



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 04:43 PM JST

PDB ID : 9XJ1 / pdb_00009xj1
EMDB ID : EMD-66925
Title : In situ structure of the PSI-LHCI supercomplex from *Oryza sativa*
Authors : Li, J.; Elias, E.; Zhang, K.; Croce, R.; Zhu, J.
Deposited on : 2025-11-04
Resolution : 2.38 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

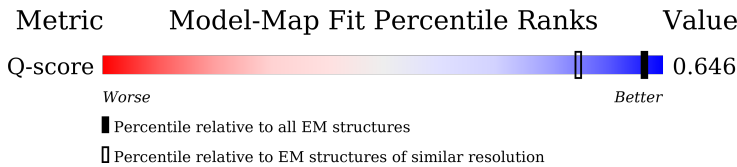
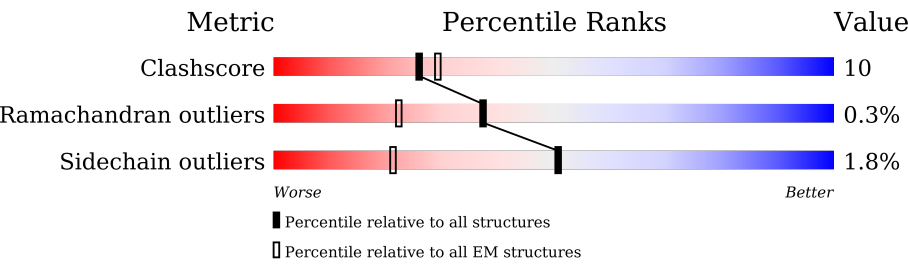
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.38 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4811 (1.88 - 2.88)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	200	78% 22%
2	2	208	85% 13% .
3	3	223	82% 18%
4	4	198	80% 18% .

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Mol	Chain	Length	Quality of chain
5	A	744	 87% 12%
6	B	734	 87% 13%
7	C	81	 94% 5% .
8	D	143	 87% 13%
9	E	68	 85% 10% .
10	F	158	 91% 9% .
11	G	97	 78% 22%
12	H	93	 88% 9% ..
13	I	30	 90% 7% .
14	J	44	 80% 20%
15	K	88	 92% 8%
16	L	163	 91% 8% .
17	N	84	 95% 5%
18	O	92	 97% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CHL	2	318	X	-	-	-
20	CLA	1	303	X	-	-	-
20	CLA	1	304	X	-	-	-
20	CLA	1	307	X	-	-	-
20	CLA	1	318	X	-	-	-
20	CLA	1	319	X	-	-	-
20	CLA	2	304	X	-	-	-
20	CLA	2	305	X	-	-	-
20	CLA	2	307	X	-	-	-
20	CLA	2	319	X	-	-	-
20	CLA	3	307	X	-	-	-
20	CLA	3	308	X	-	-	-
20	CLA	3	309	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	3	311	X	-	-	-
20	CLA	3	315	X	-	-	-
20	CLA	3	317	X	-	-	-
20	CLA	4	302	X	-	-	-
20	CLA	4	310	X	-	-	-
20	CLA	4	312	X	-	-	-
20	CLA	4	316	X	-	-	-
20	CLA	A	801	X	-	-	-
20	CLA	A	802	X	-	-	-
20	CLA	A	806	X	-	-	-
20	CLA	A	807	X	-	-	-
20	CLA	A	808	X	-	-	-
20	CLA	A	809	X	-	-	-
20	CLA	A	811	X	-	-	-
20	CLA	A	812	X	-	-	-
20	CLA	A	825	X	-	-	-
20	CLA	A	826	X	-	-	-
20	CLA	A	827	X	-	-	-
20	CLA	A	829	X	-	-	-
20	CLA	A	830	X	-	-	-
20	CLA	A	832	X	-	-	-
20	CLA	A	833	X	-	-	-
20	CLA	A	834	X	-	-	-
20	CLA	A	835	X	-	-	-
20	CLA	A	837	X	-	-	-
20	CLA	A	841	X	-	-	-
20	CLA	A	842	X	-	-	-
20	CLA	A	843	X	-	-	-
20	CLA	A	845	X	-	-	-
20	CLA	A	847	X	-	-	-
20	CLA	A	848	X	-	-	-
20	CLA	A	849	X	-	-	-
20	CLA	A	850	X	-	-	-
20	CLA	A	851	X	-	-	-
20	CLA	A	852	X	-	-	-
20	CLA	A	853	X	-	-	-
20	CLA	A	854	X	-	-	-
20	CLA	A	855	X	-	-	-
20	CLA	A	856	X	-	-	-
20	CLA	B	801	X	-	-	-
20	CLA	B	803	X	-	-	-
20	CLA	B	804	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	806	X	-	-	-
20	CLA	B	807	X	-	-	-
20	CLA	B	808	X	-	-	-
20	CLA	B	809	X	-	-	-
20	CLA	B	811	X	-	-	-
20	CLA	B	812	X	-	-	-
20	CLA	B	813	X	-	-	-
20	CLA	B	814	X	-	-	-
20	CLA	B	815	X	-	-	-
20	CLA	B	816	X	-	-	-
20	CLA	B	817	X	-	-	-
20	CLA	B	818	X	-	-	-
20	CLA	B	819	X	-	-	-
20	CLA	B	820	X	-	-	-
20	CLA	B	821	X	-	-	-
20	CLA	B	822	X	-	-	-
20	CLA	B	823	X	-	-	-
20	CLA	B	824	X	-	-	-
20	CLA	B	827	X	-	-	-
20	CLA	B	829	X	-	-	-
20	CLA	B	830	X	-	-	-
20	CLA	B	831	X	-	-	-
20	CLA	B	833	X	-	-	-
20	CLA	B	844	X	-	-	-
20	CLA	B	845	X	-	-	-
20	CLA	B	847	X	-	-	-
20	CLA	B	848	X	-	-	-
20	CLA	B	850	X	-	-	-
20	CLA	B	851	X	-	-	-
20	CLA	B	852	X	-	-	-
20	CLA	B	853	X	-	-	-
20	CLA	F	304	X	-	-	-
20	CLA	H	201	X	-	-	-
20	CLA	K	204	X	-	-	-
20	CLA	N	202	X	-	-	-
20	CLA	O	206	X	-	-	-
20	CLA	O	207	X	-	-	-
22	XAT	1	311	-	-	X	-
28	CL0	A	824	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 39160 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	200	Total	C	N	O	S	0	0
			1560	1013	258	283	6		

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	207	Total	C	N	O	S	0	0
			1612	1055	263	289	5		

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	223	Total	C	N	O	S	0	0
			1731	1138	277	310	6		

- Molecule 4 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	198	Total	C	N	O	S	0	0
			1570	1024	257	284	5		

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	742	Total	C	N	O	S	0	0
			5833	3819	991	1005	18		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	LEU	TRP	conflict	UNP P0C353

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	733	Total	C	N	O	S	0	0
			5865	3848	995	1009	13		

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			602	371	104	116	11		

- Molecule 8 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	143	Total	C	N	O	S	0	0
			1128	726	197	202	3		

- Molecule 9 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	65	Total	C	N	O	0	0
			518	329	92	97		

- Molecule 10 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	158	Total	C	N	O	S	0	0
			1236	806	210	217	3		

- Molecule 11 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	97	Total	C	N	O	S	0	0
			760	492	128	139	1		

- Molecule 12 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	H	93	Total	C	N	O	0	0
			709	465	112	132		

- Molecule 13 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	30	Total	C	N	O	S	0	0
			232	160	35	36	1		

- Molecule 14 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	44	Total	C	N	O	S	0	0
			353	241	53	58	1		

- Molecule 15 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	88	Total	C	N	O	S	0	0
			620	392	107	117	4		

- Molecule 16 is a protein called Photosystem I reaction center subunit XI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	163	Total	C	N	O	S	0	0
			1223	809	194	218	2		

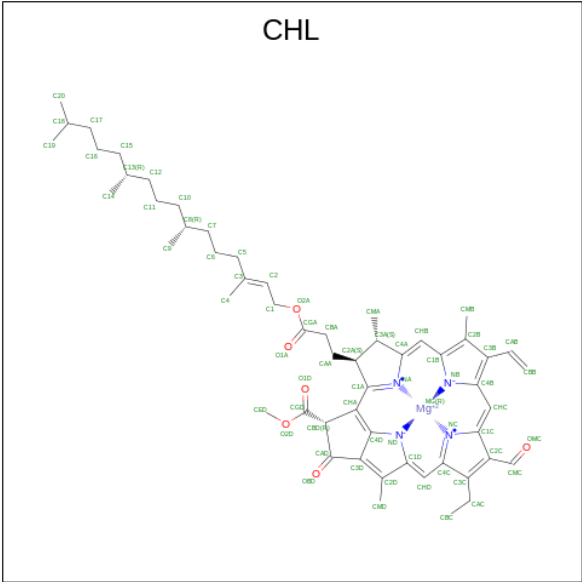
- Molecule 17 is a protein called Photosystem I reaction center subunit N, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	84	Total	C	N	O	S	0	0
			685	439	112	130	4		

- Molecule 18 is a protein called Os04g0414700 protein.

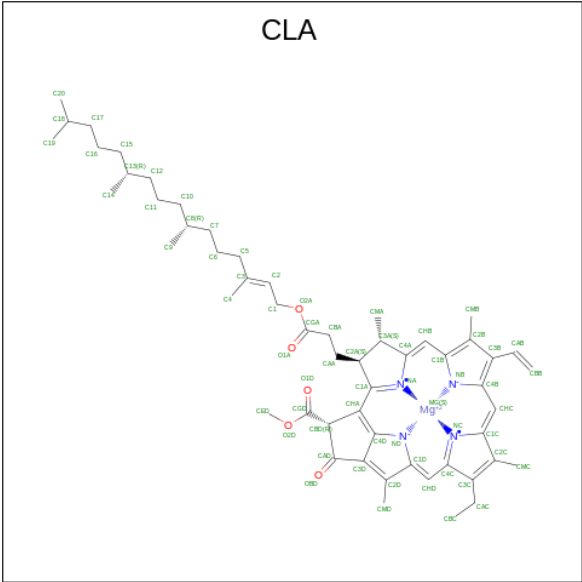
Mol	Chain	Residues	Atoms				AltConf	Trace
18	O	92	Total	C	N	O	0	0
			733	491	118	124		

- Molecule 19 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
19	1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
19	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
19	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
19	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
19	2	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
19	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
19	3	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
19	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
19	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
19	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
19	4	1	Total	C	Mg	N	O	0
			45	34	1	4	6	

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			59	51	1	4	3	
20	3	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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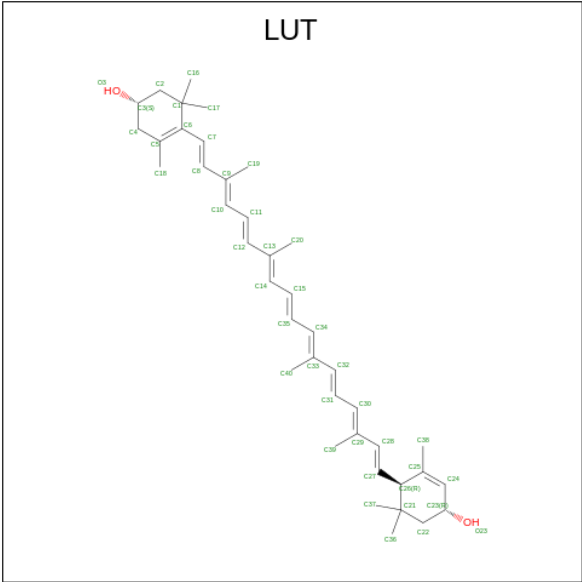
Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	H	1	Total 59	C 49	Mg 1	N 4	O 5	0

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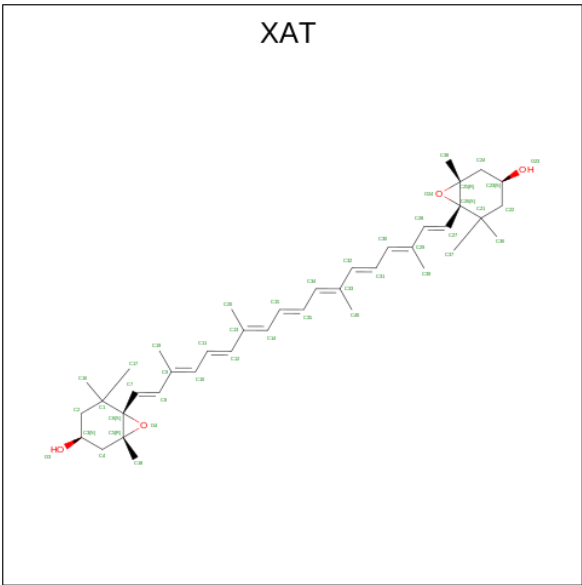
Mol	Chain	Residues	Atoms					AltConf
20	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
20	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	N	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	O	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
20	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 21 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



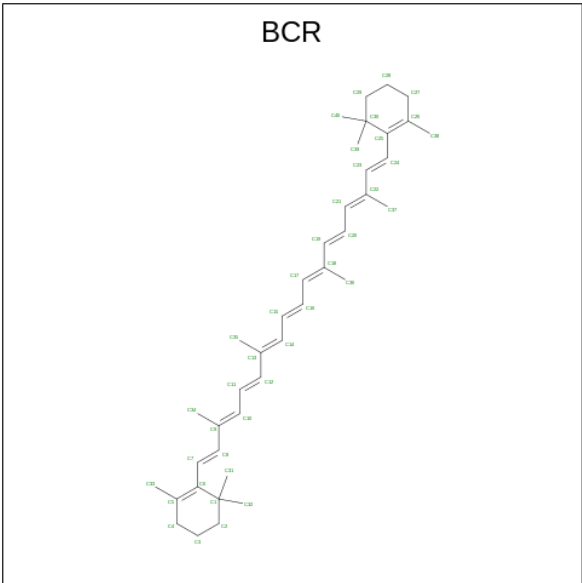
Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			42	40	2	
21	1	1	Total	C	O	0
			42	40	2	
21	2	1	Total	C	O	0
			42	40	2	
21	3	1	Total	C	O	0
			42	40	2	
21	4	1	Total	C	O	0
			42	40	2	

- Molecule 22 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
22	1	1	Total	C	O	0
			44	40	4	
22	2	1	Total	C	O	0
			44	40	4	
22	3	1	Total	C	O	0
			44	40	4	
22	4	1	Total	C	O	0
			44	40	4	

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



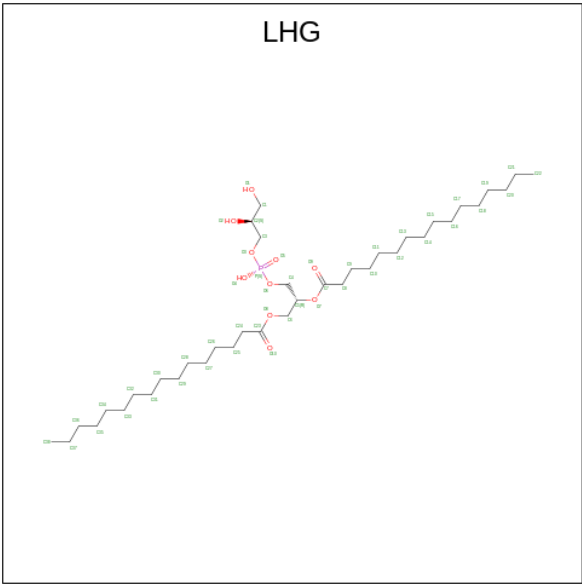
Mol	Chain	Residues	Atoms	AltConf
23	1	1	Total C 40 40	0
23	2	1	Total C 40 40	0
23	3	1	Total C 40 40	0
23	4	1	Total C 40 40	0
23	4	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 39 39	0
23	A	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 30 30	0
23	F	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	G	1	Total C 40 40	0
23	G	1	Total C 40 40	0
23	I	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
23	J	1	Total C 40 40	0
23	K	1	Total C 40 40	0
23	K	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	O	1	Total C 40 40	0
23	O	1	Total C 40 40	0

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



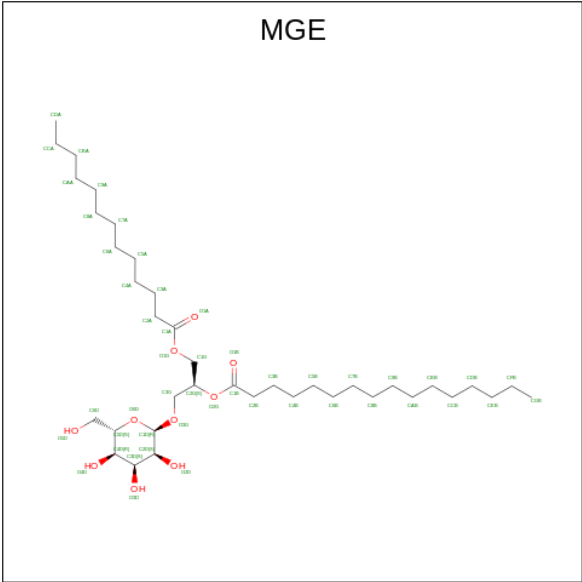
Mol	Chain	Residues	Atoms	AltConf
24	1	1	Total C O P 49 38 10 1	0
24	1	1	Total C O 33 28 5	0

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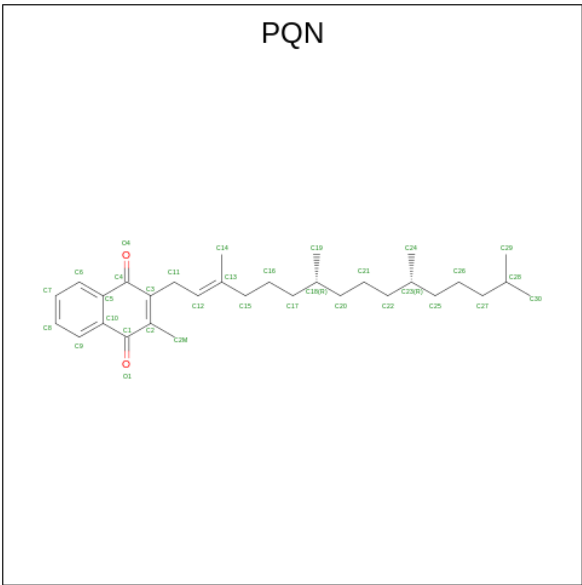
Mol	Chain	Residues	Atoms				AltConf
24	2	1	Total	C	O	P	0
			41	30	10	1	
24	2	1	Total	C	O	P	0
			40	30	9	1	
24	2	1	Total	C	O	P	0
			32	21	10	1	
24	2	1	Total	C	O	P	0
			37	28	8	1	
24	4	1	Total	C	O	P	0
			33	22	10	1	
24	4	1	Total	C	O	P	0
			49	38	10	1	
24	A	1	Total	C	O	P	0
			49	38	10	1	
24	A	1	Total	C	O	P	0
			27	18	8	1	
24	A	1	Total	C	O	P	0
			47	36	10	1	
24	A	1	Total	C	O	P	0
			42	33	8	1	
24	B	1	Total	C	O	P	0
			32	21	10	1	
24	B	1	Total	C	O	P	0
			32	23	8	1	
24	B	1	Total	C	O	P	0
			28	19	8	1	
24	I	1	Total	C	O		0
			37	33	4		
24	O	1	Total	C	O	P	0
			25	16	8	1	
24	O	1	Total	C	O	P	0
			42	33	8	1	

- Molecule 25 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (CCD ID: MGE) (formula: C₃₈H₇₂O₁₀) (labeled as "Ligand of Interest" by depositor).



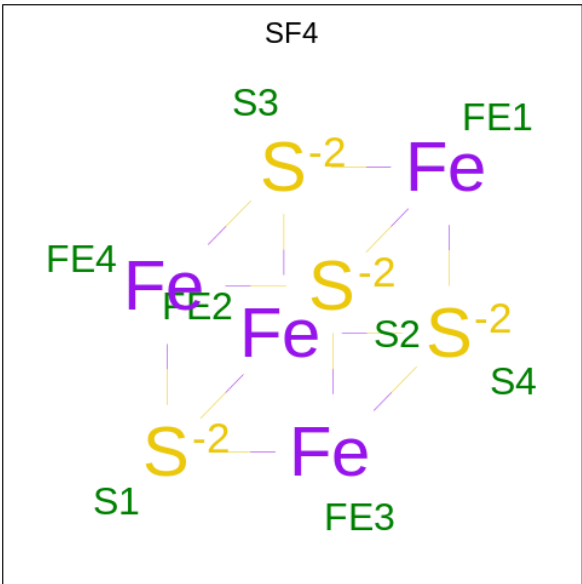
Mol	Chain	Residues	Atoms			AltConf
25	1	1	Total	C	O	0
			37	27	10	
25	1	1	Total	C	O	0
			40	30	10	
25	1	1	Total	C	O	0
			48	38	10	
25	3	1	Total	C	O	0
			33	23	10	
25	3	1	Total	C	O	0
			34	24	10	
25	3	1	Total	C	O	0
			38	28	10	
25	4	1	Total	C	O	0
			40	30	10	
25	A	1	Total	C	O	0
			34	24	10	
25	F	1	Total	C	O	0
			28	18	10	
25	G	1	Total	C	O	0
			48	38	10	
25	J	1	Total	C	O	0
			42	32	10	
25	N	1	Total	C	O	0
			40	30	10	

- Molecule 26 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Lig- and of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			33	31	2	
26	B	1	Total	C	O	0
			30	28	2	

- Molecule 27 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



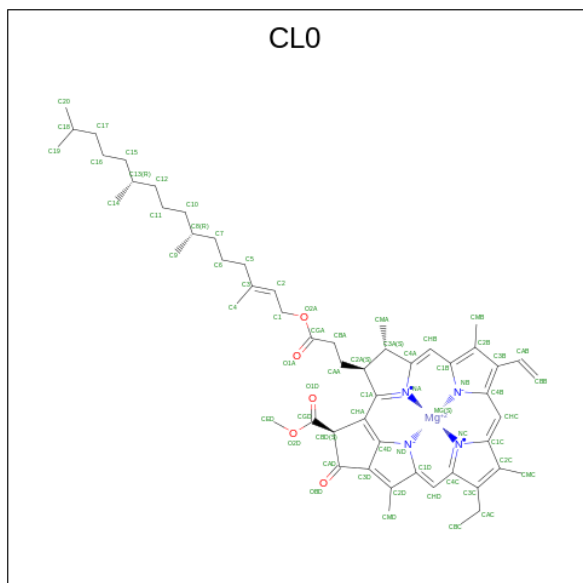
Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	Fe	S	0
			8	4	4	

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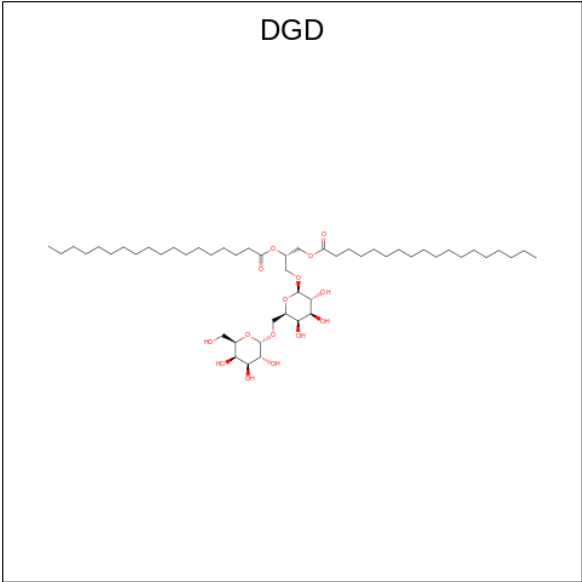
Mol	Chain	Residues	Atoms			AltConf
27	C	1	Total	Fe	S	0
			8	4	4	
27	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 28 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).

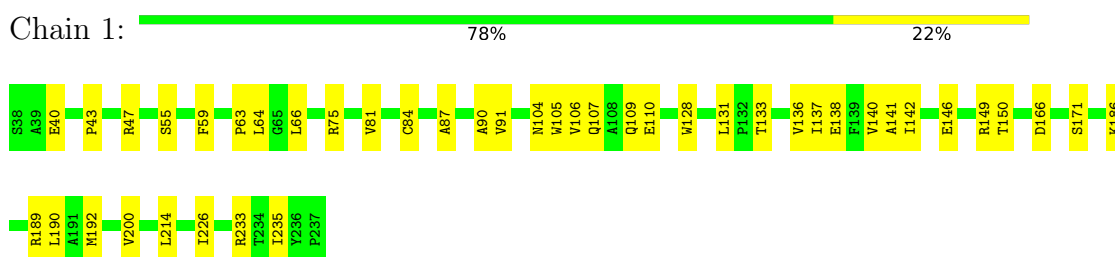


Mol	Chain	Residues	Atoms			AltConf
29	B	1	Total	C	O	0
			59	44	15	
29	G	1	Total	C	O	0
			40	31	9	
29	J	1	Total	C	O	0
			66	51	15	
29	O	1	Total	C	O	0
			53	38	15	

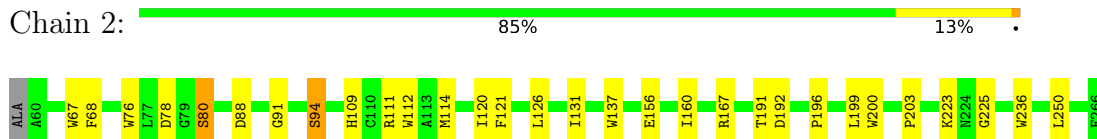
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

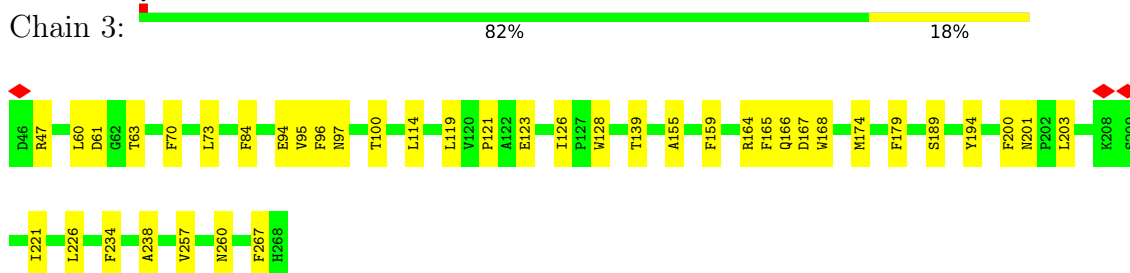
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



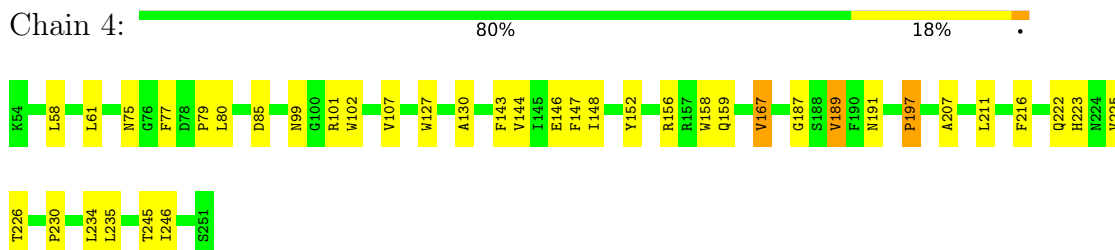
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



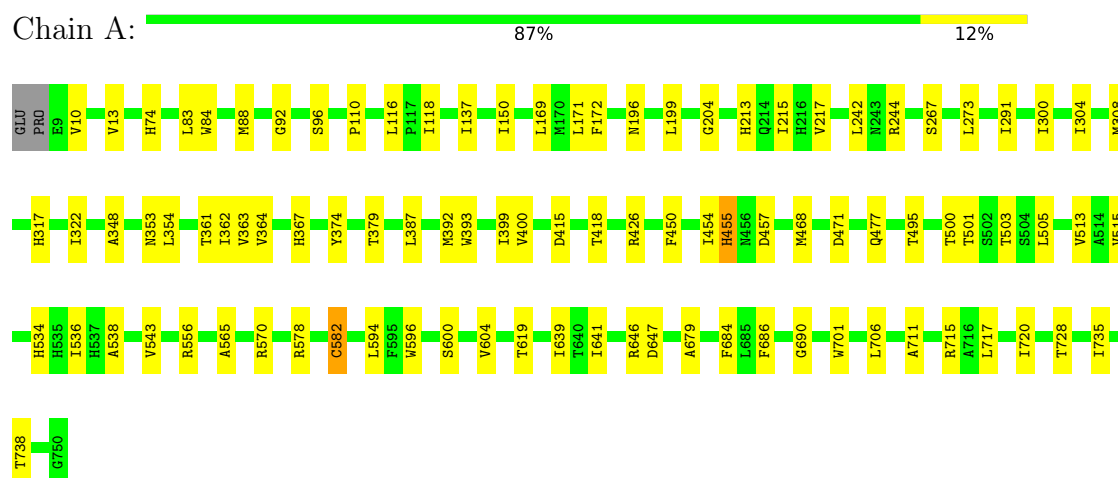
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



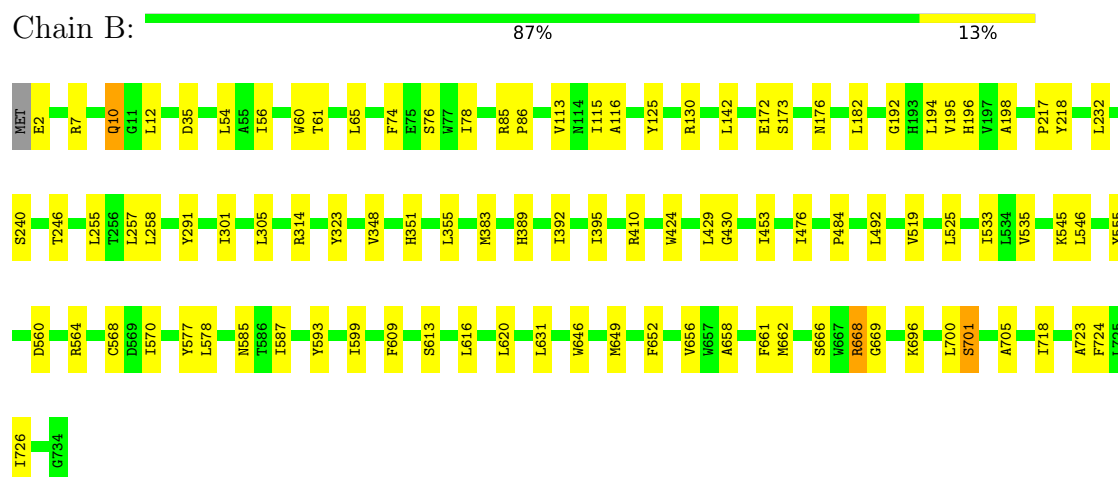
- Molecule 4: Chlorophyll a-b binding protein, chloroplastic



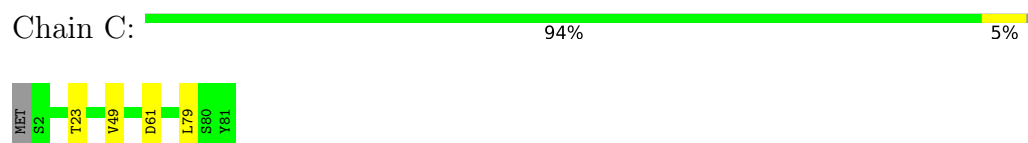
- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1



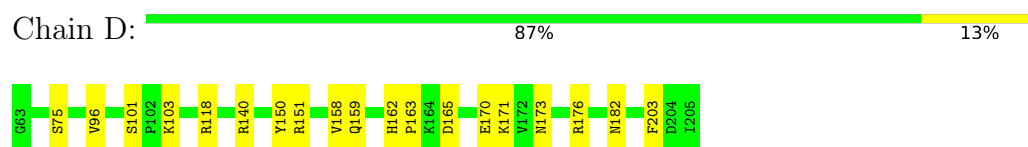
- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2



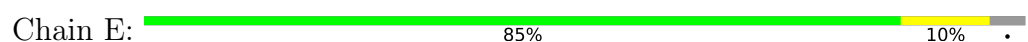
- Molecule 7: Photosystem I iron-sulfur center



- Molecule 8: Photosystem I reaction center subunit II, chloroplastic



- Molecule 9: Photosystem I reaction center subunit IV





- Molecule 10: Photosystem I reaction center subunit III

Chain F: 91% 9% .



- Molecule 11: Photosystem I reaction center subunit V, chloroplastic

Chain G: 78% 22%



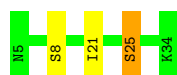
- Molecule 12: Photosystem I reaction center subunit VI, chloroplastic

Chain H: 88% 9% ..



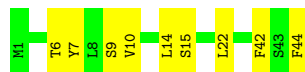
- Molecule 13: Photosystem I reaction center subunit VIII

Chain I: 90% 7% .



- Molecule 14: Photosystem I reaction center subunit IX

Chain J: 80% 20%



- Molecule 15: Photosystem I reaction center subunit psaK, chloroplastic

Chain K: 92% 8%

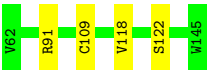


- Molecule 16: Photosystem I reaction center subunit XI, chloroplastic

Chain L: 91% 8% .



- Molecule 17: Photosystem I reaction center subunit N, chloroplastic



- Molecule 18: Os04g0414700 protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	182666	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.375	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.786	Depositor
Minimum map value	-0.971	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.14	Depositor
Map size ($\text{\AA}$)	419.84, 419.84, 419.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PQN, MGE, XAT, DGD, BCR, CHL, LHG, CLA, CL0, SF4, LUT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.18	0/1614	0.37	0/2203
2	2	0.23	0/1670	0.44	0/2286
3	3	0.20	0/1787	0.39	0/2430
4	4	0.27	1/1621 (0.1%)	0.48	1/2214 (0.0%)
5	A	0.20	0/6029	0.39	0/8222
6	B	0.20	0/6076	0.38	0/8297
7	C	0.16	0/613	0.35	0/830
8	D	0.16	0/1157	0.39	0/1564
9	E	0.16	0/530	0.38	0/722
10	F	0.17	0/1265	0.35	0/1710
11	G	0.32	0/780	0.52	0/1057
12	H	0.59	1/732 (0.1%)	0.67	2/996 (0.2%)
13	I	0.16	0/238	0.33	0/324
14	J	0.46	0/364	0.44	0/495
15	K	0.18	0/626	0.35	0/847
16	L	0.30	1/1261 (0.1%)	0.42	0/1726
17	N	0.15	0/701	0.36	0/939
18	O	0.18	0/762	0.39	0/1041
All	All	0.23	3/27826 (0.0%)	0.41	3/37903 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
8	D	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	77	SER	CA-C	-7.09	1.45	1.53
16	L	91	SER	CA-C	-6.46	1.46	1.53
4	4	197	PRO	CB-CG	5.27	1.76	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	83	GLN	N-CA-C	-8.56	92.56	110.80
4	4	197	PRO	N-CD-CG	-7.50	91.95	103.20
12	H	78	PRO	N-CA-C	-6.87	98.32	112.47

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	D	162	HIS	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1560	0	1507	49	0
2	2	1612	0	1554	32	0
3	3	1731	0	1692	41	0
4	4	1570	0	1528	46	0
5	A	5833	0	5688	88	0
6	B	5865	0	5641	81	0
7	C	602	0	585	3	0
8	D	1128	0	1135	9	0
9	E	518	0	517	4	0
10	F	1236	0	1274	12	0
11	G	760	0	734	19	0
12	H	709	0	704	12	0
13	I	232	0	252	2	0
14	J	353	0	363	9	0
15	K	620	0	647	4	0
16	L	1223	0	1228	8	0
17	N	685	0	658	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	O	733	0	710	4	0
19	1	94	0	66	16	0
19	2	241	0	173	26	0
19	3	50	0	37	11	0
19	4	184	0	121	26	0
20	1	653	0	537	37	0
20	2	565	0	469	22	0
20	3	675	0	589	17	0
20	4	577	0	497	19	0
20	A	2551	0	2555	98	0
20	B	2510	0	2547	104	0
20	F	157	0	138	9	0
20	G	142	0	104	8	0
20	H	59	0	58	2	0
20	J	46	0	33	0	0
20	K	196	0	160	5	0
20	L	144	0	109	5	0
20	N	56	0	51	4	0
20	O	169	0	163	2	0
21	1	84	0	112	27	0
21	2	42	0	56	19	0
21	3	42	0	56	15	0
21	4	42	0	56	17	0
22	1	44	0	56	25	0
22	2	44	0	56	8	0
22	3	44	0	54	12	0
22	4	44	0	56	11	0
23	1	40	0	56	4	0
23	2	40	0	56	6	0
23	3	40	0	56	2	0
23	4	80	0	112	12	0
23	A	239	0	333	24	0
23	B	230	0	319	29	0
23	F	80	0	112	10	0
23	G	80	0	112	10	0
23	I	40	0	56	2	0
23	J	40	0	56	6	0
23	K	80	0	112	6	0
23	L	160	0	224	15	0
23	O	80	0	112	8	0
24	1	82	0	121	3	0
24	2	150	0	185	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	4	82	0	110	1	0
24	A	165	0	228	7	0
24	B	92	0	100	0	0
24	I	37	0	58	0	0
24	O	67	0	83	2	0
25	1	125	0	166	32	0
25	3	105	0	123	25	0
25	4	40	0	53	6	0
25	A	34	0	38	15	0
25	F	28	0	26	5	0
25	G	48	0	72	9	0
25	J	42	0	57	13	0
25	N	40	0	50	15	0
26	A	33	0	46	11	0
26	B	30	0	37	16	0
27	A	8	0	0	0	0
27	C	16	0	0	0	0
28	A	64	0	69	13	0
29	B	59	0	79	1	0
29	G	40	0	49	13	0
29	J	66	0	96	0	0
29	O	53	0	64	0	0
All	All	39160	0	38952	800	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (800) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:197:PRO:CB	4:4:197:PRO:CG	1.76	1.40
21:1:310:LUT:H171	21:1:310:LUT:H8	1.55	0.89
21:3:301:LUT:H8	21:3:301:LUT:H171	1.53	0.89
12:H:78:PRO:HB2	20:L:305:CLA:HMD2	1.52	0.89
19:2:318:CHL:HAA2	19:2:318:CHL:HED2	1.55	0.88
23:2:312:BCR:H331	23:2:312:BCR:HC8	1.56	0.86
23:4:319:BCR:H331	23:4:319:BCR:HC8	1.58	0.84
25:1:315:MGE:H3B1	20:F:306:CLA:HED2	1.61	0.83
21:1:323:LUT:H8	21:1:323:LUT:H161	1.61	0.83
1:1:131:LEU:HD21	25:1:316:MGE:H2B1	1.62	0.82
5:A:364:VAL:HG22	20:A:843:CLA:H43	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:82:LEU:HG	20:H:201:CLA:HAC1	1.62	0.82
21:2:310:LUT:H32	21:2:310:LUT:H391	1.63	0.81
20:4:304:CLA:HMA2	19:4:305:CHL:HBC2	1.60	0.80
20:B:809:CLA:HMB2	20:B:814:CLA:HMA3	1.62	0.80
20:A:812:CLA:HMD1	28:A:824:CL0:H13	1.65	0.79
11:G:76:GLU:OE1	29:G:202:DGD:O4D	2.02	0.77
22:1:311:XAT:H182	25:1:324:MGE:H8B1	1.67	0.77
19:4:306:CHL:HBB1	22:4:318:XAT:H161	1.66	0.77
2:2:203:PRO:HD2	21:2:310:LUT:H42	1.68	0.75
25:1:316:MGE:H3G1	20:G:205:CLA:HMD2	1.66	0.75
7:C:61:ASP:N	9:E:125:ASN:OD1	2.20	0.73
5:A:578:ARG:O	6:B:668:ARG:NH2	2.22	0.73
5:A:304:ILE:O	20:A:846:CLA:HBC1	1.89	0.72
3:3:238:ALA:HB1	25:3:306:MGE:H2A2	1.72	0.72
21:2:310:LUT:H8	21:2:310:LUT:H171	1.71	0.71
23:J:101:BCR:H321	23:J:101:BCR:HC8	1.73	0.71
17:N:91:ARG:O	25:N:201:MGE:O4D	2.09	0.70
6:B:662:MET:HG3	20:B:845:CLA:NC	2.06	0.70
5:A:354:LEU:HD21	20:A:854:CLA:HBB1	1.74	0.70
25:F:303:MGE:O5D	14:J:6:THR:OG1	2.10	0.69
5:A:717:LEU:HD21	26:A:810:PQN:H152	1.74	0.69
5:A:367:HIS:ND1	20:A:842:CLA:OBD	2.25	0.69
12:H:78:PRO:HB2	20:L:305:CLA:CMD	2.22	0.69
1:1:166:ASP:OD1	21:1:310:LUT:O23	2.11	0.69
5:A:715:ARG:NH2	9:E:89:TYR:OH	2.26	0.69
25:1:315:MGE:H3A2	20:F:306:CLA:C1D	2.23	0.68
19:4:305:CHL:HBB2	19:4:306:CHL:CBB	2.24	0.68
20:1:322:CLA:HBC3	25:J:102:MGE:H5B2	1.76	0.68
20:4:312:CLA:HMA2	21:4:317:LUT:H3	1.76	0.68
4:4:191:ASN:OD1	21:4:317:LUT:O23	2.08	0.68
6:B:424:TRP:HZ3	20:B:828:CLA:HBC2	1.59	0.67
11:G:109:ASP:OD1	20:G:207:CLA:ND	2.26	0.67
23:B:838:BCR:H403	23:B:838:BCR:H23C	1.77	0.67
1:1:106:VAL:HG12	19:1:301:CHL:HED2	1.75	0.67
4:4:234:LEU:HB2	21:4:317:LUT:H22	1.77	0.67
3:3:201:ASN:OD1	21:3:301:LUT:O23	2.08	0.67
20:1:309:CLA:HBC1	25:G:204:MGE:H4B2	1.78	0.66
20:B:821:CLA:HBC2	20:B:828:CLA:HMC2	1.77	0.66
15:K:113:HIS:CD2	20:K:205:CLA:NC	2.63	0.66
20:A:806:CLA:HMD1	25:A:823:MGE:H1G1	1.77	0.66
20:1:303:CLA:C10	20:1:319:CLA:C4D	2.73	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:O:203:BCR:H363	24:O:205:LHG:H141	1.76	0.66
5:A:308:MET:HB2	20:A:846:CLA:HBC3	1.79	0.65
6:B:314:ARG:O	6:B:410:ARG:NH2	2.29	0.65
4:4:102:TRP:CE2	19:4:307:CHL:HED2	2.31	0.65
1:1:140:VAL:HG11	25:G:204:MGE:H9B1	1.78	0.65
4:4:187:GLY:O	4:4:191:ASN:N	2.29	0.65
2:2:120:ILE:HG13	22:2:311:XAT:H361	1.78	0.65
15:K:101:THR:O	15:K:105:THR:OG1	2.12	0.64
1:1:63:PRO:O	25:1:324:MGE:O5D	2.13	0.64
11:G:80:LYS:NZ	29:G:202:DGD:O3D	2.28	0.64
18:O:60:SER:OG	18:O:71:THR:OG1	2.11	0.64
1:1:90:ALA:HB2	22:1:311:XAT:C39	2.27	0.64
6:B:86:PRO:O	6:B:116:ALA:N	2.31	0.64
1:1:146:GLU:OE1	1:1:149:ARG:NE	2.28	0.64
20:A:801:CLA:HBC1	25:A:823:MGE:H9B1	1.79	0.64
28:A:824:CL0:H11	20:B:844:CLA:HAA1	1.79	0.64
6:B:351:HIS:ND1	20:B:807:CLA:OBD	2.30	0.64
1:1:66:LEU:HD12	22:1:311:XAT:H22	1.80	0.64
19:1:301:CHL:HED3	11:G:145:PHE:CZ	2.32	0.64
6:B:383:MET:HE1	23:B:837:BCR:H361	1.79	0.63
23:B:836:BCR:H391	23:B:837:BCR:H383	1.79	0.63
6:B:218:TYR:OH	6:B:232:LEU:O	2.12	0.63
20:4:302:CLA:HAB	22:4:318:XAT:H32	1.79	0.63
20:A:831:CLA:HBA2	25:N:201:MGE:H3B2	1.79	0.63
28:A:824:CL0:H14	20:B:844:CLA:C1A	2.28	0.63
6:B:348:VAL:HG22	20:B:808:CLA:H43	1.80	0.63
25:A:823:MGE:O2G	25:A:823:MGE:O2D	2.15	0.63
2:2:78:ASP:OD1	2:2:80:SER:OG	2.17	0.62
5:A:594:LEU:HD21	20:A:854:CLA:HBC1	1.80	0.62
20:1:302:CLA:H11	21:1:310:LUT:H383	1.81	0.62
10:F:193:VAL:HG21	25:F:303:MGE:H4B1	1.80	0.62
20:1:309:CLA:CBC	25:G:204:MGE:H4B2	2.29	0.62
25:3:304:MGE:H3A2	5:A:172:PHE:CE2	2.35	0.62
4:4:222:GLN:HE22	21:4:317:LUT:H42	1.64	0.62
26:A:810:PQN:H141	20:F:304:CLA:CBB	2.29	0.62
19:2:309:CHL:HAB	23:2:312:BCR:H342	1.81	0.62
20:B:844:CLA:HMB1	20:B:844:CLA:HBB1	1.82	0.62
1:1:91:VAL:HG11	21:1:310:LUT:H12	1.82	0.62
1:1:189:ARG:HB3	20:1:318:CLA:HBC3	1.81	0.62
25:3:304:MGE:H4	25:3:305:MGE:H1	1.40	0.62
25:4:322:MGE:H2A2	10:F:197:PRO:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:61:ASP:OD1	3:3:63:THR:OG1	2.13	0.61
20:A:812:CLA:H11	6:B:616:LEU:HD12	1.82	0.61
1:1:43:PRO:O	4:4:159:GLN:NE2	2.32	0.61
25:3:304:MGE:H3A2	5:A:172:PHE:CZ	2.34	0.61
25:4:322:MGE:H3A1	25:4:322:MGE:H4B1	1.82	0.61
20:B:807:CLA:HED2	20:B:808:CLA:H11	1.83	0.61
20:B:829:CLA:CBB	26:B:832:PQN:H141	2.31	0.61
2:2:76:TRP:NE1	2:2:88:ASP:OD2	2.33	0.61
20:A:801:CLA:H102	26:B:832:PQN:H211	1.82	0.61
23:L:301:BCR:HC8	23:L:301:BCR:H311	1.81	0.61
4:4:77:PHE:CE2	22:4:318:XAT:H383	2.35	0.60
5:A:171:LEU:HD13	20:A:833:CLA:H201	1.83	0.60
8:D:165:ASP:OD2	8:D:173:ASN:ND2	2.34	0.60
1:1:200:VAL:HG13	21:1:323:LUT:H26	1.82	0.60
20:2:307:CLA:HMA2	21:2:310:LUT:H23	1.82	0.60
4:4:146:GLU:OE1	19:4:306:CHL:HMC	2.02	0.60
20:A:809:CLA:H192	14:J:22:LEU:HD23	1.83	0.60
20:B:812:CLA:C2C	29:G:202:DGD:HBE2	2.32	0.60
4:4:58:LEU:CD2	25:4:322:MGE:H3B1	2.32	0.60
2:2:191:THR:OG1	2:2:192:ASP:N	2.34	0.60
20:A:809:CLA:HAC1	26:A:810:PQN:H171	1.84	0.59
20:A:812:CLA:HMA2	6:B:616:LEU:HD13	1.84	0.59
23:A:814:BCR:H321	23:A:814:BCR:HC8	1.83	0.59
1:1:105:TRP:HE3	22:1:311:XAT:H242	1.66	0.59
20:1:308:CLA:HBC1	21:1:310:LUT:H162	1.84	0.59
2:2:91:GLY:O	2:2:94:SER:OG	2.21	0.59
6:B:700:LEU:HD21	26:B:832:PQN:H152	1.84	0.59
23:A:818:BCR:H382	23:A:818:BCR:H23C	1.84	0.59
6:B:718:ILE:HD13	20:B:817:CLA:CMC	2.33	0.59
1:1:136:VAL:HG12	25:1:316:MGE:H4A2	1.84	0.59
25:1:316:MGE:H3B1	20:G:205:CLA:C1D	2.33	0.59
5:A:711:ALA:N	10:F:184:GLU:OE1	2.35	0.59
20:B:829:CLA:HBB2	26:B:832:PQN:H141	1.83	0.59
25:1:315:MGE:H3B2	25:J:102:MGE:H6B1	1.84	0.59
3:3:165:PHE:HE2	25:3:305:MGE:H6D2	1.68	0.59
4:4:234:LEU:HD13	21:4:317:LUT:H163	1.84	0.59
23:A:814:BCR:H381	20:K:205:CLA:HMC3	1.85	0.59
22:1:311:XAT:H8	22:1:311:XAT:H171	1.83	0.59
2:2:156:GLU:OE1	19:2:301:CHL:HMC	2.03	0.58
26:A:810:PQN:H201	23:F:301:BCR:H382	1.85	0.58
20:A:826:CLA:OBD	20:B:844:CLA:HMB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:60:SER:HG	18:O:71:THR:HG1	1.47	0.58
5:A:738:THR:N	28:A:824:CL0:O1D	2.35	0.58
20:A:806:CLA:CBC	25:A:823:MGE:H2A1	2.33	0.58
25:A:823:MGE:H1G2	25:A:823:MGE:O3D	2.03	0.58
20:B:810:CLA:HMB2	23:G:203:BCR:H20C	1.85	0.58
14:J:42:PHE:HB3	25:J:102:MGE:H3A1	1.85	0.58
1:1:63:PRO:HB2	25:1:324:MGE:H3B2	1.86	0.58
3:3:189:SER:OG	3:3:194:TYR:O	2.21	0.58
20:A:812:CLA:C1	6:B:616:LEU:HD12	2.33	0.58
22:1:311:XAT:H163	20:1:318:CLA:C2	2.33	0.58
21:1:323:LUT:H162	10:F:207:TYR:OH	2.03	0.58
25:3:304:MGE:H5B2	25:3:305:MGE:H4B1	1.85	0.58
3:3:238:ALA:O	25:3:306:MGE:H2A1	2.03	0.58
19:3:313:CHL:HAA1	19:3:313:CHL:HBD	1.85	0.58
23:A:857:BCR:H333	25:N:201:MGE:H8B1	1.86	0.58
8:D:171:LYS:O	8:D:176:ARG:NH2	2.37	0.58
10:F:143:GLN:O	25:J:102:MGE:H1D	2.03	0.58
23:O:203:BCR:H332	24:O:205:LHG:O10	2.03	0.58
6:B:492:LEU:HD21	11:G:140:TYR:CE2	2.39	0.57
1:1:200:VAL:CG1	21:1:323:LUT:H373	2.34	0.57
25:3:304:MGE:H6A1	20:3:309:CLA:H121	1.86	0.57
4:4:234:LEU:HD22	21:4:317:LUT:H172	1.85	0.57
5:A:582:CYS:O	6:B:669:GLY:N	2.37	0.57
20:A:812:CLA:CBB	6:B:525:LEU:HD21	2.34	0.57
1:1:128:TRP:NE1	20:1:321:CLA:OBD	2.37	0.57
5:A:83:LEU:HD21	25:N:201:MGE:H212	1.86	0.57
20:B:805:CLA:NC	23:G:201:BCR:H393	2.19	0.57
23:K:201:BCR:H331	23:K:201:BCR:C8	2.34	0.57
17:N:109:CYS:SG	25:N:201:MGE:H5D	2.44	0.57
28:A:824:CL0:H7	20:B:844:CLA:HBB1	1.86	0.57
2:2:111:ARG:NE	19:2:302:CHL:OBD	2.38	0.57
20:2:307:CLA:HMB3	21:2:310:LUT:H372	1.86	0.57
20:A:845:CLA:HMB3	20:A:849:CLA:HMA3	1.87	0.57
23:L:303:BCR:H353	23:L:304:BCR:H342	1.87	0.57
22:1:311:XAT:H403	20:1:319:CLA:HBC3	1.86	0.56
6:B:176:ASN:ND2	6:B:291:TYR:O	2.38	0.56
4:4:79:PRO:HG2	25:4:322:MGE:H7A2	1.87	0.56
5:A:534:HIS:CE1	20:A:805:CLA:NC	2.73	0.56
6:B:10:GLN:N	6:B:35:ASP:OD2	2.38	0.56
20:B:827:CLA:H93	20:B:828:CLA:HBC1	1.87	0.56
23:K:201:BCR:H383	23:K:201:BCR:H23C	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:90:ALA:HB2	22:1:311:XAT:H392	1.88	0.56
3:3:121:PRO:O	3:3:123:GLU:N	2.39	0.56
20:A:825:CLA:HMD3	6:B:533:ILE:HG12	1.86	0.56
23:B:834:BCR:H382	23:B:834:BCR:H23C	1.87	0.56
23:L:302:BCR:H23C	23:L:302:BCR:H392	1.87	0.56
23:L:303:BCR:H23C	23:L:303:BCR:H382	1.87	0.56
20:A:853:CLA:HBB1	20:A:853:CLA:HMB1	1.87	0.56
20:4:304:CLA:C2B	22:4:318:XAT:H183	2.36	0.56
20:A:831:CLA:C3D	25:N:201:MGE:H2B1	2.35	0.56
2:2:67:TRP:CH2	25:3:305:MGE:H4A1	2.41	0.56
25:3:306:MGE:H3G2	5:A:242:LEU:HD23	1.87	0.56
20:B:809:CLA:CMB	20:B:814:CLA:HMA3	2.34	0.56
6:B:519:VAL:HG21	6:B:593:TYR:HB2	1.88	0.56
23:G:201:BCR:H383	23:G:201:BCR:H23C	1.88	0.56
22:1:311:XAT:H12	20:1:318:CLA:HAB	1.88	0.56
10:F:144:ARG:HA	25:J:102:MGE:H4D	1.88	0.56
5:A:273:LEU:HD11	20:A:839:CLA:HBC1	1.88	0.56
5:A:426:ARG:NE	20:A:855:CLA:OBD	2.39	0.56
22:1:311:XAT:H381	22:1:311:XAT:C28	2.36	0.55
20:B:829:CLA:HBB2	26:B:832:PQN:H151	1.88	0.55
20:F:304:CLA:H142	14:J:14:LEU:HD22	1.87	0.55
4:4:102:TRP:CD2	19:4:307:CHL:HED2	2.41	0.55
20:4:309:CLA:HBB1	21:4:317:LUT:H32	1.88	0.55
6:B:662:MET:HG3	20:B:845:CLA:C4C	2.36	0.55
23:4:320:BCR:H23C	23:4:320:BCR:H392	1.88	0.55
1:1:137:ILE:HG13	25:G:204:MGE:H4B1	1.87	0.55
5:A:215:ILE:HD13	20:A:839:CLA:HBC2	1.88	0.55
2:2:196:PRO:HB3	19:2:302:CHL:HBC2	1.87	0.55
4:4:130:ALA:O	19:4:305:CHL:HBC1	2.07	0.55
20:A:831:CLA:ND	25:N:201:MGE:H4B1	2.22	0.55
20:B:812:CLA:C2B	29:G:202:DGD:HB52	2.37	0.55
4:4:143:PHE:HE1	25:J:102:MGE:H242	1.71	0.55
20:B:830:CLA:HHD	26:B:832:PQN:H162	1.89	0.55
23:B:837:BCR:H403	23:B:837:BCR:H23C	1.88	0.55
19:1:301:CHL:HMD1	20:G:205:CLA:CBC	2.37	0.54
5:A:83:LEU:HD11	25:N:201:MGE:H9B1	1.88	0.54
6:B:176:ASN:HB3	20:B:810:CLA:HMD2	1.88	0.54
25:N:201:MGE:H1G1	20:N:202:CLA:OBD	2.07	0.54
19:4:305:CHL:O1D	19:4:305:CHL:HBA2	2.07	0.54
1:1:235:ILE:HD13	20:1:322:CLA:HBC1	1.89	0.54
6:B:173:SER:OG	20:B:802:CLA:O1D	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:3:304:MGE:H3B2	25:3:305:MGE:H2B1	1.89	0.54
1:1:186:LYS:NZ	24:1:313:LHG:O4	2.28	0.54
22:1:311:XAT:H373	20:1:320:CLA:C2B	2.38	0.54
25:3:306:MGE:H3B1	20:A:840:CLA:HAC2	1.89	0.54
4:4:77:PHE:HE2	22:4:318:XAT:H383	1.70	0.54
5:A:477:GLN:HG2	25:A:823:MGE:H6D1	1.89	0.54
11:G:120:ALA:HB2	23:G:201:BCR:H343	1.90	0.54
25:1:315:MGE:H2B2	20:1:322:CLA:C3D	2.37	0.54
6:B:323:TYR:CE2	20:B:814:CLA:HBC1	2.43	0.54
20:B:814:CLA:CMB	20:B:816:CLA:H93	2.37	0.54
19:1:317:CHL:HMB3	20:4:314:CLA:OBD	2.08	0.54
26:A:810:PQN:H142	23:F:301:BCR:H271	1.89	0.54
26:A:810:PQN:H151	20:F:304:CLA:CBB	2.38	0.54
20:A:812:CLA:OBD	28:A:824:CL0:H13	2.07	0.54
6:B:60:TRP:NE1	20:B:817:CLA:OBD	2.41	0.54
6:B:301:ILE:HD13	20:B:814:CLA:HBC2	1.89	0.54
25:1:316:MGE:H3G1	20:G:205:CLA:CMD	2.36	0.53
19:2:318:CHL:H12	3:3:155:ALA:HA	1.90	0.53
22:3:302:XAT:C28	22:3:302:XAT:H381	2.37	0.53
23:A:857:BCR:H23C	23:A:857:BCR:H382	1.90	0.53
6:B:424:TRP:NE1	20:B:822:CLA:OBD	2.40	0.53
6:B:631:LEU:HD22	6:B:724:PHE:HA	1.89	0.53
25:1:315:MGE:H6B1	25:J:102:MGE:H7B2	1.90	0.53
2:2:250:LEU:HB2	21:2:310:LUT:H221	1.90	0.53
5:A:116:LEU:HB3	23:J:101:BCR:H323	1.89	0.53
24:A:820:LHG:H262	25:A:823:MGE:H3D	1.90	0.53
1:1:40:GLU:OE1	1:1:47:ARG:NH2	2.41	0.53
23:A:814:BCR:H381	20:K:205:CLA:CMC	2.39	0.53
1:1:142:ILE:HD13	23:1:312:BCR:H361	1.90	0.53
5:A:116:LEU:CB	23:J:101:BCR:H323	2.39	0.53
23:A:817:BCR:H392	23:A:817:BCR:H23C	1.90	0.53
23:K:201:BCR:H331	23:K:201:BCR:HC8	1.90	0.53
5:A:88:MET:HE1	20:A:832:CLA:HMA2	1.89	0.53
20:A:806:CLA:CMD	25:A:823:MGE:H1G1	2.39	0.53
20:B:814:CLA:O1A	20:B:847:CLA:H92	2.08	0.53
12:H:116:SER:OG	13:I:8:SER:O	2.24	0.53
26:B:832:PQN:H172	23:B:838:BCR:H382	1.91	0.53
23:4:319:BCR:H331	23:4:319:BCR:C8	2.36	0.53
23:B:835:BCR:H311	23:B:835:BCR:HC8	1.90	0.53
1:1:226:ILE:HG23	4:4:144:VAL:HG21	1.91	0.53
5:A:505:LEU:HD21	5:A:513:VAL:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:3:311:CLA:H111	19:3:313:CHL:HAA2	1.89	0.53
5:A:450:PHE:CZ	5:A:454:ILE:HD11	2.44	0.53
5:A:317:HIS:HB3	5:A:322:ILE:HD11	1.90	0.53
3:3:128:TRP:O	22:3:302:XAT:O23	2.26	0.52
20:A:802:CLA:HBB1	20:A:802:CLA:HMB1	1.90	0.52
11:G:120:ALA:CB	23:G:201:BCR:H343	2.39	0.52
15:K:114:ILE:HG22	20:K:204:CLA:HBC1	1.91	0.52
20:A:806:CLA:HBC1	25:A:823:MGE:H6B1	1.90	0.52
23:J:101:BCR:H392	23:J:101:BCR:H23C	1.91	0.52
20:4:304:CLA:CMA	19:4:305:CHL:HBC2	2.34	0.52
20:A:801:CLA:C3B	20:A:802:CLA:HMB2	2.40	0.52
23:A:816:BCR:H361	20:A:849:CLA:HBB2	1.91	0.52
2:2:67:TRP:HH2	25:3:305:MGE:H4A1	1.74	0.52
2:2:137:TRP:HZ3	22:2:311:XAT:H383	1.73	0.52
8:D:101:SER:OG	8:D:103:LYS:O	2.27	0.52
11:G:128:VAL:HG11	25:G:204:MGE:H7A1	1.90	0.52
3:3:165:PHE:HZ	25:3:304:MGE:H5D	1.74	0.52
4:4:225:VAL:HG23	4:4:226:THR:HG23	1.91	0.52
20:A:852:CLA:HMB1	20:A:852:CLA:HBB1	1.92	0.52
20:B:819:CLA:HBB1	20:B:819:CLA:HMB1	1.91	0.52
25:1:315:MGE:H3A2	20:F:306:CLA:ND	2.25	0.52
23:G:203:BCR:H331	23:G:203:BCR:C8	2.40	0.52
20:1:307:CLA:H2	20:1:308:CLA:HMD1	1.92	0.52
21:3:301:LUT:H383	19:3:313:CHL:H12	1.92	0.52
20:A:826:CLA:HMD1	20:B:844:CLA:HMB3	1.91	0.52
20:A:845:CLA:CMB	20:A:849:CLA:HMA3	2.40	0.52
23:B:836:BCR:H383	23:B:836:BCR:H23C	1.90	0.52
10:F:183:ARG:HH22	25:F:303:MGE:H3D	1.75	0.52
25:1:315:MGE:H2B2	20:1:322:CLA:C2D	2.39	0.52
19:2:318:CHL:HBB2	20:2:319:CLA:HH2	1.92	0.52
5:A:646:ARG:NH1	5:A:647:ASP:OD2	2.43	0.52
16:L:85:ALA:HB2	20:L:306:CLA:HMD1	1.92	0.52
25:N:201:MGE:H3A2	20:N:202:CLA:C1D	2.40	0.52
5:A:363:VAL:HG11	20:A:843:CLA:H201	1.92	0.51
23:O:202:BCR:H331	23:O:202:BCR:C8	2.40	0.51
3:3:95:VAL:HG22	3:3:221:ILE:HD13	1.91	0.51
3:3:203:LEU:O	21:3:301:LUT:O23	2.28	0.51
25:N:201:MGE:H1G1	20:N:202:CLA:CAD	2.40	0.51
1:1:166:ASP:OD2	1:1:171:SER:OG	2.25	0.51
21:3:301:LUT:H183	20:3:317:CLA:C1B	2.40	0.51
4:4:143:PHE:CE1	25:J:102:MGE:H242	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:315:MGE:H3G2	25:1:315:MGE:O2D	2.11	0.51
22:2:311:XAT:H12	20:2:319:CLA:HAB	1.93	0.51
21:3:301:LUT:H183	20:3:317:CLA:NB	2.25	0.51
20:B:812:CLA:HMB2	29:G:202:DGD:HB52	1.93	0.51
25:F:303:MGE:H1D	14:J:9:SER:OG	2.10	0.51
14:J:44:PHE:O	25:J:102:MGE:O3D	2.28	0.51
20:B:825:CLA:HMD1	11:G:144:PHE:CZ	2.46	0.51
20:4:313:CLA:O2A	23:4:320:BCR:H343	2.10	0.51
6:B:649:MET:HG2	6:B:723:ALA:HB2	1.93	0.51
25:1:315:MGE:H3B1	20:F:306:CLA:CED	2.38	0.51
14:J:7:TYR:O	14:J:10:VAL:HG12	2.11	0.51
1:1:87:ALA:CA	22:1:311:XAT:H32	2.41	0.51
4:4:85:ASP:OD1	4:4:85:ASP:N	2.44	0.51
23:A:816:BCR:H331	23:A:816:BCR:C8	2.41	0.51
20:A:826:CLA:HBB1	20:A:826:CLA:HMB1	1.93	0.51
20:B:812:CLA:C1C	29:G:202:DGD:HB91	2.40	0.51
5:A:457:ASP:OD2	5:A:641:ILE:N	2.42	0.51
20:A:812:CLA:HMD1	28:A:824:CL0:CMB	2.38	0.51
2:2:112:TRP:CD2	19:2:302:CHL:HED2	2.46	0.50
20:B:814:CLA:HBA1	20:B:814:CLA:HMA2	1.92	0.50
3:3:257:VAL:O	3:3:260:ASN:ND2	2.45	0.50
5:A:116:LEU:HG	20:A:833:CLA:HED3	1.93	0.50
20:B:829:CLA:CBB	26:B:832:PQN:H151	2.40	0.50
1:1:64:LEU:HD23	25:1:324:MGE:H3B1	1.93	0.50
1:1:190:LEU:HG	21:1:310:LUT:H11	1.92	0.50
1:1:214:LEU:HD13	20:1:308:CLA:HBC2	1.93	0.50
23:A:815:BCR:H23C	23:A:815:BCR:H382	1.92	0.50
20:A:833:CLA:HMB3	23:A:857:BCR:C22	2.42	0.50
23:K:202:BCR:H383	23:K:202:BCR:H23C	1.91	0.50
1:1:141:ALA:HB2	25:G:204:MGE:H231	1.93	0.50
3:3:179:PHE:CE2	19:3:313:CHL:HBB2	2.46	0.50
4:4:147:PHE:HD1	25:J:102:MGE:H251	1.74	0.50
5:A:686:PHE:HB2	20:A:825:CLA:HBC2	1.94	0.50
20:2:307:CLA:H121	19:2:318:CHL:H112	1.93	0.50
21:3:301:LUT:H383	19:3:313:CHL:H42	1.92	0.50
4:4:191:ASN:HA	21:4:317:LUT:H24	1.94	0.50
20:B:830:CLA:H52	20:B:830:CLA:H93	1.94	0.50
26:B:832:PQN:H142	23:B:838:BCR:H281	1.93	0.50
3:3:267:PHE:O	5:A:244:ARG:NH1	2.45	0.50
4:4:61:LEU:HG	25:4:322:MGE:H2B2	1.94	0.50
26:A:810:PQN:H172	23:F:301:BCR:H382	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:348:VAL:HG21	20:B:818:CLA:HHD	1.92	0.50
20:A:805:CLA:HBB2	20:A:850:CLA:HMD2	1.93	0.50
20:B:814:CLA:H92	20:B:816:CLA:H42	1.94	0.50
12:H:58:LEU:HD23	12:H:61:ILE:HD11	1.94	0.50
20:2:323:CLA:HBB2	20:4:302:CLA:HBC2	1.94	0.49
5:A:500:THR:HG22	5:A:501:THR:HG23	1.94	0.49
5:A:684:PHE:HA	26:A:810:PQN:H9	1.93	0.49
23:B:838:BCR:H331	23:B:838:BCR:C8	2.42	0.49
16:L:85:ALA:HB2	20:L:306:CLA:CMD	2.42	0.49
25:N:201:MGE:H3G2	20:N:202:CLA:CED	2.42	0.49
2:2:109:HIS:ND1	20:2:303:CLA:HMD1	2.28	0.49
24:4:321:LHG:H332	25:J:102:MGE:H241	1.94	0.49
23:O:203:BCR:H362	20:O:207:CLA:CAB	2.42	0.49
5:A:199:LEU:O	5:A:204:GLY:N	2.41	0.49
6:B:194:LEU:HA	6:B:198:ALA:HB3	1.94	0.49
8:D:140:ARG:NH2	8:D:170:GLU:OE2	2.41	0.49
25:1:316:MGE:H202	20:G:205:CLA:C3B	2.42	0.49
19:2:301:CHL:CAB	19:2:322:CHL:HBB2	2.42	0.49
3:3:73:LEU:HD13	20:A:836:CLA:H2	1.93	0.49
19:4:307:CHL:HBB2	19:4:315:CHL:CHC	2.43	0.49
5:A:387:LEU:HD11	20:A:853:CLA:HED3	1.93	0.49
5:A:738:THR:OG1	28:A:824:CL0:O1D	2.24	0.49
26:A:810:PQN:H111	23:F:301:BCR:H393	1.94	0.49
23:A:815:BCR:H342	20:A:853:CLA:C2	2.42	0.49
6:B:395:ILE:HD13	6:B:555:TYR:HA	1.94	0.49
1:1:200:VAL:HG11	21:1:323:LUT:H373	1.93	0.49
5:A:374:TYR:CE2	20:A:853:CLA:HED2	2.47	0.49
20:A:801:CLA:HMA2	23:I:102:BCR:H282	1.95	0.49
6:B:257:LEU:HD13	20:B:807:CLA:HMB3	1.94	0.49
20:A:847:CLA:HMB1	18:O:115:ILE:HD13	1.93	0.49
23:L:304:BCR:H15C	23:L:304:BCR:H362	1.92	0.49
6:B:348:VAL:HG22	20:B:808:CLA:C4	2.42	0.49
3:3:84:PHE:CE2	25:3:304:MGE:H2A1	2.48	0.48
28:A:824:CL0:H7	20:B:844:CLA:CBB	2.43	0.48
20:B:801:CLA:C4	20:B:801:CLA:H93	2.43	0.48
22:1:311:XAT:C18	25:1:324:MGE:H211	2.43	0.48
19:2:302:CHL:OMC	19:2:309:CHL:HAC1	2.12	0.48
21:3:301:LUT:H3	20:3:317:CLA:HMA1	1.95	0.48
5:A:88:MET:N	5:A:88:MET:HE2	2.29	0.48
5:A:213:HIS:O	5:A:217:VAL:N	2.44	0.48
20:A:831:CLA:C2D	25:N:201:MGE:H2B1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:814:CLA:HMB2	20:B:816:CLA:H93	1.94	0.48
19:1:317:CHL:H12	4:4:152:TYR:HB2	1.96	0.48
25:3:306:MGE:H9A1	20:3:312:CLA:HAC2	1.95	0.48
4:4:216:PHE:CE1	22:4:318:XAT:H10	2.48	0.48
6:B:182:LEU:HD11	20:B:803:CLA:H43	1.95	0.48
6:B:519:VAL:HG23	20:B:844:CLA:H141	1.94	0.48
6:B:545:LYS:NZ	9:E:88:SER:O	2.45	0.48
23:L:303:BCR:H372	23:L:303:BCR:H19C	1.95	0.48
1:1:59:PHE:CD2	19:1:317:CHL:HMC	2.49	0.48
20:1:304:CLA:HAB	21:1:310:LUT:H32	1.95	0.48
21:1:323:LUT:C8	21:1:323:LUT:H171	2.44	0.48
3:3:166:GLN:CB	3:3:174:MET:HE3	2.44	0.48
3:3:167:ASP:HB2	19:3:313:CHL:HAC1	1.94	0.48
19:4:305:CHL:HHB	23:4:319:BCR:H373	1.96	0.48
21:1:323:LUT:H28	21:1:323:LUT:H361	1.96	0.48
21:2:310:LUT:H391	21:2:310:LUT:C32	2.35	0.48
3:3:70:PHE:HE2	22:3:302:XAT:H183	1.78	0.48
3:3:128:TRP:HE3	22:3:302:XAT:H241	1.78	0.48
20:B:830:CLA:HBC3	26:B:832:PQN:H2M2	1.95	0.48
4:4:101:ARG:NH1	19:4:307:CHL:OBD	2.42	0.48
5:A:10:VAL:CG2	20:A:836:CLA:HMA2	2.43	0.48
6:B:255:LEU:HD11	20:B:805:CLA:HBC1	1.95	0.48
3:3:47:ARG:NH2	3:3:60:LEU:O	2.46	0.48
19:4:315:CHL:HAA2	19:4:315:CHL:HBD	1.96	0.48
5:A:118:ILE:HB	23:J:101:BCR:H322	1.96	0.48
20:B:810:CLA:HMC2	23:B:834:BCR:H312	1.96	0.48
2:2:120:ILE:CG1	22:2:311:XAT:H361	2.43	0.48
3:3:226:LEU:HG	21:3:301:LUT:H11	1.96	0.48
5:A:92:GLY:O	5:A:96:SER:OG	2.27	0.48
10:F:172:ILE:O	10:F:175:SER:OG	2.31	0.48
23:2:312:BCR:H403	23:2:312:BCR:H23C	1.95	0.47
4:4:156:ARG:NH2	19:4:315:CHL:HMC	2.29	0.47
19:2:318:CHL:HBB2	20:2:319:CLA:HAC1	1.96	0.47
3:3:234:PHE:CZ	21:3:301:LUT:H173	2.49	0.47
5:A:415:ASP:OD2	5:A:418:THR:OG1	2.29	0.47
5:A:701:TRP:CH2	20:B:821:CLA:HED3	2.50	0.47
28:A:824:CL0:H71	28:A:824:CL0:O2D	2.13	0.47
20:B:815:CLA:H43	20:B:824:CLA:HBB2	1.95	0.47
10:F:189:VAL:HG22	14:J:14:LEU:HD11	1.97	0.47
2:2:112:TRP:CE2	19:2:302:CHL:HED2	2.49	0.47
23:A:816:BCR:H362	20:A:848:CLA:HBA1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:817:BCR:H331	23:A:817:BCR:C8	2.44	0.47
24:A:820:LHG:H121	25:A:823:MGE:H2B2	1.95	0.47
20:B:830:CLA:H91	23:L:302:BCR:H353	1.97	0.47
26:B:832:PQN:H142	23:B:838:BCR:H271	1.95	0.47
12:H:82:LEU:O	12:H:83:GLN:HB2	2.15	0.47
2:2:137:TRP:CZ3	22:2:311:XAT:H383	2.48	0.47
23:L:302:BCR:C8	23:L:302:BCR:H331	2.45	0.47
23:1:312:BCR:H331	23:1:312:BCR:C8	2.45	0.47
19:2:318:CHL:HED1	3:3:159:PHE:O	2.15	0.47
20:A:831:CLA:C4D	25:N:201:MGE:H2B1	2.44	0.47
1:1:109:GLN:NE2	22:1:311:XAT:H241	2.29	0.47
22:3:302:XAT:H372	20:3:310:CLA:CHB	2.45	0.47
22:3:302:XAT:C12	20:3:309:CLA:HMB3	2.44	0.47
6:B:54:LEU:HD21	20:B:803:CLA:O1A	2.15	0.47
6:B:301:ILE:HG21	20:B:814:CLA:HBC2	1.97	0.47
6:B:696:LYS:HD2	7:C:79:LEU:HD13	1.97	0.47
1:1:43:PRO:O	19:1:317:CHL:HED1	2.14	0.47
6:B:609:PHE:O	6:B:613:SER:OG	2.23	0.47
20:B:804:CLA:H18	23:B:839:BCR:H383	1.97	0.47
10:F:143:GLN:CD	25:J:102:MGE:H2B1	2.40	0.47
11:G:58:SER:HA	25:G:204:MGE:H3A2	1.96	0.47
20:A:826:CLA:CAC	20:B:845:CLA:HMC3	2.45	0.47
29:B:840:DGD:O5D	29:B:840:DGD:O4D	2.23	0.47
1:1:104:ASN:OD1	1:1:107:GLN:NE2	2.48	0.47
22:1:311:XAT:H373	20:1:320:CLA:C1B	2.45	0.47
5:A:534:HIS:CE1	20:A:805:CLA:ND	2.82	0.47
6:B:65:LEU:HD12	6:B:142:LEU:HD12	1.96	0.47
6:B:718:ILE:HD13	20:B:817:CLA:HMC3	1.96	0.47
17:N:118:VAL:N	17:N:122:SER:OG	2.48	0.47
23:O:203:BCR:H382	23:O:203:BCR:H23C	1.97	0.47
1:1:233:ARG:NH2	25:1:315:MGE:O4D	2.48	0.46
19:1:317:CHL:HBB2	20:1:318:CLA:CHD	2.44	0.46
3:3:226:LEU:HD23	21:3:301:LUT:H203	1.97	0.46
6:B:125:TYR:O	6:B:130:ARG:NH1	2.48	0.46
22:2:311:XAT:H391	22:2:311:XAT:H31	1.35	0.46
25:3:306:MGE:H3G2	5:A:242:LEU:CD2	2.45	0.46
5:A:387:LEU:CD1	20:A:853:CLA:HED3	2.46	0.46
20:B:814:CLA:H92	20:B:816:CLA:C4	2.44	0.46
21:1:323:LUT:H41	4:4:158:TRP:CZ2	2.50	0.46
5:A:690:GLY:N	6:B:568:CYS:O	2.47	0.46
23:B:839:BCR:H382	23:B:839:BCR:H23C	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:F:301:BCR:C8	23:F:301:BCR:H331	2.45	0.46
3:3:96:PHE:CZ	19:3:313:CHL:HED2	2.51	0.46
20:A:841:CLA:H91	20:K:204:CLA:HBC3	1.96	0.46
20:4:309:CLA:CBB	21:4:317:LUT:H34	2.45	0.46
5:A:471:ASP:OD1	5:A:477:GLN:NE2	2.45	0.46
6:B:65:LEU:CD1	6:B:142:LEU:HD12	2.46	0.46
20:B:833:CLA:HMD3	20:B:846:CLA:HMA2	1.97	0.46
23:B:834:BCR:H331	23:B:834:BCR:C8	2.46	0.46
20:1:303:CLA:HMB2	29:G:202:DGD:HA22	1.98	0.46
25:3:306:MGE:C1G	25:3:306:MGE:H1D	2.46	0.46
23:A:857:BCR:H402	23:F:301:BCR:H332	1.97	0.46
20:B:801:CLA:H92	20:B:829:CLA:H43	1.98	0.46
23:B:835:BCR:H383	23:B:835:BCR:H23C	1.97	0.46
23:B:836:BCR:C39	23:B:837:BCR:H383	2.44	0.46
23:F:301:BCR:C23	23:F:301:BCR:H403	2.45	0.46
2:2:121:PHE:CD2	21:2:310:LUT:H30	2.51	0.46
1:1:106:VAL:CG1	19:1:301:CHL:HED2	2.43	0.46
3:3:234:PHE:CE1	21:3:301:LUT:H173	2.51	0.46
25:3:306:MGE:H3B1	20:A:840:CLA:CBC	2.45	0.46
5:A:74:HIS:ND1	20:A:837:CLA:OBD	2.44	0.46
15:K:94:THR:OG1	15:K:100:PHE:O	2.22	0.46
1:1:75:ARG:NH1	29:G:202:DGD:O1B	2.49	0.46
1:1:200:VAL:CG1	21:1:323:LUT:H26	2.44	0.46
20:A:825:CLA:HMD1	6:B:578:LEU:HB3	1.98	0.46
12:H:77:SER:C	12:H:78:PRO:O	2.57	0.46
4:4:222:GLN:NE2	21:4:317:LUT:H42	2.30	0.46
23:L:301:BCR:H383	23:L:301:BCR:H23C	1.97	0.46
23:O:202:BCR:H331	23:O:202:BCR:HC8	1.98	0.46
5:A:477:GLN:CG	25:A:823:MGE:H6D1	2.46	0.45
6:B:61:THR:HB	6:B:142:LEU:HD13	1.98	0.45
25:1:324:MGE:H1G2	25:1:324:MGE:H2B2	1.98	0.45
5:A:536:ILE:HD12	28:A:824:CL0:H63	1.98	0.45
22:3:302:XAT:H371	20:3:310:CLA:HMB2	1.98	0.45
21:4:317:LUT:C8	21:4:317:LUT:H181	2.45	0.45
22:4:318:XAT:H35	22:4:318:XAT:H401	1.83	0.45
22:3:302:XAT:H361	22:3:302:XAT:H27	1.62	0.45
6:B:2:GLU:OE2	6:B:7:ARG:NH2	2.48	0.45
20:B:827:CLA:C9	20:B:828:CLA:HBC1	2.46	0.45
21:2:310:LUT:C8	21:2:310:LUT:H161	2.46	0.45
5:A:455:HIS:HB2	20:A:802:CLA:C4C	2.47	0.45
23:A:815:BCR:H331	23:A:815:BCR:C8	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:83:GLN:HG3	20:H:201:CLA:C1C	2.46	0.45
21:1:323:LUT:H41	4:4:158:TRP:HZ2	1.80	0.45
23:B:837:BCR:H331	23:B:837:BCR:C8	2.46	0.45
20:A:845:CLA:H162	20:A:855:CLA:HBC1	1.97	0.45
6:B:74:PHE:CE2	6:B:78:ILE:HD11	2.52	0.45
16:L:156:SER:OG	16:L:171:ASP:O	2.31	0.45
19:1:317:CHL:HAA1	19:1:317:CHL:HBD	1.99	0.45
21:1:323:LUT:H361	21:1:323:LUT:C28	2.46	0.45
25:3:306:MGE:H1D	25:3:306:MGE:H1G1	1.97	0.45
5:A:570:ARG:NH1	24:A:819:LHG:O10	2.50	0.45
20:1:302:CLA:C1	21:1:310:LUT:H383	2.47	0.45
20:3:310:CLA:C1	20:3:311:CLA:HMD2	2.47	0.45
20:A:812:CLA:CMA	6:B:616:LEU:HD13	2.47	0.45
20:1:303:CLA:CMB	29:G:202:DGD:HA22	2.47	0.45
2:2:199:LEU:HD23	19:2:309:CHL:OBD	2.17	0.45
4:4:230:PRO:O	21:4:317:LUT:O3	2.27	0.45
23:4:319:BCR:H403	23:4:319:BCR:H23C	1.99	0.45
23:4:320:BCR:C8	23:4:320:BCR:H321	2.47	0.45
6:B:658:ALA:HB3	20:B:845:CLA:HBB2	1.98	0.45
12:H:77:SER:HA	16:L:90:VAL:HG22	1.98	0.45
25:J:102:MGE:H2A1	25:J:102:MGE:H1G2	1.73	0.45
20:1:303:CLA:HMB2	29:G:202:DGD:HA42	1.98	0.44
20:2:307:CLA:C3B	21:2:310:LUT:H383	2.47	0.44
3:3:100:THR:HB	22:3:302:XAT:H402	1.98	0.44
23:A:818:BCR:H402	20:B:822:CLA:HMB2	1.98	0.44
26:B:832:PQN:H142	23:B:838:BCR:C27	2.46	0.44
23:G:201:BCR:H331	23:G:201:BCR:C8	2.47	0.44
19:1:317:CHL:H43	4:4:148:ILE:HG22	1.98	0.44
4:4:127:TRP:HE3	22:4:318:XAT:H173	1.83	0.44
28:A:824:CL0:H72	28:A:824:CL0:H10	1.73	0.44
6:B:115:ILE:O	20:B:850:CLA:HMD3	2.18	0.44
11:G:107:SER:OG	11:G:113:PHE:O	2.25	0.44
22:1:311:XAT:H191	22:1:311:XAT:H11	1.58	0.44
3:3:165:PHE:CZ	25:3:304:MGE:H3G2	2.52	0.44
20:4:303:CLA:CBC	19:4:306:CHL:HAB	2.46	0.44
24:A:820:LHG:C13	25:A:823:MGE:H2B2	2.47	0.44
20:B:808:CLA:H201	20:B:809:CLA:H101	2.00	0.44
21:1:310:LUT:H171	21:1:310:LUT:C8	2.36	0.44
3:3:70:PHE:CE2	22:3:302:XAT:H183	2.53	0.44
19:4:305:CHL:O1D	19:4:305:CHL:H2A	2.18	0.44
6:B:718:ILE:HD13	20:B:817:CLA:HMC2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:812:CLA:CMB	29:G:202:DGD:HB52	2.47	0.44
25:F:303:MGE:H1D	25:F:303:MGE:H2G	1.79	0.44
19:2:302:CHL:HBB2	19:2:309:CHL:CMC	2.47	0.44
3:3:165:PHE:CE2	25:3:305:MGE:H6D2	2.51	0.44
3:3:238:ALA:C	25:3:306:MGE:H2A1	2.42	0.44
5:A:728:THR:HG23	24:A:819:LHG:H342	1.98	0.44
20:A:847:CLA:CMB	18:O:115:ILE:HD13	2.47	0.44
11:G:75:ARG:NH2	11:G:112:GLY:O	2.51	0.44
23:G:201:BCR:H11C	23:G:201:BCR:H341	1.88	0.44
26:B:832:PQN:H111	23:B:838:BCR:H393	2.00	0.44
19:1:317:CHL:HED1	4:4:159:GLN:HE21	1.81	0.44
2:2:250:LEU:HD22	21:2:310:LUT:H362	2.00	0.44
23:1:312:BCR:H23C	23:1:312:BCR:H403	1.99	0.44
19:4:306:CHL:H3A	19:4:306:CHL:HBA2	1.36	0.44
6:B:587:ILE:CD1	20:B:815:CLA:HMD1	2.48	0.44
20:2:308:CLA:O1A	19:2:318:CHL:H102	2.18	0.44
21:3:301:LUT:H171	21:3:301:LUT:C8	2.35	0.44
5:A:701:TRP:CD1	10:F:222:ILE:HG21	2.53	0.44
25:A:823:MGE:H1G2	25:A:823:MGE:H3	1.82	0.44
23:A:857:BCR:H321	23:A:857:BCR:C8	2.48	0.44
20:B:816:CLA:HMD1	20:B:826:CLA:CHB	2.48	0.44
24:1:314:LHG:H252	25:1:324:MGE:H4A2	2.00	0.43
5:A:393:TRP:CD1	20:A:852:CLA:HAB	2.52	0.43
24:A:820:LHG:C12	25:A:823:MGE:H2B2	2.47	0.43
20:B:801:CLA:H92	20:B:829:CLA:C4	2.48	0.43
2:2:236:TRP:CZ2	19:2:301:CHL:HBA2	2.53	0.43
20:B:809:CLA:C2	20:B:816:CLA:H91	2.48	0.43
23:L:303:BCR:H331	23:L:303:BCR:C8	2.47	0.43
3:3:114:LEU:HD23	3:3:119:LEU:HD12	2.01	0.43
19:4:305:CHL:H3A	23:4:319:BCR:C21	2.49	0.43
20:B:807:CLA:H141	20:B:825:CLA:HAA2	2.01	0.43
26:B:832:PQN:H142	23:B:838:BCR:C28	2.48	0.43
20:B:844:CLA:H121	20:B:844:CLA:H92	1.99	0.43
19:3:313:CHL:H3A	19:3:313:CHL:HBA2	1.75	0.43
4:4:80:LEU:HD12	22:4:318:XAT:H372	1.99	0.43
6:B:85:ARG:HB3	6:B:115:ILE:HD12	1.98	0.43
6:B:546:LEU:O	6:B:564:ARG:NH2	2.47	0.43
20:B:853:CLA:HBA1	11:G:97:ARG:HE	1.82	0.43
8:D:182:ASN:ND2	8:D:203:PHE:O	2.45	0.43
2:2:121:PHE:CE2	21:2:310:LUT:H28	2.52	0.43
3:3:94:GLU:HG2	3:3:221:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:543:VAL:HG11	5:A:596:TRP:CZ2	2.53	0.43
5:A:600:SER:O	5:A:604:VAL:HG23	2.18	0.43
3:3:166:GLN:HB3	3:3:174:MET:HE3	2.00	0.43
5:A:362:ILE:HG23	5:A:392:MET:SD	2.59	0.43
20:A:812:CLA:HED2	28:A:824:CL0:H15	2.00	0.43
20:B:815:CLA:HMB1	20:B:815:CLA:HBB1	2.01	0.43
7:C:23:THR:HG21	7:C:49:VAL:HG13	2.01	0.43
20:1:307:CLA:NB	21:1:310:LUT:H183	2.34	0.43
2:2:200:TRP:HZ3	19:2:302:CHL:HAB	1.84	0.43
19:4:307:CHL:H3A	19:4:307:CHL:HBA2	1.31	0.43
5:A:150:ILE:HD11	20:A:838:CLA:HMA2	2.00	0.43
20:A:833:CLA:HAA2	23:A:857:BCR:H363	2.01	0.43
1:1:110:GLU:HG3	19:1:301:CHL:HED1	2.00	0.43
23:2:312:BCR:H373	19:2:322:CHL:HHB	2.00	0.43
19:4:305:CHL:HBB1	22:4:318:XAT:H162	2.01	0.43
6:B:257:LEU:HD13	20:B:807:CLA:CMB	2.47	0.43
1:1:87:ALA:HB2	22:1:311:XAT:H32	2.01	0.43
22:2:311:XAT:H373	20:2:321:CLA:C2B	2.49	0.43
20:B:827:CLA:C8	20:B:828:CLA:HBC1	2.48	0.43
23:B:836:BCR:C8	23:B:836:BCR:H321	2.49	0.43
23:G:203:BCR:H19C	23:G:203:BCR:H373	2.01	0.43
20:2:307:CLA:C12	19:2:318:CHL:H112	2.49	0.43
23:2:312:BCR:H15C	23:2:312:BCR:H351	1.90	0.43
21:3:301:LUT:H32	20:3:315:CLA:HAB	2.01	0.43
5:A:556:ARG:O	5:A:565:ALA:N	2.52	0.43
6:B:453:ILE:HD11	20:B:823:CLA:CHB	2.49	0.43
23:F:302:BCR:H383	23:F:302:BCR:H23C	2.00	0.43
12:H:77:SER:HA	16:L:90:VAL:CG2	2.49	0.43
19:1:317:CHL:OBD	4:4:156:ARG:NH1	2.49	0.42
19:4:306:CHL:H2A	19:4:306:CHL:O2D	2.17	0.42
5:A:317:HIS:CB	5:A:322:ILE:HD11	2.49	0.42
20:A:830:CLA:HMB3	20:A:854:CLA:HBB2	2.01	0.42
1:1:138:GLU:OE1	19:1:301:CHL:HMC	2.19	0.42
4:4:189:VAL:CG1	19:4:315:CHL:HMD2	2.48	0.42
5:A:604:VAL:HG21	20:A:805:CLA:HBB2	2.01	0.42
6:B:646:TRP:CZ2	6:B:726:ILE:HG21	2.54	0.42
20:B:805:CLA:O2A	23:B:835:BCR:H333	2.19	0.42
23:F:302:BCR:H331	23:F:302:BCR:C8	2.48	0.42
25:1:316:MGE:H2A1	11:G:131:TYR:HE2	1.85	0.42
21:2:310:LUT:H7	21:2:310:LUT:H181	1.77	0.42
23:A:816:BCR:H23C	23:A:816:BCR:H392	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:560:ASP:OD2	6:B:564:ARG:NH1	2.48	0.42
11:G:135:THR:HA	11:G:138:ASN:ND2	2.34	0.42
25:G:204:MGE:O1B	25:G:204:MGE:H3G1	2.20	0.42
23:L:304:BCR:C5	23:L:304:BCR:H343	2.49	0.42
1:1:149:ARG:NH2	20:1:303:CLA:O2D	2.49	0.42
2:2:114:MET:HG3	2:2:225:GLY:HA2	2.01	0.42
19:2:301:CHL:CBB	19:2:322:CHL:HBB2	2.49	0.42
5:A:468:MET:HE2	5:A:639:ILE:HD12	2.01	0.42
20:A:848:CLA:HHC	20:A:848:CLA:HBB1	2.02	0.42
16:L:201:LEU:HG	20:L:307:CLA:HED3	2.01	0.42
22:1:311:XAT:H163	20:1:318:CLA:H2	2.00	0.42
19:4:305:CHL:CBB	22:4:318:XAT:H162	2.49	0.42
20:A:846:CLA:HMA1	20:A:847:CLA:HBD	2.00	0.42
16:L:107:LEU:HD22	16:L:134:LEU:HD23	2.01	0.42
2:2:160:ILE:HD13	23:2:312:BCR:H361	2.02	0.42
5:A:110:PRO:O	5:A:137:ILE:N	2.52	0.42
5:A:596:TRP:CH2	20:A:826:CLA:HAB	2.55	0.42
20:B:830:CLA:H91	23:L:302:BCR:C35	2.50	0.42
25:1:316:MGE:H2G	11:G:135:THR:HB	2.01	0.42
21:1:323:LUT:H391	21:1:323:LUT:H31	1.74	0.42
23:3:303:BCR:C8	23:3:303:BCR:H321	2.48	0.42
4:4:156:ARG:NH2	4:4:167:VAL:O	2.52	0.42
23:4:320:BCR:H321	23:4:320:BCR:HC8	2.02	0.42
6:B:172:GLU:OE1	6:B:172:GLU:N	2.52	0.42
20:B:825:CLA:HMB3	23:B:837:BCR:HC32	2.01	0.42
8:D:75:SER:O	8:D:118:ARG:NE	2.45	0.42
25:1:324:MGE:H2B2	25:1:324:MGE:H2G	1.79	0.42
23:4:320:BCR:C21	23:4:320:BCR:H361	2.50	0.42
23:B:834:BCR:H23C	23:B:834:BCR:C38	2.50	0.42
23:J:101:BCR:H392	23:J:101:BCR:C23	2.50	0.42
20:2:321:CLA:HMB1	20:2:321:CLA:HBB1	2.01	0.42
22:3:302:XAT:H12	20:3:308:CLA:HAB	2.02	0.42
20:A:806:CLA:HBC1	25:A:823:MGE:H2A1	2.01	0.42
20:B:803:CLA:HBD	20:B:847:CLA:H141	2.02	0.42
9:E:125:ASN:ND2	9:E:126:ASN:O	2.52	0.42
22:1:311:XAT:H7	20:1:318:CLA:H13	2.02	0.42
21:1:323:LUT:H191	21:1:323:LUT:H11	1.72	0.42
20:3:312:CLA:HMB3	20:3:312:CLA:HBB1	2.01	0.42
4:4:107:VAL:HG11	21:4:317:LUT:H12	2.01	0.42
4:4:223:HIS:ND1	20:4:316:CLA:H93	2.35	0.42
20:A:812:CLA:CED	6:B:620:LEU:HD13	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:389:HIS:HA	6:B:392:ILE:HD12	2.02	0.42
6:B:424:TRP:CZ3	20:B:828:CLA:HBC2	2.48	0.42
24:1:313:LHG:O5	19:1:317:CHL:HAC2	2.20	0.41
23:3:303:BCR:C23	23:3:303:BCR:H403	2.51	0.41
26:A:810:PQN:H111	26:A:810:PQN:H2M1	1.85	0.41
24:A:819:LHG:H221	20:A:830:CLA:HMD1	2.02	0.41
6:B:56:ILE:HD13	20:B:846:CLA:CBB	2.50	0.41
8:D:165:ASP:OD1	8:D:165:ASP:N	2.53	0.41
21:1:323:LUT:H7	21:1:323:LUT:H181	1.91	0.41
2:2:167:ARG:NH2	20:2:303:CLA:O1D	2.49	0.41
3:3:97:ASN:HD22	22:3:302:XAT:H35	1.84	0.41
4:4:207:ALA:HB3	20:4:310:CLA:OBD	2.20	0.41
5:A:291:ILE:HG23	20:A:843:CLA:HMA3	2.02	0.41
5:A:300:ILE:HG23	23:K:202:BCR:H312	2.01	0.41
5:A:399:ILE:HG23	23:A:817:BCR:C34	2.50	0.41
23:A:814:BCR:H403	23:A:814:BCR:H23C	2.02	0.41
6:B:192:GLY:O	6:B:196:HIS:ND1	2.53	0.41
6:B:535:VAL:HG13	23:B:836:BCR:C28	2.50	0.41
20:B:820:CLA:HMB2	20:B:821:CLA:C2D	2.50	0.41
8:D:96:VAL:HG21	12:H:56:PHE:CE1	2.55	0.41
21:1:323:LUT:H403	20:4:314:CLA:O2A	2.19	0.41
2:2:68:PHE:CD1	19:2:318:CHL:HMA3	2.56	0.41
20:2:304:CLA:H52	21:2:310:LUT:H10	2.01	0.41
25:3:304:MGE:H3A1	20:A:834:CLA:CMD	2.51	0.41
25:3:305:MGE:H1G2	25:3:305:MGE:H2A2	1.57	0.41
5:A:701:TRP:HH2	20:B:821:CLA:HED3	1.85	0.41
20:A:833:CLA:H41	25:N:201:MGE:H6B1	2.02	0.41
6:B:54:LEU:HD13	23:B:839:BCR:H401	2.02	0.41
6:B:430:GLY:HA2	6:B:525:LEU:HD22	2.02	0.41
20:B:803:CLA:H141	20:B:818:CLA:H93	2.03	0.41
20:B:851:CLA:HMB1	20:B:851:CLA:HBB1	2.02	0.41
23:L:302:BCR:H392	23:L:302:BCR:C23	2.50	0.41
23:1:312:BCR:H323	11:G:68:PHE:HB3	2.03	0.41
20:2:306:CLA:HMC3	21:2:310:LUT:H393	2.01	0.41
5:A:213:HIS:HB2	20:A:838:CLA:CHC	2.50	0.41
23:A:816:BCR:H361	20:A:849:CLA:CBB	2.50	0.41
20:B:809:CLA:HMD3	20:B:812:CLA:HAC1	2.03	0.41
20:B:813:CLA:HMD3	20:B:814:CLA:HHC	2.03	0.41
23:B:838:BCR:H401	20:B:845:CLA:O1D	2.20	0.41
10:F:149:PHE:O	10:F:153:GLY:N	2.50	0.41
1:1:64:LEU:HD21	25:1:324:MGE:H5B2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:311:XAT:C11	20:1:319:CLA:HMB3	2.51	0.41
2:2:223:LYS:NZ	20:2:305:CLA:O2D	2.49	0.41
19:4:315:CHL:HAB	23:4:319:BCR:C11	2.50	0.41
5:A:196:ASN:HB3	20:A:844:CLA:HMD2	2.03	0.41
6:B:355:LEU:O	20:B:807:CLA:HED1	2.20	0.41
6:B:652:PHE:O	6:B:656:VAL:HG23	2.21	0.41
26:B:832:PQN:H112	23:B:838:BCR:H281	2.03	0.41
3:3:200:PHE:HA	19:3:313:CHL:H11	2.03	0.41
4:4:75:ASN:N	20:4:302:CLA:OBD	2.47	0.41
19:4:305:CHL:HMB3	20:4:308:CLA:HBC2	2.01	0.41
21:4:317:LUT:H15	21:4:317:LUT:H201	1.94	0.41
5:A:679:ALA:HB3	20:A:825:CLA:HBB2	2.02	0.41
5:A:735:ILE:HG21	20:A:852:CLA:CMC	2.51	0.41
20:A:801:CLA:HMD3	23:L:301:BCR:H341	2.03	0.41
6:B:195:VAL:HG12	6:B:217:PRO:HB3	2.03	0.41
13:I:21:ILE:O	13:I:25:SER:OG	2.36	0.41
23:L:302:BCR:H331	23:L:302:BCR:HC8	2.01	0.41
1:1:59:PHE:HD2	20:1:318:CLA:HMD2	1.84	0.41
20:1:307:CLA:C4B	21:1:310:LUT:H183	2.51	0.41
22:1:311:XAT:H361	22:1:311:XAT:H27	1.62	0.41
20:1:319:CLA:HMD2	29:G:202:DGD:HA71	2.02	0.41
2:2:250:LEU:HD13	21:2:310:LUT:H221	2.03	0.41
5:A:353:ASN:ND2	20:A:829:CLA:OBD	2.45	0.41
5:A:717:LEU:CD2	26:A:810:PQN:H152	2.47	0.41
20:B:821:CLA:HBC2	20:B:828:CLA:CMC	2.46	0.41
20:2:304:CLA:O2A	21:2:310:LUT:H173	2.21	0.41
20:2:307:CLA:C4B	21:2:310:LUT:H383	2.51	0.41
21:2:310:LUT:H173	21:2:310:LUT:O3	2.19	0.41
3:3:226:LEU:HG	21:3:301:LUT:H191	2.03	0.41
21:4:317:LUT:H31	21:4:317:LUT:H391	1.98	0.41
12:H:56:PHE:HA	12:H:64:THR:HG23	2.03	0.41
1:1:136:VAL:CG1	25:1:316:MGE:H4A2	2.49	0.41
22:1:311:XAT:H403	20:1:319:CLA:CBC	2.51	0.41
22:1:311:XAT:H391	22:1:311:XAT:H31	1.48	0.41
25:1:315:MGE:H2D	20:F:306:CLA:CMD	2.50	0.41
22:2:311:XAT:C11	20:2:319:CLA:HMC2	2.51	0.41
19:2:318:CHL:HBC3	19:2:318:CHL:HHD	2.03	0.41
4:4:211:LEU:HG	21:4:317:LUT:H11	2.02	0.41
23:4:320:BCR:H361	23:4:320:BCR:H21C	2.02	0.41
5:A:308:MET:HE1	20:A:845:CLA:C3D	2.51	0.41
5:A:400:VAL:HG11	5:A:594:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:538:ALA:HB1	20:A:806:CLA:HMB2	2.02	0.41
6:B:195:VAL:HG21	20:B:805:CLA:HBC2	2.03	0.41
6:B:701:SER:O	6:B:705:ALA:N	2.48	0.41
2:2:109:HIS:CG	20:2:303:CLA:HMD1	2.56	0.41
20:2:308:CLA:CAD	19:2:318:CHL:H91	2.51	0.41
20:4:304:CLA:HMB1	20:4:304:CLA:HBB1	2.02	0.41
20:A:809:CLA:H43	20:A:827:CLA:HBA2	2.02	0.41
6:B:666:SER:O	26:B:832:PQN:H9	2.20	0.41
23:O:202:BCR:H341	20:O:206:CLA:HBB1	2.03	0.41
1:1:84:CYS:SG	1:1:192:MET:HE2	2.61	0.40
1:1:150:THR:OG1	20:1:303:CLA:HMA1	2.21	0.40
4:4:61:LEU:CD2	25:4:322:MGE:H2B2	2.51	0.40
20:A:809:CLA:C2D	20:A:809:CLA:H42	2.51	0.40
20:A:812:CLA:HBC2	6:B:585:ASN:HB2	2.03	0.40
20:B:808:CLA:H141	20:B:808:CLA:H172	2.02	0.40
1:1:90:ALA:HB2	22:1:311:XAT:H31	2.04	0.40
20:1:307:CLA:HMA1	21:1:310:LUT:H3	2.03	0.40
25:1:315:MGE:H6D2	25:1:315:MGE:H1D	1.87	0.40
25:1:316:MGE:H2A1	11:G:131:TYR:CE2	2.56	0.40
3:3:165:PHE:CD2	20:3:320:CLA:HBC2	2.57	0.40
4:4:99:ASN:CG	20:4:308:CLA:HMD1	2.45	0.40
20:4:312:CLA:HHB	21:4:317:LUT:H162	2.03	0.40
5:A:84:TRP:NE1	20:A:852:CLA:OBD	2.54	0.40
6:B:484:PRO:HB2	20:B:825:CLA:HMD3	2.03	0.40
20:B:852:CLA:H11	20:B:852:CLA:HMA2	2.03	0.40
11:G:128:VAL:HG21	25:G:204:MGE:H102	2.02	0.40
23:K:201:BCR:H23C	23:K:201:BCR:C38	2.51	0.40
16:L:117:LEU:O	16:L:120:THR:OG1	2.32	0.40
20:B:846:CLA:HBB1	20:B:846:CLA:HMB1	2.03	0.40
8:D:151:ARG:O	8:D:159:GLN:N	2.44	0.40
23:G:203:BCR:H372	20:G:206:CLA:C2C	2.51	0.40
23:I:102:BCR:H331	23:I:102:BCR:C8	2.51	0.40
23:O:203:BCR:H351	23:O:203:BCR:H15C	1.82	0.40
20:1:304:CLA:HMB1	20:1:304:CLA:HBB1	2.03	0.40
22:1:311:XAT:H12	20:1:318:CLA:CAB	2.52	0.40
25:1:316:MGE:H202	20:G:205:CLA:CAB	2.51	0.40
2:2:126:LEU:HD22	2:2:131:ILE:HD12	2.03	0.40
19:2:318:CHL:H62	19:2:318:CHL:H2	1.84	0.40
3:3:164:ARG:NH1	20:3:314:CLA:O1D	2.50	0.40
20:3:311:CLA:H112	19:3:313:CHL:HMA1	2.03	0.40
23:A:816:BCR:H361	23:A:816:BCR:H20C	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:661:PHE:HB3	20:B:845:CLA:HMC2	2.04	0.40
20:B:812:CLA:H42	29:G:202:DGD:HA32	2.03	0.40
20:B:823:CLA:HBB1	20:B:823:CLA:HMB3	2.04	0.40
20:3:311:CLA:H172	19:3:313:CHL:HED3	2.04	0.40
19:4:305:CHL:HBB2	19:4:306:CHL:HBB1	2.03	0.40
5:A:169:LEU:HD22	20:A:834:CLA:HBC1	2.03	0.40
5:A:379:THR:HG21	5:A:515:VAL:HB	2.02	0.40
5:A:706:LEU:CD1	23:F:302:BCR:H342	2.52	0.40
20:A:831:CLA:HMB3	20:A:832:CLA:HHB	2.03	0.40
20:F:304:CLA:H2	14:J:15:SER:OG	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	198/200 (99%)	194 (98%)	4 (2%)	0	100	100
2	2	205/208 (99%)	194 (95%)	11 (5%)	0	100	100
3	3	221/223 (99%)	210 (95%)	11 (5%)	0	100	100
4	4	196/198 (99%)	189 (96%)	7 (4%)	0	100	100
5	A	740/744 (100%)	707 (96%)	30 (4%)	3 (0%)	30	40
6	B	731/734 (100%)	709 (97%)	22 (3%)	0	100	100
7	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
8	D	141/143 (99%)	132 (94%)	7 (5%)	2 (1%)	9	11
9	E	63/68 (93%)	61 (97%)	2 (3%)	0	100	100
10	F	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
11	G	95/97 (98%)	88 (93%)	6 (6%)	1 (1%)	11	16
12	H	91/93 (98%)	81 (89%)	7 (8%)	3 (3%)	3	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	I	28/30 (93%)	28 (100%)	0	0	100	100
14	J	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
15	K	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
16	L	161/163 (99%)	154 (96%)	5 (3%)	2 (1%)	10	14
17	N	82/84 (98%)	79 (96%)	3 (4%)	0	100	100
18	O	90/92 (98%)	81 (90%)	9 (10%)	0	100	100
All	All	3404/3448 (99%)	3264 (96%)	129 (4%)	11 (0%)	37	48

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	13	VAL
5	A	348	ALA
5	A	720	ILE
8	D	163	PRO
16	L	57	ILE
12	H	83	GLN
12	H	78	PRO
12	H	79	TYR
8	D	158	VAL
16	L	52	GLN
11	G	50	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	162/162 (100%)	159 (98%)	3 (2%)	50	69
2	2	165/165 (100%)	163 (99%)	2 (1%)	63	79
3	3	177/177 (100%)	174 (98%)	3 (2%)	53	72
4	4	169/169 (100%)	164 (97%)	5 (3%)	36	56
5	A	602/604 (100%)	595 (99%)	7 (1%)	63	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	B	599/601 (100%)	584 (98%)	15 (2%)	42	61
7	C	69/71 (97%)	69 (100%)	0	100	100
8	D	121/121 (100%)	120 (99%)	1 (1%)	73	85
9	E	57/60 (95%)	54 (95%)	3 (5%)	20	33
10	F	127/127 (100%)	124 (98%)	3 (2%)	43	63
11	G	81/81 (100%)	79 (98%)	2 (2%)	42	61
12	H	76/76 (100%)	75 (99%)	1 (1%)	61	78
13	I	26/26 (100%)	25 (96%)	1 (4%)	29	46
14	J	38/38 (100%)	38 (100%)	0	100	100
15	K	64/64 (100%)	63 (98%)	1 (2%)	55	74
16	L	126/126 (100%)	123 (98%)	3 (2%)	43	63
17	N	73/73 (100%)	73 (100%)	0	100	100
18	O	77/77 (100%)	77 (100%)	0	100	100
All	All	2809/2818 (100%)	2759 (98%)	50 (2%)	51	71

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	55	SER
1	1	81	VAL
1	1	133	THR
2	2	80	SER
2	2	94	SER
3	3	126	ILE
3	3	139	THR
3	3	168	TRP
4	4	167	VAL
4	4	189	VAL
4	4	235	LEU
4	4	245	THR
4	4	246	ILE
5	A	267	SER
5	A	361	THR
5	A	455	HIS
5	A	495	THR
5	A	503	THR
5	A	582	CYS

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Mol	Chain	Res	Type
5	A	619	THR
6	B	10	GLN
6	B	12	LEU
6	B	76	SER
6	B	113	VAL
6	B	240	SER
6	B	246	THR
6	B	258	LEU
6	B	305	LEU
6	B	429	LEU
6	B	476	ILE
6	B	570	ILE
6	B	577	TYR
6	B	599	ILE
6	B	668	ARG
6	B	701	SER
8	D	150	TYR
9	E	96	SER
9	E	111	VAL
9	E	123	SER
10	F	114	LYS
10	F	175	SER
10	F	217	VAL
11	G	69	VAL
11	G	78	VAL
12	H	73	SER
13	I	25	SER
15	K	64	LEU
16	L	53	VAL
16	L	57	ILE
16	L	166	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	107	GLN
2	2	102	ASN
3	3	48	GLN
3	3	166	GLN
4	4	99	ASN
4	4	227	GLN
4	4	244	ASN

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Mol	Chain	Res	Type
5	A	704	ASN
6	B	95	HIS
6	B	231	ASN
6	B	350	GLN
8	D	177	GLN
11	G	114	ASN
11	G	126	HIS
12	H	83	GLN
16	L	55	GLN
16	L	123	HIS
18	O	68	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

244 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
20	CLA	4	302	4	64,68,73	2.22	21 (32%)	77,107,113	2.97	29 (37%)
20	CLA	K	204	-	65,69,73	2.22	21 (32%)	78,108,113	2.97	29 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	3	307	-	62,67,73	2.14	19 (30%)	76,105,113	3.06	34 (44%)
20	CLA	B	816	6	69,73,73	2.13	20 (28%)	83,113,113	2.93	34 (40%)
19	CHL	2	302	-	51,55,74	2.20	17 (33%)	57,91,114	3.10	24 (42%)
20	CLA	B	814	-	69,73,73	2.05	19 (27%)	83,113,113	3.02	32 (38%)
20	CLA	A	801	5	67,71,73	2.10	20 (29%)	83,110,113	2.84	31 (37%)
20	CLA	G	206	-	54,58,73	2.43	20 (37%)	63,94,113	3.30	29 (46%)
19	CHL	2	322	-	50,54,74	2.25	18 (36%)	56,90,114	3.18	22 (39%)
23	BCR	G	203	-	41,41,41	1.93	8 (19%)	56,56,56	1.90	15 (26%)
20	CLA	A	838	5	49,53,73	2.50	21 (42%)	59,89,113	3.27	27 (45%)
19	CHL	4	315	4	48,53,74	2.26	17 (35%)	53,89,114	3.13	21 (39%)
20	CLA	A	807	5	59,63,73	2.29	20 (33%)	71,101,113	3.12	30 (42%)
22	XAT	3	302	-	39,47,47	0.85	0	54,74,74	7.29	26 (48%)
23	BCR	L	301	-	41,41,41	1.71	7 (17%)	56,56,56	1.54	7 (12%)
26	PQN	A	810	-	34,34,34	0.38	0	42,45,45	0.41	0
20	CLA	A	840	-	50,54,73	2.48	20 (40%)	60,90,113	3.29	27 (45%)
20	CLA	L	305	16	50,54,73	2.52	21 (42%)	60,90,113	3.23	29 (48%)
20	CLA	1	319	-	59,63,73	2.31	21 (35%)	71,101,113	3.12	30 (42%)
20	CLA	B	815	-	60,64,73	2.30	20 (33%)	72,102,113	3.04	29 (40%)
20	CLA	4	311	-	50,54,73	2.52	20 (40%)	60,90,113	3.30	26 (43%)
24	LHG	4	301	-	32,32,48	0.34	0	35,38,54	0.46	0
20	CLA	G	205	-	50,54,73	2.48	20 (40%)	60,90,113	3.26	27 (45%)
21	LUT	3	301	-	42,43,43	1.59	8 (19%)	51,60,60	1.57	11 (21%)
20	CLA	B	809	-	69,73,73	2.15	20 (28%)	83,113,113	2.64	26 (31%)
20	CLA	A	806	5	69,73,73	2.12	20 (28%)	83,113,113	2.77	29 (34%)
20	CLA	4	316	-	69,73,73	2.15	20 (28%)	83,113,113	2.94	31 (37%)
23	BCR	4	320	-	41,41,41	1.87	8 (19%)	56,56,56	1.81	17 (30%)
19	CHL	1	301	1	47,51,74	2.22	16 (34%)	52,86,114	3.21	22 (42%)
21	LUT	1	323	-	42,43,43	1.66	8 (19%)	51,60,60	2.22	13 (25%)
20	CLA	G	207	11	50,54,73	2.50	20 (40%)	60,90,113	3.28	26 (43%)
20	CLA	A	805	5	58,62,73	2.37	18 (31%)	69,99,113	3.15	29 (42%)
19	CHL	4	306	-	50,54,74	2.24	16 (32%)	56,90,114	3.18	21 (37%)
20	CLA	B	817	6	62,66,73	2.21	20 (32%)	74,104,113	3.07	30 (40%)
20	CLA	4	314	4	54,58,73	2.40	20 (37%)	65,95,113	3.22	30 (46%)
20	CLA	B	813	6	61,65,73	2.27	18 (29%)	73,103,113	2.98	29 (39%)
20	CLA	B	823	6	66,70,73	2.15	20 (30%)	79,109,113	2.87	29 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	LHG	A	819	-	48,48,48	0.30	0	51,54,54	0.38	0
20	CLA	4	312	4	59,63,73	2.34	20 (33%)	71,101,113	3.05	29 (40%)
20	CLA	O	207	-	63,67,73	2.25	20 (31%)	75,105,113	2.94	30 (40%)
19	CHL	2	309	2	47,51,74	2.25	16 (34%)	52,86,114	3.30	22 (42%)
29	DGD	O	201	-	54,54,67	0.96	2 (3%)	68,68,81	0.76	3 (4%)
20	CLA	A	855	5	59,63,73	2.27	19 (32%)	71,101,113	2.98	29 (40%)
20	CLA	4	304	-	49,53,73	2.58	20 (40%)	59,89,113	3.22	26 (44%)
19	CHL	4	307	-	50,54,74	2.22	17 (34%)	56,90,114	3.06	23 (41%)
24	LHG	1	313	20	48,48,48	0.27	0	51,54,54	0.40	0
23	BCR	1	312	-	41,41,41	1.83	8 (19%)	56,56,56	1.58	13 (23%)
20	CLA	B	806	6	61,65,73	2.28	19 (31%)	73,103,113	3.11	30 (41%)
20	CLA	4	308	4	50,54,73	2.42	21 (42%)	60,90,113	3.21	29 (48%)
20	CLA	L	306	16	56,60,73	2.34	19 (33%)	67,97,113	3.16	30 (44%)
20	CLA	2	306	-	49,53,73	2.55	19 (38%)	59,89,113	3.38	26 (44%)
23	BCR	L	303	-	41,41,41	1.96	8 (19%)	56,56,56	1.63	13 (23%)
20	CLA	2	303	2	49,53,73	2.49	19 (38%)	59,89,113	3.15	29 (49%)
20	CLA	B	805	-	49,53,73	2.52	20 (40%)	59,89,113	3.29	28 (47%)
20	CLA	A	839	5	49,53,73	2.54	21 (42%)	59,89,113	3.35	29 (49%)
20	CLA	L	307	-	50,54,73	2.50	21 (42%)	60,90,113	3.28	28 (46%)
20	CLA	1	302	-	54,58,73	2.40	19 (35%)	65,95,113	3.22	29 (44%)
24	LHG	O	204	-	24,24,48	0.49	0	28,29,54	0.65	1 (3%)
25	MGE	1	315	-	37,37,48	0.25	0	45,45,56	0.48	0
20	CLA	A	848	5	69,73,73	2.13	20 (28%)	83,113,113	2.84	32 (38%)
20	CLA	1	322	1	50,54,73	2.52	20 (40%)	60,90,113	3.27	27 (45%)
20	CLA	B	851	6	69,73,73	2.07	19 (27%)	83,113,113	2.73	28 (33%)
19	CHL	4	305	-	51,55,74	2.21	18 (35%)	57,91,114	3.09	23 (40%)
20	CLA	A	826	-	69,73,73	2.05	20 (28%)	83,113,113	2.59	27 (32%)
20	CLA	1	321	-	50,54,73	2.47	21 (42%)	60,90,113	3.24	28 (46%)
20	CLA	1	303	1	57,62,73	2.34	19 (33%)	68,100,113	2.94	28 (41%)
20	CLA	F	306	-	50,54,73	2.49	19 (38%)	60,90,113	3.25	26 (43%)
20	CLA	A	852	5	69,73,73	2.12	19 (27%)	83,113,113	2.80	27 (32%)
23	BCR	L	304	-	41,41,41	1.88	8 (19%)	56,56,56	2.15	16 (28%)
24	LHG	A	821	20	46,46,48	0.29	0	49,52,54	0.38	0
25	MGE	N	201	-	40,40,48	0.23	0	48,48,56	0.41	0
20	CLA	A	842	5	65,69,73	2.22	19 (29%)	78,108,113	2.97	31 (39%)
23	BCR	A	857	-	41,41,41	1.80	7 (17%)	56,56,56	1.67	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	3	315	3	59,63,73	2.31	20 (33%)	71,101,113	3.01	29 (40%)
20	CLA	3	317	3	62,66,73	2.25	20 (32%)	74,104,113	2.99	31 (41%)
24	LHG	2	315	20	31,31,48	0.33	0	34,37,54	0.41	0
20	CLA	B	811	6	61,65,73	2.29	19 (31%)	73,103,113	3.00	29 (39%)
20	CLA	1	304	1	59,63,73	2.33	20 (33%)	71,101,113	3.02	28 (39%)
20	CLA	A	804	5	55,59,73	2.34	19 (34%)	66,96,113	3.20	31 (46%)
20	CLA	A	841	5	63,67,73	2.25	20 (31%)	75,105,113	2.95	28 (37%)
20	CLA	F	304	-	69,73,73	2.09	19 (27%)	83,113,113	2.83	29 (34%)
23	BCR	F	301	-	41,41,41	1.89	8 (19%)	56,56,56	1.74	12 (21%)
23	BCR	K	201	-	41,41,41	1.76	8 (19%)	56,56,56	1.54	9 (16%)
20	CLA	3	311	-	69,73,73	2.13	21 (30%)	83,113,113	2.85	31 (37%)
24	LHG	2	316	-	36,36,48	0.40	0	40,41,54	0.51	1 (2%)
20	CLA	B	801	-	69,73,73	2.14	21 (30%)	83,113,113	2.85	31 (37%)
20	CLA	B	825	-	49,53,73	2.52	19 (38%)	59,89,113	3.10	27 (45%)
22	XAT	1	311	-	39,47,47	0.86	1 (2%)	54,74,74	3.66	25 (46%)
20	CLA	1	305	24	50,54,73	2.54	20 (40%)	60,90,113	3.24	28 (46%)
20	CLA	2	320	2	51,55,73	2.61	23 (45%)	61,91,113	3.41	27 (44%)
25	MGE	J	102	-	42,42,48	0.23	0	50,50,56	0.27	0
20	CLA	4	309	4	58,62,73	2.36	19 (32%)	69,99,113	3.11	29 (42%)
20	CLA	B	827	6	69,73,73	2.14	19 (27%)	83,113,113	2.82	30 (36%)
20	CLA	3	318	3	45,49,73	2.64	20 (44%)	54,84,113	3.43	27 (50%)
20	CLA	A	827	5	69,73,73	2.14	21 (30%)	83,113,113	2.87	30 (36%)
20	CLA	1	309	-	45,49,73	2.65	19 (42%)	54,84,113	3.51	27 (50%)
20	CLA	3	312	3	49,53,73	2.54	21 (42%)	59,89,113	3.28	27 (45%)
20	CLA	A	809	5	69,73,73	2.14	20 (28%)	83,113,113	2.87	27 (32%)
20	CLA	1	320	-	53,57,73	2.46	20 (37%)	62,93,113	3.22	28 (45%)
24	LHG	B	843	-	27,27,48	0.46	0	31,32,54	0.59	1 (3%)
27	SF4	C	102	7	0,12,12	-	-	-	-	-
29	DGD	J	104	-	67,67,67	0.87	2 (2%)	81,81,81	1.04	5 (6%)
20	CLA	B	830	6	69,73,73	2.12	20 (28%)	83,113,113	2.86	29 (34%)
20	CLA	A	837	5	69,73,73	2.15	19 (27%)	83,113,113	2.96	29 (34%)
20	CLA	A	846	5	50,54,73	2.47	20 (40%)	60,90,113	3.28	27 (45%)
24	LHG	B	841	-	31,31,48	0.32	0	34,37,54	0.46	0
20	CLA	A	847	5	60,64,73	2.28	19 (31%)	72,102,113	3.07	30 (41%)
20	CLA	A	825	-	69,73,73	2.08	19 (27%)	83,113,113	2.74	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	803	5	64,68,73	2.16	18 (28%)	76,106,113	2.87	30 (39%)
20	CLA	B	812	6	69,73,73	2.12	19 (27%)	83,113,113	2.76	31 (37%)
20	CLA	2	308	2	55,59,73	2.43	20 (36%)	66,96,113	3.19	29 (43%)
20	CLA	K	203	15	51,55,73	2.51	21 (41%)	61,91,113	3.29	29 (47%)
23	BCR	A	817	-	41,41,41	1.67	10 (24%)	56,56,56	1.55	9 (16%)
20	CLA	A	802	5	69,73,73	2.14	21 (30%)	83,113,113	2.84	32 (38%)
20	CLA	A	836	5	56,60,73	2.39	20 (35%)	67,97,113	3.19	28 (41%)
23	BCR	G	201	-	41,41,41	1.72	8 (19%)	56,56,56	1.61	11 (19%)
24	LHG	B	842	-	31,31,48	0.46	0	35,36,54	1.37	3 (8%)
23	BCR	A	818	-	40,40,41	1.58	6 (15%)	54,54,56	1.74	9 (16%)
20	CLA	A	833	5	69,73,73	2.10	20 (28%)	83,113,113	2.78	29 (34%)
20	CLA	F	305	-	50,54,73	2.49	19 (38%)	60,90,113	3.21	26 (43%)
20	CLA	J	103	14	50,54,73	2.52	20 (40%)	60,90,113	3.26	27 (45%)
20	CLA	A	829	5	68,72,73	2.13	19 (27%)	81,111,113	2.76	28 (34%)
20	CLA	B	846	6	49,53,73	2.55	21 (42%)	59,89,113	3.33	28 (47%)
23	BCR	B	837	-	41,41,41	1.77	8 (19%)	56,56,56	1.59	12 (21%)
23	BCR	B	838	-	41,41,41	1.85	8 (19%)	56,56,56	1.63	10 (17%)
27	SF4	A	813	5,6	0,12,12	-	-	-	-	-
20	CLA	2	307	2	66,70,73	2.20	21 (31%)	79,109,113	2.90	29 (36%)
20	CLA	4	303	-	50,54,73	2.50	20 (40%)	60,90,113	3.31	27 (45%)
20	CLA	A	811	24	59,63,73	2.32	19 (32%)	71,101,113	3.06	30 (42%)
20	CLA	B	810	6	52,56,73	2.43	18 (34%)	62,92,113	3.17	28 (45%)
20	CLA	A	856	5	60,64,73	2.30	21 (35%)	72,102,113	3.09	30 (41%)
20	CLA	B	802	6	49,53,73	2.54	20 (40%)	59,89,113	3.35	28 (47%)
20	CLA	B	831	-	69,73,73	2.13	19 (27%)	83,113,113	2.92	31 (37%)
23	BCR	O	202	-	41,41,41	1.73	6 (14%)	56,56,56	2.05	13 (23%)
20	CLA	B	829	-	69,73,73	2.14	19 (27%)	83,113,113	2.80	27 (32%)
20	CLA	3	316	-	50,54,73	2.50	19 (38%)	60,90,113	3.29	27 (45%)
29	DGD	G	202	-	40,40,67	1.04	2 (5%)	48,48,81	1.12	3 (6%)
20	CLA	A	845	-	69,73,73	2.13	20 (28%)	83,113,113	2.67	30 (36%)
20	CLA	B	849	6	56,60,73	2.37	20 (35%)	67,97,113	3.21	32 (47%)
23	BCR	A	814	-	41,41,41	1.72	8 (19%)	56,56,56	1.46	9 (16%)
20	CLA	A	854	5	69,73,73	2.05	17 (24%)	83,113,113	2.62	33 (39%)
20	CLA	B	828	6	51,55,73	2.42	19 (37%)	61,91,113	3.23	26 (42%)
23	BCR	L	302	-	41,41,41	1.76	9 (21%)	56,56,56	1.58	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	LHG	A	820	-	26,26,48	0.48	0	30,31,54	1.39	4 (13%)
20	CLA	1	308	1	50,54,73	2.51	21 (42%)	60,90,113	3.29	28 (46%)
20	CLA	3	319	-	50,54,73	2.51	20 (40%)	60,90,113	3.25	26 (43%)
23	BCR	A	815	-	41,41,41	1.68	7 (17%)	56,56,56	1.57	8 (14%)
21	LUT	1	310	-	42,43,43	1.60	8 (19%)	51,60,60	1.57	11 (21%)
19	CHL	1	317	1	55,59,74	2.13	16 (29%)	62,96,114	3.08	26 (41%)
20	CLA	K	205	15	50,54,73	2.57	20 (40%)	60,90,113	3.20	23 (38%)
20	CLA	A	850	-	62,66,73	2.25	20 (32%)	74,104,113	2.95	30 (40%)
23	BCR	3	303	-	41,41,41	1.73	9 (21%)	56,56,56	1.50	11 (19%)
23	BCR	K	202	-	41,41,41	1.86	6 (14%)	56,56,56	1.56	9 (16%)
26	PQN	B	832	-	31,31,34	0.39	0	38,41,45	0.40	0
20	CLA	O	208	-	49,53,73	2.55	21 (42%)	59,89,113	3.27	28 (47%)
20	CLA	B	822	6	69,73,73	2.09	20 (28%)	83,113,113	2.78	30 (36%)
28	CL0	A	824	5	67,72,73	2.01	19 (28%)	80,112,113	2.77	31 (38%)
20	CLA	1	318	1	69,73,73	2.19	20 (28%)	83,113,113	2.86	30 (36%)
23	BCR	B	834	-	41,41,41	1.72	7 (17%)	56,56,56	1.66	10 (17%)
19	CHL	2	318	2	62,66,74	1.99	17 (27%)	70,104,114	2.93	24 (34%)
23	BCR	4	319	-	41,41,41	1.78	8 (19%)	56,56,56	1.76	10 (17%)
22	XAT	2	311	-	39,47,47	1.01	1 (2%)	54,74,74	5.69	24 (44%)
20	CLA	B	821	6	60,64,73	2.27	19 (31%)	72,102,113	3.04	30 (41%)
20	CLA	3	309	-	64,68,73	2.23	20 (31%)	77,107,113	2.94	27 (35%)
23	BCR	J	101	-	41,41,41	1.82	9 (21%)	56,56,56	1.62	12 (21%)
20	CLA	A	808	5	69,73,73	2.12	20 (28%)	83,113,113	2.82	30 (36%)
20	CLA	B	850	6	69,73,73	2.07	18 (26%)	83,113,113	2.75	29 (34%)
20	CLA	A	851	5	69,73,73	2.14	20 (28%)	83,113,113	2.88	30 (36%)
25	MGE	4	322	-	40,40,48	0.22	0	48,48,56	0.43	0
25	MGE	A	823	-	34,34,48	0.25	0	42,42,56	0.55	0
19	CHL	2	301	-	51,55,74	2.20	15 (29%)	57,91,114	3.14	23 (40%)
20	CLA	H	201	12	63,67,73	2.25	20 (31%)	75,105,113	2.98	30 (40%)
20	CLA	N	202	17	60,64,73	2.32	20 (33%)	72,102,113	3.02	28 (38%)
20	CLA	B	826	6	54,58,73	2.40	20 (37%)	65,95,113	3.21	31 (47%)
23	BCR	B	835	-	41,41,41	1.79	7 (17%)	56,56,56	1.68	12 (21%)
20	CLA	B	852	-	69,73,73	2.15	20 (28%)	83,113,113	2.85	29 (34%)
20	CLA	3	310	-	53,57,73	2.45	20 (37%)	62,93,113	3.20	28 (45%)
25	MGE	1	316	-	40,40,48	0.23	0	48,48,56	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	831	5	56,60,73	2.35	20 (35%)	67,97,113	3.19	32 (47%)
20	CLA	A	849	-	69,73,73	2.10	21 (30%)	83,113,113	2.92	29 (34%)
25	MGE	G	204	-	48,48,48	0.23	0	56,56,56	0.40	0
20	CLA	B	845	-	69,73,73	2.06	17 (24%)	83,113,113	2.75	28 (33%)
20	CLA	A	812	-	69,73,73	2.07	20 (28%)	83,113,113	2.75	31 (37%)
20	CLA	B	847	6	69,73,73	2.14	19 (27%)	83,113,113	2.92	29 (34%)
23	BCR	2	312	-	41,41,41	1.81	7 (17%)	56,56,56	1.77	12 (21%)
24	LHG	A	822	-	41,41,48	0.38	0	45,46,54	0.53	1 (2%)
21	LUT	2	310	-	42,43,43	1.64	8 (19%)	51,60,60	1.65	12 (23%)
20	CLA	A	835	5,20	69,73,73	2.13	19 (27%)	83,113,113	2.86	31 (37%)
20	CLA	1	307	1	59,63,73	2.32	20 (33%)	71,101,113	3.09	30 (42%)
20	CLA	2	321	-	54,58,73	2.44	20 (37%)	65,95,113	3.17	30 (46%)
25	MGE	1	324	-	48,48,48	0.22	0	56,56,56	0.59	1 (1%)
25	MGE	3	304	-	33,33,48	0.25	0	41,41,56	0.26	0
20	CLA	2	304	2	59,63,73	2.32	20 (33%)	71,101,113	2.90	27 (38%)
24	LHG	O	205	-	41,41,48	0.39	0	45,46,54	0.57	1 (2%)
20	CLA	A	853	5	69,73,73	2.07	20 (28%)	83,113,113	2.69	29 (34%)
20	CLA	2	317	-	51,55,73	2.53	20 (39%)	61,91,113	3.22	27 (44%)
20	CLA	B	818	6	69,73,73	2.12	18 (26%)	83,113,113	2.77	28 (33%)
20	CLA	B	844	6	69,73,73	2.07	19 (27%)	83,113,113	2.94	32 (38%)
20	CLA	B	819	6	69,73,73	2.08	18 (26%)	83,113,113	2.55	28 (33%)
27	SF4	C	101	7	0,12,12	-	-	-	-	-
20	CLA	B	848	6	69,73,73	2.12	19 (27%)	83,113,113	2.91	29 (34%)
20	CLA	A	843	5	69,73,73	2.12	20 (28%)	83,113,113	2.74	28 (33%)
25	MGE	3	305	-	34,34,48	0.25	0	42,42,56	0.41	0
24	LHG	1	314	-	32,32,48	0.29	0	34,34,54	0.48	0
20	CLA	B	833	-	65,69,73	2.24	20 (30%)	78,108,113	3.01	30 (38%)
20	CLA	3	308	3	65,69,73	2.26	20 (30%)	78,108,113	2.96	31 (39%)
24	LHG	I	101	-	36,36,48	0.25	0	38,38,54	0.28	0
20	CLA	A	828	5,20	56,60,73	2.37	20 (35%)	67,97,113	3.12	30 (44%)
23	BCR	B	839	-	30,30,41	1.92	7 (23%)	39,39,56	2.04	10 (25%)
20	CLA	B	824	6	64,68,73	2.21	20 (31%)	77,107,113	2.95	28 (36%)
20	CLA	B	803	6	69,73,73	2.12	21 (30%)	83,113,113	2.91	31 (37%)
25	MGE	F	303	-	28,28,48	0.26	0	36,36,56	0.51	0
20	CLA	2	319	2	66,70,73	2.19	21 (31%)	79,109,113	2.96	30 (37%)
20	CLA	B	853	6	59,63,73	2.33	21 (35%)	71,101,113	3.01	28 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	807	6	69,73,73	2.15	19 (27%)	83,113,113	2.93	30 (36%)
20	CLA	B	820	6	63,67,73	2.16	20 (31%)	75,105,113	2.94	30 (40%)
20	CLA	K	206	15	46,50,73	2.57	20 (43%)	55,85,113	3.40	27 (49%)
20	CLA	B	804	6	69,73,73	2.09	21 (30%)	83,113,113	2.77	28 (33%)
20	CLA	3	320	3	49,53,73	2.54	21 (42%)	59,89,113	3.26	27 (45%)
20	CLA	4	310	-	64,68,73	2.22	20 (31%)	77,107,113	2.92	29 (37%)
19	CHL	3	313	-	54,58,74	2.14	17 (31%)	59,94,114	3.04	23 (38%)
20	CLA	3	314	3	49,53,73	2.48	19 (38%)	59,89,113	3.18	27 (45%)
23	BCR	A	816	-	41,41,41	1.94	9 (21%)	56,56,56	1.77	12 (21%)
23	BCR	I	102	-	41,41,41	1.76	8 (19%)	56,56,56	1.66	11 (19%)
23	BCR	O	203	-	41,41,41	1.92	6 (14%)	56,56,56	2.41	15 (26%)
23	BCR	B	836	-	41,41,41	1.89	6 (14%)	56,56,56	1.74	15 (26%)
20	CLA	1	306	-	49,53,73	2.55	20 (40%)	59,89,113	3.30	28 (47%)
20	CLA	O	206	18	69,73,73	2.15	21 (30%)	83,113,113	2.81	29 (34%)
25	MGE	3	306	-	38,38,48	0.25	0	46,46,56	0.41	0
20	CLA	A	832	5	69,73,73	2.13	19 (27%)	83,113,113	2.76	30 (36%)
24	LHG	2	313	-	40,40,48	0.33	0	43,46,54	0.50	0
24	LHG	4	321	-	48,48,48	0.27	0	51,54,54	0.32	0
20	CLA	A	834	5	59,63,73	2.25	19 (32%)	71,101,113	3.06	27 (38%)
29	DGD	B	840	-	60,60,67	0.89	2 (3%)	74,74,81	0.93	3 (4%)
20	CLA	2	323	4	50,54,73	2.51	20 (40%)	60,90,113	3.31	28 (46%)
20	CLA	4	313	4	54,58,73	2.45	20 (37%)	65,95,113	3.19	27 (41%)
21	LUT	4	317	-	42,43,43	1.61	8 (19%)	51,60,60	1.51	10 (19%)
22	XAT	4	318	-	39,47,47	0.87	0	54,74,74	2.73	20 (37%)
23	BCR	F	302	-	41,41,41	1.71	9 (21%)	56,56,56	1.59	11 (19%)
20	CLA	A	830	5	69,73,73	2.12	20 (28%)	83,113,113	2.84	30 (36%)
20	CLA	A	844	5	50,54,73	2.44	20 (40%)	60,90,113	3.35	30 (50%)
20	CLA	2	305	24	59,63,73	2.35	20 (33%)	71,101,113	3.09	29 (40%)
24	LHG	2	314	-	38,39,48	0.31	0	41,45,54	0.48	0
20	CLA	B	808	6	69,73,73	2.14	20 (28%)	83,113,113	2.86	32 (38%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	4	302	4	1/1/14/20	5/33/109/115	-
20	CLA	K	204	-	1/1/14/20	8/35/111/115	-
20	CLA	3	307	-	1/1/13/20	7/30/106/115	-
20	CLA	B	816	6	1/1/15/20	12/39/115/115	-
20	CLA	B	814	-	1/1/15/20	10/39/115/115	-
19	CHL	2	302	-	-	8/19/95/117	-
20	CLA	A	801	5	1/1/14/20	6/35/111/115	-
20	CLA	G	206	-	-	5/21/97/115	-
19	CHL	2	322	-	-	7/17/93/117	-
23	BCR	G	203	-	-	7/29/63/63	0/2/2/2
20	CLA	A	838	5	-	7/15/91/115	-
19	CHL	4	315	4	-	5/15/91/117	-
20	CLA	A	807	5	1/1/13/20	11/27/103/115	-
22	XAT	3	302	-	-	10/31/93/93	0/4/4/4
23	BCR	L	301	-	-	7/29/63/63	0/2/2/2
26	PQN	A	810	-	-	6/23/43/43	0/2/2/2
20	CLA	A	840	-	-	1/17/93/115	-
20	CLA	L	305	16	-	1/17/93/115	-
20	CLA	1	319	-	1/1/13/20	8/27/103/115	-
20	CLA	B	815	-	1/1/13/20	6/29/105/115	-
20	CLA	4	311	-	-	2/17/93/115	-
24	LHG	4	301	-	-	6/37/37/53	-
20	CLA	G	205	-	-	3/17/93/115	-
21	LUT	3	301	-	-	0/29/67/67	0/2/2/2
20	CLA	B	809	-	1/1/15/20	14/39/115/115	-
20	CLA	A	806	5	1/1/15/20	12/39/115/115	-
20	CLA	4	316	-	1/1/15/20	16/39/115/115	-
23	BCR	4	320	-	-	6/29/63/63	0/2/2/2
19	CHL	1	301	1	-	9/14/90/117	-
21	LUT	1	323	-	-	7/29/67/67	0/2/2/2
20	CLA	G	207	11	-	4/17/93/115	-
20	CLA	A	805	5	-	7/26/102/115	-
19	CHL	4	306	-	-	14/17/93/117	-
20	CLA	B	817	6	1/1/13/20	7/31/107/115	-
20	CLA	4	314	4	-	8/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	813	6	1/1/13/20	10/30/106/115	-
20	CLA	B	823	6	1/1/14/20	11/36/112/115	-
24	LHG	A	819	-	-	5/53/53/53	-
20	CLA	4	312	4	1/1/13/20	7/27/103/115	-
20	CLA	O	207	-	1/1/13/20	8/32/108/115	-
19	CHL	2	309	2	-	5/14/90/117	-
29	DGD	O	201	-	-	9/42/82/95	0/2/2/2
20	CLA	A	855	5	1/1/13/20	4/27/103/115	-
20	CLA	4	304	-	-	8/15/91/115	-
19	CHL	4	307	-	-	7/17/93/117	-
24	LHG	1	313	20	-	8/53/53/53	-
23	BCR	1	312	-	-	8/29/63/63	0/2/2/2
20	CLA	B	806	6	1/1/13/20	12/30/106/115	-
20	CLA	4	308	4	-	2/17/93/115	-
20	CLA	L	306	16	-	3/24/100/115	-
20	CLA	2	306	-	-	2/15/91/115	-
23	BCR	L	303	-	-	7/29/63/63	0/2/2/2
20	CLA	2	303	2	-	3/15/91/115	-
20	CLA	B	805	-	-	2/15/91/115	-
20	CLA	A	839	5	-	8/15/91/115	-
20	CLA	L	307	-	-	3/17/93/115	-
20	CLA	1	302	-	-	3/21/97/115	-
24	LHG	O	204	-	-	1/26/26/53	-
25	MGE	1	315	-	-	3/32/52/63	0/1/1/1
20	CLA	A	848	5	1/1/15/20	8/39/115/115	-
20	CLA	B	851	6	1/1/15/20	11/39/115/115	-
20	CLA	1	322	1	-	3/17/93/115	-
20	CLA	A	826	-	1/1/15/20	13/39/115/115	-
19	CHL	4	305	-	-	16/19/95/117	-
20	CLA	1	321	-	-	0/17/93/115	-
20	CLA	1	303	1	1/1/13/20	8/25/101/115	-
20	CLA	F	306	-	-	6/17/93/115	-
20	CLA	A	852	5	1/1/15/20	6/39/115/115	-
23	BCR	L	304	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LHG	A	821	20	-	8/51/51/53	-
25	MGE	N	201	-	-	8/35/55/63	0/1/1/1
20	CLA	A	842	5	1/1/14/20	10/35/111/115	-
23	BCR	A	857	-	-	6/29/63/63	0/2/2/2
20	CLA	3	317	3	1/1/13/20	9/31/107/115	-
20	CLA	3	315	3	1/1/13/20	7/27/103/115	-
24	LHG	2	315	20	-	8/36/36/53	-
20	CLA	B	811	6	1/1/13/20	8/30/106/115	-
20	CLA	1	304	1	1/1/13/20	6/27/103/115	-
20	CLA	A	841	5	1/1/13/20	7/31/107/115	-
20	CLA	A	804	5	-	10/23/99/115	-
20	CLA	F	304	-	1/1/15/20	17/39/115/115	-
23	BCR	F	301	-	-	3/29/63/63	0/2/2/2
23	BCR	K	201	-	-	4/29/63/63	0/2/2/2
20	CLA	3	311	-	1/1/15/20	11/39/115/115	-
24	LHG	2	316	-	-	3/38/38/53	-
20	CLA	B	801	-	1/1/15/20	15/39/115/115	-
20	CLA	B	825	-	-	4/15/91/115	-
22	XAT	1	311	-	-	14/31/93/93	0/4/4/4
20	CLA	1	305	24	-	5/17/93/115	-
20	CLA	2	320	2	-	6/17/93/115	-
25	MGE	J	102	-	-	3/37/57/63	0/1/1/1
20	CLA	B	827	6	1/1/15/20	11/39/115/115	-
20	CLA	4	309	4	-	9/26/102/115	-
20	CLA	3	318	3	-	0/10/86/115	-
20	CLA	A	827	5	1/1/15/20	10/39/115/115	-
20	CLA	1	309	-	-	4/10/86/115	-
20	CLA	3	312	3	-	1/15/91/115	-
20	CLA	A	809	5	1/1/15/20	16/39/115/115	-
20	CLA	1	320	-	-	7/20/96/115	-
24	LHG	B	843	-	-	5/29/29/53	-
27	SF4	C	102	7	-	-	0/6/5/5
29	DGD	J	104	-	-	14/55/95/95	0/2/2/2
20	CLA	B	830	6	1/1/15/20	15/39/115/115	-
20	CLA	A	837	5	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	846	5	-	6/17/93/115	-
24	LHG	B	841	-	-	8/36/36/53	-
20	CLA	A	847	5	1/1/13/20	6/29/105/115	-
20	CLA	A	825	-	1/1/15/20	11/39/115/115	-
20	CLA	A	803	5	-	4/33/109/115	-
20	CLA	B	812	6	1/1/15/20	15/39/115/115	-
20	CLA	2	308	2	-	6/23/99/115	-
20	CLA	K	203	15	-	9/18/94/115	-
23	BCR	A	817	-	-	1/29/63/63	0/2/2/2
20	CLA	A	802	5	1/1/15/20	18/39/115/115	-
20	CLA	A	836	5	-	9/24/100/115	-
23	BCR	G	201	-	-	5/29/63/63	0/2/2/2
24	LHG	B	842	-	-	6/33/33/53	-
23	BCR	A	818	-	-	6/27/61/63	0/2/2/2
20	CLA	A	833	5	1/1/15/20	11/39/115/115	-
20	CLA	F	305	-	-	0/17/93/115	-
20	CLA	J	103	14	-	4/17/93/115	-
20	CLA	A	829	5	1/1/14/20	17/38/114/115	-
20	CLA	B	846	6	-	3/15/91/115	-
23	BCR	B	837	-	-	2/29/63/63	0/2/2/2
23	BCR	B	838	-	-	5/29/63/63	0/2/2/2
27	SF4	A	813	5,6	-	-	0/6/5/5
20	CLA	2	307	2	1/1/14/20	16/36/112/115	-
20	CLA	A	811	24	1/1/13/20	14/27/103/115	-
20	CLA	4	303	-	-	3/17/93/115	-
20	CLA	B	810	6	-	4/19/95/115	-
20	CLA	A	856	5	1/1/13/20	5/29/105/115	-
20	CLA	B	802	6	-	5/15/91/115	-
20	CLA	B	831	-	1/1/15/20	8/39/115/115	-
23	BCR	O	202	-	-	8/29/63/63	0/2/2/2
20	CLA	B	829	-	1/1/15/20	10/39/115/115	-
20	CLA	3	316	-	-	2/17/93/115	-
29	DGD	G	202	-	-	8/34/54/95	0/1/1/2
20	CLA	A	845	-	1/1/15/20	4/39/115/115	-
20	CLA	B	849	6	-	7/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	A	814	-	-	2/29/63/63	0/2/2/2
20	CLA	A	854	5	1/1/15/20	15/39/115/115	-
20	CLA	B	828	6	-	8/18/94/115	-
23	BCR	L	302	-	-	2/29/63/63	0/2/2/2
24	LHG	A	820	-	-	5/28/28/53	-
20	CLA	1	308	1	-	3/17/93/115	-
20	CLA	3	319	-	-	7/17/93/115	-
23	BCR	A	815	-	-	2/29/63/63	0/2/2/2
21	LUT	1	310	-	-	1/29/67/67	0/2/2/2
19	CHL	1	317	1	-	9/23/99/117	-
20	CLA	K	205	15	-	3/17/93/115	-
20	CLA	A	850	-	1/1/13/20	11/31/107/115	-
23	BCR	3	303	-	-	4/29/63/63	0/2/2/2
28	CL0	A	824	5	1/1/15/20	5/37/113/115	-
23	BCR	K	202	-	-	2/29/63/63	0/2/2/2
20	CLA	O	208	-	-	5/15/91/115	-
20	CLA	B	822	6	1/1/15/20	9/39/115/115	-
26	PQN	B	832	-	-	4/20/40/43	0/2/2/2
20	CLA	1	318	1	1/1/15/20	8/39/115/115	-
23	BCR	B	834	-	-	6/29/63/63	0/2/2/2
19	CHL	2	318	2	1/1/13/21	14/32/108/117	-
23	BCR	4	319	-	-	6/29/63/63	0/2/2/2
22	XAT	2	311	-	-	7/31/93/93	0/4/4/4
20	CLA	B	821	6	1/1/13/20	5/29/105/115	-
20	CLA	3	309	-	1/1/14/20	15/33/109/115	-
23	BCR	J	101	-	-	4/29/63/63	0/2/2/2
20	CLA	A	808	5	1/1/15/20	11/39/115/115	-
20	CLA	B	850	6	1/1/15/20	14/39/115/115	-
20	CLA	A	851	5	1/1/15/20	20/39/115/115	-
25	MGE	4	322	-	-	5/35/55/63	0/1/1/1
25	MGE	A	823	-	-	3/29/49/63	0/1/1/1
19	CHL	2	301	-	-	9/19/95/117	-
20	CLA	H	201	12	1/1/13/20	10/32/108/115	-
20	CLA	N	202	17	1/1/13/20	5/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	826	6	-	5/21/97/115	-
23	BCR	B	835	-	-	4/29/63/63	0/2/2/2
20	CLA	B	852	-	1/1/15/20	11/39/115/115	-
20	CLA	3	310	-	-	6/20/96/115	-
25	MGE	1	316	-	-	4/35/55/63	0/1/1/1
20	CLA	A	849	-	1/1/15/20	15/39/115/115	-
20	CLA	A	831	5	-	7/24/100/115	-
25	MGE	G	204	-	-	6/43/63/63	0/1/1/1
20	CLA	B	845	-	1/1/15/20	9/39/115/115	-
20	CLA	A	812	-	1/1/15/20	6/39/115/115	-
20	CLA	B	847	6	1/1/15/20	15/39/115/115	-
23	BCR	2	312	-	-	8/29/63/63	0/2/2/2
24	LHG	A	822	-	-	8/43/43/53	-
21	LUT	2	310	-	-	3/29/67/67	0/2/2/2
20	CLA	A	835	5,20	1/1/15/20	10/39/115/115	-
20	CLA	1	307	1	1/1/13/20	6/27/103/115	-
20	CLA	2	321	-	-	10/21/97/115	-
25	MGE	1	324	-	-	12/43/63/63	0/1/1/1
25	MGE	3	304	-	-	1/28/48/63	0/1/1/1
20	CLA	2	304	2	1/1/13/20	4/27/103/115	-
24	LHG	O	205	-	-	16/43/43/53	-
20	CLA	A	853	5	1/1/15/20	16/39/115/115	-
20	CLA	2	317	-	-	6/18/94/115	-
20	CLA	B	818	6	1/1/15/20	7/39/115/115	-
20	CLA	B	844	6	1/1/15/20	10/39/115/115	-
20	CLA	B	819	6	1/1/15/20	13/39/115/115	-
27	SF4	C	101	7	-	-	0/6/5/5
20	CLA	B	848	6	1/1/15/20	11/39/115/115	-
20	CLA	A	843	5	1/1/15/20	7/39/115/115	-
25	MGE	3	305	-	-	7/29/49/63	0/1/1/1
24	LHG	1	314	-	-	8/34/34/53	-
20	CLA	B	833	-	1/1/14/20	13/35/111/115	-
20	CLA	3	308	3	1/1/14/20	8/35/111/115	-
24	LHG	I	101	-	-	6/37/37/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	828	5,20	-	7/24/100/115	-
23	BCR	B	839	-	-	10/24/41/63	0/1/1/2
20	CLA	B	824	6	1/1/14/20	10/33/109/115	-
20	CLA	B	803	6	1/1/15/20	17/39/115/115	-
25	MGE	F	303	-	-	8/23/43/63	0/1/1/1
20	CLA	2	319	2	1/1/14/20	10/36/112/115	-
20	CLA	B	853	6	1/1/13/20	7/27/103/115	-
20	CLA	B	807	6	1/1/15/20	13/39/115/115	-
20	CLA	B	820	6	1/1/13/20	7/32/108/115	-
20	CLA	K	206	15	-	2/12/88/115	-
20	CLA	B	804	6	1/1/15/20	13/39/115/115	-
20	CLA	3	320	3	-	2/15/91/115	-
20	CLA	4	310	-	1/1/14/20	9/33/109/115	-
19	CHL	3	313	-	-	12/22/98/117	-
20	CLA	3	314	3	-	2/15/91/115	-
23	BCR	A	816	-	-	9/29/63/63	0/2/2/2
23	BCR	I	102	-	-	4/29/63/63	0/2/2/2
23	BCR	O	203	-	-	2/29/63/63	0/2/2/2
23	BCR	B	836	-	-	5/29/63/63	0/2/2/2
20	CLA	1	306	-	-	4/15/91/115	-
20	CLA	O	206	18	1/1/15/20	11/39/115/115	-
25	MGE	3	306	-	-	5/33/53/63	0/1/1/1
20	CLA	A	832	5	1/1/15/20	11/39/115/115	-
24	LHG	2	313	-	-	15/45/45/53	-
24	LHG	4	321	-	-	5/53/53/53	-
20	CLA	A	834	5	1/1/13/20	11/27/103/115	-
29	DGD	B	840	-	-	17/48/88/95	0/2/2/2
20	CLA	2	323	4	-	5/17/93/115	-
20	CLA	4	313	4	-	4/21/97/115	-
21	LUT	4	317	-	-	2/29/67/67	0/2/2/2
22	XAT	4	318	-	-	1/31/93/93	0/4/4/4
23	BCR	F	302	-	-	4/29/63/63	0/2/2/2
20	CLA	A	830	5	1/1/15/20	11/39/115/115	-
20	CLA	A	844	5	-	6/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	2	305	24	1/1/13/20	7/27/103/115	-
24	LHG	2	314	-	-	14/43/43/53	-
20	CLA	B	808	6	1/1/15/20	11/39/115/115	-

All (3517) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	805	CLA	C1D-ND	8.79	1.48	1.37
20	K	205	CLA	C1D-ND	8.65	1.48	1.37
20	1	309	CLA	C1D-ND	8.63	1.48	1.37
20	1	305	CLA	C1D-ND	8.62	1.48	1.37
20	2	308	CLA	C1D-ND	8.61	1.48	1.37
20	3	316	CLA	C1D-ND	8.60	1.48	1.37
20	2	320	CLA	C1D-ND	8.59	1.48	1.37
20	3	309	CLA	C1D-ND	8.59	1.48	1.37
20	2	317	CLA	C1D-ND	8.59	1.48	1.37
20	G	206	CLA	C1D-ND	8.58	1.48	1.37
20	N	202	CLA	C1D-ND	8.58	1.48	1.37
20	4	303	CLA	C1D-ND	8.58	1.48	1.37
20	B	848	CLA	C1D-ND	8.56	1.48	1.37
20	4	312	CLA	C1D-ND	8.56	1.48	1.37
20	2	306	CLA	C1D-ND	8.56	1.48	1.37
20	J	103	CLA	C1D-ND	8.56	1.48	1.37
20	4	311	CLA	C1D-ND	8.56	1.48	1.37
20	K	203	CLA	C1D-ND	8.54	1.48	1.37
20	4	316	CLA	C1D-ND	8.54	1.48	1.37
20	2	305	CLA	C1D-ND	8.54	1.48	1.37
20	2	323	CLA	C1D-ND	8.53	1.48	1.37
20	B	852	CLA	C1D-ND	8.53	1.48	1.37
20	B	833	CLA	C1D-ND	8.53	1.48	1.37
20	1	307	CLA	C1D-ND	8.51	1.48	1.37
20	1	306	CLA	C1D-ND	8.51	1.48	1.37
20	B	807	CLA	C1D-ND	8.51	1.48	1.37
20	4	310	CLA	C1D-ND	8.50	1.48	1.37
20	O	208	CLA	C1D-ND	8.50	1.48	1.37
20	A	836	CLA	C1D-ND	8.50	1.48	1.37
20	3	319	CLA	C1D-ND	8.49	1.48	1.37
20	A	807	CLA	C1D-ND	8.47	1.48	1.37
20	B	811	CLA	C1D-ND	8.47	1.48	1.37
20	H	201	CLA	C1D-ND	8.47	1.48	1.37
20	B	821	CLA	C1D-ND	8.46	1.48	1.37
20	3	318	CLA	C1D-ND	8.46	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	O	207	CLA	C1D-ND	8.46	1.48	1.37
20	K	206	CLA	C1D-ND	8.46	1.48	1.37
20	A	852	CLA	C1D-ND	8.45	1.48	1.37
20	K	204	CLA	C1D-ND	8.45	1.48	1.37
20	1	322	CLA	C1D-ND	8.44	1.48	1.37
20	1	320	CLA	C1D-ND	8.44	1.48	1.37
20	F	306	CLA	C1D-ND	8.44	1.48	1.37
20	4	304	CLA	C1D-ND	8.43	1.48	1.37
20	B	849	CLA	C1D-ND	8.43	1.48	1.37
20	3	310	CLA	C1D-ND	8.41	1.48	1.37
20	1	319	CLA	C1D-ND	8.41	1.48	1.37
20	A	811	CLA	C1D-ND	8.40	1.48	1.37
20	A	809	CLA	C1D-ND	8.40	1.48	1.37
20	G	207	CLA	C1D-ND	8.40	1.48	1.37
20	A	806	CLA	C1D-ND	8.40	1.48	1.37
20	A	856	CLA	C1D-ND	8.40	1.48	1.37
20	4	313	CLA	C1D-ND	8.39	1.48	1.37
20	B	806	CLA	C1D-ND	8.38	1.48	1.37
20	B	802	CLA	C1D-ND	8.38	1.48	1.37
20	A	840	CLA	C1D-ND	8.37	1.48	1.37
20	3	308	CLA	C1D-ND	8.36	1.48	1.37
20	A	848	CLA	C1D-ND	8.36	1.48	1.37
20	B	815	CLA	C1D-ND	8.36	1.48	1.37
20	2	307	CLA	C1D-ND	8.35	1.48	1.37
20	3	311	CLA	C1D-ND	8.35	1.48	1.37
20	1	303	CLA	C1D-ND	8.35	1.48	1.37
20	L	307	CLA	C1D-ND	8.34	1.48	1.37
20	1	304	CLA	C1D-ND	8.34	1.48	1.37
20	A	842	CLA	C1D-ND	8.34	1.48	1.37
20	A	849	CLA	C1D-ND	8.34	1.48	1.37
20	A	834	CLA	C1D-ND	8.33	1.48	1.37
20	B	801	CLA	C1D-ND	8.32	1.48	1.37
20	A	802	CLA	C1D-ND	8.32	1.48	1.37
20	B	846	CLA	C1D-ND	8.32	1.48	1.37
20	2	321	CLA	C1D-ND	8.32	1.48	1.37
20	1	318	CLA	C1D-ND	8.32	1.48	1.37
20	B	853	CLA	C1D-ND	8.32	1.48	1.37
20	A	847	CLA	C1D-ND	8.32	1.48	1.37
20	B	831	CLA	C1D-ND	8.31	1.48	1.37
20	A	837	CLA	C1D-ND	8.31	1.48	1.37
20	2	304	CLA	C1D-ND	8.31	1.48	1.37
20	B	824	CLA	C1D-ND	8.31	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	827	CLA	C1D-ND	8.30	1.48	1.37
20	A	808	CLA	C1D-ND	8.28	1.48	1.37
20	A	827	CLA	C1D-ND	8.28	1.48	1.37
20	A	839	CLA	C1D-ND	8.28	1.48	1.37
20	A	831	CLA	C1D-ND	8.28	1.48	1.37
20	3	320	CLA	C1D-ND	8.27	1.48	1.37
20	B	817	CLA	C1D-ND	8.27	1.48	1.37
20	1	308	CLA	C1D-ND	8.26	1.47	1.37
20	F	305	CLA	C1D-ND	8.25	1.47	1.37
20	3	312	CLA	C1D-ND	8.25	1.47	1.37
20	B	805	CLA	C1D-ND	8.24	1.47	1.37
20	2	319	CLA	C1D-ND	8.24	1.47	1.37
20	1	321	CLA	C1D-ND	8.23	1.47	1.37
20	B	803	CLA	C1D-ND	8.22	1.47	1.37
20	O	206	CLA	C1D-ND	8.22	1.47	1.37
20	1	302	CLA	C1D-ND	8.22	1.47	1.37
20	3	317	CLA	C1D-ND	8.21	1.47	1.37
20	A	855	CLA	C1D-ND	8.21	1.47	1.37
20	B	826	CLA	C1D-ND	8.20	1.47	1.37
20	3	307	CLA	C1D-ND	8.20	1.47	1.37
20	A	804	CLA	C1D-ND	8.20	1.47	1.37
20	4	309	CLA	C1D-ND	8.19	1.47	1.37
20	4	314	CLA	C1D-ND	8.19	1.47	1.37
20	L	305	CLA	C1D-ND	8.19	1.47	1.37
20	A	846	CLA	C1D-ND	8.19	1.47	1.37
20	3	315	CLA	C1D-ND	8.19	1.47	1.37
20	A	851	CLA	C1D-ND	8.17	1.47	1.37
20	A	838	CLA	C1D-ND	8.16	1.47	1.37
20	B	847	CLA	C1D-ND	8.16	1.47	1.37
20	B	808	CLA	C1D-ND	8.15	1.47	1.37
20	B	830	CLA	C1D-ND	8.15	1.47	1.37
20	B	825	CLA	C1D-ND	8.14	1.47	1.37
20	B	828	CLA	C1D-ND	8.13	1.47	1.37
20	B	829	CLA	C1D-ND	8.13	1.47	1.37
20	G	205	CLA	C1D-ND	8.13	1.47	1.37
20	A	835	CLA	C1D-ND	8.11	1.47	1.37
20	A	841	CLA	C1D-ND	8.11	1.47	1.37
20	A	829	CLA	C1D-ND	8.11	1.47	1.37
20	B	813	CLA	C1D-ND	8.10	1.47	1.37
20	F	304	CLA	C1D-ND	8.10	1.47	1.37
20	A	828	CLA	C1D-ND	8.09	1.47	1.37
20	A	850	CLA	C1D-ND	8.07	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	830	CLA	C1D-ND	8.07	1.47	1.37
20	B	810	CLA	C1D-ND	8.06	1.47	1.37
20	A	832	CLA	C1D-ND	8.06	1.47	1.37
20	4	302	CLA	C1D-ND	8.05	1.47	1.37
20	B	809	CLA	C1D-ND	8.05	1.47	1.37
20	3	314	CLA	C1D-ND	8.03	1.47	1.37
20	B	823	CLA	C1D-ND	8.03	1.47	1.37
20	A	801	CLA	C1D-ND	8.02	1.47	1.37
20	B	816	CLA	C1D-ND	8.02	1.47	1.37
20	A	833	CLA	C1D-ND	8.02	1.47	1.37
20	L	306	CLA	C1D-ND	7.98	1.47	1.37
20	B	850	CLA	C1D-ND	7.97	1.47	1.37
20	A	845	CLA	C1D-ND	7.96	1.47	1.37
20	B	804	CLA	C1D-ND	7.94	1.47	1.37
20	B	822	CLA	C1D-ND	7.93	1.47	1.37
20	A	844	CLA	C1D-ND	7.93	1.47	1.37
20	B	812	CLA	C1D-ND	7.90	1.47	1.37
20	A	843	CLA	C1D-ND	7.89	1.47	1.37
20	2	303	CLA	C1D-ND	7.88	1.47	1.37
20	B	844	CLA	C1D-ND	7.86	1.47	1.37
20	B	814	CLA	C1D-ND	7.85	1.47	1.37
20	A	803	CLA	C1D-ND	7.85	1.47	1.37
20	B	851	CLA	C1D-ND	7.83	1.47	1.37
20	B	818	CLA	C1D-ND	7.82	1.47	1.37
20	B	820	CLA	C1D-ND	7.70	1.47	1.37
20	A	854	CLA	C1D-ND	7.66	1.47	1.37
20	4	308	CLA	C1D-ND	7.64	1.47	1.37
20	A	853	CLA	C1D-ND	7.63	1.47	1.37
20	B	845	CLA	C1D-ND	7.62	1.47	1.37
20	A	812	CLA	C1D-ND	7.58	1.47	1.37
20	B	819	CLA	C1D-ND	7.51	1.47	1.37
20	A	825	CLA	C1D-ND	7.20	1.46	1.37
20	A	826	CLA	C1D-ND	7.17	1.46	1.37
28	A	824	CL0	C1D-ND	6.84	1.46	1.37
23	O	203	BCR	C14-C13	6.08	1.43	1.35
23	A	816	BCR	C10-C9	5.83	1.43	1.35
23	L	303	BCR	C10-C9	5.76	1.43	1.35
23	B	836	BCR	C10-C9	5.73	1.43	1.35
23	G	203	BCR	C14-C13	5.61	1.43	1.35
23	1	312	BCR	C10-C9	5.42	1.43	1.35
20	K	205	CLA	CHC-C1C	5.40	1.49	1.38
23	K	202	BCR	C10-C9	5.38	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	4	320	BCR	C14-C13	5.36	1.42	1.35
23	O	203	BCR	C10-C9	5.28	1.42	1.35
23	L	303	BCR	C14-C13	5.27	1.42	1.35
23	F	301	BCR	C21-C22	5.27	1.42	1.35
23	G	203	BCR	C10-C9	5.25	1.42	1.35
23	B	836	BCR	C14-C13	5.25	1.42	1.35
20	2	304	CLA	O2D-CGD	5.24	1.46	1.33
20	3	309	CLA	O2D-CGD	5.23	1.46	1.33
20	3	315	CLA	O2D-CGD	5.23	1.46	1.33
20	4	313	CLA	O2D-CGD	5.21	1.45	1.33
20	3	317	CLA	O2D-CGD	5.19	1.45	1.33
20	A	808	CLA	O2D-CGD	5.19	1.45	1.33
20	F	305	CLA	O2D-CGD	5.19	1.45	1.33
19	3	313	CHL	O2D-CGD	5.19	1.45	1.33
20	2	317	CLA	O2D-CGD	5.19	1.45	1.33
20	B	848	CLA	O2D-CGD	5.19	1.45	1.33
20	B	817	CLA	O2D-CGD	5.19	1.45	1.33
20	3	318	CLA	O2D-CGD	5.18	1.45	1.33
20	K	206	CLA	O2D-CGD	5.18	1.45	1.33
20	4	304	CLA	O2D-CGD	5.18	1.45	1.33
20	2	307	CLA	O2D-CGD	5.18	1.45	1.33
20	A	855	CLA	O2D-CGD	5.18	1.45	1.33
20	K	205	CLA	O2D-CGD	5.17	1.45	1.33
20	3	316	CLA	O2D-CGD	5.17	1.45	1.33
20	2	321	CLA	O2D-CGD	5.17	1.45	1.33
20	4	309	CLA	O2D-CGD	5.17	1.45	1.33
20	A	803	CLA	O2D-CGD	5.16	1.45	1.33
20	H	201	CLA	O2D-CGD	5.16	1.45	1.33
20	A	852	CLA	O2D-CGD	5.16	1.45	1.33
20	B	807	CLA	O2D-CGD	5.16	1.45	1.33
20	4	312	CLA	O2D-CGD	5.16	1.45	1.33
20	B	801	CLA	O2D-CGD	5.16	1.45	1.33
20	A	846	CLA	O2D-CGD	5.15	1.45	1.33
20	1	304	CLA	O2D-CGD	5.15	1.45	1.33
20	1	307	CLA	O2D-CGD	5.15	1.45	1.33
20	3	312	CLA	O2D-CGD	5.15	1.45	1.33
20	1	305	CLA	O2D-CGD	5.15	1.45	1.33
20	K	203	CLA	O2D-CGD	5.15	1.45	1.33
20	1	306	CLA	O2D-CGD	5.15	1.45	1.33
20	1	321	CLA	O2D-CGD	5.15	1.45	1.33
20	B	852	CLA	O2D-CGD	5.15	1.45	1.33
20	B	830	CLA	O2D-CGD	5.15	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	813	CLA	O2D-CGD	5.14	1.45	1.33
20	1	322	CLA	O2D-CGD	5.14	1.45	1.33
20	1	302	CLA	O2D-CGD	5.14	1.45	1.33
19	4	305	CHL	O2D-CGD	5.14	1.45	1.33
20	A	806	CLA	O2D-CGD	5.14	1.45	1.33
20	1	309	CLA	O2D-CGD	5.14	1.45	1.33
20	4	303	CLA	O2D-CGD	5.14	1.45	1.33
20	B	829	CLA	O2D-CGD	5.14	1.45	1.33
19	2	322	CHL	O2D-CGD	5.14	1.45	1.33
20	2	320	CLA	O2D-CGD	5.14	1.45	1.33
19	2	301	CHL	O2D-CGD	5.13	1.45	1.33
20	4	311	CLA	O2D-CGD	5.13	1.45	1.33
20	4	310	CLA	O2D-CGD	5.13	1.45	1.33
20	B	818	CLA	O2D-CGD	5.13	1.45	1.33
20	B	833	CLA	O2D-CGD	5.13	1.45	1.33
20	A	848	CLA	O2D-CGD	5.13	1.45	1.33
20	J	103	CLA	O2D-CGD	5.13	1.45	1.33
19	2	309	CHL	O2D-CGD	5.13	1.45	1.33
20	F	306	CLA	O2D-CGD	5.13	1.45	1.33
20	A	805	CLA	O2D-CGD	5.13	1.45	1.33
20	B	826	CLA	O2D-CGD	5.13	1.45	1.33
20	3	320	CLA	O2D-CGD	5.12	1.45	1.33
20	2	306	CLA	O2D-CGD	5.12	1.45	1.33
20	2	319	CLA	O2D-CGD	5.12	1.45	1.33
20	B	846	CLA	O2D-CGD	5.12	1.45	1.33
20	A	829	CLA	O2D-CGD	5.12	1.45	1.33
20	3	319	CLA	O2D-CGD	5.11	1.45	1.33
20	A	842	CLA	O2D-CGD	5.11	1.45	1.33
20	A	856	CLA	O2D-CGD	5.11	1.45	1.33
20	O	208	CLA	O2D-CGD	5.11	1.45	1.33
20	G	207	CLA	O2D-CGD	5.11	1.45	1.33
20	2	303	CLA	O2D-CGD	5.11	1.45	1.33
20	A	839	CLA	O2D-CGD	5.11	1.45	1.33
19	2	302	CHL	O2D-CGD	5.10	1.45	1.33
20	A	832	CLA	O2D-CGD	5.10	1.45	1.33
20	G	206	CLA	O2D-CGD	5.10	1.45	1.33
20	O	207	CLA	O2D-CGD	5.10	1.45	1.33
20	4	308	CLA	O2D-CGD	5.09	1.45	1.33
20	B	811	CLA	O2D-CGD	5.09	1.45	1.33
19	4	307	CHL	O2D-CGD	5.09	1.45	1.33
20	1	320	CLA	O2D-CGD	5.09	1.45	1.33
20	A	841	CLA	O2D-CGD	5.09	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	L	304	BCR	C14-C13	5.09	1.42	1.35
20	3	308	CLA	O2D-CGD	5.09	1.45	1.33
20	A	807	CLA	O2D-CGD	5.09	1.45	1.33
20	A	835	CLA	O2D-CGD	5.09	1.45	1.33
20	B	810	CLA	O2D-CGD	5.09	1.45	1.33
23	L	304	BCR	C10-C9	5.09	1.42	1.35
20	O	206	CLA	O2D-CGD	5.09	1.45	1.33
20	A	847	CLA	O2D-CGD	5.08	1.45	1.33
20	B	847	CLA	O2D-CGD	5.08	1.45	1.33
20	B	853	CLA	O2D-CGD	5.08	1.45	1.33
20	A	845	CLA	O2D-CGD	5.07	1.45	1.33
20	B	825	CLA	O2D-CGD	5.07	1.45	1.33
20	B	812	CLA	O2D-CGD	5.07	1.45	1.33
20	B	849	CLA	O2D-CGD	5.07	1.45	1.33
20	B	831	CLA	O2D-CGD	5.07	1.45	1.33
20	A	809	CLA	O2D-CGD	5.07	1.45	1.33
20	3	311	CLA	O2D-CGD	5.07	1.45	1.33
20	2	308	CLA	O2D-CGD	5.07	1.45	1.33
20	B	821	CLA	O2D-CGD	5.07	1.45	1.33
23	L	303	BCR	C21-C22	5.06	1.42	1.35
20	A	837	CLA	CHC-C1C	5.06	1.48	1.38
20	3	310	CLA	O2D-CGD	5.06	1.45	1.33
20	A	834	CLA	O2D-CGD	5.06	1.45	1.33
20	1	308	CLA	O2D-CGD	5.06	1.45	1.33
20	B	845	CLA	O2D-CGD	5.05	1.45	1.33
20	B	808	CLA	O2D-CGD	5.05	1.45	1.33
20	B	819	CLA	O2D-CGD	5.05	1.45	1.33
19	1	301	CHL	O2D-CGD	5.05	1.45	1.33
20	A	840	CLA	O2D-CGD	5.04	1.45	1.33
20	A	828	CLA	O2D-CGD	5.04	1.45	1.33
20	4	302	CLA	O2D-CGD	5.04	1.45	1.33
20	A	830	CLA	O2D-CGD	5.04	1.45	1.33
20	B	827	CLA	O2D-CGD	5.04	1.45	1.33
23	L	304	BCR	C17-C18	5.03	1.42	1.35
20	A	850	CLA	O2D-CGD	5.03	1.45	1.33
20	B	823	CLA	O2D-CGD	5.03	1.45	1.33
20	A	853	CLA	O2D-CGD	5.03	1.45	1.33
20	1	318	CLA	O2D-CGD	5.03	1.45	1.33
20	B	816	CLA	O2D-CGD	5.03	1.45	1.33
20	2	323	CLA	O2D-CGD	5.02	1.45	1.33
20	L	305	CLA	O2D-CGD	5.02	1.45	1.33
20	A	842	CLA	CHC-C1C	5.02	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	820	CLA	O2D-CGD	5.01	1.45	1.33
20	B	804	CLA	O2D-CGD	5.01	1.45	1.33
20	K	204	CLA	O2D-CGD	5.01	1.45	1.33
20	L	307	CLA	O2D-CGD	5.01	1.45	1.33
23	F	301	BCR	C17-C18	5.01	1.42	1.35
20	A	805	CLA	CHC-C1C	5.01	1.48	1.38
20	B	809	CLA	O2D-CGD	5.00	1.45	1.33
20	A	836	CLA	O2D-CGD	5.00	1.45	1.33
20	A	825	CLA	O2D-CGD	5.00	1.45	1.33
20	3	314	CLA	O2D-CGD	5.00	1.45	1.33
20	A	831	CLA	O2D-CGD	5.00	1.45	1.33
20	2	320	CLA	CHC-C1C	5.00	1.48	1.38
20	A	843	CLA	O2D-CGD	5.00	1.45	1.33
19	1	317	CHL	O2D-CGD	4.99	1.45	1.33
19	4	306	CHL	O2D-CGD	4.99	1.45	1.33
20	L	306	CLA	O2D-CGD	4.99	1.45	1.33
23	K	202	BCR	C14-C13	4.99	1.42	1.35
20	N	202	CLA	O2D-CGD	4.98	1.45	1.33
20	A	802	CLA	O2D-CGD	4.98	1.45	1.33
20	F	304	CLA	O2D-CGD	4.97	1.45	1.33
20	4	316	CLA	O2D-CGD	4.97	1.45	1.33
20	A	801	CLA	O2D-CGD	4.97	1.45	1.33
20	A	804	CLA	O2D-CGD	4.97	1.45	1.33
20	4	314	CLA	O2D-CGD	4.97	1.45	1.33
20	A	851	CLA	O2D-CGD	4.97	1.45	1.33
20	B	824	CLA	O2D-CGD	4.97	1.45	1.33
20	A	826	CLA	O2D-CGD	4.97	1.45	1.33
20	2	305	CLA	O2D-CGD	4.96	1.45	1.33
20	A	851	CLA	CHC-C1C	4.96	1.48	1.38
20	B	805	CLA	O2D-CGD	4.96	1.45	1.33
20	G	205	CLA	O2D-CGD	4.96	1.45	1.33
20	A	837	CLA	O2D-CGD	4.96	1.45	1.33
20	B	802	CLA	O2D-CGD	4.95	1.45	1.33
20	1	319	CLA	O2D-CGD	4.95	1.45	1.33
20	A	854	CLA	O2D-CGD	4.94	1.45	1.33
20	1	318	CLA	CHC-C1C	4.94	1.48	1.38
23	A	816	BCR	C21-C22	4.94	1.42	1.35
20	B	851	CLA	O2D-CGD	4.94	1.45	1.33
20	3	308	CLA	CHC-C1C	4.94	1.48	1.38
20	B	850	CLA	O2D-CGD	4.94	1.45	1.33
20	A	827	CLA	O2D-CGD	4.93	1.45	1.33
20	A	811	CLA	O2D-CGD	4.93	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	309	CLA	CHC-C1C	4.93	1.48	1.38
20	A	838	CLA	O2D-CGD	4.92	1.45	1.33
20	A	828	CLA	CHC-C1C	4.92	1.48	1.38
20	A	844	CLA	O2D-CGD	4.91	1.45	1.33
20	B	831	CLA	CHC-C1C	4.91	1.48	1.38
23	F	301	BCR	C10-C9	4.91	1.42	1.35
20	A	833	CLA	O2D-CGD	4.90	1.45	1.33
20	A	812	CLA	O2D-CGD	4.90	1.45	1.33
23	G	203	BCR	C17-C18	4.90	1.42	1.35
20	B	803	CLA	O2D-CGD	4.89	1.45	1.33
23	B	838	BCR	C21-C22	4.89	1.42	1.35
20	B	806	CLA	O2D-CGD	4.88	1.45	1.33
23	O	203	BCR	C17-C18	4.88	1.42	1.35
20	B	828	CLA	O2D-CGD	4.87	1.45	1.33
23	A	816	BCR	C14-C13	4.87	1.42	1.35
20	B	844	CLA	O2D-CGD	4.86	1.45	1.33
20	3	309	CLA	CHC-C1C	4.86	1.48	1.38
20	B	827	CLA	CHC-C1C	4.86	1.48	1.38
20	A	849	CLA	O2D-CGD	4.86	1.45	1.33
20	A	825	CLA	CHC-C1C	4.86	1.48	1.38
23	A	857	BCR	C10-C9	4.85	1.42	1.35
23	K	201	BCR	C10-C9	4.85	1.42	1.35
20	A	834	CLA	C3D-C4D	-4.84	1.33	1.44
20	B	829	CLA	CHC-C1C	4.84	1.48	1.38
23	J	101	BCR	C14-C13	4.83	1.42	1.35
20	B	818	CLA	C3D-C4D	-4.83	1.33	1.44
23	1	312	BCR	C14-C13	4.80	1.42	1.35
20	B	826	CLA	CHC-C1C	4.80	1.48	1.38
20	G	206	CLA	CHC-C1C	4.78	1.48	1.38
19	1	301	CHL	C3D-C4D	-4.78	1.33	1.44
20	A	811	CLA	CHC-C1C	4.78	1.48	1.38
23	4	319	BCR	C14-C13	4.77	1.42	1.35
23	B	835	BCR	C10-C9	4.77	1.42	1.35
20	1	305	CLA	CHC-C1C	4.77	1.48	1.38
20	1	322	CLA	CHC-C1C	4.77	1.48	1.38
23	O	202	BCR	C21-C22	4.77	1.42	1.35
23	B	834	BCR	C10-C9	4.77	1.42	1.35
20	N	202	CLA	CHC-C1C	4.77	1.48	1.38
23	4	320	BCR	C21-C22	4.76	1.42	1.35
20	4	303	CLA	CHC-C1C	4.75	1.48	1.38
23	2	312	BCR	C10-C9	4.75	1.42	1.35
20	3	318	CLA	CHC-C1C	4.75	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	O	207	CLA	CHC-C1C	4.75	1.48	1.38
20	1	306	CLA	CHC-C1C	4.74	1.48	1.38
20	B	815	CLA	O2D-CGD	4.74	1.44	1.33
20	2	323	CLA	CHC-C1C	4.73	1.48	1.38
20	2	306	CLA	CHC-C1C	4.73	1.48	1.38
20	1	319	CLA	C3D-C4D	-4.73	1.33	1.44
19	4	307	CHL	C3D-C4D	-4.73	1.33	1.44
20	A	841	CLA	CHC-C1C	4.72	1.48	1.38
20	4	313	CLA	CHC-C1C	4.72	1.48	1.38
20	B	819	CLA	C3D-C4D	-4.71	1.33	1.44
20	B	833	CLA	CHC-C1C	4.71	1.48	1.38
19	4	305	CHL	C3D-C4D	-4.71	1.33	1.44
23	I	102	BCR	C10-C9	4.70	1.42	1.35
20	3	320	CLA	CHC-C1C	4.70	1.48	1.38
20	4	311	CLA	CHC-C1C	4.70	1.48	1.38
20	A	847	CLA	C3D-C4D	-4.70	1.33	1.44
19	4	306	CHL	C3D-C4D	-4.70	1.33	1.44
20	1	309	CLA	CHC-C1C	4.69	1.48	1.38
19	2	309	CHL	C3D-C4D	-4.69	1.33	1.44
20	B	847	CLA	CHC-C1C	4.69	1.48	1.38
19	2	309	CHL	CHC-C1C	4.69	1.48	1.38
19	2	302	CHL	C3D-C4D	-4.69	1.33	1.44
20	2	317	CLA	CHC-C1C	4.69	1.48	1.38
20	3	316	CLA	CHC-C1C	4.69	1.48	1.38
20	A	855	CLA	C3D-C4D	-4.69	1.33	1.44
20	B	809	CLA	CHC-C1C	4.68	1.48	1.38
20	A	845	CLA	C3D-C4D	-4.68	1.33	1.44
23	O	203	BCR	C21-C22	4.68	1.42	1.35
20	2	305	CLA	CHC-C1C	4.68	1.48	1.38
20	B	845	CLA	CHC-C1C	4.68	1.48	1.38
23	L	302	BCR	C10-C9	4.67	1.42	1.35
20	B	802	CLA	CHC-C1C	4.67	1.48	1.38
20	B	815	CLA	CHC-C1C	4.67	1.48	1.38
20	3	307	CLA	O2A-CGA	4.67	1.47	1.33
20	A	812	CLA	CHC-C1C	4.67	1.48	1.38
20	2	308	CLA	CHC-C1C	4.67	1.48	1.38
23	A	857	BCR	C14-C13	4.67	1.42	1.35
20	B	803	CLA	CHC-C1C	4.67	1.48	1.38
20	B	807	CLA	CHC-C1C	4.67	1.48	1.38
20	H	201	CLA	CHC-C1C	4.67	1.48	1.38
20	B	846	CLA	CHC-C1C	4.67	1.48	1.38
20	B	814	CLA	CHC-C1C	4.67	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	301	CHL	C3D-C4D	-4.66	1.33	1.44
19	1	317	CHL	C3D-C4D	-4.66	1.33	1.44
19	2	322	CHL	C3D-C4D	-4.66	1.33	1.44
20	A	841	CLA	C3D-C4D	-4.66	1.33	1.44
20	B	804	CLA	C3D-C4D	-4.66	1.33	1.44
23	J	101	BCR	C10-C9	4.66	1.42	1.35
20	1	302	CLA	CHC-C1C	4.65	1.48	1.38
20	B	849	CLA	C3D-C4D	-4.65	1.33	1.44
20	4	302	CLA	CHC-C1C	4.65	1.48	1.38
20	A	839	CLA	C3D-C4D	-4.65	1.33	1.44
20	O	208	CLA	CHC-C1C	4.65	1.48	1.38
19	4	315	CHL	O2D-CGD	4.65	1.45	1.30
23	L	303	BCR	C17-C18	4.65	1.41	1.35
20	B	848	CLA	CHC-C1C	4.64	1.47	1.38
20	2	320	CLA	CHB-C1B	4.64	1.49	1.39
20	1	318	CLA	C3D-C4D	-4.64	1.33	1.44
20	4	304	CLA	CHC-C1C	4.64	1.47	1.38
20	B	822	CLA	O2D-CGD	4.63	1.44	1.33
20	A	827	CLA	CHC-C1C	4.63	1.47	1.38
20	B	813	CLA	CHC-C1C	4.63	1.47	1.38
19	4	315	CHL	C3D-C4D	-4.63	1.33	1.44
20	1	320	CLA	CHC-C1C	4.63	1.47	1.38
23	B	835	BCR	C14-C13	4.63	1.41	1.35
20	4	308	CLA	C3D-C4D	-4.62	1.33	1.44
20	J	103	CLA	CHC-C1C	4.62	1.47	1.38
20	L	305	CLA	C3C-C2C	4.62	1.46	1.36
20	B	827	CLA	C3D-C4D	-4.61	1.33	1.44
20	B	829	CLA	C3D-C4D	-4.61	1.33	1.44
19	3	313	CHL	C3D-C4D	-4.61	1.33	1.44
20	B	802	CLA	C3D-C4D	-4.61	1.33	1.44
20	B	811	CLA	CHC-C1C	4.61	1.47	1.38
20	B	809	CLA	C3D-C4D	-4.61	1.33	1.44
19	2	318	CHL	C3D-C4D	-4.61	1.33	1.44
23	3	303	BCR	C10-C9	4.60	1.41	1.35
20	B	814	CLA	O2D-CGD	4.60	1.44	1.33
23	K	202	BCR	C21-C22	4.60	1.41	1.35
20	A	829	CLA	CHC-C1C	4.60	1.47	1.38
20	L	305	CLA	CHC-C1C	4.60	1.47	1.38
20	B	816	CLA	C3D-C4D	-4.60	1.33	1.44
20	G	207	CLA	CHC-C1C	4.59	1.47	1.38
20	A	802	CLA	C3C-C2C	4.59	1.46	1.36
20	A	843	CLA	C3D-C4D	-4.59	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	319	CLA	CHC-C1C	4.59	1.47	1.38
20	A	853	CLA	C3D-C4D	-4.59	1.33	1.44
20	A	826	CLA	C3D-C4D	-4.59	1.33	1.44
23	4	320	BCR	C17-C18	4.59	1.41	1.35
19	2	309	CHL	C2C-C3C	4.59	1.46	1.36
23	B	838	BCR	C14-C13	4.59	1.41	1.35
20	3	312	CLA	CHC-C1C	4.58	1.47	1.38
20	A	856	CLA	C3D-C4D	-4.58	1.33	1.44
20	A	806	CLA	C3D-C4D	-4.58	1.33	1.44
20	B	848	CLA	C3D-C4D	-4.58	1.33	1.44
20	K	203	CLA	CHC-C1C	4.58	1.47	1.38
20	A	850	CLA	C3D-C4D	-4.58	1.33	1.44
19	2	318	CHL	C2C-C3C	4.58	1.46	1.36
20	1	303	CLA	O2D-CGD	4.58	1.45	1.30
20	2	320	CLA	C3C-C2C	4.58	1.45	1.36
20	L	307	CLA	CHC-C1C	4.58	1.47	1.38
20	B	824	CLA	CHC-C1C	4.58	1.47	1.38
20	F	305	CLA	CHC-C1C	4.58	1.47	1.38
20	F	306	CLA	CHC-C1C	4.57	1.47	1.38
23	2	312	BCR	C14-C13	4.57	1.41	1.35
20	K	204	CLA	CHC-C1C	4.57	1.47	1.38
20	A	836	CLA	CHC-C1C	4.57	1.47	1.38
20	B	820	CLA	C3D-C4D	-4.57	1.33	1.44
20	B	816	CLA	CHC-C1C	4.57	1.47	1.38
20	1	303	CLA	CHC-C1C	4.57	1.47	1.38
20	1	308	CLA	CHC-C1C	4.57	1.47	1.38
23	O	202	BCR	C10-C9	4.57	1.41	1.35
20	1	307	CLA	CHC-C1C	4.56	1.47	1.38
20	4	316	CLA	CHC-C1C	4.56	1.47	1.38
20	4	312	CLA	CHC-C1C	4.56	1.47	1.38
20	3	308	CLA	C3C-C2C	4.56	1.46	1.36
20	3	320	CLA	C3C-C2C	4.56	1.46	1.36
20	4	309	CLA	O2A-CGA	4.56	1.46	1.33
20	A	801	CLA	C3D-C4D	-4.56	1.33	1.44
20	B	810	CLA	CHC-C1C	4.56	1.47	1.38
20	B	828	CLA	C3D-C4D	-4.55	1.33	1.44
20	4	314	CLA	C3D-C4D	-4.55	1.33	1.44
23	B	838	BCR	C10-C9	4.55	1.41	1.35
20	A	809	CLA	C3D-C4D	-4.55	1.33	1.44
20	B	807	CLA	C3D-C4D	-4.55	1.33	1.44
20	A	803	CLA	O2A-CGA	4.55	1.46	1.33
20	B	846	CLA	C3D-C4D	-4.55	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	835	CLA	C3D-C4D	-4.55	1.33	1.44
28	A	824	CL0	O2D-CGD	4.54	1.45	1.30
20	3	310	CLA	C3D-C4D	-4.54	1.33	1.44
20	A	829	CLA	C3D-C4D	-4.54	1.33	1.44
20	B	817	CLA	CHC-C1C	4.54	1.47	1.38
20	2	321	CLA	CHC-C1C	4.54	1.47	1.38
20	B	822	CLA	C3D-C4D	-4.54	1.33	1.44
20	B	826	CLA	C3D-C4D	-4.54	1.33	1.44
20	A	854	CLA	C3D-C4D	-4.53	1.33	1.44
20	A	845	CLA	CHC-C1C	4.53	1.47	1.38
20	A	809	CLA	CHC-C1C	4.53	1.47	1.38
19	4	306	CHL	CHC-C1C	4.53	1.47	1.38
20	A	802	CLA	O2A-CGA	4.53	1.46	1.33
20	3	317	CLA	CHC-C1C	4.53	1.47	1.38
20	A	845	CLA	C3C-C2C	4.53	1.46	1.36
20	B	847	CLA	C3D-C4D	-4.52	1.34	1.44
20	A	836	CLA	O2A-CGA	4.52	1.46	1.33
20	B	806	CLA	C3D-C4D	-4.52	1.34	1.44
23	B	838	BCR	C17-C18	4.52	1.41	1.35
20	B	806	CLA	CHC-C1C	4.52	1.47	1.38
20	B	853	CLA	C3C-C2C	4.52	1.46	1.36
20	B	817	CLA	C3D-C4D	-4.52	1.34	1.44
20	A	804	CLA	C3D-C4D	-4.52	1.34	1.44
20	B	825	CLA	C3C-C2C	4.52	1.46	1.36
20	O	206	CLA	C3D-C4D	-4.52	1.34	1.44
20	A	802	CLA	C3D-C4D	-4.52	1.34	1.44
20	A	835	CLA	C3C-C2C	4.52	1.46	1.36
20	A	832	CLA	CHC-C1C	4.52	1.47	1.38
20	A	812	CLA	C3D-C4D	-4.52	1.34	1.44
23	4	319	BCR	C10-C9	4.52	1.41	1.35
20	O	207	CLA	C3C-C2C	4.51	1.46	1.36
20	4	303	CLA	C3D-C4D	-4.51	1.34	1.44
20	B	805	CLA	CHC-C1C	4.51	1.47	1.38
20	B	830	CLA	C3D-C4D	-4.51	1.34	1.44
20	B	813	CLA	C3D-C4D	-4.51	1.34	1.44
20	B	809	CLA	C3C-C2C	4.51	1.46	1.36
19	1	317	CHL	C2C-C3C	4.51	1.46	1.36
20	B	815	CLA	C3C-C2C	4.51	1.46	1.36
20	B	828	CLA	CHC-C1C	4.51	1.47	1.38
20	3	315	CLA	C3D-C4D	-4.51	1.34	1.44
20	A	842	CLA	C3D-C4D	-4.51	1.34	1.44
20	B	812	CLA	C3D-C4D	-4.50	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	825	CLA	CHC-C1C	4.50	1.47	1.38
20	A	839	CLA	O2A-CGA	4.50	1.45	1.30
20	A	830	CLA	C3D-C4D	-4.50	1.34	1.44
20	B	821	CLA	CHC-C1C	4.50	1.47	1.38
20	B	852	CLA	CHC-C1C	4.50	1.47	1.38
19	1	301	CHL	C2C-C3C	4.50	1.46	1.36
20	A	832	CLA	C3D-C4D	-4.50	1.34	1.44
20	A	851	CLA	C3D-C4D	-4.50	1.34	1.44
20	3	310	CLA	C3C-C2C	4.50	1.46	1.36
20	L	305	CLA	C3D-C4D	-4.50	1.34	1.44
19	2	302	CHL	CHC-C1C	4.50	1.47	1.38
19	4	315	CHL	C2C-C3C	4.50	1.46	1.36
20	B	805	CLA	O2A-CGA	4.50	1.45	1.30
20	2	304	CLA	CHC-C1C	4.50	1.47	1.38
20	B	824	CLA	C3D-C4D	-4.50	1.34	1.44
20	B	826	CLA	C3C-C2C	4.50	1.46	1.36
20	3	309	CLA	C3D-C4D	-4.50	1.34	1.44
20	A	849	CLA	CHC-C1C	4.50	1.47	1.38
20	2	323	CLA	C3C-C2C	4.50	1.46	1.36
20	A	807	CLA	CHC-C1C	4.50	1.47	1.38
19	4	315	CHL	O2A-CGA	4.50	1.45	1.30
19	2	322	CHL	C2C-C3C	4.50	1.46	1.36
20	B	815	CLA	C3D-C4D	-4.50	1.34	1.44
20	B	812	CLA	C3C-C2C	4.50	1.46	1.36
20	4	312	CLA	C3D-C4D	-4.50	1.34	1.44
20	B	821	CLA	C3D-C4D	-4.49	1.34	1.44
19	2	301	CHL	C2C-C3C	4.49	1.46	1.36
20	A	807	CLA	C3D-C4D	-4.49	1.34	1.44
20	1	304	CLA	CHC-C1C	4.49	1.47	1.38
20	A	846	CLA	CHC-C1C	4.49	1.47	1.38
20	1	321	CLA	C3D-C4D	-4.49	1.34	1.44
20	4	302	CLA	C3D-C4D	-4.49	1.34	1.44
20	3	308	CLA	C3D-C4D	-4.49	1.34	1.44
20	A	851	CLA	C3C-C2C	4.49	1.46	1.36
20	A	842	CLA	C3C-C2C	4.49	1.46	1.36
20	2	303	CLA	C3D-C4D	-4.49	1.34	1.44
20	3	315	CLA	CHC-C1C	4.49	1.47	1.38
19	4	305	CHL	C2C-C3C	4.49	1.46	1.36
20	B	823	CLA	C3D-C4D	-4.49	1.34	1.44
20	3	320	CLA	O2A-CGA	4.49	1.45	1.30
20	A	844	CLA	C3D-C4D	-4.49	1.34	1.44
20	B	811	CLA	C3C-C2C	4.49	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	G	206	CLA	C3D-C4D	-4.49	1.34	1.44
20	1	308	CLA	C3C-C2C	4.49	1.46	1.36
20	O	206	CLA	CHC-C1C	4.49	1.47	1.38
19	2	302	CHL	C2C-C3C	4.49	1.46	1.36
20	B	844	CLA	CHB-C1B	4.48	1.49	1.39
20	B	804	CLA	CHC-C1C	4.48	1.47	1.38
20	A	805	CLA	C3C-C2C	4.48	1.46	1.36
20	2	321	CLA	C3C-C2C	4.48	1.46	1.36
20	1	308	CLA	C3D-C4D	-4.48	1.34	1.44
20	4	304	CLA	C3C-C2C	4.48	1.46	1.36
20	2	303	CLA	CHC-C1C	4.48	1.47	1.38
20	B	812	CLA	CHC-C1C	4.48	1.47	1.38
20	4	310	CLA	C3D-C4D	-4.48	1.34	1.44
20	F	304	CLA	CHC-C1C	4.48	1.47	1.38
20	A	828	CLA	C3C-C2C	4.48	1.46	1.36
20	A	846	CLA	C3C-C2C	4.48	1.46	1.36
20	L	306	CLA	C3D-C4D	-4.48	1.34	1.44
20	K	206	CLA	CHC-C1C	4.48	1.47	1.38
20	4	304	CLA	O2A-CGA	4.47	1.45	1.30
20	K	206	CLA	C3C-C2C	4.47	1.46	1.36
20	2	305	CLA	C3D-C4D	-4.47	1.34	1.44
20	A	836	CLA	C3D-C4D	-4.47	1.34	1.44
20	1	306	CLA	O2A-CGA	4.47	1.45	1.30
20	L	307	CLA	C3C-C2C	4.47	1.46	1.36
20	A	838	CLA	C3D-C4D	-4.47	1.34	1.44
20	B	825	CLA	C3D-C4D	-4.47	1.34	1.44
20	A	850	CLA	CHC-C1C	4.47	1.47	1.38
20	3	311	CLA	C3D-C4D	-4.47	1.34	1.44
20	2	320	CLA	C3D-C4D	-4.47	1.34	1.44
20	1	318	CLA	C3C-C2C	4.47	1.46	1.36
20	B	846	CLA	O2A-CGA	4.46	1.45	1.30
20	2	317	CLA	C3C-C2C	4.46	1.46	1.36
20	B	831	CLA	C3D-C4D	-4.46	1.34	1.44
20	B	808	CLA	O2A-CGA	4.46	1.46	1.33
20	A	848	CLA	C3D-C4D	-4.46	1.34	1.44
19	4	306	CHL	O2A-CGA	4.46	1.45	1.30
20	1	303	CLA	C3D-C4D	-4.46	1.34	1.44
20	3	320	CLA	C3D-C4D	-4.46	1.34	1.44
20	1	305	CLA	C3C-C2C	4.46	1.46	1.36
20	A	849	CLA	C3D-C4D	-4.46	1.34	1.44
20	1	309	CLA	C3C-C2C	4.46	1.46	1.36
20	A	838	CLA	O2A-CGA	4.46	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	O	206	CLA	C3C-C2C	4.46	1.46	1.36
20	B	853	CLA	C3D-C4D	-4.46	1.34	1.44
23	A	816	BCR	C17-C18	4.46	1.41	1.35
23	A	818	BCR	C10-C9	4.46	1.41	1.35
20	2	321	CLA	C3D-C4D	-4.46	1.34	1.44
20	B	833	CLA	C3D-C4D	-4.46	1.34	1.44
20	G	205	CLA	CHC-C1C	4.46	1.47	1.38
20	A	812	CLA	O2A-CGA	4.46	1.46	1.33
20	K	205	CLA	C3D-C4D	-4.46	1.34	1.44
20	O	207	CLA	C3D-C4D	-4.46	1.34	1.44
19	2	322	CHL	O2A-CGA	4.45	1.45	1.30
19	4	307	CHL	O2A-CGA	4.45	1.45	1.30
20	2	306	CLA	O2A-CGA	4.45	1.45	1.30
19	2	322	CHL	CHC-C1C	4.45	1.47	1.38
20	L	306	CLA	CHC-C1C	4.45	1.47	1.38
20	A	833	CLA	C3D-C4D	-4.45	1.34	1.44
20	2	308	CLA	C3D-C4D	-4.45	1.34	1.44
20	A	852	CLA	C3D-C4D	-4.45	1.34	1.44
20	3	314	CLA	O2A-CGA	4.45	1.45	1.30
20	K	204	CLA	C3D-C4D	-4.45	1.34	1.44
20	3	319	CLA	C3D-C4D	-4.45	1.34	1.44
20	A	839	CLA	C3C-C2C	4.45	1.46	1.36
20	3	312	CLA	O2A-CGA	4.44	1.45	1.30
19	4	307	CHL	CHC-C1C	4.44	1.47	1.38
20	A	803	CLA	CHC-C1C	4.44	1.47	1.38
20	3	317	CLA	C3D-C4D	-4.44	1.34	1.44
20	B	852	CLA	C3D-C4D	-4.44	1.34	1.44
20	A	856	CLA	CHC-C1C	4.44	1.47	1.38
20	3	318	CLA	C3C-C2C	4.44	1.46	1.36
20	B	816	CLA	C3C-C2C	4.44	1.46	1.36
20	A	808	CLA	C3D-C4D	-4.44	1.34	1.44
20	1	321	CLA	CHC-C1C	4.44	1.47	1.38
19	4	306	CHL	C2C-C3C	4.44	1.46	1.36
20	2	319	CLA	C3D-C4D	-4.44	1.34	1.44
20	A	828	CLA	C3D-C4D	-4.44	1.34	1.44
23	B	839	BCR	C14-C13	4.44	1.41	1.35
20	4	314	CLA	CHC-C1C	4.44	1.47	1.38
20	1	307	CLA	C3D-C4D	-4.44	1.34	1.44
20	B	808	CLA	CHC-C1C	4.44	1.47	1.38
20	3	312	CLA	C3C-C2C	4.43	1.46	1.36
20	B	808	CLA	C3D-C4D	-4.43	1.34	1.44
20	4	313	CLA	C3D-C4D	-4.43	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	825	CLA	O2A-CGA	4.43	1.45	1.30
20	O	206	CLA	O2A-CGA	4.43	1.46	1.33
20	F	305	CLA	C3C-C2C	4.43	1.46	1.36
20	B	807	CLA	C3C-C2C	4.43	1.46	1.36
20	A	830	CLA	CHC-C1C	4.43	1.47	1.38
20	1	320	CLA	C3D-C4D	-4.43	1.34	1.44
20	A	837	CLA	C3D-C4D	-4.43	1.34	1.44
20	A	841	CLA	C3C-C2C	4.43	1.46	1.36
20	1	319	CLA	CHC-C1C	4.43	1.47	1.38
20	A	835	CLA	CHC-C1C	4.43	1.47	1.38
20	4	313	CLA	C3C-C2C	4.43	1.46	1.36
20	A	812	CLA	C3C-C2C	4.43	1.46	1.36
23	L	304	BCR	C21-C22	4.43	1.41	1.35
20	4	310	CLA	CHC-C1C	4.43	1.47	1.38
20	4	311	CLA	C3C-C2C	4.43	1.46	1.36
20	B	822	CLA	C3C-C2C	4.43	1.46	1.36
20	1	302	CLA	C3C-C2C	4.43	1.46	1.36
20	4	309	CLA	C3D-C4D	-4.42	1.34	1.44
20	B	844	CLA	C3D-C4D	-4.42	1.34	1.44
20	B	816	CLA	O2A-CGA	4.42	1.46	1.33
23	F	302	BCR	C10-C9	4.42	1.41	1.35
20	1	304	CLA	C3C-C2C	4.42	1.46	1.36
20	G	205	CLA	C3D-C4D	-4.42	1.34	1.44
20	N	202	CLA	O2A-CGA	4.42	1.46	1.33
20	2	303	CLA	O2A-CGA	4.42	1.45	1.30
20	A	850	CLA	C3C-C2C	4.42	1.46	1.36
20	3	319	CLA	CHC-C1C	4.42	1.47	1.38
20	A	847	CLA	CHC-C1C	4.42	1.47	1.38
20	A	805	CLA	C3D-C4D	-4.42	1.34	1.44
20	A	831	CLA	C3D-C4D	-4.42	1.34	1.44
20	F	306	CLA	C3D-C4D	-4.42	1.34	1.44
20	2	305	CLA	C3C-C2C	4.42	1.46	1.36
20	O	208	CLA	O2A-CGA	4.42	1.45	1.30
20	A	836	CLA	C3C-C2C	4.41	1.46	1.36
20	B	802	CLA	C3C-C2C	4.41	1.46	1.36
20	1	305	CLA	C3D-C4D	-4.41	1.34	1.44
20	4	309	CLA	C3C-C2C	4.41	1.46	1.36
20	G	205	CLA	C3C-C2C	4.41	1.46	1.36
20	K	203	CLA	C3C-C2C	4.41	1.46	1.36
20	2	323	CLA	C3D-C4D	-4.41	1.34	1.44
20	L	306	CLA	C3C-C2C	4.41	1.46	1.36
20	4	304	CLA	C3D-C4D	-4.41	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	307	CLA	C3D-C4D	-4.41	1.34	1.44
20	B	801	CLA	C3D-C4D	-4.41	1.34	1.44
20	A	843	CLA	C3C-C2C	4.41	1.46	1.36
20	H	201	CLA	O2A-CGA	4.41	1.46	1.33
20	1	320	CLA	C3C-C2C	4.41	1.46	1.36
20	A	827	CLA	C3D-C4D	-4.41	1.34	1.44
20	B	813	CLA	C3C-C2C	4.41	1.46	1.36
20	3	312	CLA	C3D-C4D	-4.40	1.34	1.44
20	B	818	CLA	C3C-C2C	4.40	1.46	1.36
19	3	313	CHL	C2C-C3C	4.40	1.46	1.36
20	1	304	CLA	C3D-C4D	-4.40	1.34	1.44
20	3	318	CLA	C3D-C4D	-4.40	1.34	1.44
19	4	307	CHL	C2C-C3C	4.40	1.46	1.36
20	L	307	CLA	C3D-C4D	-4.40	1.34	1.44
20	K	206	CLA	C3D-C4D	-4.40	1.34	1.44
20	B	802	CLA	O2A-CGA	4.40	1.45	1.30
20	B	853	CLA	CHC-C1C	4.40	1.47	1.38
20	3	314	CLA	C3D-C4D	-4.40	1.34	1.44
20	B	805	CLA	C3D-C4D	-4.40	1.34	1.44
20	A	840	CLA	CHC-C1C	4.39	1.47	1.38
20	B	810	CLA	C3C-C2C	4.39	1.46	1.36
23	B	835	BCR	C21-C22	4.39	1.41	1.35
20	A	831	CLA	C3C-C2C	4.39	1.46	1.36
23	2	312	BCR	C21-C22	4.39	1.41	1.35
20	B	833	CLA	C3C-C2C	4.39	1.46	1.36
23	3	303	BCR	C14-C13	4.39	1.41	1.35
23	4	320	BCR	C10-C9	4.39	1.41	1.35
19	1	317	CHL	CHC-C1C	4.39	1.47	1.38
23	B	837	BCR	C14-C13	4.39	1.41	1.35
20	A	803	CLA	C3D-C4D	-4.39	1.34	1.44
20	O	208	CLA	C3D-C4D	-4.39	1.34	1.44
20	J	103	CLA	C3C-C2C	4.39	1.46	1.36
20	1	306	CLA	C3D-C4D	-4.39	1.34	1.44
20	1	318	CLA	O2A-CGA	4.38	1.46	1.33
20	F	304	CLA	C3D-C4D	-4.38	1.34	1.44
20	A	855	CLA	O2A-CGA	4.38	1.46	1.33
19	2	318	CHL	O2D-CGD	4.38	1.43	1.33
20	2	307	CLA	CHC-C1C	4.38	1.47	1.38
20	3	314	CLA	CHC-C1C	4.38	1.47	1.38
20	A	806	CLA	CHC-C1C	4.38	1.47	1.38
20	A	847	CLA	C3C-C2C	4.38	1.46	1.36
23	K	202	BCR	C17-C18	4.38	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	823	CLA	C3C-C2C	4.38	1.46	1.36
20	3	308	CLA	O2A-CGA	4.38	1.46	1.33
20	J	103	CLA	C3D-C4D	-4.38	1.34	1.44
20	B	808	CLA	C3C-C2C	4.37	1.46	1.36
20	A	840	CLA	C3D-C4D	-4.37	1.34	1.44
20	2	303	CLA	C3C-C2C	4.37	1.46	1.36
20	G	207	CLA	C3C-C2C	4.37	1.46	1.36
20	N	202	CLA	C3C-C2C	4.37	1.46	1.36
19	2	309	CHL	CHD-C1D	4.37	1.46	1.38
20	L	306	CLA	O2A-CGA	4.37	1.46	1.33
20	K	204	CLA	C3C-C2C	4.37	1.46	1.36
20	B	849	CLA	C3C-C2C	4.37	1.46	1.36
20	A	811	CLA	C3D-C4D	-4.37	1.34	1.44
20	A	825	CLA	C3D-C4D	-4.37	1.34	1.44
20	G	206	CLA	C3C-C2C	4.37	1.46	1.36
20	K	203	CLA	C3D-C4D	-4.37	1.34	1.44
20	G	207	CLA	C3D-C4D	-4.37	1.34	1.44
20	B	821	CLA	C3C-C2C	4.37	1.46	1.36
19	4	305	CHL	CHC-C1C	4.36	1.47	1.38
20	A	838	CLA	C3C-C2C	4.36	1.46	1.36
20	A	833	CLA	CHC-C1C	4.36	1.47	1.38
20	B	811	CLA	O2A-CGA	4.36	1.46	1.33
20	4	316	CLA	O2A-CGA	4.36	1.46	1.33
20	A	846	CLA	C3D-C4D	-4.36	1.34	1.44
20	K	203	CLA	O2A-CGA	4.36	1.46	1.33
20	B	810	CLA	C3D-C4D	-4.36	1.34	1.44
20	B	818	CLA	CHC-C1C	4.36	1.47	1.38
23	A	814	BCR	C10-C9	4.36	1.41	1.35
20	3	317	CLA	O2A-CGA	4.36	1.46	1.33
19	2	301	CHL	CHC-C1C	4.36	1.47	1.38
20	1	302	CLA	C3D-C4D	-4.36	1.34	1.44
20	1	303	CLA	C3C-C2C	4.36	1.46	1.36
23	G	201	BCR	C10-C9	4.36	1.41	1.35
20	2	317	CLA	C3D-C4D	-4.35	1.34	1.44
23	L	301	BCR	C10-C9	4.35	1.41	1.35
20	A	832	CLA	C3C-C2C	4.35	1.46	1.36
20	A	811	CLA	C3C-C2C	4.35	1.46	1.36
20	B	849	CLA	O2A-CGA	4.35	1.46	1.33
20	4	311	CLA	C3D-C4D	-4.35	1.34	1.44
20	N	202	CLA	C3D-C4D	-4.35	1.34	1.44
20	1	309	CLA	C3D-C4D	-4.35	1.34	1.44
20	A	853	CLA	CHC-C1C	4.35	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	305	CLA	O2A-CGA	4.35	1.46	1.33
20	B	850	CLA	C3D-C4D	-4.35	1.34	1.44
20	2	321	CLA	O2A-CGA	4.35	1.46	1.33
20	1	322	CLA	C3D-C4D	-4.35	1.34	1.44
20	2	306	CLA	C3C-C2C	4.34	1.46	1.36
20	B	853	CLA	O2A-CGA	4.34	1.46	1.33
20	1	306	CLA	C3C-C2C	4.34	1.46	1.36
20	B	820	CLA	O2A-CGA	4.34	1.46	1.33
20	B	827	CLA	C3C-C2C	4.34	1.46	1.36
20	B	849	CLA	CHC-C1C	4.34	1.47	1.38
28	A	824	CL0	C3D-C4D	-4.34	1.34	1.44
20	H	201	CLA	C3D-C4D	-4.34	1.34	1.44
20	B	833	CLA	O2A-CGA	4.34	1.46	1.33
20	B	804	CLA	O2A-CGA	4.34	1.46	1.33
20	1	319	CLA	C3C-C2C	4.34	1.45	1.36
29	J	104	DGD	O2G-C1B	4.34	1.46	1.34
20	A	827	CLA	O2A-CGA	4.33	1.46	1.33
20	2	306	CLA	C3D-C4D	-4.33	1.34	1.44
29	B	840	DGD	O1G-C1A	4.33	1.46	1.33
20	B	830	CLA	CHC-C1C	4.33	1.47	1.38
20	A	853	CLA	C3C-C2C	4.33	1.45	1.36
19	1	317	CHL	O2A-CGA	4.33	1.46	1.33
21	2	310	LUT	C30-C29	4.33	1.41	1.35
20	1	303	CLA	O2A-CGA	4.33	1.46	1.33
20	A	839	CLA	CHC-C1C	4.33	1.47	1.38
20	4	310	CLA	C3C-C2C	4.33	1.45	1.36
20	4	316	CLA	C3C-C2C	4.33	1.45	1.36
20	B	810	CLA	O2A-CGA	4.33	1.46	1.33
23	F	301	BCR	C14-C13	4.33	1.41	1.35
20	F	305	CLA	C3D-C4D	-4.32	1.34	1.44
20	A	838	CLA	CHC-C1C	4.32	1.47	1.38
20	3	315	CLA	C3C-C2C	4.32	1.45	1.36
20	A	856	CLA	O2A-CGA	4.32	1.46	1.33
20	A	832	CLA	O2A-CGA	4.32	1.46	1.33
20	B	829	CLA	C3C-C2C	4.32	1.45	1.36
20	3	310	CLA	O2A-CGA	4.32	1.46	1.33
20	A	837	CLA	C3C-C2C	4.32	1.45	1.36
20	H	201	CLA	C3C-C2C	4.31	1.45	1.36
20	B	811	CLA	C3D-C4D	-4.31	1.34	1.44
20	3	317	CLA	C3C-C2C	4.31	1.45	1.36
19	1	301	CHL	CHD-C1D	4.31	1.46	1.38
20	3	319	CLA	C3C-C2C	4.31	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	302	CLA	O2A-CGA	4.31	1.45	1.33
20	3	316	CLA	C3D-C4D	-4.31	1.34	1.44
20	A	854	CLA	O2A-CGA	4.31	1.45	1.33
23	B	836	BCR	C21-C22	4.31	1.41	1.35
20	1	307	CLA	C3C-C2C	4.31	1.45	1.36
20	4	312	CLA	O2A-CGA	4.31	1.45	1.33
20	B	803	CLA	C3D-C4D	-4.31	1.34	1.44
20	3	310	CLA	CHC-C1C	4.31	1.47	1.38
19	4	305	CHL	CHD-C1D	4.31	1.46	1.38
23	L	302	BCR	C14-C13	4.31	1.41	1.35
20	3	307	CLA	C3C-C2C	4.30	1.45	1.36
20	2	317	CLA	O2A-CGA	4.30	1.45	1.33
20	A	855	CLA	C3C-C2C	4.30	1.45	1.36
23	G	201	BCR	C14-C13	4.30	1.41	1.35
23	J	101	BCR	C21-C22	4.30	1.41	1.35
20	A	848	CLA	O2A-CGA	4.30	1.45	1.33
20	2	320	CLA	C4B-NB	-4.30	1.32	1.37
20	A	840	CLA	C3C-C2C	4.30	1.45	1.36
23	O	202	BCR	C17-C18	4.30	1.41	1.35
20	4	302	CLA	C3C-C2C	4.30	1.45	1.36
20	A	807	CLA	C3C-C2C	4.30	1.45	1.36
20	A	802	CLA	CHC-C1C	4.29	1.47	1.38
20	A	811	CLA	O2A-CGA	4.29	1.45	1.33
20	A	805	CLA	O2A-CGA	4.29	1.45	1.33
20	A	844	CLA	C3C-C2C	4.29	1.45	1.36
20	1	307	CLA	O2A-CGA	4.29	1.45	1.33
20	A	825	CLA	O2A-CGA	4.29	1.45	1.33
20	B	847	CLA	C3C-C2C	4.29	1.45	1.36
20	2	304	CLA	C3D-C4D	-4.29	1.34	1.44
20	4	312	CLA	C3C-C2C	4.29	1.45	1.36
29	O	201	DGD	O2G-C1B	4.29	1.46	1.34
20	B	823	CLA	CHC-C1C	4.29	1.47	1.38
20	B	824	CLA	C3C-C2C	4.29	1.45	1.36
20	A	837	CLA	O2A-CGA	4.29	1.45	1.33
20	2	308	CLA	C3C-C2C	4.29	1.45	1.36
20	B	845	CLA	C3D-C4D	-4.28	1.34	1.44
20	2	320	CLA	O2A-CGA	4.28	1.45	1.33
20	G	206	CLA	O2A-CGA	4.28	1.45	1.33
20	B	819	CLA	C3C-C2C	4.28	1.45	1.36
20	B	824	CLA	O2A-CGA	4.28	1.45	1.33
20	B	807	CLA	O2A-CGA	4.28	1.45	1.33
20	A	830	CLA	C3C-C2C	4.28	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	851	CLA	C3D-C4D	-4.28	1.34	1.44
28	A	824	CL0	C3C-C2C	4.28	1.45	1.36
20	4	310	CLA	O2A-CGA	4.28	1.45	1.33
20	A	844	CLA	CHC-C1C	4.28	1.47	1.38
20	B	828	CLA	C3C-C2C	4.27	1.45	1.36
20	2	304	CLA	C3C-C2C	4.27	1.45	1.36
20	B	821	CLA	O2A-CGA	4.27	1.45	1.33
20	1	304	CLA	O2A-CGA	4.27	1.45	1.33
20	A	850	CLA	O2A-CGA	4.27	1.45	1.33
20	2	307	CLA	C3C-C2C	4.27	1.45	1.36
20	1	322	CLA	C3C-C2C	4.27	1.45	1.36
20	3	316	CLA	C3C-C2C	4.27	1.45	1.36
20	A	843	CLA	O2A-CGA	4.27	1.45	1.33
20	B	822	CLA	O2A-CGA	4.26	1.45	1.33
20	A	848	CLA	C3C-C2C	4.26	1.45	1.36
29	J	104	DGD	O1G-C1A	4.26	1.45	1.33
19	4	306	CHL	CHD-C1D	4.26	1.46	1.38
20	B	805	CLA	C3C-C2C	4.26	1.45	1.36
19	2	302	CHL	CHD-C1D	4.26	1.46	1.38
20	A	852	CLA	C3C-C2C	4.26	1.45	1.36
20	F	306	CLA	C3C-C2C	4.26	1.45	1.36
20	A	831	CLA	CHC-C1C	4.26	1.47	1.38
20	A	807	CLA	O2A-CGA	4.26	1.45	1.33
20	B	851	CLA	O2A-CGA	4.26	1.45	1.33
20	B	806	CLA	C3C-C2C	4.26	1.45	1.36
20	B	820	CLA	C3C-C2C	4.26	1.45	1.36
20	2	307	CLA	O2A-CGA	4.26	1.45	1.33
20	3	311	CLA	CHC-C1C	4.26	1.47	1.38
20	A	834	CLA	C3C-C2C	4.26	1.45	1.36
19	2	301	CHL	CHD-C1D	4.26	1.46	1.38
20	1	320	CLA	O2A-CGA	4.26	1.45	1.33
20	B	828	CLA	O2A-CGA	4.26	1.45	1.33
20	A	847	CLA	O2A-CGA	4.25	1.45	1.33
19	4	315	CHL	CHC-C1C	4.25	1.47	1.38
20	B	822	CLA	CHC-C1C	4.25	1.47	1.38
20	A	801	CLA	C3C-C2C	4.25	1.45	1.36
20	3	307	CLA	C3D-C4D	-4.25	1.34	1.44
20	B	830	CLA	O2A-CGA	4.25	1.45	1.33
20	A	809	CLA	O2A-CGA	4.25	1.45	1.33
20	B	817	CLA	O2A-CGA	4.25	1.45	1.33
29	O	201	DGD	O1G-C1A	4.25	1.45	1.33
20	A	825	CLA	C3C-C2C	4.25	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	317	CHL	CHD-C1D	4.25	1.46	1.38
20	A	801	CLA	CHC-C1C	4.25	1.47	1.38
20	B	801	CLA	C3C-C2C	4.24	1.45	1.36
20	3	315	CLA	O2A-CGA	4.24	1.45	1.33
20	B	818	CLA	O2A-CGA	4.24	1.45	1.33
20	A	835	CLA	O2A-CGA	4.24	1.45	1.33
20	B	809	CLA	O2A-CGA	4.24	1.45	1.33
20	A	806	CLA	C3C-C2C	4.24	1.45	1.36
20	4	313	CLA	O2A-CGA	4.24	1.45	1.33
23	B	835	BCR	C17-C18	4.24	1.41	1.35
20	B	803	CLA	O2A-CGA	4.24	1.45	1.33
20	B	826	CLA	O2A-CGA	4.24	1.45	1.33
29	G	202	DGD	O1G-C1A	4.24	1.45	1.33
19	3	313	CHL	CHC-C1C	4.24	1.47	1.38
20	B	814	CLA	C3C-C2C	4.24	1.45	1.36
20	4	308	CLA	C3C-C2C	4.23	1.45	1.36
20	B	850	CLA	CHC-C1C	4.23	1.47	1.38
20	3	314	CLA	C3C-C2C	4.23	1.45	1.36
20	2	308	CLA	O2A-CGA	4.23	1.45	1.33
20	3	311	CLA	O2A-CGA	4.23	1.45	1.33
20	4	314	CLA	C3C-C2C	4.23	1.45	1.36
20	A	826	CLA	C3C-C2C	4.23	1.45	1.36
20	A	841	CLA	O2A-CGA	4.23	1.45	1.33
20	B	830	CLA	C3C-C2C	4.23	1.45	1.36
20	2	304	CLA	O2A-CGA	4.23	1.45	1.33
19	2	318	CHL	CHC-C1C	4.23	1.47	1.38
20	O	207	CLA	O2A-CGA	4.22	1.45	1.33
20	A	843	CLA	CHC-C1C	4.22	1.47	1.38
20	3	311	CLA	C3C-C2C	4.22	1.45	1.36
19	1	301	CHL	CHC-C1C	4.22	1.47	1.38
20	B	852	CLA	C3C-C2C	4.22	1.45	1.36
20	A	848	CLA	CHC-C1C	4.22	1.47	1.38
20	K	205	CLA	C3C-C2C	4.22	1.45	1.36
20	A	829	CLA	O2A-CGA	4.22	1.45	1.33
20	B	819	CLA	O2A-CGA	4.21	1.45	1.33
20	B	801	CLA	CHC-C1C	4.21	1.47	1.38
20	A	808	CLA	C3C-C2C	4.21	1.45	1.36
23	A	857	BCR	C17-C18	4.21	1.41	1.35
20	B	831	CLA	O2A-CGA	4.20	1.45	1.33
20	4	314	CLA	O2A-CGA	4.20	1.45	1.33
20	B	812	CLA	O2A-CGA	4.20	1.45	1.33
19	3	313	CHL	O2A-CGA	4.20	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	312	CLA	CHB-C1B	4.20	1.48	1.39
20	K	204	CLA	O2A-CGA	4.20	1.45	1.33
20	A	849	CLA	CHB-C1B	4.20	1.48	1.39
20	B	829	CLA	O2A-CGA	4.19	1.45	1.33
20	O	208	CLA	C3C-C2C	4.19	1.45	1.36
20	A	842	CLA	O2A-CGA	4.19	1.45	1.33
20	B	845	CLA	O2A-CGA	4.19	1.45	1.33
20	A	828	CLA	O2A-CGA	4.19	1.45	1.33
20	B	847	CLA	O2A-CGA	4.18	1.45	1.33
19	2	322	CHL	CHD-C1D	4.18	1.46	1.38
20	B	814	CLA	C3D-C4D	-4.18	1.34	1.44
20	B	804	CLA	C3C-C2C	4.18	1.45	1.36
20	A	808	CLA	CHC-C1C	4.17	1.47	1.38
20	4	316	CLA	C3D-C4D	-4.17	1.34	1.44
19	4	315	CHL	CHD-C1D	4.17	1.46	1.38
23	I	102	BCR	C14-C13	4.17	1.41	1.35
20	B	803	CLA	C3C-C2C	4.17	1.45	1.36
23	B	834	BCR	C21-C22	4.17	1.41	1.35
20	B	850	CLA	O2A-CGA	4.17	1.45	1.33
19	4	307	CHL	CHD-C1D	4.17	1.46	1.38
19	3	313	CHL	CHD-C1D	4.16	1.46	1.38
20	A	854	CLA	C3C-C2C	4.16	1.45	1.36
20	A	826	CLA	O2A-CGA	4.16	1.45	1.33
20	A	856	CLA	C3C-C2C	4.16	1.45	1.36
20	A	831	CLA	O2A-CGA	4.16	1.45	1.33
20	A	833	CLA	O2A-CGA	4.16	1.45	1.33
19	2	318	CHL	O2A-CGA	4.16	1.45	1.33
20	A	852	CLA	O2A-CGA	4.16	1.45	1.33
20	B	806	CLA	O2A-CGA	4.15	1.45	1.33
23	I	102	BCR	C21-C22	4.15	1.41	1.35
23	2	312	BCR	C17-C18	4.14	1.41	1.35
20	A	833	CLA	C3C-C2C	4.14	1.45	1.36
20	4	308	CLA	CHC-C1C	4.14	1.46	1.38
20	2	319	CLA	O2A-CGA	4.14	1.45	1.33
28	A	824	CL0	O2A-CGA	4.14	1.45	1.33
23	L	302	BCR	C21-C22	4.14	1.41	1.35
20	A	804	CLA	CHC-C1C	4.14	1.46	1.38
20	A	804	CLA	O2A-CGA	4.14	1.45	1.33
20	A	804	CLA	C3C-C2C	4.14	1.45	1.36
20	A	834	CLA	O2A-CGA	4.13	1.45	1.33
20	B	831	CLA	C3C-C2C	4.13	1.45	1.36
20	B	814	CLA	O2A-CGA	4.13	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	321	CLA	C3C-C2C	4.13	1.45	1.36
21	1	323	LUT	C30-C29	4.13	1.41	1.35
20	B	852	CLA	O2A-CGA	4.13	1.45	1.33
20	A	806	CLA	O2A-CGA	4.12	1.45	1.33
20	F	304	CLA	O2A-CGA	4.12	1.45	1.33
20	B	846	CLA	C3C-C2C	4.12	1.45	1.36
23	K	201	BCR	C21-C22	4.12	1.41	1.35
20	A	803	CLA	C3C-C2C	4.12	1.45	1.36
21	1	323	LUT	C10-C9	4.12	1.41	1.35
23	A	818	BCR	C14-C13	4.12	1.41	1.35
20	A	845	CLA	O2A-CGA	4.12	1.45	1.33
20	B	848	CLA	O2A-CGA	4.11	1.45	1.33
20	3	309	CLA	C3C-C2C	4.11	1.45	1.36
20	A	830	CLA	O2A-CGA	4.11	1.45	1.33
20	3	307	CLA	CHC-C1C	4.11	1.46	1.38
23	G	203	BCR	C21-C22	4.11	1.41	1.35
23	B	837	BCR	C10-C9	4.10	1.41	1.35
20	4	303	CLA	C3C-C2C	4.10	1.45	1.36
29	G	202	DGD	O2G-C1B	4.10	1.45	1.34
20	A	849	CLA	C3C-C2C	4.10	1.45	1.36
23	B	836	BCR	C17-C18	4.10	1.41	1.35
23	K	201	BCR	C14-C13	4.10	1.41	1.35
20	4	302	CLA	O2A-CGA	4.09	1.45	1.33
20	3	319	CLA	O2A-CGA	4.09	1.46	1.33
20	A	809	CLA	C3C-C2C	4.08	1.45	1.36
20	A	851	CLA	O2A-CGA	4.08	1.45	1.33
20	A	855	CLA	CHC-C1C	4.07	1.46	1.38
20	2	319	CLA	C3C-C2C	4.07	1.45	1.36
21	1	323	LUT	C34-C33	4.07	1.41	1.35
20	B	815	CLA	O2A-CGA	4.07	1.45	1.33
23	L	301	BCR	C14-C13	4.07	1.41	1.35
19	4	305	CHL	O2A-CGA	4.07	1.46	1.33
23	G	201	BCR	C21-C22	4.06	1.41	1.35
20	B	847	CLA	CHB-C1B	4.06	1.48	1.39
20	B	813	CLA	O2A-CGA	4.06	1.45	1.33
21	1	323	LUT	C14-C13	4.06	1.41	1.35
20	A	801	CLA	O2A-CGA	4.06	1.45	1.33
20	B	801	CLA	O2A-CGA	4.06	1.45	1.33
20	B	848	CLA	C3C-C2C	4.05	1.45	1.36
20	K	205	CLA	CHB-C1B	4.05	1.48	1.39
20	A	833	CLA	CHB-C1B	4.05	1.48	1.39
20	A	826	CLA	CHC-C1C	4.05	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	827	CLA	O2A-CGA	4.05	1.45	1.33
19	2	309	CHL	CHD-C4C	4.05	1.48	1.39
20	L	305	CLA	O2A-CGA	4.05	1.45	1.33
23	L	301	BCR	C21-C22	4.04	1.41	1.35
20	A	852	CLA	CHC-C1C	4.04	1.46	1.38
19	2	302	CHL	O2A-CGA	4.04	1.45	1.33
20	A	846	CLA	O2A-CGA	4.04	1.45	1.33
20	3	316	CLA	O2A-CGA	4.04	1.45	1.33
20	4	303	CLA	O2A-CGA	4.04	1.45	1.33
20	B	805	CLA	CHB-C1B	4.04	1.48	1.39
20	B	817	CLA	C3C-C2C	4.04	1.45	1.36
20	K	205	CLA	O2A-CGA	4.04	1.45	1.33
28	A	824	CL0	CHC-C1C	4.03	1.46	1.38
20	2	307	CLA	CHB-C1B	4.03	1.48	1.39
20	B	816	CLA	CHB-C1B	4.03	1.48	1.39
20	F	305	CLA	O2A-CGA	4.03	1.45	1.33
20	K	205	CLA	CHC-C4B	4.03	1.48	1.39
20	3	309	CLA	O2A-CGA	4.03	1.45	1.33
19	2	318	CHL	CHD-C1D	4.03	1.46	1.38
20	B	844	CLA	CHC-C1C	4.03	1.46	1.38
20	G	205	CLA	CHB-C1B	4.02	1.48	1.39
20	F	306	CLA	O2A-CGA	4.02	1.45	1.33
20	2	306	CLA	CHB-C1B	4.02	1.48	1.39
20	A	853	CLA	O2A-CGA	4.02	1.45	1.33
20	G	207	CLA	O2A-CGA	4.02	1.45	1.33
20	B	851	CLA	CHC-C1C	4.01	1.46	1.38
20	B	845	CLA	C3C-C2C	4.01	1.45	1.36
19	2	301	CHL	O2A-CGA	4.01	1.45	1.33
20	A	827	CLA	C3C-C2C	4.01	1.45	1.36
20	4	311	CLA	O2A-CGA	4.01	1.45	1.33
20	4	303	CLA	CHB-C1B	4.01	1.48	1.39
20	B	817	CLA	CHB-C1B	4.01	1.48	1.39
20	A	840	CLA	O2A-CGA	4.01	1.45	1.33
20	G	205	CLA	O2A-CGA	4.01	1.45	1.33
20	1	308	CLA	O2A-CGA	4.00	1.45	1.33
20	B	813	CLA	CHC-C4B	4.00	1.48	1.39
20	G	206	CLA	CHB-C1B	4.00	1.48	1.39
29	B	840	DGD	O2G-C1B	4.00	1.45	1.34
20	A	849	CLA	O2A-CGA	4.00	1.45	1.33
20	1	322	CLA	O2A-CGA	3.99	1.45	1.33
20	F	304	CLA	C3C-C2C	3.99	1.45	1.36
20	1	321	CLA	O2A-CGA	3.98	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	815	BCR	C10-C9	3.97	1.41	1.35
20	L	307	CLA	O2A-CGA	3.97	1.45	1.33
20	B	823	CLA	O2A-CGA	3.97	1.45	1.33
20	B	844	CLA	C3C-C2C	3.97	1.45	1.36
20	J	103	CLA	O2A-CGA	3.97	1.45	1.33
20	1	319	CLA	O2A-CGA	3.97	1.44	1.33
20	4	308	CLA	O2A-CGA	3.97	1.45	1.33
20	K	203	CLA	CHB-C1B	3.97	1.48	1.39
23	B	839	BCR	C17-C18	3.97	1.41	1.35
20	A	803	CLA	CHB-C1B	3.97	1.48	1.39
20	1	305	CLA	O2A-CGA	3.97	1.45	1.33
20	B	851	CLA	CHB-C1B	3.97	1.48	1.39
20	B	850	CLA	C3C-C2C	3.97	1.45	1.36
20	3	318	CLA	C3A-C2A	-3.97	1.50	1.54
20	B	844	CLA	O2A-CGA	3.97	1.44	1.33
20	3	314	CLA	CHB-C1B	3.96	1.48	1.39
23	1	312	BCR	C17-C18	3.96	1.41	1.35
20	B	820	CLA	CHC-C1C	3.95	1.46	1.38
23	I	102	BCR	C17-C18	3.95	1.41	1.35
20	K	204	CLA	CHB-C1B	3.95	1.48	1.39
23	A	814	BCR	C17-C18	3.95	1.41	1.35
20	A	834	CLA	CHC-C1C	3.94	1.46	1.38
23	A	857	BCR	C21-C22	3.94	1.41	1.35
23	1	312	BCR	C21-C22	3.93	1.41	1.35
23	A	817	BCR	C10-C9	3.92	1.41	1.35
20	A	851	CLA	CHB-C1B	3.92	1.48	1.39
19	2	302	CHL	CHD-C4C	3.92	1.48	1.39
19	1	301	CHL	CHD-C4C	3.92	1.48	1.39
20	A	854	CLA	CHC-C1C	3.92	1.46	1.38
20	1	309	CLA	C3A-C2A	-3.92	1.50	1.54
23	4	319	BCR	C17-C18	3.92	1.41	1.35
21	2	310	LUT	C34-C33	3.92	1.41	1.35
20	1	309	CLA	CHB-C1B	3.92	1.48	1.39
20	B	851	CLA	C3C-C2C	3.91	1.45	1.36
19	2	322	CHL	CHD-C4C	3.91	1.48	1.39
20	A	805	CLA	CHC-C4B	3.91	1.48	1.39
20	L	307	CLA	CHB-C1B	3.91	1.48	1.39
20	A	829	CLA	C3C-C2C	3.91	1.45	1.36
19	4	306	CHL	CHD-C4C	3.91	1.48	1.39
20	1	303	CLA	CHB-C1B	3.91	1.48	1.39
20	3	316	CLA	CHB-C1B	3.91	1.48	1.39
23	4	319	BCR	C21-C22	3.90	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	317	CHL	CHD-C4C	3.89	1.48	1.39
20	1	302	CLA	CHB-C1B	3.89	1.48	1.39
23	F	302	BCR	C14-C13	3.89	1.40	1.35
23	K	201	BCR	C17-C18	3.89	1.40	1.35
19	4	305	CHL	CHD-C4C	3.88	1.48	1.39
23	B	834	BCR	C14-C13	3.88	1.40	1.35
23	J	101	BCR	C17-C18	3.87	1.40	1.35
20	2	323	CLA	O2A-CGA	3.87	1.45	1.33
20	4	302	CLA	CHB-C1B	3.87	1.48	1.39
20	3	311	CLA	CHB-C1B	3.87	1.48	1.39
19	4	315	CHL	CHD-C4C	3.87	1.48	1.39
20	2	304	CLA	CHB-C1B	3.87	1.48	1.39
19	2	301	CHL	CHD-C4C	3.86	1.48	1.39
20	A	830	CLA	CHB-C1B	3.86	1.48	1.39
20	A	827	CLA	CHB-C1B	3.86	1.48	1.39
20	1	308	CLA	CHB-C1B	3.86	1.48	1.39
23	A	814	BCR	C21-C22	3.86	1.40	1.35
20	2	321	CLA	CHB-C1B	3.86	1.48	1.39
28	A	824	CL0	CHB-C1B	3.86	1.48	1.39
20	A	829	CLA	CHB-C1B	3.86	1.48	1.39
20	B	831	CLA	CHB-C1B	3.86	1.48	1.39
20	H	201	CLA	CHB-C1B	3.85	1.48	1.39
20	1	306	CLA	CHB-C1B	3.85	1.48	1.39
20	4	309	CLA	CHC-C4B	3.85	1.48	1.39
20	B	803	CLA	CHB-C1B	3.85	1.48	1.39
20	1	304	CLA	CHB-C1B	3.85	1.48	1.39
20	A	842	CLA	CHC-C4B	3.85	1.48	1.39
23	F	302	BCR	C17-C18	3.85	1.40	1.35
20	4	311	CLA	CHB-C1B	3.84	1.48	1.39
20	A	837	CLA	CHC-C4B	3.84	1.48	1.39
20	B	826	CLA	CHB-C1B	3.84	1.48	1.39
20	O	208	CLA	CHB-C1B	3.84	1.48	1.39
23	A	815	BCR	C14-C13	3.84	1.40	1.35
20	O	206	CLA	CHB-C1B	3.84	1.48	1.39
20	3	309	CLA	CHB-C1B	3.84	1.48	1.39
20	A	805	CLA	CHB-C1B	3.84	1.48	1.39
19	3	313	CHL	CHD-C4C	3.83	1.48	1.39
20	J	103	CLA	CHB-C1B	3.83	1.48	1.39
20	3	312	CLA	CHB-C1B	3.83	1.48	1.39
23	A	815	BCR	C21-C22	3.83	1.40	1.35
20	4	313	CLA	CHB-C1B	3.83	1.48	1.39
23	A	814	BCR	C14-C13	3.82	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	802	CLA	CHB-C1B	3.82	1.48	1.39
20	2	319	CLA	CHB-C1B	3.82	1.48	1.39
20	A	828	CLA	CHC-C4B	3.82	1.48	1.39
20	3	315	CLA	CHB-C1B	3.82	1.48	1.39
20	K	206	CLA	CHB-C1B	3.82	1.48	1.39
20	A	808	CLA	O2A-CGA	3.81	1.44	1.33
23	B	834	BCR	C17-C18	3.81	1.40	1.35
20	A	809	CLA	CHB-C1B	3.81	1.47	1.39
23	B	837	BCR	C21-C22	3.80	1.40	1.35
20	B	828	CLA	CHB-C1B	3.80	1.47	1.39
20	4	316	CLA	OBD-CAD	3.80	1.29	1.22
20	B	829	CLA	CHC-C4B	3.80	1.47	1.39
21	2	310	LUT	C14-C13	3.80	1.40	1.35
20	A	846	CLA	CHB-C1B	3.80	1.47	1.39
20	2	317	CLA	CHB-C1B	3.79	1.47	1.39
20	B	810	CLA	CHB-C1B	3.79	1.47	1.39
20	A	847	CLA	CHB-C1B	3.79	1.47	1.39
20	3	319	CLA	CHB-C1B	3.79	1.47	1.39
20	1	305	CLA	CHB-C1B	3.79	1.47	1.39
20	B	811	CLA	CHB-C1B	3.79	1.47	1.39
20	3	317	CLA	CHB-C1B	3.79	1.47	1.39
20	B	804	CLA	CHB-C1B	3.78	1.47	1.39
20	B	850	CLA	CHB-C1B	3.78	1.47	1.39
23	B	837	BCR	C17-C18	3.78	1.40	1.35
20	2	304	CLA	OBD-CAD	3.78	1.29	1.22
20	B	827	CLA	CHC-C4B	3.78	1.47	1.39
20	4	316	CLA	CHB-C1B	3.78	1.47	1.39
20	A	801	CLA	CHB-C1B	3.78	1.47	1.39
20	B	801	CLA	CHB-C1B	3.78	1.47	1.39
20	F	304	CLA	CHB-C1B	3.78	1.47	1.39
20	A	856	CLA	CHB-C1B	3.77	1.47	1.39
20	A	811	CLA	CHB-C1B	3.77	1.47	1.39
20	4	310	CLA	CHB-C1B	3.77	1.47	1.39
20	B	830	CLA	CHB-C1B	3.77	1.47	1.39
20	1	319	CLA	CHB-C1B	3.77	1.47	1.39
20	A	834	CLA	CHB-C1B	3.77	1.47	1.39
20	1	321	CLA	CHB-C1B	3.77	1.47	1.39
20	F	306	CLA	CHB-C1B	3.76	1.47	1.39
20	4	308	CLA	CHB-C1B	3.76	1.47	1.39
20	G	207	CLA	CHB-C1B	3.76	1.47	1.39
20	2	308	CLA	CHB-C1B	3.76	1.47	1.39
19	4	307	CHL	CHD-C4C	3.76	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	320	CLA	CHB-C1B	3.76	1.47	1.39
20	1	322	CLA	CHB-C1B	3.76	1.47	1.39
20	A	806	CLA	CHB-C1B	3.76	1.47	1.39
20	1	305	CLA	CHC-C4B	3.76	1.47	1.39
20	A	804	CLA	CHB-C1B	3.75	1.47	1.39
23	G	201	BCR	C17-C18	3.75	1.40	1.35
20	N	202	CLA	CHB-C1B	3.75	1.47	1.39
23	O	202	BCR	C14-C13	3.75	1.40	1.35
20	A	838	CLA	CHB-C1B	3.75	1.47	1.39
20	A	844	CLA	O2A-CGA	3.75	1.45	1.33
20	O	207	CLA	OBD-CAD	3.75	1.28	1.22
20	B	827	CLA	CHB-C1B	3.75	1.47	1.39
20	A	840	CLA	CHB-C1B	3.75	1.47	1.39
20	1	309	CLA	OBD-CAD	3.75	1.28	1.22
20	4	304	CLA	OBD-CAD	3.75	1.28	1.22
20	K	206	CLA	OBD-CAD	3.75	1.28	1.22
23	B	839	BCR	C8-C9	-3.75	1.40	1.50
20	3	307	CLA	OBD-CAD	3.74	1.28	1.22
20	3	318	CLA	CHB-C1B	3.74	1.47	1.39
20	2	305	CLA	CHB-C1B	3.74	1.47	1.39
20	2	317	CLA	OBD-CAD	3.74	1.28	1.22
20	B	821	CLA	CHB-C1B	3.74	1.47	1.39
20	B	833	CLA	OBD-CAD	3.73	1.28	1.22
20	K	203	CLA	OBD-CAD	3.73	1.28	1.22
20	3	319	CLA	OBD-CAD	3.73	1.28	1.22
20	B	819	CLA	CHC-C1C	3.73	1.46	1.38
19	4	315	CHL	OBD-CAD	3.73	1.28	1.22
19	4	306	CHL	OBD-CAD	3.73	1.28	1.22
20	4	312	CLA	OBD-CAD	3.73	1.28	1.22
20	B	853	CLA	CHB-C1B	3.73	1.47	1.39
19	2	309	CHL	CHC-C4B	3.73	1.47	1.39
21	3	301	LUT	C34-C33	3.73	1.40	1.35
20	B	831	CLA	CHC-C4B	3.72	1.47	1.39
19	2	318	CHL	CHD-C4C	3.72	1.47	1.39
20	B	848	CLA	CHB-C1B	3.72	1.47	1.39
21	2	310	LUT	C10-C9	3.72	1.40	1.35
20	O	208	CLA	OBD-CAD	3.72	1.28	1.22
19	2	309	CHL	OBD-CAD	3.72	1.28	1.22
20	F	305	CLA	CHB-C1B	3.72	1.47	1.39
21	3	301	LUT	C14-C13	3.72	1.40	1.35
20	A	828	CLA	CHB-C1B	3.72	1.47	1.39
21	4	317	LUT	C34-C33	3.71	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	819	CLA	CHB-C1B	3.71	1.47	1.39
20	1	308	CLA	OBD-CAD	3.71	1.28	1.22
20	B	825	CLA	CHB-C1B	3.71	1.47	1.39
20	4	311	CLA	OBD-CAD	3.71	1.28	1.22
20	3	308	CLA	CHB-C1B	3.71	1.47	1.39
20	1	322	CLA	OBD-CAD	3.71	1.28	1.22
20	A	841	CLA	CHC-C4B	3.71	1.47	1.39
20	4	309	CLA	OBD-CAD	3.70	1.28	1.22
20	2	303	CLA	OBD-CAD	3.70	1.28	1.22
20	F	304	CLA	OBD-CAD	3.70	1.28	1.22
20	G	207	CLA	OBD-CAD	3.70	1.28	1.22
20	4	313	CLA	CHC-C4B	3.70	1.47	1.39
23	L	301	BCR	C17-C18	3.70	1.40	1.35
20	1	320	CLA	CHC-C4B	3.70	1.47	1.39
20	2	321	CLA	OBD-CAD	3.70	1.28	1.22
20	2	323	CLA	OBD-CAD	3.70	1.28	1.22
20	A	840	CLA	OBD-CAD	3.70	1.28	1.22
20	A	827	CLA	OBD-CAD	3.69	1.28	1.22
20	4	313	CLA	OBD-CAD	3.69	1.28	1.22
20	A	855	CLA	CHB-C1B	3.69	1.47	1.39
20	B	820	CLA	CHB-C1B	3.69	1.47	1.39
19	2	318	CHL	OBD-CAD	3.69	1.28	1.22
20	B	846	CLA	OBD-CAD	3.69	1.28	1.22
20	1	304	CLA	OBD-CAD	3.69	1.28	1.22
20	B	819	CLA	OBD-CAD	3.69	1.28	1.22
20	1	307	CLA	CHB-C1B	3.69	1.47	1.39
20	2	307	CLA	OBD-CAD	3.68	1.28	1.22
20	A	851	CLA	CHC-C4B	3.68	1.47	1.39
20	B	818	CLA	CHC-C4B	3.68	1.47	1.39
20	B	829	CLA	OBD-CAD	3.68	1.28	1.22
20	A	812	CLA	CHC-C4B	3.68	1.47	1.39
20	A	848	CLA	OBD-CAD	3.68	1.28	1.22
20	A	852	CLA	OBD-CAD	3.68	1.28	1.22
20	3	311	CLA	OBD-CAD	3.68	1.28	1.22
20	B	813	CLA	OBD-CAD	3.68	1.28	1.22
20	3	320	CLA	OBD-CAD	3.68	1.28	1.22
20	3	310	CLA	CHB-C1B	3.68	1.47	1.39
20	A	838	CLA	OBD-CAD	3.68	1.28	1.22
20	3	314	CLA	OBD-CAD	3.67	1.28	1.22
20	B	829	CLA	CHB-C1B	3.67	1.47	1.39
20	B	803	CLA	OBD-CAD	3.67	1.28	1.22
23	L	302	BCR	C17-C18	3.67	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	811	CLA	OBD-CAD	3.67	1.28	1.22
20	F	306	CLA	OBD-CAD	3.67	1.28	1.22
20	B	833	CLA	CHB-C1B	3.67	1.47	1.39
20	A	831	CLA	CHB-C1B	3.67	1.47	1.39
20	L	307	CLA	OBD-CAD	3.67	1.28	1.22
20	B	822	CLA	CHB-C1B	3.67	1.47	1.39
20	1	321	CLA	OBD-CAD	3.67	1.28	1.22
20	3	308	CLA	OBD-CAD	3.67	1.28	1.22
20	B	824	CLA	OBD-CAD	3.66	1.28	1.22
20	A	846	CLA	OBD-CAD	3.66	1.28	1.22
20	1	318	CLA	OBD-CAD	3.66	1.28	1.22
20	K	204	CLA	OBD-CAD	3.66	1.28	1.22
20	4	314	CLA	CHB-C1B	3.66	1.47	1.39
20	B	802	CLA	OBD-CAD	3.66	1.28	1.22
20	3	309	CLA	CHC-C4B	3.66	1.47	1.39
20	A	836	CLA	CHB-C1B	3.66	1.47	1.39
19	1	301	CHL	OBD-CAD	3.65	1.28	1.22
20	A	807	CLA	CHB-C1B	3.65	1.47	1.39
23	F	302	BCR	C21-C22	3.65	1.40	1.35
20	4	304	CLA	CHB-C1B	3.65	1.47	1.39
20	A	839	CLA	CHB-C1B	3.65	1.47	1.39
20	A	811	CLA	OBD-CAD	3.65	1.28	1.22
20	B	830	CLA	OBD-CAD	3.65	1.28	1.22
20	4	314	CLA	OBD-CAD	3.65	1.28	1.22
20	B	853	CLA	OBD-CAD	3.65	1.28	1.22
20	A	832	CLA	OBD-CAD	3.65	1.28	1.22
20	1	320	CLA	CHB-C1B	3.65	1.47	1.39
20	B	812	CLA	CHB-C1B	3.65	1.47	1.39
21	1	310	LUT	C34-C33	3.65	1.40	1.35
20	A	848	CLA	CHB-C1B	3.65	1.47	1.39
20	A	854	CLA	CHB-C1B	3.65	1.47	1.39
20	B	806	CLA	CHC-C4B	3.65	1.47	1.39
20	3	312	CLA	OBD-CAD	3.65	1.28	1.22
20	B	824	CLA	CHB-C1B	3.64	1.47	1.39
20	H	201	CLA	OBD-CAD	3.64	1.28	1.22
21	1	310	LUT	C14-C13	3.64	1.40	1.35
20	A	833	CLA	OBD-CAD	3.64	1.28	1.22
20	4	309	CLA	CHB-C1B	3.64	1.47	1.39
19	2	301	CHL	OBD-CAD	3.64	1.28	1.22
20	A	831	CLA	OBD-CAD	3.64	1.28	1.22
19	1	317	CHL	OBD-CAD	3.64	1.28	1.22
20	3	308	CLA	CHC-C4B	3.64	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	815	BCR	C17-C18	3.64	1.40	1.35
20	2	319	CLA	OBD-CAD	3.63	1.28	1.22
20	1	318	CLA	CHC-C4B	3.63	1.47	1.39
20	B	807	CLA	CHC-C4B	3.63	1.47	1.39
20	2	308	CLA	CHC-C4B	3.63	1.47	1.39
20	B	831	CLA	OBD-CAD	3.63	1.28	1.22
20	B	825	CLA	OBD-CAD	3.63	1.28	1.22
20	2	308	CLA	OBD-CAD	3.63	1.28	1.22
20	3	318	CLA	CHC-C4B	3.63	1.47	1.39
20	3	318	CLA	OBD-CAD	3.63	1.28	1.22
20	A	844	CLA	OBD-CAD	3.63	1.28	1.22
20	J	103	CLA	OBD-CAD	3.63	1.28	1.22
20	A	802	CLA	OBD-CAD	3.63	1.28	1.22
20	B	801	CLA	OBD-CAD	3.63	1.28	1.22
20	B	828	CLA	CHC-C4B	3.63	1.47	1.39
20	B	847	CLA	OBD-CAD	3.63	1.28	1.22
19	2	322	CHL	OBD-CAD	3.63	1.28	1.22
20	1	302	CLA	CHC-C4B	3.62	1.47	1.39
20	B	818	CLA	CHB-C1B	3.62	1.47	1.39
20	B	848	CLA	CHC-C4B	3.62	1.47	1.39
20	L	305	CLA	OBD-CAD	3.62	1.28	1.22
19	4	305	CHL	OBD-CAD	3.62	1.28	1.22
20	B	809	CLA	OBD-CAD	3.62	1.28	1.22
20	2	305	CLA	OBD-CAD	3.62	1.28	1.22
20	L	306	CLA	CHB-C1B	3.62	1.47	1.39
20	A	808	CLA	CHB-C1B	3.62	1.47	1.39
21	4	317	LUT	C14-C13	3.61	1.40	1.35
20	3	315	CLA	OBD-CAD	3.61	1.28	1.22
20	B	807	CLA	CHB-C1B	3.61	1.47	1.39
20	B	805	CLA	OBD-CAD	3.61	1.28	1.22
20	A	841	CLA	OBD-CAD	3.61	1.28	1.22
20	N	202	CLA	OBD-CAD	3.61	1.28	1.22
20	1	307	CLA	OBD-CAD	3.61	1.28	1.22
28	A	824	CL0	OBD-CAD	3.61	1.28	1.22
19	2	322	CHL	CHC-C4B	3.61	1.47	1.39
20	1	318	CLA	CHB-C1B	3.61	1.47	1.39
20	O	207	CLA	CHB-C1B	3.61	1.47	1.39
20	B	808	CLA	OBD-CAD	3.61	1.28	1.22
20	1	303	CLA	CHC-C4B	3.61	1.47	1.39
20	B	810	CLA	OBD-CAD	3.60	1.28	1.22
20	B	808	CLA	CHB-C1B	3.60	1.47	1.39
20	A	825	CLA	OBD-CAD	3.60	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	806	CLA	CHB-C1B	3.60	1.47	1.39
20	3	317	CLA	CHC-C4B	3.60	1.47	1.39
20	B	824	CLA	CHC-C4B	3.60	1.47	1.39
20	B	844	CLA	OBD-CAD	3.60	1.28	1.22
20	B	814	CLA	CHB-C1B	3.60	1.47	1.39
20	2	306	CLA	CHC-C4B	3.60	1.47	1.39
20	G	205	CLA	OBD-CAD	3.60	1.28	1.22
20	1	307	CLA	CHC-C4B	3.60	1.47	1.39
20	B	846	CLA	CHB-C1B	3.60	1.47	1.39
20	B	815	CLA	OBD-CAD	3.60	1.28	1.22
20	A	837	CLA	OBD-CAD	3.59	1.28	1.22
20	A	854	CLA	OBD-CAD	3.59	1.28	1.22
20	A	811	CLA	CHC-C4B	3.59	1.47	1.39
20	1	302	CLA	OBD-CAD	3.59	1.28	1.22
20	2	305	CLA	CHC-C4B	3.59	1.47	1.39
20	1	309	CLA	CHC-C4B	3.59	1.47	1.39
20	B	826	CLA	CHC-C4B	3.59	1.47	1.39
20	A	825	CLA	CHC-C4B	3.59	1.47	1.39
20	G	206	CLA	CHC-C4B	3.59	1.47	1.39
20	B	850	CLA	OBD-CAD	3.59	1.28	1.22
20	A	850	CLA	CHB-C1B	3.59	1.47	1.39
20	B	849	CLA	CHB-C1B	3.59	1.47	1.39
20	A	836	CLA	OBD-CAD	3.58	1.28	1.22
19	3	313	CHL	OBD-CAD	3.58	1.28	1.22
20	3	317	CLA	OBD-CAD	3.58	1.28	1.22
20	A	847	CLA	OBD-CAD	3.58	1.28	1.22
21	4	317	LUT	C10-C9	3.58	1.40	1.35
20	A	837	CLA	C3B-C4B	3.58	1.51	1.42
20	B	809	CLA	CHC-C4B	3.57	1.47	1.39
20	1	303	CLA	OBD-CAD	3.57	1.28	1.22
20	L	306	CLA	OBD-CAD	3.57	1.28	1.22
20	A	826	CLA	C3D-C2D	3.57	1.48	1.39
20	4	302	CLA	OBD-CAD	3.57	1.28	1.22
20	B	849	CLA	OBD-CAD	3.57	1.28	1.22
19	2	318	CHL	CHC-C4B	3.57	1.47	1.39
20	1	320	CLA	OBD-CAD	3.57	1.28	1.22
20	B	823	CLA	OBD-CAD	3.57	1.28	1.22
21	3	301	LUT	C30-C29	3.57	1.40	1.35
20	1	322	CLA	CHC-C4B	3.57	1.47	1.39
20	B	852	CLA	CHB-C1B	3.57	1.47	1.39
20	4	302	CLA	CHC-C4B	3.56	1.47	1.39
20	A	804	CLA	OBD-CAD	3.56	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	310	LUT	C30-C29	3.56	1.40	1.35
20	B	845	CLA	OBD-CAD	3.56	1.28	1.22
20	A	826	CLA	C4B-NB	-3.56	1.33	1.37
20	4	303	CLA	CHC-C4B	3.56	1.47	1.39
19	2	302	CHL	CHC-C4B	3.56	1.47	1.39
20	2	317	CLA	CHC-C4B	3.56	1.47	1.39
20	B	822	CLA	OBD-CAD	3.56	1.28	1.22
20	A	842	CLA	CHB-C1B	3.56	1.47	1.39
20	B	806	CLA	OBD-CAD	3.56	1.28	1.22
20	F	306	CLA	CHC-C4B	3.56	1.47	1.39
20	A	843	CLA	CHB-C1B	3.56	1.47	1.39
20	B	851	CLA	OBD-CAD	3.55	1.28	1.22
20	N	202	CLA	CHC-C4B	3.55	1.47	1.39
20	K	205	CLA	C3B-C4B	3.55	1.51	1.42
20	B	818	CLA	OBD-CAD	3.55	1.28	1.22
20	1	306	CLA	OBD-CAD	3.55	1.28	1.22
20	4	311	CLA	CHC-C4B	3.55	1.47	1.39
20	B	847	CLA	CHC-C4B	3.55	1.47	1.39
20	1	306	CLA	CHC-C4B	3.55	1.47	1.39
20	2	323	CLA	CHC-C4B	3.55	1.47	1.39
20	A	851	CLA	OBD-CAD	3.55	1.28	1.22
20	3	316	CLA	CHC-C4B	3.55	1.47	1.39
20	O	207	CLA	CHC-C4B	3.55	1.47	1.39
20	B	833	CLA	CHC-C4B	3.55	1.47	1.39
20	A	830	CLA	C4B-NB	-3.54	1.33	1.37
20	A	828	CLA	OBD-CAD	3.54	1.28	1.22
19	4	307	CHL	CHC-C4B	3.54	1.47	1.39
20	1	305	CLA	OBD-CAD	3.54	1.28	1.22
20	L	305	CLA	CHB-C1B	3.54	1.47	1.39
20	3	310	CLA	OBD-CAD	3.53	1.28	1.22
20	B	811	CLA	CHC-C4B	3.53	1.47	1.39
20	A	856	CLA	OBD-CAD	3.53	1.28	1.22
19	4	306	CHL	CHC-C4B	3.53	1.47	1.39
23	A	817	BCR	C21-C22	3.52	1.40	1.35
20	F	304	CLA	CHC-C4B	3.52	1.47	1.39
20	A	801	CLA	OBD-CAD	3.52	1.28	1.22
20	1	305	CLA	C3B-C4B	3.52	1.51	1.42
20	F	305	CLA	OBD-CAD	3.52	1.28	1.22
20	A	812	CLA	C4B-NB	-3.52	1.33	1.37
20	2	303	CLA	CHB-C1B	3.52	1.47	1.39
20	B	852	CLA	CHC-C4B	3.52	1.47	1.39
20	B	815	CLA	CHC-C4B	3.52	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	J	103	CLA	CHC-C4B	3.52	1.47	1.39
20	4	308	CLA	OBD-CAD	3.51	1.28	1.22
20	B	823	CLA	CHB-C1B	3.51	1.47	1.39
20	A	850	CLA	OBD-CAD	3.51	1.28	1.22
20	3	320	CLA	CHC-C4B	3.51	1.47	1.39
20	B	821	CLA	CHC-C4B	3.51	1.47	1.39
20	B	852	CLA	OBD-CAD	3.50	1.28	1.22
20	B	825	CLA	CHC-C4B	3.50	1.47	1.39
19	4	305	CHL	CHC-C4B	3.50	1.47	1.39
20	A	809	CLA	OBD-CAD	3.50	1.28	1.22
20	B	809	CLA	CHB-C1B	3.50	1.47	1.39
20	2	306	CLA	OBD-CAD	3.50	1.28	1.22
20	1	320	CLA	C3B-C4B	3.49	1.50	1.42
20	A	807	CLA	CHC-C4B	3.49	1.47	1.39
20	A	837	CLA	CHB-C1B	3.49	1.47	1.39
20	A	849	CLA	C4B-NB	-3.49	1.33	1.37
20	A	808	CLA	OBD-CAD	3.49	1.28	1.22
19	1	317	CHL	CHC-C4B	3.49	1.47	1.39
20	A	845	CLA	CHB-C1B	3.49	1.47	1.39
20	A	830	CLA	OBD-CAD	3.49	1.28	1.22
20	A	843	CLA	OBD-CAD	3.49	1.28	1.22
19	3	313	CHL	CHC-C4B	3.49	1.47	1.39
20	B	802	CLA	CHC-C4B	3.49	1.47	1.39
20	2	303	CLA	CHC-C4B	3.49	1.47	1.39
20	A	844	CLA	CHB-C1B	3.49	1.47	1.39
20	2	319	CLA	CHC-C4B	3.48	1.47	1.39
20	B	810	CLA	CHC-C4B	3.48	1.47	1.39
20	A	802	CLA	CHD-C1D	3.48	1.45	1.38
22	2	311	XAT	O4-C5	-3.48	1.41	1.46
20	A	829	CLA	OBD-CAD	3.48	1.28	1.22
20	1	318	CLA	CHD-C4C	3.48	1.47	1.39
20	B	816	CLA	OBD-CAD	3.47	1.28	1.22
20	B	849	CLA	CHC-C4B	3.47	1.47	1.39
20	A	832	CLA	CHB-C1B	3.47	1.47	1.39
20	B	813	CLA	C3B-C4B	3.47	1.50	1.42
20	A	848	CLA	CHC-C4B	3.46	1.47	1.39
20	4	312	CLA	CHC-C4B	3.46	1.47	1.39
20	A	836	CLA	CHC-C4B	3.46	1.47	1.39
20	K	206	CLA	CHC-C4B	3.46	1.47	1.39
20	O	206	CLA	OBD-CAD	3.46	1.28	1.22
20	2	308	CLA	C3B-C4B	3.46	1.50	1.42
20	A	841	CLA	CHD-C4C	3.46	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	844	CLA	CHD-C4C	3.46	1.47	1.39
20	A	851	CLA	C4B-NB	-3.46	1.33	1.37
20	G	206	CLA	OBD-CAD	3.46	1.28	1.22
20	B	812	CLA	CHC-C4B	3.46	1.47	1.39
19	2	302	CHL	OBD-CAD	3.46	1.28	1.22
20	3	307	CLA	C4B-NB	-3.46	1.33	1.37
20	3	314	CLA	CHC-C4B	3.45	1.47	1.39
20	4	309	CLA	C3B-C4B	3.45	1.50	1.42
20	A	811	CLA	C3B-C4B	3.45	1.50	1.42
19	4	307	CHL	OBD-CAD	3.45	1.28	1.22
20	B	806	CLA	C3B-C4B	3.45	1.50	1.42
20	L	305	CLA	CHD-C4C	3.44	1.47	1.39
20	4	304	CLA	CHC-C4B	3.44	1.47	1.39
20	3	310	CLA	CHD-C4C	3.44	1.47	1.39
20	A	834	CLA	C4B-NB	-3.44	1.33	1.37
20	B	813	CLA	CHB-C1B	3.44	1.47	1.39
20	1	322	CLA	C3B-C4B	3.44	1.50	1.42
20	1	308	CLA	CHC-C4B	3.44	1.47	1.39
20	3	307	CLA	CHB-C1B	3.44	1.47	1.39
20	B	833	CLA	C3B-C4B	3.44	1.50	1.42
20	A	835	CLA	CHB-C1B	3.44	1.47	1.39
20	B	812	CLA	OBD-CAD	3.44	1.28	1.22
21	1	310	LUT	C10-C9	3.43	1.40	1.35
23	A	817	BCR	C14-C13	3.43	1.40	1.35
20	K	205	CLA	OBD-CAD	3.43	1.28	1.22
19	4	315	CHL	CHC-C4B	3.43	1.47	1.39
20	2	304	CLA	CHC-C4B	3.43	1.47	1.39
20	B	831	CLA	C3B-C4B	3.43	1.50	1.42
20	A	852	CLA	CHD-C4C	3.43	1.47	1.39
20	B	812	CLA	CHD-C4C	3.43	1.47	1.39
20	A	845	CLA	CHC-C4B	3.43	1.47	1.39
20	4	310	CLA	OBD-CAD	3.43	1.28	1.22
20	B	826	CLA	C4B-NB	-3.42	1.33	1.37
20	3	318	CLA	C3B-C4B	3.42	1.50	1.42
20	4	316	CLA	C3B-C4B	3.42	1.50	1.42
20	B	846	CLA	CHC-C4B	3.42	1.47	1.39
20	B	817	CLA	OBD-CAD	3.42	1.28	1.22
20	1	319	CLA	CHD-C4C	3.42	1.47	1.39
19	1	301	CHL	CHC-C4B	3.42	1.47	1.39
20	A	843	CLA	CHD-C1D	3.42	1.45	1.38
21	3	301	LUT	C10-C9	3.42	1.40	1.35
20	4	310	CLA	CHC-C4B	3.42	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	J	103	CLA	C3B-C4B	3.42	1.50	1.42
20	N	202	CLA	C3B-C4B	3.41	1.50	1.42
20	B	845	CLA	CHB-C1B	3.41	1.47	1.39
20	B	816	CLA	CHC-C4B	3.41	1.47	1.39
20	4	314	CLA	C3B-C4B	3.41	1.50	1.42
23	A	818	BCR	C21-C22	3.41	1.40	1.35
20	B	815	CLA	CHB-C1B	3.41	1.47	1.39
20	3	310	CLA	CHD-C1D	3.41	1.45	1.38
19	2	301	CHL	CHC-C4B	3.41	1.47	1.39
20	A	809	CLA	CHC-C4B	3.41	1.47	1.39
20	B	846	CLA	CHD-C4C	3.41	1.47	1.39
21	4	317	LUT	C30-C29	3.41	1.40	1.35
20	A	849	CLA	OBD-CAD	3.41	1.28	1.22
20	H	201	CLA	CHC-C4B	3.41	1.47	1.39
20	4	316	CLA	CHC-C4B	3.41	1.47	1.39
20	A	847	CLA	CHC-C4B	3.40	1.47	1.39
20	1	309	CLA	C3B-C4B	3.40	1.50	1.42
20	A	841	CLA	C3B-C4B	3.40	1.50	1.42
20	A	825	CLA	CHB-C1B	3.40	1.47	1.39
20	F	306	CLA	C3B-C4B	3.40	1.50	1.42
20	B	820	CLA	OBD-CAD	3.40	1.28	1.22
20	A	835	CLA	CHC-C4B	3.40	1.47	1.39
20	A	836	CLA	C3B-C4B	3.40	1.50	1.42
20	3	309	CLA	C3B-C4B	3.39	1.50	1.42
20	F	305	CLA	CHC-C4B	3.39	1.47	1.39
20	3	315	CLA	CHC-C4B	3.39	1.47	1.39
20	L	305	CLA	CHC-C4B	3.39	1.47	1.39
20	A	840	CLA	CHC-C4B	3.39	1.47	1.39
20	B	814	CLA	OBD-CAD	3.39	1.28	1.22
20	A	853	CLA	CHB-C1B	3.39	1.47	1.39
20	A	842	CLA	C3B-C4B	3.39	1.50	1.42
20	4	313	CLA	C3B-C4B	3.39	1.50	1.42
20	A	803	CLA	CHC-C4B	3.39	1.47	1.39
20	B	804	CLA	CHC-C4B	3.39	1.47	1.39
20	A	806	CLA	CHC-C4B	3.39	1.47	1.39
20	2	306	CLA	C3B-C4B	3.38	1.50	1.42
20	K	203	CLA	CHC-C4B	3.38	1.47	1.39
20	A	835	CLA	C3B-C4B	3.38	1.50	1.42
20	B	827	CLA	C3B-C4B	3.38	1.50	1.42
20	A	843	CLA	CHD-C4C	3.38	1.47	1.39
20	O	207	CLA	C3B-C4B	3.38	1.50	1.42
20	A	854	CLA	C1B-NB	-3.38	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	323	CLA	C3B-C4B	3.38	1.50	1.42
20	4	304	CLA	CHD-C1D	3.38	1.44	1.38
20	3	317	CLA	C3B-C4B	3.38	1.50	1.42
20	2	305	CLA	C3B-C4B	3.38	1.50	1.42
20	B	819	CLA	CHD-C1D	3.38	1.44	1.38
20	4	304	CLA	CHD-C4C	3.38	1.46	1.39
20	4	314	CLA	CHC-C4B	3.37	1.47	1.39
20	B	817	CLA	CHC-C4B	3.37	1.47	1.39
20	3	312	CLA	CHC-C4B	3.37	1.47	1.39
20	2	317	CLA	C3B-C4B	3.37	1.50	1.42
20	B	814	CLA	C4B-NB	-3.37	1.33	1.37
20	A	835	CLA	OBD-CAD	3.37	1.28	1.22
20	A	826	CLA	CHD-C1D	3.37	1.44	1.38
20	B	821	CLA	C3B-C4B	3.37	1.50	1.42
20	A	808	CLA	C4B-NB	-3.37	1.33	1.37
20	G	206	CLA	C3B-C4B	3.36	1.50	1.42
20	A	839	CLA	OBD-CAD	3.36	1.28	1.22
20	G	207	CLA	CHC-C4B	3.36	1.46	1.39
20	B	816	CLA	C4B-NB	-3.36	1.33	1.37
20	A	809	CLA	C3B-C4B	3.36	1.50	1.42
20	A	850	CLA	CHC-C4B	3.36	1.46	1.39
20	1	306	CLA	C3B-C4B	3.36	1.50	1.42
20	A	842	CLA	OBD-CAD	3.36	1.28	1.22
20	A	845	CLA	CHD-C1D	3.36	1.44	1.38
20	B	853	CLA	CHD-C1D	3.36	1.44	1.38
20	A	827	CLA	CHC-C4B	3.36	1.46	1.39
20	A	853	CLA	OBD-CAD	3.35	1.28	1.22
20	4	308	CLA	C4B-NB	-3.35	1.33	1.37
20	B	847	CLA	MG-NA	-3.35	1.98	2.06
20	3	309	CLA	OBD-CAD	3.35	1.28	1.22
20	L	307	CLA	CHC-C4B	3.35	1.46	1.39
20	B	853	CLA	CHD-C4C	3.35	1.46	1.39
20	B	814	CLA	CHC-C4B	3.35	1.46	1.39
20	A	853	CLA	CHC-C4B	3.35	1.46	1.39
20	1	302	CLA	C3B-C4B	3.35	1.50	1.42
20	B	803	CLA	CHC-C4B	3.35	1.46	1.39
20	4	311	CLA	C3B-C4B	3.34	1.50	1.42
20	A	802	CLA	CHD-C4C	3.34	1.46	1.39
20	A	852	CLA	CHB-C1B	3.34	1.46	1.39
20	B	823	CLA	CHC-C4B	3.34	1.46	1.39
20	B	809	CLA	C3B-C4B	3.34	1.50	1.42
20	A	839	CLA	CHD-C4C	3.34	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	828	CLA	C3B-C4B	3.34	1.50	1.42
20	A	833	CLA	CHC-C4B	3.34	1.46	1.39
20	2	320	CLA	OBD-CAD	3.34	1.28	1.22
20	B	810	CLA	C3B-C4B	3.34	1.50	1.42
20	2	321	CLA	CHD-C4C	3.34	1.46	1.39
20	B	801	CLA	CHD-C1D	3.34	1.44	1.38
20	B	848	CLA	C3B-C4B	3.34	1.50	1.42
20	4	303	CLA	OBD-CAD	3.33	1.28	1.22
20	2	321	CLA	CHC-C4B	3.33	1.46	1.39
20	B	808	CLA	CHC-C4B	3.33	1.46	1.39
20	A	856	CLA	CHC-C4B	3.33	1.46	1.39
20	B	850	CLA	CHC-C4B	3.33	1.46	1.39
20	3	316	CLA	C3B-C4B	3.33	1.50	1.42
20	B	845	CLA	C4B-NB	-3.33	1.33	1.37
20	B	803	CLA	C4B-NB	-3.33	1.33	1.37
20	A	849	CLA	CHC-C4B	3.33	1.46	1.39
20	O	206	CLA	CHC-C4B	3.33	1.46	1.39
20	A	838	CLA	CHC-C4B	3.33	1.46	1.39
20	A	845	CLA	CHD-C4C	3.32	1.46	1.39
20	L	306	CLA	CHC-C4B	3.32	1.46	1.39
23	A	817	BCR	C17-C18	3.32	1.40	1.35
20	1	307	CLA	C3B-C4B	3.32	1.50	1.42
20	B	852	CLA	C3B-C4B	3.32	1.50	1.42
20	A	831	CLA	CHC-C4B	3.32	1.46	1.39
20	K	204	CLA	CHC-C4B	3.32	1.46	1.39
20	A	835	CLA	CHD-C4C	3.32	1.46	1.39
19	2	301	CHL	CHB-C1B	3.32	1.46	1.39
20	A	852	CLA	CHD-C1D	3.32	1.44	1.38
20	B	822	CLA	CHD-C4C	3.32	1.46	1.39
20	B	829	CLA	C3B-C4B	3.32	1.50	1.42
20	B	833	CLA	CHD-C4C	3.32	1.46	1.39
20	A	829	CLA	CHC-C4B	3.32	1.46	1.39
20	B	802	CLA	C3B-C4B	3.32	1.50	1.42
20	B	804	CLA	OBD-CAD	3.32	1.28	1.22
20	A	841	CLA	CHB-C1B	3.32	1.46	1.39
20	B	821	CLA	OBD-CAD	3.32	1.28	1.22
20	B	815	CLA	C4B-NB	-3.32	1.33	1.37
20	B	823	CLA	CHD-C4C	3.31	1.46	1.39
20	2	323	CLA	CHB-C1B	3.31	1.46	1.39
20	A	832	CLA	CHC-C4B	3.31	1.46	1.39
20	B	819	CLA	C1B-NB	-3.31	1.33	1.37
20	A	827	CLA	C4B-NB	-3.31	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	855	CLA	C4B-NB	-3.31	1.33	1.37
20	A	828	CLA	CHD-C4C	3.31	1.46	1.39
20	A	833	CLA	C4B-NB	-3.31	1.33	1.37
20	2	321	CLA	CHD-C1D	3.31	1.44	1.38
20	3	319	CLA	CHC-C4B	3.31	1.46	1.39
20	A	846	CLA	CHD-C4C	3.31	1.46	1.39
20	O	206	CLA	CHD-C1D	3.31	1.44	1.38
20	A	839	CLA	CHC-C4B	3.31	1.46	1.39
20	B	808	CLA	C3B-C4B	3.31	1.50	1.42
20	L	305	CLA	CHD-C1D	3.31	1.44	1.38
20	B	807	CLA	OBD-CAD	3.30	1.28	1.22
20	2	308	CLA	CHD-C1D	3.30	1.44	1.38
20	A	850	CLA	C4B-NB	-3.30	1.33	1.37
20	K	204	CLA	CHD-C4C	3.30	1.46	1.39
20	B	853	CLA	CHC-C4B	3.30	1.46	1.39
20	B	819	CLA	CHD-C4C	3.29	1.46	1.39
20	3	311	CLA	C4B-NB	-3.29	1.33	1.37
20	A	838	CLA	CHD-C4C	3.29	1.46	1.39
20	A	835	CLA	CHD-C1D	3.29	1.44	1.38
20	4	312	CLA	C3B-C4B	3.29	1.50	1.42
20	B	824	CLA	C3B-C4B	3.29	1.50	1.42
20	B	809	CLA	CHD-C1D	3.29	1.44	1.38
20	B	846	CLA	CHD-C1D	3.29	1.44	1.38
20	A	808	CLA	CHC-C4B	3.29	1.46	1.39
20	B	811	CLA	C3B-C4B	3.29	1.50	1.42
20	B	820	CLA	CHC-C4B	3.29	1.46	1.39
20	2	320	CLA	CHC-C4B	3.29	1.46	1.39
20	B	830	CLA	CHC-C4B	3.29	1.46	1.39
20	A	802	CLA	CHB-C1B	3.29	1.46	1.39
20	B	805	CLA	CHC-C4B	3.28	1.46	1.39
20	4	303	CLA	C3B-C4B	3.28	1.50	1.42
20	K	206	CLA	CHD-C4C	3.28	1.46	1.39
23	3	303	BCR	C17-C18	3.28	1.40	1.35
20	A	841	CLA	CHD-C1D	3.28	1.44	1.38
20	B	812	CLA	CHD-C1D	3.28	1.44	1.38
20	1	308	CLA	CHD-C4C	3.28	1.46	1.39
20	1	318	CLA	CHD-C1D	3.28	1.44	1.38
20	A	802	CLA	CHC-C4B	3.28	1.46	1.39
20	G	205	CLA	CHC-C4B	3.28	1.46	1.39
20	3	319	CLA	CHD-C4C	3.28	1.46	1.39
20	A	825	CLA	C4B-NB	-3.27	1.33	1.37
20	2	317	CLA	CHD-C4C	3.27	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	304	CLA	CHC-C4B	3.27	1.46	1.39
20	F	305	CLA	C3B-C4B	3.27	1.50	1.42
20	A	807	CLA	OBD-CAD	3.27	1.28	1.22
20	2	305	CLA	CHD-C4C	3.27	1.46	1.39
19	1	301	CHL	CHB-C1B	3.27	1.46	1.39
23	B	839	BCR	C23-C22	-3.26	1.38	1.45
20	B	806	CLA	CHD-C4C	3.26	1.46	1.39
20	3	316	CLA	OBD-CAD	3.26	1.28	1.22
20	H	201	CLA	C3B-C4B	3.26	1.50	1.42
20	3	320	CLA	CHD-C4C	3.26	1.46	1.39
20	B	809	CLA	CHD-C4C	3.26	1.46	1.39
20	A	806	CLA	CHD-C4C	3.26	1.46	1.39
20	A	839	CLA	CHD-C1D	3.26	1.44	1.38
20	B	818	CLA	C3B-C4B	3.26	1.50	1.42
19	4	315	CHL	CHB-C1B	3.26	1.46	1.39
20	B	801	CLA	CHC-C4B	3.26	1.46	1.39
20	B	822	CLA	CHC-C4B	3.26	1.46	1.39
19	3	313	CHL	CHB-C1B	3.25	1.46	1.39
20	O	208	CLA	CHC-C4B	3.25	1.46	1.39
20	B	806	CLA	CHD-C1D	3.25	1.44	1.38
20	2	303	CLA	C3B-C4B	3.25	1.50	1.42
20	A	855	CLA	CHC-C4B	3.25	1.46	1.39
20	B	823	CLA	CHD-C1D	3.25	1.44	1.38
20	B	827	CLA	OBD-CAD	3.25	1.28	1.22
23	3	303	BCR	C21-C22	3.25	1.40	1.35
20	B	817	CLA	C4B-NB	-3.25	1.33	1.37
20	1	303	CLA	C3B-C4B	3.25	1.50	1.42
20	G	205	CLA	CHD-C4C	3.24	1.46	1.39
20	1	319	CLA	OBD-CAD	3.24	1.28	1.22
20	B	815	CLA	CHD-C4C	3.24	1.46	1.39
20	O	206	CLA	CHD-C4C	3.24	1.46	1.39
20	2	308	CLA	CHD-C4C	3.24	1.46	1.39
20	L	307	CLA	CHD-C4C	3.24	1.46	1.39
20	1	320	CLA	CHD-C4C	3.24	1.46	1.39
20	B	823	CLA	C3D-C2D	3.23	1.47	1.39
20	B	844	CLA	C1B-C2B	3.23	1.50	1.43
20	3	315	CLA	CHD-C4C	3.23	1.46	1.39
20	A	832	CLA	C3B-C4B	3.23	1.50	1.42
20	A	846	CLA	CHC-C4B	3.23	1.46	1.39
20	O	208	CLA	C4B-NB	-3.23	1.33	1.37
20	A	847	CLA	C3B-C4B	3.23	1.50	1.42
19	2	318	CHL	CHB-C1B	3.22	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	847	CLA	C3B-C4B	3.22	1.50	1.42
20	A	848	CLA	C3B-C4B	3.22	1.50	1.42
20	4	314	CLA	CHD-C4C	3.22	1.46	1.39
20	A	807	CLA	C3B-C4B	3.22	1.50	1.42
20	A	832	CLA	CHD-C4C	3.22	1.46	1.39
20	B	845	CLA	C3D-C2D	3.21	1.47	1.39
20	B	830	CLA	C3B-C4B	3.21	1.50	1.42
20	K	203	CLA	CHD-C4C	3.21	1.46	1.39
20	A	805	CLA	C4B-NB	-3.21	1.33	1.37
20	1	319	CLA	CHC-C4B	3.21	1.46	1.39
20	2	323	CLA	CHD-C4C	3.21	1.46	1.39
20	B	818	CLA	CHD-C1D	3.21	1.44	1.38
20	1	304	CLA	CHD-C4C	3.21	1.46	1.39
19	1	317	CHL	CHB-C1B	3.21	1.46	1.39
20	A	827	CLA	CHD-C4C	3.21	1.46	1.39
20	A	847	CLA	CHD-C1D	3.21	1.44	1.38
20	2	307	CLA	CHC-C4B	3.21	1.46	1.39
20	3	308	CLA	CHD-C4C	3.21	1.46	1.39
20	A	803	CLA	OBD-CAD	3.21	1.28	1.22
20	G	207	CLA	CHD-C4C	3.21	1.46	1.39
19	2	322	CHL	CHB-C1B	3.21	1.46	1.39
20	A	845	CLA	C4B-NB	-3.20	1.33	1.37
20	A	844	CLA	CHC-C4B	3.20	1.46	1.39
20	A	845	CLA	C3D-C2D	3.20	1.47	1.39
20	4	310	CLA	C3B-C4B	3.20	1.50	1.42
20	3	318	CLA	CHD-C4C	3.20	1.46	1.39
20	B	845	CLA	CHC-C4B	3.20	1.46	1.39
20	2	323	CLA	CHD-C1D	3.20	1.44	1.38
20	A	832	CLA	CHD-C1D	3.20	1.44	1.38
20	3	319	CLA	CHD-C1D	3.20	1.44	1.38
20	B	801	CLA	CHD-C4C	3.20	1.46	1.39
20	2	305	CLA	CHD-C1D	3.20	1.44	1.38
20	B	804	CLA	CHD-C4C	3.20	1.46	1.39
20	A	846	CLA	C3B-C4B	3.20	1.50	1.42
20	A	812	CLA	CHB-C1B	3.20	1.46	1.39
20	A	825	CLA	C3D-C2D	3.20	1.47	1.39
20	1	321	CLA	CHC-C4B	3.20	1.46	1.39
20	4	313	CLA	CHD-C4C	3.20	1.46	1.39
20	B	805	CLA	C4B-NB	-3.20	1.33	1.37
20	1	320	CLA	CHD-C1D	3.19	1.44	1.38
20	A	831	CLA	C3B-C4B	3.19	1.50	1.42
20	A	806	CLA	CHD-C1D	3.19	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	803	CLA	C3D-C2D	3.19	1.47	1.39
20	A	840	CLA	C3B-C4B	3.19	1.50	1.42
20	B	801	CLA	C4B-NB	-3.19	1.33	1.37
20	A	838	CLA	CHD-C1D	3.19	1.44	1.38
20	B	850	CLA	C3D-C2D	3.19	1.47	1.39
20	3	307	CLA	CHD-C4C	3.19	1.46	1.39
20	B	808	CLA	CHD-C4C	3.19	1.46	1.39
20	A	812	CLA	C3D-C2D	3.19	1.47	1.39
20	A	854	CLA	C3D-C2D	3.19	1.47	1.39
20	3	312	CLA	CHD-C4C	3.18	1.46	1.39
23	B	837	BCR	C8-C9	-3.18	1.39	1.45
20	A	826	CLA	CHD-C4C	3.18	1.46	1.39
20	A	808	CLA	CHD-C1D	3.18	1.44	1.38
20	A	806	CLA	C3B-C4B	3.18	1.50	1.42
20	L	306	CLA	CHD-C4C	3.18	1.46	1.39
20	A	805	CLA	C3B-C4B	3.18	1.50	1.42
23	B	839	BCR	C21-C22	3.18	1.40	1.35
20	A	856	CLA	CHD-C4C	3.18	1.46	1.39
20	A	855	CLA	OBD-CAD	3.18	1.28	1.22
20	B	825	CLA	C3B-C4B	3.18	1.50	1.42
20	A	843	CLA	C3D-C2D	3.18	1.47	1.39
20	1	307	CLA	CHD-C4C	3.18	1.46	1.39
20	3	320	CLA	CHD-C1D	3.17	1.44	1.38
20	A	844	CLA	C4B-NB	-3.17	1.33	1.37
20	A	830	CLA	CHC-C4B	3.17	1.46	1.39
20	B	812	CLA	C1B-NB	-3.17	1.33	1.37
20	1	308	CLA	CHD-C1D	3.17	1.44	1.38
20	3	311	CLA	CHC-C4B	3.17	1.46	1.39
20	A	856	CLA	C4B-NB	-3.17	1.33	1.37
20	1	319	CLA	CHD-C1D	3.17	1.44	1.38
20	A	826	CLA	CHC-C4B	3.17	1.46	1.39
20	A	808	CLA	CHD-C4C	3.16	1.46	1.39
20	2	317	CLA	CHD-C1D	3.16	1.44	1.38
20	F	304	CLA	C3B-C4B	3.16	1.50	1.42
20	B	811	CLA	CHD-C4C	3.16	1.46	1.39
20	A	808	CLA	C3D-C2D	3.16	1.47	1.39
20	3	310	CLA	CHC-C4B	3.16	1.46	1.39
20	A	836	CLA	CHD-C4C	3.16	1.46	1.39
20	B	818	CLA	CHD-C4C	3.16	1.46	1.39
20	2	319	CLA	CHD-C4C	3.16	1.46	1.39
20	A	829	CLA	CHD-C4C	3.16	1.46	1.39
20	A	803	CLA	C3B-C4B	3.16	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	820	CLA	C4B-NB	-3.16	1.33	1.37
20	B	802	CLA	CHD-C4C	3.15	1.46	1.39
20	B	812	CLA	C3D-C2D	3.15	1.47	1.39
20	4	302	CLA	C4B-NB	-3.15	1.33	1.37
20	A	850	CLA	CHD-C4C	3.15	1.46	1.39
20	A	852	CLA	CHC-C4B	3.15	1.46	1.39
20	B	829	CLA	CHD-C4C	3.15	1.46	1.39
20	B	824	CLA	CHD-C4C	3.15	1.46	1.39
23	A	814	BCR	C8-C9	-3.15	1.39	1.45
20	4	308	CLA	CHC-C4B	3.15	1.46	1.39
20	O	208	CLA	CHD-C4C	3.15	1.46	1.39
20	K	206	CLA	CHD-C1D	3.15	1.44	1.38
20	3	308	CLA	C4B-NB	-3.14	1.33	1.37
20	3	311	CLA	CHD-C4C	3.14	1.46	1.39
20	A	855	CLA	CHD-C4C	3.14	1.46	1.39
20	O	207	CLA	CHD-C4C	3.14	1.46	1.39
20	A	804	CLA	CHC-C4B	3.14	1.46	1.39
20	A	844	CLA	CHD-C1D	3.14	1.44	1.38
19	4	307	CHL	CHB-C1B	3.14	1.46	1.39
20	3	308	CLA	CHD-C1D	3.14	1.44	1.38
20	A	842	CLA	CHD-C4C	3.14	1.46	1.39
20	B	807	CLA	CHD-C4C	3.14	1.46	1.39
20	3	310	CLA	C4B-NB	-3.14	1.33	1.37
20	4	313	CLA	CHD-C1D	3.14	1.44	1.38
19	2	302	CHL	CHB-C1B	3.14	1.46	1.39
20	B	833	CLA	CHD-C1D	3.14	1.44	1.38
20	1	305	CLA	CHD-C4C	3.13	1.46	1.39
20	1	321	CLA	CHD-C4C	3.13	1.46	1.39
20	A	840	CLA	CHD-C4C	3.13	1.46	1.39
20	3	315	CLA	CHD-C1D	3.13	1.44	1.38
19	4	306	CHL	CHB-C1B	3.13	1.46	1.39
20	3	307	CLA	CHD-C1D	3.13	1.44	1.38
20	A	852	CLA	C3D-C2D	3.13	1.47	1.39
20	K	204	CLA	CHD-C1D	3.13	1.44	1.38
20	B	807	CLA	CHD-C1D	3.13	1.44	1.38
20	A	845	CLA	OBD-CAD	3.13	1.27	1.22
20	B	825	CLA	CHD-C4C	3.13	1.46	1.39
20	B	827	CLA	CHD-C4C	3.13	1.46	1.39
20	B	808	CLA	CHD-C1D	3.13	1.44	1.38
20	B	815	CLA	CHD-C1D	3.13	1.44	1.38
20	B	851	CLA	C3D-C2D	3.13	1.47	1.39
20	1	309	CLA	CHD-C4C	3.13	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	303	CLA	CHD-C1D	3.13	1.44	1.38
20	B	850	CLA	C3B-C4B	3.13	1.50	1.42
20	A	801	CLA	CHD-C4C	3.13	1.46	1.39
20	B	849	CLA	CHD-C4C	3.13	1.46	1.39
20	A	847	CLA	CHD-C4C	3.13	1.46	1.39
20	3	319	CLA	C3B-C4B	3.13	1.50	1.42
20	F	305	CLA	CHD-C4C	3.12	1.46	1.39
20	A	829	CLA	C3B-C4B	3.12	1.50	1.42
20	A	841	CLA	C3D-C2D	3.12	1.47	1.39
20	A	807	CLA	CHD-C4C	3.12	1.46	1.39
20	K	204	CLA	C4B-NB	-3.12	1.34	1.37
20	A	832	CLA	C3D-C2D	3.12	1.47	1.39
20	N	202	CLA	CHD-C4C	3.12	1.46	1.39
20	A	826	CLA	CHB-C1B	3.11	1.46	1.39
20	1	322	CLA	CHD-C4C	3.11	1.46	1.39
20	B	801	CLA	C3D-C2D	3.11	1.47	1.39
20	4	314	CLA	C3D-C2D	3.11	1.47	1.39
20	1	304	CLA	CHD-C1D	3.11	1.44	1.38
20	B	851	CLA	CHD-C4C	3.11	1.46	1.39
20	B	852	CLA	CHD-C4C	3.11	1.46	1.39
20	A	804	CLA	CHD-C4C	3.11	1.46	1.39
20	B	851	CLA	C4B-NB	-3.11	1.34	1.37
20	3	311	CLA	CHD-C1D	3.10	1.44	1.38
20	B	822	CLA	CHD-C1D	3.10	1.44	1.38
20	1	304	CLA	C4B-NB	-3.10	1.34	1.37
20	B	804	CLA	CHD-C1D	3.10	1.44	1.38
20	B	844	CLA	C4B-NB	-3.10	1.34	1.37
20	B	849	CLA	C3B-C4B	3.10	1.50	1.42
20	3	318	CLA	CHD-C1D	3.10	1.44	1.38
20	2	303	CLA	C3D-C2D	3.10	1.47	1.39
23	A	817	BCR	C8-C9	-3.10	1.39	1.45
20	B	807	CLA	C3B-C4B	3.10	1.50	1.42
20	A	801	CLA	CHD-C1D	3.10	1.44	1.38
20	B	852	CLA	CHD-C1D	3.10	1.44	1.38
20	G	207	CLA	CHD-C1D	3.10	1.44	1.38
20	2	321	CLA	C4B-NB	-3.10	1.34	1.37
20	L	307	CLA	CHD-C1D	3.09	1.44	1.38
20	B	808	CLA	C3D-C2D	3.09	1.47	1.39
20	3	312	CLA	C4B-NB	-3.09	1.34	1.37
20	B	846	CLA	C4B-NB	-3.09	1.34	1.37
20	3	312	CLA	CHD-C1D	3.09	1.44	1.38
20	2	307	CLA	CHD-C4C	3.09	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	802	CLA	C4B-NB	-3.09	1.34	1.37
20	A	811	CLA	CHD-C4C	3.09	1.46	1.39
23	3	303	BCR	C23-C22	-3.09	1.39	1.45
20	B	819	CLA	C3D-C2D	3.09	1.47	1.39
20	A	853	CLA	C4B-NB	-3.09	1.34	1.37
20	A	831	CLA	CHD-C4C	3.09	1.46	1.39
20	A	850	CLA	CHD-C1D	3.09	1.44	1.38
20	2	304	CLA	CHD-C4C	3.09	1.46	1.39
20	B	810	CLA	CHD-C4C	3.09	1.46	1.39
20	B	830	CLA	CHD-C4C	3.08	1.46	1.39
28	A	824	CL0	C3D-C2D	3.08	1.47	1.39
20	3	314	CLA	C3B-C4B	3.08	1.50	1.42
20	J	103	CLA	CHD-C4C	3.08	1.46	1.39
20	2	319	CLA	CHD-C1D	3.08	1.44	1.38
20	B	809	CLA	C3D-C2D	3.08	1.47	1.39
28	A	824	CL0	MG-NA	-3.08	1.99	2.06
20	L	306	CLA	C3D-C2D	3.08	1.47	1.39
20	A	805	CLA	OBD-CAD	3.08	1.27	1.22
20	B	802	CLA	CHD-C1D	3.08	1.44	1.38
20	1	305	CLA	CHD-C1D	3.08	1.44	1.38
19	2	309	CHL	C1D-C2D	3.08	1.51	1.45
20	A	844	CLA	MG-NA	-3.08	1.99	2.06
20	1	303	CLA	CHD-C4C	3.08	1.46	1.39
20	B	825	CLA	CHD-C1D	3.08	1.44	1.38
20	A	834	CLA	OBD-CAD	3.08	1.27	1.22
20	2	307	CLA	CHD-C1D	3.08	1.44	1.38
20	1	321	CLA	CHD-C1D	3.08	1.44	1.38
20	F	305	CLA	C3D-C2D	3.07	1.47	1.39
20	A	828	CLA	CHD-C1D	3.07	1.44	1.38
19	4	305	CHL	CHB-C1B	3.07	1.46	1.39
20	B	820	CLA	CHD-C4C	3.07	1.46	1.39
20	G	206	CLA	CHD-C4C	3.07	1.46	1.39
20	L	306	CLA	C4B-NB	-3.07	1.34	1.37
20	B	844	CLA	CHC-C4B	3.07	1.46	1.39
20	4	310	CLA	CHD-C4C	3.07	1.46	1.39
20	A	806	CLA	OBD-CAD	3.07	1.27	1.22
20	A	809	CLA	CHD-C4C	3.07	1.46	1.39
20	G	207	CLA	C4B-NB	-3.06	1.34	1.37
21	1	310	LUT	C8-C9	-3.06	1.39	1.45
20	B	828	CLA	OBD-CAD	3.06	1.27	1.22
20	A	834	CLA	CHC-C4B	3.06	1.46	1.39
20	A	850	CLA	C3D-C2D	3.06	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	853	CLA	CHD-C4C	3.06	1.46	1.39
20	4	304	CLA	C4B-NB	-3.06	1.34	1.37
20	1	304	CLA	C3D-C2D	3.06	1.47	1.39
20	O	206	CLA	C4B-NB	-3.06	1.34	1.37
20	A	848	CLA	C3D-C2D	3.06	1.47	1.39
20	4	309	CLA	CHD-C4C	3.06	1.46	1.39
20	A	856	CLA	CHD-C1D	3.05	1.44	1.38
20	1	303	CLA	C3D-C2D	3.05	1.47	1.39
20	B	848	CLA	C1B-NB	-3.05	1.34	1.37
20	1	306	CLA	CHD-C4C	3.05	1.46	1.39
20	A	835	CLA	C3D-C2D	3.05	1.47	1.39
20	A	802	CLA	C3D-C2D	3.05	1.47	1.39
20	B	826	CLA	CHD-C4C	3.05	1.46	1.39
20	4	310	CLA	CHD-C1D	3.05	1.44	1.38
20	K	206	CLA	C3D-C2D	3.05	1.47	1.39
20	A	829	CLA	CHD-C1D	3.05	1.44	1.38
20	A	828	CLA	C3D-C2D	3.05	1.47	1.39
20	A	846	CLA	C3D-C2D	3.05	1.47	1.39
20	B	805	CLA	CHD-C4C	3.05	1.46	1.39
20	1	303	CLA	CHD-C1D	3.05	1.44	1.38
20	1	320	CLA	C3D-C2D	3.05	1.47	1.39
20	2	304	CLA	C3D-C2D	3.05	1.47	1.39
20	1	307	CLA	CHD-C1D	3.05	1.44	1.38
20	O	208	CLA	CHD-C1D	3.04	1.44	1.38
20	A	838	CLA	C3D-C2D	3.04	1.47	1.39
20	O	206	CLA	C3D-C2D	3.04	1.47	1.39
20	B	825	CLA	C3D-C2D	3.04	1.47	1.39
20	A	839	CLA	C4B-NB	-3.04	1.34	1.37
20	A	836	CLA	CHD-C1D	3.04	1.44	1.38
20	A	853	CLA	CHD-C1D	3.04	1.44	1.38
20	K	203	CLA	CHD-C1D	3.04	1.44	1.38
20	3	307	CLA	CHC-C4B	3.04	1.46	1.39
20	1	321	CLA	C4B-NB	-3.04	1.34	1.37
20	H	201	CLA	CHD-C4C	3.04	1.46	1.39
21	3	301	LUT	C8-C9	-3.04	1.39	1.45
20	3	309	CLA	CHD-C4C	3.03	1.46	1.39
20	B	821	CLA	CHD-C4C	3.03	1.46	1.39
20	A	839	CLA	C3D-C2D	3.03	1.47	1.39
20	1	319	CLA	C4B-NB	-3.03	1.34	1.37
20	2	303	CLA	CHD-C4C	3.03	1.46	1.39
19	4	315	CHL	C3D-C2D	3.03	1.47	1.39
20	L	305	CLA	C3D-C2D	3.03	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	308	CLA	C3D-C2D	3.03	1.47	1.39
20	B	853	CLA	C3D-C2D	3.03	1.47	1.39
20	B	829	CLA	CHD-C1D	3.02	1.44	1.38
20	4	311	CLA	CHD-C4C	3.02	1.46	1.39
20	A	811	CLA	CHD-C1D	3.02	1.44	1.38
21	4	317	LUT	C8-C9	-3.02	1.39	1.45
20	B	820	CLA	C3D-C2D	3.02	1.47	1.39
28	A	824	CL0	C4B-NB	-3.02	1.34	1.37
20	3	310	CLA	C3D-C2D	3.02	1.47	1.39
20	B	852	CLA	C3D-C2D	3.02	1.47	1.39
20	2	319	CLA	C4B-NB	-3.02	1.34	1.37
20	A	855	CLA	CHD-C1D	3.01	1.44	1.38
20	1	322	CLA	CHD-C1D	3.01	1.44	1.38
20	4	309	CLA	CHD-C1D	3.01	1.44	1.38
20	3	312	CLA	C3D-C2D	3.01	1.47	1.39
20	G	205	CLA	C4B-NB	-3.01	1.34	1.37
20	B	811	CLA	C3D-C2D	3.01	1.47	1.39
20	B	849	CLA	CHD-C1D	3.01	1.44	1.38
20	B	844	CLA	MG-NA	-3.01	1.99	2.06
20	B	820	CLA	CHD-C1D	3.01	1.44	1.38
19	2	318	CHL	C1D-C2D	3.01	1.51	1.45
20	F	305	CLA	CHD-C1D	3.01	1.44	1.38
20	A	811	CLA	C3D-C2D	3.00	1.47	1.39
20	B	822	CLA	C3D-C2D	3.00	1.47	1.39
20	H	201	CLA	C3D-C2D	3.00	1.47	1.39
20	4	302	CLA	C3D-C2D	3.00	1.47	1.39
20	4	314	CLA	CHD-C1D	3.00	1.44	1.38
20	2	319	CLA	C3D-C2D	3.00	1.47	1.39
20	F	306	CLA	CHD-C4C	3.00	1.46	1.39
20	K	206	CLA	C4B-NB	-3.00	1.34	1.37
20	2	321	CLA	C3D-C2D	3.00	1.47	1.39
20	4	309	CLA	C3D-C2D	3.00	1.47	1.39
20	A	852	CLA	C4B-NB	-3.00	1.34	1.37
19	2	309	CHL	CHB-C1B	3.00	1.46	1.39
20	B	803	CLA	CHD-C4C	3.00	1.46	1.39
19	2	309	CHL	C3D-C2D	3.00	1.47	1.39
20	A	806	CLA	C3D-C2D	3.00	1.47	1.39
20	A	801	CLA	CHC-C4B	3.00	1.46	1.39
20	3	314	CLA	CHD-C4C	3.00	1.46	1.39
20	1	318	CLA	C1D-C2D	3.00	1.51	1.45
19	4	305	CHL	C3D-C2D	3.00	1.47	1.39
20	J	103	CLA	CHD-C1D	2.99	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	827	CLA	CHD-C1D	2.99	1.44	1.38
20	B	851	CLA	C1B-NB	-2.99	1.34	1.37
20	3	308	CLA	C3D-C2D	2.99	1.47	1.39
20	3	317	CLA	CHD-C1D	2.99	1.44	1.38
20	B	845	CLA	CHD-C4C	2.99	1.46	1.39
20	1	309	CLA	CHD-C1D	2.99	1.44	1.38
20	3	317	CLA	CHD-C4C	2.99	1.46	1.39
20	B	828	CLA	CHD-C4C	2.99	1.46	1.39
20	B	806	CLA	C3D-C2D	2.99	1.47	1.39
20	1	322	CLA	C3D-C2D	2.99	1.47	1.39
20	B	853	CLA	C4B-NB	-2.99	1.34	1.37
20	B	827	CLA	CHD-C1D	2.99	1.44	1.38
20	2	304	CLA	CHD-C1D	2.99	1.44	1.38
20	A	804	CLA	CHD-C1D	2.98	1.44	1.38
20	A	804	CLA	C3B-C4B	2.98	1.49	1.42
20	A	825	CLA	MG-NA	-2.98	1.99	2.06
20	J	103	CLA	C3D-C2D	2.98	1.47	1.39
20	O	207	CLA	CHD-C1D	2.98	1.44	1.38
20	3	318	CLA	C3D-C2D	2.98	1.47	1.39
20	A	829	CLA	C3D-C2D	2.98	1.47	1.39
20	2	317	CLA	C3D-C2D	2.98	1.47	1.39
20	1	308	CLA	C3D-C2D	2.98	1.47	1.39
20	B	824	CLA	CHD-C1D	2.98	1.44	1.38
20	N	202	CLA	CHD-C1D	2.97	1.44	1.38
20	K	205	CLA	C4B-NB	-2.97	1.34	1.37
20	2	307	CLA	C3D-C2D	2.97	1.47	1.39
20	4	303	CLA	CHD-C4C	2.97	1.46	1.39
20	2	305	CLA	C3D-C2D	2.97	1.47	1.39
20	3	320	CLA	C3D-C2D	2.97	1.47	1.39
20	A	842	CLA	CHD-C1D	2.97	1.44	1.38
20	A	831	CLA	CHD-C1D	2.97	1.44	1.38
20	A	837	CLA	CHD-C4C	2.97	1.46	1.39
20	A	844	CLA	C3D-C2D	2.97	1.47	1.39
20	B	830	CLA	CHD-C1D	2.97	1.44	1.38
19	4	306	CHL	C1D-C2D	2.97	1.51	1.45
20	1	302	CLA	CHD-C4C	2.97	1.46	1.39
20	2	307	CLA	C4B-NB	-2.96	1.34	1.37
20	B	826	CLA	OBD-CAD	2.96	1.27	1.22
20	A	856	CLA	C3D-C2D	2.96	1.47	1.39
20	K	203	CLA	C4B-NB	-2.96	1.34	1.37
20	O	208	CLA	C3D-C2D	2.96	1.47	1.39
20	2	306	CLA	CHD-C4C	2.96	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	825	CLA	CHD-C4C	2.96	1.46	1.39
20	L	306	CLA	CHD-C1D	2.96	1.44	1.38
20	4	304	CLA	C3D-C2D	2.96	1.47	1.39
19	4	305	CHL	C1D-C2D	2.96	1.51	1.45
20	A	801	CLA	C4B-NB	-2.96	1.34	1.37
20	B	813	CLA	CHD-C4C	2.96	1.46	1.39
20	L	307	CLA	C3D-C2D	2.96	1.47	1.39
20	4	302	CLA	CHD-C4C	2.96	1.46	1.39
20	3	315	CLA	C4B-NB	-2.96	1.34	1.37
20	B	813	CLA	C3D-C2D	2.95	1.47	1.39
20	3	319	CLA	C3D-C2D	2.95	1.47	1.39
20	H	201	CLA	CHD-C1D	2.95	1.44	1.38
20	A	812	CLA	CHD-C4C	2.95	1.46	1.39
20	A	848	CLA	CHD-C4C	2.95	1.46	1.39
20	F	306	CLA	C3D-C2D	2.95	1.47	1.39
20	B	810	CLA	C3D-C2D	2.95	1.47	1.39
20	B	846	CLA	C3D-C2D	2.95	1.47	1.39
20	B	831	CLA	CHD-C4C	2.95	1.46	1.39
20	2	323	CLA	C3D-C2D	2.95	1.47	1.39
20	3	314	CLA	C3D-C2D	2.95	1.47	1.39
19	2	301	CHL	C3D-C2D	2.94	1.47	1.39
20	4	310	CLA	C3D-C2D	2.94	1.47	1.39
20	2	308	CLA	C1D-C2D	2.94	1.51	1.45
20	B	805	CLA	C3D-C2D	2.94	1.47	1.39
20	B	827	CLA	C3D-C2D	2.94	1.47	1.39
20	A	840	CLA	CHD-C1D	2.94	1.44	1.38
20	3	307	CLA	C3D-C2D	2.94	1.47	1.39
20	A	829	CLA	MG-NA	-2.94	1.99	2.06
20	2	320	CLA	MG-NA	-2.94	1.99	2.06
20	A	851	CLA	CHD-C4C	2.94	1.45	1.39
20	A	830	CLA	CHD-C4C	2.94	1.45	1.39
19	2	322	CHL	C1D-C2D	2.94	1.51	1.45
28	A	824	CL0	CHD-C1D	2.94	1.44	1.38
23	B	838	BCR	C8-C9	-2.94	1.39	1.45
20	1	318	CLA	C4B-NB	-2.94	1.34	1.37
23	J	101	BCR	C8-C9	-2.94	1.39	1.45
20	A	833	CLA	CHD-C4C	2.94	1.45	1.39
20	B	845	CLA	MG-NA	-2.94	1.99	2.06
20	A	843	CLA	CHC-C4B	2.93	1.46	1.39
20	4	312	CLA	CHD-C4C	2.93	1.45	1.39
20	1	318	CLA	C3D-C2D	2.93	1.47	1.39
20	A	848	CLA	CHD-C1D	2.93	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	849	CLA	C3D-C2D	2.93	1.47	1.39
20	3	315	CLA	C3D-C2D	2.93	1.47	1.39
20	G	207	CLA	C3D-C2D	2.93	1.47	1.39
20	4	308	CLA	CHD-C4C	2.93	1.45	1.39
19	2	322	CHL	C3D-C2D	2.93	1.47	1.39
19	1	317	CHL	C3D-C2D	2.93	1.47	1.39
20	1	306	CLA	C3D-C2D	2.93	1.47	1.39
20	B	805	CLA	CHD-C1D	2.93	1.44	1.38
20	B	811	CLA	CHD-C1D	2.92	1.44	1.38
20	B	824	CLA	C3D-C2D	2.92	1.47	1.39
20	4	313	CLA	C1D-C2D	2.92	1.51	1.45
20	A	825	CLA	C1B-NB	-2.92	1.34	1.37
20	K	203	CLA	C3D-C2D	2.92	1.47	1.39
20	N	202	CLA	C3D-C2D	2.92	1.47	1.39
20	A	807	CLA	CHD-C1D	2.92	1.44	1.38
19	2	302	CHL	C3D-C2D	2.92	1.47	1.39
20	4	308	CLA	CHD-C1D	2.92	1.44	1.38
20	B	815	CLA	C3D-C2D	2.92	1.47	1.39
20	B	830	CLA	C3D-C2D	2.92	1.47	1.39
20	A	855	CLA	C3D-C2D	2.92	1.47	1.39
20	G	205	CLA	C3D-C2D	2.91	1.47	1.39
19	3	313	CHL	C3D-C2D	2.91	1.47	1.39
20	A	804	CLA	C3D-C2D	2.91	1.47	1.39
20	A	805	CLA	CHD-C4C	2.91	1.45	1.39
20	L	307	CLA	C4B-NB	-2.91	1.34	1.37
19	4	306	CHL	C3D-C2D	2.91	1.47	1.39
20	A	834	CLA	CHD-C4C	2.91	1.45	1.39
20	1	306	CLA	CHD-C1D	2.91	1.44	1.38
20	4	316	CLA	CHD-C4C	2.91	1.45	1.39
20	A	801	CLA	C3D-C2D	2.91	1.47	1.39
20	A	847	CLA	C1D-C2D	2.91	1.51	1.45
20	1	305	CLA	C3D-C2D	2.91	1.47	1.39
20	3	316	CLA	CHD-C4C	2.91	1.45	1.39
20	4	312	CLA	CHD-C1D	2.90	1.44	1.38
20	4	313	CLA	C3D-C2D	2.90	1.47	1.39
20	B	822	CLA	C4B-NB	-2.90	1.34	1.37
20	4	302	CLA	CHD-C1D	2.90	1.44	1.38
20	B	821	CLA	C3D-C2D	2.90	1.47	1.39
20	2	317	CLA	C1D-C2D	2.90	1.51	1.45
20	1	309	CLA	C3D-C2D	2.90	1.47	1.39
23	B	837	BCR	C23-C22	-2.90	1.39	1.45
20	A	830	CLA	C3D-C2D	2.90	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	804	CLA	C3D-C2D	2.90	1.47	1.39
20	A	809	CLA	CHD-C1D	2.90	1.44	1.38
20	2	321	CLA	C1D-C2D	2.90	1.51	1.45
19	4	307	CHL	C3D-C2D	2.89	1.47	1.39
20	4	311	CLA	CHD-C1D	2.89	1.44	1.38
20	B	831	CLA	CHD-C1D	2.89	1.44	1.38
21	2	310	LUT	C8-C9	-2.89	1.39	1.45
20	A	843	CLA	C4B-NB	-2.89	1.34	1.37
20	A	854	CLA	CHD-C4C	2.89	1.45	1.39
20	B	851	CLA	CHD-C1D	2.89	1.44	1.38
20	B	807	CLA	C3D-C2D	2.89	1.47	1.39
20	A	830	CLA	C1B-NB	-2.89	1.34	1.37
20	B	833	CLA	C1D-C2D	2.89	1.51	1.45
20	A	853	CLA	C1B-NB	-2.89	1.34	1.37
20	B	826	CLA	C3D-C2D	2.89	1.47	1.39
20	B	816	CLA	CHD-C4C	2.88	1.45	1.39
20	1	308	CLA	C4B-NB	-2.88	1.34	1.37
20	L	305	CLA	C4B-NB	-2.88	1.34	1.37
20	2	308	CLA	C3D-C2D	2.88	1.47	1.39
19	2	301	CHL	C1D-C2D	2.88	1.51	1.45
20	B	848	CLA	C4B-NB	-2.88	1.34	1.37
20	B	831	CLA	C3D-C2D	2.88	1.47	1.39
20	B	850	CLA	MG-NA	-2.88	1.99	2.06
19	2	302	CHL	C1D-C2D	2.88	1.51	1.45
20	A	842	CLA	C3D-C2D	2.88	1.47	1.39
20	3	311	CLA	C3D-C2D	2.88	1.47	1.39
20	K	204	CLA	C3D-C2D	2.88	1.47	1.39
20	3	314	CLA	MG-NA	-2.88	1.99	2.06
19	3	313	CHL	C1D-C2D	2.88	1.51	1.45
20	O	207	CLA	C3D-C2D	2.87	1.47	1.39
20	F	304	CLA	C3D-C2D	2.87	1.47	1.39
20	2	304	CLA	C1B-NB	-2.87	1.34	1.37
20	B	810	CLA	C1B-NB	-2.87	1.34	1.37
20	A	831	CLA	C3D-C2D	2.87	1.47	1.39
20	3	310	CLA	C1D-C2D	2.87	1.51	1.45
19	1	301	CHL	C1D-C2D	2.87	1.51	1.45
20	B	814	CLA	C3D-C2D	2.87	1.46	1.39
20	A	826	CLA	C1B-NB	-2.87	1.34	1.37
20	A	827	CLA	MG-NA	-2.87	1.99	2.06
20	A	836	CLA	C3D-C2D	2.87	1.46	1.39
20	A	807	CLA	C3D-C2D	2.86	1.46	1.39
20	A	832	CLA	C1B-NB	-2.86	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	840	CLA	C3D-C2D	2.86	1.46	1.39
20	A	846	CLA	CHD-C1D	2.86	1.43	1.38
20	A	830	CLA	CHD-C1D	2.86	1.43	1.38
20	3	314	CLA	CHD-C1D	2.86	1.43	1.38
20	G	205	CLA	CHD-C1D	2.86	1.43	1.38
20	1	302	CLA	C3D-C2D	2.86	1.46	1.39
20	L	305	CLA	C1D-C2D	2.86	1.51	1.45
20	G	206	CLA	CHD-C1D	2.86	1.43	1.38
20	A	827	CLA	C3D-C2D	2.86	1.46	1.39
20	B	819	CLA	C4B-NB	-2.85	1.34	1.37
23	L	302	BCR	C8-C9	-2.85	1.39	1.45
20	B	853	CLA	C1D-C2D	2.85	1.51	1.45
19	1	301	CHL	C3D-C2D	2.85	1.46	1.39
20	B	846	CLA	C1D-C2D	2.85	1.50	1.45
23	B	839	BCR	C10-C9	2.85	1.42	1.35
20	4	311	CLA	C3D-C2D	2.85	1.46	1.39
20	B	808	CLA	C1B-NB	-2.85	1.34	1.37
20	A	843	CLA	C1D-C2D	2.85	1.50	1.45
20	A	853	CLA	C3D-C2D	2.85	1.46	1.39
19	4	315	CHL	C1D-C2D	2.85	1.50	1.45
20	1	319	CLA	C1D-C2D	2.85	1.50	1.45
20	1	321	CLA	C3D-C2D	2.85	1.46	1.39
20	4	316	CLA	CHD-C1D	2.85	1.43	1.38
20	B	817	CLA	CHD-C4C	2.85	1.45	1.39
20	B	833	CLA	C3D-C2D	2.84	1.46	1.39
23	A	817	BCR	C12-C13	-2.84	1.39	1.45
20	B	821	CLA	CHD-C1D	2.84	1.43	1.38
20	A	854	CLA	CHD-C1D	2.83	1.43	1.38
20	2	304	CLA	C4B-NB	-2.83	1.34	1.37
20	1	320	CLA	C1D-C2D	2.83	1.50	1.45
20	B	803	CLA	C3D-C2D	2.83	1.46	1.39
20	A	809	CLA	C3D-C2D	2.83	1.46	1.39
20	L	306	CLA	MG-NA	-2.83	1.99	2.06
20	B	814	CLA	CHD-C4C	2.83	1.45	1.39
20	B	818	CLA	C1B-NB	-2.83	1.34	1.37
20	3	317	CLA	C3D-C2D	2.83	1.46	1.39
20	K	206	CLA	C1D-C2D	2.83	1.50	1.45
20	F	306	CLA	CHD-C1D	2.83	1.43	1.38
20	A	838	CLA	C4B-NB	-2.82	1.34	1.37
20	A	825	CLA	C3B-C4B	2.82	1.49	1.42
20	4	312	CLA	C3D-C2D	2.82	1.46	1.39
20	B	806	CLA	C1D-C2D	2.82	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	817	BCR	C23-C22	-2.82	1.39	1.45
28	A	824	CL0	CHC-C4B	2.82	1.45	1.39
20	A	808	CLA	MG-NA	-2.82	1.99	2.06
20	A	830	CLA	MG-NA	-2.82	1.99	2.06
20	A	841	CLA	C1D-C2D	2.82	1.50	1.45
20	1	304	CLA	MG-NA	-2.82	1.99	2.06
20	A	803	CLA	MG-NA	-2.82	1.99	2.06
20	B	851	CLA	CHC-C4B	2.82	1.45	1.39
20	3	320	CLA	C4B-NB	-2.81	1.34	1.37
20	4	304	CLA	C1D-C2D	2.81	1.50	1.45
23	A	815	BCR	C8-C9	-2.81	1.39	1.45
20	B	848	CLA	CHD-C4C	2.81	1.45	1.39
19	1	317	CHL	C1D-C2D	2.81	1.50	1.45
20	B	830	CLA	MG-NA	-2.81	1.99	2.06
20	3	308	CLA	MG-NA	-2.81	1.99	2.06
19	2	318	CHL	C3D-C2D	2.81	1.46	1.39
20	A	806	CLA	C1D-C2D	2.81	1.50	1.45
20	2	306	CLA	C3D-C2D	2.81	1.46	1.39
20	A	805	CLA	C3D-C2D	2.81	1.46	1.39
20	B	808	CLA	C1D-C2D	2.81	1.50	1.45
20	3	309	CLA	CHD-C1D	2.81	1.43	1.38
20	2	303	CLA	C1B-NB	-2.81	1.34	1.37
20	A	836	CLA	C1D-C2D	2.81	1.50	1.45
20	3	316	CLA	C3D-C2D	2.81	1.46	1.39
20	F	305	CLA	MG-NA	-2.80	1.99	2.06
20	K	206	CLA	C3B-C4B	2.80	1.49	1.42
20	B	803	CLA	CHD-C1D	2.80	1.43	1.38
20	2	305	CLA	C1D-C2D	2.80	1.50	1.45
20	1	319	CLA	C3D-C2D	2.80	1.46	1.39
20	K	205	CLA	CHD-C1D	2.80	1.43	1.38
20	A	833	CLA	C1B-NB	-2.80	1.34	1.37
20	B	816	CLA	C3D-C2D	2.80	1.46	1.39
23	L	301	BCR	C8-C9	-2.79	1.39	1.45
20	A	856	CLA	MG-NA	-2.79	1.99	2.06
20	B	827	CLA	MG-NA	-2.79	1.99	2.06
20	A	839	CLA	C1D-C2D	2.79	1.50	1.45
20	4	316	CLA	C3D-C2D	2.79	1.46	1.39
20	B	823	CLA	C4B-NB	-2.79	1.34	1.37
20	1	307	CLA	C3D-C2D	2.79	1.46	1.39
20	3	308	CLA	C3B-C4B	2.79	1.49	1.42
20	1	304	CLA	C1D-C2D	2.79	1.50	1.45
20	B	844	CLA	C3D-C2D	2.79	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	319	CLA	C1D-C2D	2.79	1.50	1.45
20	1	309	CLA	C1D-C2D	2.79	1.50	1.45
23	I	102	BCR	C23-C22	-2.78	1.40	1.45
20	A	843	CLA	C1B-NB	-2.78	1.34	1.37
20	3	318	CLA	C1D-C2D	2.78	1.50	1.45
28	A	824	CL0	CHD-C4C	2.78	1.45	1.39
20	A	836	CLA	MG-NA	-2.78	1.99	2.06
20	A	835	CLA	C1D-C2D	2.78	1.50	1.45
20	3	309	CLA	C3D-C2D	2.78	1.46	1.39
20	B	815	CLA	MG-NA	-2.78	1.99	2.06
20	B	809	CLA	C1D-C2D	2.78	1.50	1.45
20	L	307	CLA	C1D-C2D	2.78	1.50	1.45
20	G	206	CLA	C3D-C2D	2.78	1.46	1.39
20	L	305	CLA	C3B-C4B	2.78	1.49	1.42
20	O	207	CLA	C1D-C2D	2.78	1.50	1.45
20	B	813	CLA	CHD-C1D	2.77	1.43	1.38
20	B	847	CLA	C3D-C2D	2.77	1.46	1.39
20	2	323	CLA	C1D-C2D	2.77	1.50	1.45
20	A	833	CLA	CHD-C1D	2.77	1.43	1.38
23	G	201	BCR	C23-C22	-2.77	1.40	1.45
20	B	816	CLA	CHD-C1D	2.77	1.43	1.38
20	A	828	CLA	C1D-C2D	2.77	1.50	1.45
20	K	205	CLA	C3D-C2D	2.77	1.46	1.39
20	B	826	CLA	CHD-C1D	2.77	1.43	1.38
19	4	307	CHL	C1D-C2D	2.77	1.50	1.45
20	O	208	CLA	MG-NA	-2.77	1.99	2.06
23	K	201	BCR	C8-C9	-2.77	1.40	1.45
20	B	828	CLA	C3D-C2D	2.77	1.46	1.39
20	O	206	CLA	C1D-C2D	2.77	1.50	1.45
20	4	316	CLA	C1B-NB	-2.77	1.34	1.37
20	J	103	CLA	C1D-C2D	2.77	1.50	1.45
20	B	848	CLA	MG-NA	-2.77	1.99	2.06
28	A	824	CL0	C1B-NB	-2.77	1.34	1.37
20	2	307	CLA	C1D-C2D	2.77	1.50	1.45
20	A	803	CLA	CHD-C4C	2.77	1.45	1.39
20	A	851	CLA	C3D-C2D	2.77	1.46	1.39
20	A	837	CLA	C3D-C2D	2.76	1.46	1.39
20	F	305	CLA	C1B-NB	-2.76	1.34	1.37
20	A	849	CLA	CHD-C4C	2.76	1.45	1.39
20	1	319	CLA	MG-NA	-2.76	1.99	2.06
20	2	320	CLA	C3D-C2D	2.76	1.46	1.39
20	F	304	CLA	CHD-C4C	2.76	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	302	CLA	C3B-C4B	2.76	1.49	1.42
20	A	854	CLA	CHC-C4B	2.76	1.45	1.39
20	A	838	CLA	C1D-C2D	2.76	1.50	1.45
20	B	850	CLA	CHD-C1D	2.76	1.43	1.38
20	1	322	CLA	C1D-C2D	2.76	1.50	1.45
20	B	802	CLA	C1D-C2D	2.76	1.50	1.45
20	K	204	CLA	C1D-C2D	2.75	1.50	1.45
20	B	809	CLA	C1B-NB	-2.75	1.34	1.37
20	B	824	CLA	C1D-C2D	2.75	1.50	1.45
20	A	851	CLA	C3B-C4B	2.75	1.49	1.42
23	G	203	BCR	C8-C9	-2.75	1.40	1.45
23	B	837	BCR	C12-C13	-2.75	1.40	1.45
20	B	822	CLA	C1D-C2D	2.75	1.50	1.45
20	4	309	CLA	MG-NA	-2.75	1.99	2.06
23	B	836	BCR	C8-C9	-2.74	1.40	1.45
20	N	202	CLA	C1D-C2D	2.74	1.50	1.45
23	4	319	BCR	C23-C22	-2.74	1.40	1.45
20	1	308	CLA	C1D-C2D	2.74	1.50	1.45
20	A	832	CLA	C1D-C2D	2.74	1.50	1.45
20	A	840	CLA	C1D-C2D	2.74	1.50	1.45
20	A	843	CLA	MG-NA	-2.74	1.99	2.06
20	4	302	CLA	C1B-NB	-2.74	1.34	1.37
20	B	813	CLA	MG-NA	-2.74	1.99	2.06
20	A	833	CLA	C3D-C2D	2.74	1.46	1.39
20	3	316	CLA	CHD-C1D	2.74	1.43	1.38
20	B	807	CLA	C4B-NB	-2.74	1.34	1.37
20	B	845	CLA	CHD-C1D	2.73	1.43	1.38
20	O	208	CLA	C1B-C2B	2.73	1.49	1.43
20	A	846	CLA	C1B-NB	-2.73	1.34	1.37
20	K	205	CLA	CHD-C4C	2.73	1.45	1.39
20	2	304	CLA	MG-NA	-2.73	1.99	2.06
20	A	856	CLA	C1D-C2D	2.73	1.50	1.45
20	A	826	CLA	OBD-CAD	2.73	1.27	1.22
20	G	207	CLA	C1D-C2D	2.73	1.50	1.45
20	B	810	CLA	CHD-C1D	2.73	1.43	1.38
20	B	847	CLA	C4B-NB	-2.72	1.34	1.37
20	B	829	CLA	C3D-C2D	2.72	1.46	1.39
20	3	309	CLA	MG-NA	-2.72	1.99	2.06
20	B	829	CLA	MG-NA	-2.72	1.99	2.06
20	4	314	CLA	MG-NA	-2.72	1.99	2.06
20	B	817	CLA	MG-NA	-2.72	1.99	2.06
20	B	818	CLA	C3D-C2D	2.72	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	303	CLA	CHD-C1D	2.72	1.43	1.38
20	A	812	CLA	CHD-C1D	2.72	1.43	1.38
23	F	302	BCR	C23-C22	-2.72	1.40	1.45
20	B	815	CLA	C1D-C2D	2.72	1.50	1.45
20	1	318	CLA	C3B-C4B	2.72	1.49	1.42
20	A	803	CLA	CHD-C1D	2.72	1.43	1.38
20	B	849	CLA	C1D-C2D	2.72	1.50	1.45
20	B	808	CLA	MG-NA	-2.72	1.99	2.06
20	K	203	CLA	C1D-C2D	2.72	1.50	1.45
20	A	826	CLA	MG-NA	-2.71	1.99	2.06
20	3	315	CLA	C1D-C2D	2.71	1.50	1.45
23	A	814	BCR	C23-C22	-2.71	1.40	1.45
20	A	842	CLA	MG-NA	-2.71	1.99	2.06
20	A	846	CLA	C1D-C2D	2.71	1.50	1.45
20	B	852	CLA	C1D-C2D	2.71	1.50	1.45
20	4	302	CLA	MG-NA	-2.71	1.99	2.06
20	A	849	CLA	C1B-C2B	2.70	1.49	1.43
20	A	847	CLA	C3D-C2D	2.70	1.46	1.39
20	B	812	CLA	C1D-C2D	2.70	1.50	1.45
20	G	205	CLA	MG-NA	-2.70	1.99	2.06
20	B	852	CLA	MG-NA	-2.70	1.99	2.06
20	G	206	CLA	C1D-C2D	2.70	1.50	1.45
23	3	303	BCR	C8-C9	-2.70	1.40	1.45
20	1	302	CLA	CHD-C1D	2.70	1.43	1.38
20	A	849	CLA	C1B-NB	-2.70	1.34	1.37
20	F	304	CLA	CHD-C1D	2.70	1.43	1.38
20	B	802	CLA	C3D-C2D	2.70	1.46	1.39
20	A	828	CLA	C3B-C4B	2.70	1.49	1.42
20	1	304	CLA	C1B-C2B	2.70	1.49	1.43
20	A	809	CLA	C1D-C2D	2.70	1.50	1.45
20	N	202	CLA	MG-NA	-2.70	1.99	2.06
20	3	308	CLA	C1D-C2D	2.70	1.50	1.45
20	B	848	CLA	OBD-CAD	2.69	1.27	1.22
20	A	805	CLA	CHD-C1D	2.69	1.43	1.38
20	1	308	CLA	C3B-C4B	2.69	1.49	1.42
20	B	801	CLA	C1D-C2D	2.69	1.50	1.45
20	2	307	CLA	C1B-C2B	2.69	1.49	1.43
20	K	204	CLA	C1B-C2B	2.69	1.49	1.43
20	B	849	CLA	MG-NA	-2.69	1.99	2.06
20	1	305	CLA	C1D-C2D	2.69	1.50	1.45
20	3	320	CLA	C1D-C2D	2.69	1.50	1.45
20	A	851	CLA	MG-NA	-2.69	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	1	312	BCR	C23-C22	-2.69	1.40	1.45
20	A	834	CLA	CHD-C1D	2.69	1.43	1.38
20	B	821	CLA	C1D-C2D	2.69	1.50	1.45
20	B	829	CLA	C1D-C2D	2.69	1.50	1.45
20	B	814	CLA	C1B-NB	-2.69	1.34	1.37
20	A	855	CLA	MG-NA	-2.69	1.99	2.06
20	1	307	CLA	C1D-C2D	2.69	1.50	1.45
20	K	203	CLA	C1B-C2B	2.69	1.49	1.43
20	A	812	CLA	C3B-C4B	2.69	1.49	1.42
20	A	837	CLA	CHD-C1D	2.69	1.43	1.38
20	B	815	CLA	C3B-C4B	2.69	1.49	1.42
20	1	308	CLA	C1B-C2B	2.69	1.49	1.43
20	B	816	CLA	MG-NA	-2.69	1.99	2.06
20	4	304	CLA	MG-NA	-2.69	1.99	2.06
20	B	850	CLA	CHD-C4C	2.68	1.45	1.39
20	3	311	CLA	C1B-C2B	2.68	1.49	1.43
20	B	847	CLA	C1D-C2D	2.68	1.50	1.45
20	A	804	CLA	MG-NA	-2.68	1.99	2.06
20	B	805	CLA	MG-NA	-2.68	1.99	2.06
20	2	320	CLA	CHD-C4C	2.68	1.45	1.39
20	B	830	CLA	C1D-C2D	2.68	1.50	1.45
20	H	201	CLA	C1D-C2D	2.68	1.50	1.45
20	A	832	CLA	MG-NA	-2.68	1.99	2.06
20	A	812	CLA	MG-NA	-2.68	1.99	2.06
20	1	319	CLA	C3B-C4B	2.68	1.49	1.42
20	A	828	CLA	C4B-NB	-2.68	1.34	1.37
20	B	827	CLA	C1D-C2D	2.68	1.50	1.45
20	A	839	CLA	MG-NA	-2.68	1.99	2.06
20	A	811	CLA	MG-NA	-2.68	1.99	2.06
20	B	802	CLA	C1B-NB	-2.68	1.34	1.37
20	2	306	CLA	CHD-C1D	2.68	1.43	1.38
20	2	320	CLA	C1B-NB	-2.68	1.34	1.37
20	1	303	CLA	MG-NA	-2.68	1.99	2.06
20	A	845	CLA	MG-NA	-2.67	1.99	2.06
20	A	807	CLA	C1D-C2D	2.67	1.50	1.45
20	B	817	CLA	C3D-C2D	2.67	1.46	1.39
20	A	804	CLA	C1B-NB	-2.67	1.34	1.37
20	3	315	CLA	MG-NA	-2.67	1.99	2.06
20	4	304	CLA	C3B-C4B	2.67	1.49	1.42
20	A	802	CLA	C1D-C2D	2.67	1.50	1.45
20	B	803	CLA	C3B-C4B	2.67	1.49	1.42
20	G	205	CLA	C1B-C2B	2.67	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	809	CLA	MG-NA	-2.67	1.99	2.06
20	O	208	CLA	C1D-C2D	2.67	1.50	1.45
21	1	310	LUT	C12-C13	-2.67	1.40	1.45
20	3	312	CLA	MG-NA	-2.67	1.99	2.06
20	2	319	CLA	C1D-C2D	2.66	1.50	1.45
20	A	840	CLA	C1B-NB	-2.66	1.34	1.37
20	B	823	CLA	C3B-C4B	2.66	1.49	1.42
23	I	102	BCR	C8-C9	-2.66	1.40	1.45
20	4	303	CLA	MG-NA	-2.66	1.99	2.06
20	L	307	CLA	MG-NA	-2.66	1.99	2.06
23	F	302	BCR	C8-C9	-2.66	1.40	1.45
20	A	801	CLA	C1B-C2B	2.66	1.49	1.43
20	B	850	CLA	C4B-NB	-2.66	1.34	1.37
23	G	203	BCR	C23-C22	-2.66	1.40	1.45
23	A	815	BCR	C12-C13	-2.66	1.40	1.45
20	A	811	CLA	C1D-C2D	2.66	1.50	1.45
20	A	831	CLA	C1D-C2D	2.66	1.50	1.45
20	H	201	CLA	MG-NA	-2.66	2.00	2.06
20	4	303	CLA	C3D-C2D	2.66	1.46	1.39
20	B	848	CLA	C3D-C2D	2.66	1.46	1.39
20	K	203	CLA	C3B-C4B	2.66	1.49	1.42
20	A	827	CLA	C1D-C2D	2.65	1.50	1.45
20	B	803	CLA	C1B-NB	-2.65	1.34	1.37
20	3	315	CLA	C3B-C4B	2.65	1.49	1.42
20	A	827	CLA	C1B-C2B	2.65	1.49	1.43
20	B	825	CLA	C1D-C2D	2.65	1.50	1.45
20	A	846	CLA	MG-NA	-2.65	2.00	2.06
21	1	323	LUT	C8-C9	-2.65	1.40	1.45
20	A	854	CLA	C3B-C4B	2.65	1.49	1.42
21	4	317	LUT	C32-C33	-2.65	1.40	1.45
20	B	813	CLA	C1B-NB	-2.65	1.34	1.37
20	A	838	CLA	C1B-C2B	2.65	1.49	1.43
20	A	842	CLA	C4B-NB	-2.65	1.34	1.37
23	G	203	BCR	C20-C19	2.65	1.41	1.34
20	B	811	CLA	MG-NA	-2.65	2.00	2.06
20	B	803	CLA	MG-NA	-2.65	2.00	2.06
20	3	319	CLA	C1B-NB	-2.65	1.34	1.37
23	A	814	BCR	C12-C13	-2.64	1.40	1.45
20	1	306	CLA	C1D-C2D	2.64	1.50	1.45
20	B	804	CLA	C4B-NB	-2.64	1.34	1.37
20	A	842	CLA	C1D-C2D	2.64	1.50	1.45
20	A	852	CLA	MG-NA	-2.64	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	848	CLA	C4B-NB	-2.64	1.34	1.37
20	3	320	CLA	C3B-C4B	2.64	1.48	1.42
23	A	818	BCR	C23-C22	-2.64	1.40	1.45
20	B	831	CLA	MG-NA	-2.64	2.00	2.06
20	2	306	CLA	MG-NA	-2.64	2.00	2.06
20	4	309	CLA	C1D-C2D	2.64	1.50	1.45
20	A	805	CLA	MG-NA	-2.64	2.00	2.06
20	3	320	CLA	C1B-C2B	2.64	1.49	1.43
20	A	829	CLA	C1D-C2D	2.64	1.50	1.45
20	B	816	CLA	C1B-C2B	2.64	1.49	1.43
20	4	308	CLA	C1B-NB	-2.64	1.34	1.37
20	A	839	CLA	C3B-C4B	2.64	1.48	1.42
20	B	817	CLA	C3B-C4B	2.63	1.48	1.42
20	F	304	CLA	MG-NA	-2.63	2.00	2.06
20	2	305	CLA	MG-NA	-2.63	2.00	2.06
20	4	309	CLA	C1C-C2C	2.63	1.49	1.44
20	3	312	CLA	C1D-C2D	2.63	1.50	1.45
20	B	847	CLA	CHD-C4C	2.63	1.45	1.39
20	A	845	CLA	C1D-C2D	2.63	1.50	1.45
20	A	849	CLA	C3D-C2D	2.63	1.46	1.39
20	3	307	CLA	C1D-C2D	2.63	1.50	1.45
20	1	322	CLA	MG-NA	-2.63	2.00	2.06
20	O	208	CLA	C3B-C4B	2.63	1.48	1.42
20	L	307	CLA	C1B-C2B	2.63	1.49	1.43
20	O	206	CLA	C1B-C2B	2.63	1.49	1.43
20	A	848	CLA	C1B-NB	-2.63	1.34	1.37
20	B	844	CLA	CHD-C4C	2.63	1.45	1.39
20	A	833	CLA	MG-NA	-2.63	2.00	2.06
20	A	844	CLA	C1D-C2D	2.63	1.50	1.45
20	A	854	CLA	MG-NA	-2.63	2.00	2.06
20	B	807	CLA	C1D-C2D	2.63	1.50	1.45
20	B	846	CLA	MG-NA	-2.63	2.00	2.06
20	B	828	CLA	MG-NA	-2.63	2.00	2.06
20	A	809	CLA	C1B-NB	-2.62	1.34	1.37
20	B	807	CLA	MG-NA	-2.62	2.00	2.06
20	A	829	CLA	C1B-NB	-2.62	1.34	1.37
20	A	805	CLA	C1C-C2C	2.62	1.49	1.44
20	2	319	CLA	C3B-C4B	2.62	1.48	1.42
20	B	851	CLA	MG-NA	-2.62	2.00	2.06
20	K	206	CLA	C1B-C2B	2.62	1.49	1.43
20	2	323	CLA	C1B-NB	-2.62	1.34	1.37
20	A	808	CLA	C1D-C2D	2.62	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	G	201	BCR	C8-C9	-2.62	1.40	1.45
20	B	826	CLA	MG-NA	-2.62	2.00	2.06
20	B	822	CLA	C1B-C2B	2.62	1.49	1.43
20	4	302	CLA	C1D-C2D	2.62	1.50	1.45
20	B	814	CLA	MG-NA	-2.62	2.00	2.06
20	4	311	CLA	MG-NA	-2.62	2.00	2.06
20	K	204	CLA	C3B-C4B	2.62	1.48	1.42
20	3	309	CLA	C1D-C2D	2.62	1.50	1.45
20	A	835	CLA	MG-NA	-2.62	2.00	2.06
20	O	206	CLA	MG-NA	-2.62	2.00	2.06
20	3	312	CLA	C1B-C2B	2.62	1.49	1.43
20	3	310	CLA	MG-NA	-2.61	2.00	2.06
20	1	308	CLA	MG-NA	-2.61	2.00	2.06
19	2	322	CHL	C3B-C4B	2.61	1.48	1.42
20	2	306	CLA	C1D-C2D	2.61	1.50	1.45
20	B	810	CLA	MG-NA	-2.61	2.00	2.06
20	B	814	CLA	C3B-C4B	2.61	1.48	1.42
20	4	311	CLA	C1D-C2D	2.61	1.50	1.45
20	B	805	CLA	C1B-C2B	2.61	1.49	1.43
20	G	205	CLA	C1D-C2D	2.61	1.50	1.45
23	A	857	BCR	C8-C9	-2.61	1.40	1.45
20	F	305	CLA	C1D-C2D	2.61	1.50	1.45
20	L	305	CLA	MG-NA	-2.61	2.00	2.06
20	B	803	CLA	C1D-C2D	2.61	1.50	1.45
20	B	803	CLA	C1B-C2B	2.61	1.49	1.43
21	4	317	LUT	C12-C13	-2.61	1.40	1.45
20	3	310	CLA	C1B-C2B	2.61	1.49	1.43
20	B	811	CLA	C1D-C2D	2.61	1.50	1.45
20	B	824	CLA	MG-NA	-2.61	2.00	2.06
20	A	850	CLA	MG-NA	-2.61	2.00	2.06
20	B	801	CLA	MG-NA	-2.61	2.00	2.06
20	1	304	CLA	C3B-C4B	2.61	1.48	1.42
20	B	846	CLA	C3B-C4B	2.61	1.48	1.42
20	A	834	CLA	C3D-C2D	2.60	1.46	1.39
20	B	819	CLA	MG-NA	-2.60	2.00	2.06
20	B	833	CLA	MG-NA	-2.60	2.00	2.06
20	O	206	CLA	C3B-C4B	2.60	1.48	1.42
20	A	837	CLA	C4B-NB	-2.60	1.34	1.37
20	B	852	CLA	C1B-NB	-2.60	1.34	1.37
20	K	206	CLA	MG-NA	-2.60	2.00	2.06
20	A	852	CLA	C3B-C4B	2.60	1.48	1.42
20	K	204	CLA	MG-NA	-2.60	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	K	201	BCR	C23-C22	-2.60	1.40	1.45
20	3	311	CLA	MG-NA	-2.60	2.00	2.06
20	2	304	CLA	C1D-C2D	2.60	1.50	1.45
20	B	820	CLA	MG-NA	-2.60	2.00	2.06
20	B	821	CLA	C1B-NB	-2.60	1.34	1.37
20	4	309	CLA	C1B-NB	-2.59	1.34	1.37
20	B	818	CLA	MG-NA	-2.59	2.00	2.06
21	4	317	LUT	C28-C29	-2.59	1.40	1.45
20	2	321	CLA	MG-NA	-2.59	2.00	2.06
20	A	812	CLA	C1B-NB	-2.59	1.34	1.37
20	1	306	CLA	MG-NA	-2.59	2.00	2.06
20	B	831	CLA	C1B-NB	-2.59	1.34	1.37
20	2	321	CLA	C3B-C4B	2.59	1.48	1.42
20	4	310	CLA	MG-NA	-2.59	2.00	2.06
20	3	308	CLA	C1B-C2B	2.59	1.49	1.43
20	L	306	CLA	C1D-C2D	2.59	1.50	1.45
20	B	852	CLA	C4B-NB	-2.59	1.34	1.37
20	B	806	CLA	C1C-C2C	2.59	1.49	1.44
20	4	314	CLA	C1D-C2D	2.59	1.50	1.45
23	L	301	BCR	C23-C22	-2.59	1.40	1.45
20	3	312	CLA	C3B-C4B	2.58	1.48	1.42
20	A	845	CLA	C3B-C4B	2.58	1.48	1.42
21	1	310	LUT	C32-C33	-2.58	1.40	1.45
20	J	103	CLA	MG-NA	-2.58	2.00	2.06
20	3	317	CLA	C1D-C2D	2.58	1.50	1.45
20	2	307	CLA	MG-NA	-2.58	2.00	2.06
20	A	808	CLA	C1B-C2B	2.58	1.49	1.43
20	B	853	CLA	C1B-C2B	2.58	1.49	1.43
20	1	302	CLA	C1B-NB	-2.58	1.34	1.37
20	A	825	CLA	CHD-C1D	2.58	1.43	1.38
23	2	312	BCR	C23-C22	-2.58	1.40	1.45
20	2	306	CLA	C1B-NB	-2.58	1.34	1.37
23	A	818	BCR	C8-C9	-2.58	1.40	1.45
20	B	820	CLA	C1D-C2D	2.58	1.50	1.45
20	1	307	CLA	MG-NA	-2.58	2.00	2.06
20	A	851	CLA	C1B-NB	-2.58	1.34	1.37
20	2	307	CLA	C3B-C4B	2.58	1.48	1.42
20	A	804	CLA	C4B-NB	-2.58	1.34	1.37
20	A	847	CLA	C1B-NB	-2.58	1.34	1.37
20	B	805	CLA	C1B-NB	-2.58	1.34	1.37
20	1	321	CLA	C3B-C4B	2.58	1.48	1.42
23	A	816	BCR	C23-C22	-2.58	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	847	CLA	C1B-NB	-2.57	1.34	1.37
20	B	828	CLA	C1B-NB	-2.57	1.34	1.37
20	1	321	CLA	C1D-C2D	2.57	1.50	1.45
20	2	317	CLA	MG-NA	-2.57	2.00	2.06
21	3	301	LUT	C12-C13	-2.57	1.40	1.45
20	A	850	CLA	C3B-C4B	2.57	1.48	1.42
20	B	844	CLA	CHD-C1D	2.57	1.43	1.38
23	A	815	BCR	C23-C22	-2.57	1.40	1.45
20	1	318	CLA	MG-NA	-2.57	2.00	2.06
20	2	319	CLA	C1B-C2B	2.57	1.49	1.43
20	B	850	CLA	C1B-NB	-2.57	1.34	1.37
20	4	302	CLA	C1B-C2B	2.57	1.49	1.43
20	A	856	CLA	C1B-C2B	2.57	1.49	1.43
23	A	857	BCR	C23-C22	-2.57	1.40	1.45
20	A	851	CLA	CHD-C1D	2.57	1.43	1.38
20	A	835	CLA	C1B-NB	-2.57	1.34	1.37
20	2	319	CLA	MG-NA	-2.57	2.00	2.06
20	B	853	CLA	MG-NA	-2.57	2.00	2.06
20	4	312	CLA	MG-NA	-2.57	2.00	2.06
20	G	206	CLA	MG-NA	-2.57	2.00	2.06
20	2	321	CLA	C1B-C2B	2.57	1.49	1.43
20	A	848	CLA	MG-NA	-2.57	2.00	2.06
20	B	826	CLA	C3B-C4B	2.57	1.48	1.42
23	B	838	BCR	C23-C22	-2.57	1.40	1.45
20	1	302	CLA	C1C-C2C	2.57	1.49	1.44
20	4	310	CLA	C1D-C2D	2.57	1.50	1.45
20	3	307	CLA	MG-NA	-2.56	2.00	2.06
23	F	301	BCR	C8-C9	-2.56	1.40	1.45
20	A	805	CLA	C1D-C2D	2.56	1.50	1.45
20	A	803	CLA	C1B-NB	-2.56	1.34	1.37
20	A	837	CLA	C1B-NB	-2.56	1.34	1.37
20	B	816	CLA	C1B-NB	-2.56	1.34	1.37
20	B	853	CLA	C3B-C4B	2.56	1.48	1.42
20	B	845	CLA	C3B-C4B	2.56	1.48	1.42
20	1	321	CLA	MG-NA	-2.56	2.00	2.06
20	B	809	CLA	MG-NA	-2.56	2.00	2.06
20	3	309	CLA	C4B-NB	-2.56	1.34	1.37
20	K	205	CLA	MG-NA	-2.56	2.00	2.06
20	3	309	CLA	C1B-NB	-2.56	1.34	1.37
20	B	822	CLA	C3B-C4B	2.56	1.48	1.42
20	3	311	CLA	C1D-C2D	2.56	1.50	1.45
20	A	852	CLA	C1D-C2D	2.56	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	1	312	BCR	C8-C9	-2.56	1.40	1.45
20	1	309	CLA	MG-NA	-2.56	2.00	2.06
20	A	830	CLA	C1B-C2B	2.55	1.49	1.43
20	4	313	CLA	MG-NA	-2.55	2.00	2.06
20	G	207	CLA	C3B-C4B	2.55	1.48	1.42
19	2	309	CHL	C3B-C4B	2.55	1.48	1.42
20	1	321	CLA	C1B-C2B	2.55	1.49	1.43
20	2	320	CLA	C1D-C2D	2.55	1.50	1.45
20	2	320	CLA	C3B-C4B	2.55	1.48	1.42
20	L	307	CLA	C3B-C4B	2.55	1.48	1.42
20	A	850	CLA	C1D-C2D	2.55	1.50	1.45
20	A	839	CLA	C1B-C2B	2.55	1.49	1.43
20	B	823	CLA	C1B-C2B	2.55	1.49	1.43
20	F	306	CLA	C1B-NB	-2.55	1.34	1.37
20	B	813	CLA	C1C-C2C	2.55	1.49	1.44
20	A	837	CLA	MG-NA	-2.55	2.00	2.06
20	2	308	CLA	C1B-NB	-2.55	1.34	1.37
20	2	303	CLA	MG-NA	-2.55	2.00	2.06
20	A	855	CLA	C1D-C2D	2.55	1.50	1.45
20	1	320	CLA	MG-NA	-2.55	2.00	2.06
20	4	303	CLA	C1D-C2D	2.54	1.50	1.45
20	4	308	CLA	MG-NA	-2.54	2.00	2.06
20	A	834	CLA	C1B-C2B	2.54	1.49	1.43
20	F	304	CLA	C1C-C2C	2.54	1.49	1.44
20	A	837	CLA	C1D-C2D	2.54	1.50	1.45
20	A	837	CLA	C1C-C2C	2.54	1.49	1.44
20	A	833	CLA	C3B-C4B	2.54	1.48	1.42
20	A	806	CLA	MG-NA	-2.54	2.00	2.06
20	G	205	CLA	C3B-C4B	2.54	1.48	1.42
20	G	207	CLA	MG-NA	-2.54	2.00	2.06
19	2	301	CHL	C3B-C4B	2.54	1.48	1.42
20	4	316	CLA	C1C-C2C	2.54	1.49	1.44
21	1	310	LUT	C28-C29	-2.54	1.40	1.45
20	B	828	CLA	CHD-C1D	2.54	1.43	1.38
20	B	848	CLA	CHD-C1D	2.54	1.43	1.38
20	A	807	CLA	MG-NA	-2.54	2.00	2.06
20	A	827	CLA	C3B-C4B	2.54	1.48	1.42
20	4	312	CLA	C1D-C2D	2.54	1.50	1.45
20	1	302	CLA	C1D-C2D	2.54	1.50	1.45
20	1	321	CLA	C1B-NB	-2.54	1.34	1.37
20	A	847	CLA	MG-NA	-2.54	2.00	2.06
20	1	302	CLA	MG-NA	-2.54	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	822	CLA	MG-NA	-2.54	2.00	2.06
20	2	305	CLA	C1B-NB	-2.54	1.34	1.37
20	3	316	CLA	C1B-NB	-2.54	1.34	1.37
20	H	201	CLA	C1B-NB	-2.54	1.34	1.37
20	3	316	CLA	MG-NA	-2.53	2.00	2.06
20	B	825	CLA	MG-NA	-2.53	2.00	2.06
20	B	805	CLA	C3B-C4B	2.53	1.48	1.42
20	4	311	CLA	C1B-NB	-2.53	1.34	1.37
20	L	305	CLA	C1B-NB	-2.53	1.34	1.37
20	A	829	CLA	C4B-NB	-2.53	1.34	1.37
20	3	307	CLA	C4C-C3C	2.53	1.49	1.45
20	4	308	CLA	C1B-C2B	2.53	1.49	1.43
20	F	306	CLA	MG-NA	-2.53	2.00	2.06
20	3	318	CLA	MG-NA	-2.53	2.00	2.06
23	L	302	BCR	C12-C13	-2.53	1.40	1.45
20	A	834	CLA	C1B-NB	-2.53	1.34	1.37
20	1	305	CLA	C1C-C2C	2.53	1.49	1.44
20	A	836	CLA	C1B-NB	-2.53	1.34	1.37
19	4	306	CHL	C3B-C4B	2.53	1.48	1.42
20	A	804	CLA	C1D-C2D	2.53	1.50	1.45
20	4	303	CLA	C1B-NB	-2.53	1.34	1.37
20	4	311	CLA	C4B-NB	-2.52	1.34	1.37
20	L	306	CLA	C1B-C2B	2.52	1.49	1.43
20	F	306	CLA	C1C-C2C	2.52	1.49	1.44
20	4	316	CLA	C1D-C2D	2.52	1.50	1.45
20	G	207	CLA	C1B-C2B	2.52	1.49	1.43
20	N	202	CLA	C1B-NB	-2.52	1.34	1.37
20	2	320	CLA	MG-NB	-2.52	2.00	2.05
20	3	317	CLA	MG-NA	-2.52	2.00	2.06
20	A	827	CLA	C1B-NB	-2.52	1.34	1.37
19	1	301	CHL	C1B-C2B	2.52	1.49	1.43
20	2	317	CLA	C1B-NB	-2.52	1.34	1.37
20	B	805	CLA	C1D-C2D	2.52	1.50	1.45
20	1	303	CLA	C1C-C2C	2.52	1.49	1.44
20	K	203	CLA	MG-NA	-2.52	2.00	2.06
19	4	307	CHL	C3B-C4B	2.52	1.48	1.42
20	B	844	CLA	C1B-NB	-2.52	1.34	1.37
20	B	825	CLA	C1B-NB	-2.52	1.34	1.37
20	F	304	CLA	C1B-NB	-2.52	1.34	1.37
20	1	305	CLA	MG-NA	-2.51	2.00	2.06
20	4	303	CLA	C4B-NB	-2.51	1.34	1.37
20	B	804	CLA	C1B-C2B	2.51	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	802	CLA	MG-NA	-2.51	2.00	2.06
20	4	312	CLA	C1B-C2B	2.51	1.49	1.43
20	3	319	CLA	MG-NA	-2.51	2.00	2.06
20	1	322	CLA	C1B-NB	-2.51	1.34	1.37
20	A	853	CLA	MG-NA	-2.51	2.00	2.06
19	2	301	CHL	C1B-C2B	2.51	1.49	1.43
20	A	849	CLA	MG-NA	-2.51	2.00	2.06
21	3	301	LUT	C28-C29	-2.51	1.40	1.45
20	1	319	CLA	C1B-NB	-2.51	1.34	1.37
20	B	826	CLA	C1B-C2B	2.51	1.49	1.43
20	2	308	CLA	MG-NA	-2.51	2.00	2.06
20	B	847	CLA	CHD-C1D	2.51	1.43	1.38
20	B	801	CLA	C1B-C2B	2.51	1.49	1.43
20	3	316	CLA	C1C-C2C	2.51	1.49	1.44
20	2	304	CLA	C1B-C2B	2.51	1.49	1.43
20	A	831	CLA	C4C-C3C	2.51	1.49	1.45
20	B	823	CLA	C1D-C2D	2.50	1.50	1.45
20	B	817	CLA	C1B-C2B	2.50	1.49	1.43
20	A	845	CLA	C1B-NB	-2.50	1.34	1.37
20	A	856	CLA	C3B-C4B	2.50	1.48	1.42
20	A	851	CLA	C1C-C2C	2.50	1.49	1.44
20	3	316	CLA	C1D-C2D	2.50	1.50	1.45
20	3	315	CLA	C1B-C2B	2.50	1.49	1.43
20	B	845	CLA	C1B-NB	-2.50	1.34	1.37
20	1	320	CLA	C1B-NB	-2.50	1.34	1.37
21	2	310	LUT	C32-C33	-2.50	1.40	1.45
20	B	830	CLA	C1B-NB	-2.50	1.34	1.37
20	B	828	CLA	C1D-C2D	2.50	1.50	1.45
20	O	207	CLA	MG-NA	-2.50	2.00	2.06
20	1	306	CLA	C1C-C2C	2.50	1.49	1.44
20	A	812	CLA	OBD-CAD	2.50	1.26	1.22
20	2	320	CLA	C1B-C2B	2.50	1.49	1.43
23	B	837	BCR	C19-C18	-2.50	1.40	1.45
20	A	850	CLA	C1B-NB	-2.50	1.34	1.37
20	2	320	CLA	CHD-C1D	2.50	1.43	1.38
23	2	312	BCR	C8-C9	-2.49	1.40	1.45
20	G	206	CLA	C1C-C2C	2.49	1.49	1.44
20	A	852	CLA	C1B-C2B	2.49	1.49	1.43
20	A	842	CLA	C1C-C2C	2.49	1.49	1.44
20	A	844	CLA	C1B-NB	-2.49	1.34	1.37
20	A	834	CLA	MG-NA	-2.49	2.00	2.06
20	3	314	CLA	C4B-NB	-2.49	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	O	207	CLA	C1B-NB	-2.49	1.34	1.37
19	4	315	CHL	C3B-C4B	2.49	1.48	1.42
20	B	846	CLA	C1B-NB	-2.49	1.34	1.37
19	4	305	CHL	C3B-C4B	2.48	1.48	1.42
20	2	319	CLA	C1C-C2C	2.48	1.49	1.44
19	4	315	CHL	C1B-C2B	2.48	1.49	1.43
19	3	313	CHL	C1B-C2B	2.48	1.49	1.43
20	L	306	CLA	C3B-C4B	2.48	1.48	1.42
21	3	301	LUT	C32-C33	-2.48	1.40	1.45
20	B	820	CLA	C1B-C2B	2.48	1.49	1.43
20	1	306	CLA	C1B-NB	-2.48	1.34	1.37
20	A	801	CLA	C1D-C2D	2.48	1.50	1.45
23	K	202	BCR	C8-C9	-2.48	1.40	1.45
20	B	826	CLA	C1C-C2C	2.47	1.49	1.44
20	2	304	CLA	C3B-C4B	2.47	1.48	1.42
23	A	817	BCR	C19-C18	-2.47	1.40	1.45
20	A	828	CLA	MG-NA	-2.47	2.00	2.06
20	B	819	CLA	CHC-C4B	2.47	1.44	1.39
20	1	303	CLA	C1B-NB	-2.47	1.34	1.37
20	A	831	CLA	C4B-NB	-2.47	1.34	1.37
20	A	831	CLA	MG-NA	-2.47	2.00	2.06
20	A	812	CLA	C1C-C2C	2.47	1.49	1.44
20	3	307	CLA	C1B-C2B	2.47	1.49	1.43
20	A	833	CLA	C1B-C2B	2.47	1.49	1.43
20	B	849	CLA	C4B-NB	-2.47	1.34	1.37
20	A	808	CLA	C1B-NB	-2.47	1.34	1.37
20	A	811	CLA	C1B-NB	-2.47	1.34	1.37
20	B	806	CLA	C1B-NB	-2.47	1.34	1.37
20	3	315	CLA	C1B-NB	-2.47	1.34	1.37
20	B	851	CLA	C1B-C2B	2.46	1.49	1.43
23	J	101	BCR	C23-C22	-2.46	1.40	1.45
20	4	310	CLA	C1B-NB	-2.46	1.34	1.37
20	B	829	CLA	C1B-NB	-2.46	1.34	1.37
19	2	318	CHL	C1B-C2B	2.46	1.49	1.43
20	3	314	CLA	C1B-NB	-2.46	1.34	1.37
19	2	322	CHL	C1B-C2B	2.46	1.49	1.43
20	3	310	CLA	C3B-C4B	2.46	1.48	1.42
20	3	308	CLA	C1C-C2C	2.46	1.49	1.44
20	3	318	CLA	C1C-C2C	2.46	1.49	1.44
20	3	319	CLA	C4C-C3C	2.46	1.49	1.45
20	A	832	CLA	C1C-C2C	2.46	1.49	1.44
20	B	812	CLA	C3B-C4B	2.46	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	813	CLA	C4B-NB	-2.46	1.34	1.37
20	A	840	CLA	MG-NA	-2.46	2.00	2.06
20	A	842	CLA	C1B-NB	-2.45	1.34	1.37
20	K	205	CLA	C1D-C2D	2.45	1.50	1.45
20	B	833	CLA	C1B-NB	-2.45	1.34	1.37
20	B	806	CLA	MG-NA	-2.45	2.00	2.06
19	1	301	CHL	C4C-C3C	2.45	1.49	1.45
20	2	306	CLA	C1C-C2C	2.45	1.49	1.44
20	A	807	CLA	C1C-C2C	2.45	1.49	1.44
19	2	318	CHL	C3B-C4B	2.45	1.48	1.42
20	K	205	CLA	C1B-NB	-2.45	1.34	1.37
20	3	317	CLA	C1C-C2C	2.45	1.49	1.44
20	3	319	CLA	C4B-NB	-2.45	1.34	1.37
23	F	302	BCR	C19-C18	-2.45	1.40	1.45
19	1	317	CHL	C3B-C4B	2.44	1.48	1.42
20	A	830	CLA	C3B-C4B	2.44	1.48	1.42
20	2	303	CLA	C1D-C2D	2.44	1.50	1.45
20	A	841	CLA	C1C-C2C	2.44	1.49	1.44
20	B	824	CLA	C1C-C2C	2.44	1.49	1.44
20	4	310	CLA	C4B-NB	-2.44	1.34	1.37
20	B	818	CLA	C4B-NB	-2.44	1.34	1.37
20	4	312	CLA	C1C-C2C	2.44	1.49	1.44
20	B	816	CLA	C3B-C4B	2.44	1.48	1.42
20	B	829	CLA	C1C-C2C	2.44	1.49	1.44
20	A	831	CLA	C1C-C2C	2.44	1.49	1.44
20	B	815	CLA	C1B-C2B	2.44	1.49	1.43
20	B	821	CLA	C1C-C2C	2.44	1.49	1.44
23	B	838	BCR	C12-C13	-2.44	1.40	1.45
20	B	817	CLA	C1B-NB	-2.44	1.34	1.37
20	A	849	CLA	C3B-C4B	2.43	1.48	1.42
20	2	307	CLA	C1B-NB	-2.43	1.34	1.37
20	A	841	CLA	MG-NA	-2.43	2.00	2.06
20	A	801	CLA	MG-NA	-2.43	2.00	2.06
20	A	850	CLA	C1C-C2C	2.43	1.49	1.44
20	4	314	CLA	C1B-NB	-2.43	1.34	1.37
20	O	207	CLA	C1C-C2C	2.43	1.49	1.44
20	2	317	CLA	C1C-C2C	2.43	1.49	1.44
20	B	810	CLA	C1D-C2D	2.43	1.50	1.45
20	2	319	CLA	C1B-NB	-2.43	1.34	1.37
20	G	205	CLA	C1B-NB	-2.43	1.34	1.37
20	3	317	CLA	C1B-NB	-2.43	1.34	1.37
20	1	307	CLA	C1C-C2C	2.43	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	303	CLA	C1C-C2C	2.43	1.49	1.44
20	B	804	CLA	C1D-C2D	2.43	1.50	1.45
23	3	303	BCR	C12-C13	-2.43	1.40	1.45
20	A	843	CLA	C3B-C4B	2.43	1.48	1.42
20	A	853	CLA	C1C-C2C	2.43	1.49	1.44
20	A	849	CLA	CHD-C1D	2.43	1.43	1.38
23	L	303	BCR	C23-C22	-2.43	1.40	1.45
19	1	317	CHL	C1B-C2B	2.42	1.49	1.43
20	1	320	CLA	C1C-C2C	2.42	1.49	1.44
20	3	311	CLA	C1B-NB	-2.42	1.34	1.37
20	1	309	CLA	C1C-C2C	2.42	1.49	1.44
20	B	847	CLA	C1C-C2C	2.42	1.49	1.44
20	B	846	CLA	C1B-C2B	2.42	1.49	1.43
20	1	309	CLA	C1B-NB	-2.42	1.34	1.37
20	4	304	CLA	C1B-NB	-2.42	1.34	1.37
20	B	851	CLA	C1D-C2D	2.42	1.50	1.45
23	I	102	BCR	C12-C13	-2.42	1.40	1.45
20	B	814	CLA	C1C-C2C	2.42	1.49	1.44
20	A	825	CLA	C1C-C2C	2.42	1.49	1.44
20	1	303	CLA	C1D-C2D	2.42	1.50	1.45
20	B	802	CLA	C4C-C3C	2.42	1.49	1.45
28	A	824	CL0	C1D-C2D	2.42	1.50	1.45
20	2	323	CLA	MG-NA	-2.42	2.00	2.06
20	B	824	CLA	C1B-NB	-2.41	1.34	1.37
20	B	828	CLA	C1C-C2C	2.41	1.49	1.44
20	A	840	CLA	C4C-C3C	2.41	1.49	1.45
19	3	313	CHL	C3B-C4B	2.41	1.48	1.42
20	A	850	CLA	C1B-C2B	2.41	1.48	1.43
20	G	206	CLA	C1B-C2B	2.41	1.48	1.43
20	B	815	CLA	C1B-NB	-2.41	1.34	1.37
20	2	323	CLA	C4B-NB	-2.41	1.34	1.37
20	B	811	CLA	C1C-C2C	2.41	1.49	1.44
21	2	310	LUT	C12-C13	-2.41	1.40	1.45
20	J	103	CLA	C1B-NB	-2.41	1.34	1.37
20	F	304	CLA	C1D-C2D	2.41	1.50	1.45
20	1	304	CLA	C1B-NB	-2.41	1.34	1.37
20	A	843	CLA	C4C-C3C	2.40	1.49	1.45
20	4	313	CLA	C1C-C2C	2.40	1.49	1.44
20	B	825	CLA	C1C-C2C	2.40	1.49	1.44
20	2	320	CLA	C4D-ND	2.40	1.41	1.37
20	B	807	CLA	C1B-NB	-2.40	1.34	1.37
20	A	826	CLA	CHB-C4A	-2.40	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	312	CLA	C4B-NB	-2.40	1.34	1.37
20	B	850	CLA	C1B-C2B	2.40	1.48	1.43
20	2	308	CLA	C1C-C2C	2.40	1.49	1.44
20	A	838	CLA	C3B-C4B	2.40	1.48	1.42
20	B	801	CLA	C3B-C4B	2.40	1.48	1.42
20	A	855	CLA	C1B-C2B	2.40	1.48	1.43
20	A	808	CLA	C1C-C2C	2.40	1.49	1.44
20	1	307	CLA	C1B-NB	-2.40	1.34	1.37
20	B	821	CLA	MG-NA	-2.40	2.00	2.06
20	4	310	CLA	C1C-C2C	2.40	1.49	1.44
20	A	851	CLA	C1B-C2B	2.40	1.48	1.43
20	4	304	CLA	C1B-C2B	2.39	1.48	1.43
20	2	323	CLA	C1C-C2C	2.39	1.49	1.44
20	B	831	CLA	C1C-C2C	2.39	1.49	1.44
20	A	840	CLA	C4B-NB	-2.39	1.34	1.37
20	J	103	CLA	C1C-C2C	2.39	1.49	1.44
20	3	316	CLA	C4B-NB	-2.39	1.34	1.37
21	2	310	LUT	C28-C29	-2.39	1.40	1.45
23	J	101	BCR	C12-C13	-2.39	1.40	1.45
20	1	318	CLA	C1C-C2C	2.39	1.49	1.44
20	B	804	CLA	C3B-C4B	2.39	1.48	1.42
23	B	834	BCR	C23-C22	-2.39	1.40	1.45
20	A	809	CLA	C4B-NB	-2.39	1.34	1.37
20	B	848	CLA	C1C-C2C	2.39	1.49	1.44
20	A	847	CLA	C1C-C2C	2.39	1.49	1.44
20	1	322	CLA	C4B-NB	-2.38	1.34	1.37
20	A	855	CLA	C1B-NB	-2.38	1.34	1.37
20	3	311	CLA	C3B-C4B	2.38	1.48	1.42
20	B	817	CLA	CHD-C1D	2.38	1.43	1.38
20	3	312	CLA	C1B-NB	-2.38	1.34	1.37
20	A	807	CLA	C1B-NB	-2.38	1.34	1.37
20	1	319	CLA	C1B-C2B	2.38	1.48	1.43
23	3	303	BCR	C19-C18	-2.38	1.40	1.45
19	4	306	CHL	C1B-C2B	2.38	1.48	1.43
20	3	310	CLA	C1B-NB	-2.38	1.34	1.37
20	K	206	CLA	C1B-NB	-2.38	1.34	1.37
20	B	848	CLA	C1D-C2D	2.38	1.50	1.45
23	L	302	BCR	C23-C22	-2.38	1.40	1.45
20	A	828	CLA	C1B-C2B	2.38	1.48	1.43
20	B	845	CLA	C1B-C2B	2.38	1.48	1.43
20	A	831	CLA	C1B-NB	-2.38	1.34	1.37
20	B	818	CLA	C1C-C2C	2.38	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	820	CLA	C4C-C3C	2.38	1.49	1.45
20	B	829	CLA	C4B-NB	-2.38	1.34	1.37
20	B	826	CLA	C1D-C2D	2.37	1.50	1.45
20	A	826	CLA	C1D-C2D	2.37	1.50	1.45
20	A	835	CLA	C1C-C2C	2.37	1.49	1.44
20	B	831	CLA	C1D-C2D	2.37	1.50	1.45
20	1	305	CLA	C1B-NB	-2.37	1.34	1.37
20	1	305	CLA	C4B-NB	-2.37	1.34	1.37
20	A	802	CLA	C3B-C4B	2.37	1.48	1.42
20	1	318	CLA	C1B-C2B	2.37	1.48	1.43
19	2	302	CHL	C3B-C4B	2.37	1.48	1.42
20	3	307	CLA	C1B-NB	-2.37	1.34	1.37
20	4	316	CLA	MG-NA	-2.37	2.00	2.06
20	3	320	CLA	MG-NA	-2.37	2.00	2.06
20	A	806	CLA	C1B-NB	-2.37	1.34	1.37
20	2	304	CLA	C1C-C2C	2.37	1.49	1.44
20	L	307	CLA	C1B-NB	-2.37	1.34	1.37
20	4	302	CLA	C1C-C2C	2.37	1.49	1.44
20	F	304	CLA	C4B-NB	-2.36	1.34	1.37
20	A	844	CLA	C1B-C2B	2.36	1.48	1.43
28	A	824	CL0	C1B-C2B	2.36	1.48	1.43
20	3	314	CLA	C1C-C2C	2.36	1.49	1.44
20	1	318	CLA	C4C-C3C	2.36	1.49	1.45
20	A	803	CLA	C1C-C2C	2.36	1.49	1.44
20	G	207	CLA	C1B-NB	-2.36	1.34	1.37
20	A	806	CLA	C4C-C3C	2.36	1.49	1.45
20	G	207	CLA	C1C-C2C	2.35	1.49	1.44
20	B	814	CLA	C1B-C2B	2.35	1.48	1.43
20	H	201	CLA	C4B-NB	-2.35	1.34	1.37
20	A	802	CLA	C1B-C2B	2.35	1.48	1.43
20	B	804	CLA	C1B-NB	-2.35	1.34	1.37
20	B	823	CLA	MG-NA	-2.35	2.00	2.06
20	B	818	CLA	C1D-C2D	2.35	1.50	1.45
20	A	848	CLA	C1C-C2C	2.35	1.49	1.44
20	4	313	CLA	C1B-NB	-2.35	1.34	1.37
20	L	306	CLA	C1B-NB	-2.35	1.34	1.37
20	O	206	CLA	C1B-NB	-2.35	1.34	1.37
20	4	311	CLA	C1C-C2C	2.35	1.49	1.44
20	B	827	CLA	C1B-NB	-2.35	1.34	1.37
20	K	204	CLA	C1B-NB	-2.35	1.34	1.37
20	B	812	CLA	MG-NA	-2.35	2.00	2.06
20	A	848	CLA	C4C-C3C	2.34	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	308	CLA	C1C-C2C	2.34	1.49	1.44
20	B	812	CLA	C1C-C2C	2.34	1.49	1.44
20	A	844	CLA	C3B-C4B	2.34	1.48	1.42
20	B	812	CLA	C1B-C2B	2.34	1.48	1.43
20	B	844	CLA	C3B-C4B	2.34	1.48	1.42
19	2	302	CHL	C1B-C2B	2.34	1.48	1.43
20	A	848	CLA	C1D-C2D	2.34	1.49	1.45
20	1	306	CLA	C4B-NB	-2.34	1.34	1.37
20	A	849	CLA	C1C-C2C	2.34	1.49	1.44
20	A	808	CLA	C3B-C4B	2.34	1.48	1.42
20	2	320	CLA	C1C-C2C	2.34	1.49	1.44
20	3	314	CLA	C1D-C2D	2.34	1.49	1.45
20	K	203	CLA	C1B-NB	-2.34	1.34	1.37
20	K	206	CLA	C1C-C2C	2.34	1.49	1.44
20	4	308	CLA	C4C-C3C	2.33	1.49	1.45
20	B	815	CLA	C1C-C2C	2.33	1.49	1.44
20	A	852	CLA	C1B-NB	-2.33	1.34	1.37
20	B	833	CLA	C1C-C2C	2.33	1.49	1.44
19	2	301	CHL	C4C-C3C	2.33	1.49	1.45
23	F	301	BCR	C23-C22	-2.33	1.40	1.45
20	B	833	CLA	C4C-C3C	2.33	1.49	1.45
20	3	315	CLA	C1C-C2C	2.33	1.49	1.44
20	B	846	CLA	C1C-C2C	2.33	1.49	1.44
20	B	831	CLA	C4B-NB	-2.33	1.34	1.37
20	K	203	CLA	C1C-C2C	2.33	1.49	1.44
20	3	318	CLA	C1B-NB	-2.33	1.34	1.37
20	B	808	CLA	C4B-NB	-2.33	1.34	1.37
20	A	828	CLA	C1B-NB	-2.33	1.34	1.37
20	A	836	CLA	C4B-NB	-2.32	1.34	1.37
20	2	320	CLA	C3B-C2B	2.32	1.49	1.41
20	B	807	CLA	C1C-C2C	2.32	1.49	1.44
20	B	801	CLA	C1B-NB	-2.32	1.34	1.37
20	B	804	CLA	MG-NA	-2.32	2.00	2.06
20	1	318	CLA	C1B-NB	-2.32	1.34	1.37
20	A	830	CLA	C1D-C2D	2.32	1.49	1.45
20	B	808	CLA	C1B-C2B	2.32	1.48	1.43
23	A	816	BCR	C8-C9	-2.32	1.41	1.45
23	O	202	BCR	C8-C9	-2.32	1.41	1.45
20	B	809	CLA	C1C-C2C	2.32	1.49	1.44
19	4	305	CHL	C1B-C2B	2.32	1.48	1.43
20	B	833	CLA	C4B-NB	-2.32	1.34	1.37
20	4	303	CLA	C1C-C2C	2.32	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	321	CLA	C1B-NB	-2.32	1.34	1.37
20	B	849	CLA	C1B-NB	-2.32	1.34	1.37
20	B	849	CLA	C1C-C2C	2.32	1.49	1.44
20	B	830	CLA	C4C-C3C	2.31	1.49	1.45
20	4	316	CLA	C1B-C2B	2.31	1.48	1.43
20	K	204	CLA	C1C-C2C	2.31	1.49	1.44
20	4	308	CLA	C3B-C4B	2.31	1.48	1.42
20	L	305	CLA	C1B-C2B	2.31	1.48	1.43
23	A	818	BCR	C12-C13	-2.31	1.41	1.45
20	A	853	CLA	C3B-C4B	2.31	1.48	1.42
20	1	309	CLA	C1B-C2B	2.31	1.48	1.43
20	A	831	CLA	C1B-C2B	2.31	1.48	1.43
20	L	306	CLA	C1C-C2C	2.31	1.49	1.44
19	4	306	CHL	C4C-C3C	2.31	1.49	1.45
20	B	811	CLA	C1B-NB	-2.31	1.34	1.37
20	B	810	CLA	C1C-C2C	2.31	1.49	1.44
20	G	206	CLA	C4B-NB	-2.31	1.34	1.37
20	2	306	CLA	C4B-NB	-2.31	1.34	1.37
20	3	308	CLA	C1B-NB	-2.30	1.35	1.37
20	F	305	CLA	C4B-NB	-2.30	1.35	1.37
20	A	853	CLA	C1B-C2B	2.30	1.48	1.43
20	A	807	CLA	C4B-NB	-2.30	1.35	1.37
20	2	305	CLA	C1C-C2C	2.30	1.49	1.44
20	2	307	CLA	C4C-C3C	2.30	1.49	1.45
20	1	303	CLA	C1B-C2B	2.30	1.48	1.43
20	B	852	CLA	C1C-C2C	2.30	1.49	1.44
20	J	103	CLA	C1B-C2B	2.30	1.48	1.43
19	2	302	CHL	C4C-C3C	2.30	1.49	1.45
23	L	303	BCR	C8-C9	-2.30	1.41	1.45
20	B	827	CLA	C1C-C2C	2.30	1.49	1.44
20	G	205	CLA	C1C-C2C	2.30	1.49	1.44
20	B	801	CLA	C1C-C2C	2.30	1.49	1.44
20	B	804	CLA	C1C-C2C	2.30	1.49	1.44
20	B	825	CLA	C4B-NB	-2.30	1.35	1.37
20	O	207	CLA	C4B-NB	-2.30	1.35	1.37
20	B	809	CLA	C4B-NB	-2.29	1.35	1.37
20	A	811	CLA	C1C-C2C	2.29	1.49	1.44
20	A	843	CLA	C1B-C2B	2.29	1.48	1.43
20	3	320	CLA	C1C-C2C	2.29	1.49	1.44
20	1	303	CLA	C4B-NB	-2.29	1.35	1.37
20	1	320	CLA	C4B-NB	-2.29	1.35	1.37
20	A	828	CLA	C1C-C2C	2.29	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	N	202	CLA	C4B-NB	-2.29	1.35	1.37
20	L	305	CLA	C1C-C2C	2.29	1.49	1.44
20	A	832	CLA	C4B-NB	-2.29	1.35	1.37
20	A	839	CLA	C1B-NB	-2.29	1.35	1.37
20	3	310	CLA	C4C-C3C	2.29	1.49	1.45
23	B	834	BCR	C8-C9	-2.29	1.41	1.45
19	1	317	CHL	C4C-C3C	2.29	1.49	1.45
20	2	307	CLA	C1C-C2C	2.29	1.49	1.44
20	3	312	CLA	C1C-C2C	2.29	1.49	1.44
20	B	827	CLA	C4B-NB	-2.29	1.35	1.37
20	B	802	CLA	C4B-NB	-2.29	1.35	1.37
20	F	306	CLA	C1D-C2D	2.29	1.49	1.45
20	1	322	CLA	C1C-C2C	2.28	1.49	1.44
20	2	306	CLA	C1B-C2B	2.28	1.48	1.43
20	B	817	CLA	C1D-C2D	2.28	1.49	1.45
20	B	824	CLA	C4B-NB	-2.28	1.35	1.37
20	3	318	CLA	C1B-C2B	2.28	1.48	1.43
20	4	312	CLA	C1B-NB	-2.28	1.35	1.37
20	B	828	CLA	C4B-NB	-2.28	1.35	1.37
20	A	846	CLA	C4B-NB	-2.28	1.35	1.37
20	A	845	CLA	C4C-C3C	2.28	1.49	1.45
20	B	833	CLA	C1B-C2B	2.28	1.48	1.43
20	4	316	CLA	C4B-NB	-2.28	1.35	1.37
20	4	314	CLA	C1B-C2B	2.28	1.48	1.43
23	B	836	BCR	C23-C22	-2.28	1.41	1.45
20	4	302	CLA	C3B-C2B	2.27	1.48	1.41
20	A	840	CLA	C1C-C2C	2.27	1.49	1.44
20	4	304	CLA	C1C-C2C	2.27	1.49	1.44
20	A	834	CLA	C1C-C2C	2.27	1.49	1.44
20	B	811	CLA	C1B-C2B	2.27	1.48	1.43
20	3	317	CLA	C1B-C2B	2.27	1.48	1.43
20	B	853	CLA	C4C-C3C	2.27	1.49	1.45
23	4	319	BCR	C8-C9	-2.27	1.41	1.45
23	B	835	BCR	C23-C22	-2.27	1.41	1.45
20	B	826	CLA	C1B-NB	-2.27	1.35	1.37
20	4	310	CLA	C1B-C2B	2.27	1.48	1.43
20	B	822	CLA	C1C-C2C	2.27	1.49	1.44
20	4	313	CLA	C4C-C3C	2.27	1.48	1.45
20	B	823	CLA	C1C-C2C	2.27	1.49	1.44
20	3	317	CLA	C4B-NB	-2.27	1.35	1.37
20	A	841	CLA	C1B-NB	-2.27	1.35	1.37
20	B	819	CLA	C1D-C2D	2.26	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	319	CLA	C1C-C2C	2.26	1.48	1.44
20	H	201	CLA	C1C-C2C	2.26	1.48	1.44
20	B	853	CLA	C1B-NB	-2.26	1.35	1.37
20	B	852	CLA	C4C-C3C	2.26	1.48	1.45
20	N	202	CLA	C1C-C2C	2.26	1.48	1.44
20	B	849	CLA	C1B-C2B	2.26	1.48	1.43
20	B	807	CLA	C4C-C3C	2.26	1.48	1.45
20	B	803	CLA	C1C-C2C	2.26	1.48	1.44
20	4	314	CLA	C1C-C2C	2.26	1.48	1.44
20	O	206	CLA	C4C-C3C	2.26	1.48	1.45
20	A	838	CLA	MG-NA	-2.25	2.00	2.06
20	F	305	CLA	C1C-C2C	2.25	1.48	1.44
20	A	806	CLA	C4B-NB	-2.25	1.35	1.37
20	B	820	CLA	C1C-C2C	2.25	1.48	1.44
20	A	837	CLA	C4C-C3C	2.25	1.48	1.45
20	2	305	CLA	C4C-C3C	2.25	1.48	1.45
20	2	303	CLA	C4B-NB	-2.25	1.35	1.37
20	A	851	CLA	C1D-C2D	2.25	1.49	1.45
20	B	805	CLA	C1C-C2C	2.25	1.48	1.44
20	A	839	CLA	C4C-C3C	2.25	1.48	1.45
20	4	304	CLA	C4C-C3C	2.25	1.48	1.45
20	4	313	CLA	C1B-C2B	2.25	1.48	1.43
20	B	821	CLA	C4B-NB	-2.25	1.35	1.37
19	4	307	CHL	C1B-C2B	2.25	1.48	1.43
20	O	207	CLA	C4C-C3C	2.25	1.48	1.45
20	B	810	CLA	C4B-NB	-2.25	1.35	1.37
20	1	322	CLA	C4C-C3C	2.25	1.48	1.45
20	1	302	CLA	C1B-C2B	2.24	1.48	1.43
20	3	316	CLA	C1B-C2B	2.24	1.48	1.43
19	1	301	CHL	C3B-C4B	2.24	1.48	1.42
20	N	202	CLA	C1B-C2B	2.24	1.48	1.43
20	A	805	CLA	C1B-NB	-2.24	1.35	1.37
20	3	307	CLA	C1C-C2C	2.24	1.48	1.44
20	O	206	CLA	C1C-C2C	2.24	1.48	1.44
20	3	310	CLA	C1C-C2C	2.24	1.48	1.44
20	B	828	CLA	C1B-C2B	2.24	1.48	1.43
20	B	819	CLA	C4C-C3C	2.24	1.48	1.45
20	A	856	CLA	C1B-NB	-2.24	1.35	1.37
20	A	833	CLA	C1C-C2C	2.24	1.48	1.44
20	1	308	CLA	C1B-NB	-2.23	1.35	1.37
20	O	208	CLA	C1B-NB	-2.23	1.35	1.37
20	B	816	CLA	C1C-C2C	2.23	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	809	CLA	C1B-C2B	2.23	1.48	1.43
20	A	806	CLA	C1C-C2C	2.23	1.48	1.44
20	L	307	CLA	C1C-C2C	2.23	1.48	1.44
20	B	811	CLA	C4B-NB	-2.23	1.35	1.37
23	L	303	BCR	C20-C19	2.23	1.40	1.34
20	H	201	CLA	C1B-C2B	2.23	1.48	1.43
20	A	839	CLA	C1C-C2C	2.23	1.48	1.44
23	F	301	BCR	C12-C13	-2.23	1.41	1.45
20	O	207	CLA	C1B-C2B	2.23	1.48	1.43
20	B	830	CLA	C1B-C2B	2.23	1.48	1.43
20	1	319	CLA	C4C-C3C	2.23	1.48	1.45
20	2	305	CLA	C4B-NB	-2.23	1.35	1.37
20	B	813	CLA	C1D-C2D	2.23	1.49	1.45
20	B	801	CLA	C4C-C3C	2.23	1.48	1.45
20	J	103	CLA	C4B-NB	-2.23	1.35	1.37
20	4	303	CLA	C1B-C2B	2.23	1.48	1.43
28	A	824	CL0	C3B-C4B	2.23	1.48	1.42
20	2	305	CLA	C1B-C2B	2.22	1.48	1.43
20	B	844	CLA	C1C-C2C	2.22	1.48	1.44
20	4	311	CLA	C1B-C2B	2.22	1.48	1.43
20	A	809	CLA	C1C-C2C	2.22	1.48	1.44
20	2	321	CLA	C1C-C2C	2.22	1.48	1.44
20	A	803	CLA	C4B-NB	-2.22	1.35	1.37
20	A	833	CLA	C3B-C2B	2.22	1.48	1.41
20	B	812	CLA	C4C-C3C	2.22	1.48	1.45
20	K	203	CLA	C4C-C3C	2.22	1.48	1.45
20	3	320	CLA	C1B-NB	-2.22	1.35	1.37
20	1	322	CLA	C1B-C2B	2.21	1.48	1.43
20	A	836	CLA	C1B-C2B	2.21	1.48	1.43
19	2	309	CHL	CHB-C4A	-2.21	1.32	1.37
20	B	821	CLA	C1B-C2B	2.21	1.48	1.43
20	B	803	CLA	C4C-C3C	2.21	1.48	1.45
20	A	801	CLA	C1C-C2C	2.21	1.48	1.44
20	B	851	CLA	C3B-C4B	2.21	1.47	1.42
19	2	318	CHL	MG-NA	-2.21	2.01	2.06
20	1	307	CLA	C4B-NB	-2.21	1.35	1.37
20	A	802	CLA	MG-NA	-2.21	2.01	2.06
20	A	836	CLA	C1C-C2C	2.21	1.48	1.44
20	F	306	CLA	C4B-NB	-2.20	1.35	1.37
20	B	808	CLA	C1C-C2C	2.20	1.48	1.44
20	2	308	CLA	C4B-NB	-2.20	1.35	1.37
20	A	802	CLA	C1B-NB	-2.20	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	317	CLA	C4C-C3C	2.20	1.48	1.45
23	F	302	BCR	C29-C28	-2.20	1.47	1.52
20	A	855	CLA	C1C-C2C	2.20	1.48	1.44
20	A	801	CLA	C1B-NB	-2.20	1.35	1.37
20	B	822	CLA	C1B-NB	-2.20	1.35	1.37
20	A	829	CLA	C1B-C2B	2.20	1.48	1.43
19	2	309	CHL	C4C-C3C	2.20	1.48	1.45
20	1	321	CLA	C4C-C3C	2.20	1.48	1.45
20	B	831	CLA	C1B-C2B	2.20	1.48	1.43
20	B	802	CLA	C1C-C2C	2.19	1.48	1.44
20	4	314	CLA	C4C-C3C	2.19	1.48	1.45
20	G	206	CLA	C1B-NB	-2.19	1.35	1.37
19	4	305	CHL	C4C-C3C	2.19	1.48	1.45
19	4	305	CHL	C1B-NB	-2.19	1.35	1.37
20	4	308	CLA	C1C-C2C	2.19	1.48	1.44
20	B	830	CLA	C1C-C2C	2.19	1.48	1.44
20	A	807	CLA	C1B-C2B	2.19	1.48	1.43
20	K	206	CLA	C3B-C2B	2.19	1.48	1.41
20	2	321	CLA	C4C-C3C	2.19	1.48	1.45
20	B	806	CLA	C1B-C2B	2.19	1.48	1.43
23	1	312	BCR	C12-C13	-2.19	1.41	1.45
20	2	323	CLA	C4C-C3C	2.19	1.48	1.45
20	A	854	CLA	CHB-C4A	-2.19	1.32	1.37
20	1	302	CLA	C4B-NB	-2.18	1.35	1.37
23	4	320	BCR	C23-C22	-2.18	1.41	1.45
20	F	305	CLA	C1B-C2B	2.18	1.48	1.43
20	2	317	CLA	C4B-NB	-2.18	1.35	1.37
23	4	320	BCR	C8-C9	-2.18	1.41	1.45
19	4	315	CHL	C4C-C3C	2.18	1.48	1.45
20	A	812	CLA	C1D-C2D	2.18	1.49	1.45
20	A	846	CLA	C1B-C2B	2.18	1.48	1.43
20	3	311	CLA	C1C-C2C	2.18	1.48	1.44
23	B	835	BCR	C8-C9	-2.18	1.41	1.45
20	A	855	CLA	C3B-C4B	2.18	1.47	1.42
20	2	319	CLA	C3B-C2B	2.18	1.48	1.41
19	2	309	CHL	C1B-C2B	2.18	1.48	1.43
20	2	308	CLA	C1B-C2B	2.18	1.48	1.43
20	A	845	CLA	C1C-C2C	2.18	1.48	1.44
20	A	848	CLA	C1B-C2B	2.18	1.48	1.43
21	1	323	LUT	C28-C29	-2.18	1.41	1.45
23	4	319	BCR	C12-C13	-2.18	1.41	1.45
20	B	819	CLA	CHB-C4A	-2.18	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	317	CLA	C4C-C3C	2.18	1.48	1.45
21	1	323	LUT	C32-C33	-2.18	1.41	1.45
20	A	808	CLA	C4C-C3C	2.17	1.48	1.45
20	4	308	CLA	C3B-C2B	2.17	1.48	1.41
20	B	814	CLA	CHD-C1D	2.17	1.42	1.38
20	L	305	CLA	C4C-C3C	2.17	1.48	1.45
20	B	820	CLA	C3B-C4B	2.17	1.47	1.42
20	B	817	CLA	C3B-C2B	2.17	1.48	1.41
20	1	305	CLA	C1B-C2B	2.17	1.48	1.43
20	1	307	CLA	C1B-C2B	2.17	1.48	1.43
20	1	321	CLA	C1C-C2C	2.17	1.48	1.44
23	G	203	BCR	C11-C12	2.17	1.40	1.34
20	F	306	CLA	C1B-C2B	2.17	1.48	1.43
20	B	817	CLA	C1C-C2C	2.17	1.48	1.44
20	A	812	CLA	C1B-C2B	2.17	1.48	1.43
20	G	207	CLA	C4C-C3C	2.17	1.48	1.45
20	A	856	CLA	C1C-C2C	2.16	1.48	1.44
20	J	103	CLA	C4C-C3C	2.16	1.48	1.45
20	A	834	CLA	C1D-C2D	2.16	1.49	1.45
20	1	306	CLA	C1B-C2B	2.16	1.48	1.43
19	4	307	CHL	C4C-C3C	2.16	1.48	1.45
20	B	853	CLA	C1C-C2C	2.16	1.48	1.44
20	A	835	CLA	C4B-NB	-2.16	1.35	1.37
19	4	307	CHL	C1B-NB	-2.16	1.35	1.37
20	3	307	CLA	C3B-C4B	2.16	1.47	1.42
20	K	206	CLA	C4C-C3C	2.16	1.48	1.45
20	A	807	CLA	C4C-C3C	2.16	1.48	1.45
20	K	204	CLA	C4C-C3C	2.16	1.48	1.45
20	4	309	CLA	C4B-NB	-2.16	1.35	1.37
20	A	841	CLA	C1B-C2B	2.16	1.48	1.43
23	B	839	BCR	C11-C12	2.16	1.40	1.34
20	G	206	CLA	C4C-C3C	2.16	1.48	1.45
20	B	814	CLA	C1D-C2D	2.16	1.49	1.45
20	4	316	CLA	C4C-C3C	2.15	1.48	1.45
20	A	804	CLA	C1C-C2C	2.15	1.48	1.44
20	B	816	CLA	C1D-C2D	2.15	1.49	1.45
20	A	838	CLA	C1C-C2C	2.15	1.48	1.44
20	A	849	CLA	C1D-C2D	2.15	1.49	1.45
20	1	304	CLA	C1C-C2C	2.15	1.48	1.44
20	2	303	CLA	C4C-C3C	2.15	1.48	1.45
20	2	308	CLA	C4C-C3C	2.15	1.48	1.45
20	3	318	CLA	C4B-NB	-2.15	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	834	CLA	C3B-C4B	2.15	1.47	1.42
23	4	320	BCR	C12-C13	-2.15	1.41	1.45
20	3	309	CLA	C1C-C2C	2.15	1.48	1.44
20	B	825	CLA	C4C-C3C	2.15	1.48	1.45
20	A	845	CLA	C1B-C2B	2.15	1.48	1.43
20	2	307	CLA	C3B-C2B	2.15	1.48	1.41
23	O	203	BCR	C11-C12	2.15	1.40	1.34
20	3	319	CLA	C1B-C2B	2.15	1.48	1.43
20	A	801	CLA	C4B-C3B	2.15	1.48	1.43
20	4	313	CLA	C4B-NB	-2.14	1.35	1.37
23	L	304	BCR	C23-C22	-2.14	1.41	1.45
20	2	317	CLA	C1B-C2B	2.14	1.48	1.43
20	A	802	CLA	C4C-C3C	2.14	1.48	1.45
20	B	830	CLA	C4B-NB	-2.14	1.35	1.37
20	B	816	CLA	C3B-C2B	2.14	1.48	1.41
20	3	314	CLA	C1B-C2B	2.14	1.48	1.43
20	A	838	CLA	C4C-C3C	2.14	1.48	1.45
20	B	852	CLA	C1B-C2B	2.14	1.48	1.43
23	G	201	BCR	C19-C18	-2.14	1.41	1.45
23	A	816	BCR	C29-C28	-2.14	1.47	1.52
20	A	854	CLA	C4B-NB	-2.14	1.35	1.37
20	A	836	CLA	C4C-C3C	2.14	1.48	1.45
20	A	826	CLA	C1C-C2C	2.14	1.48	1.44
20	A	841	CLA	C4C-C3C	2.13	1.48	1.45
20	A	835	CLA	C1B-C2B	2.13	1.48	1.43
20	A	811	CLA	C4B-NB	-2.13	1.35	1.37
19	4	305	CHL	CHB-C4A	-2.13	1.32	1.37
20	A	809	CLA	C4C-C3C	2.13	1.48	1.45
20	A	801	CLA	C4C-C3C	2.13	1.48	1.45
20	A	826	CLA	C4C-C3C	2.13	1.48	1.45
23	K	201	BCR	C12-C13	-2.13	1.41	1.45
20	A	829	CLA	C1C-C2C	2.13	1.48	1.44
20	B	802	CLA	C1B-C2B	2.12	1.48	1.43
20	1	319	CLA	C3B-C2B	2.12	1.48	1.41
20	B	846	CLA	C3B-C2B	2.12	1.48	1.41
20	4	310	CLA	C4C-C3C	2.12	1.48	1.45
20	B	822	CLA	C4C-C3C	2.12	1.48	1.45
23	O	203	BCR	C23-C22	-2.12	1.41	1.45
20	B	809	CLA	C4C-C3C	2.12	1.48	1.45
20	L	307	CLA	C4C-C3C	2.12	1.48	1.45
20	A	811	CLA	C1B-C2B	2.12	1.48	1.43
20	A	833	CLA	C1D-C2D	2.12	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	802	CLA	CHB-C4A	-2.12	1.32	1.37
20	A	830	CLA	C1C-C2C	2.11	1.48	1.44
23	A	857	BCR	C29-C28	-2.11	1.47	1.52
20	3	311	CLA	C3B-C2B	2.11	1.48	1.41
20	1	308	CLA	C3B-C2B	2.11	1.48	1.41
20	A	847	CLA	C4C-C3C	2.11	1.48	1.45
20	A	839	CLA	C3B-C2B	2.11	1.48	1.41
20	A	851	CLA	C3B-C2B	2.11	1.48	1.41
23	2	312	BCR	C2-C3	-2.11	1.47	1.52
20	A	850	CLA	C3B-C2B	2.11	1.48	1.41
20	2	319	CLA	C4C-C3C	2.11	1.48	1.45
20	A	827	CLA	C3B-C2B	2.11	1.48	1.41
20	B	844	CLA	C1D-C2D	2.11	1.49	1.45
20	A	852	CLA	CHB-C4A	-2.11	1.32	1.37
20	1	308	CLA	C4C-C3C	2.11	1.48	1.45
20	4	303	CLA	C4C-C3C	2.11	1.48	1.45
20	3	309	CLA	C4C-C3C	2.10	1.48	1.45
20	B	829	CLA	C4C-C3C	2.10	1.48	1.45
20	A	840	CLA	C1B-C2B	2.10	1.48	1.43
20	B	851	CLA	C4C-C3C	2.10	1.48	1.45
20	B	849	CLA	C4C-C3C	2.10	1.48	1.45
20	O	208	CLA	C4C-C3C	2.10	1.48	1.45
20	3	308	CLA	C3B-C2B	2.10	1.48	1.41
20	3	312	CLA	C3B-C2B	2.10	1.48	1.41
19	4	315	CHL	MG-NA	-2.10	2.01	2.06
21	1	323	LUT	C12-C13	-2.10	1.41	1.45
20	A	827	CLA	C4C-C3C	2.10	1.48	1.45
20	B	805	CLA	C3B-C2B	2.10	1.48	1.41
20	A	847	CLA	C1B-C2B	2.10	1.48	1.43
20	B	803	CLA	C3B-C2B	2.10	1.48	1.41
20	A	826	CLA	C3B-C4B	2.10	1.47	1.42
20	O	208	CLA	C1C-C2C	2.10	1.48	1.44
20	K	203	CLA	C3B-C2B	2.10	1.48	1.41
20	O	208	CLA	C3B-C2B	2.10	1.48	1.41
19	1	301	CHL	C4B-NB	-2.10	1.35	1.37
20	1	309	CLA	C4B-NB	-2.09	1.35	1.37
20	1	320	CLA	C4C-C3C	2.09	1.48	1.45
20	1	304	CLA	C3B-C2B	2.09	1.48	1.41
20	2	320	CLA	C4C-C3C	2.09	1.48	1.44
20	F	304	CLA	C1B-C2B	2.09	1.48	1.43
20	4	311	CLA	C4C-C3C	2.09	1.48	1.45
20	G	205	CLA	C3B-C2B	2.09	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	824	CLA	C1B-C2B	2.09	1.48	1.43
20	K	204	CLA	C3B-C2B	2.09	1.48	1.41
23	F	301	BCR	C29-C28	-2.09	1.47	1.52
20	B	823	CLA	C1B-NB	-2.09	1.35	1.37
20	A	806	CLA	C1B-C2B	2.09	1.48	1.43
20	A	812	CLA	CHB-C4A	-2.09	1.32	1.37
23	O	202	BCR	C23-C22	-2.09	1.41	1.45
19	2	318	CHL	C4C-C3C	2.08	1.48	1.45
23	B	838	BCR	C29-C28	-2.08	1.47	1.52
20	B	847	CLA	C1B-C2B	2.08	1.48	1.43
20	A	849	CLA	C3B-C2B	2.08	1.48	1.41
23	I	102	BCR	C19-C18	-2.08	1.41	1.45
20	4	314	CLA	C4B-NB	-2.08	1.35	1.37
20	B	846	CLA	C4C-C3C	2.08	1.48	1.45
23	L	303	BCR	C11-C12	2.08	1.39	1.34
20	B	808	CLA	C4C-C3C	2.08	1.48	1.45
20	3	311	CLA	C4C-C3C	2.08	1.48	1.45
23	4	319	BCR	C2-C3	-2.08	1.47	1.52
23	G	201	BCR	C12-C13	-2.08	1.41	1.45
20	O	206	CLA	C3B-C2B	2.08	1.48	1.41
20	A	825	CLA	C1B-C2B	2.08	1.48	1.43
19	3	313	CHL	C1B-NB	-2.08	1.35	1.37
20	A	825	CLA	C3B-C2B	2.08	1.48	1.41
23	J	101	BCR	C19-C18	-2.08	1.41	1.45
23	F	302	BCR	C12-C13	-2.08	1.41	1.45
20	B	820	CLA	C1B-NB	-2.07	1.35	1.37
20	1	305	CLA	C4C-C3C	2.07	1.48	1.45
23	B	834	BCR	C19-C18	-2.07	1.41	1.45
20	K	205	CLA	C1B-C2B	2.07	1.48	1.43
20	B	804	CLA	C4C-C3C	2.07	1.48	1.45
23	A	814	BCR	C19-C18	-2.07	1.41	1.45
20	A	843	CLA	CHB-C4A	-2.07	1.32	1.37
23	A	816	BCR	C11-C12	2.07	1.39	1.34
20	3	318	CLA	C4C-C3C	2.07	1.48	1.45
23	L	304	BCR	C11-C12	2.06	1.39	1.34
20	4	308	CLA	C1D-C2D	2.06	1.49	1.45
23	K	202	BCR	C23-C22	-2.06	1.41	1.45
20	A	838	CLA	C3B-C2B	2.06	1.48	1.41
20	3	309	CLA	C1B-C2B	2.06	1.48	1.43
20	A	856	CLA	C4C-C3C	2.06	1.48	1.45
23	A	816	BCR	C20-C19	2.06	1.39	1.34
20	B	848	CLA	C1B-C2B	2.06	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	823	CLA	C4C-C3C	2.06	1.48	1.45
20	A	804	CLA	C1B-C2B	2.06	1.48	1.43
20	A	844	CLA	C1C-C2C	2.06	1.48	1.44
20	A	803	CLA	C1D-C2D	2.06	1.49	1.45
20	B	809	CLA	CHB-C4A	-2.06	1.32	1.37
20	A	841	CLA	C4B-NB	-2.06	1.35	1.37
19	3	313	CHL	C4C-C3C	2.06	1.48	1.45
28	A	824	CL0	C1C-C2C	2.06	1.48	1.44
19	4	315	CHL	C1B-NB	-2.06	1.35	1.37
20	A	856	CLA	C3B-C2B	2.06	1.48	1.41
20	L	305	CLA	C3B-C2B	2.05	1.48	1.41
23	L	302	BCR	C19-C18	-2.05	1.41	1.45
20	A	849	CLA	C4C-C3C	2.05	1.48	1.45
23	A	817	BCR	C29-C28	-2.05	1.47	1.52
19	1	317	CHL	MG-NA	-2.05	2.01	2.06
20	A	802	CLA	C1C-C2C	2.05	1.48	1.44
23	L	302	BCR	C29-C28	-2.05	1.47	1.52
20	A	846	CLA	C4C-C3C	2.05	1.48	1.45
20	4	309	CLA	C1B-C2B	2.05	1.48	1.43
20	N	202	CLA	C4C-C3C	2.05	1.48	1.45
19	1	301	CHL	MG-NA	-2.05	2.01	2.06
19	2	322	CHL	MG-NA	-2.05	2.01	2.06
20	K	205	CLA	C1C-C2C	2.05	1.48	1.44
20	3	320	CLA	C3B-C2B	2.05	1.48	1.41
19	2	322	CHL	C4C-C3C	2.05	1.48	1.45
19	4	307	CHL	CHB-C4A	-2.05	1.32	1.37
20	1	319	CLA	C1C-C2C	2.05	1.48	1.44
19	2	322	CHL	C1B-NB	-2.04	1.35	1.37
20	1	306	CLA	C4C-C3C	2.04	1.48	1.45
20	1	321	CLA	C3B-C2B	2.04	1.48	1.41
20	2	304	CLA	C3B-C2B	2.04	1.48	1.41
20	4	302	CLA	C4C-C3C	2.04	1.48	1.45
20	1	320	CLA	C1B-C2B	2.04	1.48	1.43
20	3	312	CLA	C4C-C3C	2.04	1.48	1.45
20	3	320	CLA	C4C-C3C	2.04	1.48	1.45
20	K	205	CLA	MG-NB	-2.04	2.01	2.05
22	1	311	XAT	O4-C5	-2.04	1.43	1.46
19	4	306	CHL	MG-NA	-2.04	2.01	2.06
23	B	835	BCR	C2-C3	-2.04	1.47	1.52
20	2	323	CLA	C1B-C2B	2.03	1.48	1.43
19	3	313	CHL	MG-NA	-2.03	2.01	2.06
20	B	824	CLA	C4C-C3C	2.03	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	804	CLA	C3B-C2B	2.03	1.48	1.41
19	2	302	CHL	CHB-C4A	-2.03	1.32	1.37
19	2	322	CHL	CHB-C4A	-2.03	1.32	1.37
20	B	826	CLA	C3B-C2B	2.03	1.48	1.41
19	2	302	CHL	MG-NA	-2.03	2.01	2.06
20	B	827	CLA	C1B-C2B	2.03	1.48	1.43
20	B	853	CLA	C3B-C2B	2.03	1.48	1.41
20	3	315	CLA	C3B-C2B	2.03	1.48	1.41
20	A	828	CLA	C3B-C2B	2.03	1.48	1.41
20	A	827	CLA	C1C-C2C	2.03	1.48	1.44
20	A	853	CLA	C1D-C2D	2.03	1.49	1.45
20	A	842	CLA	C4C-C3C	2.03	1.48	1.45
23	A	817	BCR	C16-C17	-2.03	1.37	1.43
20	A	838	CLA	C1B-NB	-2.03	1.35	1.37
20	A	830	CLA	C3B-C2B	2.03	1.48	1.41
23	L	301	BCR	C2-C3	-2.03	1.47	1.52
23	L	304	BCR	C19-C18	-2.03	1.41	1.45
20	A	846	CLA	C1C-C2C	2.03	1.48	1.44
20	A	844	CLA	C3B-C2B	2.02	1.48	1.41
20	L	307	CLA	C3B-C2B	2.02	1.48	1.41
20	B	815	CLA	C4C-C3C	2.02	1.48	1.45
23	K	201	BCR	C29-C28	-2.02	1.47	1.52
20	B	801	CLA	C3B-C2B	2.02	1.48	1.41
23	1	312	BCR	C19-C18	-2.02	1.41	1.45
20	B	806	CLA	C4B-NB	-2.01	1.35	1.37
23	4	320	BCR	C29-C28	-2.01	1.47	1.52
20	A	832	CLA	C4C-C3C	2.01	1.48	1.45
19	2	309	CHL	MG-NA	-2.01	2.01	2.06
23	L	304	BCR	C8-C9	-2.01	1.41	1.45
19	4	305	CHL	MG-NA	-2.01	2.01	2.06
23	J	101	BCR	C29-C28	-2.01	1.47	1.52
20	4	312	CLA	C4C-C3C	2.00	1.48	1.45
20	H	201	CLA	C4C-C3C	2.00	1.48	1.45
23	3	303	BCR	C2-C3	-2.00	1.47	1.52
20	B	850	CLA	C1C-C2C	2.00	1.48	1.44
20	1	307	CLA	C4C-C3C	2.00	1.48	1.45
20	A	853	CLA	C4C-C3C	2.00	1.48	1.45
19	2	318	CHL	C1D-ND	-2.00	1.35	1.37

All (5231) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	302	XAT	C40-C33-C34	-33.63	75.82	122.92
22	3	302	XAT	C40-C33-C32	-26.40	76.48	118.08
22	2	311	XAT	O4-C5-C4	-23.89	95.43	113.38
22	3	302	XAT	C32-C33-C34	21.58	152.06	118.94
22	2	311	XAT	O4-C5-C18	-18.69	92.66	115.06
19	2	309	CHL	C2B-C1B-NB	10.55	117.31	110.23
22	2	311	XAT	C35-C34-C33	10.54	142.35	127.31
20	3	309	CLA	C1D-ND-C4D	-10.42	98.93	106.33
20	A	846	CLA	C1D-ND-C4D	-10.41	98.94	106.33
20	B	806	CLA	C1D-ND-C4D	-10.35	98.98	106.33
20	4	303	CLA	C1D-ND-C4D	-10.33	98.99	106.33
20	B	828	CLA	C1D-ND-C4D	-10.30	99.02	106.33
20	2	320	CLA	C1D-ND-C4D	-10.29	99.02	106.33
20	B	814	CLA	C1D-ND-C4D	-10.29	99.03	106.33
20	K	205	CLA	C1D-ND-C4D	-10.28	99.03	106.33
20	A	809	CLA	C1D-ND-C4D	-10.28	99.03	106.33
20	B	827	CLA	C1D-ND-C4D	-10.27	99.04	106.33
22	1	311	XAT	C31-C30-C29	-10.27	112.65	127.31
20	2	306	CLA	C1D-ND-C4D	-10.25	99.05	106.33
20	G	206	CLA	C1D-ND-C4D	-10.24	99.06	106.33
20	B	831	CLA	C1D-ND-C4D	-10.23	99.06	106.33
19	2	322	CHL	C2B-C1B-NB	10.21	117.08	110.23
20	B	848	CLA	C1D-ND-C4D	-10.21	99.08	106.33
20	B	845	CLA	C2B-C1B-NB	10.20	117.07	110.23
20	4	312	CLA	C1D-ND-C4D	-10.20	99.09	106.33
20	1	302	CLA	C1D-ND-C4D	-10.18	99.10	106.33
19	4	306	CHL	C2B-C1B-NB	10.12	117.02	110.23
20	A	852	CLA	C2B-C1B-NB	10.08	116.99	110.23
19	4	305	CHL	C2B-C1B-NB	10.08	116.99	110.23
20	1	309	CLA	C1D-ND-C4D	-10.07	99.18	106.33
20	4	313	CLA	C1D-ND-C4D	-10.05	99.20	106.33
20	A	805	CLA	C1D-ND-C4D	-10.01	99.22	106.33
20	B	830	CLA	C1D-ND-C4D	-10.00	99.23	106.33
20	4	311	CLA	C1D-ND-C4D	-10.00	99.23	106.33
19	2	318	CHL	C2B-C1B-NB	10.00	116.93	110.23
20	1	306	CLA	C1D-ND-C4D	-9.99	99.24	106.33
20	A	836	CLA	C1D-ND-C4D	-9.99	99.24	106.33
20	B	811	CLA	C1D-ND-C4D	-9.98	99.24	106.33
20	B	847	CLA	C1D-ND-C4D	-9.97	99.25	106.33
19	2	302	CHL	C2B-C1B-NB	9.96	116.91	110.23
20	3	316	CLA	C1D-ND-C4D	-9.96	99.26	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	315	CHL	C2B-C1B-NB	9.94	116.90	110.23
20	N	202	CLA	C1D-ND-C4D	-9.92	99.29	106.33
20	B	817	CLA	C1D-ND-C4D	-9.91	99.30	106.33
20	3	308	CLA	C1D-ND-C4D	-9.90	99.30	106.33
20	B	813	CLA	C1D-ND-C4D	-9.89	99.31	106.33
20	B	849	CLA	C1D-ND-C4D	-9.89	99.31	106.33
22	1	311	XAT	C27-C28-C29	-9.88	110.20	125.53
20	B	833	CLA	C1D-ND-C4D	-9.87	99.32	106.33
20	B	802	CLA	C1D-ND-C4D	-9.87	99.32	106.33
20	A	807	CLA	C1D-ND-C4D	-9.87	99.32	106.33
20	4	309	CLA	C1D-ND-C4D	-9.87	99.32	106.33
19	2	301	CHL	C2B-C1B-NB	9.86	116.84	110.23
20	A	851	CLA	C1D-ND-C4D	-9.85	99.34	106.33
20	3	318	CLA	C1D-ND-C4D	-9.85	99.34	106.33
20	A	849	CLA	C1D-ND-C4D	-9.82	99.36	106.33
20	B	844	CLA	C1D-ND-C4D	-9.80	99.37	106.33
20	O	207	CLA	C1D-ND-C4D	-9.78	99.39	106.33
20	1	322	CLA	C1D-ND-C4D	-9.78	99.39	106.33
19	3	313	CHL	C2B-C1B-NB	9.77	116.78	110.23
20	4	302	CLA	C1D-ND-C4D	-9.76	99.40	106.33
20	A	837	CLA	C1D-ND-C4D	-9.76	99.40	106.33
20	L	306	CLA	C1D-ND-C4D	-9.76	99.40	106.33
19	1	301	CHL	C2B-C1B-NB	9.75	116.77	110.23
20	B	829	CLA	C1D-ND-C4D	-9.75	99.41	106.33
19	4	307	CHL	C2B-C1B-NB	9.74	116.76	110.23
20	B	805	CLA	C1D-ND-C4D	-9.74	99.42	106.33
20	1	305	CLA	C1D-ND-C4D	-9.74	99.42	106.33
20	F	304	CLA	C1D-ND-C4D	-9.74	99.42	106.33
20	A	803	CLA	C1D-ND-C4D	-9.73	99.42	106.33
20	2	304	CLA	C1D-ND-C4D	-9.72	99.43	106.33
20	B	810	CLA	C1D-ND-C4D	-9.72	99.43	106.33
20	4	314	CLA	C1D-ND-C4D	-9.71	99.43	106.33
20	A	827	CLA	C1D-ND-C4D	-9.69	99.45	106.33
20	A	811	CLA	C1D-ND-C4D	-9.69	99.45	106.33
20	B	852	CLA	C1D-ND-C4D	-9.69	99.45	106.33
20	3	317	CLA	C1D-ND-C4D	-9.69	99.45	106.33
20	B	824	CLA	C1D-ND-C4D	-9.69	99.45	106.33
20	B	826	CLA	C1D-ND-C4D	-9.67	99.47	106.33
22	2	311	XAT	C32-C33-C34	9.66	133.77	118.94
20	2	323	CLA	C2B-C1B-NB	9.65	116.70	110.23
19	1	317	CHL	C2B-C1B-NB	9.64	116.70	110.23
20	H	201	CLA	C1D-ND-C4D	-9.64	99.49	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	840	CLA	C1D-ND-C4D	-9.63	99.49	106.33
20	2	317	CLA	C1D-ND-C4D	-9.63	99.49	106.33
20	2	305	CLA	C1D-ND-C4D	-9.63	99.50	106.33
20	G	205	CLA	C1D-ND-C4D	-9.63	99.50	106.33
20	B	803	CLA	C1D-ND-C4D	-9.62	99.50	106.33
20	A	812	CLA	C2B-C1B-NB	9.62	116.68	110.23
20	A	825	CLA	C2B-C1B-NB	9.62	116.68	110.23
20	A	831	CLA	C1D-ND-C4D	-9.61	99.51	106.33
20	B	823	CLA	C2B-C1B-NB	9.59	116.66	110.23
20	A	842	CLA	C1D-ND-C4D	-9.58	99.53	106.33
20	2	308	CLA	C1D-ND-C4D	-9.54	99.56	106.33
20	1	318	CLA	C1D-ND-C4D	-9.54	99.56	106.33
20	A	844	CLA	C2B-C1B-NB	9.52	116.61	110.23
20	B	850	CLA	C1D-ND-C4D	-9.52	99.58	106.33
20	1	320	CLA	C1D-ND-C4D	-9.50	99.59	106.33
20	L	307	CLA	C1D-ND-C4D	-9.49	99.59	106.33
20	B	815	CLA	C2B-C1B-NB	9.49	116.59	110.23
20	L	305	CLA	C2B-C1B-NB	9.48	116.59	110.23
20	A	841	CLA	C1D-ND-C4D	-9.48	99.60	106.33
20	B	821	CLA	C1D-ND-C4D	-9.47	99.60	106.33
20	K	204	CLA	C1D-ND-C4D	-9.47	99.61	106.33
20	A	835	CLA	C1D-ND-C4D	-9.46	99.61	106.33
20	A	856	CLA	C1D-ND-C4D	-9.46	99.61	106.33
20	B	846	CLA	C1D-ND-C4D	-9.46	99.61	106.33
20	1	308	CLA	C1D-ND-C4D	-9.45	99.62	106.33
20	1	307	CLA	C1D-ND-C4D	-9.43	99.63	106.33
20	F	305	CLA	C1D-ND-C4D	-9.43	99.64	106.33
20	J	103	CLA	C1D-ND-C4D	-9.42	99.64	106.33
20	3	307	CLA	C2B-C1B-NB	9.42	116.55	110.23
20	3	312	CLA	C1D-ND-C4D	-9.41	99.65	106.33
20	B	816	CLA	C1D-ND-C4D	-9.41	99.65	106.33
20	A	839	CLA	C1D-ND-C4D	-9.41	99.65	106.33
20	A	842	CLA	C2B-C1B-NB	9.39	116.53	110.23
20	A	802	CLA	C1D-ND-C4D	-9.38	99.67	106.33
20	O	208	CLA	C1D-ND-C4D	-9.38	99.67	106.33
20	A	833	CLA	C1D-ND-C4D	-9.37	99.68	106.33
20	F	306	CLA	C1D-ND-C4D	-9.35	99.69	106.33
20	K	203	CLA	C1D-ND-C4D	-9.35	99.69	106.33
20	1	303	CLA	C1D-ND-C4D	-9.35	99.70	106.33
20	A	802	CLA	C2B-C1B-NB	9.35	116.50	110.23
20	A	847	CLA	C1D-ND-C4D	-9.33	99.71	106.33
20	G	207	CLA	C1D-ND-C4D	-9.32	99.71	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	304	CLA	C1D-ND-C4D	-9.31	99.72	106.33
22	2	311	XAT	C31-C30-C29	-9.31	114.03	127.31
20	A	841	CLA	C2B-C1B-NB	9.29	116.46	110.23
20	2	307	CLA	C1D-ND-C4D	-9.29	99.73	106.33
20	3	319	CLA	C1D-ND-C4D	-9.28	99.74	106.33
20	A	839	CLA	C2B-C1B-NB	9.28	116.45	110.23
20	2	319	CLA	C1D-ND-C4D	-9.26	99.75	106.33
20	B	846	CLA	C2B-C1B-NB	9.25	116.43	110.23
20	3	314	CLA	C1D-ND-C4D	-9.22	99.78	106.33
20	2	321	CLA	C1D-ND-C4D	-9.22	99.79	106.33
20	B	807	CLA	C2B-C1B-NB	9.21	116.41	110.23
20	A	825	CLA	C1D-ND-C4D	-9.19	99.81	106.33
20	A	806	CLA	C1D-ND-C4D	-9.18	99.81	106.33
20	A	835	CLA	C2B-C1B-NB	9.18	116.38	110.23
20	2	323	CLA	C1D-ND-C4D	-9.17	99.82	106.33
20	4	316	CLA	C1D-ND-C4D	-9.15	99.83	106.33
20	A	844	CLA	C1D-ND-C4D	-9.15	99.83	106.33
20	A	847	CLA	CMD-C2D-C1D	9.14	140.81	124.71
20	4	310	CLA	C1D-ND-C4D	-9.14	99.84	106.33
20	B	853	CLA	C1D-ND-C4D	-9.12	99.85	106.33
20	A	828	CLA	C2B-C1B-NB	9.12	116.35	110.23
20	K	206	CLA	C1D-ND-C4D	-9.11	99.86	106.33
20	A	850	CLA	C2B-C1B-NB	9.10	116.33	110.23
20	A	848	CLA	C1D-ND-C4D	-9.09	99.88	106.33
20	A	830	CLA	C1D-ND-C4D	-9.09	99.88	106.33
20	B	807	CLA	C1D-ND-C4D	-9.08	99.88	106.33
20	4	314	CLA	C2B-C1B-NB	9.08	116.32	110.23
20	B	825	CLA	C1D-ND-C4D	-9.08	99.88	106.33
20	3	315	CLA	C1D-ND-C4D	-9.08	99.89	106.33
20	B	815	CLA	C1D-ND-C4D	-9.05	99.91	106.33
20	A	804	CLA	C1D-ND-C4D	-9.05	99.91	106.33
20	3	320	CLA	C2B-C1B-NB	9.00	116.27	110.23
20	3	310	CLA	C2B-C1B-NB	8.99	116.26	110.23
20	K	206	CLA	C2B-C1B-NB	8.99	116.26	110.23
20	3	320	CLA	C1D-ND-C4D	-8.98	99.95	106.33
20	1	319	CLA	C2B-C1B-NB	8.98	116.25	110.23
20	2	319	CLA	C2B-C1B-NB	8.97	116.25	110.23
20	A	828	CLA	C1D-ND-C4D	-8.96	99.97	106.33
20	B	808	CLA	C1D-ND-C4D	-8.95	99.98	106.33
20	1	321	CLA	C1D-ND-C4D	-8.92	100.00	106.33
20	4	302	CLA	C2B-C1B-NB	8.90	116.20	110.23
28	A	824	CL0	C2C-C1C-NC	8.87	118.29	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	837	CLA	C2B-C1B-NB	8.87	116.18	110.23
20	A	826	CLA	C2B-C1B-NB	8.85	116.16	110.23
20	B	814	CLA	C2B-C1B-NB	8.85	116.16	110.23
20	A	838	CLA	C1D-ND-C4D	-8.83	100.06	106.33
20	A	808	CLA	C2B-C1B-NB	8.82	116.15	110.23
20	B	802	CLA	CMD-C2D-C1D	8.81	140.24	124.71
20	B	809	CLA	C1D-ND-C4D	-8.81	100.08	106.33
20	3	311	CLA	C1D-ND-C4D	-8.79	100.09	106.33
20	A	838	CLA	C2B-C1B-NB	8.78	116.12	110.23
20	O	206	CLA	C2B-C1B-NB	8.78	116.12	110.23
20	L	306	CLA	C2B-C1B-NB	8.78	116.11	110.23
20	3	315	CLA	C2B-C1B-NB	8.77	116.11	110.23
20	1	318	CLA	C2B-C1B-NB	8.77	116.11	110.23
20	B	803	CLA	C2B-C1B-NB	8.76	116.11	110.23
20	1	304	CLA	C2B-C1B-NB	8.76	116.10	110.23
20	1	319	CLA	CMD-C2D-C1D	8.76	140.15	124.71
20	A	832	CLA	C1D-ND-C4D	-8.76	100.11	106.33
20	A	845	CLA	C2B-C1B-NB	8.71	116.07	110.23
20	1	319	CLA	C1D-ND-C4D	-8.70	100.16	106.33
20	A	808	CLA	C1D-ND-C4D	-8.69	100.16	106.33
20	B	818	CLA	C1D-ND-C4D	-8.69	100.16	106.33
20	A	850	CLA	C1D-ND-C4D	-8.69	100.16	106.33
20	B	852	CLA	C2B-C1B-NB	8.68	116.05	110.23
20	B	804	CLA	C2B-C1B-NB	8.67	116.05	110.23
20	3	308	CLA	C2B-C1B-NB	8.67	116.04	110.23
20	4	304	CLA	C1D-ND-C4D	-8.67	100.18	106.33
20	B	822	CLA	C1D-ND-C4D	-8.67	100.18	106.33
20	L	305	CLA	C1D-ND-C4D	-8.66	100.18	106.33
20	B	813	CLA	C2B-C1B-NB	8.66	116.04	110.23
20	B	851	CLA	C2C-C1C-NC	8.64	118.07	109.97
20	4	304	CLA	C2B-C1B-NB	8.64	116.03	110.23
20	2	303	CLA	C1D-ND-C4D	-8.64	100.20	106.33
20	4	309	CLA	C2B-C1B-NB	8.63	116.02	110.23
20	B	806	CLA	C2B-C1B-NB	8.63	116.02	110.23
20	A	836	CLA	C2B-C1B-NB	8.62	116.01	110.23
20	B	845	CLA	C1D-ND-C4D	-8.62	100.21	106.33
20	2	308	CLA	C2B-C1B-NB	8.62	116.01	110.23
20	B	820	CLA	C1D-ND-C4D	-8.61	100.22	106.33
20	3	312	CLA	C2B-C1B-NB	8.59	115.99	110.23
20	B	822	CLA	C2B-C1B-NB	8.59	115.99	110.23
20	B	824	CLA	C2B-C1B-NB	8.59	115.99	110.23
20	3	311	CLA	C2B-C1B-NB	8.57	115.98	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	316	CLA	C2B-C1B-NB	8.57	115.98	110.23
20	3	307	CLA	C2C-C1C-NC	8.57	118.00	109.97
20	A	834	CLA	C2C-C1C-NC	8.56	117.99	109.97
20	1	321	CLA	C2B-C1B-NB	8.55	115.96	110.23
20	A	855	CLA	C1D-ND-C4D	-8.55	100.26	106.33
20	1	308	CLA	C2B-C1B-NB	8.55	115.96	110.23
20	A	848	CLA	C2B-C1B-NB	8.54	115.96	110.23
20	2	321	CLA	C2B-C1B-NB	8.52	115.94	110.23
20	B	808	CLA	C2B-C1B-NB	8.51	115.94	110.23
20	B	851	CLA	C1D-ND-C4D	-8.51	100.29	106.33
20	K	204	CLA	C2B-C1B-NB	8.51	115.94	110.23
20	4	308	CLA	C2C-C1C-NC	8.51	117.94	109.97
20	B	833	CLA	CMD-C2D-C1D	8.51	139.70	124.71
20	1	305	CLA	C2B-C1B-NB	8.49	115.92	110.23
20	B	833	CLA	C2B-C1B-NB	8.49	115.92	110.23
20	B	812	CLA	C1D-ND-C4D	-8.49	100.31	106.33
20	F	306	CLA	C2B-C1B-NB	8.48	115.92	110.23
20	2	305	CLA	C2B-C1B-NB	8.48	115.92	110.23
20	2	308	CLA	CMD-C2D-C1D	8.47	139.64	124.71
20	3	310	CLA	C1D-ND-C4D	-8.47	100.32	106.33
20	4	308	CLA	C2B-C1B-NB	8.46	115.91	110.23
20	1	307	CLA	C2B-C1B-NB	8.46	115.90	110.23
20	B	801	CLA	C1D-ND-C4D	-8.46	100.33	106.33
20	B	804	CLA	C1D-ND-C4D	-8.45	100.33	106.33
19	2	318	CHL	CMD-C2D-C1D	8.44	139.59	124.71
20	A	829	CLA	C1D-ND-C4D	-8.43	100.34	106.33
20	A	826	CLA	C2C-C1C-NC	8.43	117.87	109.97
20	A	843	CLA	C2B-C1B-NB	8.43	115.89	110.23
20	A	845	CLA	C1D-ND-C4D	-8.43	100.35	106.33
20	B	823	CLA	C1D-ND-C4D	-8.43	100.35	106.33
20	N	202	CLA	C2B-C1B-NB	8.43	115.88	110.23
20	A	834	CLA	C1D-ND-C4D	-8.42	100.36	106.33
20	1	320	CLA	C2B-C1B-NB	8.41	115.87	110.23
20	G	207	CLA	C2B-C1B-NB	8.41	115.87	110.23
20	A	811	CLA	C2B-C1B-NB	8.41	115.87	110.23
20	A	804	CLA	C2C-C1C-NC	8.40	117.84	109.97
20	A	834	CLA	CMD-C2D-C1D	8.40	139.51	124.71
20	A	856	CLA	C2B-C1B-NB	8.39	115.86	110.23
20	O	206	CLA	C1D-ND-C4D	-8.38	100.38	106.33
20	B	844	CLA	C2C-C1C-NC	8.38	117.82	109.97
20	1	322	CLA	C2B-C1B-NB	8.38	115.85	110.23
20	O	208	CLA	C2B-C1B-NB	8.38	115.85	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	318	CLA	CMD-C2D-C1D	8.38	139.48	124.71
20	K	203	CLA	C2B-C1B-NB	8.37	115.84	110.23
20	O	207	CLA	C2B-C1B-NB	8.37	115.84	110.23
20	B	826	CLA	C2B-C1B-NB	8.36	115.84	110.23
20	A	853	CLA	C2B-C1B-NB	8.35	115.83	110.23
20	B	819	CLA	C2C-C1C-NC	8.35	117.79	109.97
20	B	853	CLA	C2B-C1B-NB	8.34	115.82	110.23
20	A	855	CLA	C2C-C1C-NC	8.34	117.78	109.97
20	A	832	CLA	C2B-C1B-NB	8.34	115.82	110.23
20	4	303	CLA	CMD-C2D-C1D	8.34	139.41	124.71
20	4	313	CLA	CMD-C2D-C1D	8.33	139.40	124.71
20	G	206	CLA	CMD-C2D-C1D	8.33	139.39	124.71
20	B	817	CLA	C2B-C1B-NB	8.33	115.82	110.23
20	B	820	CLA	C2C-C1C-NC	8.33	117.77	109.97
20	B	809	CLA	C2B-C1B-NB	8.32	115.81	110.23
20	J	103	CLA	C2B-C1B-NB	8.32	115.81	110.23
20	B	817	CLA	CMD-C2D-C1D	8.32	139.37	124.71
20	B	801	CLA	C2B-C1B-NB	8.31	115.80	110.23
20	B	848	CLA	CMD-C2D-C1D	8.30	139.34	124.71
20	A	827	CLA	C2B-C1B-NB	8.30	115.80	110.23
20	A	836	CLA	CMD-C2D-C1D	8.29	139.32	124.71
19	1	301	CHL	CMD-C2D-C1D	8.29	139.32	124.71
20	L	307	CLA	C2B-C1B-NB	8.27	115.78	110.23
20	A	830	CLA	C2B-C1B-NB	8.27	115.77	110.23
19	4	306	CHL	CMD-C2D-C1D	8.26	139.28	124.71
20	4	316	CLA	C2C-C1C-NC	8.26	117.71	109.97
19	2	309	CHL	CMD-C2D-C1D	8.26	139.27	124.71
20	3	311	CLA	C2C-C1C-NC	8.26	117.71	109.97
20	B	818	CLA	C2B-C1B-NB	8.25	115.77	110.23
20	1	307	CLA	CMD-C2D-C1D	8.24	139.24	124.71
20	A	852	CLA	C1D-ND-C4D	-8.23	100.49	106.33
20	A	851	CLA	C2B-C1B-NB	8.22	115.75	110.23
20	4	313	CLA	C2B-C1B-NB	8.21	115.74	110.23
20	2	317	CLA	C2B-C1B-NB	8.21	115.73	110.23
20	A	848	CLA	C2C-C1C-NC	8.20	117.66	109.97
20	B	812	CLA	C2B-C1B-NB	8.20	115.73	110.23
20	B	801	CLA	C2C-C1C-NC	8.20	117.66	109.97
20	4	310	CLA	C2B-C1B-NB	8.20	115.73	110.23
20	A	808	CLA	C2C-C1C-NC	8.19	117.64	109.97
20	B	829	CLA	CMD-C2D-C1D	8.19	139.15	124.71
20	A	801	CLA	C2C-C1C-NC	8.19	117.64	109.97
20	B	847	CLA	CMD-C2D-C1D	8.18	139.13	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	849	CLA	C2B-C1B-NB	8.18	115.71	110.23
20	B	829	CLA	C2B-C1B-NB	8.17	115.71	110.23
20	F	305	CLA	C2B-C1B-NB	8.17	115.71	110.23
20	B	846	CLA	CMD-C2D-C1D	8.17	139.11	124.71
20	A	854	CLA	C1D-ND-C4D	-8.16	100.53	106.33
22	2	311	XAT	C35-C15-C14	-8.16	106.76	123.47
20	2	320	CLA	C2C-C1C-NC	8.16	117.61	109.97
19	3	313	CHL	CMD-C2D-C1D	8.16	139.09	124.71
20	A	801	CLA	C1D-ND-C4D	-8.15	100.54	106.33
20	4	316	CLA	CMD-C2D-C1D	8.15	139.08	124.71
20	2	307	CLA	C2B-C1B-NB	8.14	115.69	110.23
20	3	318	CLA	C2B-C1B-NB	8.14	115.69	110.23
20	A	831	CLA	C2C-C1C-NC	8.13	117.59	109.97
19	2	302	CHL	CMD-C2D-C1D	8.12	139.03	124.71
20	3	310	CLA	CMD-C2D-C1D	8.12	139.03	124.71
20	B	811	CLA	C2B-C1B-NB	8.12	115.68	110.23
19	4	306	CHL	C2C-C3C-C4C	-8.12	100.70	106.49
20	1	309	CLA	C2B-C1B-NB	8.12	115.67	110.23
20	A	805	CLA	CMD-C2D-C1D	8.12	139.02	124.71
19	2	322	CHL	CMD-C2D-C1D	8.12	139.02	124.71
20	A	840	CLA	CMD-C2D-C1D	8.12	139.01	124.71
20	A	809	CLA	C2B-C1B-NB	8.11	115.67	110.23
20	3	309	CLA	CMD-C2D-C1D	8.11	139.00	124.71
20	A	801	CLA	C2B-C1B-NB	8.10	115.67	110.23
19	2	301	CHL	CMD-C2D-C1D	8.10	138.99	124.71
20	2	323	CLA	CMD-C2D-C1D	8.10	138.99	124.71
20	A	853	CLA	C1D-ND-C4D	-8.10	100.58	106.33
20	K	204	CLA	CMD-C2D-C1D	8.10	138.98	124.71
20	3	319	CLA	C2B-C1B-NB	8.10	115.66	110.23
20	J	103	CLA	CMD-C2D-C1D	8.09	138.97	124.71
20	B	807	CLA	CMD-C2D-C1D	8.09	138.97	124.71
20	A	849	CLA	C2C-C1C-NC	8.08	117.54	109.97
20	A	831	CLA	C2B-C1B-NB	8.07	115.64	110.23
20	A	840	CLA	C2C-C1C-NC	8.07	117.53	109.97
20	G	205	CLA	C2B-C1B-NB	8.07	115.64	110.23
20	3	317	CLA	C2B-C1B-NB	8.07	115.64	110.23
20	B	821	CLA	C2B-C1B-NB	8.06	115.64	110.23
20	A	831	CLA	CMD-C2D-C1D	8.06	138.91	124.71
20	K	203	CLA	CMD-C2D-C1D	8.06	138.91	124.71
20	A	807	CLA	CMD-C2D-C1D	8.05	138.90	124.71
20	2	320	CLA	CMD-C2D-C1D	8.04	138.89	124.71
20	A	805	CLA	C2B-C1B-NB	8.04	115.62	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	307	CLA	CMD-C2D-C1D	8.04	138.89	124.71
20	O	207	CLA	CMD-C2D-C1D	8.04	138.89	124.71
20	A	837	CLA	CMD-C2D-C1D	8.03	138.87	124.71
20	1	309	CLA	CMD-C2D-C1D	8.03	138.87	124.71
20	B	828	CLA	CMD-C2D-C1D	8.03	138.86	124.71
20	3	319	CLA	C2C-C1C-NC	8.03	117.49	109.97
20	L	307	CLA	CMD-C2D-C1D	8.02	138.85	124.71
20	B	803	CLA	CMD-C2D-C1D	8.02	138.84	124.71
19	4	305	CHL	CMD-C2D-C1D	8.01	138.84	124.71
20	1	321	CLA	CMD-C2D-C1D	8.01	138.84	124.71
19	4	315	CHL	CMD-C2D-C1D	8.01	138.82	124.71
20	B	818	CLA	CMD-C2D-C1D	8.00	138.81	124.71
20	A	807	CLA	C2B-C1B-NB	8.00	115.59	110.23
20	2	321	CLA	CMD-C2D-C1D	8.00	138.81	124.71
20	2	306	CLA	CMD-C2D-C1D	7.99	138.80	124.71
20	3	319	CLA	CMD-C2D-C1D	7.99	138.80	124.71
20	A	830	CLA	C2C-C1C-NC	7.99	117.46	109.97
20	B	820	CLA	C2B-C1B-NB	7.99	115.59	110.23
20	2	303	CLA	C2B-C1B-NB	7.99	115.59	110.23
20	3	320	CLA	CMD-C2D-C1D	7.99	138.79	124.71
20	A	843	CLA	C2C-C1C-NC	7.98	117.45	109.97
20	1	302	CLA	C2B-C1B-NB	7.98	115.58	110.23
20	B	821	CLA	CMD-C2D-C1D	7.97	138.77	124.71
19	4	307	CHL	CMD-C2D-C1D	7.97	138.77	124.71
20	3	314	CLA	C2C-C1C-NC	7.97	117.44	109.97
20	B	831	CLA	C2B-C1B-NB	7.97	115.57	110.23
19	2	301	CHL	C2C-C3C-C4C	-7.97	100.81	106.49
20	4	312	CLA	CMD-C2D-C1D	7.96	138.75	124.71
20	L	305	CLA	CMD-C2D-C1D	7.96	138.75	124.71
20	A	809	CLA	CMD-C2D-C1D	7.96	138.74	124.71
20	A	856	CLA	CMD-C2D-C1D	7.96	138.74	124.71
20	A	806	CLA	CMD-C2D-C1D	7.95	138.73	124.71
20	B	853	CLA	CMD-C2D-C1D	7.95	138.72	124.71
20	4	304	CLA	CMD-C2D-C1D	7.95	138.72	124.71
20	A	834	CLA	C2B-C1B-NB	7.94	115.56	110.23
20	B	824	CLA	CMD-C2D-C1D	7.94	138.71	124.71
20	B	830	CLA	C2C-C1C-NC	7.94	117.41	109.97
20	B	822	CLA	C2C-C1C-NC	7.93	117.40	109.97
20	A	833	CLA	C2B-C1B-NB	7.93	115.55	110.23
20	B	847	CLA	C2C-C1C-NC	7.93	117.40	109.97
20	B	802	CLA	C2B-C1B-NB	7.93	115.55	110.23
20	3	317	CLA	CMD-C2D-C1D	7.93	138.68	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	815	CLA	CMD-C2D-C1D	7.92	138.68	124.71
20	F	304	CLA	C2B-C1B-NB	7.92	115.54	110.23
20	G	207	CLA	CMD-C2D-C1D	7.92	138.67	124.71
20	1	308	CLA	CMD-C2D-C1D	7.92	138.66	124.71
20	3	318	CLA	CMD-C2D-C1D	7.91	138.66	124.71
20	B	816	CLA	C2B-C1B-NB	7.91	115.53	110.23
20	2	307	CLA	C2C-C1C-NC	7.90	117.37	109.97
20	B	849	CLA	CMD-C2D-C1D	7.90	138.63	124.71
20	A	854	CLA	C2C-C1C-NC	7.90	117.37	109.97
20	3	309	CLA	C2B-C1B-NB	7.90	115.53	110.23
20	3	311	CLA	CMD-C2D-C1D	7.89	138.62	124.71
20	A	840	CLA	C2B-C1B-NB	7.89	115.52	110.23
20	O	206	CLA	C2C-C1C-NC	7.89	117.36	109.97
20	1	320	CLA	CMD-C2D-C1D	7.89	138.61	124.71
20	3	307	CLA	CMD-C2D-C1D	7.89	138.61	124.71
20	A	828	CLA	CMD-C2D-C1D	7.88	138.61	124.71
20	A	833	CLA	C2C-C1C-NC	7.88	117.36	109.97
20	K	206	CLA	CMD-C2D-C1D	7.88	138.60	124.71
20	A	842	CLA	CMD-C2D-C1D	7.88	138.60	124.71
20	2	317	CLA	CMD-C2D-C1D	7.88	138.60	124.71
20	4	308	CLA	C1D-ND-C4D	-7.88	100.74	106.33
20	2	305	CLA	CMD-C2D-C1D	7.88	138.59	124.71
20	A	829	CLA	C2C-C1C-NC	7.87	117.35	109.97
20	1	306	CLA	C2B-C1B-NB	7.87	115.51	110.23
20	O	206	CLA	CMD-C2D-C1D	7.87	138.58	124.71
20	B	830	CLA	CMD-C2D-C1D	7.87	138.58	124.71
20	B	810	CLA	C2B-C1B-NB	7.87	115.50	110.23
20	4	311	CLA	C2B-C1B-NB	7.86	115.50	110.23
20	A	827	CLA	CMD-C2D-C1D	7.86	138.56	124.71
20	O	208	CLA	CMD-C2D-C1D	7.85	138.56	124.71
20	F	305	CLA	C2C-C1C-NC	7.85	117.33	109.97
20	B	816	CLA	C2C-C1C-NC	7.85	117.32	109.97
20	B	849	CLA	C2C-C1C-NC	7.84	117.32	109.97
20	3	315	CLA	CMD-C2D-C1D	7.84	138.53	124.71
20	1	302	CLA	CMD-C2D-C1D	7.84	138.53	124.71
20	3	310	CLA	C2C-C1C-NC	7.84	117.31	109.97
20	A	847	CLA	C2C-C1C-NC	7.84	117.31	109.97
20	B	823	CLA	C2C-C1C-NC	7.83	117.31	109.97
20	A	855	CLA	CMD-C2D-C1D	7.83	138.51	124.71
19	1	317	CHL	CMD-C2D-C1D	7.82	138.49	124.71
20	K	205	CLA	CMD-C2D-C1D	7.81	138.48	124.71
22	1	311	XAT	C11-C10-C9	-7.81	116.17	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	305	CLA	CMD-C2D-C1D	7.80	138.47	124.71
20	A	849	CLA	CMD-C2D-C1D	7.80	138.47	124.71
20	2	303	CLA	C2C-C1C-NC	7.80	117.28	109.97
20	B	808	CLA	C2C-C1C-NC	7.79	117.27	109.97
20	3	316	CLA	CMD-C2D-C1D	7.79	138.44	124.71
20	A	838	CLA	C2C-C1C-NC	7.79	117.27	109.97
22	2	311	XAT	C40-C33-C34	-7.79	112.02	122.92
20	A	806	CLA	C2C-C1C-NC	7.78	117.27	109.97
20	K	203	CLA	C2C-C1C-NC	7.78	117.26	109.97
20	A	804	CLA	CMD-C2D-C1D	7.78	138.43	124.71
22	2	311	XAT	O24-C25-C24	7.78	119.23	113.38
20	B	848	CLA	C2B-C1B-NB	7.78	115.45	110.23
20	G	205	CLA	CMD-C2D-C1D	7.78	138.42	124.71
20	4	311	CLA	CMD-C2D-C1D	7.78	138.42	124.71
19	1	317	CHL	C2C-C3C-C4C	-7.77	100.95	106.49
20	A	807	CLA	C2C-C1C-NC	7.77	117.25	109.97
20	4	310	CLA	C2C-C1C-NC	7.77	117.25	109.97
20	B	822	CLA	CMD-C2D-C1D	7.77	138.41	124.71
20	N	202	CLA	CMD-C2D-C1D	7.77	138.41	124.71
20	B	804	CLA	CMD-C2D-C1D	7.77	138.41	124.71
20	B	852	CLA	CMD-C2D-C1D	7.77	138.40	124.71
20	2	319	CLA	CMD-C2D-C1D	7.77	138.40	124.71
20	4	310	CLA	CMD-C2D-C1D	7.77	138.40	124.71
20	A	812	CLA	C1D-ND-C4D	-7.76	100.82	106.33
20	B	805	CLA	C2B-C1B-NB	7.76	115.44	110.23
20	J	103	CLA	C2C-C1C-NC	7.76	117.24	109.97
20	A	838	CLA	CMD-C2D-C1D	7.76	138.39	124.71
20	3	316	CLA	C2B-C1B-NB	7.76	115.43	110.23
20	2	306	CLA	C2B-C1B-NB	7.76	115.43	110.23
20	1	303	CLA	C2C-C1C-NC	7.75	117.24	109.97
20	4	312	CLA	C2C-C1C-NC	7.75	117.24	109.97
20	A	801	CLA	CMD-C2D-C1D	7.75	138.38	124.71
20	B	806	CLA	CMD-C2D-C1D	7.75	138.38	124.71
19	2	318	CHL	C2C-C3C-C4C	-7.75	100.96	106.49
20	H	201	CLA	C2B-C1B-NB	7.74	115.42	110.23
20	3	316	CLA	C2C-C1C-NC	7.74	117.22	109.97
20	B	853	CLA	C2C-C1C-NC	7.74	117.22	109.97
19	2	302	CHL	C2C-C3C-C4C	-7.74	100.97	106.49
20	A	843	CLA	C1D-ND-C4D	-7.74	100.84	106.33
20	A	850	CLA	C2C-C1C-NC	7.74	117.22	109.97
20	A	806	CLA	C2B-C1B-NB	7.73	115.42	110.23
20	G	205	CLA	C2C-C1C-NC	7.73	117.21	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	318	XAT	O4-C5-C4	7.73	119.19	113.38
20	A	811	CLA	CMD-C2D-C1D	7.72	138.31	124.71
20	A	839	CLA	CMD-C2D-C1D	7.72	138.31	124.71
20	2	306	CLA	C2C-C1C-NC	7.72	117.20	109.97
20	K	206	CLA	C2C-C1C-NC	7.71	117.20	109.97
20	B	827	CLA	CMD-C2D-C1D	7.71	138.30	124.71
20	1	306	CLA	CMD-C2D-C1D	7.71	138.30	124.71
22	3	302	XAT	C27-C28-C29	-7.71	113.57	125.53
20	1	322	CLA	CMD-C2D-C1D	7.71	138.30	124.71
20	4	311	CLA	C2C-C1C-NC	7.69	117.18	109.97
20	B	821	CLA	C2C-C1C-NC	7.69	117.18	109.97
20	2	321	CLA	C2C-C1C-NC	7.69	117.18	109.97
20	B	825	CLA	C2C-C1C-NC	7.68	117.16	109.97
20	3	315	CLA	C2C-C1C-NC	7.68	117.16	109.97
20	L	307	CLA	C2C-C1C-NC	7.67	117.16	109.97
20	A	847	CLA	C2B-C1B-NB	7.67	115.37	110.23
20	H	201	CLA	CMD-C2D-C1D	7.66	138.22	124.71
20	B	827	CLA	C2B-C1B-NB	7.66	115.37	110.23
20	A	804	CLA	C2B-C1B-NB	7.66	115.36	110.23
19	4	315	CHL	C2C-C3C-C4C	-7.65	101.03	106.49
20	1	319	CLA	C2C-C1C-NC	7.65	117.14	109.97
20	A	852	CLA	C2C-C1C-NC	7.65	117.14	109.97
20	G	207	CLA	C2C-C1C-NC	7.65	117.14	109.97
22	3	302	XAT	C35-C15-C14	-7.64	107.82	123.47
19	1	301	CHL	C2C-C3C-C4C	-7.64	101.04	106.49
20	3	308	CLA	CMD-C2D-C1D	7.64	138.18	124.71
20	F	306	CLA	C2C-C1C-NC	7.63	117.12	109.97
20	B	804	CLA	C2C-C1C-NC	7.63	117.12	109.97
20	A	846	CLA	C2B-C1B-NB	7.63	115.35	110.23
20	A	839	CLA	C2C-C1C-NC	7.63	117.12	109.97
20	B	824	CLA	C2C-C1C-NC	7.63	117.12	109.97
20	B	810	CLA	C2C-C1C-NC	7.63	117.12	109.97
20	1	321	CLA	C2C-C1C-NC	7.62	117.11	109.97
20	1	302	CLA	C2C-C1C-NC	7.62	117.11	109.97
20	A	851	CLA	CMD-C2D-C1D	7.62	138.15	124.71
20	B	830	CLA	C2B-C1B-NB	7.61	115.34	110.23
20	1	303	CLA	C2B-C1B-NB	7.61	115.33	110.23
22	1	311	XAT	O24-C25-C38	7.61	124.17	115.06
20	A	841	CLA	CMD-C2D-C1D	7.60	138.11	124.71
20	B	828	CLA	C2C-C1C-NC	7.59	117.09	109.97
20	1	304	CLA	CMD-C2D-C1D	7.59	138.10	124.71
20	A	832	CLA	C2C-C1C-NC	7.59	117.09	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	846	CLA	C2C-C1C-NC	7.59	117.09	109.97
20	B	831	CLA	CMD-C2D-C1D	7.59	138.09	124.71
20	A	835	CLA	CMD-C2D-C1D	7.59	138.09	124.71
20	B	811	CLA	CMD-C2D-C1D	7.59	138.08	124.71
20	A	846	CLA	CMD-C2D-C1D	7.58	138.08	124.71
20	B	808	CLA	CMD-C2D-C1D	7.58	138.07	124.71
20	3	307	CLA	C1D-ND-C4D	-7.58	100.95	106.33
20	A	843	CLA	CMD-C2D-C1D	7.57	138.06	124.71
20	2	317	CLA	C2C-C1C-NC	7.57	117.07	109.97
20	B	828	CLA	C2B-C1B-NB	7.57	115.31	110.23
20	3	312	CLA	CMD-C2D-C1D	7.57	138.05	124.71
20	B	805	CLA	C2C-C1C-NC	7.56	117.06	109.97
20	B	811	CLA	C2C-C1C-NC	7.56	117.06	109.97
20	B	805	CLA	CMD-C2D-C1D	7.56	138.04	124.71
20	3	312	CLA	C2C-C1C-NC	7.56	117.06	109.97
20	F	306	CLA	CMD-C2D-C1D	7.56	138.03	124.71
20	K	204	CLA	C2C-C1C-NC	7.56	117.05	109.97
20	A	855	CLA	C2B-C1B-NB	7.55	115.30	110.23
20	A	829	CLA	CMD-C2D-C1D	7.55	138.02	124.71
20	B	850	CLA	C2B-C1B-NB	7.55	115.29	110.23
20	1	309	CLA	C2C-C1C-NC	7.54	117.04	109.97
20	2	304	CLA	C2C-C1C-NC	7.54	117.03	109.97
20	B	807	CLA	C2C-C1C-NC	7.54	117.03	109.97
20	F	304	CLA	CMD-C2D-C1D	7.54	137.99	124.71
20	A	829	CLA	C2B-C1B-NB	7.53	115.28	110.23
20	B	826	CLA	CMD-C2D-C1D	7.53	137.99	124.71
20	4	314	CLA	C2C-C1C-NC	7.53	117.03	109.97
20	2	308	CLA	C2C-C1C-NC	7.53	117.03	109.97
20	A	803	CLA	C2C-C1C-NC	7.53	117.02	109.97
20	B	801	CLA	CMD-C2D-C1D	7.53	137.98	124.71
20	1	306	CLA	C2C-C1C-NC	7.53	117.02	109.97
20	B	850	CLA	C2C-C1C-NC	7.51	117.01	109.97
19	2	309	CHL	C2C-C3C-C4C	-7.51	101.14	106.49
20	G	206	CLA	C2C-C1C-NC	7.51	117.01	109.97
20	B	809	CLA	CMD-C2D-C1D	7.51	137.94	124.71
19	4	307	CHL	C2C-C3C-C4C	-7.50	101.14	106.49
20	B	818	CLA	C2C-C1C-NC	7.50	117.00	109.97
20	L	306	CLA	C2C-C1C-NC	7.50	117.00	109.97
20	F	304	CLA	C2C-C1C-NC	7.49	116.99	109.97
20	A	844	CLA	C2C-C1C-NC	7.49	116.99	109.97
20	1	320	CLA	C2C-C1C-NC	7.48	116.98	109.97
20	H	201	CLA	C2C-C1C-NC	7.48	116.98	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	853	CLA	C2C-C1C-NC	7.48	116.98	109.97
20	1	304	CLA	C2C-C1C-NC	7.47	116.97	109.97
20	B	820	CLA	CMD-C2D-C1D	7.46	137.86	124.71
20	3	314	CLA	CMD-C2D-C1D	7.46	137.85	124.71
20	G	206	CLA	C2B-C1B-NB	7.45	115.23	110.23
20	4	302	CLA	CMD-C2D-C1D	7.45	137.84	124.71
20	A	850	CLA	CMD-C2D-C1D	7.45	137.84	124.71
22	2	311	XAT	C38-C25-C26	-7.44	109.78	122.26
20	3	317	CLA	C2C-C1C-NC	7.44	116.94	109.97
20	A	849	CLA	C2B-C1B-NB	7.44	115.22	110.23
20	A	844	CLA	CMD-C2D-C1D	7.43	137.81	124.71
20	A	845	CLA	C2C-C1C-NC	7.43	116.93	109.97
20	1	307	CLA	C2C-C1C-NC	7.42	116.93	109.97
20	A	856	CLA	C2C-C1C-NC	7.42	116.93	109.97
20	1	308	CLA	C2C-C1C-NC	7.42	116.92	109.97
19	2	322	CHL	C2C-C3C-C4C	-7.42	101.20	106.49
20	4	304	CLA	C2C-C1C-NC	7.41	116.91	109.97
20	4	309	CLA	CMD-C2D-C1D	7.40	137.76	124.71
20	A	832	CLA	CMD-C2D-C1D	7.40	137.75	124.71
20	A	830	CLA	CMD-C2D-C1D	7.40	137.75	124.71
20	A	802	CLA	CMD-C2D-C1D	7.40	137.75	124.71
20	B	852	CLA	C2C-C1C-NC	7.40	116.90	109.97
20	B	825	CLA	CMD-C2D-C1D	7.40	137.75	124.71
20	3	314	CLA	C2B-C1B-NB	7.38	115.18	110.23
20	B	806	CLA	C2C-C1C-NC	7.38	116.89	109.97
20	4	303	CLA	C2B-C1B-NB	7.37	115.17	110.23
20	A	802	CLA	C2C-C1C-NC	7.36	116.87	109.97
20	3	318	CLA	C2C-C1C-NC	7.36	116.87	109.97
20	O	207	CLA	C2C-C1C-NC	7.36	116.86	109.97
20	B	833	CLA	C2C-C1C-NC	7.35	116.86	109.97
20	B	810	CLA	CMD-C2D-C1D	7.35	137.66	124.71
20	B	816	CLA	CMD-C2D-C1D	7.35	137.66	124.71
20	A	852	CLA	CMD-C2D-C1D	7.34	137.65	124.71
20	4	313	CLA	C2C-C1C-NC	7.32	116.83	109.97
20	F	305	CLA	CMD-C2D-C1D	7.32	137.62	124.71
20	B	848	CLA	C2C-C1C-NC	7.32	116.83	109.97
20	B	803	CLA	C2C-C1C-NC	7.32	116.83	109.97
20	B	812	CLA	CMD-C2D-C1D	7.31	137.60	124.71
20	1	322	CLA	C2C-C1C-NC	7.31	116.82	109.97
20	B	812	CLA	C2C-C1C-NC	7.31	116.82	109.97
20	2	305	CLA	C2C-C1C-NC	7.31	116.82	109.97
19	4	305	CHL	C2C-C3C-C4C	-7.30	101.28	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	320	CLA	C2C-C1C-NC	7.30	116.81	109.97
20	2	304	CLA	CMD-C2D-C1D	7.30	137.58	124.71
20	B	847	CLA	C2B-C1B-NB	7.30	115.12	110.23
20	A	805	CLA	C2C-C1C-NC	7.29	116.81	109.97
20	A	808	CLA	CMD-C2D-C1D	7.29	137.57	124.71
20	A	809	CLA	C2C-C1C-NC	7.29	116.80	109.97
20	B	826	CLA	C2C-C1C-NC	7.29	116.80	109.97
20	4	303	CLA	C2C-C1C-NC	7.29	116.80	109.97
20	A	848	CLA	CMD-C2D-C1D	7.28	137.54	124.71
20	4	302	CLA	C2C-C1C-NC	7.28	116.79	109.97
20	2	323	CLA	C2C-C1C-NC	7.27	116.79	109.97
20	L	305	CLA	C2C-C1C-NC	7.27	116.79	109.97
20	B	802	CLA	C2C-C1C-NC	7.27	116.78	109.97
20	B	851	CLA	C2B-C1B-NB	7.25	115.09	110.23
20	4	314	CLA	CMD-C2D-C1D	7.25	137.50	124.71
20	B	814	CLA	C2C-C1C-NC	7.25	116.76	109.97
20	A	836	CLA	C2C-C1C-NC	7.24	116.75	109.97
20	2	319	CLA	C2C-C1C-NC	7.23	116.75	109.97
20	B	817	CLA	C2C-C1C-NC	7.23	116.75	109.97
20	L	306	CLA	CMD-C2D-C1D	7.23	137.46	124.71
20	A	835	CLA	C2C-C1C-NC	7.23	116.74	109.97
28	A	824	CL0	CMD-C2D-C1D	7.22	137.44	124.71
20	N	202	CLA	C2C-C1C-NC	7.21	116.72	109.97
20	K	205	CLA	C2B-C1B-NB	7.21	115.06	110.23
20	A	833	CLA	CMD-C2D-C1D	7.18	137.38	124.71
23	O	203	BCR	C16-C15-C14	7.18	138.19	123.47
20	O	208	CLA	C2C-C1C-NC	7.18	116.70	109.97
20	B	814	CLA	CMD-C2D-C1D	7.18	137.36	124.71
20	A	851	CLA	C2C-C1C-NC	7.17	116.69	109.97
20	A	803	CLA	C2B-C1B-NB	7.17	115.04	110.23
22	1	311	XAT	C18-C5-C6	-7.16	110.25	122.26
20	B	813	CLA	C2C-C1C-NC	7.16	116.68	109.97
20	B	819	CLA	CMD-C2D-C1D	7.16	137.33	124.71
20	A	828	CLA	C2C-C1C-NC	7.16	116.68	109.97
20	1	305	CLA	C2C-C1C-NC	7.15	116.67	109.97
20	B	844	CLA	CMD-C2D-C1D	7.15	137.32	124.71
20	A	827	CLA	C2C-C1C-NC	7.15	116.67	109.97
20	B	825	CLA	C2B-C1B-NB	7.15	115.02	110.23
20	1	303	CLA	CMD-C2D-C1D	7.12	137.26	124.71
20	B	823	CLA	CMD-C2D-C1D	7.09	137.22	124.71
20	B	809	CLA	C2C-C1C-NC	7.09	116.61	109.97
20	B	813	CLA	CMD-C2D-C1D	7.09	137.21	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	824	CL0	C2B-C1B-NB	7.08	114.98	110.23
20	B	831	CLA	C2C-C1C-NC	7.06	116.58	109.97
20	A	845	CLA	CMD-C2D-C1D	7.05	137.13	124.71
20	4	312	CLA	C2B-C1B-NB	7.04	114.95	110.23
20	2	320	CLA	C3C-C4C-NC	7.04	118.26	110.57
22	3	302	XAT	C18-C5-C6	-7.02	110.50	122.26
20	A	812	CLA	C2C-C1C-NC	7.02	116.54	109.97
20	B	815	CLA	C2C-C1C-NC	7.00	116.53	109.97
19	3	313	CHL	C2C-C3C-C4C	-6.99	101.50	106.49
20	A	811	CLA	C2C-C1C-NC	6.99	116.52	109.97
20	B	846	CLA	C2C-C1C-NC	6.96	116.49	109.97
20	B	819	CLA	C1D-ND-C4D	-6.96	101.39	106.33
22	2	311	XAT	C15-C35-C34	6.96	137.73	123.47
19	2	318	CHL	CHD-C1D-ND	-6.95	118.07	124.45
20	2	303	CLA	CMD-C2D-C1D	6.91	136.89	124.71
20	B	829	CLA	C2C-C1C-NC	6.91	116.44	109.97
28	A	824	CL0	C1D-ND-C4D	-6.90	101.43	106.33
20	A	841	CLA	C2C-C1C-NC	6.89	116.42	109.97
20	A	842	CLA	C2C-C1C-NC	6.89	116.42	109.97
20	B	847	CLA	C3C-C4C-NC	6.86	118.27	110.57
22	4	318	XAT	C38-C25-C26	-6.85	110.78	122.26
20	B	845	CLA	C2C-C1C-NC	6.85	116.39	109.97
20	B	851	CLA	CMD-C2D-C1D	6.82	136.74	124.71
23	B	839	BCR	C15-C16-C17	6.81	137.43	123.47
22	4	318	XAT	C18-C5-C6	-6.79	110.89	122.26
20	3	309	CLA	C2C-C1C-NC	6.75	116.30	109.97
20	4	308	CLA	CMD-C2D-C1D	6.75	136.61	124.71
20	B	827	CLA	C2C-C1C-NC	6.75	116.29	109.97
20	B	844	CLA	C3C-C4C-NC	6.73	118.12	110.57
19	2	309	CHL	CHD-C1D-ND	-6.72	118.28	124.45
20	B	814	CLA	C3C-C4C-NC	6.72	118.10	110.57
22	4	318	XAT	O24-C25-C24	6.71	118.42	113.38
22	1	311	XAT	C38-C25-C26	-6.71	111.02	122.26
20	4	309	CLA	C2C-C1C-NC	6.69	116.24	109.97
20	4	316	CLA	C3C-C4C-NC	6.68	118.06	110.57
20	B	807	CLA	C4-C3-C5	6.68	126.51	115.27
20	A	812	CLA	CMD-C2D-C1D	6.68	136.48	124.71
20	A	849	CLA	C3C-C4C-NC	6.67	118.06	110.57
28	A	824	CL0	C3C-C4C-NC	6.67	118.05	110.57
20	A	801	CLA	C1B-C2B-C3B	-6.67	100.70	107.03
20	3	308	CLA	C2C-C1C-NC	6.65	116.20	109.97
20	A	853	CLA	CMD-C2D-C1D	6.64	136.42	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	837	CLA	C2C-C1C-NC	6.64	116.19	109.97
20	A	834	CLA	C3C-C4C-NC	6.62	118.00	110.57
20	2	320	CLA	C2B-C1B-NB	6.55	114.62	110.23
20	2	304	CLA	C2B-C1B-NB	6.53	114.61	110.23
20	A	825	CLA	C2C-C1C-NC	6.52	116.08	109.97
20	A	803	CLA	C3C-C4C-NC	6.51	117.87	110.57
20	A	812	CLA	C3C-C4C-NC	6.50	117.86	110.57
20	1	318	CLA	C2C-C1C-NC	6.49	116.05	109.97
20	A	851	CLA	C3C-C4C-NC	6.49	117.85	110.57
20	A	805	CLA	C3C-C4C-NC	6.49	117.84	110.57
20	3	316	CLA	C3C-C4C-NC	6.43	117.78	110.57
22	3	302	XAT	C28-C29-C30	6.43	128.80	118.94
24	B	842	LHG	O7-C7-C8	6.42	125.34	111.50
22	2	311	XAT	C31-C32-C33	-6.42	108.39	126.42
20	A	804	CLA	O2D-CGD-CBD	6.42	122.67	111.27
20	B	850	CLA	C3C-C4C-NC	6.41	117.76	110.57
20	B	816	CLA	C3C-C4C-NC	6.40	117.75	110.57
20	2	306	CLA	C3C-C4C-NC	6.39	117.73	110.57
19	2	322	CHL	CHD-C1D-ND	-6.38	118.59	124.45
20	A	812	CLA	C3B-C2B-C1B	-6.37	99.47	107.16
20	2	305	CLA	O2D-CGD-CBD	6.35	122.55	111.27
19	4	305	CHL	CHD-C1D-ND	-6.33	118.64	124.45
20	B	816	CLA	C4-C3-C5	6.32	125.91	115.27
20	B	821	CLA	C3C-C4C-NC	6.31	117.64	110.57
20	F	304	CLA	C3C-C4C-NC	6.31	117.64	110.57
19	3	313	CHL	CHD-C1D-ND	-6.30	118.66	124.45
20	B	844	CLA	C2B-C1B-NB	6.29	114.45	110.23
19	2	302	CHL	CHD-C1D-ND	-6.29	118.67	124.45
20	1	302	CLA	C3C-C4C-NC	6.29	117.62	110.57
19	4	306	CHL	CHD-C1D-ND	-6.29	118.68	124.45
20	B	826	CLA	C3C-C4C-NC	6.29	117.62	110.57
20	B	848	CLA	C3C-C4C-NC	6.28	117.62	110.57
20	B	831	CLA	C3C-C4C-NC	6.28	117.61	110.57
20	A	826	CLA	C1D-ND-C4D	-6.26	101.89	106.33
20	A	837	CLA	C3C-C4C-NC	6.26	117.59	110.57
20	4	311	CLA	C3C-C4C-NC	6.26	117.59	110.57
20	B	831	CLA	O2D-CGD-CBD	6.26	122.39	111.27
20	F	306	CLA	C3C-C4C-NC	6.25	117.58	110.57
20	4	312	CLA	C3C-C4C-NC	6.22	117.55	110.57
20	A	854	CLA	C3C-C4C-NC	6.22	117.55	110.57
20	A	854	CLA	CMD-C2D-C1D	6.22	135.67	124.71
20	B	845	CLA	C3C-C4C-NC	6.21	117.54	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	K	205	CLA	C3C-C4C-NC	6.20	117.52	110.57
19	1	317	CHL	CHD-C1D-ND	-6.19	118.77	124.45
28	A	824	CL0	CHD-C4C-C3C	-6.19	115.74	124.84
20	4	308	CLA	C3C-C4C-NC	6.19	117.51	110.57
20	B	845	CLA	CMD-C2D-C1D	6.18	135.61	124.71
20	G	206	CLA	C3C-C4C-NC	6.17	117.49	110.57
20	H	201	CLA	C3C-C4C-NC	6.17	117.49	110.57
20	A	842	CLA	C3C-C4C-NC	6.17	117.49	110.57
20	J	103	CLA	C3C-C4C-NC	6.16	117.48	110.57
19	2	301	CHL	CHD-C1D-ND	-6.16	118.79	124.45
20	A	831	CLA	C3C-C4C-NC	6.15	117.47	110.57
20	B	813	CLA	C3C-C4C-NC	6.14	117.46	110.57
20	B	803	CLA	C3C-C4C-NC	6.14	117.46	110.57
20	1	306	CLA	C3C-C4C-NC	6.13	117.45	110.57
20	3	317	CLA	C3C-C4C-NC	6.13	117.44	110.57
20	3	307	CLA	C3B-C2B-C1B	-6.12	99.77	107.16
20	A	830	CLA	C3C-C4C-NC	6.11	117.43	110.57
19	4	315	CHL	CHD-C1D-ND	-6.11	118.84	124.45
20	4	303	CLA	C3C-C4C-NC	6.11	117.42	110.57
20	A	847	CLA	C3C-C4C-NC	6.11	117.42	110.57
20	A	801	CLA	C3C-C4C-NC	6.09	117.40	110.57
20	2	303	CLA	C3C-C4C-NC	6.08	117.39	110.57
20	B	845	CLA	C3B-C2B-C1B	-6.08	99.82	107.16
20	3	307	CLA	C3C-C4C-NC	6.07	117.38	110.57
20	B	820	CLA	C3C-C4C-NC	6.07	117.38	110.57
20	A	807	CLA	C3C-C4C-NC	6.07	117.38	110.57
20	B	814	CLA	CHD-C4C-C3C	-6.06	115.93	124.84
20	B	805	CLA	C3C-C4C-NC	6.05	117.36	110.57
20	B	828	CLA	C3C-C4C-NC	6.04	117.35	110.57
20	A	825	CLA	C3C-C4C-NC	6.04	117.35	110.57
20	K	203	CLA	C3C-C4C-NC	6.03	117.34	110.57
20	4	310	CLA	C3C-C4C-NC	6.03	117.34	110.57
20	B	825	CLA	C3C-C4C-NC	6.03	117.33	110.57
20	A	850	CLA	C3C-C4C-NC	6.02	117.33	110.57
20	A	833	CLA	C3C-C4C-NC	6.02	117.32	110.57
20	1	303	CLA	C3C-C4C-NC	6.02	117.32	110.57
20	A	848	CLA	C3C-C4C-NC	6.02	117.32	110.57
20	1	309	CLA	C3C-C4C-NC	6.01	117.31	110.57
20	B	819	CLA	C2B-C1B-NB	6.01	114.26	110.23
19	1	301	CHL	CHD-C1D-ND	-6.00	118.94	124.45
20	B	815	CLA	C3B-C2B-C1B	-5.99	99.93	107.16
20	A	853	CLA	C3C-C4C-NC	5.99	117.29	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	817	CLA	C3C-C4C-NC	5.98	117.28	110.57
20	A	851	CLA	O2D-CGD-CBD	5.97	121.88	111.27
20	A	809	CLA	C3C-C4C-NC	5.96	117.26	110.57
20	1	305	CLA	C3C-C4C-NC	5.96	117.25	110.57
20	A	852	CLA	C3B-C2B-C1B	-5.96	99.97	107.16
20	N	202	CLA	C3C-C4C-NC	5.95	117.25	110.57
20	A	844	CLA	O2D-CGD-CBD	5.95	121.85	111.27
20	O	207	CLA	C3C-C4C-NC	5.95	117.25	110.57
20	3	314	CLA	C3C-C4C-NC	5.95	117.24	110.57
20	2	304	CLA	C3C-C4C-NC	5.94	117.23	110.57
19	4	307	CHL	CHD-C1D-ND	-5.93	119.00	124.45
20	A	834	CLA	CHD-C4C-C3C	-5.92	116.13	124.84
19	2	309	CHL	C3B-C2B-C1B	-5.92	100.01	107.16
20	2	307	CLA	C3C-C4C-NC	5.91	117.20	110.57
20	B	802	CLA	C3C-C4C-NC	5.91	117.20	110.57
20	A	808	CLA	C3C-C4C-NC	5.91	117.20	110.57
23	L	304	BCR	C1-C6-C5	-5.91	114.29	122.61
20	A	802	CLA	C3B-C2B-C1B	-5.91	100.03	107.16
20	B	807	CLA	C3C-C4C-NC	5.90	117.19	110.57
20	B	844	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
20	G	207	CLA	C3C-C4C-NC	5.90	117.19	110.57
20	1	321	CLA	C3C-C4C-NC	5.90	117.18	110.57
20	3	312	CLA	C3C-C4C-NC	5.89	117.18	110.57
20	B	849	CLA	C3C-C4C-NC	5.89	117.18	110.57
20	B	810	CLA	C3C-C4C-NC	5.89	117.18	110.57
24	A	820	LHG	O7-C7-C8	5.89	124.20	111.50
20	A	812	CLA	CHD-C4C-C3C	-5.88	116.19	124.84
20	2	317	CLA	C3C-C4C-NC	5.87	117.15	110.57
20	3	311	CLA	C3C-C4C-NC	5.87	117.15	110.57
20	4	316	CLA	CHD-C4C-C3C	-5.87	116.22	124.84
20	A	844	CLA	C3B-C2B-C1B	-5.86	100.09	107.16
20	1	307	CLA	C3C-C4C-NC	5.86	117.14	110.57
20	1	320	CLA	C3C-C4C-NC	5.86	117.14	110.57
20	3	318	CLA	C3C-C4C-NC	5.86	117.14	110.57
20	3	316	CLA	CHD-C4C-C3C	-5.85	116.23	124.84
20	B	821	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
20	K	205	CLA	C2C-C1C-NC	5.85	115.45	109.97
20	1	309	CLA	O2D-CGD-CBD	5.85	121.66	111.27
20	A	855	CLA	C3C-C4C-NC	5.84	117.13	110.57
23	O	203	BCR	C1-C6-C5	-5.84	114.38	122.61
20	A	811	CLA	C3C-C4C-NC	5.84	117.12	110.57
20	A	838	CLA	C3C-C4C-NC	5.84	117.12	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	814	CLA	C4-C3-C5	5.84	125.09	115.27
20	2	306	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
20	B	824	CLA	C3C-C4C-NC	5.81	117.08	110.57
20	A	826	CLA	C3B-C2B-C1B	-5.81	100.15	107.16
20	A	840	CLA	C3C-C4C-NC	5.80	117.08	110.57
20	A	826	CLA	CMD-C2D-C1D	5.80	134.94	124.71
20	B	848	CLA	CHD-C4C-C3C	-5.80	116.31	124.84
20	3	309	CLA	C3C-C4C-NC	5.80	117.08	110.57
20	B	806	CLA	C3C-C4C-NC	5.80	117.08	110.57
20	A	836	CLA	C3C-C4C-NC	5.80	117.07	110.57
20	L	306	CLA	O2D-CGD-CBD	5.80	121.57	111.27
20	A	850	CLA	C3B-C2B-C1B	-5.79	100.17	107.16
20	4	309	CLA	C3C-C4C-NC	5.79	117.06	110.57
20	B	804	CLA	C3C-C4C-NC	5.78	117.06	110.57
20	4	302	CLA	C3C-C4C-NC	5.78	117.06	110.57
20	K	206	CLA	C3C-C4C-NC	5.78	117.06	110.57
20	A	825	CLA	C3B-C2B-C1B	-5.78	100.18	107.16
20	B	826	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
20	A	803	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
20	L	306	CLA	C3C-C4C-NC	5.76	117.03	110.57
20	A	808	CLA	C3B-C2B-C1B	-5.76	100.21	107.16
20	B	826	CLA	C3B-C2B-C1B	-5.76	100.21	107.16
23	O	203	BCR	C12-C13-C14	5.76	127.78	118.94
20	B	847	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
20	B	852	CLA	C3C-C4C-NC	5.75	117.02	110.57
20	B	851	CLA	C3C-C4C-NC	5.75	117.01	110.57
20	O	206	CLA	C3C-C4C-NC	5.74	117.01	110.57
20	B	823	CLA	C3C-C4C-NC	5.74	117.01	110.57
20	3	311	CLA	C3B-C2B-C1B	-5.74	100.23	107.16
20	B	830	CLA	C3C-C4C-NC	5.74	117.00	110.57
20	B	850	CLA	CMD-C2D-C1D	5.74	134.82	124.71
20	A	849	CLA	CHD-C4C-C3C	-5.74	116.41	124.84
20	B	823	CLA	C3B-C2B-C1B	-5.73	100.24	107.16
20	2	319	CLA	C3B-C2B-C1B	-5.73	100.24	107.16
20	F	305	CLA	C3C-C4C-NC	5.73	116.99	110.57
20	L	307	CLA	C3C-C4C-NC	5.73	116.99	110.57
20	A	851	CLA	CHD-C4C-C3C	-5.73	116.42	124.84
20	B	822	CLA	C3C-C4C-NC	5.72	116.99	110.57
20	2	321	CLA	C3C-C4C-NC	5.72	116.99	110.57
20	A	839	CLA	C3B-C2B-C1B	-5.72	100.26	107.16
20	B	823	CLA	O2D-CGD-CBD	5.72	121.42	111.27
20	2	323	CLA	C3C-C4C-NC	5.71	116.98	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	O	208	CLA	C3C-C4C-NC	5.71	116.97	110.57
20	A	826	CLA	C3C-C4C-NC	5.71	116.97	110.57
20	A	837	CLA	C4-C3-C5	5.71	124.87	115.27
20	A	825	CLA	CMD-C2D-C1D	5.70	134.76	124.71
20	A	828	CLA	O2D-CGD-CBD	5.70	121.40	111.27
23	A	818	BCR	C1-C6-C5	-5.70	114.58	122.61
20	B	811	CLA	C3C-C4C-NC	5.70	116.96	110.57
20	A	854	CLA	O2D-CGD-CBD	5.69	121.38	111.27
20	A	854	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
20	B	809	CLA	C3C-C4C-NC	5.68	116.94	110.57
20	3	320	CLA	C3C-C4C-NC	5.68	116.94	110.57
20	F	306	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
20	A	841	CLA	C3C-C4C-NC	5.68	116.94	110.57
20	B	816	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
19	2	302	CHL	C3B-C2B-C1B	-5.67	100.31	107.16
20	B	815	CLA	C3C-C4C-NC	5.67	116.93	110.57
20	3	310	CLA	C3C-C4C-NC	5.67	116.93	110.57
20	1	308	CLA	C3C-C4C-NC	5.66	116.92	110.57
20	A	807	CLA	O2D-CGD-CBD	5.66	121.33	111.27
20	2	308	CLA	C3C-C4C-NC	5.66	116.92	110.57
20	B	827	CLA	C3C-C4C-NC	5.66	116.92	110.57
20	B	817	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
20	B	801	CLA	C3C-C4C-NC	5.65	116.91	110.57
20	L	306	CLA	C3B-C2B-C1B	-5.65	100.34	107.16
20	A	849	CLA	O2D-CGD-CBD	5.65	121.31	111.27
20	1	322	CLA	C3C-C4C-NC	5.65	116.91	110.57
20	B	827	CLA	O2D-CGD-CBD	5.65	121.31	111.27
20	2	319	CLA	C3C-C4C-NC	5.65	116.91	110.57
21	1	323	LUT	C7-C8-C9	5.65	134.77	126.23
20	B	814	CLA	C3B-C2B-C1B	-5.65	100.34	107.16
20	A	825	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
20	B	808	CLA	O2D-CGD-CBD	5.64	121.29	111.27
20	B	808	CLA	C3C-C4C-NC	5.64	116.90	110.57
20	G	205	CLA	C3C-C4C-NC	5.64	116.89	110.57
20	3	319	CLA	C3C-C4C-NC	5.64	116.89	110.57
20	4	314	CLA	C3C-C4C-NC	5.63	116.89	110.57
19	1	301	CHL	C3B-C2B-C1B	-5.63	100.37	107.16
20	B	831	CLA	CHD-C4C-C3C	-5.62	116.57	124.84
20	B	803	CLA	C3B-C2B-C1B	-5.62	100.38	107.16
20	A	804	CLA	C3C-C4C-NC	5.62	116.87	110.57
20	1	302	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
20	4	313	CLA	C3C-C4C-NC	5.61	116.86	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	828	CLA	C3B-C2B-C1B	-5.61	100.39	107.16
20	2	320	CLA	CHD-C4C-C3C	-5.61	116.22	124.98
20	A	830	CLA	O2D-CGD-CBD	5.61	121.23	111.27
20	A	803	CLA	CMD-C2D-C1D	5.61	134.59	124.71
20	B	828	CLA	CHD-C4C-C3C	-5.61	116.60	124.84
20	3	320	CLA	C3B-C2B-C1B	-5.61	100.39	107.16
20	4	308	CLA	C3B-C2B-C1B	-5.60	100.40	107.16
20	F	304	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
22	1	311	XAT	C15-C35-C34	-5.60	112.00	123.47
20	A	854	CLA	C2B-C1B-NB	5.60	113.99	110.23
20	1	304	CLA	C3C-C4C-NC	5.60	116.85	110.57
19	2	318	CHL	C3B-C2B-C1B	-5.60	100.40	107.16
20	A	838	CLA	C3B-C2B-C1B	-5.60	100.40	107.16
20	B	846	CLA	C3B-C2B-C1B	-5.59	100.41	107.16
20	K	204	CLA	C3C-C4C-NC	5.59	116.84	110.57
20	A	805	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
20	3	308	CLA	C3B-C2B-C1B	-5.59	100.42	107.16
20	3	315	CLA	C3C-C4C-NC	5.59	116.83	110.57
20	A	828	CLA	C3C-C4C-NC	5.58	116.83	110.57
20	4	302	CLA	C3B-C2B-C1B	-5.58	100.43	107.16
20	3	310	CLA	C3B-C2B-C1B	-5.57	100.44	107.16
20	A	851	CLA	C3B-C2B-C1B	-5.57	100.44	107.16
20	A	827	CLA	C3C-C4C-NC	5.56	116.81	110.57
20	A	829	CLA	C3C-C4C-NC	5.56	116.80	110.57
20	A	832	CLA	O2D-CGD-CBD	5.55	121.14	111.27
22	2	311	XAT	C26-C27-C28	-5.55	114.25	125.99
20	1	304	CLA	C3B-C2B-C1B	-5.55	100.46	107.16
20	1	318	CLA	C3B-C2B-C1B	-5.55	100.46	107.16
20	A	856	CLA	C3B-C2B-C1B	-5.55	100.46	107.16
20	A	845	CLA	C3C-C4C-NC	5.55	116.79	110.57
20	L	306	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
20	A	827	CLA	O2D-CGD-CBD	5.55	121.12	111.27
20	1	309	CLA	CHD-C4C-C3C	-5.54	116.69	124.84
20	B	805	CLA	CHD-C4C-C3C	-5.54	116.69	124.84
20	A	842	CLA	CHD-C4C-C3C	-5.54	116.69	124.84
20	B	818	CLA	C3C-C4C-NC	5.54	116.78	110.57
20	B	829	CLA	C3C-C4C-NC	5.54	116.78	110.57
20	3	312	CLA	C3B-C2B-C1B	-5.54	100.48	107.16
20	B	820	CLA	C3B-C2B-C1B	-5.54	100.48	107.16
19	4	306	CHL	C3B-C2B-C1B	-5.54	100.48	107.16
20	1	306	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
19	2	322	CHL	C3B-C2B-C1B	-5.53	100.49	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	312	CLA	CHD-C4C-C3C	-5.53	116.72	124.84
20	B	816	CLA	C3B-C2B-C1B	-5.52	100.49	107.16
20	A	832	CLA	C3C-C4C-NC	5.52	116.77	110.57
20	A	807	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
20	B	810	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
20	B	812	CLA	C3C-C4C-NC	5.51	116.75	110.57
20	B	850	CLA	O2D-CGD-CBD	5.51	121.06	111.27
20	B	811	CLA	CHD-C4C-C3C	-5.51	116.75	124.84
20	K	206	CLA	C3B-C2B-C1B	-5.50	100.52	107.16
20	A	830	CLA	C3B-C2B-C1B	-5.49	100.53	107.16
20	B	850	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
20	4	311	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
20	A	856	CLA	C3C-C4C-NC	5.49	116.72	110.57
20	B	805	CLA	O2D-CGD-CBD	5.48	121.01	111.27
20	A	842	CLA	C3B-C2B-C1B	-5.48	100.55	107.16
20	3	308	CLA	C3C-C4C-NC	5.47	116.71	110.57
19	4	305	CHL	C3B-C2B-C1B	-5.47	100.56	107.16
20	1	308	CLA	C3B-C2B-C1B	-5.47	100.56	107.16
20	B	817	CLA	C3B-C2B-C1B	-5.47	100.56	107.16
20	A	806	CLA	C3C-C4C-NC	5.47	116.70	110.57
20	A	827	CLA	C3B-C2B-C1B	-5.47	100.56	107.16
20	K	203	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
20	A	853	CLA	C3B-C2B-C1B	-5.46	100.57	107.16
20	B	824	CLA	CHD-C4C-C3C	-5.46	116.82	124.84
20	B	853	CLA	C3C-C4C-NC	5.46	116.69	110.57
20	N	202	CLA	CHD-C4C-C3C	-5.45	116.82	124.84
20	O	206	CLA	C3B-C2B-C1B	-5.45	100.58	107.16
20	K	204	CLA	C3B-C2B-C1B	-5.45	100.58	107.16
22	3	302	XAT	O4-C5-C4	5.45	117.47	113.38
20	O	206	CLA	O2D-CGD-CBD	5.45	120.95	111.27
20	B	827	CLA	CHD-C4C-C3C	-5.45	116.84	124.84
20	J	103	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
20	L	305	CLA	C3C-C4C-NC	5.44	116.67	110.57
20	B	810	CLA	O2D-CGD-CBD	5.44	120.94	111.27
20	A	847	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
20	B	807	CLA	C3B-C2B-C1B	-5.44	100.60	107.16
20	A	850	CLA	CHD-C4C-C3C	-5.44	116.85	124.84
20	L	305	CLA	C3B-C2B-C1B	-5.44	100.60	107.16
20	A	855	CLA	CHD-C4C-C3C	-5.44	116.85	124.84
20	H	201	CLA	CHD-C4C-C3C	-5.44	116.85	124.84
20	2	305	CLA	C3C-C4C-NC	5.44	116.67	110.57
20	1	321	CLA	C3B-C2B-C1B	-5.43	100.60	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	833	CLA	C3C-C4C-NC	5.42	116.65	110.57
22	3	302	XAT	O24-C25-C38	5.42	121.55	115.06
20	B	813	CLA	CHD-C4C-C3C	-5.42	116.88	124.84
20	B	801	CLA	C3B-C2B-C1B	-5.42	100.62	107.16
20	B	849	CLA	O2D-CGD-CBD	5.41	120.89	111.27
19	4	315	CHL	C3B-C2B-C1B	-5.41	100.63	107.16
20	B	804	CLA	C3B-C2B-C1B	-5.41	100.63	107.16
20	A	828	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
20	A	830	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
20	2	321	CLA	C3B-C2B-C1B	-5.41	100.63	107.16
20	4	304	CLA	C3C-C4C-NC	5.41	116.64	110.57
20	A	839	CLA	C3C-C4C-NC	5.41	116.64	110.57
20	G	207	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
20	O	208	CLA	C3B-C2B-C1B	-5.41	100.64	107.16
23	O	202	BCR	C37-C22-C21	-5.40	115.35	122.92
20	4	303	CLA	CHD-C4C-C3C	-5.40	116.90	124.84
20	B	822	CLA	C3B-C2B-C1B	-5.40	100.64	107.16
20	A	834	CLA	C3B-C2B-C1B	-5.39	100.65	107.16
20	G	207	CLA	C3B-C2B-C1B	-5.39	100.65	107.16
20	G	206	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
20	A	811	CLA	O2D-CGD-CBD	5.39	120.85	111.27
19	3	313	CHL	C3B-C2B-C1B	-5.39	100.66	107.16
20	4	309	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
20	B	825	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
20	3	312	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
20	3	315	CLA	C3B-C2B-C1B	-5.39	100.66	107.16
20	B	823	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
23	F	301	BCR	C15-C16-C17	5.38	134.50	123.47
20	A	805	CLA	C3B-C2B-C1B	-5.38	100.67	107.16
20	B	803	CLA	O2D-CGD-CBD	5.38	120.83	111.27
20	A	801	CLA	CHD-C4C-C3C	-5.38	116.94	124.84
20	G	205	CLA	CHD-C4C-C3C	-5.37	116.94	124.84
20	3	318	CLA	CHD-C4C-C3C	-5.37	116.94	124.84
20	1	307	CLA	CHD-C4C-C3C	-5.37	116.95	124.84
20	A	843	CLA	C3C-C4C-NC	5.37	116.59	110.57
20	G	207	CLA	O2D-CGD-CBD	5.37	120.80	111.27
19	1	317	CHL	O2D-CGD-CBD	5.36	120.80	111.27
20	A	845	CLA	C3B-C2B-C1B	-5.36	100.69	107.16
20	B	812	CLA	O2D-CGD-CBD	5.36	120.79	111.27
20	2	317	CLA	CHD-C4C-C3C	-5.36	116.97	124.84
20	1	308	CLA	O2D-CGD-CBD	5.36	120.79	111.27
20	L	307	CLA	CHD-C4C-C3C	-5.35	116.97	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	319	CLA	O2D-CGD-CBD	5.35	120.78	111.27
20	B	849	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
20	A	835	CLA	C3C-C4C-NC	5.35	116.57	110.57
20	4	310	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
19	2	301	CHL	C3B-C2B-C1B	-5.34	100.71	107.16
20	3	308	CLA	O2D-CGD-CBD	5.34	120.76	111.27
20	B	801	CLA	C4-C3-C5	5.34	124.25	115.27
20	A	811	CLA	CHD-C4C-C3C	-5.34	117.00	124.84
20	1	320	CLA	O2D-CGD-CBD	5.34	120.75	111.27
19	1	317	CHL	C3B-C2B-C1B	-5.34	100.72	107.16
23	O	203	BCR	C7-C8-C9	5.33	134.29	126.23
20	A	836	CLA	CHD-C4C-C3C	-5.33	117.00	124.84
23	L	304	BCR	C37-C22-C21	-5.33	115.46	122.92
20	A	838	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
22	4	318	XAT	C26-C27-C28	-5.32	114.74	125.99
19	2	318	CHL	C3C-C4C-NC	5.32	116.54	110.57
20	K	205	CLA	CHC-C4B-NB	-5.32	118.63	124.26
20	K	206	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
20	O	207	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
20	2	323	CLA	C3B-C2B-C1B	-5.31	100.75	107.16
20	K	203	CLA	C3B-C2B-C1B	-5.30	100.76	107.16
20	A	846	CLA	C3C-C4C-NC	5.30	116.52	110.57
22	3	302	XAT	C30-C31-C32	-5.30	106.68	123.22
20	A	849	CLA	C3B-C2B-C1B	-5.29	100.78	107.16
20	B	819	CLA	C3C-C4C-NC	5.29	116.50	110.57
20	4	304	CLA	C3B-C2B-C1B	-5.29	100.78	107.16
20	3	314	CLA	CHD-C4C-C3C	-5.28	117.07	124.84
20	3	315	CLA	CHD-C4C-C3C	-5.28	117.07	124.84
20	B	822	CLA	CHD-C4C-C3C	-5.28	117.08	124.84
20	B	806	CLA	C4-C3-C5	5.28	124.15	115.27
20	A	809	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
20	2	304	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
20	2	303	CLA	CHD-C4C-C3C	-5.27	117.10	124.84
19	4	307	CHL	C3B-C2B-C1B	-5.26	100.81	107.16
20	B	815	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
20	B	806	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
20	A	855	CLA	C3B-C2B-C1B	-5.25	100.82	107.16
20	2	319	CLA	O2D-CGD-CBD	5.25	120.60	111.27
19	2	309	CHL	O2D-CGD-CBD	5.25	120.60	111.27
20	2	319	CLA	CHD-C4C-C3C	-5.25	117.13	124.84
20	A	843	CLA	O2D-CGD-CBD	5.24	120.58	111.27
20	L	307	CLA	C3B-C2B-C1B	-5.24	100.83	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	317	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
20	3	311	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
20	1	320	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
20	2	321	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
20	1	318	CLA	O2D-CGD-CBD	5.23	120.57	111.27
20	4	311	CLA	O2D-CGD-CBD	5.23	120.56	111.27
20	O	206	CLA	CHD-C4C-C3C	-5.23	117.16	124.84
20	B	853	CLA	C3B-C2B-C1B	-5.23	100.85	107.16
20	1	305	CLA	CHD-C4C-C3C	-5.23	117.16	124.84
20	1	308	CLA	CHD-C4C-C3C	-5.23	117.16	124.84
20	B	803	CLA	CHD-C4C-C3C	-5.23	117.16	124.84
19	4	307	CHL	C3C-C4C-NC	5.23	116.43	110.57
20	A	852	CLA	CHD-C1D-ND	-5.22	119.65	124.45
20	B	803	CLA	CAC-C3C-C4C	5.22	131.59	124.81
20	B	808	CLA	CHD-C4C-C3C	-5.21	117.18	124.84
20	1	321	CLA	CHD-C4C-C3C	-5.21	117.18	124.84
23	O	202	BCR	C1-C6-C5	-5.21	115.28	122.61
20	2	308	CLA	CHD-C4C-C3C	-5.21	117.19	124.84
20	B	804	CLA	CHD-C4C-C3C	-5.21	117.19	124.84
20	A	833	CLA	CHD-C4C-C3C	-5.20	117.19	124.84
20	1	303	CLA	CHD-C4C-C3C	-5.20	117.19	124.84
20	G	205	CLA	C3B-C2B-C1B	-5.20	100.88	107.16
20	F	305	CLA	CHD-C4C-C3C	-5.20	117.20	124.84
20	A	801	CLA	C3B-C4B-NB	5.19	113.71	110.23
19	2	301	CHL	C3C-C4C-NC	5.19	116.39	110.57
20	K	203	CLA	O2D-CGD-CBD	5.19	120.49	111.27
19	4	315	CHL	C3C-C4C-NC	5.19	116.39	110.57
20	2	307	CLA	CHD-C4C-C3C	-5.19	117.22	124.84
20	1	318	CLA	C3C-C4C-NC	5.19	116.39	110.57
22	3	302	XAT	O24-C25-C24	5.18	117.28	113.38
20	A	841	CLA	CHD-C4C-C3C	-5.18	117.22	124.84
20	2	320	CLA	C4A-NA-C1A	5.18	109.03	106.71
21	1	323	LUT	C8-C9-C10	5.18	126.89	118.94
20	A	847	CLA	CHD-C1D-ND	-5.18	119.69	124.45
22	3	302	XAT	C15-C35-C34	5.18	134.08	123.47
20	B	816	CLA	O2D-CGD-CBD	5.18	120.47	111.27
20	A	808	CLA	CHD-C4C-C3C	-5.18	117.23	124.84
20	B	805	CLA	C3B-C2B-C1B	-5.18	100.91	107.16
20	K	205	CLA	O2D-CGD-CBD	5.17	120.45	111.27
20	3	310	CLA	CHD-C4C-C3C	-5.17	117.24	124.84
20	B	814	CLA	C2D-C1D-ND	5.17	113.91	110.10
20	1	304	CLA	CHD-C4C-C3C	-5.17	117.25	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	829	CLA	CHD-C4C-C3C	-5.16	117.25	124.84
20	3	319	CLA	O2D-CGD-CBD	5.16	120.44	111.27
20	A	837	CLA	CHD-C4C-C3C	-5.16	117.25	124.84
20	3	308	CLA	CHD-C4C-C3C	-5.16	117.26	124.84
20	K	204	CLA	O2D-CGD-CBD	5.15	120.42	111.27
20	A	804	CLA	CHD-C4C-C3C	-5.15	117.28	124.84
20	4	314	CLA	O2D-CGD-CBD	5.14	120.41	111.27
19	2	302	CHL	C3C-C4C-NC	5.14	116.34	110.57
20	B	806	CLA	C3D-C4D-ND	5.14	118.56	110.24
20	B	809	CLA	CHD-C4C-C3C	-5.14	117.28	124.84
19	2	322	CHL	C3C-C4C-NC	5.14	116.34	110.57
20	A	806	CLA	O2D-CGD-CBD	5.14	120.40	111.27
20	K	204	CLA	CHD-C4C-C3C	-5.14	117.29	124.84
20	4	310	CLA	O2D-CGD-CBD	5.13	120.39	111.27
20	A	853	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
20	1	319	CLA	C3C-C4C-NC	5.13	116.33	110.57
20	A	835	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
20	A	841	CLA	C3B-C2B-C1B	-5.13	100.97	107.16
19	4	306	CHL	C3C-C4C-NC	5.13	116.32	110.57
20	3	320	CLA	CHD-C4C-C3C	-5.12	117.31	124.84
20	B	833	CLA	O2D-CGD-CBD	5.12	120.37	111.27
20	B	813	CLA	C3B-C2B-C1B	-5.11	100.99	107.16
20	A	805	CLA	O2D-CGD-CBD	5.11	120.35	111.27
20	A	852	CLA	CHD-C4C-C3C	-5.11	117.34	124.84
20	1	319	CLA	C3B-C2B-C1B	-5.10	101.00	107.16
20	2	320	CLA	C3B-C2B-C1B	-5.10	101.00	107.16
20	2	307	CLA	C3B-C2B-C1B	-5.10	101.00	107.16
20	A	833	CLA	C3B-C2B-C1B	-5.10	101.00	107.16
20	2	323	CLA	CHD-C4C-C3C	-5.10	117.34	124.84
20	A	826	CLA	O2D-CGD-CBD	5.10	120.32	111.27
20	B	826	CLA	O2D-CGD-CBD	5.10	120.32	111.27
19	1	317	CHL	C3C-C4C-NC	5.10	116.28	110.57
20	A	802	CLA	O2D-CGD-CBD	5.09	120.32	111.27
20	1	318	CLA	C3D-C4D-ND	5.09	118.47	110.24
20	A	837	CLA	C3B-C2B-C1B	-5.09	101.02	107.16
20	B	802	CLA	O2D-CGD-CBD	5.08	120.29	111.27
19	1	301	CHL	C3C-C4C-NC	5.07	116.26	110.57
20	O	208	CLA	CHD-C4C-C3C	-5.07	117.39	124.84
19	2	322	CHL	O2D-CGD-CBD	5.07	120.28	111.27
20	H	201	CLA	O2D-CGD-CBD	5.07	120.28	111.27
20	3	309	CLA	CHD-C4C-C3C	-5.07	117.39	124.84
20	B	845	CLA	CHD-C4C-C3C	-5.07	117.39	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	846	CLA	C3C-C4C-NC	5.07	116.25	110.57
20	A	846	CLA	C3D-C4D-ND	5.06	118.42	110.24
20	B	852	CLA	O2D-CGD-CBD	5.05	120.25	111.27
20	B	807	CLA	CHD-C4C-C3C	-5.05	117.42	124.84
20	1	306	CLA	O2D-CGD-CBD	5.05	120.24	111.27
20	1	322	CLA	CAC-C3C-C4C	5.05	131.36	124.81
20	A	832	CLA	CHD-C4C-C3C	-5.05	117.42	124.84
20	2	320	CLA	C4C-C3C-C2C	-5.04	102.44	107.07
20	A	839	CLA	CHD-C4C-C3C	-5.04	117.43	124.84
19	3	313	CHL	C3C-C4C-NC	5.04	116.23	110.57
20	L	305	CLA	CHD-C4C-C3C	-5.04	117.43	124.84
20	3	320	CLA	O2D-CGD-CBD	5.04	120.23	111.27
20	A	856	CLA	CHD-C4C-C3C	-5.04	117.43	124.84
20	A	844	CLA	CHD-C4C-C3C	-5.04	117.44	124.84
20	4	314	CLA	CHD-C4C-C3C	-5.04	117.44	124.84
20	B	848	CLA	CHC-C4B-NB	-5.03	118.93	124.26
20	3	307	CLA	CHD-C4C-C3C	-5.03	117.44	124.84
20	A	841	CLA	C3D-C4D-ND	5.03	118.38	110.24
23	L	304	BCR	C15-C16-C17	5.03	133.77	123.47
20	4	302	CLA	CHD-C4C-C3C	-5.02	117.45	124.84
20	B	827	CLA	C3D-C4D-ND	5.02	118.36	110.24
20	1	319	CLA	CHD-C1D-ND	-5.02	119.84	124.45
20	A	827	CLA	CAC-C3C-C4C	5.02	131.32	124.81
20	B	851	CLA	O2D-CGD-CBD	5.01	120.18	111.27
20	A	831	CLA	CHD-C4C-C3C	-5.01	117.48	124.84
20	A	847	CLA	O2D-CGD-CBD	5.01	120.17	111.27
20	A	844	CLA	C1C-C2C-C3C	-5.00	101.69	106.96
20	B	813	CLA	C3D-C4D-ND	5.00	118.33	110.24
19	4	305	CHL	C3C-C4C-NC	5.00	116.18	110.57
20	A	806	CLA	CAC-C3C-C4C	5.00	131.30	124.81
20	B	801	CLA	CHD-C4C-C3C	-4.99	117.50	124.84
22	3	302	XAT	C39-C29-C30	-4.99	115.93	122.92
20	B	807	CLA	O2D-CGD-CBD	4.99	120.13	111.27
19	2	309	CHL	C3C-C4C-NC	4.99	116.16	110.57
20	2	306	CLA	O2D-CGD-CBD	4.98	120.12	111.27
20	A	837	CLA	CAC-C3C-C4C	4.98	131.27	124.81
20	B	812	CLA	CHD-C4C-C3C	-4.98	117.52	124.84
20	A	837	CLA	CHC-C4B-NB	-4.98	118.99	124.26
20	3	309	CLA	CAC-C3C-C4C	4.97	131.26	124.81
20	B	852	CLA	CHD-C4C-C3C	-4.97	117.53	124.84
20	2	308	CLA	O2D-CGD-CBD	4.97	120.10	111.27
20	B	829	CLA	C3D-C4D-ND	4.97	118.28	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	308	CLA	C3D-C4D-ND	4.97	118.27	110.24
20	B	849	CLA	C3B-C2B-C1B	-4.97	101.17	107.16
20	4	308	CLA	CHD-C4C-C3C	-4.97	117.54	124.84
20	A	839	CLA	O2D-CGD-CBD	4.96	120.09	111.27
20	L	306	CLA	C3D-C4D-ND	4.95	118.25	110.24
20	2	323	CLA	O2D-CGD-CBD	4.95	120.07	111.27
20	A	827	CLA	CHD-C4C-C3C	-4.95	117.56	124.84
20	B	853	CLA	CHD-C4C-C3C	-4.95	117.56	124.84
20	B	824	CLA	C3B-C2B-C1B	-4.95	101.19	107.16
20	3	309	CLA	CHC-C4B-NB	-4.94	119.02	124.26
20	A	809	CLA	O2D-CGD-CBD	4.94	120.05	111.27
23	4	319	BCR	C1-C6-C5	-4.94	115.66	122.61
20	3	318	CLA	O2D-CGD-CBD	4.94	120.04	111.27
20	A	826	CLA	CHD-C4C-C3C	-4.93	117.59	124.84
20	A	831	CLA	CAC-C3C-C4C	4.93	131.21	124.81
20	3	307	CLA	CBD-CHA-C1A	4.93	135.33	127.43
20	K	205	CLA	CHD-C4C-C3C	-4.93	117.59	124.84
22	1	311	XAT	O4-C5-C4	4.93	117.08	113.38
20	B	830	CLA	CHD-C4C-C3C	-4.93	117.60	124.84
20	L	307	CLA	O2D-CGD-CBD	4.93	120.02	111.27
20	A	852	CLA	C3C-C4C-NC	4.93	116.09	110.57
20	3	309	CLA	C3D-C4D-ND	4.92	118.20	110.24
20	A	841	CLA	O2D-CGD-CBD	4.92	120.01	111.27
20	A	840	CLA	CAC-C3C-C4C	4.92	131.19	124.81
19	4	305	CHL	O2D-CGD-CBD	4.92	120.01	111.27
19	4	306	CHL	O2D-CGD-CBD	4.92	120.00	111.27
22	1	311	XAT	O4-C5-C18	4.91	120.94	115.06
20	4	313	CLA	C3D-C4D-ND	4.91	118.19	110.24
20	B	802	CLA	C3D-C4D-ND	4.91	118.19	110.24
20	B	820	CLA	CHD-C4C-C3C	-4.91	117.62	124.84
20	A	848	CLA	C3B-C2B-C1B	-4.91	101.24	107.16
20	4	302	CLA	O2D-CGD-CBD	4.90	119.98	111.27
20	A	804	CLA	C1C-C2C-C3C	-4.90	101.81	106.96
20	3	307	CLA	CAC-C3C-C4C	4.89	131.16	124.81
20	3	319	CLA	CAC-C3C-C4C	4.89	131.16	124.81
20	B	852	CLA	C3B-C2B-C1B	-4.89	101.26	107.16
23	B	835	BCR	C37-C22-C21	-4.89	116.08	122.92
20	A	802	CLA	C3C-C4C-NC	4.89	116.05	110.57
20	4	313	CLA	CHD-C4C-C3C	-4.89	117.66	124.84
20	A	843	CLA	CHD-C1D-ND	-4.88	119.97	124.45
20	4	314	CLA	C3D-C4D-ND	4.88	118.14	110.24
20	B	831	CLA	C3D-C4D-ND	4.88	118.13	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	G	206	CLA	O2D-CGD-CBD	4.88	119.93	111.27
20	1	318	CLA	CHD-C1D-ND	-4.88	119.97	124.45
22	3	302	XAT	C6-C7-C8	-4.87	115.69	125.99
20	4	309	CLA	C3B-C2B-C1B	-4.87	101.28	107.16
20	B	845	CLA	CHB-C4A-NA	4.87	131.25	124.51
20	B	829	CLA	CHD-C4C-C3C	-4.87	117.68	124.84
20	B	851	CLA	CHD-C4C-C3C	-4.86	117.69	124.84
20	B	830	CLA	CAC-C3C-C4C	4.86	131.12	124.81
20	N	202	CLA	O2D-CGD-CBD	4.86	119.90	111.27
20	A	839	CLA	C3D-C4D-ND	4.86	118.10	110.24
20	B	802	CLA	CAC-C3C-C4C	4.86	131.11	124.81
20	2	319	CLA	CMC-C2C-C1C	4.86	132.44	125.04
19	2	318	CHL	C3D-C2D-C1D	-4.86	99.20	105.83
20	4	302	CLA	C3D-C4D-ND	4.85	118.08	110.24
20	B	847	CLA	O2D-CGD-CBD	4.85	119.88	111.27
20	B	818	CLA	C4D-CHA-C1A	-4.85	115.35	121.25
20	4	308	CLA	CAC-C3C-C4C	4.85	131.10	124.81
20	A	840	CLA	CHD-C4C-C3C	-4.85	117.72	124.84
20	K	205	CLA	C3D-C4D-ND	4.84	118.07	110.24
20	B	820	CLA	O2D-CGD-CBD	4.84	119.87	111.27
20	A	835	CLA	CHD-C1D-ND	-4.83	120.01	124.45
20	A	802	CLA	C3D-C4D-ND	4.83	118.06	110.24
20	L	305	CLA	CHD-C1D-ND	-4.83	120.01	124.45
20	2	320	CLA	C1C-C2C-C3C	-4.83	102.64	107.07
20	A	835	CLA	O2D-CGD-CBD	4.82	119.84	111.27
20	4	313	CLA	CHD-C1D-ND	-4.82	120.02	124.45
20	A	809	CLA	C3D-C4D-ND	4.82	118.04	110.24
20	A	844	CLA	C3D-C4D-ND	4.82	118.04	110.24
19	1	317	CHL	C1-C2-C3	-4.82	118.95	126.75
20	A	855	CLA	O2D-CGD-CBD	4.82	119.83	111.27
20	A	856	CLA	C4-C3-C5	4.81	123.37	115.27
20	A	848	CLA	CHD-C4C-C3C	-4.81	117.77	124.84
20	A	855	CLA	C1C-C2C-C3C	-4.81	101.90	106.96
20	K	205	CLA	C3B-C2B-C1B	-4.81	101.36	107.16
20	B	819	CLA	C3B-C4B-NB	4.80	114.97	110.52
20	B	847	CLA	CHD-C1D-ND	-4.80	120.04	124.45
20	B	821	CLA	O2D-CGD-CBD	4.80	119.80	111.27
20	2	321	CLA	CHD-C1D-ND	-4.80	120.04	124.45
20	A	827	CLA	C3D-C4D-ND	4.80	118.01	110.24
22	1	311	XAT	C28-C29-C30	4.80	126.31	118.94
20	A	844	CLA	CHD-C1D-ND	-4.80	120.04	124.45
20	1	322	CLA	CHD-C4C-C3C	-4.79	117.79	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	314	CLA	C3B-C2B-C1B	-4.79	101.37	107.16
20	A	846	CLA	O2D-CGD-CBD	4.79	119.79	111.27
20	A	847	CLA	C3D-C4D-ND	4.79	117.99	110.24
20	A	838	CLA	O2D-CGD-CBD	4.79	119.78	111.27
20	A	839	CLA	CHD-C1D-ND	-4.79	120.05	124.45
20	2	319	CLA	CAC-C3C-C4C	4.79	131.03	124.81
20	1	306	CLA	C3D-C4D-ND	4.79	117.99	110.24
20	B	849	CLA	C3D-C4D-ND	4.79	117.99	110.24
20	B	819	CLA	O2D-CGD-CBD	4.79	119.78	111.27
23	O	202	BCR	C34-C9-C10	-4.79	116.21	122.92
22	2	311	XAT	O24-C25-C38	4.79	120.79	115.06
20	4	309	CLA	C3D-C4D-ND	4.79	117.98	110.24
20	A	836	CLA	C3D-C4D-ND	4.79	117.98	110.24
21	1	323	LUT	C19-C9-C10	-4.78	116.22	122.92
20	1	319	CLA	CHD-C4C-C3C	-4.78	117.81	124.84
20	B	847	CLA	CHC-C4B-NB	-4.78	119.19	124.26
20	A	846	CLA	CHD-C4C-C3C	-4.78	117.81	124.84
20	B	846	CLA	C3D-C4D-ND	4.78	117.97	110.24
20	A	805	CLA	CHC-C4B-NB	-4.78	119.20	124.26
20	B	830	CLA	C3D-C4D-ND	4.78	117.97	110.24
20	B	817	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
20	O	207	CLA	C3D-C4D-ND	4.78	117.97	110.24
20	2	317	CLA	C3D-C4D-ND	4.78	117.96	110.24
20	N	202	CLA	CHC-C4B-NB	-4.77	119.21	124.26
20	1	305	CLA	C3B-C2B-C1B	-4.77	101.41	107.16
20	G	206	CLA	C3D-C4D-ND	4.77	117.95	110.24
20	4	303	CLA	CHC-C4B-NB	-4.77	119.21	124.26
20	B	805	CLA	C3D-C4D-ND	4.77	117.95	110.24
20	1	308	CLA	C3D-C4D-ND	4.77	117.95	110.24
20	A	848	CLA	CAC-C3C-C4C	4.76	130.99	124.81
20	B	818	CLA	CHD-C4C-C3C	-4.76	117.84	124.84
20	G	205	CLA	O2D-CGD-CBD	4.76	119.73	111.27
20	B	819	CLA	CHD-C4C-C3C	-4.76	117.84	124.84
20	2	306	CLA	CHC-C4B-NB	-4.76	119.22	124.26
28	A	824	CL0	C1C-C2C-C3C	-4.76	101.95	106.96
20	A	843	CLA	CHD-C4C-C3C	-4.76	117.85	124.84
20	B	844	CLA	C3B-C2B-C1B	-4.76	101.42	107.16
22	3	302	XAT	C38-C25-C26	-4.76	114.29	122.26
20	A	803	CLA	C3D-C4D-ND	4.75	117.93	110.24
20	A	844	CLA	C3C-C4C-NC	4.75	115.90	110.57
20	2	305	CLA	CHD-C4C-C3C	-4.75	117.85	124.84
20	3	318	CLA	C3D-C4D-ND	4.75	117.92	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	835	CLA	C3D-C4D-ND	4.75	117.92	110.24
20	1	322	CLA	CHC-C4B-NB	-4.74	119.23	124.26
20	A	826	CLA	C1C-C2C-C3C	-4.74	101.97	106.96
28	A	824	CL0	C3B-C2B-C1B	-4.74	101.44	107.16
20	4	308	CLA	O2D-CGD-CBD	4.74	119.69	111.27
20	3	319	CLA	CHD-C4C-C3C	-4.74	117.87	124.84
20	B	814	CLA	C3D-C2D-C1D	-4.74	99.37	105.83
20	4	312	CLA	C3D-C4D-ND	4.74	117.90	110.24
20	A	845	CLA	CHD-C4C-C3C	-4.74	117.88	124.84
20	B	802	CLA	CHD-C4C-C3C	-4.74	117.88	124.84
20	A	846	CLA	CHD-C1D-ND	-4.73	120.10	124.45
20	3	314	CLA	C1C-C2C-C3C	-4.73	101.98	106.96
20	B	851	CLA	C1C-C2C-C3C	-4.73	101.98	106.96
20	4	311	CLA	CHC-C4B-NB	-4.73	119.25	124.26
20	B	822	CLA	O2D-CGD-CBD	4.73	119.67	111.27
20	4	312	CLA	O2D-CGD-CBD	4.73	119.67	111.27
20	B	833	CLA	C3D-C4D-ND	4.73	117.88	110.24
20	A	843	CLA	C3B-C2B-C1B	-4.73	101.46	107.16
20	A	856	CLA	C3D-C4D-ND	4.73	117.88	110.24
19	2	301	CHL	O2D-CGD-CBD	4.72	119.66	111.27
20	A	856	CLA	O2D-CGD-CBD	4.72	119.66	111.27
20	1	320	CLA	CHC-C4B-NB	-4.72	119.26	124.26
20	4	310	CLA	C3B-C2B-C1B	-4.72	101.47	107.16
20	A	835	CLA	C3B-C2B-C1B	-4.72	101.47	107.16
20	B	852	CLA	C3D-C4D-ND	4.72	117.87	110.24
23	A	817	BCR	C37-C22-C23	4.72	125.51	118.08
20	3	310	CLA	CHD-C1D-ND	-4.71	120.12	124.45
20	A	806	CLA	CHD-C4C-C3C	-4.71	117.91	124.84
23	L	304	BCR	C16-C15-C14	4.71	133.13	123.47
20	4	303	CLA	C3D-C4D-ND	4.71	117.86	110.24
20	B	811	CLA	C3D-C4D-ND	4.71	117.86	110.24
20	4	316	CLA	CHC-C4B-NB	-4.71	119.27	124.26
20	B	831	CLA	C3B-C2B-C1B	-4.71	101.48	107.16
23	I	102	BCR	C30-C25-C26	-4.71	115.98	122.61
20	2	319	CLA	C3D-C4D-ND	4.71	117.85	110.24
20	B	853	CLA	CHD-C1D-ND	-4.71	120.13	124.45
19	2	322	CHL	C3D-C2D-C1D	-4.71	99.41	105.83
20	1	320	CLA	C3D-C4D-ND	4.70	117.85	110.24
20	4	304	CLA	CHD-C4C-C3C	-4.70	117.93	124.84
20	L	307	CLA	CHD-C1D-ND	-4.70	120.13	124.45
20	3	312	CLA	O2D-CGD-CBD	4.70	119.62	111.27
20	3	317	CLA	C3D-C4D-ND	4.70	117.84	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	853	CLA	O2D-CGD-CBD	4.70	119.62	111.27
20	B	822	CLA	CHD-C1D-ND	-4.70	120.14	124.45
20	A	834	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
20	B	848	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
20	B	824	CLA	C3D-C4D-ND	4.70	117.83	110.24
20	O	207	CLA	C3B-C2B-C1B	-4.70	101.49	107.16
20	B	804	CLA	O2D-CGD-CBD	4.70	119.61	111.27
20	1	307	CLA	C3B-C2B-C1B	-4.69	101.50	107.16
20	2	321	CLA	C3D-C4D-ND	4.69	117.83	110.24
20	G	205	CLA	C1C-C2C-C3C	-4.69	102.02	106.96
20	B	809	CLA	C3D-C4D-ND	4.69	117.83	110.24
19	1	301	CHL	O2D-CGD-CBD	4.69	119.61	111.27
20	B	830	CLA	O2D-CGD-CBD	4.69	119.61	111.27
20	B	808	CLA	CHC-C4B-NB	-4.69	119.29	124.26
20	B	852	CLA	CAC-C3C-C4C	4.69	130.89	124.81
20	1	322	CLA	C3D-C4D-ND	4.68	117.81	110.24
20	2	305	CLA	C3D-C4D-ND	4.68	117.81	110.24
19	2	318	CHL	C2D-C1D-ND	4.68	113.55	110.10
20	B	853	CLA	O2D-CGD-CBD	4.68	119.58	111.27
20	2	305	CLA	C3B-C2B-C1B	-4.68	101.51	107.16
20	B	833	CLA	CHC-C4B-NB	-4.68	119.31	124.26
20	B	801	CLA	C1C-C2C-C3C	-4.68	102.04	106.96
20	N	202	CLA	C3D-C4D-ND	4.67	117.80	110.24
20	1	309	CLA	C3D-C4D-ND	4.67	117.80	110.24
20	B	853	CLA	C3D-C4D-ND	4.67	117.80	110.24
20	L	307	CLA	C3D-C4D-ND	4.67	117.80	110.24
20	A	841	CLA	CHD-C1D-ND	-4.67	120.16	124.45
20	2	308	CLA	C3B-C2B-C1B	-4.67	101.52	107.16
20	F	306	CLA	C3B-C2B-C1B	-4.67	101.53	107.16
20	1	305	CLA	CHC-C4B-NB	-4.67	119.32	124.26
20	B	817	CLA	CAC-C3C-C4C	4.67	130.87	124.81
19	3	313	CHL	C3D-C2D-C1D	-4.67	99.46	105.83
20	B	829	CLA	C3B-C2B-C1B	-4.66	101.53	107.16
20	B	820	CLA	CAC-C3C-C4C	4.66	130.86	124.81
20	2	308	CLA	CHD-C1D-ND	-4.66	120.17	124.45
20	A	825	CLA	C3D-C4D-ND	4.66	117.78	110.24
20	A	803	CLA	C1-O2A-CGA	4.66	128.67	116.44
20	1	318	CLA	CAC-C3C-C4C	4.66	130.86	124.81
20	B	820	CLA	CHD-C1D-ND	-4.66	120.17	124.45
20	B	848	CLA	C3B-C2B-C1B	-4.66	101.54	107.16
20	4	314	CLA	CAC-C3C-C4C	4.66	130.85	124.81
19	2	301	CHL	C3D-C2D-C1D	-4.66	99.48	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	308	CLA	C3D-C4D-ND	4.65	117.77	110.24
20	K	204	CLA	C3D-C4D-ND	4.65	117.77	110.24
20	B	806	CLA	C3B-C2B-C1B	-4.65	101.54	107.16
20	A	836	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
20	B	833	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
20	F	304	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
20	N	202	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
20	3	316	CLA	CHC-C4B-NB	-4.65	119.33	124.26
20	1	322	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
20	A	811	CLA	C3D-C4D-ND	4.65	117.76	110.24
20	B	806	CLA	CHD-C1D-ND	-4.65	120.18	124.45
20	B	812	CLA	C3B-C4B-NB	4.65	114.83	110.52
20	1	302	CLA	C3D-C4D-ND	4.65	117.75	110.24
20	B	818	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
23	B	836	BCR	C16-C15-C14	4.65	132.99	123.47
22	1	311	XAT	C6-C7-C8	-4.64	116.17	125.99
23	L	304	BCR	C34-C9-C10	-4.64	116.42	122.92
20	B	808	CLA	CHD-C1D-ND	-4.64	120.19	124.45
20	B	818	CLA	C3D-C4D-ND	4.64	117.75	110.24
22	3	302	XAT	C31-C30-C29	4.64	133.93	127.31
21	1	323	LUT	C32-C33-C34	4.64	126.06	118.94
20	B	815	CLA	O2D-CGD-CBD	4.64	119.51	111.27
20	B	833	CLA	CHD-C4C-C3C	-4.64	118.02	124.84
20	B	846	CLA	CHD-C4C-C3C	-4.64	118.02	124.84
20	1	304	CLA	C3D-C4D-ND	4.64	117.74	110.24
20	A	842	CLA	C3D-C4D-ND	4.63	117.73	110.24
20	A	840	CLA	O2D-CGD-CBD	4.63	119.50	111.27
20	4	313	CLA	C3B-C2B-C1B	-4.63	101.57	107.16
20	2	319	CLA	CHD-C1D-ND	-4.63	120.20	124.45
20	A	809	CLA	CAC-C3C-C4C	4.63	130.81	124.81
20	2	307	CLA	CHD-C1D-ND	-4.63	120.20	124.45
20	B	852	CLA	CHC-C4B-NB	-4.62	119.36	124.26
20	A	836	CLA	CHC-C4B-NB	-4.62	119.36	124.26
20	A	848	CLA	CHC-C4B-NB	-4.62	119.36	124.26
20	L	305	CLA	O2D-CGD-CBD	4.62	119.48	111.27
20	3	312	CLA	C3D-C4D-ND	4.62	117.71	110.24
20	G	205	CLA	C3D-C4D-ND	4.61	117.70	110.24
20	3	318	CLA	C3B-C2B-C1B	-4.61	101.59	107.16
20	J	103	CLA	CHC-C4B-NB	-4.61	119.37	124.26
20	4	311	CLA	C3D-C4D-ND	4.61	117.70	110.24
20	2	305	CLA	CHC-C4B-NB	-4.61	119.38	124.26
20	B	830	CLA	CHD-C1D-ND	-4.61	120.22	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	832	CLA	CHC-C4B-NB	-4.61	119.38	124.26
20	B	814	CLA	O2D-CGD-CBD	4.61	119.46	111.27
20	1	321	CLA	CAC-C3C-C4C	4.61	130.79	124.81
20	A	836	CLA	CHD-C1D-ND	-4.61	120.22	124.45
20	A	845	CLA	C3D-C4D-ND	4.61	117.69	110.24
20	B	846	CLA	CHD-C1D-ND	-4.61	120.22	124.45
20	B	811	CLA	CHD-C1D-ND	-4.60	120.22	124.45
20	B	828	CLA	C3D-C4D-ND	4.60	117.68	110.24
20	A	828	CLA	CHD-C1D-ND	-4.60	120.22	124.45
19	4	315	CHL	C3D-C2D-C1D	-4.60	99.55	105.83
20	A	807	CLA	C3B-C2B-C1B	-4.60	101.61	107.16
20	A	832	CLA	C1C-C2C-C3C	-4.60	102.12	106.96
20	F	305	CLA	C1C-C2C-C3C	-4.60	102.12	106.96
20	B	808	CLA	C3B-C2B-C1B	-4.60	101.61	107.16
20	F	306	CLA	CHC-C4B-NB	-4.60	119.39	124.26
20	O	206	CLA	CHD-C1D-ND	-4.60	120.23	124.45
29	B	840	DGD	O2G-C1B-C2B	4.60	121.41	111.50
20	1	318	CLA	CHD-C4C-C3C	-4.60	118.08	124.84
20	B	813	CLA	CHC-C4B-NB	-4.60	119.39	124.26
20	A	802	CLA	CHD-C1D-ND	-4.60	120.23	124.45
20	B	811	CLA	C3B-C2B-C1B	-4.59	101.62	107.16
20	L	305	CLA	C3D-C4D-ND	4.59	117.67	110.24
19	2	318	CHL	C1D-ND-C4D	-4.59	103.07	106.33
19	4	306	CHL	C3D-C2D-C1D	-4.59	99.56	105.83
20	B	850	CLA	C3B-C2B-C1B	-4.59	101.62	107.16
20	H	201	CLA	C3D-C4D-ND	4.59	117.66	110.24
20	4	316	CLA	C3B-C2B-C1B	-4.59	101.62	107.16
20	2	307	CLA	C3D-C4D-ND	4.59	117.66	110.24
23	4	320	BCR	C34-C9-C10	-4.59	116.50	122.92
20	K	205	CLA	CAC-C3C-C4C	4.58	130.76	124.81
23	O	202	BCR	C24-C23-C22	4.58	133.16	126.23
20	J	103	CLA	C3B-C2B-C1B	-4.58	101.63	107.16
20	B	847	CLA	C3D-C4D-ND	4.58	117.65	110.24
20	1	320	CLA	C3B-C2B-C1B	-4.58	101.63	107.16
20	3	315	CLA	C3D-C4D-ND	4.58	117.65	110.24
20	K	206	CLA	C3D-C4D-ND	4.58	117.64	110.24
20	A	852	CLA	C1C-C2C-C3C	-4.58	102.14	106.96
20	K	206	CLA	O2D-CGD-CBD	4.58	119.40	111.27
19	4	305	CHL	C3D-C2D-C1D	-4.57	99.59	105.83
20	1	309	CLA	CHC-C4B-NB	-4.57	119.42	124.26
20	2	317	CLA	CHC-C4B-NB	-4.57	119.42	124.26
20	2	304	CLA	C3D-C4D-ND	4.57	117.63	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	826	CLA	C3D-C4D-ND	4.57	117.63	110.24
20	B	848	CLA	O2D-CGD-CBD	4.57	119.39	111.27
20	G	207	CLA	C3D-C4D-ND	4.57	117.63	110.24
20	B	802	CLA	CHC-C4B-NB	-4.57	119.42	124.26
20	K	204	CLA	CHD-C1D-ND	-4.57	120.26	124.45
20	L	306	CLA	CHD-C1D-ND	-4.57	120.26	124.45
22	3	302	XAT	O4-C5-C18	4.56	120.52	115.06
20	B	829	CLA	C4D-CHA-C1A	-4.56	115.70	121.25
20	B	824	CLA	CHD-C1D-ND	-4.56	120.26	124.45
20	A	840	CLA	C3D-C4D-ND	4.56	117.62	110.24
20	3	319	CLA	C3B-C2B-C1B	-4.56	101.66	107.16
20	3	315	CLA	C1C-C2C-C3C	-4.56	102.16	106.96
20	A	811	CLA	CHC-C4B-NB	-4.56	119.43	124.26
20	B	831	CLA	CHC-C4B-NB	-4.56	119.43	124.26
20	A	842	CLA	O2D-CGD-CBD	4.56	119.37	111.27
20	2	308	CLA	CHC-C4B-NB	-4.56	119.43	124.26
20	F	305	CLA	CHC-C4B-NB	-4.56	119.43	124.26
20	A	809	CLA	CHC-C4B-NB	-4.55	119.44	124.26
20	A	840	CLA	CHC-C4B-NB	-4.55	119.44	124.26
20	A	806	CLA	C3D-C4D-ND	4.55	117.61	110.24
20	B	812	CLA	CHD-C1D-ND	-4.55	120.27	124.45
20	2	306	CLA	C3D-C4D-ND	4.55	117.60	110.24
20	1	306	CLA	CHC-C4B-NB	-4.55	119.44	124.26
20	B	818	CLA	C1C-C2C-C3C	-4.55	102.17	106.96
19	4	307	CHL	C3D-C2D-C1D	-4.55	99.63	105.83
20	3	317	CLA	C3B-C2B-C1B	-4.54	101.68	107.16
20	A	831	CLA	C3B-C2B-C1B	-4.54	101.68	107.16
20	4	316	CLA	O2D-CGD-CBD	4.54	119.34	111.27
19	2	309	CHL	C3D-C2D-C1D	-4.54	99.63	105.83
20	1	302	CLA	C3B-C2B-C1B	-4.54	101.68	107.16
20	A	802	CLA	CHD-C4C-C3C	-4.54	118.17	124.84
20	3	311	CLA	O2D-CGD-CBD	4.54	119.33	111.27
20	O	207	CLA	CHC-C4B-NB	-4.54	119.45	124.26
20	A	808	CLA	C1C-C2C-C3C	-4.54	102.19	106.96
20	1	305	CLA	C3D-C4D-ND	4.54	117.58	110.24
20	B	823	CLA	C3D-C4D-ND	4.53	117.57	110.24
20	1	309	CLA	C3B-C2B-C1B	-4.53	101.69	107.16
20	B	833	CLA	CAC-C3C-C4C	4.53	130.69	124.81
20	B	846	CLA	CAC-C3C-C4C	4.53	130.69	124.81
20	A	807	CLA	C3D-C4D-ND	4.53	117.57	110.24
20	A	831	CLA	C3D-C4D-ND	4.53	117.57	110.24
20	A	833	CLA	C3D-C4D-ND	4.53	117.57	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	807	CLA	CHD-C1D-ND	-4.53	120.29	124.45
19	2	322	CHL	CHD-C4C-C3C	-4.53	118.18	124.84
20	2	303	CLA	O2D-CGD-CBD	4.53	119.31	111.27
20	F	305	CLA	O2D-CGD-CBD	4.53	119.31	111.27
20	F	306	CLA	O2D-CGD-CBD	4.53	119.31	111.27
20	B	822	CLA	C3D-C4D-ND	4.53	117.56	110.24
20	A	848	CLA	C3D-C4D-ND	4.53	117.56	110.24
20	F	304	CLA	C3D-C4D-ND	4.52	117.56	110.24
20	3	311	CLA	C1C-C2C-C3C	-4.52	102.20	106.96
20	B	821	CLA	C3B-C2B-C1B	-4.52	101.70	107.16
20	O	208	CLA	CAC-C3C-C4C	4.52	130.68	124.81
20	2	305	CLA	CAC-C3C-C4C	4.52	130.68	124.81
20	4	311	CLA	C3B-C2B-C1B	-4.52	101.70	107.16
20	B	810	CLA	C3D-C4D-ND	4.52	117.55	110.24
20	B	851	CLA	C3B-C2B-C1B	-4.52	101.70	107.16
20	B	810	CLA	CHC-C4B-NB	-4.52	119.47	124.26
20	1	303	CLA	CHC-C4B-NB	-4.52	119.47	124.26
20	1	303	CLA	C3D-C4D-ND	4.52	117.54	110.24
20	1	319	CLA	CAC-C3C-C4C	4.52	130.67	124.81
20	1	308	CLA	CHD-C1D-ND	-4.51	120.31	124.45
20	B	816	CLA	C3D-C4D-ND	4.51	117.53	110.24
20	B	822	CLA	C1C-C2C-C3C	-4.51	102.22	106.96
20	3	316	CLA	O2D-CGD-CBD	4.51	119.28	111.27
19	2	302	CHL	C3D-C2D-C1D	-4.51	99.68	105.83
20	B	814	CLA	C3D-C4D-ND	4.51	117.53	110.24
20	B	820	CLA	C3D-C4D-ND	4.51	117.53	110.24
20	B	848	CLA	C2D-C1D-ND	4.51	113.42	110.10
20	A	829	CLA	CHD-C1D-ND	-4.50	120.32	124.45
20	3	319	CLA	C3D-C4D-ND	4.50	117.52	110.24
20	A	825	CLA	CHB-C4A-NA	4.50	130.73	124.51
19	2	318	CHL	CHD-C4C-C3C	-4.49	118.23	124.84
19	4	307	CHL	CHD-C4C-C3C	-4.49	118.24	124.84
20	3	320	CLA	C3D-C4D-ND	4.49	117.50	110.24
20	3	309	CLA	C3B-C2B-C1B	-4.49	101.74	107.16
20	B	819	CLA	C1C-C2C-C3C	-4.49	102.23	106.96
21	1	323	LUT	C39-C29-C30	-4.49	116.63	122.92
20	A	842	CLA	CHC-C4B-NB	-4.49	119.50	124.26
23	A	818	BCR	C37-C22-C23	4.49	125.15	118.08
20	A	856	CLA	CHD-C1D-ND	-4.49	120.33	124.45
20	B	825	CLA	C3D-C4D-ND	4.49	117.50	110.24
20	B	802	CLA	CHD-C1D-ND	-4.49	120.33	124.45
20	2	307	CLA	CAC-C3C-C4C	4.49	130.63	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	319	CLA	C3D-C4D-ND	4.49	117.50	110.24
19	3	313	CHL	O2D-CGD-CBD	4.49	119.24	111.27
20	1	306	CLA	C3B-C2B-C1B	-4.48	101.75	107.16
20	A	832	CLA	C3D-C4D-ND	4.48	117.49	110.24
20	A	851	CLA	C3D-C4D-ND	4.48	117.48	110.24
20	O	208	CLA	C3D-C4D-ND	4.48	117.48	110.24
20	A	856	CLA	CAC-C3C-C4C	4.48	130.62	124.81
20	A	811	CLA	C3B-C2B-C1B	-4.48	101.76	107.16
20	A	809	CLA	C3B-C2B-C1B	-4.47	101.76	107.16
20	1	303	CLA	C1C-C2C-C3C	-4.47	102.25	106.96
20	3	315	CLA	CHD-C1D-ND	-4.47	120.34	124.45
20	B	827	CLA	C3B-C2B-C1B	-4.47	101.77	107.16
20	2	304	CLA	C3B-C2B-C1B	-4.47	101.77	107.16
20	A	812	CLA	C4-C3-C5	4.47	122.78	115.27
19	1	317	CHL	C3D-C2D-C1D	-4.47	99.74	105.83
20	A	829	CLA	O2D-CGD-CBD	4.47	119.20	111.27
20	A	829	CLA	CHC-C4B-NB	-4.47	119.53	124.26
20	A	853	CLA	C4D-CHA-C1A	-4.47	115.81	121.25
20	B	808	CLA	C3D-C4D-ND	4.46	117.46	110.24
20	A	836	CLA	O2D-CGD-CBD	4.46	119.20	111.27
20	A	805	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
20	4	314	CLA	CHC-C4B-NB	-4.46	119.53	124.26
20	A	834	CLA	C1C-C2C-C3C	-4.46	102.27	106.96
20	G	206	CLA	CHC-C4B-NB	-4.46	119.53	124.26
20	3	316	CLA	C3B-C2B-C1B	-4.46	101.78	107.16
20	1	303	CLA	C4D-CHA-C1A	-4.46	115.82	121.25
20	4	303	CLA	CAC-C3C-C4C	4.46	130.60	124.81
20	2	317	CLA	O2D-CGD-CBD	4.46	119.20	111.27
20	K	206	CLA	CHD-C1D-ND	-4.46	120.35	124.45
20	1	305	CLA	O2D-CGD-CBD	4.46	119.19	111.27
20	G	206	CLA	C3B-C2B-C1B	-4.46	101.78	107.16
19	3	313	CHL	CHD-C4C-C3C	-4.46	118.29	124.84
20	2	323	CLA	CHC-C4B-NB	-4.46	119.54	124.26
23	G	203	BCR	C8-C9-C10	4.46	125.78	118.94
20	B	812	CLA	C4-C3-C5	4.46	122.77	115.27
20	A	806	CLA	CHD-C1D-ND	-4.45	120.36	124.45
20	B	815	CLA	C3D-C4D-ND	4.45	117.44	110.24
20	K	203	CLA	C3D-C4D-ND	4.45	117.44	110.24
20	B	851	CLA	CAC-C3C-C4C	4.45	130.59	124.81
20	A	837	CLA	O2D-CGD-CBD	4.45	119.18	111.27
20	1	303	CLA	C3B-C2B-C1B	-4.45	101.79	107.16
20	B	828	CLA	C3B-C2B-C1B	-4.45	101.79	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	317	CLA	CHD-C1D-ND	-4.45	120.37	124.45
20	A	838	CLA	CHD-C1D-ND	-4.45	120.37	124.45
23	B	838	BCR	C15-C16-C17	4.45	132.58	123.47
20	B	823	CLA	CHD-C1D-ND	-4.45	120.37	124.45
20	A	829	CLA	CMC-C2C-C1C	4.44	131.81	125.04
20	3	318	CLA	CHD-C1D-ND	-4.44	120.37	124.45
20	3	308	CLA	C4D-CHA-C1A	-4.44	115.84	121.25
20	A	812	CLA	CHB-C4A-NA	4.44	130.66	124.51
20	2	306	CLA	C3B-C2B-C1B	-4.44	101.80	107.16
20	B	844	CLA	O2D-CGD-CBD	4.44	119.16	111.27
20	4	304	CLA	C3D-C4D-ND	4.44	117.42	110.24
20	2	323	CLA	C3D-C4D-ND	4.44	117.42	110.24
23	O	203	BCR	C30-C25-C26	-4.44	116.36	122.61
20	F	305	CLA	C3D-C4D-ND	4.44	117.42	110.24
20	G	207	CLA	CHD-C1D-ND	-4.44	120.37	124.45
20	B	812	CLA	C3D-C4D-ND	4.44	117.42	110.24
20	B	844	CLA	C4D-CHA-C1A	-4.44	115.85	121.25
22	2	311	XAT	C28-C29-C30	4.44	125.75	118.94
22	1	311	XAT	C18-C5-C4	4.44	119.27	114.28
23	B	835	BCR	C34-C9-C10	-4.44	116.71	122.92
20	B	829	CLA	CHC-C4B-NB	-4.43	119.56	124.26
20	A	802	CLA	C4D-CHA-C1A	-4.43	115.85	121.25
20	B	808	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
20	B	847	CLA	C3B-C2B-C1B	-4.43	101.81	107.16
20	B	821	CLA	C3D-C4D-ND	4.43	117.41	110.24
20	B	803	CLA	C3D-C4D-ND	4.43	117.40	110.24
20	O	207	CLA	CHD-C1D-ND	-4.43	120.38	124.45
20	2	317	CLA	C3B-C2B-C1B	-4.43	101.82	107.16
20	B	815	CLA	CHD-C1D-ND	-4.43	120.39	124.45
20	A	846	CLA	CHC-C4B-NB	-4.43	119.57	124.26
20	A	850	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
20	A	844	CLA	C4D-CHA-C1A	-4.42	115.86	121.25
20	4	308	CLA	C1C-C2C-C3C	-4.42	102.31	106.96
20	A	833	CLA	CAC-C3C-C4C	4.42	130.55	124.81
20	F	306	CLA	C3D-C4D-ND	4.42	117.39	110.24
20	A	829	CLA	C1C-C2C-C3C	-4.42	102.31	106.96
20	2	320	CLA	C3D-C4D-ND	4.42	117.38	110.24
20	4	313	CLA	CHC-C4B-NB	-4.42	119.58	124.26
20	B	810	CLA	C1C-C2C-C3C	-4.42	102.31	106.96
20	A	835	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
20	A	843	CLA	C3B-C4B-NB	4.41	114.61	110.52
20	4	309	CLA	C4D-CHA-C1A	-4.41	115.88	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	320	CLA	CHD-C1D-ND	-4.41	120.40	124.45
20	3	318	CLA	CHC-C4B-NB	-4.41	119.59	124.26
20	4	309	CLA	CHC-C4B-NB	-4.41	119.59	124.26
20	4	304	CLA	C4D-CHA-C1A	-4.41	115.89	121.25
20	H	201	CLA	CHC-C4B-NB	-4.41	119.59	124.26
20	B	849	CLA	CHD-C1D-ND	-4.41	120.40	124.45
20	1	302	CLA	CHC-C4B-NB	-4.41	119.59	124.26
20	G	205	CLA	CHD-C1D-ND	-4.40	120.41	124.45
20	2	307	CLA	O2D-CGD-CBD	4.40	119.09	111.27
19	2	309	CHL	CHD-C4C-C3C	-4.40	118.37	124.84
20	B	820	CLA	C1C-C2C-C3C	-4.40	102.33	106.96
20	A	837	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
23	A	816	BCR	C36-C18-C17	-4.40	116.77	122.92
20	3	314	CLA	C3D-C4D-ND	4.40	117.35	110.24
20	H	201	CLA	C3B-C2B-C1B	-4.39	101.86	107.16
23	A	815	BCR	C37-C22-C21	-4.39	116.77	122.92
20	B	809	CLA	CHD-C1D-ND	-4.39	120.42	124.45
20	A	805	CLA	C3D-C4D-ND	4.39	117.34	110.24
20	4	312	CLA	CHC-C4B-NB	-4.39	119.61	124.26
20	4	304	CLA	O2D-CGD-CBD	4.39	119.06	111.27
20	A	835	CLA	C4D-CHA-C1A	-4.38	115.92	121.25
20	B	828	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
22	4	318	XAT	C6-C7-C8	-4.38	116.74	125.99
20	B	817	CLA	O2D-CGD-CBD	4.37	119.04	111.27
20	A	808	CLA	C3D-C4D-ND	4.37	117.31	110.24
20	1	304	CLA	CHD-C1D-ND	-4.37	120.44	124.45
20	1	307	CLA	C3D-C4D-ND	4.37	117.31	110.24
23	2	312	BCR	C16-C15-C14	4.37	132.43	123.47
23	K	202	BCR	C37-C22-C21	-4.37	116.80	122.92
20	A	848	CLA	O2D-CGD-CBD	4.37	119.04	111.27
20	F	305	CLA	C3B-C2B-C1B	-4.37	101.89	107.16
20	1	304	CLA	O2D-CGD-CBD	4.37	119.03	111.27
20	A	843	CLA	CAC-C3C-C4C	4.37	130.48	124.81
20	B	821	CLA	CHC-C4B-NB	-4.37	119.63	124.26
20	2	303	CLA	C3D-C4D-ND	4.37	117.30	110.24
20	4	316	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
20	A	830	CLA	C3D-C4D-ND	4.37	117.30	110.24
20	3	307	CLA	C1C-C2C-C3C	-4.37	102.37	106.96
20	B	824	CLA	C1C-C2C-C3C	-4.36	102.37	106.96
20	1	302	CLA	C1C-C2C-C3C	-4.36	102.37	106.96
23	4	319	BCR	C34-C9-C10	-4.36	116.81	122.92
20	B	851	CLA	C3B-C4B-NB	4.36	114.56	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	804	CLA	C3D-C4D-ND	4.36	117.29	110.24
20	3	316	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
20	K	203	CLA	CHD-C1D-ND	-4.36	120.45	124.45
20	B	848	CLA	C3D-C4D-ND	4.36	117.29	110.24
20	1	307	CLA	CHC-C4B-NB	-4.36	119.64	124.26
20	B	824	CLA	CHC-C4B-NB	-4.35	119.65	124.26
20	A	846	CLA	C2D-C1D-ND	4.35	113.31	110.10
23	L	302	BCR	C37-C22-C21	-4.35	116.82	122.92
20	3	316	CLA	C3D-C4D-ND	4.35	117.28	110.24
20	B	811	CLA	C1C-C2C-C3C	-4.35	102.38	106.96
19	2	302	CHL	CHD-C4C-C3C	-4.35	118.45	124.84
23	4	320	BCR	C37-C22-C21	-4.35	116.83	122.92
20	3	310	CLA	C3D-C4D-ND	4.34	117.27	110.24
20	A	812	CLA	O2D-CGD-CBD	4.34	118.99	111.27
20	2	306	CLA	C3D-C2D-C1D	-4.34	99.90	105.83
20	A	832	CLA	CHD-C1D-ND	-4.34	120.46	124.45
19	4	315	CHL	CHD-C4C-C3C	-4.34	118.46	124.84
20	A	840	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
20	A	829	CLA	C3D-C4D-ND	4.34	117.26	110.24
20	3	310	CLA	O2D-CGD-CBD	4.34	118.98	111.27
20	4	316	CLA	C4D-CHA-C1A	-4.34	115.97	121.25
20	4	316	CLA	C1C-C2C-C3C	-4.34	102.39	106.96
19	4	305	CHL	CHD-C4C-C3C	-4.34	118.46	124.84
20	A	828	CLA	C3D-C4D-ND	4.34	117.26	110.24
20	A	803	CLA	O2D-CGD-CBD	4.34	118.98	111.27
20	A	837	CLA	C3D-C4D-ND	4.34	117.26	110.24
20	A	838	CLA	C3D-C4D-ND	4.34	117.25	110.24
20	3	314	CLA	C3B-C2B-C1B	-4.34	101.93	107.16
20	B	811	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
20	B	847	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
19	4	306	CHL	CHD-C4C-C3C	-4.34	118.47	124.84
20	B	823	CLA	C1C-C2C-C3C	-4.33	102.40	106.96
20	1	319	CLA	C3B-C4B-NB	4.33	114.53	110.52
20	4	303	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
20	4	314	CLA	CHD-C1D-ND	-4.33	120.48	124.45
19	1	317	CHL	CHD-C4C-C3C	-4.33	118.48	124.84
20	3	317	CLA	CHC-C4B-NB	-4.33	119.68	124.26
20	A	847	CLA	C1C-C2C-C3C	-4.33	102.41	106.96
20	J	103	CLA	CHD-C1D-ND	-4.33	120.48	124.45
23	O	203	BCR	C37-C22-C21	-4.33	116.86	122.92
20	A	850	CLA	O2D-CGD-CBD	4.33	118.95	111.27
23	G	203	BCR	C21-C20-C19	4.33	136.72	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	826	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
20	B	828	CLA	CHD-C1D-ND	-4.32	120.48	124.45
20	J	103	CLA	C3D-C4D-ND	4.32	117.23	110.24
20	B	833	CLA	CHD-C1D-ND	-4.32	120.48	124.45
20	2	323	CLA	CHD-C1D-ND	-4.32	120.48	124.45
20	3	308	CLA	CHD-C1D-ND	-4.32	120.48	124.45
20	3	317	CLA	CHD-C1D-ND	-4.32	120.48	124.45
20	B	828	CLA	CHC-C4B-NB	-4.32	119.68	124.26
20	B	827	CLA	CHC-C4B-NB	-4.32	119.69	124.26
20	A	804	CLA	C3D-C4D-ND	4.32	117.22	110.24
20	B	827	CLA	CHD-C1D-ND	-4.32	120.49	124.45
20	A	849	CLA	C3D-C4D-ND	4.32	117.22	110.24
20	A	830	CLA	C1C-C2C-C3C	-4.31	102.42	106.96
20	B	828	CLA	C1C-C2C-C3C	-4.31	102.42	106.96
20	A	846	CLA	C3D-C2D-C1D	-4.31	99.94	105.83
23	O	203	BCR	C35-C13-C14	-4.31	116.88	122.92
23	B	834	BCR	C37-C22-C23	4.31	124.87	118.08
20	B	807	CLA	C3D-C4D-ND	4.31	117.22	110.24
20	B	846	CLA	C4D-CHA-C1A	-4.31	116.00	121.25
20	B	829	CLA	CAC-C3C-C4C	4.31	130.41	124.81
20	1	309	CLA	CHD-C1D-ND	-4.31	120.49	124.45
20	2	321	CLA	O2D-CGD-CBD	4.31	118.93	111.27
20	B	850	CLA	C3D-C4D-ND	4.31	117.21	110.24
19	4	307	CHL	O2D-CGD-CBD	4.31	118.93	111.27
20	F	304	CLA	CHD-C1D-ND	-4.31	120.50	124.45
20	1	307	CLA	O2D-CGD-CBD	4.31	118.92	111.27
20	2	305	CLA	CHD-C1D-ND	-4.31	120.50	124.45
23	O	203	BCR	C11-C10-C9	4.31	133.45	127.31
23	A	816	BCR	C19-C18-C17	4.30	125.55	118.94
20	4	303	CLA	C3B-C2B-C1B	-4.30	101.97	107.16
20	4	310	CLA	CHC-C4B-NB	-4.30	119.70	124.26
20	3	310	CLA	C1C-C2C-C3C	-4.30	102.43	106.96
20	A	849	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
20	A	807	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
20	B	844	CLA	C1C-C2C-C3C	-4.30	102.44	106.96
20	1	307	CLA	C4D-CHA-C1A	-4.30	116.02	121.25
20	A	842	CLA	CHD-C1D-ND	-4.29	120.51	124.45
20	B	802	CLA	C3B-C2B-C1B	-4.29	101.98	107.16
20	N	202	CLA	CHD-C1D-ND	-4.29	120.51	124.45
23	A	818	BCR	C37-C22-C21	-4.29	116.91	122.92
20	4	316	CLA	C4A-NA-C1A	4.29	108.64	106.71
20	B	801	CLA	C3D-C4D-ND	4.29	117.18	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	302	CHL	O2D-CGD-CBD	4.29	118.89	111.27
20	A	828	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
20	2	303	CLA	CHC-C4B-NB	-4.29	119.72	124.26
20	A	801	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
19	1	301	CHL	C3D-C2D-C1D	-4.29	99.98	105.83
20	K	206	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
20	O	206	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
19	3	313	CHL	C2D-C1D-ND	4.29	113.26	110.10
20	A	837	CLA	CHB-C4A-NA	4.29	130.44	124.51
20	4	312	CLA	C3B-C2B-C1B	-4.29	101.99	107.16
20	A	846	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
20	2	320	CLA	C2D-C1D-ND	4.28	113.26	110.10
20	3	317	CLA	O2D-CGD-CBD	4.28	118.88	111.27
23	G	203	BCR	C37-C22-C21	-4.28	116.92	122.92
20	2	303	CLA	C3B-C2B-C1B	-4.28	102.00	107.16
20	A	855	CLA	CHD-C1D-ND	-4.28	120.52	124.45
20	B	803	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
20	A	806	CLA	C3B-C2B-C1B	-4.28	102.00	107.16
20	B	844	CLA	CHB-C4A-NA	4.28	130.43	124.51
20	3	307	CLA	C4D-CHA-C1A	-4.28	116.05	121.25
20	A	827	CLA	CHD-C1D-ND	-4.27	120.53	124.45
20	B	803	CLA	CHD-C1D-ND	-4.27	120.53	124.45
20	B	819	CLA	C3D-C4D-ND	4.27	117.15	110.24
20	2	304	CLA	C1C-C2C-C3C	-4.27	102.46	106.96
20	A	848	CLA	C1C-C2C-C3C	-4.27	102.46	106.96
20	B	853	CLA	C1C-C2C-C3C	-4.27	102.46	106.96
20	B	850	CLA	C4D-CHA-C1A	-4.27	116.05	121.25
20	L	306	CLA	C1C-C2C-C3C	-4.27	102.47	106.96
20	1	307	CLA	CHD-C1D-ND	-4.27	120.53	124.45
20	B	818	CLA	CHC-C4B-NB	-4.27	119.74	124.26
20	A	804	CLA	C3B-C2B-C1B	-4.27	102.01	107.16
20	A	831	CLA	C3D-C2D-C1D	-4.26	100.01	105.83
20	1	305	CLA	CHD-C1D-ND	-4.26	120.54	124.45
20	3	309	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
20	F	304	CLA	C1C-C2C-C3C	-4.26	102.48	106.96
20	L	307	CLA	C1C-C2C-C3C	-4.26	102.48	106.96
20	A	829	CLA	C3B-C2B-C1B	-4.26	102.02	107.16
20	B	846	CLA	CMC-C2C-C1C	4.26	131.52	125.04
20	3	311	CLA	C3D-C4D-ND	4.26	117.12	110.24
20	K	204	CLA	C1C-C2C-C3C	-4.26	102.48	106.96
20	B	806	CLA	CHC-C4B-NB	-4.25	119.75	124.26
20	B	849	CLA	C1C-C2C-C3C	-4.25	102.48	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	O	203	BCR	C34-C9-C8	4.25	124.78	118.08
20	3	307	CLA	C2A-C3A-C4A	-4.25	95.01	101.87
19	2	301	CHL	C2D-C1D-ND	4.24	113.23	110.10
19	2	322	CHL	C2D-C1D-ND	4.24	113.23	110.10
20	1	319	CLA	C1C-C2C-C3C	-4.24	102.50	106.96
20	B	806	CLA	CMC-C2C-C1C	4.24	131.50	125.04
20	B	804	CLA	CAC-C3C-C4C	4.24	130.31	124.81
19	2	301	CHL	CHD-C4C-C3C	-4.24	118.60	124.84
20	B	811	CLA	CHC-C4B-NB	-4.24	119.77	124.26
20	1	322	CLA	O2D-CGD-CBD	4.24	118.81	111.27
20	B	849	CLA	CMB-C2B-C1B	4.24	131.83	125.37
23	A	857	BCR	C37-C22-C21	-4.24	116.98	122.92
23	O	202	BCR	C10-C11-C12	4.24	136.44	123.22
20	1	302	CLA	C3D-C2D-C1D	-4.24	100.05	105.83
20	B	818	CLA	O2D-CGD-CBD	4.24	118.80	111.27
20	B	821	CLA	C3D-C2D-C1D	-4.24	100.05	105.83
20	A	839	CLA	C1C-C2C-C3C	-4.24	102.50	106.96
20	2	303	CLA	C1C-C2C-C3C	-4.23	102.50	106.96
20	A	837	CLA	C4-C3-C2	-4.23	112.82	123.68
20	G	206	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
23	G	201	BCR	C34-C9-C10	-4.23	117.00	122.92
20	A	849	CLA	CAC-C3C-C4C	4.23	130.30	124.81
20	A	802	CLA	C1C-C2C-C3C	-4.23	102.51	106.96
20	A	853	CLA	C1C-C2C-C3C	-4.23	102.51	106.96
20	3	312	CLA	CHD-C1D-ND	-4.23	120.57	124.45
20	A	831	CLA	CHC-C4B-NB	-4.23	119.78	124.26
20	3	319	CLA	CHD-C1D-ND	-4.23	120.57	124.45
20	2	321	CLA	C1C-C2C-C3C	-4.23	102.51	106.96
20	A	840	CLA	CHD-C1D-ND	-4.23	120.57	124.45
20	A	833	CLA	C1C-C2C-C3C	-4.23	102.51	106.96
20	A	831	CLA	CHD-C1D-ND	-4.23	120.57	124.45
23	F	301	BCR	C37-C22-C21	-4.22	117.00	122.92
20	3	309	CLA	CHD-C1D-ND	-4.22	120.57	124.45
20	O	206	CLA	C3D-C4D-ND	4.22	117.07	110.24
20	B	821	CLA	CHD-C1D-ND	-4.22	120.57	124.45
20	B	852	CLA	CHD-C1D-ND	-4.22	120.58	124.45
20	A	809	CLA	CHD-C1D-ND	-4.22	120.58	124.45
20	B	830	CLA	C1C-C2C-C3C	-4.22	102.52	106.96
20	B	833	CLA	C4D-CHA-C1A	-4.22	116.12	121.25
20	B	812	CLA	C3B-C2B-C1B	-4.22	102.07	107.16
20	3	315	CLA	O2D-CGD-CBD	4.22	118.76	111.27
20	4	310	CLA	C1C-C2C-C3C	-4.22	102.53	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	321	CLA	C3D-C4D-ND	4.21	117.06	110.24
20	B	813	CLA	C4D-CHA-C1A	-4.21	116.12	121.25
19	4	315	CHL	C2D-C1D-ND	4.21	113.21	110.10
23	L	302	BCR	C37-C22-C23	4.21	124.71	118.08
20	A	843	CLA	C1C-C2C-C3C	-4.21	102.53	106.96
20	1	309	CLA	C1C-C2C-C3C	-4.20	102.54	106.96
20	3	319	CLA	C1C-C2C-C3C	-4.20	102.54	106.96
20	B	801	CLA	O2D-CGD-CBD	4.20	118.73	111.27
21	1	323	LUT	C40-C33-C34	-4.20	117.04	122.92
20	A	840	CLA	C1C-C2C-C3C	-4.20	102.54	106.96
20	A	835	CLA	CHC-C4B-NB	-4.20	119.81	124.26
20	1	308	CLA	C1C-C2C-C3C	-4.20	102.54	106.96
20	B	821	CLA	C1C-C2C-C3C	-4.20	102.54	106.96
20	3	320	CLA	CHD-C1D-ND	-4.20	120.60	124.45
20	B	816	CLA	C1C-C2C-C3C	-4.19	102.55	106.96
20	2	305	CLA	C4D-CHA-C1A	-4.19	116.14	121.25
20	A	851	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
20	B	825	CLA	C1C-C2C-C3C	-4.19	102.55	106.96
20	1	309	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
20	B	809	CLA	C3B-C2B-C1B	-4.19	102.10	107.16
20	G	206	CLA	CHD-C1D-ND	-4.19	120.60	124.45
22	3	302	XAT	C35-C34-C33	4.19	133.29	127.31
20	4	310	CLA	C3D-C4D-ND	4.19	117.02	110.24
20	1	302	CLA	CHD-C1D-ND	-4.19	120.60	124.45
20	B	844	CLA	C4A-NA-C1A	4.19	108.59	106.71
20	2	306	CLA	C2D-C1D-ND	4.19	113.19	110.10
20	3	312	CLA	C1C-C2C-C3C	-4.19	102.55	106.96
20	2	320	CLA	C3D-C2D-C1D	-4.19	100.12	105.83
20	B	804	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
20	1	307	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
20	A	806	CLA	CHC-C4B-NB	-4.18	119.83	124.26
20	B	806	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
20	A	807	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
20	A	832	CLA	C3B-C2B-C1B	-4.18	102.12	107.16
20	A	843	CLA	C3D-C4D-ND	4.17	116.99	110.24
20	A	850	CLA	C3D-C4D-ND	4.17	116.99	110.24
20	2	307	CLA	C3B-C4B-NB	4.17	114.38	110.52
20	F	304	CLA	CMC-C2C-C1C	4.17	131.38	125.04
20	4	304	CLA	C1C-C2C-C3C	-4.16	102.58	106.96
20	A	812	CLA	C3D-C2D-C1D	-4.16	100.15	105.83
20	B	815	CLA	CHB-C4A-NA	4.16	130.27	124.51
20	A	855	CLA	C3D-C4D-ND	4.16	116.97	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	303	CLA	C2D-C1D-ND	4.16	113.17	110.10
20	A	811	CLA	C4D-CHA-C1A	-4.16	116.19	121.25
20	F	305	CLA	CHD-C1D-ND	-4.16	120.63	124.45
20	B	806	CLA	CAC-C3C-C4C	4.16	130.21	124.81
20	G	206	CLA	CAC-C3C-C4C	4.16	130.21	124.81
20	A	809	CLA	C3D-C2D-C1D	-4.16	100.16	105.83
23	F	302	BCR	C37-C22-C21	-4.16	117.10	122.92
23	2	312	BCR	C10-C11-C12	4.15	136.18	123.22
23	B	834	BCR	C37-C22-C21	-4.15	117.10	122.92
20	A	855	CLA	C3D-C2D-C1D	-4.15	100.16	105.83
20	A	853	CLA	C3D-C4D-ND	4.15	116.95	110.24
20	A	851	CLA	C4D-CHA-C1A	-4.15	116.20	121.25
20	A	805	CLA	C2D-C1D-ND	4.15	113.16	110.10
20	1	304	CLA	C1C-C2C-C3C	-4.15	102.59	106.96
20	2	308	CLA	C1C-C2C-C3C	-4.15	102.59	106.96
20	2	317	CLA	C1C-C2C-C3C	-4.15	102.60	106.96
20	A	850	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
20	B	845	CLA	C3D-C4D-ND	4.15	116.95	110.24
20	4	302	CLA	CHD-C1D-ND	-4.15	120.64	124.45
20	1	320	CLA	C1C-C2C-C3C	-4.15	102.60	106.96
20	3	317	CLA	CAC-C3C-C4C	4.15	130.19	124.81
20	A	806	CLA	C1C-C2C-C3C	-4.15	102.60	106.96
20	F	306	CLA	C1C-C2C-C3C	-4.15	102.60	106.96
20	1	306	CLA	CHD-C1D-ND	-4.14	120.64	124.45
20	B	830	CLA	C3D-C2D-C1D	-4.14	100.17	105.83
23	K	201	BCR	C37-C22-C21	-4.14	117.12	122.92
20	1	307	CLA	C3D-C2D-C1D	-4.14	100.18	105.83
20	1	321	CLA	CHD-C1D-ND	-4.14	120.65	124.45
20	L	305	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
20	A	840	CLA	C3D-C2D-C1D	-4.14	100.18	105.83
20	B	807	CLA	CHC-C4B-NB	-4.14	119.87	124.26
20	B	810	CLA	C3D-C2D-C1D	-4.14	100.19	105.83
22	1	311	XAT	C30-C31-C32	4.13	136.12	123.22
20	B	850	CLA	CAC-C3C-C4C	4.13	130.17	124.81
20	B	829	CLA	CHD-C1D-ND	-4.13	120.66	124.45
20	3	319	CLA	CHC-C4B-NB	-4.13	119.88	124.26
20	A	836	CLA	C3D-C2D-C1D	-4.13	100.19	105.83
20	4	312	CLA	C1C-C2C-C3C	-4.13	102.61	106.96
20	B	848	CLA	CMC-C2C-C1C	4.13	131.33	125.04
20	B	812	CLA	C1C-C2C-C3C	-4.13	102.62	106.96
20	4	303	CLA	CHD-C1D-ND	-4.13	120.66	124.45
20	B	809	CLA	CHC-C4B-NB	-4.13	119.89	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	805	CLA	CHD-C1D-ND	-4.13	120.66	124.45
20	B	849	CLA	C3D-C2D-C1D	-4.13	100.20	105.83
20	2	307	CLA	C1C-C2C-C3C	-4.13	102.62	106.96
20	3	309	CLA	C2D-C1D-ND	4.13	113.14	110.10
20	A	854	CLA	C3D-C4D-ND	4.13	116.91	110.24
20	3	314	CLA	CHC-C4B-NB	-4.13	119.89	124.26
20	4	302	CLA	C4D-CHA-C1A	-4.12	116.23	121.25
20	3	320	CLA	C1C-C2C-C3C	-4.12	102.62	106.96
20	B	844	CLA	C3D-C4D-ND	4.12	116.91	110.24
20	B	814	CLA	CHD-C1D-ND	-4.12	120.67	124.45
20	B	830	CLA	C3B-C2B-C1B	-4.12	102.19	107.16
20	4	310	CLA	C3D-C2D-C1D	-4.12	100.21	105.83
20	K	203	CLA	C3D-C2D-C1D	-4.12	100.21	105.83
21	1	323	LUT	C28-C29-C30	4.12	125.26	118.94
20	A	811	CLA	CHD-C1D-ND	-4.12	120.67	124.45
20	1	302	CLA	O2D-CGD-CBD	4.12	118.58	111.27
20	F	304	CLA	CAC-C3C-C4C	4.12	130.15	124.81
20	4	303	CLA	O2D-CGD-CBD	4.11	118.58	111.27
20	B	810	CLA	CHD-C1D-ND	-4.11	120.68	124.45
20	A	836	CLA	C4D-CHA-C1A	-4.11	116.25	121.25
20	A	833	CLA	O2D-CGD-CBD	4.11	118.57	111.27
20	A	829	CLA	CAC-C3C-C4C	4.11	130.14	124.81
20	F	305	CLA	C3D-C2D-C1D	-4.11	100.22	105.83
20	4	304	CLA	CHB-C4A-NA	4.11	130.19	124.51
20	1	321	CLA	O2D-CGD-CBD	4.11	118.57	111.27
20	O	208	CLA	C4D-CHA-C1A	-4.11	116.25	121.25
20	A	807	CLA	CAC-C3C-C4C	4.11	130.14	124.81
23	J	101	BCR	C37-C22-C21	-4.10	117.17	122.92
20	4	309	CLA	O2D-CGD-CBD	4.10	118.56	111.27
20	A	847	CLA	CHC-C4B-NB	-4.10	119.91	124.26
20	1	322	CLA	C4D-CHA-C1A	-4.10	116.25	121.25
20	G	205	CLA	C3D-C2D-C1D	-4.10	100.23	105.83
20	N	202	CLA	C3D-C2D-C1D	-4.10	100.23	105.83
20	A	808	CLA	CHD-C1D-ND	-4.10	120.68	124.45
20	3	318	CLA	C1C-C2C-C3C	-4.10	102.64	106.96
20	2	306	CLA	C1C-C2C-C3C	-4.10	102.65	106.96
19	2	301	CHL	C1D-ND-C4D	-4.10	103.42	106.33
20	B	852	CLA	C3D-C2D-C1D	-4.10	100.24	105.83
20	K	203	CLA	C1C-C2C-C3C	-4.10	102.65	106.96
20	4	304	CLA	CHD-C1D-ND	-4.10	120.69	124.45
20	A	838	CLA	C3D-C2D-C1D	-4.10	100.24	105.83
20	G	207	CLA	C3D-C2D-C1D	-4.10	100.24	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	319	CLA	C1C-C2C-C3C	-4.10	102.65	106.96
20	A	854	CLA	C1C-C2C-C3C	-4.10	102.65	106.96
20	A	856	CLA	C1C-C2C-C3C	-4.10	102.65	106.96
20	A	845	CLA	CHD-C1D-ND	-4.10	120.69	124.45
20	F	304	CLA	C3D-C2D-C1D	-4.10	100.24	105.83
20	B	847	CLA	C1C-C2C-C3C	-4.09	102.65	106.96
20	B	827	CLA	C4D-CHA-C1A	-4.09	116.27	121.25
20	J	103	CLA	C1C-C2C-C3C	-4.09	102.65	106.96
20	A	841	CLA	CHC-C4B-NB	-4.09	119.93	124.26
19	2	322	CHL	C1D-ND-C4D	-4.09	103.43	106.33
20	A	856	CLA	C3D-C2D-C1D	-4.09	100.25	105.83
20	A	838	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
20	1	309	CLA	C4D-CHA-C1A	-4.09	116.27	121.25
20	B	844	CLA	CHB-C1B-NB	-4.09	119.93	124.26
20	L	307	CLA	C3D-C2D-C1D	-4.09	100.26	105.83
20	3	307	CLA	C3D-C2D-C1D	-4.08	100.26	105.83
23	B	837	BCR	C37-C22-C23	4.08	124.51	118.08
20	B	807	CLA	CHD-C1D-ND	-4.08	120.70	124.45
20	G	207	CLA	C1C-C2C-C3C	-4.08	102.67	106.96
19	1	317	CHL	C1D-ND-C4D	-4.08	103.44	106.33
19	4	306	CHL	C1D-ND-C4D	-4.08	103.44	106.33
20	1	302	CLA	C4D-CHA-C1A	-4.08	116.28	121.25
20	2	307	CLA	C3D-C2D-C1D	-4.08	100.26	105.83
23	B	836	BCR	C37-C22-C21	-4.08	117.21	122.92
19	1	317	CHL	C2D-C1D-ND	4.08	113.11	110.10
20	B	829	CLA	O2D-CGD-CBD	4.08	118.51	111.27
19	3	313	CHL	C1D-ND-C4D	-4.08	103.44	106.33
19	1	301	CHL	CHD-C4C-C3C	-4.07	118.85	124.84
20	A	808	CLA	CAC-C3C-C4C	4.07	130.09	124.81
20	2	320	CLA	C1D-CHD-C4C	-4.07	117.27	126.06
20	4	302	CLA	C1C-C2C-C3C	-4.07	102.68	106.96
20	B	846	CLA	C1C-C2C-C3C	-4.07	102.68	106.96
20	4	313	CLA	CAC-C3C-C4C	4.07	130.09	124.81
20	A	825	CLA	CMC-C2C-C1C	4.07	131.23	125.04
20	B	813	CLA	C1C-C2C-C3C	-4.07	102.68	106.96
20	A	804	CLA	CHD-C1D-ND	-4.07	120.72	124.45
20	4	311	CLA	C3D-C2D-C1D	-4.07	100.28	105.83
20	1	306	CLA	C1C-C2C-C3C	-4.07	102.68	106.96
20	3	316	CLA	C1C-C2C-C3C	-4.07	102.68	106.96
20	A	803	CLA	CHC-C4B-NB	-4.07	119.95	124.26
20	A	849	CLA	C2D-C1D-ND	4.06	113.10	110.10
20	B	811	CLA	C2D-C1D-ND	4.06	113.10	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	845	CLA	CAC-C3C-C4C	4.06	130.08	124.81
20	B	826	CLA	CHD-C1D-ND	-4.06	120.72	124.45
20	A	850	CLA	CHD-C1D-ND	-4.06	120.72	124.45
20	3	314	CLA	C4D-CHA-C1A	-4.06	116.31	121.25
20	B	820	CLA	C3D-C2D-C1D	-4.06	100.29	105.83
20	A	808	CLA	CHB-C4A-NA	4.06	130.13	124.51
23	B	838	BCR	C37-C22-C21	-4.06	117.24	122.92
20	A	811	CLA	C3D-C2D-C1D	-4.06	100.29	105.83
20	H	201	CLA	CHD-C1D-ND	-4.06	120.72	124.45
20	L	306	CLA	C3D-C2D-C1D	-4.06	100.29	105.83
20	B	807	CLA	C3D-C2D-C1D	-4.06	100.30	105.83
20	A	846	CLA	CAC-C3C-C4C	4.05	130.07	124.81
20	B	848	CLA	CHD-C1D-ND	-4.05	120.73	124.45
20	J	103	CLA	C3D-C2D-C1D	-4.05	100.30	105.83
20	H	201	CLA	C3D-C2D-C1D	-4.05	100.30	105.83
20	B	801	CLA	CHD-C1D-ND	-4.05	120.73	124.45
20	A	847	CLA	CMD-C2D-C3D	-4.05	118.30	127.61
20	2	306	CLA	CHD-C1D-ND	-4.05	120.73	124.45
23	B	837	BCR	C16-C15-C14	4.05	131.77	123.47
20	A	828	CLA	C3D-C2D-C1D	-4.05	100.31	105.83
20	A	846	CLA	C3B-C2B-C1B	-4.05	102.28	107.16
20	B	817	CLA	CHD-C1D-ND	-4.05	120.73	124.45
20	B	825	CLA	CHD-C1D-ND	-4.05	120.74	124.45
20	A	847	CLA	C3B-C2B-C1B	-4.05	102.28	107.16
20	B	844	CLA	C3B-C4B-NB	4.05	114.27	110.52
20	1	305	CLA	C3D-C2D-C1D	-4.04	100.31	105.83
21	2	310	LUT	C19-C9-C10	-4.04	117.26	122.92
20	B	850	CLA	CHC-C4B-NB	-4.04	119.98	124.26
20	4	313	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
20	4	311	CLA	CHD-C1D-ND	-4.04	120.74	124.45
19	4	315	CHL	C1D-ND-C4D	-4.04	103.46	106.33
20	B	819	CLA	CAC-C3C-C4C	4.04	130.05	124.81
19	4	306	CHL	C2D-C1D-ND	4.04	113.08	110.10
23	A	814	BCR	C37-C22-C21	-4.04	117.27	122.92
20	F	304	CLA	CHC-C4B-NB	-4.04	119.98	124.26
20	2	305	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
20	4	312	CLA	C3D-C2D-C1D	-4.04	100.32	105.83
20	4	309	CLA	CHD-C1D-ND	-4.04	120.74	124.45
20	3	316	CLA	C2D-C1D-ND	4.04	113.08	110.10
20	4	309	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
20	K	205	CLA	C4D-CHA-C1A	-4.04	116.34	121.25
23	B	834	BCR	C34-C9-C10	-4.03	117.27	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	851	CLA	C3D-C4D-ND	4.03	116.76	110.24
23	A	857	BCR	C8-C9-C10	4.03	125.13	118.94
23	2	312	BCR	C11-C10-C9	4.03	133.06	127.31
20	1	302	CLA	C2D-C1D-ND	4.03	113.07	110.10
23	L	304	BCR	C7-C8-C9	4.03	132.32	126.23
20	4	312	CLA	CHD-C1D-ND	-4.03	120.75	124.45
20	3	317	CLA	C4D-CHA-C1A	-4.03	116.35	121.25
20	1	322	CLA	CHD-C1D-ND	-4.03	120.75	124.45
19	2	309	CHL	C1D-ND-C4D	-4.03	103.47	106.33
20	B	830	CLA	CHC-C4B-NB	-4.03	120.00	124.26
20	K	204	CLA	C3D-C2D-C1D	-4.03	100.34	105.83
20	3	314	CLA	CHB-C4A-NA	4.03	130.08	124.51
20	A	833	CLA	C4D-CHA-C1A	-4.02	116.35	121.25
20	4	302	CLA	C3D-C2D-C1D	-4.02	100.34	105.83
20	B	825	CLA	C3B-C2B-C1B	-4.02	102.31	107.16
20	A	831	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
20	A	854	CLA	C4D-CHA-C1A	-4.02	116.36	121.25
20	A	807	CLA	CHC-C4B-NB	-4.02	120.00	124.26
20	B	805	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
20	3	308	CLA	CHB-C4A-NA	4.02	130.07	124.51
20	A	804	CLA	C3D-C2D-C1D	-4.02	100.35	105.83
20	B	810	CLA	C3B-C2B-C1B	-4.02	102.31	107.16
20	1	306	CLA	C3D-C2D-C1D	-4.02	100.35	105.83
20	4	310	CLA	CHD-C1D-ND	-4.02	120.76	124.45
20	4	314	CLA	C3D-C2D-C1D	-4.01	100.35	105.83
29	G	202	DGD	O2G-C1B-C2B	4.01	120.15	111.50
20	A	806	CLA	C3D-C2D-C1D	-4.01	100.35	105.83
20	O	208	CLA	CHD-C1D-ND	-4.01	120.77	124.45
20	1	319	CLA	C3D-C2D-C1D	-4.01	100.36	105.83
20	B	825	CLA	O2D-CGD-CBD	4.01	118.39	111.27
20	B	833	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
19	4	305	CHL	C2D-C1D-ND	4.01	113.06	110.10
20	4	314	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
20	A	836	CLA	CAC-C3C-C4C	4.00	130.00	124.81
20	3	316	CLA	CHD-C1D-ND	-4.00	120.78	124.45
20	O	208	CLA	C3D-C2D-C1D	-4.00	100.37	105.83
20	B	822	CLA	C3D-C2D-C1D	-4.00	100.37	105.83
20	A	808	CLA	CMC-C2C-C1C	4.00	131.13	125.04
20	4	313	CLA	O2D-CGD-CBD	4.00	118.37	111.27
20	B	815	CLA	C3D-C2D-C1D	-4.00	100.38	105.83
20	B	806	CLA	O2D-CGD-CBD	4.00	118.37	111.27
20	A	838	CLA	CAC-C3C-C4C	3.99	129.99	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	817	CLA	C3D-C4D-ND	3.99	116.70	110.24
20	A	837	CLA	CMC-C2C-C1C	3.99	131.12	125.04
20	B	833	CLA	C3D-C2D-C1D	-3.99	100.38	105.83
20	A	801	CLA	CHB-C4A-NA	3.99	130.03	124.51
20	B	824	CLA	C3D-C2D-C1D	-3.99	100.39	105.83
20	3	310	CLA	C3B-C4B-NB	3.99	114.22	110.52
20	O	207	CLA	O2D-CGD-CBD	3.99	118.36	111.27
21	1	323	LUT	C35-C15-C14	3.99	131.64	123.47
23	L	301	BCR	C37-C22-C21	-3.99	117.34	122.92
20	A	851	CLA	CHB-C4A-NA	3.99	130.02	124.51
20	2	323	CLA	C1C-C2C-C3C	-3.99	102.77	106.96
23	A	857	BCR	C34-C9-C10	-3.98	117.34	122.92
20	3	318	CLA	C3D-C2D-C1D	-3.98	100.39	105.83
20	4	308	CLA	C3D-C4D-ND	3.98	116.68	110.24
20	B	844	CLA	C3D-C2D-C1D	-3.98	100.40	105.83
20	1	320	CLA	C3D-C2D-C1D	-3.98	100.40	105.83
23	J	101	BCR	C37-C22-C23	3.98	124.35	118.08
28	A	824	CL0	C3D-C4D-ND	3.98	116.67	110.24
21	2	310	LUT	C15-C35-C34	3.98	131.62	123.47
20	2	304	CLA	C3D-C2D-C1D	-3.98	100.40	105.83
20	B	827	CLA	C3D-C2D-C1D	-3.98	100.41	105.83
20	4	313	CLA	C3D-C2D-C1D	-3.98	100.41	105.83
20	A	805	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
19	2	301	CHL	C3B-C4B-NB	3.97	114.20	110.52
20	2	305	CLA	C3D-C2D-C1D	-3.97	100.41	105.83
23	F	301	BCR	C23-C22-C21	3.97	125.03	118.94
20	B	805	CLA	C3D-C2D-C1D	-3.97	100.41	105.83
20	3	308	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
23	O	202	BCR	C37-C22-C23	3.97	124.33	118.08
20	1	304	CLA	C3D-C2D-C1D	-3.96	100.42	105.83
20	2	317	CLA	C3D-C2D-C1D	-3.96	100.42	105.83
20	A	852	CLA	C3D-C4D-ND	3.96	116.65	110.24
20	B	817	CLA	C2D-C1D-ND	3.96	113.02	110.10
20	A	825	CLA	O2D-CGD-CBD	3.96	118.30	111.27
20	A	852	CLA	CHB-C4A-NA	3.96	129.98	124.51
20	3	309	CLA	O2D-CGD-CBD	3.96	118.30	111.27
20	A	801	CLA	CAC-C3C-C4C	3.95	129.94	124.81
20	2	320	CLA	O2D-CGD-CBD	3.95	118.29	111.27
23	B	839	BCR	C37-C22-C23	3.95	124.31	118.08
20	1	321	CLA	C3D-C2D-C1D	-3.95	100.44	105.83
20	3	317	CLA	C3D-C2D-C1D	-3.95	100.44	105.83
20	B	853	CLA	C3D-C2D-C1D	-3.95	100.44	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	323	CLA	C3D-C2D-C1D	-3.95	100.45	105.83
20	3	310	CLA	C3D-C2D-C1D	-3.95	100.45	105.83
20	A	839	CLA	C3D-C2D-C1D	-3.95	100.45	105.83
20	K	206	CLA	C3D-C2D-C1D	-3.95	100.45	105.83
23	I	102	BCR	C37-C22-C21	-3.94	117.40	122.92
20	A	803	CLA	CAC-C3C-C4C	3.94	129.93	124.81
20	G	205	CLA	C4D-CHA-C1A	-3.94	116.45	121.25
20	A	845	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
19	4	307	CHL	C2D-C1D-ND	3.94	113.01	110.10
20	A	849	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
20	B	826	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
20	A	801	CLA	C3D-C2D-C1D	-3.94	100.45	105.83
20	O	206	CLA	C3D-C2D-C1D	-3.94	100.45	105.83
20	4	311	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
20	2	320	CLA	CHB-C4A-NA	3.94	129.96	124.51
20	2	308	CLA	C3D-C2D-C1D	-3.94	100.45	105.83
20	B	816	CLA	C4D-CHA-C1A	-3.94	116.45	121.25
20	A	842	CLA	C3D-C2D-C1D	-3.94	100.46	105.83
20	G	206	CLA	C1C-C2C-C3C	-3.94	102.82	106.96
20	3	308	CLA	C3D-C2D-C1D	-3.94	100.46	105.83
20	1	322	CLA	C3D-C2D-C1D	-3.94	100.46	105.83
20	O	207	CLA	C1C-C2C-C3C	-3.94	102.82	106.96
20	2	320	CLA	CHC-C1C-C2C	-3.94	115.80	126.73
20	B	804	CLA	C4D-CHA-C1A	-3.93	116.46	121.25
20	3	312	CLA	C3D-C2D-C1D	-3.93	100.46	105.83
20	B	850	CLA	C3D-C2D-C1D	-3.93	100.47	105.83
20	A	832	CLA	C4D-CHA-C1A	-3.93	116.46	121.25
20	3	311	CLA	CHD-C1D-ND	-3.93	120.84	124.45
20	B	806	CLA	C3D-C2D-C1D	-3.93	100.47	105.83
19	4	315	CHL	C3B-C4B-NB	3.93	114.16	110.52
20	B	801	CLA	CHB-C4A-NA	3.93	129.94	124.51
20	A	835	CLA	C4-C3-C5	3.93	121.88	115.27
20	B	847	CLA	CHB-C4A-NA	3.93	129.94	124.51
20	A	852	CLA	O2D-CGD-CBD	3.93	118.24	111.27
20	3	319	CLA	C3D-C2D-C1D	-3.92	100.47	105.83
19	2	302	CHL	C2D-C1D-ND	3.92	112.99	110.10
20	O	206	CLA	C3B-C4B-NB	3.92	114.15	110.52
20	A	830	CLA	C4D-CHA-C1A	-3.92	116.48	121.25
20	A	801	CLA	C3D-C4D-ND	3.92	116.58	110.24
20	O	208	CLA	CHB-C4A-NA	3.92	129.93	124.51
23	4	320	BCR	C21-C20-C19	3.92	135.44	123.22
20	A	808	CLA	C3D-C2D-C1D	-3.91	100.49	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	318	CLA	C3D-C2D-C1D	-3.91	100.49	105.83
19	2	309	CHL	C2D-C1D-ND	3.91	112.99	110.10
20	4	313	CLA	C4D-CHA-C1A	-3.91	116.49	121.25
19	3	313	CHL	C3B-C4B-NB	3.91	114.14	110.52
20	A	835	CLA	C3D-C2D-C1D	-3.91	100.50	105.83
20	B	804	CLA	CHD-C1D-ND	-3.91	120.86	124.45
20	A	851	CLA	C2D-C1D-ND	3.91	112.98	110.10
20	B	807	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
23	F	301	BCR	C15-C14-C13	3.91	132.89	127.31
20	4	310	CLA	CAC-C3C-C4C	3.91	129.88	124.81
20	G	207	CLA	CAC-C3C-C4C	3.91	129.88	124.81
20	O	207	CLA	C3D-C2D-C1D	-3.91	100.50	105.83
20	B	847	CLA	C4A-NA-C1A	3.91	108.46	106.71
20	1	318	CLA	C4D-CHA-C1A	-3.90	116.50	121.25
20	4	302	CLA	CAC-C3C-C4C	3.90	129.87	124.81
20	B	851	CLA	C3D-C2D-C1D	-3.90	100.50	105.83
20	3	309	CLA	C4D-CHA-C1A	-3.90	116.50	121.25
19	4	306	CHL	CAC-C3C-C4C	3.90	129.87	124.81
23	A	816	BCR	C35-C13-C14	-3.90	117.46	122.92
20	B	807	CLA	CAC-C3C-C4C	3.90	129.87	124.81
20	A	852	CLA	C3B-C4B-NB	3.90	114.13	110.52
20	B	815	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
19	1	301	CHL	C3B-C4B-NB	3.90	114.13	110.52
19	2	302	CHL	C1D-ND-C4D	-3.90	103.57	106.33
22	2	311	XAT	C39-C29-C30	-3.90	117.47	122.92
23	A	817	BCR	C37-C22-C21	-3.90	117.47	122.92
20	A	839	CLA	C3B-C4B-NB	3.89	114.13	110.52
20	B	826	CLA	C2D-C1D-ND	3.89	112.97	110.10
20	1	322	CLA	CHB-C4A-NA	3.89	129.90	124.51
20	4	309	CLA	CMC-C2C-C1C	3.89	130.96	125.04
20	A	837	CLA	C2D-C1D-ND	3.89	112.97	110.10
20	B	847	CLA	C2D-C1D-ND	3.89	112.97	110.10
19	4	305	CHL	C1D-ND-C4D	-3.89	103.57	106.33
20	4	302	CLA	CMC-C2C-C1C	3.89	130.96	125.04
20	A	853	CLA	CHB-C4A-NA	3.89	129.88	124.51
20	1	321	CLA	C1C-C2C-C3C	-3.88	102.87	106.96
20	B	850	CLA	CHB-C4A-NA	3.88	129.88	124.51
20	4	309	CLA	C3D-C2D-C1D	-3.88	100.53	105.83
20	B	846	CLA	O2D-CGD-CBD	3.88	118.17	111.27
20	4	310	CLA	C4D-CHA-C1A	-3.88	116.53	121.25
20	B	808	CLA	C3D-C2D-C1D	-3.88	100.53	105.83
20	F	306	CLA	C3D-C2D-C1D	-3.88	100.53	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2	312	BCR	C37-C22-C21	-3.88	117.49	122.92
20	A	852	CLA	C3D-C2D-C1D	-3.88	100.54	105.83
20	B	830	CLA	C4D-CHA-C1A	-3.88	116.53	121.25
20	B	819	CLA	CHD-C1D-ND	-3.87	120.89	124.45
23	O	203	BCR	C16-C17-C18	3.87	132.84	127.31
20	B	801	CLA	C5-C3-C2	-3.87	113.28	121.12
20	A	805	CLA	CHD-C1D-ND	-3.87	120.90	124.45
20	A	803	CLA	C2D-C1D-ND	3.87	112.96	110.10
20	K	205	CLA	C3D-C2D-C1D	-3.87	100.55	105.83
20	O	208	CLA	C3B-C4B-NB	3.87	114.11	110.52
20	B	803	CLA	CMC-C2C-C1C	3.87	130.93	125.04
20	B	851	CLA	CHC-C1C-C2C	-3.87	115.98	126.73
20	B	812	CLA	C3D-C2D-C1D	-3.87	100.55	105.83
20	2	304	CLA	O2D-CGD-CBD	3.87	118.14	111.27
20	B	811	CLA	O2D-CGD-CBD	3.87	118.14	111.27
20	F	304	CLA	O2D-CGD-CBD	3.86	118.13	111.27
20	A	825	CLA	C4D-CHA-C1A	-3.86	116.55	121.25
20	2	320	CLA	CHC-C4B-NB	-3.86	120.17	124.26
23	A	818	BCR	C34-C9-C10	-3.86	117.51	122.92
20	1	305	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
20	O	208	CLA	O2D-CGD-CBD	3.86	118.13	111.27
20	B	824	CLA	O2D-CGD-CBD	3.86	118.13	111.27
20	B	846	CLA	C3D-C2D-C1D	-3.86	100.56	105.83
20	A	803	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
20	B	853	CLA	C3B-C4B-NB	3.86	114.10	110.52
20	3	311	CLA	C3D-C2D-C1D	-3.86	100.57	105.83
20	B	801	CLA	CAC-C3C-C4C	3.86	129.81	124.81
20	A	804	CLA	CHC-C4B-NB	-3.85	120.18	124.26
23	4	319	BCR	C34-C9-C8	3.85	124.15	118.08
20	A	837	CLA	CHD-C1D-ND	-3.85	120.91	124.45
20	2	304	CLA	CHB-C4A-NA	3.85	129.84	124.51
20	A	809	CLA	CHB-C4A-NA	3.85	129.84	124.51
20	B	833	CLA	CHB-C4A-NA	3.85	129.83	124.51
23	A	816	BCR	C37-C22-C21	-3.85	117.53	122.92
20	F	306	CLA	CHD-C1D-ND	-3.85	120.92	124.45
20	4	309	CLA	CHB-C4A-NA	3.85	129.83	124.51
20	B	802	CLA	C3D-C2D-C1D	-3.85	100.58	105.83
20	A	851	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
20	B	807	CLA	CHB-C4A-NA	3.84	129.82	124.51
20	3	320	CLA	C3D-C2D-C1D	-3.84	100.59	105.83
20	J	103	CLA	O2D-CGD-CBD	3.84	118.09	111.27
20	A	844	CLA	C3D-C2D-C1D	-3.84	100.59	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	809	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
20	1	304	CLA	C3B-C4B-NB	3.84	114.08	110.52
20	3	311	CLA	CHB-C4A-NA	3.84	129.82	124.51
23	1	312	BCR	C16-C15-C14	3.84	131.34	123.47
20	F	306	CLA	CHB-C4A-NA	3.84	129.82	124.51
20	1	308	CLA	C3D-C2D-C1D	-3.84	100.59	105.83
20	B	831	CLA	C4D-CHA-C1A	-3.84	116.58	121.25
20	B	808	CLA	O2A-C1-C2	3.84	118.72	108.64
20	B	825	CLA	CHC-C4B-NB	-3.84	120.19	124.26
20	A	830	CLA	C3D-C2D-C1D	-3.84	100.59	105.83
19	2	318	CHL	C3D-C4D-ND	3.84	116.44	110.24
20	2	323	CLA	C4D-CHA-C1A	-3.83	116.58	121.25
20	K	203	CLA	C3B-C4B-NB	3.83	114.07	110.52
20	A	803	CLA	C3D-C2D-C1D	-3.83	100.60	105.83
20	A	827	CLA	CHB-C4A-NA	3.83	129.81	124.51
23	3	303	BCR	C37-C22-C23	3.83	124.12	118.08
20	B	829	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
23	B	836	BCR	C37-C22-C23	3.83	124.11	118.08
20	B	853	CLA	CAC-C3C-C4C	3.83	129.78	124.81
20	2	321	CLA	C3D-C2D-C1D	-3.83	100.61	105.83
20	G	206	CLA	C2D-C1D-ND	3.83	112.92	110.10
20	A	843	CLA	C3D-C2D-C1D	-3.83	100.61	105.83
20	F	306	CLA	CMC-C2C-C1C	3.83	130.87	125.04
20	3	317	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
20	2	319	CLA	C3D-C2D-C1D	-3.83	100.61	105.83
20	H	201	CLA	C1C-C2C-C3C	-3.83	102.94	106.96
20	L	305	CLA	C3D-C2D-C1D	-3.82	100.61	105.83
20	4	312	CLA	C4D-CHA-C1A	-3.82	116.59	121.25
20	B	817	CLA	CHB-C4A-NA	3.82	129.80	124.51
20	A	804	CLA	CAC-C3C-C4C	3.82	129.77	124.81
20	B	823	CLA	C3D-C2D-C1D	-3.82	100.61	105.83
20	B	848	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
20	4	308	CLA	CHB-C4A-NA	3.82	129.79	124.51
19	2	309	CHL	C3D-C4D-ND	3.82	116.42	110.24
20	A	803	CLA	C3B-C2B-C1B	-3.82	102.55	107.16
23	A	814	BCR	C15-C16-C17	3.82	131.30	123.47
20	1	304	CLA	CHB-C4A-NA	3.82	129.79	124.51
28	A	824	CL0	C3D-C2D-C1D	-3.82	100.62	105.83
20	A	856	CLA	C4D-CHA-C1A	-3.82	116.60	121.25
20	3	314	CLA	C3D-C2D-C1D	-3.82	100.62	105.83
20	B	831	CLA	C3D-C2D-C1D	-3.81	100.63	105.83
20	B	845	CLA	C3B-C4B-NB	3.81	114.05	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	801	CLA	C3D-C2D-C1D	-3.81	100.63	105.83
20	B	847	CLA	C4D-CHA-C1A	-3.81	116.61	121.25
20	1	322	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
20	B	825	CLA	C3D-C2D-C1D	-3.81	100.64	105.83
20	1	319	CLA	C1-C2-C3	-3.81	119.46	126.04
23	F	302	BCR	C37-C22-C23	3.80	124.07	118.08
20	B	849	CLA	CHC-C4B-NB	-3.80	120.23	124.26
20	3	312	CLA	CHB-C4A-NA	3.80	129.77	124.51
20	B	849	CLA	CAC-C3C-C4C	3.80	129.75	124.81
20	2	304	CLA	CHD-C1D-ND	-3.80	120.96	124.45
20	A	838	CLA	C3B-C4B-NB	3.80	114.04	110.52
20	2	308	CLA	CAC-C3C-C4C	3.80	129.74	124.81
20	B	828	CLA	C2D-C1D-ND	3.80	112.91	110.10
20	A	832	CLA	C3D-C2D-C1D	-3.80	100.64	105.83
19	1	301	CHL	CAC-C3C-C4C	3.80	129.74	124.81
20	B	801	CLA	C4D-CHA-C1A	-3.80	116.63	121.25
20	B	806	CLA	C4D-CHA-C1A	-3.80	116.63	121.25
20	B	804	CLA	CMC-C2C-C1C	3.80	130.82	125.04
20	A	844	CLA	CHB-C4A-NA	3.80	129.76	124.51
20	4	303	CLA	C4D-CHA-C1A	-3.80	116.63	121.25
20	A	825	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
23	4	319	BCR	C37-C22-C21	-3.79	117.61	122.92
28	A	824	CL0	C1-C2-C3	-3.79	119.48	126.04
20	B	846	CLA	CHB-C4A-NA	3.79	129.76	124.51
20	B	816	CLA	CHB-C4A-NA	3.79	129.76	124.51
23	B	839	BCR	C35-C13-C14	-3.79	117.61	122.92
22	4	318	XAT	C35-C34-C33	-3.79	121.90	127.31
23	1	312	BCR	C37-C22-C23	3.79	124.05	118.08
20	B	827	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
20	A	853	CLA	CMC-C2C-C1C	3.78	130.80	125.04
20	B	802	CLA	C4D-CHA-C1A	-3.78	116.64	121.25
20	A	832	CLA	CMC-C2C-C1C	3.78	130.80	125.04
20	B	844	CLA	C4-C3-C5	3.78	121.63	115.27
20	A	827	CLA	C3D-C2D-C1D	-3.78	100.67	105.83
20	K	205	CLA	C4C-C3C-C2C	-3.78	101.39	106.90
20	B	848	CLA	CAC-C3C-C4C	3.77	129.71	124.81
19	2	301	CHL	CAC-C3C-C4C	3.77	129.71	124.81
20	2	323	CLA	CHB-C4A-NA	3.77	129.73	124.51
20	3	320	CLA	CHB-C4A-NA	3.77	129.73	124.51
21	1	323	LUT	C12-C13-C14	3.77	124.73	118.94
20	K	205	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
21	1	323	LUT	C20-C13-C14	-3.77	117.64	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	834	CLA	C3B-C4B-NB	3.77	114.01	110.52
20	A	805	CLA	CHB-C4A-NA	3.77	129.72	124.51
22	4	318	XAT	C38-C25-C24	3.77	118.52	114.28
23	1	312	BCR	C37-C22-C21	-3.77	117.64	122.92
20	B	853	CLA	C4D-CHA-C1A	-3.77	116.66	121.25
20	A	849	CLA	C4A-NA-C1A	3.77	108.40	106.71
20	3	318	CLA	C4D-CHA-C1A	-3.77	116.66	121.25
20	B	819	CLA	C4D-CHA-C1A	-3.77	116.66	121.25
20	2	304	CLA	CMC-C2C-C1C	3.77	130.77	125.04
20	A	831	CLA	O2D-CGD-CBD	3.76	117.96	111.27
20	1	305	CLA	C4D-CHA-C1A	-3.76	116.67	121.25
22	2	311	XAT	C6-C7-C8	-3.76	118.04	125.99
20	B	831	CLA	CAC-C3C-C4C	3.76	129.69	124.81
20	K	205	CLA	C2D-C1D-ND	3.76	112.88	110.10
20	A	848	CLA	C3D-C2D-C1D	-3.76	100.70	105.83
20	K	206	CLA	C3B-C4B-NB	3.76	114.00	110.52
20	B	852	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
20	3	311	CLA	CAC-C3C-C4C	3.76	129.69	124.81
29	J	104	DGD	C1E-O6E-C5E	3.76	121.07	113.69
19	4	307	CHL	C1D-ND-C4D	-3.76	103.67	106.33
20	A	808	CLA	C3B-C4B-NB	3.76	114.00	110.52
20	A	804	CLA	C4D-CHA-C1A	-3.76	116.68	121.25
20	A	803	CLA	C4D-CHA-C1A	-3.75	116.68	121.25
20	A	850	CLA	CHB-C4A-NA	3.75	129.70	124.51
28	A	824	CL0	CHC-C1C-C2C	-3.75	116.32	126.73
20	3	308	CLA	O2A-CGA-CBA	3.75	123.67	111.91
20	G	205	CLA	C3B-C4B-NB	3.75	113.99	110.52
20	A	854	CLA	C3D-C2D-C1D	-3.75	100.72	105.83
20	A	834	CLA	CHD-C1D-ND	-3.74	121.01	124.45
20	B	817	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
20	1	303	CLA	CHB-C4A-NA	3.74	129.69	124.51
23	G	203	BCR	C23-C22-C21	3.74	124.69	118.94
20	2	323	CLA	CAC-C3C-C4C	3.74	129.67	124.81
20	B	823	CLA	C3B-C4B-NB	3.74	113.99	110.52
20	F	305	CLA	CHB-C4A-NA	3.74	129.68	124.51
20	A	802	CLA	C3D-C2D-C1D	-3.74	100.73	105.83
20	A	833	CLA	C3D-C2D-C1D	-3.74	100.73	105.83
20	1	303	CLA	C3D-C2D-C1D	-3.74	100.73	105.83
20	A	811	CLA	CHB-C4A-NA	3.74	129.68	124.51
20	A	804	CLA	CHC-C1C-C2C	-3.74	116.35	126.73
20	B	819	CLA	CHC-C1C-C2C	-3.74	116.36	126.73
20	1	309	CLA	C2D-C1D-ND	3.73	112.86	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	828	CLA	CHB-C4A-NA	3.73	129.68	124.51
20	H	201	CLA	CHB-C4A-NA	3.73	129.67	124.51
20	3	311	CLA	C3B-C4B-NB	3.73	113.98	110.52
20	4	316	CLA	CHC-C1C-C2C	-3.73	116.36	126.73
20	4	308	CLA	C3B-C4B-NB	3.73	113.98	110.52
20	B	801	CLA	C3B-C4B-NB	3.73	113.98	110.52
20	B	852	CLA	C4D-CHA-C1A	-3.73	116.71	121.25
20	2	304	CLA	C4D-CHA-C1A	-3.73	116.71	121.25
20	A	834	CLA	O2D-CGD-CBD	3.73	117.89	111.27
20	A	830	CLA	CHB-C4A-NA	3.73	129.67	124.51
20	1	304	CLA	C4D-CHA-C1A	-3.73	116.71	121.25
20	2	303	CLA	CAC-C3C-C4C	3.73	129.65	124.81
20	A	841	CLA	CAC-C3C-C4C	3.73	129.65	124.81
23	G	203	BCR	C36-C18-C17	-3.73	117.70	122.92
20	1	308	CLA	C4D-CHA-C1A	-3.73	116.72	121.25
20	3	310	CLA	CHB-C4A-NA	3.72	129.66	124.51
20	4	304	CLA	C3D-C2D-C1D	-3.72	100.75	105.83
20	A	836	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
20	A	848	CLA	CHD-C1D-ND	-3.72	121.03	124.45
23	A	816	BCR	C12-C13-C14	3.72	124.66	118.94
20	B	845	CLA	C3D-C2D-C1D	-3.72	100.75	105.83
20	1	322	CLA	CMC-C2C-C1C	3.72	130.71	125.04
20	L	305	CLA	C3B-C4B-NB	3.72	113.97	110.52
20	4	311	CLA	CHB-C4A-NA	3.72	129.66	124.51
20	B	810	CLA	C2D-C1D-ND	3.72	112.84	110.10
23	G	203	BCR	C34-C9-C10	-3.72	117.71	122.92
20	3	320	CLA	C4D-CHA-C1A	-3.72	116.72	121.25
21	1	310	LUT	C39-C29-C30	-3.72	117.72	122.92
20	A	849	CLA	CMC-C2C-C1C	3.72	130.70	125.04
20	A	812	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
20	B	822	CLA	C3B-C4B-NB	3.71	113.96	110.52
19	4	306	CHL	C3D-C4D-ND	3.71	116.24	110.24
20	N	202	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
23	A	815	BCR	C34-C9-C10	-3.71	117.73	122.92
19	1	317	CHL	C3D-C4D-ND	3.71	116.24	110.24
20	A	829	CLA	CHC-C1C-C2C	-3.71	116.43	126.73
20	G	206	CLA	C4D-CHA-C1A	-3.71	116.74	121.25
20	3	317	CLA	C4-C3-C5	3.71	121.50	115.27
20	B	816	CLA	C3D-C2D-C1D	-3.70	100.78	105.83
20	4	304	CLA	CAC-C3C-C4C	3.70	129.62	124.81
23	G	203	BCR	C15-C16-C17	3.70	131.06	123.47
20	L	307	CLA	C3B-C4B-NB	3.70	113.95	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	848	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
20	4	312	CLA	CAC-C3C-C4C	3.70	129.61	124.81
20	A	849	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
23	L	301	BCR	C16-C15-C14	3.70	131.05	123.47
20	K	204	CLA	C3B-C4B-NB	3.70	113.95	110.52
20	B	851	CLA	CHB-C4A-NA	3.70	129.63	124.51
20	A	826	CLA	CHB-C4A-NA	3.70	129.62	124.51
20	A	839	CLA	CHB-C4A-NA	3.70	129.62	124.51
20	B	846	CLA	C3B-C4B-NB	3.70	113.94	110.52
20	H	201	CLA	C4D-CHA-C1A	-3.70	116.75	121.25
20	1	307	CLA	CHB-C4A-NA	3.70	129.62	124.51
20	A	801	CLA	CHD-C1D-ND	-3.69	121.06	124.45
20	A	846	CLA	CHC-C1C-C2C	-3.69	116.47	126.73
20	F	304	CLA	C2D-C1D-ND	3.69	112.83	110.10
22	1	311	XAT	C35-C15-C14	3.69	131.04	123.47
20	3	307	CLA	CHD-C1D-ND	-3.69	121.06	124.45
20	B	830	CLA	C2D-C1D-ND	3.69	112.82	110.10
20	2	317	CLA	C4D-CHA-C1A	-3.69	116.76	121.25
19	4	315	CHL	C3D-C4D-ND	3.69	116.21	110.24
20	K	204	CLA	CHB-C4A-NA	3.69	129.61	124.51
20	L	305	CLA	C4D-CHA-C1A	-3.69	116.76	121.25
20	A	842	CLA	CHB-C4A-NA	3.69	129.61	124.51
20	A	833	CLA	C3B-C4B-NB	3.69	113.94	110.52
20	B	831	CLA	C2D-C1D-ND	3.69	112.82	110.10
20	3	308	CLA	CMC-C2C-C1C	3.68	130.65	125.04
21	1	310	LUT	C19-C9-C8	3.68	123.88	118.08
20	A	829	CLA	CHB-C4A-NA	3.68	129.60	124.51
20	B	812	CLA	CHB-C4A-NA	3.68	129.60	124.51
20	A	811	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
20	B	802	CLA	CMD-C2D-C3D	-3.68	119.15	127.61
23	B	837	BCR	C37-C22-C21	-3.68	117.77	122.92
20	3	315	CLA	C3D-C2D-C1D	-3.68	100.81	105.83
20	4	311	CLA	C2D-C1D-ND	3.68	112.81	110.10
20	A	841	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
20	B	845	CLA	C4C-C3C-C2C	-3.68	101.54	106.90
20	L	306	CLA	C2D-C1D-ND	3.67	112.81	110.10
23	B	837	BCR	C16-C17-C18	3.67	132.55	127.31
20	2	321	CLA	CHB-C4A-NA	3.67	129.59	124.51
21	3	301	LUT	C39-C29-C30	-3.67	117.78	122.92
20	B	824	CLA	CHB-C4A-NA	3.67	129.59	124.51
20	A	844	CLA	C3B-C4B-NB	3.67	113.92	110.52
20	F	304	CLA	C4D-CHA-C1A	-3.67	116.78	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	813	CLA	CHB-C4A-NA	3.67	129.59	124.51
20	B	809	CLA	C3D-C2D-C1D	-3.67	100.82	105.83
20	H	201	CLA	CAC-C3C-C4C	3.67	129.57	124.81
20	A	809	CLA	C2D-C1D-ND	3.67	112.81	110.10
23	A	816	BCR	C16-C15-C14	3.67	130.99	123.47
20	A	840	CLA	CHC-C1C-C2C	-3.67	116.53	126.73
23	B	836	BCR	C8-C9-C10	3.67	124.57	118.94
20	B	830	CLA	CHB-C4A-NA	3.67	129.59	124.51
23	A	815	BCR	C34-C9-C8	3.67	123.86	118.08
23	K	201	BCR	C36-C18-C17	-3.67	117.78	122.92
19	2	302	CHL	CAC-C3C-C4C	3.67	129.57	124.81
20	B	807	CLA	C4D-CHA-C1A	-3.66	116.79	121.25
20	4	316	CLA	C3D-C4D-ND	3.66	116.16	110.24
22	3	302	XAT	C18-C5-C4	3.66	118.40	114.28
20	2	308	CLA	C4D-CHA-C1A	-3.66	116.80	121.25
20	A	828	CLA	C4D-CHA-C1A	-3.66	116.80	121.25
19	4	305	CHL	C3D-C4D-ND	3.66	116.16	110.24
20	A	855	CLA	CHB-C4A-NA	3.66	129.57	124.51
20	N	202	CLA	CHB-C4A-NA	3.66	129.57	124.51
20	F	305	CLA	C4D-CHA-C1A	-3.66	116.80	121.25
23	B	839	BCR	C12-C13-C14	3.66	124.55	118.94
20	4	314	CLA	CHB-C4A-NA	3.66	129.57	124.51
20	1	318	CLA	CMC-C2C-C1C	3.66	130.61	125.04
28	A	824	CL0	C4A-NA-C1A	3.65	108.35	106.71
20	B	803	CLA	C2D-C1D-ND	3.65	112.80	110.10
20	A	803	CLA	CMC-C2C-C1C	3.65	130.60	125.04
19	2	322	CHL	C3B-C4B-NB	3.65	113.90	110.52
23	F	302	BCR	C35-C13-C14	-3.65	117.81	122.92
20	3	319	CLA	CHC-C1C-C2C	-3.65	116.59	126.73
20	A	845	CLA	CHB-C4A-NA	3.65	129.56	124.51
20	3	312	CLA	C4D-CHA-C1A	-3.65	116.81	121.25
20	B	848	CLA	C4D-CHA-C1A	-3.65	116.81	121.25
20	1	306	CLA	C2D-C1D-ND	3.64	112.79	110.10
20	O	206	CLA	CAC-C3C-C4C	3.64	129.54	124.81
19	2	322	CHL	C3D-C4D-ND	3.64	116.13	110.24
23	K	201	BCR	C37-C22-C23	3.64	123.81	118.08
20	B	844	CLA	CAC-C3C-C4C	3.64	129.53	124.81
20	A	841	CLA	C3D-C2D-C1D	-3.64	100.86	105.83
20	A	805	CLA	C1D-CHD-C4C	-3.64	118.21	126.06
20	4	302	CLA	CHB-C4A-NA	3.64	129.54	124.51
19	2	318	CHL	C3B-C4B-NB	3.64	113.89	110.52
20	A	801	CLA	O2D-CGD-CBD	3.64	117.73	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	315	CLA	C3B-C4B-NB	3.64	113.89	110.52
20	K	206	CLA	CHB-C4A-NA	3.64	129.54	124.51
20	B	845	CLA	O2D-CGD-CBD	3.64	117.73	111.27
20	3	307	CLA	CHC-C1C-C2C	-3.64	116.63	126.73
23	3	303	BCR	C37-C22-C21	-3.63	117.83	122.92
20	B	849	CLA	C4D-CHA-C1A	-3.63	116.83	121.25
20	J	103	CLA	C4D-CHA-C1A	-3.63	116.83	121.25
22	1	311	XAT	C19-C9-C10	-3.63	117.84	122.92
19	2	302	CHL	C3D-C4D-ND	3.63	116.11	110.24
20	1	308	CLA	CHB-C4A-NA	3.63	129.53	124.51
20	2	319	CLA	CHB-C4A-NA	3.63	129.53	124.51
20	3	319	CLA	C4D-CHA-C1A	-3.63	116.83	121.25
20	N	202	CLA	C4D-CHA-C1A	-3.63	116.83	121.25
20	A	807	CLA	CMC-C2C-C1C	3.63	130.56	125.04
20	A	838	CLA	CHB-C4A-NA	3.63	129.53	124.51
20	B	801	CLA	CMC-C2C-C1C	3.63	130.56	125.04
20	B	851	CLA	CMC-C2C-C1C	3.63	130.56	125.04
19	2	301	CHL	C3D-C4D-ND	3.63	116.10	110.24
20	B	831	CLA	CHD-C1D-ND	-3.62	121.12	124.45
20	A	847	CLA	C3D-C2D-C1D	-3.62	100.89	105.83
21	2	310	LUT	C30-C31-C32	3.62	134.53	123.22
20	4	316	CLA	CHD-C1D-ND	-3.62	121.12	124.45
20	A	809	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
20	3	311	CLA	CHC-C1C-C2C	-3.62	116.67	126.73
20	A	830	CLA	CHC-C1C-C2C	-3.62	116.67	126.73
19	1	301	CHL	C1D-ND-C4D	-3.62	103.76	106.33
20	K	203	CLA	CAC-C3C-C4C	3.62	129.51	124.81
20	B	826	CLA	CHB-C4A-NA	3.62	129.52	124.51
21	4	317	LUT	C39-C29-C30	-3.62	117.85	122.92
19	1	301	CHL	C3D-C4D-ND	3.62	116.09	110.24
20	4	308	CLA	CHC-C1C-C2C	-3.62	116.69	126.73
20	3	312	CLA	C3B-C4B-NB	3.62	113.87	110.52
22	1	311	XAT	O24-C25-C24	3.62	116.10	113.38
20	F	305	CLA	CHC-C1C-C2C	-3.61	116.69	126.73
20	B	803	CLA	CHB-C4A-NA	3.61	129.51	124.51
20	O	208	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
20	4	309	CLA	C4-C3-C5	3.61	121.34	115.27
20	B	850	CLA	C4C-C3C-C2C	-3.61	101.64	106.90
20	K	204	CLA	CAC-C3C-C4C	3.61	129.49	124.81
20	4	312	CLA	C2D-C1D-ND	3.61	112.76	110.10
20	B	829	CLA	C3D-C2D-C1D	-3.61	100.91	105.83
20	A	843	CLA	CHC-C1C-C2C	-3.60	116.72	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	829	CLA	C3D-C2D-C1D	-3.60	100.91	105.83
20	1	318	CLA	CHB-C4A-NA	3.60	129.50	124.51
20	1	321	CLA	CHB-C4A-NA	3.60	129.50	124.51
20	4	310	CLA	CHB-C4A-NA	3.60	129.50	124.51
20	B	829	CLA	CMC-C2C-C1C	3.60	130.53	125.04
20	B	815	CLA	C4D-CHA-C1A	-3.60	116.86	121.25
20	A	856	CLA	CHB-C4A-NA	3.60	129.49	124.51
23	L	301	BCR	C34-C9-C10	-3.60	117.88	122.92
20	O	206	CLA	CHB-C4A-NA	3.60	129.49	124.51
19	3	313	CHL	C3D-C4D-ND	3.60	116.06	110.24
20	A	805	CLA	C4D-CHA-C1A	-3.60	116.87	121.25
20	2	303	CLA	CHB-C4A-NA	3.60	129.49	124.51
20	B	805	CLA	C3B-C4B-NB	3.60	113.85	110.52
20	O	207	CLA	C4D-CHA-C1A	-3.60	116.87	121.25
20	B	847	CLA	CHC-C1C-C2C	-3.60	116.73	126.73
22	4	318	XAT	O24-C25-C38	3.60	119.37	115.06
20	B	818	CLA	CHB-C4A-NA	3.60	129.49	124.51
20	G	205	CLA	CHB-C4A-NA	3.60	129.48	124.51
20	A	854	CLA	CAC-C3C-C4C	3.60	129.47	124.81
20	B	804	CLA	CHB-C4A-NA	3.59	129.48	124.51
20	A	837	CLA	C4C-C3C-C2C	-3.59	101.66	106.90
20	B	817	CLA	CMC-C2C-C1C	3.59	130.51	125.04
20	A	811	CLA	CAC-C3C-C4C	3.59	129.47	124.81
23	B	839	BCR	C37-C22-C21	-3.59	117.89	122.92
20	B	831	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
20	K	203	CLA	CHB-C4A-NA	3.59	129.48	124.51
20	1	308	CLA	C3B-C4B-NB	3.59	113.84	110.52
20	K	204	CLA	C4D-CHA-C1A	-3.59	116.88	121.25
20	A	802	CLA	C3B-C4B-NB	3.59	113.84	110.52
20	2	320	CLA	CHD-C1D-ND	-3.59	121.16	124.45
20	B	830	CLA	CHC-C1C-C2C	-3.59	116.77	126.73
20	A	847	CLA	C4D-CHA-C1A	-3.59	116.88	121.25
23	A	815	BCR	C37-C22-C23	3.59	123.73	118.08
20	B	844	CLA	CHC-C1C-C2C	-3.59	116.77	126.73
20	2	303	CLA	CHD-C1D-ND	-3.59	121.16	124.45
20	2	303	CLA	C3D-C2D-C1D	-3.59	100.94	105.83
20	B	851	CLA	CHD-C1D-ND	-3.58	121.16	124.45
20	1	321	CLA	C3B-C4B-NB	3.58	113.84	110.52
20	B	806	CLA	C2D-C1D-ND	3.58	112.74	110.10
23	B	838	BCR	C23-C22-C21	3.58	124.43	118.94
20	J	103	CLA	CHB-C4A-NA	3.58	129.46	124.51
20	1	318	CLA	C1C-C2C-C3C	-3.58	103.19	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	827	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
20	B	814	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
20	A	804	CLA	CMC-C2C-C1C	3.58	130.49	125.04
20	A	827	CLA	C3B-C4B-NB	3.58	113.83	110.52
20	A	845	CLA	C3D-C2D-C1D	-3.58	100.95	105.83
20	B	804	CLA	C3B-C4B-NB	3.58	113.83	110.52
20	A	806	CLA	CHC-C1C-C2C	-3.58	116.80	126.73
20	F	304	CLA	CHB-C4A-NA	3.58	129.46	124.51
20	3	315	CLA	C4D-CHA-C1A	-3.58	116.90	121.25
20	4	311	CLA	CHC-C1C-C2C	-3.58	116.80	126.73
20	A	853	CLA	CAC-C3C-C4C	3.57	129.45	124.81
20	A	842	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
20	3	307	CLA	CAA-C2A-C1A	3.57	123.69	111.97
20	4	314	CLA	C2D-C1D-ND	3.57	112.74	110.10
20	2	306	CLA	C4D-CHA-C1A	-3.57	116.90	121.25
20	A	854	CLA	CHC-C1C-C2C	-3.57	116.81	126.73
20	2	306	CLA	CHC-C1C-C2C	-3.57	116.82	126.73
19	1	317	CHL	CAC-C3C-C4C	3.57	129.44	124.81
20	1	320	CLA	C4D-CHA-C1A	-3.57	116.91	121.25
20	A	837	CLA	C4D-CHA-C1A	-3.57	116.91	121.25
20	A	826	CLA	C3D-C4D-ND	3.57	116.01	110.24
20	B	808	CLA	CHC-C1C-C2C	-3.57	116.82	126.73
20	A	848	CLA	CHC-C1C-C2C	-3.57	116.82	126.73
21	1	310	LUT	C19-C9-C10	-3.57	117.93	122.92
20	B	804	CLA	C3D-C2D-C1D	-3.57	100.97	105.83
20	4	312	CLA	CHC-C1C-C2C	-3.56	116.83	126.73
20	J	103	CLA	CHC-C1C-C2C	-3.56	116.83	126.73
20	1	305	CLA	CAC-C3C-C4C	3.56	129.43	124.81
20	A	848	CLA	CHB-C4A-NA	3.56	129.44	124.51
23	B	838	BCR	C11-C10-C9	3.56	132.39	127.31
20	A	804	CLA	CHB-C4A-NA	3.56	129.44	124.51
20	B	824	CLA	CMC-C2C-C1C	3.56	130.46	125.04
20	4	303	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
20	B	809	CLA	O2D-CGD-CBD	3.56	117.59	111.27
20	L	306	CLA	CHB-C4A-NA	3.56	129.43	124.51
20	A	830	CLA	C3B-C4B-NB	3.56	113.82	110.52
23	2	312	BCR	C35-C13-C14	-3.56	117.94	122.92
20	4	311	CLA	CAC-C3C-C4C	3.56	129.43	124.81
20	1	321	CLA	C4D-CHA-C1A	-3.56	116.92	121.25
20	A	850	CLA	C4D-CHA-C1A	-3.56	116.92	121.25
23	G	201	BCR	C8-C9-C10	3.56	124.40	118.94
20	B	805	CLA	CHB-C4A-NA	3.56	129.43	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	320	CLA	C3B-C4B-NB	3.55	113.81	110.52
20	3	316	CLA	CMC-C2C-C1C	3.55	130.45	125.04
19	4	306	CHL	C3B-C4B-NB	3.55	113.81	110.52
20	2	308	CLA	CMC-C2C-C1C	3.55	130.45	125.04
23	K	202	BCR	C37-C22-C23	3.55	123.67	118.08
20	4	316	CLA	CAC-C3C-C4C	3.55	129.42	124.81
20	B	817	CLA	C4D-CHA-C1A	-3.55	116.93	121.25
20	A	852	CLA	CAC-C3C-C4C	3.55	129.42	124.81
21	1	323	LUT	C30-C31-C32	3.55	134.29	123.22
20	A	841	CLA	CHB-C4A-NA	3.55	129.42	124.51
20	2	321	CLA	CAC-C3C-C4C	3.55	129.41	124.81
20	B	820	CLA	CMC-C2C-C1C	3.55	130.44	125.04
19	1	317	CHL	C3B-C4B-NB	3.55	113.81	110.52
20	3	315	CLA	CHB-C4A-NA	3.55	129.42	124.51
20	B	814	CLA	C4C-C3C-C2C	-3.55	101.73	106.90
20	3	314	CLA	CMC-C2C-C1C	3.55	130.44	125.04
20	2	305	CLA	CHB-C4A-NA	3.54	129.41	124.51
20	A	835	CLA	C2A-C1A-CHA	-3.54	117.66	123.86
20	B	805	CLA	C4D-CHA-C1A	-3.54	116.94	121.25
20	A	830	CLA	CHD-C1D-ND	-3.54	121.20	124.45
20	A	846	CLA	C4D-CHA-C1A	-3.54	116.94	121.25
23	1	312	BCR	C8-C9-C10	3.54	124.38	118.94
20	B	844	CLA	C4-C3-C2	-3.54	114.59	123.68
20	3	307	CLA	C3B-C4B-NB	3.54	113.80	110.52
23	L	303	BCR	C15-C16-C17	3.54	130.72	123.47
20	1	319	CLA	CMD-C2D-C3D	-3.54	119.47	127.61
20	B	813	CLA	O2D-CGD-CBD	3.54	117.56	111.27
20	1	302	CLA	CHB-C4A-NA	3.54	129.41	124.51
20	K	205	CLA	CHB-C4A-NA	3.54	129.41	124.51
20	1	320	CLA	CAC-C3C-C4C	3.54	129.40	124.81
23	F	302	BCR	C16-C15-C14	3.54	130.72	123.47
20	A	826	CLA	CAC-C3C-C4C	3.54	129.40	124.81
20	1	319	CLA	C4D-CHA-C1A	-3.54	116.95	121.25
19	4	307	CHL	C3D-C4D-ND	3.54	115.96	110.24
20	B	831	CLA	CMC-C2C-C1C	3.54	130.42	125.04
20	J	103	CLA	CAC-C3C-C4C	3.54	129.40	124.81
20	A	834	CLA	CHB-C4A-NA	3.53	129.40	124.51
20	H	201	CLA	CHC-C1C-C2C	-3.53	116.92	126.73
20	A	807	CLA	C2D-C1D-ND	3.53	112.71	110.10
20	N	202	CLA	C2D-C1D-ND	3.53	112.71	110.10
20	A	803	CLA	CHB-C4A-NA	3.53	129.40	124.51
20	B	831	CLA	CHB-C4A-NA	3.53	129.40	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	849	CLA	CHC-C1C-C2C	-3.53	116.93	126.73
20	A	809	CLA	CHC-C1C-C2C	-3.53	116.93	126.73
23	A	857	BCR	C37-C22-C23	3.53	123.63	118.08
20	B	813	CLA	C3D-C2D-C1D	-3.53	101.02	105.83
20	L	307	CLA	C4D-CHA-C1A	-3.52	116.96	121.25
20	2	321	CLA	C3B-C4B-NB	3.52	113.78	110.52
20	2	306	CLA	CMC-C2C-C1C	3.52	130.40	125.04
29	J	104	DGD	O2G-C1B-C2B	3.52	119.09	111.50
20	B	844	CLA	CMC-C2C-C1C	3.52	130.40	125.04
20	L	307	CLA	CHB-C4A-NA	3.52	129.38	124.51
23	O	202	BCR	C35-C13-C14	-3.52	117.99	122.92
20	4	302	CLA	C2D-C1D-ND	3.52	112.70	110.10
20	B	825	CLA	C4D-CHA-C1A	-3.52	116.97	121.25
20	2	306	CLA	CHB-C4A-NA	3.52	129.38	124.51
20	B	802	CLA	C4C-C3C-C2C	-3.52	101.77	106.90
20	4	308	CLA	C4D-CHA-C1A	-3.52	116.97	121.25
23	G	201	BCR	C16-C15-C14	3.52	130.68	123.47
20	B	849	CLA	CHC-C1C-C2C	-3.52	116.96	126.73
23	4	319	BCR	C37-C22-C23	3.51	123.61	118.08
20	A	851	CLA	CHD-C1D-ND	-3.51	121.22	124.45
20	G	206	CLA	CHB-C4A-NA	3.51	129.37	124.51
20	B	850	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
20	N	202	CLA	CAC-C3C-C4C	3.51	129.37	124.81
21	3	301	LUT	C19-C9-C10	-3.51	118.00	122.92
20	B	803	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
20	B	805	CLA	C2D-C1D-ND	3.51	112.69	110.10
20	4	302	CLA	C3B-C4B-NB	3.51	113.77	110.52
20	A	825	CLA	C3D-C2D-C1D	-3.51	101.04	105.83
20	3	314	CLA	CHC-C1C-C2C	-3.51	116.98	126.73
20	2	304	CLA	CAC-C3C-C4C	3.51	129.36	124.81
20	B	810	CLA	CHC-C1C-C2C	-3.51	116.98	126.73
20	1	305	CLA	CHB-C4A-NA	3.51	129.36	124.51
20	A	808	CLA	O2D-CGD-CBD	3.51	117.50	111.27
23	G	201	BCR	C37-C22-C21	-3.51	118.01	122.92
20	G	205	CLA	C2D-C1D-ND	3.51	112.69	110.10
20	B	818	CLA	CMC-C2C-C1C	3.50	130.38	125.04
20	B	853	CLA	CHB-C4A-NA	3.50	129.36	124.51
21	4	317	LUT	C19-C9-C8	3.50	123.60	118.08
20	G	207	CLA	CHB-C4A-NA	3.50	129.36	124.51
20	A	827	CLA	C4D-CHA-C1A	-3.50	116.99	121.25
21	4	317	LUT	C19-C9-C10	-3.50	118.02	122.92
20	A	856	CLA	CMC-C2C-C1C	3.50	130.37	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	G	206	CLA	CHC-C1C-C2C	-3.50	117.01	126.73
20	B	833	CLA	CHC-C1C-C2C	-3.50	117.01	126.73
20	B	808	CLA	CAC-C3C-C4C	3.50	129.35	124.81
20	4	314	CLA	CHC-C1C-C2C	-3.50	117.02	126.73
20	B	813	CLA	C4-C3-C5	3.50	121.15	115.27
20	1	319	CLA	CHC-C1C-C2C	-3.50	117.02	126.73
20	B	845	CLA	CHB-C1B-NB	-3.50	120.56	124.26
20	B	828	CLA	C4D-CHA-C1A	-3.50	117.00	121.25
23	B	838	BCR	C15-C14-C13	3.49	132.30	127.31
20	A	802	CLA	CHB-C4A-NA	3.49	129.34	124.51
20	A	833	CLA	CHC-C1C-C2C	-3.49	117.03	126.73
20	F	306	CLA	C4D-CHA-C1A	-3.49	117.00	121.25
20	A	834	CLA	CHC-C1C-C2C	-3.49	117.03	126.73
22	2	311	XAT	O4-C5-C6	-3.49	56.07	58.96
20	4	303	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
20	4	310	CLA	CHC-C1C-C2C	-3.49	117.04	126.73
20	1	306	CLA	CHB-C4A-NA	3.49	129.34	124.51
20	4	316	CLA	C2D-C1D-ND	3.49	112.67	110.10
20	B	827	CLA	C2D-C1D-ND	3.49	112.67	110.10
19	2	318	CHL	C1-C2-C3	-3.49	120.01	126.04
20	A	832	CLA	CHB-C4A-NA	3.48	129.33	124.51
20	1	303	CLA	CMC-C2C-C1C	3.48	130.34	125.04
20	A	809	CLA	CMC-C2C-C1C	3.48	130.34	125.04
20	O	207	CLA	CAC-C3C-C4C	3.48	129.33	124.81
20	B	850	CLA	C2D-C1D-ND	3.48	112.67	110.10
20	4	308	CLA	C3D-C2D-C1D	-3.48	101.08	105.83
20	4	303	CLA	CHC-C1C-C2C	-3.48	117.06	126.73
20	A	856	CLA	C3B-C4B-NB	3.48	113.74	110.52
21	1	323	LUT	C10-C11-C12	3.48	134.07	123.22
20	3	316	CLA	CHC-C1C-C2C	-3.48	117.07	126.73
20	B	818	CLA	CMD-C2D-C3D	-3.48	119.61	127.61
20	1	320	CLA	CHB-C4A-NA	3.48	129.32	124.51
23	I	102	BCR	C15-C16-C17	3.48	130.60	123.47
23	4	320	BCR	C34-C9-C8	3.48	123.55	118.08
20	1	321	CLA	CHC-C1C-C2C	-3.48	117.08	126.73
20	1	318	CLA	O2A-CGA-CBA	3.47	122.81	111.91
20	1	322	CLA	CHC-C1C-C2C	-3.47	117.08	126.73
20	3	314	CLA	CHD-C1D-ND	-3.47	121.26	124.45
20	B	822	CLA	O2A-CGA-CBA	3.47	122.81	111.91
23	F	301	BCR	C11-C10-C9	3.47	132.27	127.31
20	O	206	CLA	CHC-C1C-C2C	-3.47	117.08	126.73
19	4	307	CHL	CAC-C3C-C4C	3.47	129.31	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	843	CLA	C4-C3-C5	3.47	121.11	115.27
23	G	201	BCR	C37-C22-C23	3.47	123.55	118.08
23	A	857	BCR	C16-C15-C14	3.47	130.58	123.47
20	A	827	CLA	CHC-C1C-C2C	-3.47	117.09	126.73
20	A	847	CLA	CHC-C1C-C2C	-3.47	117.09	126.73
20	A	801	CLA	CHC-C1C-C2C	-3.47	117.10	126.73
23	L	303	BCR	C37-C22-C21	-3.47	118.07	122.92
20	L	305	CLA	CHB-C4A-NA	3.46	129.30	124.51
20	B	852	CLA	CHC-C1C-C2C	-3.46	117.11	126.73
20	4	310	CLA	CMC-C2C-C1C	3.46	130.31	125.04
20	A	806	CLA	CMC-C2C-C1C	3.46	130.31	125.04
20	3	316	CLA	C1D-CHD-C4C	-3.46	118.58	126.06
20	B	823	CLA	CHB-C4A-NA	3.46	129.30	124.51
20	2	305	CLA	CHC-C1C-C2C	-3.46	117.11	126.73
20	A	831	CLA	CHC-C1C-C2C	-3.46	117.11	126.73
20	A	842	CLA	C4D-CHA-C1A	-3.46	117.04	121.25
20	1	302	CLA	CMC-C2C-C1C	3.46	130.31	125.04
20	2	307	CLA	CHC-C1C-C2C	-3.46	117.13	126.73
20	1	309	CLA	CHC-C1C-C2C	-3.45	117.14	126.73
20	A	855	CLA	C4D-CHA-C1A	-3.45	117.05	121.25
20	A	831	CLA	C2D-C1D-ND	3.45	112.65	110.10
20	3	311	CLA	C4D-CHA-C1A	-3.45	117.05	121.25
20	B	814	CLA	C4-C3-C2	-3.45	114.82	123.68
20	B	809	CLA	C4D-CHA-C1A	-3.45	117.05	121.25
20	A	826	CLA	CHD-C1D-ND	-3.45	121.28	124.45
20	B	848	CLA	CHC-C1C-C2C	-3.45	117.14	126.73
20	2	306	CLA	C1D-CHD-C4C	-3.45	118.61	126.06
20	A	845	CLA	O2D-CGD-CBD	3.45	117.40	111.27
20	H	201	CLA	C2D-C1D-ND	3.45	112.65	110.10
20	A	807	CLA	CHC-C1C-C2C	-3.45	117.15	126.73
20	B	803	CLA	C3B-C4B-NB	3.45	113.71	110.52
20	N	202	CLA	CHC-C1C-C2C	-3.45	117.15	126.73
20	2	303	CLA	CHC-C1C-C2C	-3.45	117.15	126.73
23	L	304	BCR	C19-C18-C17	3.45	124.23	118.94
20	2	308	CLA	CHC-C1C-C2C	-3.45	117.16	126.73
20	1	307	CLA	O2A-CGA-CBA	3.44	122.72	111.91
20	B	815	CLA	C4-C3-C5	3.44	121.06	115.27
20	A	831	CLA	CHB-C4A-NA	3.44	129.27	124.51
20	K	203	CLA	CHC-C1C-C2C	-3.44	117.17	126.73
20	2	317	CLA	CHC-C1C-C2C	-3.44	117.17	126.73
20	B	802	CLA	CHC-C1C-C2C	-3.44	117.17	126.73
20	B	810	CLA	C4D-CHA-C1A	-3.44	117.06	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	824	CL0	C4D-CHA-C1A	-3.44	117.06	121.25
20	B	802	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
20	3	310	CLA	C4D-CHA-C1A	-3.44	117.06	121.25
20	3	314	CLA	O2D-CGD-CBD	3.44	117.38	111.27
20	A	812	CLA	C4C-C3C-C2C	-3.44	101.89	106.90
20	A	831	CLA	C4C-C3C-C2C	-3.44	101.89	106.90
23	L	303	BCR	C16-C15-C14	3.44	130.51	123.47
23	L	301	BCR	C36-C18-C17	-3.44	118.11	122.92
20	2	321	CLA	CHC-C1C-C2C	-3.44	117.19	126.73
20	B	847	CLA	CAC-C3C-C4C	3.43	129.26	124.81
20	2	303	CLA	C4D-CHA-C1A	-3.43	117.07	121.25
20	A	834	CLA	C3D-C4D-ND	3.43	115.79	110.24
20	B	813	CLA	CHD-C1D-ND	-3.43	121.30	124.45
20	B	814	CLA	O2A-CGA-CBA	3.43	122.68	111.91
19	1	301	CHL	C2D-C1D-ND	3.43	112.63	110.10
20	B	821	CLA	CHC-C1C-C2C	-3.43	117.20	126.73
20	A	805	CLA	CMC-C2C-C1C	3.43	130.26	125.04
20	K	206	CLA	C4D-CHA-C1A	-3.43	117.08	121.25
20	1	306	CLA	CHC-C1C-C2C	-3.43	117.21	126.73
20	A	838	CLA	CHC-C1C-C2C	-3.43	117.21	126.73
20	B	823	CLA	CAC-C3C-C4C	3.43	129.26	124.81
20	A	854	CLA	CHC-C4B-NB	-3.43	120.63	124.26
20	B	850	CLA	CHC-C1C-C2C	-3.43	117.21	126.73
20	A	841	CLA	CMB-C2B-C1B	3.42	130.58	125.37
20	3	309	CLA	CHB-C4A-NA	3.42	129.25	124.51
20	B	814	CLA	CAC-C3C-C4C	3.42	129.25	124.81
20	O	207	CLA	CHC-C1C-C2C	-3.42	117.22	126.73
20	B	807	CLA	C4-C3-C2	-3.42	114.90	123.68
20	2	307	CLA	CMC-C2C-C1C	3.42	130.25	125.04
20	1	303	CLA	CHC-C1C-C2C	-3.42	117.23	126.73
22	4	318	XAT	O4-C5-C18	3.42	119.15	115.06
20	A	852	CLA	CMC-C2C-C1C	3.42	130.25	125.04
20	1	303	CLA	CHD-C1D-ND	-3.42	121.31	124.45
20	1	306	CLA	CAC-C3C-C4C	3.42	129.25	124.81
20	B	811	CLA	CHC-C1C-C2C	-3.42	117.24	126.73
20	A	809	CLA	C4D-CHA-C1A	-3.42	117.09	121.25
20	1	306	CLA	CMC-C2C-C1C	3.42	130.24	125.04
23	A	815	BCR	C16-C15-C14	3.42	130.47	123.47
19	4	305	CHL	C3B-C4B-NB	3.41	113.68	110.52
20	B	816	CLA	C1D-CHD-C4C	-3.41	118.69	126.06
20	A	807	CLA	C4D-CHA-C1A	-3.41	117.09	121.25
20	1	319	CLA	CHB-C4A-NA	3.41	129.23	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	308	CLA	CMC-C2C-C1C	3.41	130.24	125.04
20	B	801	CLA	CHC-C1C-C2C	-3.41	117.25	126.73
20	2	307	CLA	C4D-CHA-C1A	-3.41	117.10	121.25
20	B	831	CLA	C1D-CHD-C4C	-3.41	118.70	126.06
20	4	313	CLA	CHB-C4A-NA	3.41	129.23	124.51
20	1	307	CLA	CMC-C2C-C1C	3.41	130.23	125.04
20	A	848	CLA	CMC-C2C-C1C	3.41	130.23	125.04
20	3	319	CLA	CHB-C4A-NA	3.41	129.22	124.51
20	A	855	CLA	CHC-C1C-C2C	-3.41	117.27	126.73
20	2	319	CLA	C3B-C4B-NB	3.41	113.68	110.52
20	4	304	CLA	C3B-C4B-NB	3.41	113.67	110.52
20	4	312	CLA	CMC-C2C-C1C	3.40	130.22	125.04
20	A	847	CLA	CAC-C3C-C4C	3.40	129.22	124.81
20	A	848	CLA	C4D-CHA-C1A	-3.40	117.11	121.25
20	3	309	CLA	CHC-C1C-C2C	-3.40	117.28	126.73
20	4	316	CLA	CMC-C2C-C1C	3.40	130.22	125.04
28	A	824	CL0	CHD-C1D-ND	-3.40	121.33	124.45
20	3	316	CLA	CHB-C4A-NA	3.40	129.21	124.51
20	B	822	CLA	CHB-C4A-NA	3.40	129.21	124.51
20	A	803	CLA	C4C-C3C-C2C	-3.40	101.94	106.90
20	B	828	CLA	O2D-CGD-CBD	3.40	117.31	111.27
20	1	306	CLA	C4D-CHA-C1A	-3.40	117.11	121.25
20	B	829	CLA	CHB-C4A-NA	3.40	129.21	124.51
20	B	824	CLA	CHC-C1C-C2C	-3.40	117.30	126.73
20	B	845	CLA	CAC-C3C-C4C	3.40	129.22	124.81
20	3	307	CLA	C3D-C4D-ND	3.40	115.73	110.24
20	B	821	CLA	CHB-C4A-NA	3.40	129.21	124.51
20	A	836	CLA	C2D-C1D-ND	3.40	112.61	110.10
20	A	840	CLA	C2D-C1D-ND	3.40	112.61	110.10
20	A	833	CLA	CHB-C4A-NA	3.39	129.21	124.51
20	B	849	CLA	CHB-C4A-NA	3.39	129.20	124.51
20	A	843	CLA	CHB-C4A-NA	3.39	129.20	124.51
20	2	323	CLA	CHC-C1C-C2C	-3.39	117.31	126.73
20	K	204	CLA	CHC-C1C-C2C	-3.39	117.31	126.73
23	I	102	BCR	C15-C14-C13	3.39	132.15	127.31
20	B	816	CLA	CHC-C1C-C2C	-3.39	117.31	126.73
19	1	317	CHL	CMB-C2B-C1B	3.39	130.53	125.37
20	B	852	CLA	C2D-C1D-ND	3.39	112.60	110.10
20	A	839	CLA	CAC-C3C-C4C	3.39	129.21	124.81
20	A	840	CLA	C4D-CHA-C1A	-3.39	117.12	121.25
20	A	804	CLA	C4-C3-C5	3.39	119.86	115.98
20	A	833	CLA	C2D-C1D-ND	3.39	112.60	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	836	CLA	CHC-C1C-C2C	-3.39	117.32	126.73
20	A	850	CLA	C3B-C4B-NB	3.39	113.66	110.52
20	A	833	CLA	CMC-C2C-C1C	3.39	130.20	125.04
20	A	803	CLA	CHC-C1C-C2C	-3.39	117.32	126.73
20	A	806	CLA	C4D-CHA-C1A	-3.39	117.13	121.25
20	L	307	CLA	CHC-C1C-C2C	-3.39	117.32	126.73
20	B	805	CLA	CHC-C1C-C2C	-3.39	117.32	126.73
20	2	303	CLA	CMC-C2C-C1C	3.39	130.20	125.04
20	B	806	CLA	CHB-C4A-NA	3.39	129.19	124.51
20	3	317	CLA	C2D-C1D-ND	3.39	112.60	110.10
20	A	842	CLA	CAC-C3C-C4C	3.38	129.20	124.81
20	A	835	CLA	CMC-C2C-C1C	3.38	130.19	125.04
20	3	309	CLA	C1D-CHD-C4C	-3.38	118.76	126.06
20	A	826	CLA	CHC-C1C-C2C	-3.38	117.33	126.73
20	4	311	CLA	C1D-CHD-C4C	-3.38	118.76	126.06
20	B	828	CLA	CHC-C1C-C2C	-3.38	117.34	126.73
20	3	318	CLA	CAC-C3C-C4C	3.38	129.20	124.81
22	1	311	XAT	C31-C32-C33	3.38	135.91	126.42
20	B	826	CLA	C4D-CHA-C1A	-3.38	117.14	121.25
20	A	849	CLA	C3B-C4B-NB	3.38	113.65	110.52
20	K	206	CLA	CHC-C1C-C2C	-3.38	117.35	126.73
20	A	811	CLA	C2D-C1D-ND	3.38	112.59	110.10
20	B	817	CLA	C3B-C4B-NB	3.38	113.65	110.52
20	G	207	CLA	CHC-C1C-C2C	-3.38	117.35	126.73
20	B	825	CLA	CHC-C1C-C2C	-3.37	117.36	126.73
20	3	316	CLA	CAC-C3C-C4C	3.37	129.19	124.81
20	B	818	CLA	CHD-C1D-ND	-3.37	121.35	124.45
23	L	303	BCR	C23-C22-C21	3.37	124.12	118.94
20	3	315	CLA	CMC-C2C-C1C	3.37	130.18	125.04
20	3	318	CLA	CHB-C4A-NA	3.37	129.18	124.51
20	B	849	CLA	C2D-C1D-ND	3.37	112.59	110.10
20	1	302	CLA	CHC-C1C-C2C	-3.37	117.37	126.73
20	B	820	CLA	C4D-CHA-C1A	-3.37	117.15	121.25
20	B	809	CLA	CAC-C3C-C4C	3.37	129.18	124.81
20	A	852	CLA	CHC-C1C-C2C	-3.37	117.37	126.73
20	A	849	CLA	CHB-C4A-NA	3.37	129.17	124.51
20	G	205	CLA	CHC-C1C-C2C	-3.37	117.38	126.73
20	1	320	CLA	CHC-C1C-C2C	-3.37	117.38	126.73
20	A	825	CLA	CHD-C1D-ND	-3.37	121.36	124.45
20	L	306	CLA	C4D-CHA-C1A	-3.37	117.15	121.25
20	B	822	CLA	CHC-C1C-C2C	-3.37	117.38	126.73
20	1	309	CLA	CHB-C4A-NA	3.36	129.16	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	813	CLA	CMC-C2C-C1C	3.36	130.16	125.04
20	2	308	CLA	CMD-C2D-C3D	-3.36	119.87	127.61
20	4	311	CLA	C4D-CHA-C1A	-3.36	117.16	121.25
20	A	812	CLA	C3D-C4D-ND	3.36	115.68	110.24
20	3	307	CLA	C4A-NA-C1A	3.36	108.22	106.71
23	B	838	BCR	C36-C18-C17	-3.36	118.21	122.92
20	A	841	CLA	C4D-CHA-C1A	-3.36	117.16	121.25
20	1	321	CLA	CMC-C2C-C1C	3.36	130.16	125.04
20	B	847	CLA	C4C-C3C-C2C	-3.36	102.00	106.90
20	B	812	CLA	C4D-CHA-C1A	-3.36	117.16	121.25
19	1	301	CHL	C2A-C1A-CHA	-3.36	117.99	123.86
20	4	312	CLA	C1D-CHD-C4C	-3.36	118.81	126.06
20	F	306	CLA	CHC-C1C-C2C	-3.36	117.40	126.73
20	1	307	CLA	C2D-C1D-ND	3.36	112.58	110.10
20	A	828	CLA	CMC-C2C-C1C	3.36	130.15	125.04
20	4	303	CLA	CHB-C4A-NA	3.36	129.15	124.51
20	1	307	CLA	CHC-C1C-C2C	-3.36	117.41	126.73
20	A	854	CLA	C4C-C3C-C2C	-3.35	102.01	106.90
20	G	207	CLA	C3B-C4B-NB	3.35	113.63	110.52
20	3	316	CLA	C4D-CHA-C1A	-3.35	117.17	121.25
20	A	807	CLA	CHB-C4A-NA	3.35	129.15	124.51
20	3	318	CLA	CHC-C1C-C2C	-3.35	117.42	126.73
20	B	815	CLA	O2A-CGA-CBA	3.35	122.43	111.91
20	4	309	CLA	C2D-C1D-ND	3.35	112.57	110.10
20	A	833	CLA	C1D-CHD-C4C	-3.35	118.83	126.06
20	B	833	CLA	CMD-C2D-C3D	-3.35	119.91	127.61
20	4	314	CLA	CMC-C2C-C1C	3.35	130.14	125.04
20	A	840	CLA	CHB-C4A-NA	3.35	129.14	124.51
20	A	826	CLA	C3D-C2D-C1D	-3.35	101.26	105.83
20	3	307	CLA	CHB-C4A-NA	3.35	129.14	124.51
20	1	304	CLA	CHC-C1C-C2C	-3.35	117.43	126.73
20	B	853	CLA	CHC-C1C-C2C	-3.35	117.43	126.73
20	3	309	CLA	C4C-C3C-C2C	-3.35	102.02	106.90
20	A	801	CLA	CMC-C2C-C1C	3.35	130.13	125.04
20	A	839	CLA	CHC-C1C-C2C	-3.35	117.44	126.73
20	A	842	CLA	C4C-C3C-C2C	-3.35	102.02	106.90
20	4	312	CLA	CHB-C4A-NA	3.35	129.14	124.51
21	3	301	LUT	C19-C9-C8	3.34	123.35	118.08
20	K	203	CLA	C4D-CHA-C1A	-3.34	117.18	121.25
20	A	805	CLA	CHC-C1C-C2C	-3.34	117.44	126.73
20	F	304	CLA	C4-C3-C2	-3.34	115.10	123.68
20	B	812	CLA	CAC-C3C-C4C	3.34	129.15	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	834	CLA	C1D-CHD-C4C	-3.34	118.85	126.06
20	3	315	CLA	CHC-C1C-C2C	-3.34	117.45	126.73
20	3	317	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
20	B	829	CLA	CMD-C2D-C3D	-3.34	119.93	127.61
20	2	308	CLA	CHB-C4A-NA	3.34	129.13	124.51
19	2	309	CHL	CAC-C3C-C4C	3.34	129.14	124.81
23	B	834	BCR	C36-C18-C17	-3.34	118.25	122.92
19	1	317	CHL	C2A-C1A-CHA	-3.34	118.02	123.86
20	B	847	CLA	CMC-C2C-C1C	3.34	130.12	125.04
20	B	814	CLA	CMC-C2C-C1C	3.34	130.12	125.04
20	B	817	CLA	CHC-C1C-C2C	-3.34	117.46	126.73
20	B	811	CLA	C4-C3-C5	3.34	120.88	115.27
20	4	316	CLA	CHB-C4A-NA	3.34	129.12	124.51
20	B	803	CLA	C4C-C3C-C2C	-3.34	102.04	106.90
20	A	825	CLA	C2D-C1D-ND	3.34	112.56	110.10
20	G	207	CLA	C2D-C1D-ND	3.33	112.56	110.10
20	A	831	CLA	CMC-C2C-C1C	3.33	130.12	125.04
20	A	853	CLA	C3D-C2D-C1D	-3.33	101.28	105.83
20	L	307	CLA	CAC-C3C-C4C	3.33	129.13	124.81
23	F	302	BCR	C12-C13-C14	3.33	124.05	118.94
20	B	807	CLA	CHC-C1C-C2C	-3.33	117.48	126.73
20	A	832	CLA	CHC-C1C-C2C	-3.33	117.48	126.73
20	A	836	CLA	CHB-C4A-NA	3.33	129.12	124.51
20	A	834	CLA	OBD-CAD-C3D	-3.33	120.51	128.52
20	4	313	CLA	CMC-C2C-C1C	3.33	130.11	125.04
20	A	856	CLA	CHC-C1C-C2C	-3.33	117.49	126.73
20	3	308	CLA	C2D-C1D-ND	3.33	112.56	110.10
20	A	851	CLA	C1D-CHD-C4C	-3.33	118.88	126.06
20	B	850	CLA	C1D-CHD-C4C	-3.33	118.88	126.06
20	B	844	CLA	C1D-CHD-C4C	-3.32	118.89	126.06
20	B	831	CLA	CHC-C1C-C2C	-3.32	117.50	126.73
20	4	313	CLA	CHC-C1C-C2C	-3.32	117.50	126.73
20	A	834	CLA	C4C-C3C-C2C	-3.32	102.06	106.90
20	3	312	CLA	CHC-C1C-C2C	-3.32	117.50	126.73
20	A	834	CLA	C4D-CHA-C1A	-3.32	117.21	121.25
20	1	322	CLA	C2D-C1D-ND	3.32	112.55	110.10
20	3	317	CLA	CHC-C1C-C2C	-3.32	117.51	126.73
20	A	845	CLA	C4D-CHA-C1A	-3.32	117.21	121.25
20	O	208	CLA	CHC-C1C-C2C	-3.32	117.51	126.73
23	K	202	BCR	C15-C16-C17	3.32	130.27	123.47
20	1	306	CLA	C1D-CHD-C4C	-3.32	118.90	126.06
19	4	307	CHL	C3B-C4B-NB	3.32	113.59	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	K	206	CLA	CAC-C3C-C4C	3.32	129.11	124.81
20	A	807	CLA	CMB-C2B-C1B	3.32	130.42	125.37
20	B	810	CLA	CHB-C4A-NA	3.32	129.10	124.51
20	B	826	CLA	C1D-CHD-C4C	-3.32	118.90	126.06
20	3	310	CLA	CHC-C1C-C2C	-3.32	117.52	126.73
20	A	811	CLA	CHC-C1C-C2C	-3.32	117.52	126.73
22	4	318	XAT	C18-C5-C4	3.31	118.01	114.28
20	2	307	CLA	CHB-C4A-NA	3.31	129.09	124.51
20	A	811	CLA	CMC-C2C-C1C	3.31	130.08	125.04
20	B	808	CLA	CHB-C4A-NA	3.31	129.09	124.51
20	A	840	CLA	CMC-C2C-C1C	3.31	130.08	125.04
20	B	809	CLA	CHB-C4A-NA	3.31	129.09	124.51
20	1	318	CLA	CMD-C2D-C3D	-3.31	120.00	127.61
20	O	206	CLA	C4D-CHA-C1A	-3.31	117.23	121.25
20	A	850	CLA	CMC-C2C-C1C	3.31	130.07	125.04
20	B	828	CLA	CMC-C2C-C1C	3.30	130.07	125.04
20	B	803	CLA	CHC-C1C-C2C	-3.30	117.55	126.73
20	A	831	CLA	O2A-CGA-CBA	3.30	122.28	111.91
20	B	851	CLA	C4D-CHA-C1A	-3.30	117.23	121.25
23	B	835	BCR	C15-C16-C17	3.30	130.24	123.47
20	B	852	CLA	CHB-C4A-NA	3.30	129.08	124.51
20	F	306	CLA	CAC-C3C-C4C	3.30	129.09	124.81
23	B	839	BCR	C16-C17-C18	3.30	132.02	127.31
20	B	845	CLA	CHD-C1D-ND	-3.30	121.42	124.45
20	B	828	CLA	CHB-C4A-NA	3.30	129.08	124.51
20	B	830	CLA	CMC-C2C-C1C	3.30	130.06	125.04
20	1	308	CLA	CAC-C3C-C4C	3.30	129.09	124.81
20	A	830	CLA	C1D-CHD-C4C	-3.30	118.94	126.06
20	L	306	CLA	C3B-C4B-NB	3.30	113.58	110.52
20	A	844	CLA	CHC-C1C-C2C	-3.30	117.57	126.73
20	G	207	CLA	CMC-C2C-C1C	3.30	130.06	125.04
20	2	317	CLA	CAC-C3C-C4C	3.30	129.09	124.81
20	B	820	CLA	CHC-C1C-C2C	-3.30	117.58	126.73
20	A	849	CLA	C4C-C3C-C2C	-3.29	102.10	106.90
20	B	827	CLA	CHB-C4A-NA	3.29	129.07	124.51
20	A	851	CLA	C4C-C3C-C2C	-3.29	102.10	106.90
20	2	317	CLA	CHB-C4A-NA	3.29	129.06	124.51
20	A	825	CLA	CMB-C2B-C3B	3.29	134.56	126.59
20	A	847	CLA	C1-C2-C3	-3.29	120.35	126.04
20	3	310	CLA	CAC-C3C-C4C	3.29	129.08	124.81
20	A	854	CLA	O2A-CGA-CBA	3.29	122.23	111.91
20	A	827	CLA	CMC-C2C-C1C	3.29	130.05	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	309	CLA	O2A-CGA-CBA	3.29	122.23	111.91
23	B	837	BCR	C34-C9-C8	3.29	123.26	118.08
20	A	836	CLA	C4C-C3C-C2C	-3.29	102.11	106.90
20	B	802	CLA	CHB-C4A-NA	3.29	129.06	124.51
23	F	302	BCR	C34-C9-C10	-3.29	118.32	122.92
20	F	305	CLA	C2D-C1D-ND	3.29	112.53	110.10
20	A	833	CLA	CMB-C2B-C3B	3.29	134.54	126.59
20	B	805	CLA	CAC-C3C-C4C	3.28	129.07	124.81
20	3	309	CLA	CMC-C2C-C1C	3.28	130.04	125.04
20	B	844	CLA	C4C-C3C-C2C	-3.28	102.11	106.90
20	A	801	CLA	C4D-CHA-C1A	-3.28	117.26	121.25
20	4	304	CLA	CHC-C1C-C2C	-3.28	117.62	126.73
19	2	309	CHL	C2A-C1A-CHA	-3.28	118.12	123.86
20	N	202	CLA	C4C-C3C-C2C	-3.28	102.12	106.90
20	3	319	CLA	CMC-C2C-C1C	3.28	130.03	125.04
20	G	205	CLA	CMC-C2C-C1C	3.28	130.03	125.04
20	B	849	CLA	CMC-C2C-C1C	3.28	130.03	125.04
20	B	821	CLA	C4D-CHA-C1A	-3.28	117.26	121.25
20	A	808	CLA	CHC-C1C-C2C	-3.28	117.63	126.73
23	L	304	BCR	C35-C13-C14	-3.27	118.34	122.92
20	4	303	CLA	C4C-C3C-C2C	-3.27	102.12	106.90
20	F	306	CLA	C2D-C1D-ND	3.27	112.52	110.10
20	1	305	CLA	CHC-C1C-C2C	-3.27	117.64	126.73
20	B	806	CLA	CHC-C1C-C2C	-3.27	117.64	126.73
20	A	839	CLA	C4D-CHA-C1A	-3.27	117.27	121.25
20	G	206	CLA	C1D-CHD-C4C	-3.27	119.00	126.06
20	2	306	CLA	CAC-C3C-C4C	3.27	129.06	124.81
20	B	818	CLA	CHC-C1C-C2C	-3.27	117.64	126.73
20	F	304	CLA	CHC-C1C-C2C	-3.27	117.64	126.73
20	K	203	CLA	C2D-C1D-ND	3.27	112.51	110.10
20	B	818	CLA	C4-C3-C5	3.27	120.77	115.27
20	A	809	CLA	C4C-C3C-C2C	-3.27	102.13	106.90
20	B	831	CLA	C4C-C3C-C2C	-3.27	102.13	106.90
20	4	302	CLA	CMB-C2B-C3B	3.27	134.50	126.59
19	4	315	CHL	CAC-C3C-C4C	3.27	129.05	124.81
28	A	824	CL0	CHB-C4A-NA	3.27	129.03	124.51
23	I	102	BCR	C23-C22-C21	3.27	123.95	118.94
20	2	305	CLA	CMC-C2C-C1C	3.27	130.01	125.04
20	B	813	CLA	C2D-C1D-ND	3.26	112.51	110.10
20	H	201	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
23	L	301	BCR	C37-C22-C23	3.26	123.22	118.08
20	B	817	CLA	C1D-CHD-C4C	-3.26	119.02	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	814	CLA	C4A-NA-C1A	3.26	108.17	106.71
20	A	829	CLA	C1D-CHD-C4C	-3.26	119.02	126.06
21	4	317	LUT	C39-C29-C28	3.26	123.21	118.08
20	1	308	CLA	CHC-C1C-C2C	-3.26	117.67	126.73
20	3	311	CLA	CMC-C2C-C1C	3.26	130.00	125.04
20	A	849	CLA	CHD-C1D-ND	-3.26	121.46	124.45
20	2	304	CLA	CHC-C1C-C2C	-3.26	117.67	126.73
19	2	302	CHL	C2A-C1A-CHA	-3.26	118.16	123.86
20	B	845	CLA	C4D-CHA-C1A	-3.26	117.28	121.25
19	2	302	CHL	C3B-C4B-NB	3.26	113.54	110.52
23	K	202	BCR	C36-C18-C17	-3.26	118.36	122.92
20	B	846	CLA	C2A-C1A-CHA	-3.26	118.16	123.86
20	K	204	CLA	C2D-C1D-ND	3.26	112.50	110.10
20	2	319	CLA	C4D-CHA-C1A	-3.26	117.29	121.25
20	L	307	CLA	C2D-C1D-ND	3.26	112.50	110.10
20	B	820	CLA	C3B-C4B-NB	3.26	113.53	110.52
20	G	207	CLA	C4D-CHA-C1A	-3.25	117.29	121.25
23	F	301	BCR	C36-C18-C17	-3.25	118.36	122.92
20	B	844	CLA	C2D-C1D-ND	3.25	112.50	110.10
20	B	811	CLA	C4D-CHA-C1A	-3.25	117.29	121.25
20	B	852	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
20	A	835	CLA	CHC-C1C-C2C	-3.25	117.70	126.73
20	1	305	CLA	CMC-C2C-C1C	3.25	129.99	125.04
20	A	855	CLA	C3B-C4B-NB	3.25	113.53	110.52
20	2	320	CLA	CMC-C2C-C1C	3.25	129.99	125.04
20	A	831	CLA	C4D-CHA-C1A	-3.25	117.30	121.25
23	G	203	BCR	C16-C15-C14	3.25	130.13	123.47
20	B	825	CLA	CAC-C3C-C4C	3.25	129.02	124.81
20	1	319	CLA	CMB-C2B-C3B	3.25	134.45	126.59
20	2	304	CLA	C2D-C1D-ND	3.24	112.50	110.10
20	A	826	CLA	CMC-C2C-C1C	3.24	129.98	125.04
23	L	302	BCR	C11-C10-C9	3.24	131.94	127.31
20	B	845	CLA	CHC-C1C-C2C	-3.24	117.72	126.73
20	2	304	CLA	C3B-C4B-NB	3.24	113.52	110.52
21	4	317	LUT	C15-C35-C34	3.24	130.12	123.47
20	4	311	CLA	C4C-C3C-C2C	-3.24	102.17	106.90
20	O	207	CLA	CHB-C4A-NA	3.24	129.00	124.51
20	3	317	CLA	CHB-C4A-NA	3.24	128.99	124.51
20	4	313	CLA	CMD-C2D-C3D	-3.24	120.16	127.61
20	A	803	CLA	C1D-CHD-C4C	-3.24	119.07	126.06
20	4	313	CLA	C2D-C1D-ND	3.24	112.49	110.10
20	F	306	CLA	C1D-CHD-C4C	-3.24	119.07	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	316	CLA	C1D-CHD-C4C	-3.24	119.07	126.06
20	B	811	CLA	CHB-C4A-NA	3.24	128.99	124.51
19	4	315	CHL	C2A-C1A-CHA	-3.24	118.20	123.86
20	A	847	CLA	CHB-C4A-NA	3.24	128.99	124.51
20	G	206	CLA	CMC-C2C-C1C	3.24	129.97	125.04
20	A	801	CLA	CMB-C2B-C1B	3.24	130.30	125.37
20	A	842	CLA	O2A-CGA-CBA	3.24	122.07	111.91
20	B	822	CLA	CAC-C3C-C4C	3.24	129.01	124.81
20	B	826	CLA	C4C-C3C-C2C	-3.23	102.18	106.90
20	A	835	CLA	CHB-C4A-NA	3.23	128.98	124.51
20	G	206	CLA	C4C-C3C-C2C	-3.23	102.18	106.90
20	F	305	CLA	CAC-C3C-C4C	3.23	129.00	124.81
23	B	835	BCR	C36-C18-C17	-3.23	118.40	122.92
19	2	318	CHL	C2A-C1A-CHA	-3.23	118.21	123.86
21	2	310	LUT	C31-C30-C29	3.23	131.92	127.31
20	A	850	CLA	CHC-C1C-C2C	-3.23	117.76	126.73
20	B	804	CLA	CHC-C1C-C2C	-3.23	117.76	126.73
20	A	834	CLA	CMC-C2C-C1C	3.23	129.96	125.04
20	B	809	CLA	CHC-C1C-C2C	-3.23	117.76	126.73
23	O	202	BCR	C16-C15-C14	3.23	130.09	123.47
20	A	845	CLA	CHC-C1C-C2C	-3.23	117.76	126.73
20	3	320	CLA	CHC-C1C-C2C	-3.23	117.77	126.73
22	1	311	XAT	C39-C29-C30	-3.22	118.41	122.92
20	A	834	CLA	CAC-C3C-C4C	3.22	128.99	124.81
20	3	317	CLA	CMC-C2C-C1C	3.22	129.95	125.04
20	A	832	CLA	CAC-C3C-C4C	3.22	128.99	124.81
20	A	853	CLA	C3B-C4B-NB	3.22	113.50	110.52
20	L	306	CLA	CHC-C1C-C2C	-3.22	117.78	126.73
20	B	814	CLA	C1D-CHD-C4C	-3.22	119.11	126.06
22	4	318	XAT	C10-C11-C12	-3.22	113.16	123.22
20	1	320	CLA	CMC-C2C-C1C	3.22	129.94	125.04
20	4	303	CLA	CMC-C2C-C1C	3.22	129.94	125.04
23	3	303	BCR	C16-C15-C14	3.22	130.07	123.47
20	B	820	CLA	CHB-C4A-NA	3.22	128.97	124.51
20	B	833	CLA	C2D-C1D-ND	3.22	112.48	110.10
20	1	318	CLA	C2A-C1A-CHA	-3.22	118.23	123.86
20	3	312	CLA	CAC-C3C-C4C	3.21	128.98	124.81
21	1	310	LUT	C15-C35-C34	3.21	130.06	123.47
20	A	811	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
20	B	850	CLA	CMC-C2C-C1C	3.21	129.93	125.04
20	K	205	CLA	CHC-C1C-C2C	-3.21	117.81	126.73
20	B	821	CLA	C2D-C1D-ND	3.21	112.47	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	844	CLA	CMC-C2C-C1C	3.21	129.93	125.04
20	B	852	CLA	CMC-C2C-C1C	3.21	129.93	125.04
20	1	308	CLA	C2A-C1A-CHA	-3.21	118.25	123.86
20	B	816	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
19	4	305	CHL	CMB-C2B-C1B	3.21	130.25	125.37
20	K	204	CLA	C4-C3-C5	3.21	120.67	115.27
20	B	813	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
20	4	314	CLA	C1-C2-C3	-3.21	121.56	126.75
20	2	307	CLA	C2D-C1D-ND	3.21	112.47	110.10
20	3	318	CLA	CMC-C2C-C1C	3.21	129.92	125.04
20	B	807	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
20	B	812	CLA	CHC-C1C-C2C	-3.20	117.84	126.73
20	1	305	CLA	C2D-C1D-ND	3.20	112.46	110.10
20	B	820	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
20	4	316	CLA	O2A-CGA-CBA	3.20	121.95	111.91
20	A	838	CLA	CMC-C2C-C1C	3.20	129.91	125.04
20	3	318	CLA	C2D-C1D-ND	3.20	112.46	110.10
20	O	207	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
20	O	208	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
20	B	827	CLA	CHC-C1C-C2C	-3.20	117.84	126.73
20	B	824	CLA	C4D-CHA-C1A	-3.20	117.36	121.25
19	4	305	CHL	CAC-C3C-C4C	3.20	128.96	124.81
20	B	829	CLA	CHC-C1C-C2C	-3.20	117.85	126.73
20	2	321	CLA	C4D-CHA-C1A	-3.20	117.36	121.25
20	N	202	CLA	C1D-CHD-C4C	-3.20	119.16	126.06
20	3	307	CLA	O2A-CGA-CBA	3.19	121.93	111.91
23	4	319	BCR	C16-C15-C14	3.19	130.02	123.47
20	L	305	CLA	CHC-C1C-C2C	-3.19	117.86	126.73
23	K	201	BCR	C15-C16-C17	3.19	130.01	123.47
20	4	314	CLA	C4D-CHA-C1A	-3.19	117.37	121.25
19	2	301	CHL	C2A-C1A-CHA	-3.19	118.28	123.86
20	2	323	CLA	CMC-C2C-C1C	3.19	129.90	125.04
28	A	824	CL0	C3B-C4B-NB	3.19	113.47	110.52
20	1	304	CLA	CAC-C3C-C4C	3.19	128.95	124.81
20	B	821	CLA	C1D-CHD-C4C	-3.19	119.18	126.06
20	B	826	CLA	CMC-C2C-C1C	3.19	129.89	125.04
20	A	841	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
20	B	811	CLA	C1D-CHD-C4C	-3.18	119.19	126.06
20	H	201	CLA	C1D-CHD-C4C	-3.18	119.19	126.06
20	1	307	CLA	CAC-C3C-C4C	3.18	128.94	124.81
20	1	309	CLA	C1D-CHD-C4C	-3.18	119.20	126.06
20	B	816	CLA	C3B-C4B-NB	3.18	113.47	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	825	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
20	A	837	CLA	CHC-C1C-C2C	-3.18	117.90	126.73
20	B	805	CLA	C1D-CHD-C4C	-3.18	119.20	126.06
20	4	316	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
20	A	841	CLA	CHC-C1C-C2C	-3.18	117.91	126.73
20	B	846	CLA	CMD-C2D-C3D	-3.18	120.31	127.61
20	1	305	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
20	A	803	CLA	CHD-C1D-ND	-3.18	121.54	124.45
20	A	841	CLA	CMC-C2C-C1C	3.17	129.87	125.04
20	A	845	CLA	C4C-C3C-C2C	-3.17	102.27	106.90
20	A	854	CLA	C1D-CHD-C4C	-3.17	119.21	126.06
20	B	827	CLA	CAC-C3C-C4C	3.17	128.93	124.81
20	B	810	CLA	CMC-C2C-C1C	3.17	129.87	125.04
29	J	104	DGD	O6E-C5E-C4E	3.17	115.45	109.69
20	B	827	CLA	C1D-CHD-C4C	-3.17	119.22	126.06
20	3	312	CLA	C2D-C1D-ND	3.17	112.44	110.10
23	L	303	BCR	C36-C18-C17	-3.17	118.48	122.92
20	3	316	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
20	A	855	CLA	CMC-C2C-C1C	3.17	129.86	125.04
20	B	813	CLA	C1D-CHD-C4C	-3.17	119.22	126.06
20	2	317	CLA	C2D-C1D-ND	3.17	112.44	110.10
20	A	827	CLA	C2D-C1D-ND	3.17	112.44	110.10
19	3	313	CHL	C2A-C1A-CHA	-3.16	118.33	123.86
20	A	849	CLA	C4D-CHA-C1A	-3.16	117.40	121.25
20	B	808	CLA	CMC-C2C-C1C	3.16	129.85	125.04
20	A	856	CLA	C2D-C1D-ND	3.16	112.43	110.10
20	3	308	CLA	C3B-C4B-NB	3.16	113.45	110.52
20	B	808	CLA	C4D-CHA-C1A	-3.16	117.40	121.25
20	A	804	CLA	C1D-CHD-C4C	-3.16	119.24	126.06
20	3	307	CLA	CMC-C2C-C1C	3.16	129.85	125.04
20	B	816	CLA	CHD-C1D-ND	-3.16	121.55	124.45
20	A	808	CLA	C4D-CHA-C1A	-3.16	117.41	121.25
20	A	812	CLA	C4D-CHA-C1A	-3.16	117.41	121.25
20	B	811	CLA	CMC-C2C-C1C	3.16	129.85	125.04
20	A	848	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
20	B	809	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
20	B	821	CLA	CMC-C2C-C1C	3.16	129.85	125.04
20	B	808	CLA	O2A-CGA-CBA	3.16	121.82	111.91
20	A	842	CLA	CHC-C1C-C2C	-3.16	117.96	126.73
20	K	204	CLA	CMC-C2C-C1C	3.16	129.84	125.04
20	A	833	CLA	CHD-C1D-ND	-3.16	121.55	124.45
20	B	821	CLA	C4C-C3C-C2C	-3.15	102.30	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	311	CLA	C1D-CHD-C4C	-3.15	119.25	126.06
20	J	103	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
20	A	809	CLA	C1D-CHD-C4C	-3.15	119.26	126.06
20	A	851	CLA	CHC-C1C-C2C	-3.15	117.98	126.73
22	3	302	XAT	C24-C23-C22	-3.15	104.69	110.77
20	B	816	CLA	CHB-C1B-NB	-3.15	120.92	124.26
20	A	804	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
23	A	814	BCR	C30-C25-C26	-3.15	118.18	122.61
20	A	846	CLA	CMC-C2C-C1C	3.15	129.83	125.04
20	B	848	CLA	CHB-C4A-NA	3.14	128.86	124.51
19	2	322	CHL	CAC-C3C-C4C	3.14	128.89	124.81
20	B	821	CLA	C4-C3-C5	3.14	120.56	115.27
20	B	812	CLA	C4-C3-C2	-3.14	115.62	123.68
20	2	319	CLA	CHC-C1C-C2C	-3.14	118.00	126.73
20	4	302	CLA	CHC-C1C-C2C	-3.14	118.00	126.73
20	B	813	CLA	CHC-C1C-C2C	-3.14	118.00	126.73
20	A	827	CLA	CHB-C1B-NB	-3.14	120.93	124.26
20	B	827	CLA	C2A-C1A-CHA	-3.14	118.37	123.86
20	A	846	CLA	CHB-C4A-NA	3.14	128.86	124.51
20	A	827	CLA	C1D-CHD-C4C	-3.14	119.28	126.06
20	A	804	CLA	C3B-C4B-NB	3.14	113.43	110.52
20	A	850	CLA	CAC-C3C-C4C	3.14	128.88	124.81
20	B	815	CLA	C3B-C4B-NB	3.14	113.43	110.52
20	B	811	CLA	CAC-C3C-C4C	3.14	128.88	124.81
20	A	808	CLA	CHB-C1B-NB	-3.14	120.93	124.26
20	O	207	CLA	C2D-C1D-ND	3.14	112.42	110.10
20	B	826	CLA	CHC-C1C-C2C	-3.14	118.01	126.73
20	B	815	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
20	3	309	CLA	C1C-C2C-C3C	-3.14	103.66	106.96
20	1	319	CLA	CMC-C2C-C1C	3.14	129.82	125.04
20	3	314	CLA	C1D-CHD-C4C	-3.14	119.29	126.06
20	B	815	CLA	CHC-C1C-C2C	-3.14	118.02	126.73
20	B	810	CLA	CAC-C3C-C4C	3.14	128.88	124.81
20	2	306	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
20	O	208	CLA	CHB-C1B-NB	-3.13	120.94	124.26
20	B	823	CLA	CHC-C1C-C2C	-3.13	118.03	126.73
19	2	322	CHL	C2A-C1A-CHA	-3.13	118.38	123.86
20	B	810	CLA	C1D-CHD-C4C	-3.13	119.30	126.06
20	4	308	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
20	A	854	CLA	C3B-C4B-NB	3.13	113.42	110.52
20	A	852	CLA	C4D-CHA-C1A	-3.13	117.44	121.25
20	J	103	CLA	CMC-C2C-C1C	3.13	129.80	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	827	CLA	CMC-C2C-C1C	3.12	129.80	125.04
20	A	836	CLA	C2A-C1A-CHA	-3.12	118.39	123.86
20	2	303	CLA	C4C-C3C-C2C	-3.12	102.34	106.90
20	B	818	CLA	C3D-C2D-C1D	-3.12	101.57	105.83
19	4	306	CHL	C2A-C1A-CHA	-3.12	118.40	123.86
20	B	833	CLA	CMC-C2C-C1C	3.12	129.79	125.04
20	B	830	CLA	O2A-CGA-CBA	3.12	121.71	111.91
20	3	318	CLA	C2A-C1A-CHA	-3.12	118.41	123.85
23	L	304	BCR	C23-C22-C21	3.12	123.72	118.94
20	B	827	CLA	C1-C2-C3	-3.12	120.65	126.04
28	A	824	CL0	C1D-CHD-C4C	-3.12	119.34	126.06
20	B	805	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
20	4	312	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
20	A	842	CLA	C1D-CHD-C4C	-3.11	119.34	126.06
20	B	825	CLA	CHB-C4A-NA	3.11	128.82	124.51
20	1	303	CLA	C1D-CHD-C4C	-3.11	119.34	126.06
20	B	817	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
20	K	203	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
20	O	208	CLA	C2D-C1D-ND	3.11	112.40	110.10
20	B	848	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
19	2	301	CHL	CHB-C1B-NB	-3.11	120.97	124.26
20	A	831	CLA	C4-C3-C5	3.11	120.50	115.27
20	B	852	CLA	C1D-CHD-C4C	-3.11	119.35	126.06
19	4	315	CHL	CHB-C1B-NB	-3.11	120.97	124.26
20	A	847	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
23	L	301	BCR	C35-C13-C14	-3.11	118.57	122.92
23	L	303	BCR	C21-C20-C19	3.11	132.92	123.22
20	B	814	CLA	CHC-C1C-C2C	-3.11	118.10	126.73
28	A	824	CL0	C4C-C3C-C2C	-3.11	102.37	106.90
20	B	815	CLA	CHB-C1B-NB	-3.11	120.97	124.26
20	1	304	CLA	CHB-C1B-NB	-3.11	120.97	124.26
21	3	301	LUT	C15-C35-C34	3.11	129.84	123.47
20	B	823	CLA	CMC-C2C-C1C	3.11	129.77	125.04
20	K	203	CLA	CMC-C2C-C1C	3.11	129.77	125.04
20	A	805	CLA	C4C-C3C-C2C	-3.10	102.37	106.90
20	B	818	CLA	CAC-C3C-C4C	3.10	128.84	124.81
20	A	836	CLA	CMD-C2D-C3D	-3.10	120.48	127.61
20	3	307	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
20	A	806	CLA	C2A-C1A-CHA	-3.10	118.44	123.86
20	A	812	CLA	CHD-C1D-ND	-3.10	121.61	124.45
20	A	807	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
20	B	825	CLA	CMC-C2C-C1C	3.10	129.76	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	838	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
23	A	815	BCR	C36-C18-C17	-3.10	118.58	122.92
20	A	847	CLA	CMC-C2C-C1C	3.10	129.76	125.04
20	A	854	CLA	CHD-C1D-ND	-3.10	121.61	124.45
21	2	310	LUT	C39-C29-C30	-3.10	118.58	122.92
20	A	853	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
20	B	831	CLA	C1-C2-C3	-3.10	120.69	126.04
22	2	311	XAT	C30-C31-C32	3.10	132.88	123.22
20	1	321	CLA	C4C-C3C-C2C	-3.10	102.39	106.90
20	A	837	CLA	C1D-CHD-C4C	-3.09	119.38	126.06
20	A	854	CLA	CMC-C2C-C1C	3.09	129.75	125.04
20	B	828	CLA	C1D-CHD-C4C	-3.09	119.39	126.06
19	1	301	CHL	CHB-C1B-NB	-3.09	120.98	124.26
20	2	307	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
23	B	837	BCR	C11-C10-C9	3.09	131.72	127.31
20	2	306	CLA	C4A-NA-C1A	3.09	108.09	106.71
20	A	803	CLA	O2A-C1-C2	3.09	116.75	108.64
20	3	310	CLA	CMD-C2D-C3D	-3.09	120.51	127.61
20	A	834	CLA	C2D-C1D-ND	3.09	112.38	110.10
20	B	807	CLA	C1D-CHD-C4C	-3.08	119.40	126.06
20	2	305	CLA	C2D-C1D-ND	3.08	112.38	110.10
20	2	305	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
20	4	310	CLA	C4C-C3C-C2C	-3.08	102.40	106.90
22	2	311	XAT	C15-C14-C13	3.08	131.71	127.31
20	2	317	CLA	C1D-CHD-C4C	-3.08	119.41	126.06
20	A	830	CLA	CHB-C1B-NB	-3.08	121.00	124.26
20	A	830	CLA	C2D-C1D-ND	3.08	112.37	110.10
20	A	844	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
20	F	306	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
20	4	304	CLA	CMD-C2D-C3D	-3.08	120.53	127.61
20	A	812	CLA	C1D-CHD-C4C	-3.08	119.42	126.06
19	4	307	CHL	C2A-C1A-CHA	-3.08	118.48	123.86
20	B	816	CLA	CMC-C2C-C1C	3.08	129.73	125.04
20	B	805	CLA	CMC-C2C-C1C	3.08	129.73	125.04
20	F	305	CLA	CMC-C2C-C1C	3.08	129.73	125.04
20	G	206	CLA	CMD-C2D-C3D	-3.08	120.53	127.61
20	A	825	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
20	A	851	CLA	CMC-C2C-C1C	3.08	129.72	125.04
20	A	806	CLA	CHB-C4A-NA	3.08	128.76	124.51
23	2	312	BCR	C36-C18-C17	-3.07	118.62	122.92
19	4	305	CHL	C2A-C1A-CHA	-3.07	118.48	123.86
20	A	842	CLA	CMC-C2C-C1C	3.07	129.72	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	308	CLA	CMC-C2C-C1C	3.07	129.72	125.04
20	A	836	CLA	CMC-C2C-C1C	3.07	129.72	125.04
20	L	307	CLA	CMC-C2C-C1C	3.07	129.72	125.04
20	2	323	CLA	CMD-C2D-C3D	-3.07	120.55	127.61
20	3	311	CLA	CHB-C1B-NB	-3.07	121.01	124.26
20	1	322	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
20	4	310	CLA	C1D-CHD-C4C	-3.07	119.43	126.06
20	4	309	CLA	C1-C2-C3	-3.07	120.73	126.04
20	K	206	CLA	CMC-C2C-C1C	3.07	129.71	125.04
20	1	302	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
20	A	846	CLA	C3B-C4B-NB	3.07	113.36	110.52
20	B	830	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
20	3	308	CLA	CHB-C1B-NB	-3.07	121.01	124.26
20	A	801	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
20	1	320	CLA	C2D-C1D-ND	3.06	112.36	110.10
20	A	839	CLA	C2A-C1A-CHA	-3.06	118.50	123.86
20	1	309	CLA	CMC-C2C-C1C	3.06	129.70	125.04
23	4	320	BCR	C15-C14-C13	3.06	131.68	127.31
20	1	307	CLA	CMD-C2D-C3D	-3.06	120.58	127.61
20	2	317	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
20	2	321	CLA	CMD-C2D-C3D	-3.06	120.58	127.61
20	B	807	CLA	CMC-C2C-C1C	3.06	129.70	125.04
23	G	201	BCR	C36-C18-C17	-3.06	118.64	122.92
20	1	306	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
20	3	308	CLA	CAC-C3C-C4C	3.06	128.78	124.81
19	2	309	CHL	CMB-C2B-C1B	3.06	130.02	125.37
20	J	103	CLA	C1D-CHD-C4C	-3.06	119.47	126.06
20	B	849	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
20	2	320	CLA	C4D-CHA-C1A	-3.05	117.53	121.25
20	A	827	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
20	A	851	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
20	2	320	CLA	CMB-C2B-C3B	3.05	133.98	126.59
20	B	826	CLA	CAC-C3C-C4C	3.05	128.77	124.81
20	O	207	CLA	CMD-C2D-C3D	-3.05	120.60	127.61
20	3	314	CLA	C2D-C1D-ND	3.05	112.35	110.10
20	B	849	CLA	C1D-CHD-C4C	-3.05	119.48	126.06
20	K	203	CLA	C1D-CHD-C4C	-3.05	119.48	126.06
20	A	840	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
20	G	207	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
23	O	203	BCR	C37-C22-C23	3.05	122.88	118.08
20	B	812	CLA	C4C-C3C-C2C	-3.04	102.46	106.90
20	3	320	CLA	CMD-C2D-C3D	-3.04	120.61	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	323	CLA	C4C-C3C-C2C	-3.04	102.46	106.90
20	B	804	CLA	CMD-C2D-C3D	-3.04	120.61	127.61
20	3	318	CLA	C4C-C3C-C2C	-3.04	102.46	106.90
20	L	305	CLA	CMD-C2D-C3D	-3.04	120.62	127.61
20	B	819	CLA	C3D-C2D-C1D	-3.04	101.68	105.83
20	3	312	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
20	1	320	CLA	C1D-CHD-C4C	-3.04	119.50	126.06
20	4	309	CLA	CHC-C1C-C2C	-3.04	118.30	126.73
20	B	824	CLA	CAC-C3C-C4C	3.04	128.75	124.81
20	G	207	CLA	C1D-CHD-C4C	-3.04	119.51	126.06
20	1	320	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
20	2	308	CLA	C1D-CHD-C4C	-3.03	119.51	126.06
20	A	836	CLA	C1D-CHD-C4C	-3.03	119.51	126.06
20	3	315	CLA	CMD-C2D-C3D	-3.03	120.64	127.61
20	4	314	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
20	B	806	CLA	C2A-C1A-CHA	-3.03	118.56	123.86
20	A	830	CLA	CAC-C3C-C4C	3.03	128.74	124.81
20	A	837	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
20	1	308	CLA	CHB-C1B-NB	-3.03	121.05	124.26
25	1	324	MGE	O2G-C1B-C2B	3.03	118.03	111.50
23	I	102	BCR	C11-C10-C9	3.03	131.63	127.31
20	1	307	CLA	C4-C3-C5	3.03	120.36	115.27
20	A	842	CLA	C2D-C1D-ND	3.03	112.33	110.10
20	B	829	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
20	A	812	CLA	CMC-C2C-C1C	3.03	129.65	125.04
20	B	827	CLA	C4C-C3C-C2C	-3.03	102.49	106.90
20	1	318	CLA	C4C-C3C-C2C	-3.03	102.49	106.90
20	4	303	CLA	CMD-C2D-C3D	-3.03	120.66	127.61
20	A	831	CLA	C3B-C4B-NB	3.02	113.32	110.52
19	2	318	CHL	CHB-C1B-NB	-3.02	121.06	124.26
19	2	318	CHL	CMB-C2B-C1B	3.02	129.97	125.37
20	B	812	CLA	CMB-C2B-C3B	3.02	133.91	126.59
20	1	304	CLA	CMC-C2C-C1C	3.02	129.64	125.04
20	1	307	CLA	C1D-CHD-C4C	-3.02	119.54	126.06
20	O	207	CLA	C1D-CHD-C4C	-3.02	119.54	126.06
20	2	317	CLA	CMC-C2C-C1C	3.02	129.64	125.04
20	K	205	CLA	CHD-C1D-ND	-3.02	121.68	124.45
20	3	307	CLA	C1-O2A-CGA	3.02	124.36	116.44
19	2	302	CHL	CMB-C2B-C1B	3.02	129.97	125.37
20	A	802	CLA	C1-C2-C3	-3.02	120.82	126.04
23	F	302	BCR	C34-C9-C8	3.02	122.83	118.08
20	A	830	CLA	C4A-NA-C1A	3.02	108.06	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	318	CLA	C1D-CHD-C4C	-3.02	119.55	126.06
20	A	843	CLA	C4D-CHA-C1A	-3.02	117.58	121.25
20	K	204	CLA	CMD-C2D-C3D	-3.02	120.67	127.61
20	3	320	CLA	CHB-C1B-NB	-3.02	121.06	124.26
20	A	833	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
20	A	832	CLA	C4-C3-C5	3.02	120.34	115.27
20	1	309	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
20	B	824	CLA	C1D-CHD-C4C	-3.02	119.55	126.06
20	L	305	CLA	CMB-C2B-C3B	3.02	133.89	126.59
20	1	307	CLA	C4C-C3C-C2C	-3.01	102.50	106.90
20	O	208	CLA	C1D-CHD-C4C	-3.01	119.56	126.06
20	4	313	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
21	3	301	LUT	C39-C29-C28	3.01	122.82	118.08
20	3	319	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
20	L	306	CLA	CMC-C2C-C1C	3.01	129.62	125.04
20	A	850	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
23	A	817	BCR	C11-C10-C9	3.01	131.61	127.31
19	2	322	CHL	CHB-C1B-NB	-3.01	121.07	124.26
20	F	304	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
20	A	844	CLA	C2D-C1D-ND	3.01	112.32	110.10
20	A	830	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
20	B	826	CLA	C1-C2-C3	-3.01	121.89	126.75
20	A	840	CLA	C1D-CHD-C4C	-3.01	119.57	126.06
20	A	835	CLA	C3B-C4B-NB	3.01	113.30	110.52
20	B	823	CLA	C4C-C3C-C2C	-3.01	102.52	106.90
20	B	816	CLA	C2D-C1D-ND	3.01	112.32	110.10
23	O	202	BCR	C15-C16-C17	3.01	129.63	123.47
19	1	301	CHL	CMD-C2D-C3D	-3.01	120.70	127.61
20	3	319	CLA	CMD-C2D-C3D	-3.01	120.70	127.61
20	3	312	CLA	C1D-CHD-C4C	-3.01	119.58	126.06
20	B	817	CLA	CHB-C1B-NB	-3.00	121.08	124.26
23	L	304	BCR	C36-C18-C17	-3.00	118.71	122.92
20	J	103	CLA	CMD-C2D-C3D	-3.00	120.70	127.61
20	1	305	CLA	C1D-CHD-C4C	-3.00	119.58	126.06
20	B	814	CLA	CHB-C4A-NA	3.00	128.66	124.51
23	B	834	BCR	C15-C16-C17	3.00	129.62	123.47
20	A	853	CLA	CHC-C1C-C2C	-3.00	118.39	126.73
20	A	845	CLA	C3B-C4B-NB	3.00	113.30	110.52
20	A	830	CLA	CMC-C2C-C1C	3.00	129.61	125.04
20	3	317	CLA	C2A-C1A-CHA	-3.00	118.61	123.86
20	A	807	CLA	C1D-CHD-C4C	-3.00	119.59	126.06
20	1	304	CLA	C2D-C1D-ND	3.00	112.31	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	G	202	DGD	O1G-C1A-C2A	3.00	121.31	111.91
20	A	854	CLA	C2D-C1D-ND	3.00	112.31	110.10
20	1	321	CLA	CMD-C2D-C3D	-3.00	120.72	127.61
20	1	302	CLA	C1D-CHD-C4C	-3.00	119.59	126.06
20	A	848	CLA	C1D-CHD-C4C	-3.00	119.59	126.06
20	O	206	CLA	CMC-C2C-C1C	3.00	129.60	125.04
20	3	310	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
20	A	843	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
20	1	308	CLA	CMD-C2D-C3D	-3.00	120.72	127.61
20	B	845	CLA	O2A-CGA-CBA	2.99	121.31	111.91
20	L	305	CLA	C4C-C3C-C2C	-2.99	102.53	106.90
20	4	311	CLA	CMC-C2C-C1C	2.99	129.60	125.04
20	B	824	CLA	C2D-C1D-ND	2.99	112.31	110.10
20	B	807	CLA	CMD-C2D-C3D	-2.99	120.73	127.61
20	F	305	CLA	C1D-CHD-C4C	-2.99	119.61	126.06
20	G	205	CLA	CHB-C1B-NB	-2.99	121.09	124.26
20	K	204	CLA	C1D-CHD-C4C	-2.99	119.61	126.06
20	L	305	CLA	CAC-C3C-C4C	2.99	128.69	124.81
20	B	803	CLA	C1D-CHD-C4C	-2.99	119.61	126.06
20	B	847	CLA	C1D-CHD-C4C	-2.99	119.61	126.06
20	3	312	CLA	CHB-C1B-NB	-2.99	121.09	124.26
20	2	308	CLA	C4-C3-C5	2.98	119.39	115.98
20	B	803	CLA	C4D-CHA-C1A	-2.98	117.62	121.25
19	4	306	CHL	CMB-C2B-C1B	2.98	129.91	125.37
20	B	825	CLA	C1D-CHD-C4C	-2.98	119.62	126.06
20	A	827	CLA	CMD-C2D-C3D	-2.98	120.75	127.61
20	A	811	CLA	C1D-CHD-C4C	-2.98	119.63	126.06
20	3	320	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
22	2	311	XAT	C27-C28-C29	2.98	130.15	125.53
20	B	812	CLA	C2A-C1A-CHA	-2.98	118.65	123.86
20	B	851	CLA	C4A-NA-C1A	2.98	108.05	106.71
20	4	302	CLA	CHC-C4B-NB	-2.98	121.10	124.26
20	B	829	CLA	C1D-CHD-C4C	-2.98	119.63	126.06
20	B	844	CLA	O2A-CGA-CBA	2.98	121.25	111.91
20	1	322	CLA	C1D-CHD-C4C	-2.98	119.64	126.06
20	2	304	CLA	C1D-CHD-C4C	-2.98	119.64	126.06
20	K	204	CLA	CHB-C1B-NB	-2.98	121.11	124.26
20	1	321	CLA	C1D-CHD-C4C	-2.98	119.64	126.06
20	2	321	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
20	B	853	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
19	3	313	CHL	CHB-C1B-NB	-2.97	121.11	124.26
23	K	202	BCR	C16-C15-C14	2.97	129.57	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	304	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
20	3	319	CLA	C1D-CHD-C4C	-2.97	119.64	126.06
23	J	101	BCR	C16-C15-C14	2.97	129.56	123.47
20	4	308	CLA	C1D-CHD-C4C	-2.97	119.65	126.06
20	B	820	CLA	O2A-CGA-CBA	2.97	121.22	111.91
20	A	840	CLA	CMD-C2D-C3D	-2.97	120.78	127.61
20	L	306	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
20	B	802	CLA	C2A-C1A-CHA	-2.97	118.67	123.86
20	2	319	CLA	C2D-C1D-ND	2.97	112.29	110.10
20	4	302	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
23	L	302	BCR	C36-C18-C17	-2.97	118.77	122.92
23	L	303	BCR	C11-C10-C9	2.97	131.54	127.31
20	3	311	CLA	CMD-C2D-C3D	-2.97	120.79	127.61
20	B	814	CLA	C3B-C4B-NB	2.97	113.27	110.52
20	A	843	CLA	O2A-CGA-CBA	2.97	121.22	111.91
20	A	856	CLA	CHB-C1B-NB	-2.97	121.12	124.26
20	A	804	CLA	O2A-CGA-CBA	2.97	121.21	111.91
20	B	802	CLA	C2D-C1D-ND	2.96	112.29	110.10
19	3	313	CHL	CAC-C3C-C4C	2.96	128.66	124.81
28	A	824	CL0	O2A-CGA-CBA	2.96	121.21	111.91
20	2	320	CLA	CAC-C3C-C4C	2.96	129.55	125.04
22	2	311	XAT	C11-C10-C9	-2.96	123.08	127.31
20	B	853	CLA	O2A-CGA-CBA	2.96	121.21	111.91
20	B	828	CLA	C2A-C1A-CHA	-2.96	118.68	123.86
20	B	830	CLA	C3B-C4B-NB	2.96	113.26	110.52
20	B	803	CLA	CHB-C1B-NB	-2.96	121.12	124.26
20	2	303	CLA	C1D-CHD-C4C	-2.96	119.67	126.06
20	B	820	CLA	C2D-C1D-ND	2.96	112.29	110.10
20	1	308	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
23	A	814	BCR	C37-C22-C23	2.96	122.74	118.08
20	B	831	CLA	O2A-CGA-CBA	2.96	121.20	111.91
20	B	833	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
20	H	201	CLA	CMC-C2C-C1C	2.96	129.55	125.04
20	B	828	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
20	A	848	CLA	C2D-C1D-ND	2.96	112.28	110.10
20	2	305	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
20	A	845	CLA	C2A-C1A-CHA	-2.96	118.69	123.86
20	O	206	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
20	B	853	CLA	CMD-C2D-C3D	-2.96	120.81	127.61
23	I	102	BCR	C27-C26-C25	-2.95	118.44	122.73
19	2	322	CHL	CMB-C2B-C1B	2.95	129.87	125.37
21	2	310	LUT	C40-C33-C34	-2.95	118.79	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	847	CLA	C2A-C1A-CHA	-2.95	118.70	123.86
20	A	855	CLA	C1D-CHD-C4C	-2.95	119.69	126.06
20	K	206	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
20	L	307	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
19	2	301	CHL	CMB-C2B-C1B	2.95	129.86	125.37
20	B	808	CLA	C3B-C4B-NB	2.95	113.25	110.52
20	B	809	CLA	CMC-C2C-C1C	2.95	129.53	125.04
20	B	851	CLA	C1D-CHD-C4C	-2.95	119.70	126.06
20	A	802	CLA	CAC-C3C-C4C	2.95	128.63	124.81
23	4	320	BCR	C15-C16-C17	2.95	129.51	123.47
23	L	304	BCR	C34-C9-C8	2.95	122.72	118.08
20	A	849	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
20	3	315	CLA	CAC-C3C-C4C	2.94	128.63	124.81
20	2	307	CLA	CMD-C2D-C3D	-2.94	120.84	127.61
20	F	305	CLA	C3B-C4B-NB	2.94	113.25	110.52
20	A	801	CLA	C1D-CHD-C4C	-2.94	119.71	126.06
20	4	310	CLA	C2D-C1D-ND	2.94	112.27	110.10
20	A	802	CLA	C2D-C1D-ND	2.94	112.27	110.10
20	G	205	CLA	C1D-CHD-C4C	-2.94	119.71	126.06
20	B	806	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
19	1	317	CHL	CHB-C1B-NB	-2.94	121.14	124.26
24	B	842	LHG	O7-C7-O9	-2.94	116.60	123.70
20	A	850	CLA	C1D-CHD-C4C	-2.94	119.72	126.06
20	1	304	CLA	O2A-CGA-CBA	2.94	121.13	111.91
20	1	318	CLA	CHC-C1C-C2C	-2.94	118.57	126.73
20	A	828	CLA	C3B-C4B-NB	2.94	113.24	110.52
20	B	833	CLA	C2A-C1A-CHA	-2.94	118.72	123.86
20	A	839	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
20	O	207	CLA	CMC-C2C-C1C	2.94	129.51	125.04
20	A	828	CLA	CHC-C1C-C2C	-2.94	118.57	126.73
20	A	804	CLA	C2D-C1D-ND	2.94	112.27	110.10
20	A	846	CLA	C1D-CHD-C4C	-2.94	119.72	126.06
20	1	303	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
20	K	203	CLA	CMD-C2D-C3D	-2.93	120.86	127.61
20	A	854	CLA	C4-C3-C5	2.93	120.21	115.27
20	2	323	CLA	C1D-CHD-C4C	-2.93	119.73	126.06
20	3	308	CLA	C2A-C1A-CHA	-2.93	118.73	123.86
20	K	206	CLA	C1D-CHD-C4C	-2.93	119.73	126.06
20	1	303	CLA	C2D-C1D-ND	2.93	112.27	110.10
20	B	819	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
20	B	822	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
20	1	304	CLA	C1D-CHD-C4C	-2.93	119.73	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	323	CLA	C2D-C1D-ND	2.93	112.26	110.10
20	J	103	CLA	C2D-C1D-ND	2.93	112.26	110.10
20	3	317	CLA	CMD-C2D-C3D	-2.93	120.88	127.61
20	4	313	CLA	C2A-C1A-CHA	-2.93	118.74	123.86
20	4	314	CLA	C1D-CHD-C4C	-2.93	119.74	126.06
20	2	321	CLA	CMC-C2C-C1C	2.93	129.50	125.04
20	L	307	CLA	CMD-C2D-C3D	-2.93	120.88	127.61
20	2	305	CLA	C2A-C1A-CHA	-2.93	118.74	123.86
20	B	802	CLA	CMC-C2C-C1C	2.93	129.50	125.04
20	B	822	CLA	CMC-C2C-C1C	2.93	129.50	125.04
20	4	304	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
20	4	309	CLA	C1D-CHD-C4C	-2.93	119.75	126.06
20	B	824	CLA	CMD-C2D-C3D	-2.93	120.89	127.61
20	1	304	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
20	A	853	CLA	C1-C2-C3	-2.92	120.98	126.04
20	N	202	CLA	CMC-C2C-C1C	2.92	129.49	125.04
20	A	808	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
20	B	816	CLA	CAC-C3C-C4C	2.92	128.60	124.81
20	A	839	CLA	C2D-C1D-ND	2.92	112.26	110.10
20	B	804	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
20	4	308	CLA	CMB-C2B-C3B	2.92	133.66	126.59
20	3	312	CLA	CMC-C2C-C1C	2.92	129.49	125.04
20	A	806	CLA	CMD-C2D-C3D	-2.92	120.90	127.61
20	O	208	CLA	CMC-C2C-C1C	2.92	129.48	125.04
20	A	801	CLA	CHB-C1B-NB	-2.92	121.17	124.26
23	4	320	BCR	C12-C13-C14	2.91	123.41	118.94
20	A	806	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
20	2	321	CLA	C1-C2-C3	-2.91	122.04	126.75
23	A	814	BCR	C15-C14-C13	2.91	131.47	127.31
20	B	818	CLA	C1D-CHD-C4C	-2.91	119.78	126.06
20	K	203	CLA	CHB-C1B-NB	-2.91	121.17	124.26
20	A	808	CLA	C1D-CHD-C4C	-2.91	119.78	126.06
20	4	312	CLA	CMD-C2D-C3D	-2.91	120.92	127.61
19	2	318	CHL	O2A-CGA-CBA	2.91	121.04	111.91
23	L	303	BCR	C20-C21-C22	2.91	131.46	127.31
20	F	304	CLA	C4-C3-C5	2.91	120.17	115.27
20	L	307	CLA	C1D-CHD-C4C	-2.91	119.78	126.06
20	3	318	CLA	CMD-C2D-C3D	-2.91	120.92	127.61
20	B	845	CLA	C1C-C2C-C3C	-2.91	103.90	106.96
23	2	312	BCR	C37-C22-C23	2.91	122.66	118.08
20	B	814	CLA	C1-C2-C3	-2.91	121.02	126.04
20	A	838	CLA	C4D-CHA-C1A	-2.91	117.71	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	828	CLA	CMB-C2B-C3B	2.90	133.62	126.59
20	B	804	CLA	C2A-C1A-CHA	-2.90	118.78	123.86
20	A	825	CLA	C1D-CHD-C4C	-2.90	119.79	126.06
20	L	306	CLA	C1D-CHD-C4C	-2.90	119.80	126.06
20	B	815	CLA	CMD-C2D-C3D	-2.90	120.94	127.61
20	1	319	CLA	C1D-CHD-C4C	-2.90	119.80	126.06
20	K	206	CLA	CMD-C2D-C3D	-2.90	120.94	127.61
20	B	833	CLA	C1D-CHD-C4C	-2.90	119.80	126.06
20	B	847	CLA	CMD-C2D-C3D	-2.90	120.94	127.61
23	J	101	BCR	C11-C10-C9	2.90	131.45	127.31
20	A	842	CLA	CMD-C2D-C3D	-2.90	120.94	127.61
20	A	851	CLA	CAC-C3C-C4C	2.90	128.57	124.81
21	1	310	LUT	C39-C29-C28	2.90	122.64	118.08
20	2	308	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
20	4	309	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
20	A	835	CLA	C2D-C1D-ND	2.90	112.24	110.10
20	3	308	CLA	CHC-C1C-C2C	-2.90	118.68	126.73
20	3	308	CLA	C4C-C3C-C2C	-2.90	102.68	106.90
20	A	841	CLA	C2A-C1A-CHA	-2.90	118.80	123.86
20	4	302	CLA	CHB-C1B-NB	-2.90	121.19	124.26
20	B	819	CLA	C3B-C2B-C1B	-2.89	103.67	107.16
20	A	806	CLA	C1D-CHD-C4C	-2.89	119.81	126.06
20	O	206	CLA	CMD-C2D-C3D	-2.89	120.96	127.61
19	2	318	CHL	CAC-C3C-C4C	2.89	128.56	124.81
20	3	320	CLA	CAC-C3C-C4C	2.89	128.56	124.81
20	K	205	CLA	CMD-C2D-C3D	-2.89	120.96	127.61
20	A	856	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
20	3	309	CLA	CMD-C2D-C3D	-2.89	120.96	127.61
20	B	807	CLA	C2D-C1D-ND	2.89	112.23	110.10
20	2	317	CLA	CMD-C2D-C3D	-2.89	120.96	127.61
20	2	305	CLA	C1D-CHD-C4C	-2.89	119.82	126.06
19	2	318	CHL	CHB-C4A-NA	2.89	128.51	124.51
20	A	848	CLA	C4-C3-C5	2.89	120.13	115.27
20	1	320	CLA	CMD-C2D-C3D	-2.89	120.97	127.61
20	B	845	CLA	C1D-CHD-C4C	-2.89	119.83	126.06
20	1	318	CLA	C3B-C4B-NB	2.89	113.19	110.52
20	O	206	CLA	C1D-CHD-C4C	-2.89	119.83	126.06
20	B	831	CLA	C4-C3-C5	2.89	120.13	115.27
23	4	319	BCR	C36-C18-C17	-2.89	118.88	122.92
20	1	303	CLA	CAC-C3C-C4C	2.89	128.56	124.81
20	B	812	CLA	CMC-C2C-C1C	2.89	129.44	125.04
23	A	818	BCR	C17-C16-C15	2.89	131.23	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	811	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
20	2	319	CLA	CMD-C2D-C3D	-2.88	120.98	127.61
20	B	853	CLA	CMC-C2C-C1C	2.88	129.43	125.04
20	4	314	CLA	C3B-C4B-NB	2.88	113.19	110.52
20	B	819	CLA	CMD-C2D-C3D	-2.88	120.98	127.61
20	A	812	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
20	B	826	CLA	O2A-CGA-CBA	2.88	120.95	111.91
20	2	321	CLA	C1D-CHD-C4C	-2.88	119.84	126.06
20	3	308	CLA	C1D-CHD-C4C	-2.88	119.84	126.06
20	A	838	CLA	C2D-C1D-ND	2.88	112.23	110.10
20	B	824	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
20	2	305	CLA	CMD-C2D-C3D	-2.88	120.98	127.61
20	A	856	CLA	C1D-CHD-C4C	-2.88	119.84	126.06
20	2	320	CLA	CMD-C2D-C3D	-2.88	120.99	127.61
19	3	313	CHL	CMB-C2B-C1B	2.88	129.75	125.37
21	2	310	LUT	C20-C13-C14	-2.88	118.89	122.92
20	B	851	CLA	O2A-CGA-CBA	2.88	120.94	111.91
20	A	829	CLA	C4D-CHA-C1A	-2.88	117.75	121.25
28	A	824	CL0	CHB-C1B-NB	-2.88	121.21	124.26
20	4	316	CLA	C3B-C4B-NB	2.88	113.18	110.52
20	1	321	CLA	CHB-C1B-NB	-2.88	121.21	124.26
20	1	309	CLA	CMD-C2D-C3D	-2.87	121.00	127.61
20	A	845	CLA	CMC-C2C-C1C	2.87	129.42	125.04
20	K	204	CLA	O2A-CGA-CBA	2.87	120.93	111.91
20	2	320	CLA	C3B-C4B-NB	2.87	113.18	110.52
20	3	310	CLA	CHB-C1B-NB	-2.87	121.22	124.26
20	1	319	CLA	CHC-C4B-NB	-2.87	121.22	124.26
20	A	856	CLA	CMD-C2D-C3D	-2.87	121.01	127.61
20	A	802	CLA	O2A-CGA-CBA	2.87	120.92	111.91
23	A	814	BCR	C36-C18-C17	-2.87	118.90	122.92
20	K	206	CLA	CMB-C2B-C3B	2.87	133.54	126.59
20	L	307	CLA	CHB-C1B-NB	-2.87	121.22	124.26
21	1	310	LUT	C40-C33-C34	-2.87	118.90	122.92
19	3	313	CHL	C1C-C2C-C3C	-2.87	104.84	107.11
20	A	849	CLA	CHC-C4B-NB	-2.87	121.22	124.26
20	4	316	CLA	CMD-C2D-C3D	-2.87	121.01	127.61
20	B	801	CLA	CHB-C1B-NB	-2.87	121.22	124.26
20	1	308	CLA	C2D-C1D-ND	2.87	112.22	110.10
20	B	810	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
20	B	808	CLA	C1D-CHD-C4C	-2.86	119.88	126.06
20	B	808	CLA	C4C-C3C-C2C	-2.86	102.72	106.90
19	1	301	CHL	CMB-C2B-C1B	2.86	129.73	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	841	CLA	CMD-C2D-C3D	-2.86	121.03	127.61
20	2	319	CLA	C1D-CHD-C4C	-2.86	119.88	126.06
20	3	315	CLA	C1D-CHD-C4C	-2.86	119.88	126.06
20	A	831	CLA	C1D-CHD-C4C	-2.86	119.89	126.06
29	O	201	DGD	O2G-C1B-C2B	2.86	117.66	111.50
20	A	852	CLA	CHB-C1B-NB	-2.86	121.23	124.26
20	A	842	CLA	CAA-C2A-C3A	2.86	120.60	112.78
20	A	825	CLA	CAC-C3C-C4C	2.86	128.52	124.81
20	3	311	CLA	C4-C3-C5	2.86	120.08	115.27
20	B	846	CLA	CMB-C2B-C3B	2.85	133.50	126.59
20	A	802	CLA	CHC-C1C-C2C	-2.85	118.80	126.73
20	A	839	CLA	CMC-C2C-C1C	2.85	129.38	125.04
20	A	829	CLA	CMD-C2D-C3D	-2.85	121.06	127.61
20	A	831	CLA	CMD-C2D-C3D	-2.85	121.06	127.61
20	3	320	CLA	C1D-CHD-C4C	-2.85	119.91	126.06
20	1	308	CLA	C1D-CHD-C4C	-2.85	119.91	126.06
20	O	208	CLA	CMD-C2D-C3D	-2.85	121.06	127.61
20	A	834	CLA	CMD-C2D-C3D	-2.85	121.06	127.61
20	3	311	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
20	A	853	CLA	C1D-CHD-C4C	-2.85	119.92	126.06
20	B	815	CLA	C1D-CHD-C4C	-2.85	119.92	126.06
23	L	302	BCR	C15-C16-C17	2.85	129.31	123.47
20	K	204	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
20	B	846	CLA	CHC-C4B-NB	-2.85	121.24	124.26
20	A	829	CLA	C3B-C4B-NB	2.85	113.16	110.52
21	3	301	LUT	C40-C33-C34	-2.85	118.94	122.92
20	4	313	CLA	O2A-CGA-CBA	2.85	120.84	111.91
20	B	824	CLA	C2A-C1A-CHA	-2.84	118.89	123.86
20	A	850	CLA	C2D-C1D-ND	2.84	112.20	110.10
20	B	803	CLA	CHC-C4B-NB	-2.84	121.25	124.26
19	3	313	CHL	CHB-C4A-NA	2.84	128.44	124.51
20	B	806	CLA	C5-C3-C2	-2.84	115.36	121.12
20	A	825	CLA	CHC-C4B-NB	-2.84	121.25	124.26
20	K	206	CLA	C2D-C1D-ND	2.84	112.20	110.10
20	B	817	CLA	C4A-NA-C1A	2.84	107.98	106.71
20	A	828	CLA	CMD-C2D-C3D	-2.84	121.08	127.61
20	3	319	CLA	C2D-C1D-ND	2.84	112.20	110.10
20	A	835	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
20	3	317	CLA	C1D-CHD-C4C	-2.84	119.93	126.06
20	G	207	CLA	CMD-C2D-C3D	-2.84	121.08	127.61
20	1	318	CLA	C2D-C1D-ND	2.84	112.20	110.10
20	2	308	CLA	C2D-C1D-ND	2.84	112.20	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	201	CLA	C4-C3-C5	2.84	120.05	115.27
23	1	312	BCR	C11-C10-C9	2.84	131.36	127.31
20	2	307	CLA	C1D-CHD-C4C	-2.84	119.94	126.06
20	3	314	CLA	CMB-C2B-C1B	2.84	129.69	125.37
20	A	809	CLA	CMD-C2D-C3D	-2.84	121.09	127.61
19	2	301	CHL	CHB-C4A-NA	2.84	128.44	124.51
23	B	836	BCR	C30-C25-C26	-2.84	118.62	122.61
20	A	827	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	3	302	XAT	C4-C3-C2	-2.84	105.30	110.77
20	3	307	CLA	CMD-C2D-C3D	-2.84	121.09	127.61
20	B	815	CLA	CAC-C3C-C4C	2.83	128.49	124.81
19	2	309	CHL	CMD-C2D-C3D	-2.83	121.09	127.61
21	4	317	LUT	C40-C33-C34	-2.83	118.95	122.92
20	B	844	CLA	C2A-C1A-CHA	-2.83	118.90	123.86
20	F	304	CLA	C1D-CHD-C4C	-2.83	119.94	126.06
20	A	850	CLA	CMB-C2B-C3B	2.83	133.45	126.59
23	B	835	BCR	C8-C9-C10	2.83	123.29	118.94
20	A	827	CLA	CHC-C4B-NB	-2.83	121.26	124.26
20	B	818	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
20	B	848	CLA	C6-C5-C3	-2.83	106.03	113.45
20	A	825	CLA	C3B-C4B-NB	2.83	113.14	110.52
20	A	836	CLA	C3B-C4B-NB	2.83	113.14	110.52
20	A	825	CLA	CHC-C1C-C2C	-2.82	118.88	126.73
20	A	807	CLA	CMD-C2D-C3D	-2.82	121.12	127.61
20	2	321	CLA	C2A-C1A-CHA	-2.82	118.92	123.86
20	A	851	CLA	CHC-C4B-NB	-2.82	121.27	124.26
20	B	826	CLA	CHB-C1B-NB	-2.82	121.27	124.26
20	B	823	CLA	C4D-CHA-C1A	-2.82	117.82	121.25
20	4	302	CLA	O2A-CGA-CBA	2.82	120.75	111.91
23	K	201	BCR	C16-C15-C14	2.82	129.25	123.47
23	I	102	BCR	C36-C18-C17	-2.82	118.98	122.92
23	A	817	BCR	C15-C14-C13	2.82	131.33	127.31
20	B	846	CLA	CHC-C1C-C2C	-2.82	118.91	126.73
20	2	319	CLA	CHB-C1B-NB	-2.81	121.28	124.26
20	A	841	CLA	C2D-C1D-ND	2.81	112.18	110.10
23	A	816	BCR	C21-C20-C19	2.81	132.00	123.22
23	A	817	BCR	C15-C16-C17	2.81	129.24	123.47
20	L	306	CLA	C2A-C1A-CHA	-2.81	118.94	123.86
20	B	806	CLA	CMD-C2D-C3D	-2.81	121.14	127.61
19	4	307	CHL	CMB-C2B-C1B	2.81	129.65	125.37
20	B	801	CLA	C1D-CHD-C4C	-2.81	119.99	126.06
20	4	304	CLA	CMC-C2C-C1C	2.81	129.32	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	832	CLA	C1D-CHD-C4C	-2.81	119.99	126.06
19	1	301	CHL	CHB-C4A-NA	2.81	128.40	124.51
20	B	821	CLA	CAC-C3C-C4C	2.81	128.46	124.81
23	B	839	BCR	C10-C11-C12	2.81	131.99	123.22
20	4	302	CLA	C1D-CHD-C4C	-2.81	119.99	126.06
20	B	853	CLA	C2D-C1D-ND	2.81	112.17	110.10
28	A	824	CL0	C4-C3-C5	2.81	120.00	115.27
20	B	803	CLA	CMD-C2D-C3D	-2.81	121.16	127.61
20	B	821	CLA	CMD-C2D-C3D	-2.81	121.16	127.61
20	A	801	CLA	CMD-C2D-C3D	-2.81	121.16	127.61
19	4	306	CHL	CMD-C2D-C3D	-2.81	121.16	127.61
20	B	849	CLA	CMD-C2D-C3D	-2.81	121.16	127.61
23	G	203	BCR	C10-C11-C12	2.81	131.98	123.22
20	A	846	CLA	C2A-C1A-CHA	-2.81	118.95	123.86
20	B	815	CLA	C2D-C1D-ND	2.81	112.17	110.10
20	B	802	CLA	C1D-CHD-C4C	-2.81	120.00	126.06
20	3	319	CLA	C3B-C4B-NB	2.80	113.12	110.52
20	A	846	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
20	A	807	CLA	O2A-CGA-CBA	2.80	120.70	111.91
20	A	850	CLA	C4-C3-C2	-2.80	116.49	123.68
20	B	809	CLA	C1D-CHD-C4C	-2.80	120.02	126.06
20	A	834	CLA	C1-C2-C3	-2.80	121.20	126.04
20	A	828	CLA	CAC-C3C-C4C	2.80	128.44	124.81
20	1	309	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
20	4	310	CLA	O2A-CGA-CBA	2.80	120.69	111.91
20	K	206	CLA	CHC-C4B-NB	-2.80	121.30	124.26
20	1	302	CLA	CAC-C3C-C4C	2.80	128.44	124.81
23	A	818	BCR	C15-C14-C13	2.80	131.30	127.31
20	B	806	CLA	C1D-CHD-C4C	-2.80	120.03	126.06
20	B	822	CLA	CHB-C1B-NB	-2.80	121.30	124.26
19	4	315	CHL	CMB-C2B-C1B	2.80	129.63	125.37
20	B	829	CLA	C2D-C1D-ND	2.80	112.16	110.10
20	A	847	CLA	C3B-C4B-NB	2.80	113.11	110.52
21	3	301	LUT	C35-C15-C14	2.79	129.20	123.47
20	B	845	CLA	C2D-C1D-ND	2.79	112.16	110.10
20	A	855	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
20	A	838	CLA	C1D-CHD-C4C	-2.79	120.03	126.06
19	4	305	CHL	CHB-C1B-NB	-2.79	121.30	124.26
23	J	101	BCR	C36-C18-C17	-2.79	119.01	122.92
20	3	307	CLA	C1D-CHD-C4C	-2.79	120.04	126.06
20	A	844	CLA	CAA-C2A-C1A	-2.79	102.83	111.97
23	O	203	BCR	C34-C9-C10	-2.79	119.02	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	811	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
20	A	804	CLA	CMD-C2D-C3D	-2.79	121.20	127.61
20	A	844	CLA	C1D-CHD-C4C	-2.79	120.04	126.06
23	B	834	BCR	C35-C13-C14	-2.79	119.02	122.92
19	2	318	CHL	CMD-C2D-C3D	-2.79	121.20	127.61
20	4	312	CLA	C2A-C1A-CHA	-2.79	118.99	123.86
20	B	822	CLA	C2A-C1A-CHA	-2.79	118.99	123.86
19	4	306	CHL	CHB-C1B-NB	-2.79	121.31	124.26
20	A	826	CLA	C4C-C3C-C2C	-2.79	102.84	106.90
20	2	319	CLA	C4C-C3C-C2C	-2.79	102.84	106.90
20	L	306	CLA	CAC-C3C-C4C	2.79	128.42	124.81
20	B	822	CLA	CMD-C2D-C3D	-2.79	121.21	127.61
20	A	854	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
20	1	305	CLA	CMD-C2D-C3D	-2.78	121.21	127.61
20	A	807	CLA	C1-O2A-CGA	2.78	123.75	116.44
20	B	853	CLA	CHB-C1B-NB	-2.78	121.31	124.26
23	J	101	BCR	C15-C14-C13	2.78	131.28	127.31
20	2	304	CLA	O2A-CGA-CBA	2.78	120.64	111.91
20	1	308	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
20	A	825	CLA	C1-O2A-CGA	2.78	123.74	116.44
20	A	839	CLA	CHB-C1B-NB	-2.78	121.31	124.26
19	2	302	CHL	CHB-C4A-NA	2.78	128.35	124.51
20	1	302	CLA	C1-C2-C3	-2.78	122.26	126.75
20	A	839	CLA	CMD-C2D-C3D	-2.78	121.23	127.61
20	B	848	CLA	CMD-C2D-C3D	-2.78	121.23	127.61
19	1	317	CHL	CHB-C4A-NA	2.78	128.35	124.51
20	A	850	CLA	CHB-C1B-NB	-2.78	121.32	124.26
20	1	322	CLA	CMD-C2D-C3D	-2.78	121.23	127.61
20	B	809	CLA	CMD-C2D-C3D	-2.78	121.23	127.61
20	L	306	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
22	1	311	XAT	C5-C4-C3	-2.77	107.26	112.75
20	B	803	CLA	C4-C3-C5	2.77	119.94	115.27
20	4	314	CLA	O2A-CGA-CBA	2.77	120.61	111.91
20	B	850	CLA	C1-C2-C3	-2.77	121.25	126.04
20	G	206	CLA	O2A-CGA-CBA	2.77	120.61	111.91
22	3	302	XAT	C31-C32-C33	2.77	134.21	126.42
20	A	805	CLA	CMD-C2D-C3D	-2.77	121.24	127.61
20	B	830	CLA	CMD-C2D-C3D	-2.77	121.24	127.61
20	B	828	CLA	CMD-C2D-C3D	-2.77	121.24	127.61
20	A	853	CLA	CHD-C1D-ND	-2.77	121.91	124.45
20	2	321	CLA	CHB-C1B-NB	-2.77	121.32	124.26
23	4	320	BCR	C37-C22-C23	2.77	122.44	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	820	CLA	C2A-C1A-CHA	-2.77	119.01	123.86
20	B	805	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
20	2	307	CLA	C2A-C1A-CHA	-2.77	119.02	123.86
20	B	850	CLA	CHD-C1D-ND	-2.77	121.91	124.45
20	A	829	CLA	C4A-NA-C1A	2.77	107.95	106.71
20	A	826	CLA	C4-C3-C5	2.77	119.93	115.27
20	4	308	CLA	CHD-C1D-ND	-2.77	121.91	124.45
20	A	828	CLA	C2D-C1D-ND	2.77	112.14	110.10
20	B	801	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
20	4	309	CLA	CAC-C3C-C4C	2.77	128.40	124.81
19	4	306	CHL	CHB-C4A-NA	2.77	128.34	124.51
19	4	315	CHL	CHB-C4A-NA	2.77	128.34	124.51
20	B	814	CLA	CHC-C4B-NB	-2.77	121.33	124.26
20	4	311	CLA	CMD-C2D-C3D	-2.76	121.25	127.61
20	A	805	CLA	CAC-C3C-C4C	2.76	128.40	124.81
19	1	317	CHL	O2A-CGA-CBA	2.76	120.58	111.91
20	3	320	CLA	CMC-C2C-C1C	2.76	129.25	125.04
23	A	857	BCR	C15-C16-C17	2.76	129.13	123.47
20	O	206	CLA	O2A-CGA-CBA	2.76	120.58	111.91
23	4	319	BCR	C15-C16-C17	2.76	129.13	123.47
20	1	321	CLA	C2D-C1D-ND	2.76	112.14	110.10
20	A	855	CLA	CAC-C3C-C4C	2.76	128.39	124.81
20	3	310	CLA	C1D-CHD-C4C	-2.76	120.10	126.06
23	2	312	BCR	C34-C9-C8	2.76	122.42	118.08
22	4	318	XAT	C4-C3-C2	-2.76	105.44	110.77
20	B	823	CLA	C1D-CHD-C4C	-2.76	120.11	126.06
19	2	322	CHL	CHB-C4A-NA	2.76	128.33	124.51
23	2	312	BCR	C34-C9-C10	-2.76	119.06	122.92
23	B	836	BCR	C36-C18-C17	-2.76	119.06	122.92
20	B	801	CLA	O2A-CGA-CBA	2.76	120.56	111.91
23	B	834	BCR	C16-C15-C14	2.76	129.12	123.47
20	B	817	CLA	CMD-C2D-C3D	-2.76	121.27	127.61
20	G	206	CLA	CMB-C2B-C1B	2.76	129.57	125.37
20	B	804	CLA	C1D-CHD-C4C	-2.76	120.11	126.06
20	O	206	CLA	CHB-C1B-NB	-2.76	121.34	124.26
23	4	320	BCR	C16-C15-C14	2.75	129.12	123.47
20	B	850	CLA	C3B-C4B-NB	2.75	113.07	110.52
23	L	302	BCR	C16-C15-C14	2.75	129.11	123.47
20	B	830	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
20	A	832	CLA	C3B-C4B-NB	2.75	113.07	110.52
20	B	826	CLA	C3B-C4B-NB	2.75	113.07	110.52
20	B	827	CLA	CMD-C2D-C3D	-2.75	121.28	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	K	206	CLA	CHB-C1B-NB	-2.75	121.34	124.26
20	1	309	CLA	CAC-C3C-C4C	2.75	128.38	124.81
20	2	306	CLA	CMD-C2D-C3D	-2.75	121.28	127.61
20	B	831	CLA	CMD-C2D-C3D	-2.75	121.28	127.61
20	B	833	CLA	C1-C2-C3	-2.75	121.28	126.04
23	O	202	BCR	C8-C9-C10	2.75	123.16	118.94
19	2	309	CHL	CHB-C4A-NA	2.75	128.31	124.51
20	3	311	CLA	O2A-CGA-CBA	2.75	120.53	111.91
19	2	302	CHL	CMD-C2D-C3D	-2.75	121.29	127.61
20	A	837	CLA	CMD-C2D-C3D	-2.75	121.29	127.61
20	A	828	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
23	G	203	BCR	C19-C18-C17	2.75	123.16	118.94
20	B	809	CLA	O2A-CGA-CBA	2.75	120.52	111.91
23	F	301	BCR	C19-C18-C17	2.75	123.15	118.94
20	4	304	CLA	C1D-CHD-C4C	-2.75	120.14	126.06
20	A	849	CLA	O2A-CGA-CBA	2.74	120.52	111.91
20	A	835	CLA	CAC-C3C-C4C	2.74	128.37	124.81
20	A	853	CLA	C4-C3-C5	2.74	119.89	115.27
20	A	802	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
23	B	835	BCR	C16-C15-C14	2.74	129.09	123.47
20	A	850	CLA	C4-C3-C5	2.74	119.89	115.27
20	1	318	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
20	B	844	CLA	CMB-C2B-C1B	2.74	129.54	125.37
23	3	303	BCR	C34-C9-C10	-2.74	119.08	122.92
20	B	822	CLA	C4D-CHA-C1A	-2.74	117.91	121.25
20	1	320	CLA	O2A-CGA-CBA	2.74	120.51	111.91
20	A	843	CLA	CMD-C2D-C3D	-2.74	121.31	127.61
20	A	808	CLA	O2A-CGA-O1A	-2.74	116.68	123.59
20	A	855	CLA	CMD-C2D-C3D	-2.74	121.31	127.61
20	B	829	CLA	C4-C3-C5	2.74	119.88	115.27
22	4	318	XAT	C15-C14-C13	-2.74	123.40	127.31
20	2	303	CLA	CAA-C2A-C3A	2.74	120.27	112.78
20	B	833	CLA	C3B-C4B-NB	2.74	113.05	110.52
20	B	851	CLA	C2D-C1D-ND	2.74	112.12	110.10
20	L	306	CLA	CHB-C1B-NB	-2.74	121.36	124.26
20	A	808	CLA	O2A-CGA-CBA	2.74	120.49	111.91
20	2	319	CLA	CMB-C2B-C3B	2.74	133.21	126.59
20	A	826	CLA	C1D-CHD-C4C	-2.74	120.16	126.06
20	A	845	CLA	C1D-CHD-C4C	-2.74	120.16	126.06
20	B	805	CLA	CHB-C1B-NB	-2.73	121.36	124.26
23	B	836	BCR	C24-C23-C22	2.73	130.37	126.23
20	1	306	CLA	CMD-C2D-C3D	-2.73	121.33	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	G	205	CLA	CMD-C2D-C3D	-2.73	121.33	127.61
20	4	308	CLA	CHB-C1B-NB	-2.73	121.36	124.26
20	B	851	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
21	4	317	LUT	C20-C13-C14	-2.73	119.10	122.92
28	A	824	CL0	CMB-C2B-C1B	2.73	129.53	125.37
19	1	317	CHL	OMC-CMC-C2C	-2.73	119.52	125.69
28	A	824	CL0	CAC-C3C-C4C	2.73	128.35	124.81
20	B	846	CLA	CHB-C1B-NB	-2.73	121.37	124.26
20	B	831	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
20	F	305	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
20	A	830	CLA	CHC-C4B-NB	-2.73	121.37	124.26
20	4	302	CLA	C2A-C1A-CHA	-2.73	119.09	123.86
20	G	205	CLA	CAC-C3C-C4C	2.73	128.35	124.81
20	3	320	CLA	C2A-C1A-CHA	-2.73	119.09	123.86
23	O	202	BCR	C12-C13-C14	2.73	123.12	118.94
20	A	856	CLA	C2A-C1A-CHA	-2.73	119.09	123.86
20	B	852	CLA	CMD-C2D-C3D	-2.72	121.35	127.61
20	N	202	CLA	CMD-C2D-C3D	-2.72	121.35	127.61
20	A	811	CLA	C4-C3-C5	2.72	119.85	115.27
21	4	317	LUT	C35-C15-C14	2.72	129.05	123.47
20	B	808	CLA	CMD-C2D-C3D	-2.72	121.35	127.61
20	B	812	CLA	CHC-C4B-NB	-2.72	121.37	124.26
20	1	320	CLA	C2A-C1A-CHA	-2.72	119.10	123.86
20	1	319	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
20	3	308	CLA	CMD-C2D-C3D	-2.72	121.36	127.61
23	B	835	BCR	C1-C6-C5	-2.72	118.78	122.61
20	A	838	CLA	CMD-C2D-C3D	-2.72	121.36	127.61
22	4	318	XAT	C24-C23-C22	-2.72	105.52	110.77
20	B	818	CLA	O2A-CGA-CBA	2.72	120.44	111.91
20	B	805	CLA	C2A-C1A-CHA	-2.72	119.11	123.86
20	A	809	CLA	C3B-C4B-NB	2.72	113.04	110.52
20	1	307	CLA	CAA-C2A-C3A	-2.72	105.34	112.78
20	3	310	CLA	CMC-C2C-C1C	2.72	129.18	125.04
23	G	203	BCR	C15-C14-C13	2.72	131.19	127.31
20	1	319	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
20	A	839	CLA	CMB-C2B-C3B	2.72	133.17	126.59
20	B	817	CLA	CMB-C2B-C3B	2.72	133.17	126.59
23	2	312	BCR	C12-C13-C14	2.72	123.11	118.94
20	A	851	CLA	CHB-C1B-NB	-2.72	121.38	124.26
20	J	103	CLA	C3B-C4B-NB	2.72	113.03	110.52
20	4	310	CLA	CMD-C2D-C3D	-2.71	121.37	127.61
20	A	811	CLA	CMD-C2D-C3D	-2.71	121.37	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	307	CLA	CHB-C1B-NB	-2.71	121.38	124.26
23	K	202	BCR	C15-C14-C13	2.71	131.18	127.31
20	A	839	CLA	C1D-CHD-C4C	-2.71	120.20	126.06
20	A	849	CLA	CHB-C1B-NB	-2.71	121.39	124.26
20	B	845	CLA	CMB-C2B-C3B	2.71	133.15	126.59
20	B	853	CLA	C1D-CHD-C4C	-2.71	120.21	126.06
20	1	302	CLA	C2A-C1A-CHA	-2.71	119.12	123.86
20	A	841	CLA	C1D-CHD-C4C	-2.71	120.21	126.06
23	3	303	BCR	C36-C18-C17	-2.71	119.13	122.92
20	H	201	CLA	O2A-CGA-CBA	2.71	120.41	111.91
20	A	807	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
20	B	801	CLA	CMD-C2D-C3D	-2.71	121.39	127.61
20	B	827	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
23	B	837	BCR	C20-C21-C22	2.71	131.17	127.31
20	2	321	CLA	C2D-C1D-ND	2.71	112.10	110.10
20	2	308	CLA	C2A-C1A-CHA	-2.71	119.13	123.86
20	F	306	CLA	CMD-C2D-C3D	-2.71	121.39	127.61
20	A	812	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
20	A	834	CLA	O2A-CGA-CBA	2.71	120.40	111.91
20	B	818	CLA	C2A-C1A-CHA	-2.71	119.13	123.86
23	A	817	BCR	C34-C9-C8	2.70	122.34	118.08
20	B	802	CLA	C3B-C4B-NB	2.70	113.02	110.52
20	1	302	CLA	CMD-C2D-C3D	-2.70	121.39	127.61
20	L	305	CLA	C2A-C1A-CHA	-2.70	119.13	123.86
20	A	855	CLA	C2D-C1D-ND	2.70	112.10	110.10
20	1	320	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
23	G	203	BCR	C12-C13-C14	2.70	123.08	118.94
20	2	305	CLA	O2A-CGA-CBA	2.70	120.38	111.91
20	B	808	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
19	4	305	CHL	O2D-CGD-O1D	-2.70	118.56	123.84
20	L	307	CLA	C2A-C1A-CHA	-2.70	119.14	123.86
20	G	205	CLA	C2A-C1A-CHA	-2.70	119.14	123.86
20	A	835	CLA	CMD-C2D-C3D	-2.70	121.41	127.61
23	4	320	BCR	C30-C25-C26	-2.70	118.82	122.61
19	2	322	CHL	OMC-CMC-C2C	-2.70	119.59	125.69
20	A	806	CLA	O2A-CGA-CBA	2.70	120.37	111.91
20	A	844	CLA	CHB-C1B-NB	-2.69	121.40	124.26
23	L	304	BCR	C20-C21-C22	2.69	131.16	127.31
20	A	840	CLA	C3B-C4B-NB	2.69	113.02	110.52
20	O	206	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
20	3	310	CLA	O2A-CGA-CBA	2.69	120.36	111.91
20	B	846	CLA	C2D-C1D-ND	2.69	112.09	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	838	CLA	CHB-C1B-NB	-2.69	121.41	124.26
19	4	306	CHL	O2D-CGD-O1D	-2.69	118.58	123.84
20	A	828	CLA	C4C-C3C-C2C	-2.69	102.97	106.90
20	3	308	CLA	C4-C3-C5	2.69	119.80	115.27
20	B	851	CLA	CHB-C1B-NB	-2.69	121.41	124.26
20	B	815	CLA	CMC-C2C-C1C	2.69	129.14	125.04
20	A	806	CLA	C2D-C1D-ND	2.69	112.08	110.10
20	A	848	CLA	O2A-CGA-CBA	2.69	120.34	111.91
20	B	813	CLA	O2A-CGA-CBA	2.69	120.34	111.91
20	B	828	CLA	CAC-C3C-C4C	2.69	128.29	124.81
21	3	301	LUT	C20-C13-C14	-2.68	119.16	122.92
20	A	855	CLA	O2A-CGA-CBA	2.68	120.33	111.91
23	B	836	BCR	C11-C10-C9	2.68	131.14	127.31
19	4	307	CHL	CHB-C4A-NA	2.68	128.22	124.51
20	3	314	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
19	3	313	CHL	CMD-C2D-C3D	-2.68	121.45	127.61
23	L	304	BCR	C12-C13-C14	2.68	123.05	118.94
20	4	310	CLA	C3B-C4B-NB	2.68	113.00	110.52
20	B	822	CLA	C4-C3-C5	2.68	119.78	115.27
20	B	819	CLA	C1D-CHD-C4C	-2.68	120.28	126.06
23	G	203	BCR	C20-C21-C22	2.67	131.13	127.31
20	1	304	CLA	CMD-C2D-C3D	-2.67	121.47	127.61
20	L	305	CLA	CHC-C4B-NB	-2.67	121.43	124.26
20	2	303	CLA	C2A-C1A-CHA	-2.67	119.19	123.86
20	H	201	CLA	CMD-C2D-C3D	-2.67	121.47	127.61
19	2	302	CHL	CHB-C1B-NB	-2.67	121.43	124.26
20	1	322	CLA	C2A-C1A-CHA	-2.67	119.19	123.86
20	B	826	CLA	C2A-C1A-CHA	-2.67	119.19	123.86
20	A	802	CLA	CMC-C2C-C1C	2.67	129.10	125.04
20	B	817	CLA	CHC-C4B-NB	-2.67	121.43	124.26
20	A	832	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
20	B	830	CLA	C1D-CHD-C4C	-2.67	120.30	126.06
20	3	314	CLA	CMD-C2D-C3D	-2.67	121.48	127.61
20	4	313	CLA	C1D-CHD-C4C	-2.67	120.31	126.06
20	3	320	CLA	C2D-C1D-ND	2.67	112.07	110.10
20	3	312	CLA	CMD-C2D-C3D	-2.66	121.49	127.61
29	J	104	DGD	O1G-C1A-C2A	2.66	120.26	111.91
20	B	825	CLA	C2A-C1A-CHA	-2.66	119.20	123.86
20	4	312	CLA	C3B-C4B-NB	2.66	112.98	110.52
20	4	304	CLA	CHB-C1B-NB	-2.66	121.44	124.26
20	B	844	CLA	CHD-C1D-ND	-2.66	122.01	124.45
20	B	814	CLA	CMA-C3A-C4A	2.66	118.93	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	849	CLA	C2A-C1A-CHA	-2.66	119.21	123.86
23	A	857	BCR	C36-C18-C17	-2.66	119.20	122.92
20	B	851	CLA	C4C-C3C-C2C	-2.66	103.02	106.90
20	2	304	CLA	CHB-C1B-NB	-2.66	121.44	124.26
19	3	313	CHL	O2A-CGA-CBA	2.66	120.24	111.91
20	B	846	CLA	C4C-C3C-C2C	-2.65	103.03	106.90
20	G	205	CLA	C4C-C3C-C2C	-2.65	103.03	106.90
20	B	824	CLA	C1-O2A-CGA	2.65	123.41	116.44
23	K	202	BCR	C11-C10-C9	2.65	131.10	127.31
19	2	309	CHL	C3B-C4B-NB	2.65	112.98	110.52
20	B	808	CLA	CAA-C2A-C3A	2.65	120.04	112.78
20	A	841	CLA	C7-C6-C5	-2.65	108.72	114.49
20	B	805	CLA	CMD-C2D-C3D	-2.65	121.51	127.61
23	L	303	BCR	C15-C14-C13	2.65	131.10	127.31
20	B	847	CLA	C4-C3-C5	2.65	119.73	115.27
23	B	838	BCR	C34-C9-C8	2.65	122.25	118.08
20	4	309	CLA	C2A-C1A-CHA	-2.65	119.22	123.86
20	A	852	CLA	O2A-CGA-CBA	2.65	120.22	111.91
20	A	852	CLA	C2A-C1A-CHA	-2.65	119.23	123.86
20	A	829	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
20	A	802	CLA	CMD-C2D-C3D	-2.65	121.52	127.61
20	O	206	CLA	C2A-C1A-CHA	-2.65	119.23	123.86
20	4	311	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
20	K	205	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
23	A	814	BCR	C11-C10-C9	2.64	131.08	127.31
20	O	208	CLA	CHC-C4B-NB	-2.64	121.46	124.26
20	B	813	CLA	CAC-C3C-C4C	2.64	128.24	124.81
20	A	854	CLA	CAA-CBA-CGA	-2.64	105.53	113.25
20	B	825	CLA	C2D-C1D-ND	2.64	112.05	110.10
20	G	207	CLA	CHB-C1B-NB	-2.64	121.46	124.26
20	A	803	CLA	C2A-C1A-CHA	-2.64	119.24	123.86
19	2	301	CHL	CMD-C2D-C3D	-2.64	121.53	127.61
22	1	311	XAT	C35-C34-C33	-2.64	123.54	127.31
23	O	202	BCR	C36-C18-C17	-2.64	119.22	122.92
28	A	824	CL0	CMC-C2C-C1C	2.64	129.06	125.04
20	A	844	CLA	C2A-C1A-CHA	-2.64	119.24	123.86
20	A	832	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
20	A	849	CLA	CMD-C2D-C3D	-2.64	121.54	127.61
20	B	801	CLA	CED-O2D-CGD	2.64	121.90	115.94
23	G	201	BCR	C1-C6-C5	-2.64	118.90	122.61
20	B	822	CLA	C1D-CHD-C4C	-2.64	120.37	126.06
23	B	837	BCR	C24-C23-C22	2.64	130.22	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	847	CLA	O2A-CGA-CBA	2.64	120.18	111.91
23	A	816	BCR	C11-C10-C9	2.64	131.07	127.31
20	A	842	CLA	C2A-C1A-CHA	-2.64	119.25	123.86
20	B	816	CLA	CMD-C2D-C3D	-2.64	121.55	127.61
20	3	315	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
20	B	820	CLA	CMB-C2B-C1B	2.63	129.38	125.37
20	3	311	CLA	C4A-NA-C1A	2.63	107.89	106.71
20	3	315	CLA	CHB-C1B-NB	-2.63	121.47	124.26
20	3	312	CLA	C2A-C1A-CHA	-2.63	119.25	123.86
23	3	303	BCR	C15-C14-C13	2.63	131.07	127.31
19	4	305	CHL	CHB-C4A-NA	2.63	128.15	124.51
20	B	821	CLA	C1-C2-C3	-2.63	121.49	126.04
21	1	323	LUT	C15-C35-C34	2.63	128.86	123.47
20	B	810	CLA	C3B-C4B-NB	2.63	112.95	110.52
20	A	847	CLA	C1D-CHD-C4C	-2.63	120.39	126.06
20	A	856	CLA	O2A-CGA-CBA	2.63	120.16	111.91
20	B	816	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
19	2	322	CHL	CMD-C2D-C3D	-2.63	121.57	127.61
20	K	206	CLA	C2A-C1A-CHA	-2.63	119.27	123.86
20	B	831	CLA	O1D-CGD-CBD	-2.63	119.11	124.48
20	A	828	CLA	O2A-CGA-CBA	2.63	120.15	111.91
19	2	318	CHL	OMC-CMC-C2C	-2.63	119.75	125.69
20	A	811	CLA	O2A-CGA-CBA	2.63	120.15	111.91
19	4	305	CHL	CMD-C2D-C3D	-2.63	121.58	127.61
20	B	809	CLA	C2A-C1A-CHA	-2.62	119.27	123.86
20	A	831	CLA	C1-C2-C3	-2.62	121.51	126.04
20	B	850	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
20	B	819	CLA	O2A-CGA-CBA	2.62	120.14	111.91
20	4	308	CLA	CAA-C2A-C3A	2.62	119.95	112.78
20	3	308	CLA	CHC-C4B-NB	-2.62	121.48	124.26
20	3	315	CLA	CMB-C2B-C3B	2.62	132.93	126.59
20	A	844	CLA	CMD-C2D-C3D	-2.62	121.59	127.61
20	1	304	CLA	CHC-C4B-NB	-2.62	121.48	124.26
20	B	804	CLA	CHB-C1B-NB	-2.62	121.48	124.26
20	A	851	CLA	CMB-C2B-C3B	2.62	132.93	126.59
20	A	851	CLA	C3B-C4B-NB	2.62	112.94	110.52
24	A	820	LHG	O7-C7-O9	-2.62	117.38	123.70
20	A	827	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
20	A	832	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
20	A	844	CLA	CMB-C2B-C3B	2.62	132.93	126.59
20	A	832	CLA	CMD-C2D-C3D	-2.62	121.60	127.61
20	A	827	CLA	C1-O2A-CGA	2.62	123.31	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	855	CLA	C1-C2-C3	-2.61	121.52	126.04
20	1	318	CLA	C1D-CHD-C4C	-2.61	120.42	126.06
20	G	207	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
20	2	317	CLA	C3B-C4B-NB	2.61	112.94	110.52
23	L	304	BCR	C1-C6-C7	2.61	123.17	115.78
20	B	812	CLA	CHB-C1B-NB	-2.61	121.49	124.26
19	4	307	CHL	CMD-C2D-C3D	-2.61	121.61	127.61
20	A	843	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
20	A	802	CLA	C2A-C1A-CHA	-2.61	119.29	123.86
20	B	831	CLA	C2A-C1A-CHA	-2.61	119.29	123.86
20	K	203	CLA	O2A-CGA-CBA	2.61	120.10	111.91
20	G	206	CLA	C2A-C1A-CHA	-2.61	119.30	123.86
20	L	305	CLA	CMC-C2C-C1C	2.61	129.01	125.04
23	1	312	BCR	C36-C18-C17	-2.61	119.27	122.92
20	A	811	CLA	C2A-C1A-CHA	-2.61	119.30	123.86
20	A	807	CLA	C2A-C1A-CHA	-2.61	119.30	123.86
20	B	815	CLA	CHC-C4B-NB	-2.61	121.50	124.26
20	3	310	CLA	C2A-C1A-CHA	-2.61	119.30	123.86
20	B	825	CLA	CMD-C2D-C3D	-2.61	121.62	127.61
20	2	317	CLA	C2A-C1A-CHA	-2.61	119.30	123.86
20	A	830	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
20	A	835	CLA	C1D-CHD-C4C	-2.60	120.44	126.06
19	4	315	CHL	CMD-C2D-C3D	-2.60	121.62	127.61
20	O	206	CLA	CHC-C4B-NB	-2.60	121.50	124.26
23	A	817	BCR	C36-C18-C17	-2.60	119.28	122.92
20	A	828	CLA	C1D-CHD-C4C	-2.60	120.44	126.06
20	B	816	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
20	B	849	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
20	A	830	CLA	CMB-C2B-C3B	2.60	132.88	126.59
20	K	203	CLA	CHC-C4B-NB	-2.60	121.51	124.26
20	3	315	CLA	C2A-C1A-CHA	-2.60	119.32	123.86
20	A	808	CLA	CED-O2D-CGD	2.60	121.81	115.94
20	A	830	CLA	CMD-C2D-C3D	-2.60	121.64	127.61
20	A	831	CLA	C2A-C1A-CHA	-2.60	119.32	123.86
20	1	302	CLA	O2A-CGA-CBA	2.59	120.05	111.91
20	B	810	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
20	A	809	CLA	C4A-NA-C1A	2.59	107.87	106.71
20	2	319	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
20	1	319	CLA	C2A-C1A-CHA	-2.59	119.33	123.86
20	B	823	CLA	C2D-C1D-ND	2.59	112.01	110.10
20	3	316	CLA	C4A-NA-C1A	2.59	107.87	106.71
20	A	802	CLA	CMB-C2B-C1B	2.59	129.31	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	811	CLA	C1-C2-C3	-2.59	121.56	126.04
20	N	202	CLA	C3B-C4B-NB	2.59	112.92	110.52
20	A	843	CLA	CMC-C2C-C1C	2.59	128.98	125.04
20	A	833	CLA	CHC-C4B-NB	-2.59	121.52	124.26
20	B	827	CLA	C4-C3-C5	2.59	119.63	115.27
20	A	806	CLA	CMB-C2B-C1B	2.59	129.31	125.37
20	4	310	CLA	C4-C3-C5	2.59	119.62	115.27
20	2	319	CLA	CAA-C2A-C3A	2.59	119.86	112.78
20	B	809	CLA	CHB-C1B-C2B	-2.59	119.94	127.24
20	3	316	CLA	CMD-C2D-C3D	-2.59	121.67	127.61
20	3	314	CLA	CAC-C3C-C4C	2.58	128.16	124.81
20	B	811	CLA	C3B-C4B-NB	2.58	112.91	110.52
23	L	301	BCR	C15-C16-C17	2.58	128.76	123.47
20	A	837	CLA	C1-O2A-CGA	2.58	123.22	116.44
20	G	206	CLA	CAA-C2A-C3A	2.58	119.85	112.78
20	B	825	CLA	CMB-C2B-C1B	2.58	129.30	125.37
20	G	206	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
20	1	309	CLA	C2A-C1A-CHA	-2.58	119.35	123.85
20	3	319	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
20	A	804	CLA	C4C-C3C-C2C	-2.58	103.14	106.90
20	B	846	CLA	C1D-CHD-C4C	-2.58	120.50	126.06
20	4	312	CLA	C4A-NA-C1A	2.58	107.86	106.71
20	A	834	CLA	CHB-C1B-NB	-2.58	121.53	124.26
20	A	806	CLA	C3B-C4B-NB	2.58	112.91	110.52
20	4	309	CLA	CMD-C2D-C3D	-2.57	121.69	127.61
20	A	826	CLA	C2A-C1A-CHA	-2.57	119.36	123.86
20	B	853	CLA	C2A-C1A-CHA	-2.57	119.36	123.86
20	A	837	CLA	CMB-C2B-C1B	2.57	129.29	125.37
20	B	822	CLA	C2D-C1D-ND	2.57	112.00	110.10
19	2	318	CHL	C4-C3-C5	2.57	119.60	115.27
20	B	833	CLA	O2A-CGA-CBA	2.57	119.98	111.91
23	4	319	BCR	C15-C14-C13	2.57	130.98	127.31
20	2	305	CLA	C3B-C4B-NB	2.57	112.90	110.52
20	A	805	CLA	O2A-CGA-CBA	2.57	119.98	111.91
20	A	845	CLA	C1-O2A-CGA	2.57	123.18	116.44
20	B	819	CLA	C1-O2A-CGA	2.57	123.18	116.44
23	B	835	BCR	C15-C14-C13	2.57	130.97	127.31
20	B	823	CLA	CHB-C1B-NB	-2.56	121.54	124.26
23	O	203	BCR	C11-C12-C13	2.56	133.62	126.42
23	J	101	BCR	C1-C6-C7	2.56	123.03	115.78
20	2	307	CLA	CMB-C2B-C3B	2.56	132.79	126.59
20	1	309	CLA	C3B-C4B-NB	2.56	112.89	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	851	CLA	CMD-C2D-C3D	-2.56	121.73	127.61
20	B	813	CLA	C2A-C1A-CHA	-2.56	119.39	123.86
23	G	201	BCR	C35-C13-C14	-2.56	119.34	122.92
19	1	317	CHL	C5-C3-C4	2.56	120.25	114.60
20	B	816	CLA	C4-C3-C2	-2.56	117.12	123.68
20	B	852	CLA	C2A-C1A-CHA	-2.56	119.39	123.86
20	A	839	CLA	CAA-C2A-C3A	2.55	119.77	112.78
23	L	303	BCR	C34-C9-C10	-2.55	119.34	122.92
20	3	311	CLA	C2D-C1D-ND	2.55	111.99	110.10
20	1	318	CLA	CHC-C4B-NB	-2.55	121.55	124.26
20	B	802	CLA	O2A-CGA-CBA	2.55	122.23	114.03
20	N	202	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
19	2	301	CHL	OMC-CMC-C2C	-2.55	119.92	125.69
20	A	852	CLA	CMD-C2D-C3D	-2.55	121.75	127.61
20	A	831	CLA	CMB-C2B-C1B	2.55	129.25	125.37
20	A	848	CLA	CMD-C2D-C3D	-2.55	121.75	127.61
23	2	312	BCR	C33-C5-C6	2.55	127.39	124.53
20	1	318	CLA	CHB-C1B-NB	-2.55	121.56	124.26
21	1	310	LUT	C20-C13-C14	-2.55	119.36	122.92
21	1	310	LUT	C35-C15-C14	2.55	128.69	123.47
20	B	816	CLA	C1-C2-C3	-2.55	121.64	126.04
20	A	845	CLA	CED-O2D-CGD	2.54	121.69	115.94
20	F	304	CLA	CMD-C2D-C3D	-2.54	121.76	127.61
20	B	816	CLA	O2A-CGA-CBA	2.54	119.89	111.91
20	A	855	CLA	C4-C3-C5	2.54	119.55	115.27
20	A	835	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
20	A	812	CLA	O2A-CGA-CBA	2.54	119.89	111.91
22	4	318	XAT	C35-C15-C14	-2.54	118.27	123.47
21	3	301	LUT	C11-C10-C9	2.54	130.94	127.31
20	A	802	CLA	CHB-C1B-NB	-2.54	121.57	124.26
20	B	849	CLA	O2A-CGA-CBA	2.54	119.88	111.91
20	2	319	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
19	1	317	CHL	CMD-C2D-C3D	-2.54	121.77	127.61
20	A	831	CLA	O2A-CGA-O1A	-2.54	117.18	123.59
20	B	815	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
20	A	836	CLA	O2A-CGA-CBA	2.54	119.88	111.91
20	3	308	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
23	J	101	BCR	C1-C6-C5	-2.54	119.04	122.61
20	L	305	CLA	C1D-CHD-C4C	-2.54	120.58	126.06
20	A	832	CLA	C2D-C1D-ND	2.54	111.97	110.10
20	B	813	CLA	CMD-C2D-C3D	-2.54	121.77	127.61
20	B	850	CLA	CMB-C2B-C1B	2.54	129.23	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	828	CLA	CMB-C2B-C1B	2.54	129.23	125.37
20	3	317	CLA	C3B-C4B-NB	2.54	112.87	110.52
28	A	824	CL0	CHC-C4B-NB	-2.54	121.57	124.26
20	A	829	CLA	O2A-CGA-CBA	2.53	119.86	111.91
20	B	819	CLA	CHB-C4A-NA	2.53	128.01	124.51
20	4	302	CLA	CMD-C2D-C3D	-2.53	121.79	127.61
20	4	303	CLA	C2A-C1A-CHA	-2.53	119.43	123.86
20	A	835	CLA	O2A-CGA-CBA	2.53	119.85	111.91
20	2	307	CLA	CHC-C4B-NB	-2.53	121.58	124.26
20	H	201	CLA	C1-C2-C3	-2.53	121.67	126.04
20	1	305	CLA	C2A-C1A-CHA	-2.53	119.43	123.86
20	B	819	CLA	CMC-C2C-C1C	2.53	128.89	125.04
20	A	852	CLA	C1D-CHD-C4C	-2.53	120.60	126.06
20	4	310	CLA	C1-C2-C3	-2.53	121.67	126.04
20	B	853	CLA	C4-C3-C5	2.53	119.52	115.27
20	A	831	CLA	C6-C5-C3	-2.53	110.49	114.62
20	3	320	CLA	CHC-C4B-NB	-2.53	121.58	124.26
20	1	306	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
23	F	301	BCR	C34-C9-C10	-2.52	119.39	122.92
20	A	852	CLA	C4C-C3C-C2C	-2.52	103.22	106.90
23	J	101	BCR	C15-C16-C17	2.52	128.64	123.47
20	B	812	CLA	CMD-C2D-C3D	-2.52	121.81	127.61
20	1	303	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
23	K	201	BCR	C11-C10-C9	2.52	130.91	127.31
23	B	838	BCR	C29-C30-C25	2.52	114.36	110.48
20	4	302	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
20	2	308	CLA	O2A-CGA-CBA	2.52	119.81	111.91
20	A	802	CLA	C1D-CHD-C4C	-2.52	120.63	126.06
20	A	808	CLA	C2A-C1A-CHA	-2.52	119.46	123.86
20	F	305	CLA	C2A-C1A-CHA	-2.51	119.46	123.86
20	A	802	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
20	B	852	CLA	C3B-C4B-NB	2.51	112.85	110.52
22	1	311	XAT	C8-C9-C10	2.51	122.80	118.94
20	B	820	CLA	CMD-C2D-C3D	-2.51	121.83	127.61
20	A	826	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
20	A	843	CLA	C1D-CHD-C4C	-2.51	120.64	126.06
20	A	828	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
20	B	828	CLA	O2A-CGA-CBA	2.51	119.78	111.91
20	A	808	CLA	C2D-C1D-ND	2.51	111.95	110.10
20	A	802	CLA	C4A-NA-C1A	-2.51	105.58	106.71
20	O	207	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
20	1	307	CLA	C1-C2-C3	-2.51	121.70	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	319	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
23	4	320	BCR	C1-C6-C5	-2.51	119.08	122.61
20	A	854	CLA	CHB-C4A-NA	2.51	127.98	124.51
20	K	204	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
20	B	817	CLA	O2A-CGA-CBA	2.51	119.77	111.91
20	K	203	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
20	A	829	CLA	C4C-C3C-C2C	-2.50	103.25	106.90
20	3	315	CLA	CHC-C4B-NB	-2.50	121.61	124.26
20	A	833	CLA	CHB-C1B-NB	-2.50	121.61	124.26
23	L	304	BCR	C10-C11-C12	2.50	131.02	123.22
20	4	314	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
20	A	833	CLA	CMD-C2D-C3D	-2.50	121.86	127.61
20	B	833	CLA	C4-C3-C5	2.50	119.48	115.27
20	J	103	CLA	C2A-C1A-CHA	-2.50	119.49	123.86
23	K	201	BCR	C35-C13-C14	-2.50	119.42	122.92
20	1	319	CLA	C2D-C1D-ND	2.50	111.94	110.10
23	L	302	BCR	C15-C14-C13	2.50	130.88	127.31
20	B	852	CLA	C4-C3-C2	-2.50	117.27	123.68
23	I	102	BCR	C34-C9-C10	-2.50	119.43	122.92
20	2	308	CLA	C3B-C4B-NB	2.50	112.83	110.52
23	A	816	BCR	C34-C9-C10	-2.49	119.43	122.92
20	N	202	CLA	O2A-CGA-CBA	2.49	119.73	111.91
20	A	848	CLA	C3B-C4B-NB	2.49	112.83	110.52
20	2	319	CLA	CHC-C4B-NB	-2.49	121.62	124.26
20	B	823	CLA	O1D-CGD-CBD	-2.49	119.39	124.48
20	A	847	CLA	O2A-CGA-CBA	2.49	119.72	111.91
20	A	803	CLA	C3B-C4B-NB	2.49	112.82	110.52
20	3	311	CLA	C1-C2-C3	-2.49	121.74	126.04
20	A	842	CLA	C4-C3-C5	2.49	119.46	115.27
20	H	201	CLA	C3B-C4B-NB	2.49	112.82	110.52
20	B	801	CLA	C2D-C1D-ND	2.49	111.94	110.10
20	A	855	CLA	CMB-C2B-C1B	2.49	129.16	125.37
19	2	309	CHL	O2D-CGD-O1D	-2.49	118.98	123.84
20	O	207	CLA	CMB-C2B-C1B	2.48	129.15	125.37
20	1	307	CLA	C3B-C4B-NB	2.48	112.82	110.52
20	A	808	CLA	CMD-C2D-C3D	-2.48	121.91	127.61
20	A	845	CLA	CMD-C2D-C3D	-2.48	121.91	127.61
19	4	307	CHL	CHB-C1B-NB	-2.48	121.64	124.26
23	B	837	BCR	C34-C9-C10	-2.48	119.46	122.92
20	B	806	CLA	C3B-C4B-NB	2.47	112.81	110.52
20	4	304	CLA	CHC-C4B-NB	-2.47	121.64	124.26
20	2	323	CLA	CHB-C1B-C2B	-2.47	120.25	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	851	CLA	C4-C3-C5	2.47	119.43	115.27
23	O	202	BCR	C21-C20-C19	2.47	130.93	123.22
20	B	811	CLA	O2A-CGA-CBA	2.47	119.66	111.91
20	4	304	CLA	C2D-C1D-ND	2.47	111.92	110.10
20	A	806	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
28	A	824	CL0	CMD-C2D-C3D	-2.47	121.94	127.61
20	B	845	CLA	C1-C2-C3	-2.47	121.78	126.04
20	B	808	CLA	C2A-C1A-CHA	-2.47	119.55	123.86
20	B	819	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
20	B	844	CLA	O2A-CGA-O1A	-2.46	117.37	123.59
19	2	318	CHL	C1C-C2C-C3C	-2.46	105.16	107.11
21	1	310	LUT	C7-C8-C9	2.46	129.96	126.23
23	L	302	BCR	C30-C25-C26	-2.46	119.15	122.61
20	1	306	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
20	B	826	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
20	F	304	CLA	O2A-CGA-CBA	2.46	119.63	111.91
20	B	814	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
20	B	847	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
22	2	311	XAT	C40-C33-C32	-2.46	114.20	118.08
20	1	304	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
20	1	322	CLA	C3B-C4B-NB	2.46	112.80	110.52
29	B	840	DGD	O2G-C1B-O1B	-2.46	117.76	123.70
20	3	312	CLA	CHC-C4B-NB	-2.46	121.66	124.26
20	A	828	CLA	CHC-C4B-NB	-2.46	121.66	124.26
20	2	308	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
20	A	842	CLA	CHB-C1B-C2B	-2.46	120.30	127.24
20	H	201	CLA	CMB-C2B-C1B	2.46	129.11	125.37
20	L	307	CLA	CHC-C4B-NB	-2.46	121.66	124.26
21	4	317	LUT	C11-C10-C9	2.45	130.81	127.31
20	1	303	CLA	CMD-C2D-C3D	-2.45	121.97	127.61
20	B	817	CLA	C2A-C1A-CHA	-2.45	119.57	123.86
20	B	833	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
20	B	812	CLA	O1D-CGD-CBD	-2.45	119.47	124.48
20	A	808	CLA	CMB-C2B-C3B	2.45	132.53	126.59
20	B	833	CLA	CAA-C2A-C3A	2.45	119.49	112.78
20	A	826	CLA	C3B-C4B-NB	2.45	112.79	110.52
20	4	310	CLA	C2A-C1A-CHA	-2.45	119.58	123.86
20	2	304	CLA	CMD-C2D-C3D	-2.45	121.98	127.61
20	4	316	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
23	J	101	BCR	C30-C25-C26	-2.45	119.16	122.61
20	A	846	CLA	CMD-C2D-C3D	-2.45	121.98	127.61
20	A	812	CLA	CAC-C3C-C4C	2.45	127.99	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	316	CLA	C4-C3-C2	-2.45	117.40	123.68
20	A	850	CLA	CMD-C2D-C3D	-2.45	121.98	127.61
20	A	830	CLA	O2A-CGA-CBA	2.45	119.58	111.91
23	B	839	BCR	C36-C18-C17	-2.45	119.50	122.92
20	B	808	CLA	C2D-C1D-ND	2.45	111.91	110.10
20	A	832	CLA	O2A-CGA-CBA	2.44	119.58	111.91
20	A	803	CLA	O2A-CGA-CBA	2.44	119.58	111.91
20	2	305	CLA	C4-C3-C5	2.44	119.38	115.27
20	B	806	CLA	O2A-CGA-CBA	2.44	119.57	111.91
23	B	836	BCR	C35-C13-C14	-2.44	119.50	122.92
20	B	812	CLA	C1D-CHD-C4C	-2.44	120.79	126.06
20	N	202	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
19	4	305	CHL	OMC-CMC-C2C	-2.44	120.17	125.69
20	3	309	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
20	A	812	CLA	C1-O2A-CGA	2.44	122.84	116.44
20	B	811	CLA	CMD-C2D-C3D	-2.44	122.00	127.61
20	A	840	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
20	4	303	CLA	C3B-C4B-NB	2.44	112.78	110.52
20	B	812	CLA	O2A-CGA-CBA	2.44	119.56	111.91
20	K	204	CLA	CHC-C4B-NB	-2.44	121.68	124.26
20	2	321	CLA	CHC-C4B-NB	-2.44	121.68	124.26
20	B	821	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
20	1	303	CLA	C3B-C4B-NB	2.44	112.77	110.52
20	4	311	CLA	C3B-C4B-NB	2.43	112.77	110.52
23	G	201	BCR	C7-C8-C9	2.43	129.91	126.23
19	2	318	CHL	O2D-CGD-CBD	2.43	115.59	111.27
20	B	820	CLA	C4-C3-C5	2.43	119.36	115.27
20	2	320	CLA	O2A-CGA-CBA	2.43	119.53	111.91
20	4	311	CLA	C4A-NA-C1A	2.43	107.80	106.71
20	4	316	CLA	C5-C3-C2	2.43	126.03	121.12
20	A	825	CLA	CHB-C1B-NB	-2.43	121.69	124.26
20	A	825	CLA	C2A-C1A-CHA	-2.42	119.62	123.86
20	B	826	CLA	CHC-C4B-NB	-2.42	121.69	124.26
20	4	308	CLA	C2A-C1A-CHA	-2.42	119.62	123.86
20	B	845	CLA	CHC-C4B-NB	-2.42	121.69	124.26
20	B	801	CLA	C6-C5-C3	2.42	119.80	113.45
20	A	809	CLA	C2A-C1A-CHA	-2.42	119.63	123.86
20	B	823	CLA	CMD-C2D-C3D	-2.42	122.05	127.61
23	F	301	BCR	C34-C9-C8	2.42	121.89	118.08
23	1	312	BCR	C34-C9-C10	-2.42	119.54	122.92
20	4	313	CLA	C3B-C4B-NB	2.42	112.76	110.52
20	A	850	CLA	CHC-C4B-NB	-2.42	121.70	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	4	320	BCR	C16-C17-C18	2.42	130.76	127.31
20	A	811	CLA	C3B-C4B-NB	2.42	112.76	110.52
20	A	855	CLA	CHB-C1B-NB	-2.42	121.70	124.26
20	2	306	CLA	O2D-CGD-O1D	-2.42	119.12	123.84
20	A	839	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
20	4	312	CLA	O2A-CGA-CBA	2.41	119.48	111.91
22	1	311	XAT	C24-C23-C22	-2.41	106.12	110.77
20	A	841	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
20	O	208	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
20	B	814	CLA	C4D-CHA-C1A	-2.41	118.32	121.25
20	4	304	CLA	CMB-C2B-C3B	2.41	132.42	126.59
20	B	826	CLA	CMD-C2D-C3D	-2.41	122.08	127.61
23	F	301	BCR	C21-C20-C19	2.41	130.73	123.22
21	2	310	LUT	C35-C15-C14	2.41	128.41	123.47
20	B	821	CLA	C3B-C4B-NB	2.41	112.75	110.52
20	2	303	CLA	CMD-C2D-C3D	-2.41	122.08	127.61
20	4	302	CLA	O2A-CGA-O1A	-2.41	117.52	123.59
20	2	304	CLA	CED-O2D-CGD	2.40	121.38	115.94
20	2	323	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
20	B	820	CLA	CHB-C1B-NB	-2.40	121.71	124.26
20	A	809	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
20	B	804	CLA	O2A-CGA-CBA	2.40	119.45	111.91
24	A	822	LHG	O4-P-O5	2.40	120.09	110.68
20	B	848	CLA	C4-C3-C2	-2.40	117.52	123.68
20	3	315	CLA	C2D-C1D-ND	2.40	111.87	110.10
20	A	848	CLA	C1-C2-C3	-2.40	121.89	126.04
20	1	303	CLA	C1-O2A-CGA	2.40	122.75	116.44
20	A	852	CLA	CED-O2D-CGD	2.40	121.37	115.94
23	B	837	BCR	C7-C8-C9	2.40	129.86	126.23
20	B	821	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
22	1	311	XAT	C26-C27-C28	2.40	131.07	125.99
20	B	802	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
23	B	834	BCR	C8-C9-C10	2.40	122.62	118.94
19	4	305	CHL	C1C-C2C-C3C	-2.40	105.21	107.11
19	4	315	CHL	C1C-C2C-C3C	-2.40	105.21	107.11
20	H	201	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
20	B	813	CLA	CMB-C2B-C1B	2.40	129.02	125.37
23	G	203	BCR	C35-C13-C14	-2.40	119.57	122.92
20	1	308	CLA	CHC-C4B-NB	-2.39	121.72	124.26
20	A	848	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
20	A	855	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
20	A	855	CLA	O2D-CGD-O1D	-2.39	119.16	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	823	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
20	B	821	CLA	O2A-CGA-CBA	2.39	119.41	111.91
20	3	320	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
20	4	312	CLA	CMB-C2B-C1B	2.39	129.01	125.37
23	L	303	BCR	C35-C13-C14	-2.39	119.58	122.92
21	1	310	LUT	C11-C10-C9	2.39	130.72	127.31
20	B	852	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
20	A	833	CLA	C1-C2-C3	-2.39	121.92	126.04
19	1	317	CHL	O2D-CGD-O1D	-2.39	119.17	123.84
20	1	321	CLA	CHC-C4B-NB	-2.39	121.73	124.26
20	A	841	CLA	O2A-CGA-CBA	2.38	119.39	111.91
20	A	812	CLA	CHB-C1B-NB	-2.38	121.73	124.26
22	2	311	XAT	C38-C25-C24	2.38	116.96	114.28
23	A	815	BCR	C15-C16-C17	2.38	128.35	123.47
20	B	816	CLA	C4A-NA-C1A	2.38	107.78	106.71
20	3	316	CLA	C3B-C4B-NB	2.38	112.72	110.52
20	B	824	CLA	C1-C2-C3	-2.38	121.92	126.04
20	B	810	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
23	A	816	BCR	C16-C17-C18	2.38	130.71	127.31
20	B	823	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
20	4	314	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
20	F	305	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
20	3	318	CLA	C3B-C4B-NB	2.38	112.72	110.52
20	4	314	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
23	A	816	BCR	C15-C16-C17	2.38	128.34	123.47
20	B	829	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
19	2	322	CHL	O2D-CGD-O1D	-2.38	119.19	123.84
20	2	305	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
19	2	322	CHL	C1C-C2C-C3C	-2.38	105.23	107.11
20	1	302	CLA	C3B-C4B-NB	2.37	112.72	110.52
20	3	317	CLA	C1-C2-C3	-2.37	121.94	126.04
24	2	316	LHG	O4-P-O5	2.37	119.97	110.68
20	2	303	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
20	A	856	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
20	4	310	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
20	O	206	CLA	CMB-C2B-C3B	2.37	132.33	126.59
23	B	835	BCR	C37-C22-C23	2.37	121.81	118.08
20	B	807	CLA	CED-O2D-CGD	2.37	121.30	115.94
20	B	805	CLA	CHC-C4B-NB	-2.37	121.75	124.26
20	A	841	CLA	CHB-C1B-C2B	-2.37	120.54	127.24
19	4	307	CHL	OMC-CMC-C2C	-2.37	120.33	125.69
24	B	842	LHG	O4-P-O5	2.37	119.96	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	103	CLA	C4A-NA-C1A	2.37	107.77	106.71
20	4	308	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
20	A	801	CLA	C4B-C3B-C2B	-2.37	104.78	107.03
20	A	836	CLA	C1-O2A-CGA	2.37	122.65	116.44
20	2	304	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
29	B	840	DGD	O1G-C1A-C2A	2.37	119.33	111.91
21	2	310	LUT	C39-C29-C28	2.37	121.81	118.08
20	1	319	CLA	O2A-CGA-CBA	2.37	119.33	111.91
20	B	852	CLA	C5-C3-C2	2.37	125.90	121.12
24	A	820	LHG	O4-P-O5	2.36	119.94	110.68
20	3	307	CLA	C4-C3-C5	2.36	119.25	115.27
20	H	201	CLA	C2A-C1A-CHA	-2.36	119.72	123.86
23	B	836	BCR	C1-C6-C5	-2.36	119.28	122.61
23	O	203	BCR	C29-C30-C25	2.36	114.12	110.48
20	3	308	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
20	A	804	CLA	O1D-CGD-CBD	-2.36	119.65	124.48
20	A	801	CLA	C4-C3-C5	2.36	119.24	115.27
20	A	847	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
20	4	313	CLA	CED-O2D-CGD	2.36	121.28	115.94
20	3	312	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
20	2	306	CLA	C3B-C4B-NB	2.36	112.70	110.52
28	A	824	CL0	O2D-CGD-O1D	-2.36	118.74	124.09
20	3	309	CLA	C1-C2-C3	-2.35	121.97	126.04
23	A	814	BCR	C34-C9-C10	-2.35	119.63	122.92
20	A	828	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
20	O	206	CLA	C2D-C1D-ND	2.35	111.83	110.10
20	B	811	CLA	CED-O2D-CGD	2.35	121.25	115.94
20	L	306	CLA	O2A-CGA-CBA	2.35	119.28	111.91
20	L	306	CLA	CMD-C2D-C3D	-2.35	122.22	127.61
20	A	849	CLA	CMB-C2B-C3B	2.35	132.27	126.59
20	A	826	CLA	CHB-C1B-C2B	-2.35	120.61	127.24
19	2	302	CHL	OMC-CMC-C2C	-2.35	120.38	125.69
20	F	306	CLA	C3B-C4B-NB	2.34	112.69	110.52
20	B	810	CLA	C2A-C1A-CHA	-2.34	119.76	123.86
23	L	304	BCR	C16-C17-C18	2.34	130.65	127.31
21	2	310	LUT	C22-C23-C24	-2.34	109.08	111.74
20	B	850	CLA	O2A-CGA-CBA	2.34	119.25	111.91
20	A	805	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
20	1	321	CLA	C2A-C1A-CHA	-2.34	119.77	123.86
20	G	207	CLA	C2A-C1A-CHA	-2.34	119.77	123.86
24	B	843	LHG	O4-P-O5	2.34	119.84	110.68
24	O	205	LHG	O4-P-O5	2.34	119.83	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	845	CLA	C1-C2-C3	-2.34	122.00	126.04
23	A	857	BCR	C35-C13-C14	-2.33	119.65	122.92
20	A	843	CLA	CHC-C4B-NB	-2.33	121.79	124.26
20	B	849	CLA	C4-C3-C5	2.33	119.20	115.27
23	F	302	BCR	C16-C17-C18	2.33	130.64	127.31
20	4	308	CLA	CMD-C2D-C3D	-2.33	122.25	127.61
20	G	205	CLA	CHC-C4B-NB	-2.33	121.79	124.26
23	B	836	BCR	C20-C21-C22	2.33	130.64	127.31
21	2	310	LUT	C32-C33-C34	2.33	122.52	118.94
23	B	836	BCR	C16-C17-C18	2.33	130.63	127.31
20	L	307	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
24	O	204	LHG	O4-P-O5	2.33	119.79	110.68
20	A	835	CLA	CHB-C1B-C2B	-2.33	120.67	127.24
20	B	844	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
20	A	833	CLA	CBC-CAC-C3C	-2.32	106.02	112.43
20	A	837	CLA	O2A-CGA-CBA	2.32	119.20	111.91
23	B	834	BCR	C38-C26-C25	2.32	127.14	124.53
20	3	311	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
20	3	307	CLA	CMA-C3A-C4A	2.32	118.02	111.77
20	A	805	CLA	CMB-C2B-C1B	2.32	128.91	125.37
20	G	207	CLA	CHC-C4B-NB	-2.32	121.80	124.26
22	3	302	XAT	C38-C25-C24	2.32	116.89	114.28
22	4	318	XAT	C20-C13-C12	2.32	121.73	118.08
20	3	310	CLA	C2D-C1D-ND	2.32	111.81	110.10
20	B	807	CLA	CHB-C1B-C2B	-2.32	120.68	127.24
20	B	803	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
23	4	320	BCR	C36-C18-C17	-2.32	119.67	122.92
20	B	830	CLA	CMB-C2B-C1B	2.32	128.90	125.37
20	A	829	CLA	CMB-C2B-C1B	2.32	128.90	125.37
20	A	853	CLA	CMD-C2D-C3D	-2.32	122.28	127.61
20	B	848	CLA	C1-C2-C3	-2.32	122.04	126.04
20	B	829	CLA	CED-O2D-CGD	2.32	121.17	115.94
20	A	801	CLA	C2D-C1D-ND	2.31	111.81	110.10
20	B	845	CLA	C4-C3-C5	2.31	119.17	115.27
29	O	201	DGD	O1G-C1A-C2A	2.31	119.17	111.91
20	B	850	CLA	CHB-C1B-NB	-2.31	121.81	124.26
20	B	813	CLA	C5-C3-C2	-2.31	116.44	121.12
20	B	813	CLA	CED-O2D-CGD	2.31	121.16	115.94
20	3	314	CLA	C3B-C4B-NB	2.31	112.66	110.52
20	2	319	CLA	O2A-CGA-CBA	2.31	119.15	111.91
28	A	824	CL0	C2D-C1D-ND	2.31	111.81	110.10
20	O	207	CLA	C3B-C4B-NB	2.31	112.66	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	F	301	BCR	C30-C25-C26	-2.31	119.36	122.61
19	1	301	CHL	C1C-C2C-C3C	-2.31	105.28	107.11
20	B	812	CLA	C2D-C1D-ND	2.31	111.80	110.10
20	3	307	CLA	CHB-C1B-NB	-2.31	121.81	124.26
20	B	827	CLA	CMB-C2B-C1B	2.31	128.88	125.37
20	K	205	CLA	CMC-C2C-C1C	2.31	128.55	125.04
23	G	201	BCR	C15-C16-C17	2.30	128.19	123.47
20	A	847	CLA	C2D-C1D-ND	2.30	111.80	110.10
20	A	846	CLA	CMB-C2B-C1B	2.30	128.88	125.37
20	F	304	CLA	CMB-C2B-C1B	2.30	128.88	125.37
20	A	850	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
20	1	318	CLA	CMB-C2B-C3B	2.30	132.16	126.59
22	3	302	XAT	C10-C11-C12	-2.30	116.03	123.22
20	B	814	CLA	CHB-C1B-NB	-2.30	121.82	124.26
20	B	823	CLA	O2A-CGA-CBA	2.30	119.13	111.91
20	A	853	CLA	CHB-C1B-NB	-2.30	121.82	124.26
20	L	305	CLA	C2D-C1D-ND	2.30	111.80	110.10
20	F	304	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
20	B	820	CLA	C1D-CHD-C4C	-2.30	121.10	126.06
20	A	842	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
20	2	317	CLA	O2A-CGA-CBA	2.30	119.12	111.91
20	2	303	CLA	CHB-C1B-C2B	-2.30	120.75	127.24
20	A	840	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
23	B	839	BCR	C34-C9-C8	2.30	119.67	114.60
23	K	202	BCR	C34-C9-C10	-2.30	119.71	122.92
20	B	853	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
20	A	845	CLA	C4-C3-C5	2.29	119.13	115.27
20	G	206	CLA	C3B-C4B-NB	2.29	112.64	110.52
20	1	304	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
20	B	808	CLA	C4-C3-C5	2.29	119.13	115.27
23	A	815	BCR	C35-C13-C14	-2.29	119.71	122.92
20	A	842	CLA	C6-C5-C3	-2.29	107.45	113.45
20	1	321	CLA	CED-O2D-CGD	2.29	121.12	115.94
20	A	827	CLA	O2A-CGA-CBA	2.29	119.09	111.91
20	K	203	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
19	2	309	CHL	CHB-C1B-C2B	-2.29	120.78	127.24
20	A	804	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
20	3	317	CLA	O2A-CGA-CBA	2.29	119.08	111.91
20	B	830	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
20	1	305	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
20	A	826	CLA	C4D-CHA-C1A	-2.28	118.47	121.25
20	A	842	CLA	O2D-CGD-O1D	-2.28	119.37	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	832	CLA	CHB-C1B-C2B	-2.28	120.79	127.24
19	4	307	CHL	C1C-C2C-C3C	-2.28	105.30	107.11
23	A	857	BCR	C1-C6-C5	-2.28	119.40	122.61
20	B	851	CLA	CHC-C4B-NB	-2.28	121.84	124.26
20	A	838	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
20	A	844	CLA	CAC-C3C-C4C	2.28	127.77	124.81
20	A	854	CLA	C7-C6-C5	-2.28	107.17	113.36
20	3	308	CLA	CMB-C2B-C3B	2.28	132.11	126.59
20	3	316	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
20	B	809	CLA	C2D-C1D-ND	2.28	111.78	110.10
20	4	314	CLA	CHB-C1B-C2B	-2.28	120.81	127.24
20	G	205	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
20	2	307	CLA	O2A-CGA-CBA	2.28	119.05	111.91
20	B	816	CLA	CHC-C4B-NB	-2.28	121.85	124.26
20	3	311	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
23	B	836	BCR	C12-C13-C14	2.27	122.43	118.94
20	B	831	CLA	C11-C10-C8	-2.27	108.57	115.92
20	3	311	CLA	CMB-C2B-C3B	2.27	132.10	126.59
20	4	316	CLA	C1-O2A-CGA	2.27	122.41	116.44
23	F	301	BCR	C1-C6-C5	-2.27	119.41	122.61
23	K	202	BCR	C1-C6-C5	-2.27	119.41	122.61
20	A	850	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
20	A	854	CLA	C2A-C3A-C4A	-2.27	98.20	101.87
20	A	854	CLA	CHB-C1B-C2B	-2.27	120.82	127.24
20	4	311	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
20	B	804	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
20	1	320	CLA	CHB-C1B-C2B	-2.27	120.82	127.24
20	A	811	CLA	CMB-C2B-C1B	2.27	128.82	125.37
20	1	321	CLA	CMB-C2B-C3B	2.27	132.08	126.59
20	B	805	CLA	CMB-C2B-C3B	2.27	132.08	126.59
20	B	819	CLA	C4-C3-C5	2.27	119.08	115.27
20	A	845	CLA	CHC-C4B-NB	-2.27	121.86	124.26
23	J	101	BCR	C34-C9-C10	-2.27	119.75	122.92
20	B	820	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
20	B	805	CLA	C4A-NA-C1A	2.26	107.72	106.71
20	A	812	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
20	3	309	CLA	O2A-CGA-CBA	2.26	119.00	111.91
20	A	853	CLA	O2A-CGA-CBA	2.26	119.00	111.91
20	B	820	CLA	C1-C2-C3	-2.26	122.13	126.04
20	4	309	CLA	CHB-C1B-C2B	-2.26	120.85	127.24
20	B	822	CLA	C1-C2-C3	-2.26	122.13	126.04
20	A	838	CLA	O2D-CGD-O1D	-2.26	119.42	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	824	CLA	CBA-CAA-C2A	2.26	120.53	113.86
19	1	301	CHL	O2D-CGD-O1D	-2.26	119.42	123.84
23	K	201	BCR	C38-C26-C25	2.25	127.06	124.53
20	B	803	CLA	O1D-CGD-CBD	-2.25	119.87	124.48
20	1	306	CLA	C3B-C4B-NB	2.25	112.61	110.52
20	B	810	CLA	O2A-CGA-CBA	2.25	118.98	111.91
20	A	838	CLA	CMB-C2B-C3B	2.25	132.04	126.59
29	G	202	DGD	C2G-O2G-C1B	-2.25	112.25	117.79
20	1	303	CLA	O2A-CGA-CBA	2.25	118.96	111.91
20	B	803	CLA	C2A-C1A-CHA	-2.25	119.93	123.86
20	B	851	CLA	C1-C2-C3	-2.25	122.16	126.04
20	4	309	CLA	CAA-C2A-C3A	2.25	118.93	112.78
20	A	843	CLA	CMB-C2B-C3B	2.25	132.03	126.59
21	2	310	LUT	C12-C13-C14	2.25	122.39	118.94
20	A	805	CLA	CBA-CAA-C2A	-2.24	107.24	113.86
20	A	812	CLA	CHB-C1B-C2B	-2.24	120.90	127.24
20	B	806	CLA	CHB-C1B-C2B	-2.24	120.90	127.24
20	A	853	CLA	CED-O2D-CGD	2.24	121.01	115.94
20	1	319	CLA	CHB-C1B-NB	-2.24	121.88	124.26
20	B	808	CLA	CHB-C1B-C2B	-2.24	120.91	127.24
20	A	837	CLA	CHB-C1B-C2B	-2.24	120.91	127.24
20	3	318	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
23	L	302	BCR	C34-C9-C8	2.24	121.61	118.08
20	A	812	CLA	CHC-C4B-NB	-2.24	121.89	124.26
23	A	818	BCR	C18-C19-C20	2.24	129.79	124.81
20	A	845	CLA	CMB-C2B-C3B	2.24	132.01	126.59
20	K	204	CLA	CAA-C2A-C3A	-2.24	106.65	112.78
20	B	848	CLA	CMB-C2B-C1B	2.24	128.78	125.37
23	I	102	BCR	C34-C9-C8	2.24	121.60	118.08
29	O	201	DGD	O6D-C5D-C6D	2.24	111.18	106.67
19	1	301	CHL	OMC-CMC-C2C	-2.24	120.63	125.69
20	A	846	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
20	1	303	CLA	O2D-CGD-O1D	-2.24	119.01	124.09
20	2	308	CLA	CHB-C1B-C2B	-2.24	120.92	127.24
20	3	312	CLA	CMB-C2B-C3B	2.24	132.00	126.59
23	1	312	BCR	C15-C14-C13	2.23	130.50	127.31
23	3	303	BCR	C20-C21-C22	2.23	130.50	127.31
19	2	301	CHL	O2D-CGD-O1D	-2.23	119.47	123.84
20	L	305	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
20	B	819	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
20	A	826	CLA	O2A-CGA-CBA	2.23	118.91	111.91
23	B	838	BCR	C34-C9-C10	-2.23	119.80	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	318	XAT	C19-C9-C8	2.23	121.59	118.08
22	2	311	XAT	C25-C24-C23	2.23	117.16	112.75
20	2	306	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
23	L	303	BCR	C1-C6-C5	-2.23	119.48	122.61
20	2	321	CLA	CMB-C2B-C3B	2.23	131.98	126.59
20	3	307	CLA	CMB-C2B-C3B	2.23	131.98	126.59
20	A	832	CLA	C1-O2A-CGA	2.22	122.28	116.44
20	2	320	CLA	CHB-C1B-NB	-2.22	121.90	124.26
20	A	801	CLA	C4-C3-C2	-2.22	117.97	123.68
20	A	827	CLA	CMB-C2B-C3B	2.22	131.97	126.59
20	2	323	CLA	C2A-C1A-CHA	-2.22	119.97	123.86
20	4	308	CLA	CHC-C4B-NB	-2.22	121.91	124.26
20	B	824	CLA	CAA-C2A-C1A	2.22	119.25	111.97
20	B	818	CLA	CHB-C1B-C2B	-2.22	120.96	127.24
20	3	310	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
20	1	305	CLA	CHB-C1B-C2B	-2.22	120.97	127.24
20	B	827	CLA	O2A-CGA-CBA	2.22	118.88	111.91
20	A	801	CLA	C2A-C1A-CHA	-2.22	119.98	123.86
23	K	201	BCR	C34-C9-C10	-2.22	119.81	122.92
23	1	312	BCR	C16-C17-C18	2.22	130.47	127.31
23	A	817	BCR	C34-C9-C10	-2.22	119.82	122.92
20	L	305	CLA	CHB-C1B-NB	-2.22	121.91	124.26
20	3	309	CLA	C3B-C4B-NB	2.22	112.57	110.52
23	A	818	BCR	C16-C15-C14	2.22	128.01	123.47
20	B	807	CLA	O1D-CGD-CBD	-2.21	119.95	124.48
20	A	836	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
20	1	307	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
20	B	850	CLA	C4-C3-C5	2.21	118.99	115.27
20	L	306	CLA	CMB-C2B-C3B	2.21	131.95	126.59
20	A	839	CLA	CHC-C4B-NB	-2.21	121.92	124.26
20	3	314	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
20	B	829	CLA	CHB-C1B-C2B	-2.21	120.99	127.24
20	A	808	CLA	CHC-C4B-NB	-2.21	121.92	124.26
20	B	849	CLA	C6-C5-C3	-2.21	111.00	114.62
24	A	820	LHG	C5-O7-C7	2.21	123.23	117.79
19	2	309	CHL	CHB-C1B-NB	-2.21	121.92	124.26
20	B	813	CLA	CHB-C1B-C2B	-2.21	121.00	127.24
20	F	306	CLA	C2A-C1A-CHA	-2.21	120.00	123.86
20	A	802	CLA	C2A-C3A-C4A	-2.21	98.30	101.87
23	4	319	BCR	C32-C1-C6	2.21	113.88	110.30
23	3	303	BCR	C24-C23-C22	2.21	129.57	126.23
20	4	309	CLA	CED-O2D-CGD	2.21	120.93	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	K	203	CLA	C4A-NA-C1A	2.21	107.70	106.71
19	4	315	CHL	O2D-CGD-O1D	-2.21	119.08	124.09
20	B	810	CLA	CHB-C1B-C2B	-2.21	121.01	127.24
22	3	302	XAT	C20-C13-C12	2.21	121.55	118.08
20	B	816	CLA	C6-C5-C3	2.21	119.24	113.45
20	K	206	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
20	A	852	CLA	CHB-C1B-C2B	-2.20	121.01	127.24
20	B	803	CLA	CMB-C2B-C3B	2.20	131.92	126.59
20	B	824	CLA	CHB-C1B-C2B	-2.20	121.02	127.24
20	A	854	CLA	C3B-C2B-C1B	-2.20	104.50	107.16
20	1	309	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
20	B	820	CLA	C6-C5-C3	-2.20	107.68	113.45
20	L	305	CLA	CHB-C1B-C2B	-2.20	121.02	127.24
20	A	856	CLA	C5-C3-C2	-2.20	116.67	121.12
23	O	203	BCR	C1-C6-C7	2.20	122.00	115.78
20	B	849	CLA	CHB-C1B-NB	-2.20	121.93	124.26
20	A	848	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
20	1	305	CLA	C3B-C4B-NB	2.20	112.56	110.52
20	A	843	CLA	C2A-C1A-CHA	-2.20	120.02	123.86
20	A	804	CLA	C4A-NA-C1A	2.20	107.69	106.71
20	A	830	CLA	C2A-C1A-CHA	-2.20	120.02	123.86
20	A	802	CLA	CHB-C1B-C2B	-2.20	121.03	127.24
20	A	835	CLA	C6-C7-C8	-2.20	108.82	115.92
20	A	826	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
20	B	847	CLA	C1-C2-C3	-2.19	122.25	126.04
23	A	857	BCR	C16-C17-C18	2.19	130.44	127.31
20	A	825	CLA	O2A-CGA-CBA	2.19	118.79	111.91
20	A	844	CLA	C4C-C3C-C2C	-2.19	103.70	106.90
20	F	305	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
20	A	805	CLA	C4A-NA-C1A	2.19	107.69	106.71
20	1	305	CLA	O2A-CGA-CBA	2.19	120.90	112.23
20	3	315	CLA	CAA-C2A-C3A	2.19	118.78	112.78
20	2	321	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
20	2	303	CLA	C3B-C4B-NB	2.19	112.55	110.52
20	1	322	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
20	3	318	CLA	CMB-C2B-C1B	2.19	128.70	125.37
20	L	306	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
20	3	314	CLA	CBC-CAC-C3C	-2.19	106.40	112.43
20	3	320	CLA	CMB-C2B-C3B	2.19	131.88	126.59
20	L	307	CLA	O2A-CGA-CBA	2.19	120.87	112.23
19	2	301	CHL	O2A-CGA-CBA	2.18	120.87	112.23
20	A	853	CLA	CMB-C2B-C3B	2.18	131.88	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	846	CLA	C4A-NA-C1A	2.18	107.69	106.71
20	B	807	CLA	C6-C5-C3	2.18	119.18	113.45
23	A	857	BCR	C12-C13-C14	2.18	122.29	118.94
20	A	825	CLA	CHB-C1B-C2B	-2.18	121.08	127.24
20	B	801	CLA	CMB-C2B-C3B	2.18	131.87	126.59
23	A	817	BCR	C30-C25-C26	-2.18	119.54	122.61
20	3	311	CLA	CHC-C4B-NB	-2.18	121.95	124.26
20	B	816	CLA	CMB-C2B-C3B	2.18	131.87	126.59
20	A	830	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
20	B	823	CLA	CMB-C2B-C3B	2.18	131.86	126.59
20	B	804	CLA	CMB-C2B-C3B	2.18	131.86	126.59
20	3	310	CLA	CMB-C2B-C3B	2.18	131.86	126.59
20	B	830	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
20	1	304	CLA	CMB-C2B-C3B	2.18	131.86	126.59
19	1	317	CHL	O1D-CGD-CBD	-2.18	120.03	124.48
20	A	835	CLA	C1-C2-C3	-2.17	122.28	126.04
23	A	814	BCR	C30-C25-C24	2.17	121.93	115.78
20	A	812	CLA	CMB-C2B-C1B	2.17	128.68	125.37
20	A	856	CLA	CHC-C4B-NB	-2.17	121.96	124.26
20	4	316	CLA	CHB-C1B-C2B	-2.17	121.10	127.24
20	B	803	CLA	C4A-NA-C1A	2.17	107.68	106.71
23	2	312	BCR	C15-C16-C17	2.17	127.92	123.47
20	A	828	CLA	CHB-C1B-NB	-2.17	121.96	124.26
20	N	202	CLA	C4-C3-C5	2.17	118.92	115.27
22	3	302	XAT	C12-C13-C14	-2.17	115.61	118.94
20	A	812	CLA	O2A-C1-C2	2.17	114.34	108.64
23	A	857	BCR	C15-C14-C13	2.17	130.41	127.31
20	A	807	CLA	C3B-C4B-NB	2.17	112.53	110.52
20	2	307	CLA	C11-C10-C8	-2.17	108.92	115.92
20	A	851	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
20	B	830	CLA	C4A-NA-C1A	2.16	107.68	106.71
20	A	803	CLA	C4-C3-C5	2.16	118.91	115.27
20	B	852	CLA	CHB-C1B-C2B	-2.16	121.13	127.24
20	A	812	CLA	CMB-C2B-C3B	2.16	131.82	126.59
20	3	310	CLA	CHC-C4B-NB	-2.16	121.97	124.26
20	2	317	CLA	CHB-C1B-C2B	-2.16	121.14	127.24
20	L	305	CLA	O2A-CGA-CBA	2.16	120.75	112.23
20	3	307	CLA	C2D-C1D-ND	2.16	111.69	110.10
20	G	205	CLA	CMB-C2B-C3B	2.16	131.81	126.59
20	B	817	CLA	CED-O2D-CGD	2.16	120.81	115.94
23	B	835	BCR	C35-C13-C14	-2.15	119.91	122.92
23	4	320	BCR	C30-C25-C24	2.15	121.86	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	308	CLA	C1-C2-C3	-2.15	122.32	126.04
22	1	311	XAT	C38-C25-C24	2.15	116.70	114.28
20	2	319	CLA	C4-C3-C5	2.15	118.89	115.27
20	A	801	CLA	CED-O2D-CGD	2.15	120.80	115.94
22	4	318	XAT	C31-C30-C29	-2.15	124.24	127.31
20	K	205	CLA	C1C-C2C-C3C	-2.15	104.70	106.96
20	1	307	CLA	CHB-C1B-C2B	-2.15	121.17	127.24
20	B	846	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
20	A	826	CLA	CMB-C2B-C3B	2.15	131.79	126.59
20	O	208	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
20	A	845	CLA	CHB-C1B-NB	-2.15	121.98	124.26
20	2	303	CLA	C2D-C1D-ND	2.15	111.69	110.10
20	A	853	CLA	C2D-C1D-ND	2.15	111.69	110.10
20	B	814	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
20	F	306	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
20	B	831	CLA	C7-C6-C5	-2.14	107.53	113.36
20	B	826	CLA	CMB-C2B-C3B	2.14	131.78	126.59
20	1	308	CLA	CMB-C2B-C3B	2.14	131.78	126.59
20	A	856	CLA	CMB-C2B-C3B	2.14	131.78	126.59
19	4	307	CHL	O2A-CGA-CBA	2.14	120.92	114.03
23	3	303	BCR	C30-C25-C26	-2.14	119.60	122.61
19	4	307	CHL	O2D-CGD-O1D	-2.14	119.65	123.84
20	1	302	CLA	C5-C3-C4	2.14	119.33	114.60
20	1	318	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
20	K	204	CLA	CMB-C2B-C3B	2.14	131.77	126.59
20	A	847	CLA	C4-C3-C5	2.14	118.87	115.27
23	3	303	BCR	C1-C6-C5	-2.14	119.60	122.61
23	A	816	BCR	C30-C25-C26	-2.14	119.60	122.61
20	4	303	CLA	CED-O2D-CGD	2.14	120.77	115.94
20	2	321	CLA	CED-O2D-CGD	2.14	120.77	115.94
20	B	804	CLA	C4-C3-C5	2.14	118.87	115.27
20	3	315	CLA	CED-O2D-CGD	2.14	120.77	115.94
23	I	102	BCR	C29-C30-C25	2.13	113.77	110.48
23	4	320	BCR	C35-C13-C14	-2.13	119.93	122.92
20	3	315	CLA	O2A-CGA-CBA	2.13	118.61	111.91
20	A	836	CLA	CHB-C1B-C2B	-2.13	121.21	127.24
20	B	815	CLA	CMB-C2B-C3B	2.13	131.76	126.59
20	L	306	CLA	C6-C5-C3	-2.13	111.13	114.62
20	A	837	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
20	A	854	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
20	A	849	CLA	C4-C3-C5	2.13	118.86	115.27
20	B	853	CLA	CHC-C4B-NB	-2.13	122.00	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	807	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
20	B	808	CLA	C6-C7-C8	-2.13	109.04	115.92
20	1	302	CLA	C4A-NA-C1A	2.13	107.66	106.71
20	A	803	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
20	B	803	CLA	O2A-CGA-CBA	2.13	118.58	111.91
20	A	838	CLA	O2A-CGA-CBA	2.13	120.86	114.03
20	A	828	CLA	CHB-C1B-C2B	-2.13	121.23	127.24
20	B	811	CLA	CHB-C1B-C2B	-2.13	121.23	127.24
20	2	307	CLA	C4A-NA-C1A	2.13	107.66	106.71
20	L	307	CLA	CMB-C2B-C3B	2.13	131.74	126.59
20	B	823	CLA	CHB-C1B-C2B	-2.13	121.23	127.24
20	O	207	CLA	CBA-CAA-C2A	2.12	120.14	113.86
20	4	313	CLA	CHB-C1B-C2B	-2.12	121.24	127.24
20	B	821	CLA	CHB-C1B-C2B	-2.12	121.24	127.24
20	A	827	CLA	C4A-NA-C1A	2.12	107.66	106.71
22	4	318	XAT	O4-C5-C6	-2.12	57.20	58.96
20	O	206	CLA	C1-O2A-CGA	2.12	122.02	116.44
23	B	838	BCR	C30-C25-C26	-2.12	119.62	122.61
23	L	302	BCR	C34-C9-C10	-2.12	119.95	122.92
19	2	309	CHL	OMC-CMC-C2C	-2.12	120.89	125.69
20	3	307	CLA	CGD-CBD-CAD	-2.12	105.60	114.30
20	B	825	CLA	C3B-C4B-NB	2.12	112.48	110.52
20	O	208	CLA	CMB-C2B-C3B	2.12	131.72	126.59
20	B	808	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
20	B	851	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
20	A	848	CLA	CED-O2D-CGD	2.12	120.73	115.94
20	B	825	CLA	CHB-C1B-C2B	-2.12	121.25	127.24
20	B	827	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
20	4	316	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
20	3	319	CLA	CHB-C1B-C2B	-2.12	121.25	127.24
20	4	314	CLA	C5-C3-C4	2.12	119.28	114.60
21	1	310	LUT	C32-C33-C34	2.12	122.19	118.94
20	1	308	CLA	O2A-CGA-CBA	2.12	120.60	112.23
20	B	811	CLA	CMB-C2B-C1B	2.12	128.59	125.37
23	G	201	BCR	C20-C21-C22	2.12	130.33	127.31
20	H	201	CLA	C4A-NA-C1A	2.12	107.66	106.71
20	A	843	CLA	CHB-C1B-C2B	-2.11	121.26	127.24
19	3	313	CHL	CED-O2D-CGD	2.11	120.72	115.94
20	A	847	CLA	CHB-C1B-C2B	-2.11	121.27	127.24
20	B	827	CLA	CHB-C1B-C2B	-2.11	121.27	127.24
23	A	818	BCR	C1-C6-C7	2.11	121.76	115.78
20	B	818	CLA	CBC-CAC-C3C	-2.11	106.61	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	825	CLA	CED-O2D-CGD	2.11	120.72	115.94
20	1	320	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
20	F	305	CLA	CED-O2D-CGD	2.11	120.71	115.94
23	B	835	BCR	C1-C6-C7	2.11	121.75	115.78
19	4	306	CHL	OMC-CMC-C2C	-2.11	120.92	125.69
20	B	804	CLA	C2D-C1D-ND	2.11	111.66	110.10
20	A	832	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
20	2	321	CLA	CBA-CAA-C2A	2.11	120.08	113.86
20	1	322	CLA	CED-O2D-CGD	2.11	120.70	115.94
20	2	305	CLA	CHB-C1B-C2B	-2.11	121.29	127.24
20	2	323	CLA	O2A-CGA-CBA	2.11	120.55	112.23
20	1	320	CLA	C3B-C4B-NB	2.10	112.47	110.52
28	A	824	CL0	C2A-C1A-CHA	-2.10	120.18	123.86
20	A	851	CLA	C1-C2-C3	-2.10	122.41	126.04
20	F	306	CLA	CHB-C1B-C2B	-2.10	121.30	127.24
19	3	313	CHL	OMC-CMC-C2C	-2.10	120.94	125.69
20	4	303	CLA	C4A-NA-C1A	2.10	107.65	106.71
20	A	854	CLA	C1-C2-C3	-2.10	122.41	126.04
20	B	812	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
20	3	307	CLA	CHB-C1B-C2B	-2.10	121.32	127.24
20	4	312	CLA	CHB-C1B-NB	-2.10	122.04	124.26
20	A	848	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
29	J	104	DGD	O1G-C1A-O1A	-2.10	118.30	123.59
20	B	848	CLA	CED-O2D-CGD	2.09	120.67	115.94
23	B	837	BCR	C30-C25-C26	-2.09	119.67	122.61
20	B	806	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
20	3	318	CLA	CHB-C1B-C2B	-2.09	121.33	127.24
20	O	207	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
20	2	317	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
21	3	301	LUT	C31-C30-C29	2.09	130.29	127.31
23	4	320	BCR	C1-C6-C7	2.09	121.69	115.78
20	A	806	CLA	CHB-C1B-C2B	-2.09	121.33	127.24
21	3	301	LUT	C32-C33-C34	2.09	122.15	118.94
23	B	839	BCR	C15-C14-C13	2.09	130.29	127.31
20	B	848	CLA	O2A-CGA-CBA	2.09	118.46	111.91
20	K	203	CLA	CMB-C2B-C3B	2.09	131.64	126.59
20	A	801	CLA	CMB-C2B-C3B	2.09	129.00	123.59
20	A	803	CLA	CED-O2D-CGD	2.09	120.65	115.94
23	F	302	BCR	C36-C18-C17	-2.09	120.00	122.92
20	B	848	CLA	C2A-C1A-CHA	-2.08	120.21	123.86
22	1	311	XAT	C10-C11-C12	-2.08	116.71	123.22
20	3	307	CLA	O2A-CGA-O1A	-2.08	118.33	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	309	CLA	CHB-C1B-C2B	-2.08	121.35	127.24
20	N	202	CLA	CHB-C1B-C2B	-2.08	121.35	127.24
20	B	822	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
20	B	846	CLA	CED-O2D-CGD	2.08	120.65	115.94
20	3	317	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
20	A	829	CLA	C2D-C1D-ND	2.08	111.64	110.10
20	A	854	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
23	B	836	BCR	C34-C9-C10	-2.08	120.01	122.92
23	B	837	BCR	C15-C14-C13	2.08	130.28	127.31
20	B	811	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
20	A	844	CLA	CBC-CAC-C3C	-2.08	106.70	112.43
20	B	850	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
20	A	804	CLA	CBC-CAC-C3C	-2.08	106.70	112.43
20	B	826	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
19	2	302	CHL	CBB-CAB-C3B	-2.08	117.28	127.62
20	A	854	CLA	O2A-C1-C2	2.08	114.10	108.64
20	O	208	CLA	O2A-CGA-CBA	2.08	120.70	114.03
20	A	831	CLA	CED-O2D-CGD	2.08	120.64	115.94
21	4	317	LUT	C32-C33-C34	2.08	122.13	118.94
20	A	850	CLA	O2A-CGA-CBA	2.08	118.42	111.91
20	2	304	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
19	4	315	CHL	OMC-CMC-C2C	-2.08	120.99	125.69
20	1	302	CLA	O2D-CGD-O1D	-2.07	119.78	123.84
20	A	851	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
20	3	317	CLA	C1-O2A-CGA	2.07	121.88	116.44
20	B	844	CLA	CBC-CAC-C3C	-2.07	106.72	112.43
20	B	845	CLA	C4A-NA-C1A	2.07	107.64	106.71
20	O	207	CLA	CHB-C1B-C2B	-2.07	121.39	127.24
20	A	840	CLA	O2A-CGA-CBA	2.07	120.41	112.23
20	A	840	CLA	CHB-C1B-C2B	-2.07	121.40	127.24
20	A	852	CLA	CMB-C2B-C3B	2.07	131.59	126.59
23	F	302	BCR	C15-C16-C17	2.07	127.71	123.47
20	O	207	CLA	CAA-C2A-C3A	2.07	118.43	112.78
20	3	316	CLA	CED-O2D-CGD	2.07	120.61	115.94
23	1	312	BCR	C15-C16-C17	2.06	127.70	123.47
19	2	302	CHL	O2D-CGD-O1D	-2.06	119.80	123.84
20	2	323	CLA	CED-O2D-CGD	2.06	120.60	115.94
23	1	312	BCR	C20-C21-C22	2.06	130.25	127.31
20	B	818	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
20	A	835	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
20	B	802	CLA	CHB-C1B-C2B	-2.06	121.42	127.24
20	J	103	CLA	O2D-CGD-O1D	-2.06	119.81	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	317	CLA	CED-O2D-CGD	2.06	120.59	115.94
20	A	833	CLA	O2D-CGD-O1D	-2.06	119.82	123.84
20	2	323	CLA	C3B-C4B-NB	2.06	112.42	110.52
20	F	304	CLA	C3B-C4B-NB	2.06	112.42	110.52
20	B	814	CLA	CMB-C2B-C3B	2.05	131.56	126.59
23	B	835	BCR	C23-C22-C21	2.05	122.09	118.94
20	A	844	CLA	CAA-CBA-CGA	-2.05	107.25	113.25
20	A	807	CLA	CHB-C1B-C2B	-2.05	121.44	127.24
23	4	320	BCR	C20-C19-C18	2.05	132.18	126.42
20	1	303	CLA	C4-C3-C5	2.05	118.72	115.27
20	B	810	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
20	A	845	CLA	CHB-C1B-C2B	-2.05	121.44	127.24
20	4	314	CLA	CMB-C2B-C1B	2.05	128.49	125.37
20	4	308	CLA	O2A-CGA-CBA	2.05	120.33	112.23
20	A	853	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
20	O	207	CLA	C1-C2-C3	-2.05	122.50	126.04
20	B	816	CLA	C5-C3-C2	-2.05	116.97	121.12
20	A	802	CLA	C1-O2A-CGA	2.05	121.82	116.44
20	B	801	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
20	B	801	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
20	2	303	CLA	O2A-CGA-CBA	2.05	120.61	114.03
20	3	317	CLA	CHB-C1B-C2B	-2.05	121.46	127.24
23	B	836	BCR	C20-C19-C18	2.05	132.16	126.42
19	4	305	CHL	O2A-CGA-CBA	2.04	120.31	112.23
20	3	316	CLA	C2A-C1A-CHA	-2.04	120.28	123.86
20	B	833	CLA	CHB-C1B-C2B	-2.04	121.46	127.24
20	B	818	CLA	C3B-C4B-NB	2.04	112.41	110.52
20	B	807	CLA	CMB-C2B-C3B	2.04	131.53	126.59
20	1	319	CLA	CHB-C1B-C2B	-2.04	121.47	127.24
20	B	852	CLA	C6-C5-C3	-2.04	108.11	113.45
20	B	826	CLA	C5-C3-C4	2.04	119.11	114.60
23	L	303	BCR	C12-C13-C14	2.04	122.07	118.94
20	1	318	CLA	C1-C2-C3	-2.04	122.52	126.04
20	B	822	CLA	CMB-C2B-C3B	2.04	131.52	126.59
20	1	306	CLA	CMB-C2B-C1B	2.04	128.47	125.37
20	1	306	CLA	O2A-CGA-CBA	2.04	120.57	114.03
20	L	306	CLA	CHC-C4B-NB	-2.04	122.10	124.26
20	B	817	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
20	J	103	CLA	CHB-C1B-C2B	-2.04	121.49	127.24
20	B	819	CLA	C2A-C1A-CHA	-2.04	120.30	123.86
20	4	308	CLA	C4A-NA-C1A	2.04	107.62	106.71
20	A	809	CLA	CHB-C1B-NB	-2.03	122.10	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	3	303	BCR	C1-C6-C7	2.03	121.53	115.78
28	A	824	CL0	O2A-CGA-O1A	-2.03	118.46	123.59
20	B	849	CLA	C1-O2A-CGA	2.03	121.78	116.44
20	F	304	CLA	CHB-C1B-C2B	-2.03	121.50	127.24
20	A	848	CLA	CHB-C1B-C2B	-2.03	121.50	127.24
19	2	301	CHL	C1C-C2C-C3C	-2.03	105.50	107.11
20	B	845	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
20	B	822	CLA	CHC-C4B-NB	-2.03	122.11	124.26
20	A	844	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
20	1	307	CLA	CED-O2D-CGD	2.03	120.53	115.94
20	A	808	CLA	C6-C7-C8	-2.03	109.36	115.92
20	B	815	CLA	C2A-C1A-CHA	-2.03	120.31	123.86
20	B	844	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
20	A	812	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
20	A	806	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
20	A	829	CLA	C2A-C1A-CHA	-2.03	120.32	123.86
20	4	303	CLA	O2D-CGD-O1D	-2.03	119.88	123.84
19	2	302	CHL	O2A-CGA-CBA	2.03	120.23	112.23
20	B	831	CLA	CHB-C1B-C2B	-2.02	121.52	127.24
20	A	801	CLA	O2A-CGA-CBA	2.02	118.26	111.91
20	A	848	CLA	CHB-C1B-NB	-2.02	122.11	124.26
20	1	306	CLA	C4A-NA-C1A	2.02	107.62	106.71
20	4	310	CLA	CHB-C1B-C2B	-2.02	121.52	127.24
20	B	829	CLA	C1-C2-C3	-2.02	122.54	126.04
20	1	305	CLA	CED-O2D-CGD	2.02	120.51	115.94
20	B	849	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
19	2	302	CHL	C1C-C2C-C3C	-2.02	105.51	107.11
20	2	303	CLA	CBA-CAA-C2A	2.02	119.83	113.86
20	1	309	CLA	CHB-C1B-C2B	-2.02	121.53	127.24
23	1	312	BCR	C7-C8-C9	2.02	129.29	126.23
23	1	312	BCR	C1-C6-C5	-2.02	119.77	122.61
20	A	831	CLA	CHB-C1B-C2B	-2.02	121.54	127.24
20	A	842	CLA	CED-O2D-CGD	2.02	120.50	115.94
23	J	101	BCR	C24-C23-C22	2.02	129.28	126.23
20	A	833	CLA	O2A-CGA-CBA	2.02	118.23	111.91
20	A	847	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
20	3	308	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
20	A	805	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
20	4	304	CLA	O2D-CGD-O1D	-2.01	119.90	123.84
23	B	834	BCR	C20-C21-C22	2.01	130.18	127.31
20	G	206	CLA	CHB-C1B-NB	-2.01	122.13	124.26
20	B	809	CLA	C3B-C4B-NB	2.01	112.38	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	847	CLA	C3B-C4B-NB	2.01	112.38	110.52
20	A	811	CLA	CHB-C1B-C2B	-2.01	121.56	127.24
19	1	317	CHL	C1C-C2C-C3C	-2.01	105.52	107.11
20	B	807	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
23	F	302	BCR	C11-C10-C9	2.01	130.17	127.31
20	A	839	CLA	CHB-C1B-C2B	-2.01	121.57	127.24
20	1	303	CLA	CMB-C2B-C1B	2.01	128.42	125.37
20	A	834	CLA	CMB-C2B-C3B	2.01	131.45	126.59
20	A	804	CLA	CHB-C1B-C2B	-2.01	121.57	127.24
20	A	825	CLA	C4-C3-C5	2.01	118.64	115.27
20	B	828	CLA	C3B-C4B-NB	2.00	112.38	110.52
20	4	312	CLA	O1D-CGD-CBD	-2.00	120.38	124.48
20	B	819	CLA	CHB-C1B-C2B	-2.00	121.58	127.24
20	3	314	CLA	CED-O2D-CGD	2.00	120.47	115.94
20	A	803	CLA	C4A-NA-C1A	2.00	107.61	106.71
20	B	847	CLA	CMB-C2B-C1B	2.00	128.42	125.37
20	A	805	CLA	C2A-C1A-CHA	-2.00	120.36	123.86
20	B	802	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
20	B	821	CLA	CBA-CAA-C2A	2.00	119.77	113.86
20	1	322	CLA	CHB-C1B-C2B	-2.00	121.58	127.24
20	B	806	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
23	G	203	BCR	C7-C8-C9	2.00	129.26	126.23
20	1	321	CLA	O2A-CGA-CBA	2.00	120.14	112.23
20	B	849	CLA	C3B-C4B-NB	2.00	112.37	110.52

All (93) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	2	318	CHL	C8
20	1	303	CLA	C8
20	1	304	CLA	C8
20	1	307	CLA	C8
20	1	318	CLA	C8
20	1	319	CLA	C8
20	2	304	CLA	C8
20	2	305	CLA	C8
20	2	307	CLA	C8
20	2	319	CLA	C8
20	3	307	CLA	C8
20	3	308	CLA	C8
20	3	309	CLA	C8
20	3	311	CLA	C8

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Mol	Chain	Res	Type	Atom
20	3	315	CLA	C8
20	3	317	CLA	C8
20	4	302	CLA	C8
20	4	310	CLA	C8
20	4	312	CLA	C8
20	4	316	CLA	C8
20	A	801	CLA	C8
20	A	802	CLA	C8
20	A	806	CLA	C8
20	A	807	CLA	C8
20	A	808	CLA	C8
20	A	809	CLA	C8
20	A	811	CLA	C8
20	A	812	CLA	C8
20	A	825	CLA	C8
20	A	826	CLA	C8
20	A	827	CLA	C8
20	A	829	CLA	C8
20	A	830	CLA	C8
20	A	832	CLA	C8
20	A	833	CLA	C8
20	A	834	CLA	C8
20	A	835	CLA	C8
20	A	837	CLA	C8
20	A	841	CLA	C8
20	A	842	CLA	C8
20	A	843	CLA	C8
20	A	845	CLA	C8
20	A	847	CLA	C8
20	A	848	CLA	C8
20	A	849	CLA	C8
20	A	850	CLA	C8
20	A	851	CLA	C8
20	A	852	CLA	C8
20	A	853	CLA	C8
20	A	854	CLA	C8
20	A	855	CLA	C8
20	A	856	CLA	C8
20	B	801	CLA	C8
20	B	803	CLA	C8
20	B	804	CLA	C8
20	B	806	CLA	C8

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Mol	Chain	Res	Type	Atom
20	B	807	CLA	C8
20	B	808	CLA	C8
20	B	809	CLA	C8
20	B	811	CLA	C8
20	B	812	CLA	C8
20	B	813	CLA	C8
20	B	814	CLA	C8
20	B	815	CLA	C8
20	B	816	CLA	C8
20	B	817	CLA	C8
20	B	818	CLA	C8
20	B	819	CLA	C8
20	B	820	CLA	C8
20	B	821	CLA	C8
20	B	822	CLA	C8
20	B	823	CLA	C8
20	B	824	CLA	C8
20	B	827	CLA	C8
20	B	829	CLA	C8
20	B	830	CLA	C8
20	B	831	CLA	C8
20	B	833	CLA	C8
20	B	844	CLA	C8
20	B	845	CLA	C8
20	B	847	CLA	C8
20	B	848	CLA	C8
20	B	850	CLA	C8
20	B	851	CLA	C8
20	B	852	CLA	C8
20	B	853	CLA	C8
20	F	304	CLA	C8
20	H	201	CLA	C8
20	K	204	CLA	C8
20	N	202	CLA	C8
20	O	206	CLA	C8
20	O	207	CLA	C8
28	A	824	CL0	CBD

All (1804) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	1	301	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	1	317	CHL	C2B-C3B-CAB-CBB
19	1	317	CHL	C4B-C3B-CAB-CBB
19	1	317	CHL	C3C-C2C-CMC-OMC
19	2	301	CHL	C3A-C2A-CAA-CBA
19	2	301	CHL	C2A-CAA-CBA-CGA
19	2	318	CHL	C3A-C2A-CAA-CBA
19	2	318	CHL	C3C-C2C-CMC-OMC
19	2	318	CHL	CBD-CGD-O2D-CED
19	2	322	CHL	C1C-C2C-CMC-OMC
19	3	313	CHL	C1A-C2A-CAA-CBA
19	4	305	CHL	CHA-CBD-CGD-O1D
19	4	305	CHL	CHA-CBD-CGD-O2D
19	4	305	CHL	CAD-CBD-CGD-O1D
19	4	305	CHL	CAD-CBD-CGD-O2D
19	4	306	CHL	C1A-C2A-CAA-CBA
19	4	306	CHL	C3A-C2A-CAA-CBA
19	4	306	CHL	C2B-C3B-CAB-CBB
19	4	306	CHL	C4B-C3B-CAB-CBB
19	4	306	CHL	CBD-CGD-O2D-CED
19	4	307	CHL	C1A-C2A-CAA-CBA
19	4	307	CHL	C3A-C2A-CAA-CBA
20	1	302	CLA	CBD-CGD-O2D-CED
20	1	304	CLA	CBD-CGD-O2D-CED
20	1	308	CLA	CHA-CBD-CGD-O1D
20	1	308	CLA	CHA-CBD-CGD-O2D
20	2	303	CLA	C3A-C2A-CAA-CBA
20	2	307	CLA	CHA-CBD-CGD-O1D
20	2	308	CLA	C4-C3-C5-C6
20	2	319	CLA	C1A-C2A-CAA-CBA
20	2	319	CLA	C3A-C2A-CAA-CBA
20	2	320	CLA	CBD-CGD-O2D-CED
20	2	321	CLA	C1A-C2A-CAA-CBA
20	2	323	CLA	CHA-CBD-CGD-O1D
20	2	323	CLA	CHA-CBD-CGD-O2D
20	3	307	CLA	O1A-CGA-O2A-C1
20	3	309	CLA	CBD-CGD-O2D-CED
20	3	310	CLA	CBD-CGD-O2D-CED
20	3	311	CLA	CBD-CGD-O2D-CED
20	3	315	CLA	C1A-C2A-CAA-CBA
20	3	315	CLA	C3A-C2A-CAA-CBA
20	3	315	CLA	CBD-CGD-O2D-CED
20	3	319	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
20	3	319	CLA	CHA-CBD-CGD-O2D
20	4	304	CLA	C1A-C2A-CAA-CBA
20	4	304	CLA	CBD-CGD-O2D-CED
20	4	308	CLA	C3A-C2A-CAA-CBA
20	4	309	CLA	CBD-CGD-O2D-CED
20	4	310	CLA	CHA-CBD-CGD-O1D
20	4	310	CLA	CHA-CBD-CGD-O2D
20	4	313	CLA	C1A-C2A-CAA-CBA
20	4	313	CLA	C3A-C2A-CAA-CBA
20	4	316	CLA	CBD-CGD-O2D-CED
20	A	802	CLA	C1A-C2A-CAA-CBA
20	A	802	CLA	CHA-CBD-CGD-O1D
20	A	802	CLA	CHA-CBD-CGD-O2D
20	A	803	CLA	C2-C1-O2A-CGA
20	A	804	CLA	C2-C3-C5-C6
20	A	804	CLA	C4-C3-C5-C6
20	A	807	CLA	C2-C1-O2A-CGA
20	A	807	CLA	CHA-CBD-CGD-O1D
20	A	807	CLA	CHA-CBD-CGD-O2D
20	A	809	CLA	C1A-C2A-CAA-CBA
20	A	811	CLA	CHA-CBD-CGD-O1D
20	A	811	CLA	CHA-CBD-CGD-O2D
20	A	811	CLA	CAD-CBD-CGD-O1D
20	A	825	CLA	CBD-CGD-O2D-CED
20	A	829	CLA	CHA-CBD-CGD-O1D
20	A	829	CLA	CHA-CBD-CGD-O2D
20	A	829	CLA	CAD-CBD-CGD-O1D
20	A	833	CLA	CBD-CGD-O2D-CED
20	A	835	CLA	C2-C3-C5-C6
20	A	835	CLA	C4-C3-C5-C6
20	A	836	CLA	C3-C5-C6-C7
20	A	837	CLA	C2-C3-C5-C6
20	A	837	CLA	C4-C3-C5-C6
20	A	838	CLA	C1A-C2A-CAA-CBA
20	A	839	CLA	C1A-C2A-CAA-CBA
20	A	842	CLA	C3A-C2A-CAA-CBA
20	A	843	CLA	O2A-C1-C2-C3
20	A	843	CLA	C2-C3-C5-C6
20	A	843	CLA	C4-C3-C5-C6
20	A	844	CLA	CBA-CGA-O2A-C1
20	A	846	CLA	CBA-CGA-O2A-C1
20	A	851	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	A	851	CLA	CHA-CBD-CGD-O1D
20	A	851	CLA	CHA-CBD-CGD-O2D
20	A	853	CLA	C1A-C2A-CAA-CBA
20	A	853	CLA	CBD-CGD-O2D-CED
20	A	854	CLA	C1A-C2A-CAA-CBA
20	A	856	CLA	C2-C3-C5-C6
20	A	856	CLA	C4-C3-C5-C6
20	B	801	CLA	C1A-C2A-CAA-CBA
20	B	802	CLA	C1A-C2A-CAA-CBA
20	B	806	CLA	O2A-C1-C2-C3
20	B	808	CLA	C3A-C2A-CAA-CBA
20	B	808	CLA	O2A-C1-C2-C3
20	B	809	CLA	CHA-CBD-CGD-O1D
20	B	809	CLA	CBD-CGD-O2D-CED
20	B	812	CLA	C2-C3-C5-C6
20	B	812	CLA	C4-C3-C5-C6
20	B	812	CLA	C6-C7-C8-C9
20	B	821	CLA	C1A-C2A-CAA-CBA
20	B	823	CLA	C1A-C2A-CAA-CBA
20	B	823	CLA	C3A-C2A-CAA-CBA
20	B	823	CLA	CHA-CBD-CGD-O1D
20	B	823	CLA	CHA-CBD-CGD-O2D
20	B	824	CLA	C1A-C2A-CAA-CBA
20	B	827	CLA	C14-C13-C15-C16
20	B	831	CLA	C6-C7-C8-C9
20	B	833	CLA	C1A-C2A-CAA-CBA
20	B	833	CLA	CHA-CBD-CGD-O1D
20	B	833	CLA	CHA-CBD-CGD-O2D
20	B	844	CLA	CBD-CGD-O2D-CED
20	B	845	CLA	CBD-CGD-O2D-CED
20	B	846	CLA	CBD-CGD-O2D-CED
20	B	850	CLA	C1A-C2A-CAA-CBA
20	F	306	CLA	C2A-CAA-CBA-CGA
20	G	206	CLA	C1A-C2A-CAA-CBA
20	G	206	CLA	C3A-C2A-CAA-CBA
20	G	207	CLA	CHA-CBD-CGD-O1D
20	G	207	CLA	CHA-CBD-CGD-O2D
20	K	203	CLA	C1A-C2A-CAA-CBA
20	K	203	CLA	C3A-C2A-CAA-CBA
20	K	203	CLA	CHA-CBD-CGD-O1D
20	K	203	CLA	CHA-CBD-CGD-O2D
20	O	207	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	O	207	CLA	C3A-C2A-CAA-CBA
21	1	323	LUT	C21-C26-C27-C28
21	1	323	LUT	C25-C26-C27-C28
21	2	310	LUT	C31-C32-C33-C34
21	2	310	LUT	C31-C32-C33-C40
21	4	317	LUT	C7-C8-C9-C19
22	1	311	XAT	C5-C6-C7-C8
22	1	311	XAT	O4-C6-C7-C8
22	1	311	XAT	C7-C8-C9-C10
22	1	311	XAT	C7-C8-C9-C19
22	1	311	XAT	C13-C14-C15-C35
22	1	311	XAT	C21-C26-C27-C28
22	1	311	XAT	C25-C26-C27-C28
22	2	311	XAT	C1-C6-C7-C8
22	3	302	XAT	C21-C26-C27-C28
22	3	302	XAT	C25-C26-C27-C28
22	3	302	XAT	C27-C28-C29-C30
22	3	302	XAT	C27-C28-C29-C39
22	3	302	XAT	C31-C32-C33-C34
23	1	312	BCR	C7-C8-C9-C10
23	1	312	BCR	C37-C22-C23-C24
23	2	312	BCR	C1-C6-C7-C8
23	2	312	BCR	C5-C6-C7-C8
23	2	312	BCR	C9-C10-C11-C12
23	2	312	BCR	C37-C22-C23-C24
23	4	319	BCR	C37-C22-C23-C24
23	4	320	BCR	C11-C12-C13-C35
23	A	816	BCR	C37-C22-C23-C24
23	A	816	BCR	C23-C24-C25-C30
23	B	834	BCR	C23-C24-C25-C26
23	B	834	BCR	C23-C24-C25-C30
23	B	839	BCR	C17-C18-C19-C20
23	B	839	BCR	C36-C18-C19-C20
23	B	839	BCR	C18-C19-C20-C21
23	B	839	BCR	C37-C22-C23-C24
23	F	301	BCR	C21-C22-C23-C24
23	F	301	BCR	C37-C22-C23-C24
23	G	201	BCR	C7-C8-C9-C10
23	G	201	BCR	C7-C8-C9-C34
23	G	203	BCR	C21-C22-C23-C24
23	G	203	BCR	C37-C22-C23-C24
23	J	101	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
23	L	301	BCR	C7-C8-C9-C10
23	L	301	BCR	C7-C8-C9-C34
23	L	303	BCR	C19-C20-C21-C22
23	L	303	BCR	C37-C22-C23-C24
23	L	304	BCR	C17-C18-C19-C20
23	L	304	BCR	C36-C18-C19-C20
23	O	202	BCR	C11-C12-C13-C35
23	O	202	BCR	C23-C24-C25-C26
23	O	203	BCR	C11-C12-C13-C14
23	O	203	BCR	C11-C12-C13-C35
24	1	313	LHG	C4-O6-P-O5
24	1	313	LHG	O10-C23-O8-C6
24	1	313	LHG	C24-C23-O8-C6
24	2	313	LHG	C3-O3-P-O6
24	2	313	LHG	C5-C4-O6-P
24	2	313	LHG	O10-C23-O8-C6
24	2	314	LHG	C3-O3-P-O5
24	2	315	LHG	C1-C2-C3-O3
24	2	315	LHG	C2-C3-O3-P
24	4	301	LHG	C4-O6-P-O3
24	4	321	LHG	C2-C3-O3-P
24	A	820	LHG	C5-C4-O6-P
24	A	820	LHG	O9-C7-O7-C5
24	A	820	LHG	C8-C7-O7-C5
24	B	842	LHG	O9-C7-O7-C5
24	B	842	LHG	C8-C7-O7-C5
24	B	843	LHG	O6-C4-C5-O7
24	I	101	LHG	C4-C5-C6-O8
24	I	101	LHG	O7-C5-C6-O8
24	O	205	LHG	O10-C23-O8-C6
25	1	316	MGE	O6D-C1D-O3G-C3G
25	1	324	MGE	C2A-C1A-O1G-C1G
25	1	324	MGE	O1A-C1A-O1G-C1G
25	1	324	MGE	C2B-C1B-O2G-C2G
25	1	324	MGE	O1B-C1B-O2G-C2G
25	3	305	MGE	C2A-C1A-O1G-C1G
25	3	305	MGE	O1A-C1A-O1G-C1G
25	A	823	MGE	C2D-C1D-O3G-C3G
25	A	823	MGE	O6D-C1D-O3G-C3G
25	J	102	MGE	C2A-C1A-O1G-C1G
25	J	102	MGE	O1A-C1A-O1G-C1G
25	N	201	MGE	O6D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
29	B	840	DGD	O1B-C1B-O2G-C2G
29	J	104	DGD	O6D-C1D-O3G-C3G
20	2	320	CLA	O1D-CGD-O2D-CED
20	A	825	CLA	O1D-CGD-O2D-CED
20	F	304	CLA	O1D-CGD-O2D-CED
20	O	208	CLA	O1D-CGD-O2D-CED
19	4	306	CHL	O1D-CGD-O2D-CED
20	1	304	CLA	O1D-CGD-O2D-CED
20	3	309	CLA	O1D-CGD-O2D-CED
20	B	821	CLA	O1D-CGD-O2D-CED
20	B	844	CLA	O1D-CGD-O2D-CED
20	B	845	CLA	O1D-CGD-O2D-CED
20	J	103	CLA	O1D-CGD-O2D-CED
19	1	301	CHL	CBD-CGD-O2D-CED
19	1	317	CHL	CBD-CGD-O2D-CED
19	2	302	CHL	CBD-CGD-O2D-CED
19	4	307	CHL	CBD-CGD-O2D-CED
20	2	304	CLA	CBD-CGD-O2D-CED
20	2	317	CLA	CBD-CGD-O2D-CED
20	3	319	CLA	CBD-CGD-O2D-CED
20	4	303	CLA	CBD-CGD-O2D-CED
20	B	802	CLA	CBD-CGD-O2D-CED
20	B	806	CLA	CBD-CGD-O2D-CED
20	B	821	CLA	CBD-CGD-O2D-CED
20	B	828	CLA	CBD-CGD-O2D-CED
20	B	848	CLA	CBD-CGD-O2D-CED
20	F	304	CLA	CBD-CGD-O2D-CED
20	J	103	CLA	CBD-CGD-O2D-CED
20	O	207	CLA	CBD-CGD-O2D-CED
20	O	208	CLA	CBD-CGD-O2D-CED
19	1	317	CHL	O1A-CGA-O2A-C1
20	3	309	CLA	O1A-CGA-O2A-C1
20	A	809	CLA	O1A-CGA-O2A-C1
20	B	847	CLA	O1A-CGA-O2A-C1
20	A	844	CLA	O1A-CGA-O2A-C1
20	4	304	CLA	O1D-CGD-O2D-CED
20	B	828	CLA	O1D-CGD-O2D-CED
20	O	207	CLA	O1D-CGD-O2D-CED
19	2	302	CHL	O1D-CGD-O2D-CED
19	2	318	CHL	O1D-CGD-O2D-CED
19	4	307	CHL	O1D-CGD-O2D-CED
20	1	302	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	3	310	CLA	O1D-CGD-O2D-CED
20	3	315	CLA	O1D-CGD-O2D-CED
20	4	309	CLA	O1D-CGD-O2D-CED
20	4	316	CLA	O1D-CGD-O2D-CED
20	A	833	CLA	O1D-CGD-O2D-CED
20	A	853	CLA	O1D-CGD-O2D-CED
20	B	809	CLA	O1D-CGD-O2D-CED
24	2	313	LHG	C24-C23-O8-C6
24	O	205	LHG	C24-C23-O8-C6
19	2	301	CHL	CBD-CGD-O2D-CED
20	2	307	CLA	CBD-CGD-O2D-CED
20	4	314	CLA	CBD-CGD-O2D-CED
20	A	834	CLA	CBD-CGD-O2D-CED
20	A	851	CLA	CBD-CGD-O2D-CED
20	A	852	CLA	CBD-CGD-O2D-CED
20	B	804	CLA	CBD-CGD-O2D-CED
20	B	819	CLA	CBD-CGD-O2D-CED
20	B	827	CLA	CBD-CGD-O2D-CED
20	B	853	CLA	CBD-CGD-O2D-CED
20	F	306	CLA	CBD-CGD-O2D-CED
20	A	850	CLA	O1A-CGA-O2A-C1
20	B	803	CLA	O1A-CGA-O2A-C1
20	B	814	CLA	O1A-CGA-O2A-C1
20	B	833	CLA	O1A-CGA-O2A-C1
20	O	207	CLA	O1A-CGA-O2A-C1
20	B	846	CLA	O1D-CGD-O2D-CED
19	4	305	CHL	CBD-CGD-O2D-CED
20	3	317	CLA	CBD-CGD-O2D-CED
20	A	811	CLA	CBD-CGD-O2D-CED
20	A	838	CLA	CBD-CGD-O2D-CED
20	K	206	CLA	CBD-CGD-O2D-CED
20	B	844	CLA	O1A-CGA-O2A-C1
20	3	311	CLA	O1D-CGD-O2D-CED
20	1	307	CLA	C3-C5-C6-C7
20	4	302	CLA	C3-C5-C6-C7
20	4	310	CLA	C3-C5-C6-C7
20	A	803	CLA	C3-C5-C6-C7
20	A	805	CLA	C3-C5-C6-C7
20	A	825	CLA	C3-C5-C6-C7
20	A	829	CLA	C3-C5-C6-C7
20	A	842	CLA	C3-C5-C6-C7
20	B	801	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
20	B	807	CLA	C3-C5-C6-C7
20	B	820	CLA	C3-C5-C6-C7
20	B	823	CLA	C3-C5-C6-C7
20	B	833	CLA	C3-C5-C6-C7
20	B	844	CLA	C3-C5-C6-C7
19	1	317	CHL	CBA-CGA-O2A-C1
20	3	307	CLA	CBA-CGA-O2A-C1
20	3	309	CLA	CBA-CGA-O2A-C1
20	3	315	CLA	CBA-CGA-O2A-C1
20	A	809	CLA	CBA-CGA-O2A-C1
20	A	833	CLA	CBA-CGA-O2A-C1
20	B	803	CLA	CBA-CGA-O2A-C1
20	B	833	CLA	CBA-CGA-O2A-C1
20	B	847	CLA	CBA-CGA-O2A-C1
29	B	840	DGD	C2B-C1B-O2G-C2G
20	2	321	CLA	CBD-CGD-O2D-CED
20	A	808	CLA	CBD-CGD-O2D-CED
20	B	848	CLA	O1D-CGD-O2D-CED
20	B	813	CLA	C4-C3-C5-C6
20	B	813	CLA	C2-C3-C5-C6
19	2	309	CHL	CBD-CGD-O2D-CED
20	B	817	CLA	CBD-CGD-O2D-CED
19	3	313	CHL	C2A-CAA-CBA-CGA
19	4	315	CHL	C2A-CAA-CBA-CGA
20	1	305	CLA	C2A-CAA-CBA-CGA
20	2	308	CLA	C2A-CAA-CBA-CGA
20	A	832	CLA	C2A-CAA-CBA-CGA
20	A	844	CLA	C2A-CAA-CBA-CGA
20	A	851	CLA	C2A-CAA-CBA-CGA
20	K	203	CLA	C2A-CAA-CBA-CGA
20	4	303	CLA	O1D-CGD-O2D-CED
20	A	846	CLA	O1A-CGA-O2A-C1
20	3	317	CLA	C3-C5-C6-C7
20	4	316	CLA	C3-C5-C6-C7
20	A	811	CLA	C3-C5-C6-C7
20	A	832	CLA	C3-C5-C6-C7
20	B	804	CLA	C3-C5-C6-C7
20	B	809	CLA	C3-C5-C6-C7
20	2	319	CLA	CBA-CGA-O2A-C1
20	2	321	CLA	CBA-CGA-O2A-C1
20	A	850	CLA	CBA-CGA-O2A-C1
20	B	808	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	B	814	CLA	CBA-CGA-O2A-C1
20	B	820	CLA	CBA-CGA-O2A-C1
20	B	823	CLA	CBA-CGA-O2A-C1
20	B	848	CLA	CBA-CGA-O2A-C1
20	O	207	CLA	CBA-CGA-O2A-C1
29	O	201	DGD	C2A-C1A-O1G-C1G
20	A	832	CLA	CBD-CGD-O2D-CED
20	3	315	CLA	O1A-CGA-O2A-C1
20	A	801	CLA	O1A-CGA-O2A-C1
20	A	833	CLA	O1A-CGA-O2A-C1
20	B	820	CLA	O1A-CGA-O2A-C1
20	B	848	CLA	O1A-CGA-O2A-C1
29	O	201	DGD	O1A-C1A-O1G-C1G
20	2	317	CLA	O1D-CGD-O2D-CED
21	2	310	LUT	C29-C30-C31-C32
22	3	302	XAT	C33-C34-C35-C15
23	B	839	BCR	C15-C16-C17-C18
23	G	203	BCR	C19-C20-C21-C22
23	L	304	BCR	C15-C16-C17-C18
20	1	322	CLA	CBD-CGD-O2D-CED
20	3	316	CLA	CBD-CGD-O2D-CED
20	A	802	CLA	CBD-CGD-O2D-CED
20	A	806	CLA	CBD-CGD-O2D-CED
20	A	848	CLA	CBD-CGD-O2D-CED
20	L	307	CLA	CBD-CGD-O2D-CED
20	3	319	CLA	O1D-CGD-O2D-CED
24	2	315	LHG	O2-C2-C3-O3
20	3	309	CLA	C3-C5-C6-C7
20	A	806	CLA	C3-C5-C6-C7
20	A	826	CLA	C3-C5-C6-C7
20	A	849	CLA	C3-C5-C6-C7
20	B	813	CLA	C3-C5-C6-C7
20	B	829	CLA	C3-C5-C6-C7
20	2	305	CLA	CBA-CGA-O2A-C1
20	B	802	CLA	O1D-CGD-O2D-CED
20	B	806	CLA	O1D-CGD-O2D-CED
20	F	306	CLA	CBA-CGA-O2A-C1
20	B	824	CLA	CBD-CGD-O2D-CED
20	B	825	CLA	CBD-CGD-O2D-CED
20	K	203	CLA	CBD-CGD-O2D-CED
19	4	305	CHL	C2C-C3C-CAC-CBC
19	1	301	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	A	851	CLA	C3-C5-C6-C7
20	A	801	CLA	CBA-CGA-O2A-C1
20	A	841	CLA	CBA-CGA-O2A-C1
20	B	844	CLA	CBA-CGA-O2A-C1
24	1	313	LHG	C5-C4-O6-P
20	2	319	CLA	O1A-CGA-O2A-C1
20	2	321	CLA	O1A-CGA-O2A-C1
20	B	808	CLA	O1A-CGA-O2A-C1
20	B	823	CLA	O1A-CGA-O2A-C1
20	B	801	CLA	C4-C3-C5-C6
20	B	806	CLA	C4-C3-C5-C6
20	B	807	CLA	C4-C3-C5-C6
20	B	814	CLA	C4-C3-C5-C6
20	B	816	CLA	C4-C3-C5-C6
20	B	801	CLA	C2-C3-C5-C6
20	B	806	CLA	C2-C3-C5-C6
20	B	807	CLA	C2-C3-C5-C6
20	B	814	CLA	C2-C3-C5-C6
20	B	816	CLA	C2-C3-C5-C6
29	O	201	DGD	O6D-C5D-C6D-O5D
19	4	307	CHL	C2A-CAA-CBA-CGA
20	B	851	CLA	C2A-CAA-CBA-CGA
20	A	841	CLA	O1A-CGA-O2A-C1
25	1	315	MGE	O6D-C1D-O3G-C3G
20	1	320	CLA	CBA-CGA-O2A-C1
20	2	308	CLA	CBA-CGA-O2A-C1
20	A	828	CLA	CBA-CGA-O2A-C1
19	1	317	CHL	O1D-CGD-O2D-CED
20	2	304	CLA	O1D-CGD-O2D-CED
20	2	307	CLA	O1D-CGD-O2D-CED
20	2	305	CLA	O1A-CGA-O2A-C1
20	2	308	CLA	O1A-CGA-O2A-C1
29	O	201	DGD	C4D-C5D-C6D-O5D
20	A	852	CLA	O1D-CGD-O2D-CED
20	B	819	CLA	O1D-CGD-O2D-CED
20	B	853	CLA	O1D-CGD-O2D-CED
20	A	828	CLA	O1A-CGA-O2A-C1
20	3	308	CLA	C3-C5-C6-C7
20	B	816	CLA	C3-C5-C6-C7
20	F	306	CLA	O1D-CGD-O2D-CED
20	4	310	CLA	CBA-CGA-O2A-C1
20	A	807	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	A	830	CLA	CBA-CGA-O2A-C1
20	A	834	CLA	CBA-CGA-O2A-C1
20	A	847	CLA	CBA-CGA-O2A-C1
20	F	304	CLA	CBA-CGA-O2A-C1
20	A	842	CLA	CBD-CGD-O2D-CED
20	A	827	CLA	C5-C6-C7-C8
20	A	853	CLA	C15-C16-C17-C18
20	A	812	CLA	C15-C16-C17-C18
20	A	841	CLA	C8-C10-C11-C12
20	A	855	CLA	C5-C6-C7-C8
20	B	804	CLA	C15-C16-C17-C18
20	O	206	CLA	C10-C11-C12-C13
20	B	849	CLA	C3-C5-C6-C7
20	L	306	CLA	C3-C5-C6-C7
25	1	315	MGE	C2D-C1D-O3G-C3G
25	1	316	MGE	C2D-C1D-O3G-C3G
25	N	201	MGE	C2D-C1D-O3G-C3G
20	A	846	CLA	C2C-C3C-CAC-CBC
20	A	834	CLA	O1A-CGA-O2A-C1
20	A	802	CLA	C11-C10-C8-C9
20	A	808	CLA	C11-C10-C8-C9
20	A	809	CLA	C14-C13-C15-C16
20	A	827	CLA	C11-C12-C13-C14
20	A	841	CLA	C6-C7-C8-C9
20	A	848	CLA	C6-C7-C8-C9
20	A	850	CLA	C11-C10-C8-C9
20	A	851	CLA	C14-C13-C15-C16
20	A	854	CLA	C6-C7-C8-C9
20	B	804	CLA	C14-C13-C15-C16
20	B	816	CLA	C6-C7-C8-C9
20	B	820	CLA	C6-C7-C8-C9
20	B	822	CLA	C11-C10-C8-C9
20	B	829	CLA	C11-C10-C8-C9
20	B	830	CLA	C11-C10-C8-C9
20	B	850	CLA	C6-C7-C8-C9
20	F	304	CLA	C14-C13-C15-C16
20	O	206	CLA	C11-C10-C8-C9
20	B	827	CLA	O1D-CGD-O2D-CED
20	B	822	CLA	CBD-CGD-O2D-CED
19	2	322	CHL	C2A-CAA-CBA-CGA
20	A	847	CLA	C2A-CAA-CBA-CGA
20	B	801	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
20	B	824	CLA	C2A-CAA-CBA-CGA
21	1	323	LUT	C7-C8-C9-C19
22	1	311	XAT	C27-C28-C29-C39
22	1	311	XAT	C31-C32-C33-C40
23	1	312	BCR	C7-C8-C9-C34
23	A	857	BCR	C7-C8-C9-C34
23	B	836	BCR	C7-C8-C9-C34
23	B	838	BCR	C37-C22-C23-C24
23	B	839	BCR	C11-C12-C13-C35
23	I	102	BCR	C37-C22-C23-C24
21	1	323	LUT	C7-C8-C9-C10
22	1	311	XAT	C27-C28-C29-C30
22	1	311	XAT	C31-C32-C33-C34
23	4	320	BCR	C11-C12-C13-C14
23	A	857	BCR	C7-C8-C9-C10
23	B	836	BCR	C7-C8-C9-C10
23	B	838	BCR	C21-C22-C23-C24
23	B	839	BCR	C11-C12-C13-C14
23	G	203	BCR	C7-C8-C9-C10
23	I	102	BCR	C21-C22-C23-C24
23	L	303	BCR	C21-C22-C23-C24
20	A	807	CLA	O1A-CGA-O2A-C1
20	A	830	CLA	O1A-CGA-O2A-C1
20	A	847	CLA	O1A-CGA-O2A-C1
20	1	318	CLA	C8-C10-C11-C12
20	A	835	CLA	C8-C10-C11-C12
20	B	847	CLA	C5-C6-C7-C8
20	A	809	CLA	C3-C5-C6-C7
20	B	803	CLA	C3-C5-C6-C7
20	B	817	CLA	CBA-CGA-O2A-C1
20	B	850	CLA	CBA-CGA-O2A-C1
20	B	852	CLA	CBA-CGA-O2A-C1
20	3	311	CLA	C8-C10-C11-C12
20	A	845	CLA	C15-C16-C17-C18
20	A	848	CLA	C13-C15-C16-C17
20	B	820	CLA	C8-C10-C11-C12
20	N	202	CLA	C5-C6-C7-C8
25	1	316	MGE	C1A-C2A-C3A-C4A
20	A	806	CLA	C8-C10-C11-C12
20	A	842	CLA	C10-C11-C12-C13
20	A	851	CLA	C8-C10-C11-C12
20	B	845	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
19	2	301	CHL	O1D-CGD-O2D-CED
20	F	304	CLA	O1A-CGA-O2A-C1
24	4	301	LHG	C7-C8-C9-C10
29	O	201	DGD	C1A-C2A-C3A-C4A
20	B	813	CLA	CBD-CGD-O2D-CED
20	A	851	CLA	O1D-CGD-O2D-CED
20	2	307	CLA	C5-C6-C7-C8
20	A	841	CLA	C10-C11-C12-C13
20	B	847	CLA	C13-C15-C16-C17
26	B	832	PQN	C15-C16-C17-C18
20	A	834	CLA	O1D-CGD-O2D-CED
20	B	848	CLA	C13-C15-C16-C17
20	4	313	CLA	CBD-CGD-O2D-CED
20	2	307	CLA	C13-C15-C16-C17
20	B	822	CLA	C15-C16-C17-C18
20	A	802	CLA	C12-C13-C15-C16
20	A	829	CLA	C6-C7-C8-C10
20	A	851	CLA	C12-C13-C15-C16
20	B	830	CLA	C11-C10-C8-C7
20	B	844	CLA	C12-C13-C15-C16
20	F	304	CLA	C12-C13-C15-C16
20	B	819	CLA	C3-C5-C6-C7
19	4	306	CHL	C2A-CAA-CBA-CGA
20	B	833	CLA	C2A-CAA-CBA-CGA
19	4	305	CHL	O1D-CGD-O2D-CED
20	4	314	CLA	O1D-CGD-O2D-CED
20	B	804	CLA	O1D-CGD-O2D-CED
20	4	316	CLA	C13-C15-C16-C17
20	B	833	CLA	C10-C11-C12-C13
20	O	206	CLA	C5-C6-C7-C8
20	1	320	CLA	O1A-CGA-O2A-C1
20	4	310	CLA	O1A-CGA-O2A-C1
20	B	817	CLA	O1A-CGA-O2A-C1
20	1	309	CLA	CBD-CGD-O2D-CED
19	2	318	CHL	C5-C6-C7-C8
20	A	825	CLA	C13-C15-C16-C17
20	B	850	CLA	C10-C11-C12-C13
20	F	306	CLA	O1A-CGA-O2A-C1
20	H	201	CLA	C3-C5-C6-C7
20	3	317	CLA	C8-C10-C11-C12
20	A	830	CLA	C5-C6-C7-C8
20	B	827	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	B	803	CLA	C2C-C3C-CAC-CBC
20	4	302	CLA	C10-C11-C12-C13
20	A	809	CLA	C5-C6-C7-C8
20	A	849	CLA	C8-C10-C11-C12
20	A	851	CLA	C10-C11-C12-C13
20	A	852	CLA	C8-C10-C11-C12
20	B	816	CLA	C10-C11-C12-C13
20	B	852	CLA	C15-C16-C17-C18
20	H	201	CLA	C5-C6-C7-C8
20	O	206	CLA	C13-C15-C16-C17
20	B	852	CLA	O1A-CGA-O2A-C1
20	2	321	CLA	O1D-CGD-O2D-CED
20	B	807	CLA	C15-C16-C17-C18
20	B	852	CLA	C8-C10-C11-C12
20	B	826	CLA	CBA-CGA-O2A-C1
19	3	313	CHL	CBD-CGD-O2D-CED
20	4	310	CLA	C10-C11-C12-C13
20	A	837	CLA	C13-C15-C16-C17
20	3	317	CLA	O1D-CGD-O2D-CED
20	A	812	CLA	C4-C3-C5-C6
20	3	308	CLA	C10-C11-C12-C13
20	K	206	CLA	O1D-CGD-O2D-CED
20	B	848	CLA	C3-C5-C6-C7
20	A	804	CLA	CBA-CGA-O2A-C1
20	B	830	CLA	CBA-CGA-O2A-C1
20	B	851	CLA	CBA-CGA-O2A-C1
20	K	203	CLA	CBA-CGA-O2A-C1
20	B	851	CLA	CBD-CGD-O2D-CED
20	A	829	CLA	C10-C11-C12-C13
23	4	320	BCR	C20-C21-C22-C37
23	B	839	BCR	C20-C21-C22-C37
23	O	202	BCR	C11-C10-C9-C34
20	A	838	CLA	O1D-CGD-O2D-CED
20	B	801	CLA	C16-C17-C18-C20
20	A	801	CLA	C12-C13-C15-C16
19	2	309	CHL	O1D-CGD-O2D-CED
20	A	808	CLA	O1D-CGD-O2D-CED
20	A	856	CLA	C5-C6-C7-C8
24	O	205	LHG	C15-C16-C17-C18
20	3	316	CLA	O1D-CGD-O2D-CED
20	A	831	CLA	C2C-C3C-CAC-CBC
20	B	818	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	4	320	BCR	C20-C21-C22-C23
20	1	318	CLA	CBA-CGA-O2A-C1
20	A	851	CLA	CBA-CGA-O2A-C1
20	B	818	CLA	CBA-CGA-O2A-C1
24	1	313	LHG	C18-C19-C20-C21
25	4	322	MGE	C2A-C3A-C4A-C5A
20	A	852	CLA	C15-C16-C17-C18
20	K	203	CLA	O1A-CGA-O2A-C1
20	A	806	CLA	O1D-CGD-O2D-CED
20	A	811	CLA	O1D-CGD-O2D-CED
20	2	307	CLA	C4-C3-C5-C6
20	A	809	CLA	C4-C3-C5-C6
20	A	834	CLA	C4-C3-C5-C6
20	B	809	CLA	C4-C3-C5-C6
20	2	307	CLA	C2-C3-C5-C6
20	A	812	CLA	C2-C3-C5-C6
20	A	806	CLA	C14-C13-C15-C16
20	A	808	CLA	C6-C7-C8-C9
20	A	825	CLA	C14-C13-C15-C16
20	A	833	CLA	C11-C10-C8-C9
20	A	845	CLA	C11-C12-C13-C14
20	B	816	CLA	C14-C13-C15-C16
20	F	304	CLA	C11-C10-C8-C9
20	A	803	CLA	C11-C10-C8-C7
24	B	841	LHG	C11-C10-C9-C8
20	4	316	CLA	C5-C6-C7-C8
20	4	316	CLA	C10-C11-C12-C13
20	A	803	CLA	C2A-CAA-CBA-CGA
20	B	803	CLA	C2A-CAA-CBA-CGA
20	B	830	CLA	O1A-CGA-O2A-C1
20	B	850	CLA	O1A-CGA-O2A-C1
23	G	203	BCR	C7-C8-C9-C34
22	2	311	XAT	C27-C28-C29-C30
20	B	847	CLA	C3-C5-C6-C7
20	N	202	CLA	C3-C5-C6-C7
20	O	206	CLA	C3-C5-C6-C7
25	G	204	MGE	C1A-C2A-C3A-C4A
24	2	314	LHG	C27-C28-C29-C30
25	3	306	MGE	C2A-C3A-C4A-C5A
20	A	849	CLA	C16-C17-C18-C20
20	A	801	CLA	C15-C16-C17-C18
20	A	806	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
20	A	807	CLA	CBD-CGD-O2D-CED
20	A	847	CLA	CBD-CGD-O2D-CED
20	1	322	CLA	O1D-CGD-O2D-CED
20	A	832	CLA	O1D-CGD-O2D-CED
20	B	817	CLA	O1D-CGD-O2D-CED
24	4	321	LHG	C30-C31-C32-C33
29	J	104	DGD	CCB-CDB-CEB-CFB
24	O	205	LHG	C7-C8-C9-C10
20	B	830	CLA	C8-C10-C11-C12
19	4	305	CHL	C4C-C3C-CAC-CBC
20	A	802	CLA	O1D-CGD-O2D-CED
20	3	311	CLA	CBA-CGA-O2A-C1
20	B	853	CLA	CBA-CGA-O2A-C1
24	B	841	LHG	C10-C11-C12-C13
20	L	307	CLA	O1D-CGD-O2D-CED
19	4	305	CHL	C3A-C2A-CAA-CBA
20	1	306	CLA	C3A-C2A-CAA-CBA
20	3	307	CLA	C3A-C2A-CAA-CBA
20	3	309	CLA	C3A-C2A-CAA-CBA
20	3	319	CLA	C3A-C2A-CAA-CBA
20	4	311	CLA	C3A-C2A-CAA-CBA
20	A	802	CLA	C3A-C2A-CAA-CBA
20	A	839	CLA	C3A-C2A-CAA-CBA
20	A	851	CLA	C3A-C2A-CAA-CBA
20	B	811	CLA	C3A-C2A-CAA-CBA
20	B	824	CLA	C3A-C2A-CAA-CBA
20	B	833	CLA	C3A-C2A-CAA-CBA
20	B	848	CLA	C3A-C2A-CAA-CBA
20	B	850	CLA	C3A-C2A-CAA-CBA
20	B	852	CLA	C3A-C2A-CAA-CBA
20	K	205	CLA	C3A-C2A-CAA-CBA
20	B	801	CLA	C15-C16-C17-C18
25	3	306	MGE	C2G-C1G-O1G-C1A
29	O	201	DGD	C8A-C9A-CAA-CBA
20	A	848	CLA	O1D-CGD-O2D-CED
20	A	834	CLA	C6-C7-C8-C9
24	2	314	LHG	C9-C10-C11-C12
24	I	101	LHG	C32-C33-C34-C35
24	A	822	LHG	C4-C5-C6-O8
20	G	207	CLA	CBD-CGD-O2D-CED
20	3	317	CLA	O2A-C1-C2-C3
20	B	824	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
20	3	311	CLA	C5-C6-C7-C8
20	4	312	CLA	C2-C3-C5-C6
20	A	809	CLA	C2-C3-C5-C6
20	A	834	CLA	C2-C3-C5-C6
20	A	804	CLA	O1A-CGA-O2A-C1
20	B	818	CLA	O1A-CGA-O2A-C1
20	B	826	CLA	O1A-CGA-O2A-C1
20	B	851	CLA	O1A-CGA-O2A-C1
20	B	801	CLA	C16-C17-C18-C19
20	3	311	CLA	C13-C15-C16-C17
20	B	819	CLA	C5-C6-C7-C8
20	4	302	CLA	CBA-CGA-O2A-C1
20	4	316	CLA	CBA-CGA-O2A-C1
20	A	835	CLA	CBA-CGA-O2A-C1
20	B	807	CLA	CBA-CGA-O2A-C1
20	B	801	CLA	C8-C10-C11-C12
24	O	205	LHG	C11-C12-C13-C14
29	J	104	DGD	C7B-C8B-C9B-CAB
20	B	813	CLA	C2-C1-O2A-CGA
29	B	840	DGD	C5B-C6B-C7B-C8B
20	A	837	CLA	C5-C6-C7-C8
20	B	851	CLA	C15-C16-C17-C18
20	1	318	CLA	O1A-CGA-O2A-C1
20	A	851	CLA	O1A-CGA-O2A-C1
20	B	853	CLA	O1A-CGA-O2A-C1
24	1	313	LHG	C27-C28-C29-C30
23	1	312	BCR	C1-C6-C7-C8
23	1	312	BCR	C5-C6-C7-C8
23	1	312	BCR	C23-C24-C25-C30
23	2	312	BCR	C23-C24-C25-C30
23	3	303	BCR	C23-C24-C25-C30
23	4	319	BCR	C1-C6-C7-C8
23	4	319	BCR	C5-C6-C7-C8
23	4	319	BCR	C23-C24-C25-C30
23	A	814	BCR	C1-C6-C7-C8
23	A	814	BCR	C5-C6-C7-C8
23	A	815	BCR	C23-C24-C25-C26
23	A	816	BCR	C23-C24-C25-C26
23	A	818	BCR	C23-C24-C25-C26
23	A	818	BCR	C23-C24-C25-C30
23	A	857	BCR	C23-C24-C25-C26
23	B	834	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	B	834	BCR	C5-C6-C7-C8
23	B	836	BCR	C23-C24-C25-C26
23	B	837	BCR	C23-C24-C25-C26
23	B	837	BCR	C23-C24-C25-C30
23	B	838	BCR	C23-C24-C25-C30
23	F	302	BCR	C23-C24-C25-C26
23	G	201	BCR	C1-C6-C7-C8
23	G	201	BCR	C23-C24-C25-C26
23	J	101	BCR	C5-C6-C7-C8
23	K	201	BCR	C1-C6-C7-C8
23	K	201	BCR	C5-C6-C7-C8
23	K	201	BCR	C23-C24-C25-C26
23	K	201	BCR	C23-C24-C25-C30
23	K	202	BCR	C23-C24-C25-C26
23	L	301	BCR	C5-C6-C7-C8
23	L	302	BCR	C1-C6-C7-C8
23	L	302	BCR	C5-C6-C7-C8
23	L	303	BCR	C23-C24-C25-C26
23	L	304	BCR	C23-C24-C25-C26
23	L	304	BCR	C23-C24-C25-C30
23	O	202	BCR	C1-C6-C7-C8
23	O	202	BCR	C23-C24-C25-C30
24	O	205	LHG	C32-C33-C34-C35
20	B	829	CLA	CBA-CGA-O2A-C1
20	H	201	CLA	CBA-CGA-O2A-C1
20	G	206	CLA	C2-C3-C5-C6
20	A	825	CLA	C12-C13-C15-C16
20	A	827	CLA	C11-C10-C8-C7
20	A	833	CLA	C11-C10-C8-C7
20	A	841	CLA	C6-C7-C8-C10
20	A	845	CLA	C11-C12-C13-C15
20	B	809	CLA	C2-C3-C5-C6
20	B	812	CLA	C12-C13-C15-C16
20	B	816	CLA	C12-C13-C15-C16
20	B	822	CLA	C11-C10-C8-C7
20	B	824	CLA	C2-C3-C5-C6
20	B	830	CLA	C11-C12-C13-C15
20	B	850	CLA	C6-C7-C8-C10
20	2	319	CLA	C3-C5-C6-C7
20	3	311	CLA	O1A-CGA-O2A-C1
20	4	302	CLA	O1A-CGA-O2A-C1
20	B	807	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	B	829	CLA	O1A-CGA-O2A-C1
20	B	808	CLA	C8-C10-C11-C12
20	B	830	CLA	C16-C17-C18-C19
20	A	805	CLA	CBA-CGA-O2A-C1
20	B	828	CLA	CBA-CGA-O2A-C1
20	K	204	CLA	CBA-CGA-O2A-C1
19	4	305	CHL	C2A-CAA-CBA-CGA
20	G	206	CLA	C2A-CAA-CBA-CGA
20	B	825	CLA	O1D-CGD-O2D-CED
20	A	812	CLA	C8-C10-C11-C12
20	B	824	CLA	O1D-CGD-O2D-CED
20	A	805	CLA	C5-C6-C7-C8
29	J	104	DGD	C7A-C8A-C9A-CAA
25	1	324	MGE	C1B-C2B-C3B-C4B
29	J	104	DGD	C1A-C2A-C3A-C4A
20	A	851	CLA	C5-C6-C7-C8
24	A	819	LHG	C13-C14-C15-C16
24	A	822	LHG	C31-C32-C33-C34
19	2	318	CHL	CBA-CGA-O2A-C1
20	B	801	CLA	CBA-CGA-O2A-C1
20	A	830	CLA	C15-C16-C17-C18
20	A	832	CLA	C10-C11-C12-C13
26	A	810	PQN	C15-C16-C17-C18
23	4	320	BCR	C18-C19-C20-C21
20	B	823	CLA	C8-C10-C11-C12
20	2	319	CLA	CBD-CGD-O2D-CED
20	4	316	CLA	O1A-CGA-O2A-C1
20	A	855	CLA	C3-C5-C6-C7
20	A	828	CLA	C3-C5-C6-C7
20	3	309	CLA	C8-C10-C11-C12
20	A	825	CLA	C15-C16-C17-C18
20	B	814	CLA	C10-C11-C12-C13
20	B	816	CLA	C15-C16-C17-C18
24	A	822	LHG	O7-C5-C6-O8
20	B	830	CLA	CBD-CGD-O2D-CED
20	A	835	CLA	O1A-CGA-O2A-C1
20	H	201	CLA	O1A-CGA-O2A-C1
20	3	311	CLA	C16-C17-C18-C19
20	A	802	CLA	C16-C17-C18-C20
20	A	849	CLA	C16-C17-C18-C19
20	3	307	CLA	C5-C6-C7-C8
20	B	803	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
20	4	312	CLA	C4-C3-C5-C6
20	B	824	CLA	C4-C3-C5-C6
20	A	802	CLA	C14-C13-C15-C16
20	B	844	CLA	C14-C13-C15-C16
20	B	851	CLA	C11-C10-C8-C9
24	O	205	LHG	C5-C6-O8-C23
20	1	307	CLA	CBD-CGD-O2D-CED
20	3	308	CLA	C2A-CAA-CBA-CGA
20	B	810	CLA	C2A-CAA-CBA-CGA
29	B	840	DGD	C4A-C5A-C6A-C7A
22	2	311	XAT	C27-C28-C29-C39
19	2	301	CHL	C1A-C2A-CAA-CBA
19	2	318	CHL	C1A-C2A-CAA-CBA
19	4	305	CHL	C1A-C2A-CAA-CBA
20	1	305	CLA	C1A-C2A-CAA-CBA
20	1	306	CLA	C1A-C2A-CAA-CBA
20	2	303	CLA	C1A-C2A-CAA-CBA
20	3	307	CLA	C1A-C2A-CAA-CBA
20	3	309	CLA	C1A-C2A-CAA-CBA
20	3	319	CLA	C1A-C2A-CAA-CBA
20	4	308	CLA	C1A-C2A-CAA-CBA
20	4	309	CLA	C1A-C2A-CAA-CBA
20	4	311	CLA	C1A-C2A-CAA-CBA
20	A	834	CLA	C1A-C2A-CAA-CBA
20	A	842	CLA	C1A-C2A-CAA-CBA
20	A	846	CLA	C1A-C2A-CAA-CBA
20	A	848	CLA	C1A-C2A-CAA-CBA
20	B	808	CLA	C1A-C2A-CAA-CBA
20	B	811	CLA	C1A-C2A-CAA-CBA
20	B	828	CLA	C1A-C2A-CAA-CBA
20	B	831	CLA	C1A-C2A-CAA-CBA
20	B	848	CLA	C1A-C2A-CAA-CBA
20	B	852	CLA	C1A-C2A-CAA-CBA
20	J	103	CLA	C1A-C2A-CAA-CBA
20	K	205	CLA	C1A-C2A-CAA-CBA
29	O	201	DGD	O6E-C5E-C6E-O5E
20	A	834	CLA	C6-C7-C8-C10
20	A	853	CLA	C16-C17-C18-C19
20	B	808	CLA	C13-C15-C16-C17
20	A	846	CLA	C4C-C3C-CAC-CBC
29	G	202	DGD	C3B-C4B-C5B-C6B
20	B	807	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	A	835	CLA	C3-C5-C6-C7
20	B	853	CLA	C3-C5-C6-C7
24	2	314	LHG	C5-C4-O6-P
24	O	204	LHG	C5-C4-O6-P
20	K	203	CLA	O1D-CGD-O2D-CED
20	B	803	CLA	C4C-C3C-CAC-CBC
20	A	853	CLA	CBA-CGA-O2A-C1
20	B	812	CLA	CBA-CGA-O2A-C1
24	B	843	LHG	O6-C4-C5-C6
24	2	313	LHG	C31-C32-C33-C34
20	A	830	CLA	C13-C15-C16-C17
20	B	801	CLA	C5-C6-C7-C8
20	B	812	CLA	C15-C16-C17-C18
20	B	830	CLA	C16-C17-C18-C20
24	B	842	LHG	C28-C29-C30-C31
20	A	830	CLA	C8-C10-C11-C12
20	A	854	CLA	C13-C15-C16-C17
19	1	301	CHL	C3A-C2A-CAA-CBA
20	B	828	CLA	O1A-CGA-O2A-C1
20	K	204	CLA	O1A-CGA-O2A-C1
20	A	837	CLA	C2C-C3C-CAC-CBC
24	2	315	LHG	C4-C5-C6-O8
24	A	820	LHG	C4-C5-C6-O8
25	F	303	MGE	O1G-C1G-C2G-C3G
25	F	303	MGE	C1G-C2G-C3G-O3G
24	2	314	LHG	C10-C11-C12-C13
20	A	805	CLA	O1A-CGA-O2A-C1
25	A	823	MGE	C2G-C3G-O3G-C1D
25	F	303	MGE	C2G-C3G-O3G-C1D
19	2	318	CHL	C8-C10-C11-C12
20	A	802	CLA	C5-C6-C7-C8
20	F	304	CLA	C13-C15-C16-C17
29	B	840	DGD	C1B-C2B-C3B-C4B
20	A	842	CLA	O1D-CGD-O2D-CED
20	3	308	CLA	CBA-CGA-O2A-C1
20	A	839	CLA	CBD-CGD-O2D-CED
20	B	812	CLA	O1A-CGA-O2A-C1
24	A	821	LHG	C14-C15-C16-C17
20	B	822	CLA	O1D-CGD-O2D-CED
20	B	816	CLA	C13-C15-C16-C17
20	3	309	CLA	C4-C3-C5-C6
20	A	802	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	A	807	CLA	C4-C3-C5-C6
26	B	832	PQN	C14-C13-C15-C16
29	G	202	DGD	C9B-CAB-CBB-CCB
20	2	305	CLA	C6-C7-C8-C10
20	B	801	CLA	C13-C15-C16-C17
20	1	318	CLA	C2A-CAA-CBA-CGA
20	4	310	CLA	C2-C1-O2A-CGA
20	A	826	CLA	C2-C1-O2A-CGA
20	A	831	CLA	C2-C1-O2A-CGA
20	A	847	CLA	C3-C5-C6-C7
29	O	201	DGD	C3A-C4A-C5A-C6A
20	1	309	CLA	O1D-CGD-O2D-CED
20	A	829	CLA	C15-C16-C17-C18
24	B	842	LHG	C24-C25-C26-C27
20	1	303	CLA	CBA-CGA-O2A-C1
19	2	318	CHL	O1A-CGA-O2A-C1
20	A	802	CLA	C16-C17-C18-C19
20	A	853	CLA	C16-C17-C18-C20
20	A	854	CLA	C10-C11-C12-C13
20	B	801	CLA	O1A-CGA-O2A-C1
29	B	840	DGD	C4E-C5E-C6E-O5E
29	B	840	DGD	O2G-C2G-C3G-O3G
20	A	808	CLA	C10-C11-C12-C13
20	A	853	CLA	O1A-CGA-O2A-C1
24	A	822	LHG	C13-C14-C15-C16
29	J	104	DGD	C1B-C2B-C3B-C4B
20	A	829	CLA	C4-C3-C5-C6
26	A	810	PQN	C14-C13-C15-C16
24	1	313	LHG	C11-C10-C9-C8
20	3	309	CLA	C2-C3-C5-C6
20	A	806	CLA	C6-C7-C8-C10
20	A	809	CLA	C12-C13-C15-C16
20	A	827	CLA	C12-C13-C15-C16
20	A	837	CLA	C12-C13-C15-C16
20	A	843	CLA	C12-C13-C15-C16
20	A	848	CLA	C6-C7-C8-C10
20	A	850	CLA	C11-C10-C8-C7
20	B	801	CLA	C11-C12-C13-C15
20	B	804	CLA	C12-C13-C15-C16
20	B	816	CLA	C6-C7-C8-C10
20	B	824	CLA	C11-C10-C8-C7
20	B	845	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
20	B	851	CLA	C11-C10-C8-C7
20	F	304	CLA	C11-C10-C8-C7
20	O	206	CLA	C11-C10-C8-C7
26	A	810	PQN	C12-C13-C15-C16
20	1	318	CLA	CAA-CBA-CGA-O2A
25	G	204	MGE	O2G-C1B-C2B-C3B
20	A	806	CLA	C6-C7-C8-C9
20	A	829	CLA	C6-C7-C8-C9
20	A	837	CLA	C14-C13-C15-C16
20	A	852	CLA	C6-C7-C8-C9
20	B	812	CLA	C14-C13-C15-C16
20	B	817	CLA	C11-C10-C8-C9
20	B	824	CLA	C11-C10-C8-C9
20	B	830	CLA	C11-C12-C13-C14
20	B	845	CLA	C11-C10-C8-C9
20	B	850	CLA	C11-C12-C13-C14
22	2	311	XAT	C33-C34-C35-C15
20	B	804	CLA	CBA-CGA-O2A-C1
22	3	302	XAT	C31-C32-C33-C40
20	A	830	CLA	C10-C11-C12-C13
20	2	305	CLA	C6-C7-C8-C9
24	4	321	LHG	C29-C30-C31-C32
23	O	202	BCR	C11-C12-C13-C14
25	G	204	MGE	CAB-CBB-CCB-CDB
20	A	843	CLA	C15-C16-C17-C18
20	A	806	CLA	CBA-CGA-O2A-C1
20	B	809	CLA	C13-C15-C16-C17
23	L	304	BCR	C6-C7-C8-C9
19	2	309	CHL	C4B-C3B-CAB-CBB
20	A	827	CLA	C13-C15-C16-C17
20	B	830	CLA	C13-C15-C16-C17
20	1	303	CLA	C3-C5-C6-C7
20	A	843	CLA	C10-C11-C12-C13
20	A	802	CLA	C2-C3-C5-C6
20	A	807	CLA	C2-C3-C5-C6
26	B	832	PQN	C12-C13-C15-C16
20	A	826	CLA	C16-C17-C18-C19
20	F	304	CLA	C5-C6-C7-C8
20	1	319	CLA	CBA-CGA-O2A-C1
20	2	323	CLA	CAA-CBA-CGA-O2A
19	3	313	CHL	C3A-C2A-CAA-CBA
20	2	321	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	4	309	CLA	C3A-C2A-CAA-CBA
20	A	809	CLA	C3A-C2A-CAA-CBA
20	A	838	CLA	C3A-C2A-CAA-CBA
20	A	849	CLA	C3A-C2A-CAA-CBA
20	B	802	CLA	C3A-C2A-CAA-CBA
20	B	803	CLA	C3A-C2A-CAA-CBA
20	B	821	CLA	C3A-C2A-CAA-CBA
24	2	313	LHG	C35-C36-C37-C38
29	B	840	DGD	C4B-C5B-C6B-C7B
20	3	311	CLA	C16-C17-C18-C20
20	A	850	CLA	C10-C11-C12-C13
24	A	821	LHG	C29-C30-C31-C32
20	1	318	CLA	C13-C15-C16-C17
24	B	843	LHG	C4-C5-C6-O8
24	O	205	LHG	C4-C5-C6-O8
25	3	305	MGE	O1G-C1G-C2G-C3G
29	J	104	DGD	C1G-C2G-C3G-O3G
20	3	308	CLA	O1A-CGA-O2A-C1
20	A	835	CLA	O2A-C1-C2-C3
20	B	847	CLA	C10-C11-C12-C13
20	B	819	CLA	C13-C15-C16-C17
20	A	849	CLA	C4-C3-C5-C6
19	2	301	CHL	C3C-C2C-CMC-OMC
19	2	322	CHL	C3C-C2C-CMC-OMC
19	4	305	CHL	C3C-C2C-CMC-OMC
19	4	306	CHL	C3C-C2C-CMC-OMC
24	1	314	LHG	O7-C7-C8-C9
24	A	819	LHG	O8-C23-C24-C25
20	1	303	CLA	O1A-CGA-O2A-C1
20	B	804	CLA	O1A-CGA-O2A-C1
25	4	322	MGE	C6A-C7A-C8A-C9A
20	A	853	CLA	C2A-CAA-CBA-CGA
24	2	314	LHG	O6-C4-C5-O7
20	4	316	CLA	C15-C16-C17-C18
20	B	814	CLA	C13-C15-C16-C17
20	A	802	CLA	C3-C5-C6-C7
24	1	314	LHG	O7-C5-C6-O8
24	2	313	LHG	O7-C5-C6-O8
20	3	310	CLA	CAA-CBA-CGA-O2A
20	A	826	CLA	C16-C17-C18-C20
25	3	305	MGE	O6D-C1D-O3G-C3G
20	2	307	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
20	2	321	CLA	C2-C1-O2A-CGA
20	A	802	CLA	C2-C1-O2A-CGA
20	A	825	CLA	C2-C1-O2A-CGA
20	B	849	CLA	C2-C1-O2A-CGA
20	A	829	CLA	C2-C3-C5-C6
20	B	819	CLA	C15-C16-C17-C18
20	1	307	CLA	CAA-CBA-CGA-O2A
20	A	854	CLA	C14-C13-C15-C16
20	B	806	CLA	C6-C7-C8-C9
20	B	814	CLA	C11-C10-C8-C9
20	B	833	CLA	C11-C10-C8-C9
20	B	852	CLA	C11-C10-C8-C9
20	A	826	CLA	C10-C11-C12-C13
20	O	206	CLA	C15-C16-C17-C18
24	B	841	LHG	C2-C3-O3-P
24	B	843	LHG	C5-C4-O6-P
23	1	312	BCR	C23-C24-C25-C26
23	2	312	BCR	C23-C24-C25-C26
23	3	303	BCR	C23-C24-C25-C26
23	A	816	BCR	C1-C6-C7-C8
23	A	818	BCR	C1-C6-C7-C8
23	A	857	BCR	C23-C24-C25-C30
23	F	301	BCR	C1-C6-C7-C8
23	I	102	BCR	C1-C6-C7-C8
23	K	202	BCR	C23-C24-C25-C30
23	L	303	BCR	C1-C6-C7-C8
23	L	303	BCR	C23-C24-C25-C30
23	2	312	BCR	C11-C12-C13-C35
21	4	317	LUT	C7-C8-C9-C10
23	2	312	BCR	C21-C22-C23-C24
23	4	319	BCR	C21-C22-C23-C24
23	A	816	BCR	C21-C22-C23-C24
20	B	827	CLA	C8-C10-C11-C12
24	2	314	LHG	C23-C24-C25-C26
20	A	807	CLA	O1D-CGD-O2D-CED
20	B	807	CLA	O1D-CGD-O2D-CED
24	2	313	LHG	O6-C4-C5-C6
20	3	311	CLA	C6-C7-C8-C10
20	A	827	CLA	C11-C12-C13-C15
20	A	835	CLA	C6-C7-C8-C10
20	A	851	CLA	C11-C12-C13-C15
20	A	852	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
20	A	853	CLA	C11-C12-C13-C15
20	A	854	CLA	C6-C7-C8-C10
20	A	854	CLA	C11-C10-C8-C7
20	A	854	CLA	C12-C13-C15-C16
20	B	807	CLA	C11-C12-C13-C15
20	B	814	CLA	C11-C10-C8-C7
20	B	817	CLA	C11-C10-C8-C7
20	B	819	CLA	C11-C10-C8-C7
20	B	827	CLA	C12-C13-C15-C16
20	B	831	CLA	C6-C7-C8-C10
20	B	850	CLA	C11-C12-C13-C15
20	A	847	CLA	O1D-CGD-O2D-CED
20	B	851	CLA	O1D-CGD-O2D-CED
20	B	809	CLA	C15-C16-C17-C18
20	4	313	CLA	O1D-CGD-O2D-CED
20	A	804	CLA	C2A-CAA-CBA-CGA
23	L	303	BCR	C20-C21-C22-C37
25	N	201	MGE	C1A-C2A-C3A-C4A
20	A	831	CLA	C4C-C3C-CAC-CBC
19	1	317	CHL	CAD-CBD-CGD-O2D
20	1	302	CLA	CAD-CBD-CGD-O2D
20	1	319	CLA	CAD-CBD-CGD-O2D
20	2	305	CLA	CAD-CBD-CGD-O2D
20	2	319	CLA	CAD-CBD-CGD-O2D
20	3	315	CLA	CAD-CBD-CGD-O2D
20	4	309	CLA	CAD-CBD-CGD-O2D
20	A	804	CLA	CAD-CBD-CGD-O2D
20	A	809	CLA	CAD-CBD-CGD-O2D
20	A	811	CLA	CAD-CBD-CGD-O2D
20	A	827	CLA	CAD-CBD-CGD-O2D
20	A	830	CLA	CAD-CBD-CGD-O2D
20	A	831	CLA	CAD-CBD-CGD-O2D
20	A	835	CLA	CAD-CBD-CGD-O2D
20	A	836	CLA	CAD-CBD-CGD-O2D
20	A	850	CLA	CAD-CBD-CGD-O2D
20	B	804	CLA	CAD-CBD-CGD-O2D
20	B	808	CLA	CAD-CBD-CGD-O2D
20	B	811	CLA	CAD-CBD-CGD-O2D
20	B	815	CLA	CAD-CBD-CGD-O2D
20	B	819	CLA	CAD-CBD-CGD-O2D
20	B	828	CLA	CAD-CBD-CGD-O2D
20	N	202	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	A	850	CLA	C3-C5-C6-C7
20	A	837	CLA	C4C-C3C-CAC-CBC
23	G	203	BCR	C22-C23-C24-C25
20	4	314	CLA	CBA-CGA-O2A-C1
20	A	836	CLA	CBA-CGA-O2A-C1
20	L	306	CLA	CBA-CGA-O2A-C1
20	A	849	CLA	C2-C3-C5-C6
29	G	202	DGD	C4B-C5B-C6B-C7B
24	2	313	LHG	C4-C5-C6-O8
29	B	840	DGD	C1G-C2G-C3G-O3G
29	J	104	DGD	O1G-C1G-C2G-C3G
20	A	805	CLA	CBD-CGD-O2D-CED
20	4	314	CLA	O1A-CGA-O2A-C1
20	A	806	CLA	O1A-CGA-O2A-C1
29	G	202	DGD	C5B-C6B-C7B-C8B
24	2	313	LHG	O6-C4-C5-O7
20	B	822	CLA	CAA-CBA-CGA-O2A
19	2	302	CHL	CBA-CGA-O2A-C1
19	1	301	CHL	CHA-CBD-CGD-O1D
19	4	306	CHL	CHA-CBD-CGD-O1D
19	4	306	CHL	CHA-CBD-CGD-O2D
20	1	320	CLA	CHA-CBD-CGD-O1D
20	1	320	CLA	CHA-CBD-CGD-O2D
20	3	317	CLA	CHA-CBD-CGD-O1D
20	4	304	CLA	CHA-CBD-CGD-O1D
20	4	316	CLA	CHA-CBD-CGD-O1D
20	4	316	CLA	CHA-CBD-CGD-O2D
20	A	804	CLA	CHA-CBD-CGD-O1D
20	A	832	CLA	CHA-CBD-CGD-O1D
20	A	832	CLA	CHA-CBD-CGD-O2D
20	B	831	CLA	CHA-CBD-CGD-O1D
20	B	831	CLA	CHA-CBD-CGD-O2D
20	B	844	CLA	CHA-CBD-CGD-O1D
20	B	844	CLA	CHA-CBD-CGD-O2D
20	B	847	CLA	CHA-CBD-CGD-O1D
20	B	847	CLA	CHA-CBD-CGD-O2D
20	B	850	CLA	CHA-CBD-CGD-O1D
20	B	850	CLA	CHA-CBD-CGD-O2D
20	B	852	CLA	CHA-CBD-CGD-O1D
20	1	319	CLA	O1A-CGA-O2A-C1
20	A	836	CLA	O1A-CGA-O2A-C1
20	B	813	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	O	202	BCR	C11-C10-C9-C8
24	2	315	LHG	O7-C5-C6-O8
24	4	301	LHG	O7-C5-C6-O8
24	O	205	LHG	O7-C5-C6-O8
25	F	303	MGE	O1G-C1G-C2G-O2G
25	N	201	MGE	O2G-C2G-C3G-O3G
29	J	104	DGD	O2G-C2G-C3G-O3G
20	2	307	CLA	CBA-CGA-O2A-C1
24	O	205	LHG	C13-C14-C15-C16
20	1	303	CLA	C4-C3-C5-C6
20	A	828	CLA	C4-C3-C5-C6
20	A	831	CLA	C4-C3-C5-C6
20	1	319	CLA	C2-C3-C5-C6
20	A	826	CLA	C11-C10-C8-C9
24	4	301	LHG	C5-C6-O8-C23
20	L	306	CLA	O1A-CGA-O2A-C1
20	O	207	CLA	C3-C5-C6-C7
20	B	819	CLA	O1A-CGA-O2A-C1
24	I	101	LHG	C5-C6-O8-C23
20	B	830	CLA	C5-C6-C7-C8
19	2	322	CHL	CBD-CGD-O2D-CED
23	1	312	BCR	C21-C22-C23-C24
23	B	839	BCR	C21-C22-C23-C24
20	G	207	CLA	O1D-CGD-O2D-CED
20	1	308	CLA	C1A-C2A-CAA-CBA
20	A	831	CLA	C1A-C2A-CAA-CBA
20	1	303	CLA	C2-C1-O2A-CGA
20	A	829	CLA	C2-C1-O2A-CGA
20	B	815	CLA	C2-C1-O2A-CGA
20	F	304	CLA	C2-C1-O2A-CGA
20	2	317	CLA	CBA-CGA-O2A-C1
25	F	303	MGE	C2G-C1G-O1G-C1A
24	1	313	LHG	C4-O6-P-O3
24	2	314	LHG	C3-O3-P-O6
24	B	841	LHG	C4-O6-P-O3
19	2	302	CHL	C4B-C3B-CAB-CBB
24	2	313	LHG	C3-O3-P-O4
24	4	301	LHG	C4-O6-P-O4
20	A	851	CLA	C15-C16-C17-C18
20	A	849	CLA	CBA-CGA-O2A-C1
20	B	810	CLA	CBA-CGA-O2A-C1
20	B	819	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	A	827	CLA	CBD-CGD-O2D-CED
24	2	314	LHG	O6-C4-C5-C6
19	2	322	CHL	O1D-CGD-O2D-CED
24	O	205	LHG	C27-C28-C29-C30
20	2	307	CLA	O1A-CGA-O2A-C1
20	B	812	CLA	C3-C5-C6-C7
29	O	201	DGD	C6A-C7A-C8A-C9A
19	1	301	CHL	CAD-CBD-CGD-O1D
20	1	320	CLA	CAD-CBD-CGD-O1D
20	2	308	CLA	C2-C3-C5-C6
20	2	323	CLA	CAD-CBD-CGD-O1D
20	4	316	CLA	CAD-CBD-CGD-O1D
20	A	837	CLA	CAD-CBD-CGD-O1D
20	B	831	CLA	CAD-CBD-CGD-O1D
20	B	847	CLA	CAD-CBD-CGD-O1D
20	A	802	CLA	CAA-CBA-CGA-O2A
20	G	205	CLA	CBA-CGA-O2A-C1
20	A	849	CLA	C15-C16-C17-C18
19	2	318	CHL	C3-C5-C6-C7
25	1	324	MGE	C2A-C3A-C4A-C5A
19	4	305	CHL	CBA-CGA-O2A-C1
20	1	305	CLA	C3A-C2A-CAA-CBA
20	2	307	CLA	C11-C10-C8-C7
20	2	319	CLA	C11-C12-C13-C15
20	3	307	CLA	C12-C13-C15-C16
20	A	802	CLA	C11-C10-C8-C7
20	A	808	CLA	C11-C10-C8-C7
20	A	829	CLA	C12-C13-C15-C16
20	B	803	CLA	C12-C13-C15-C16
20	B	820	CLA	C6-C7-C8-C10
20	B	847	CLA	C11-C12-C13-C15
25	4	322	MGE	C1B-C2B-C3B-C4B
20	B	852	CLA	C13-C15-C16-C17
20	2	317	CLA	O1A-CGA-O2A-C1
20	3	308	CLA	CAA-CBA-CGA-O2A
20	A	832	CLA	C13-C15-C16-C17
19	3	313	CHL	O1D-CGD-O2D-CED
24	2	316	LHG	C12-C13-C14-C15
20	4	316	CLA	C8-C10-C11-C12
20	4	304	CLA	C2A-CAA-CBA-CGA
20	4	310	CLA	C2A-CAA-CBA-CGA
29	B	840	DGD	C1A-C2A-C3A-C4A

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Mol	Chain	Res	Type	Atoms
19	1	317	CHL	C1C-C2C-CMC-OMC
19	2	301	CHL	C1C-C2C-CMC-OMC
19	2	318	CHL	C1C-C2C-CMC-OMC
19	4	305	CHL	C1C-C2C-CMC-OMC
19	4	306	CHL	C1C-C2C-CMC-OMC
25	N	201	MGE	C1G-C2G-C3G-O3G
29	J	104	DGD	CAA-CBA-CCA-CDA
25	F	303	MGE	O2G-C2G-C3G-O3G
20	B	818	CLA	C5-C6-C7-C8
25	3	306	MGE	C2G-C3G-O3G-C1D
20	A	849	CLA	C10-C11-C12-C13
20	1	307	CLA	O1D-CGD-O2D-CED
20	B	830	CLA	O1D-CGD-O2D-CED
20	A	850	CLA	C5-C6-C7-C8
20	B	804	CLA	C4-C3-C5-C6
20	B	827	CLA	C4-C3-C5-C6
20	B	849	CLA	C4-C3-C5-C6
19	3	313	CHL	CBA-CGA-O2A-C1
20	A	842	CLA	CBA-CGA-O2A-C1
24	O	205	LHG	C24-C25-C26-C27
24	B	842	LHG	C10-C11-C12-C13
20	A	833	CLA	C10-C11-C12-C13
20	3	311	CLA	C6-C7-C8-C9
20	A	835	CLA	C6-C7-C8-C9
20	A	851	CLA	C11-C12-C13-C14
20	A	853	CLA	C11-C12-C13-C14
20	B	801	CLA	C11-C12-C13-C14
20	B	807	CLA	C11-C12-C13-C14
20	B	819	CLA	C11-C10-C8-C9
20	B	823	CLA	C14-C13-C15-C16
24	O	205	LHG	C29-C30-C31-C32
20	B	810	CLA	O1A-CGA-O2A-C1
22	1	311	XAT	C30-C31-C32-C33
23	B	839	BCR	C10-C11-C12-C13
23	A	817	BCR	C7-C8-C9-C34
20	B	823	CLA	C10-C11-C12-C13
20	K	204	CLA	C5-C6-C7-C8
19	2	309	CHL	C2B-C3B-CAB-CBB
20	B	822	CLA	C4-C3-C5-C6
20	1	303	CLA	C2-C3-C5-C6
20	A	837	CLA	C8-C10-C11-C12
19	3	313	CHL	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
20	1	320	CLA	C1-C2-C3-C4
20	A	849	CLA	O1A-CGA-O2A-C1
29	B	840	DGD	C6A-C7A-C8A-C9A
20	2	320	CLA	O2A-C1-C2-C3
20	A	828	CLA	C2-C1-O2A-CGA
20	A	836	CLA	C2-C1-O2A-CGA
20	H	201	CLA	C2-C1-O2A-CGA
24	A	822	LHG	C30-C31-C32-C33
29	J	104	DGD	C4B-C5B-C6B-C7B
20	B	853	CLA	CAA-CBA-CGA-O2A
19	3	313	CHL	O1A-CGA-O2A-C1
20	B	811	CLA	CAA-CBA-CGA-O2A
20	A	808	CLA	C15-C16-C17-C18
20	B	818	CLA	C4-C3-C5-C6
23	4	319	BCR	C23-C24-C25-C26
23	B	836	BCR	C5-C6-C7-C8
20	2	319	CLA	O1D-CGD-O2D-CED
24	4	321	LHG	C34-C35-C36-C37
20	3	309	CLA	C5-C6-C7-C8
20	1	303	CLA	C6-C7-C8-C9
24	A	820	LHG	O7-C5-C6-O8
24	B	843	LHG	O7-C5-C6-O8
25	3	305	MGE	O1G-C1G-C2G-O2G
24	O	205	LHG	C26-C27-C28-C29
24	2	313	LHG	C4-O6-P-O3
24	2	315	LHG	C3-O3-P-O6
24	A	819	LHG	C4-O6-P-O3
24	A	821	LHG	C3-O3-P-O6
24	2	316	LHG	C23-C24-C25-C26
24	A	822	LHG	C33-C34-C35-C36
20	B	814	CLA	C2C-C3C-CAC-CBC
20	2	317	CLA	C2-C1-O2A-CGA
20	B	818	CLA	C8-C10-C11-C12
20	A	828	CLA	C2-C3-C5-C6
20	A	831	CLA	C2-C3-C5-C6
20	A	833	CLA	C11-C12-C13-C15
20	B	806	CLA	C6-C7-C8-C10
20	B	818	CLA	C2-C3-C5-C6
20	A	827	CLA	C14-C13-C15-C16
20	A	854	CLA	C11-C10-C8-C9
20	B	803	CLA	C14-C13-C15-C16
20	B	847	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	J	104	DGD	CFB-CGB-CHB-CIB
23	3	303	BCR	C37-C22-C23-C24
19	2	301	CHL	CBA-CGA-O2A-C1
20	B	803	CLA	C13-C15-C16-C17
29	G	202	DGD	C5A-C6A-C7A-C8A
20	1	319	CLA	C4-C3-C5-C6
20	K	204	CLA	C4-C3-C5-C6
28	A	824	CL0	CAA-CBA-CGA-O2A
20	3	310	CLA	CBA-CGA-O2A-C1
20	4	312	CLA	CBA-CGA-O2A-C1
20	4	316	CLA	CAA-CBA-CGA-O2A
20	A	839	CLA	O1D-CGD-O2D-CED
20	A	842	CLA	O1A-CGA-O2A-C1
20	B	806	CLA	C2A-CAA-CBA-CGA
22	1	311	XAT	C29-C30-C31-C32
20	A	833	CLA	C3-C5-C6-C7
20	A	856	CLA	O1A-CGA-O2A-C1
20	B	809	CLA	C10-C11-C12-C13
20	B	803	CLA	C4-C3-C5-C6
20	3	310	CLA	O1A-CGA-O2A-C1
20	4	312	CLA	O1A-CGA-O2A-C1
20	3	314	CLA	CAA-CBA-CGA-O2A
20	4	312	CLA	C2-C1-O2A-CGA
20	B	811	CLA	C2-C1-O2A-CGA
20	B	833	CLA	C2-C1-O2A-CGA
24	A	821	LHG	C24-C25-C26-C27
20	O	206	CLA	C8-C10-C11-C12
20	3	317	CLA	C2A-CAA-CBA-CGA
25	1	324	MGE	O2G-C2G-C3G-O3G
25	3	306	MGE	O1G-C1G-C2G-O2G
24	4	321	LHG	C27-C28-C29-C30
20	B	815	CLA	CBA-CGA-O2A-C1
20	A	834	CLA	C3A-C2A-CAA-CBA
20	A	853	CLA	C3A-C2A-CAA-CBA
20	A	854	CLA	C3A-C2A-CAA-CBA
20	B	847	CLA	C3A-C2A-CAA-CBA
20	B	829	CLA	C4-C3-C5-C6
20	A	850	CLA	CBD-CGD-O2D-CED
20	B	804	CLA	C2-C3-C5-C6
20	3	307	CLA	C14-C13-C15-C16
20	A	854	CLA	C11-C12-C13-C14
26	A	810	PQN	C19-C18-C20-C21

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Mol	Chain	Res	Type	Atoms
20	B	848	CLA	C16-C17-C18-C19
21	1	323	LUT	C40-C33-C34-C35
22	2	311	XAT	C40-C33-C34-C35
22	3	302	XAT	C39-C29-C30-C31
22	3	302	XAT	C40-C33-C34-C35
23	A	816	BCR	C35-C13-C14-C15
23	A	816	BCR	C16-C17-C18-C36
23	A	857	BCR	C20-C21-C22-C37
23	B	835	BCR	C11-C10-C9-C34
23	B	835	BCR	C20-C21-C22-C37
23	L	301	BCR	C11-C10-C9-C34
23	L	304	BCR	C16-C17-C18-C36
24	1	314	LHG	C4-C5-C6-O8
20	2	307	CLA	C2A-CAA-CBA-CGA
19	2	318	CHL	O2A-C1-C2-C3
21	1	310	LUT	C7-C8-C9-C19
20	B	813	CLA	CAA-CBA-CGA-O2A
25	G	204	MGE	O1B-C1B-C2B-C3B
25	1	316	MGE	C2A-C3A-C4A-C5A
24	A	821	LHG	C13-C14-C15-C16
29	G	202	DGD	C7A-C8A-C9A-CAA
20	1	306	CLA	CAA-CBA-CGA-O1A
25	4	322	MGE	C3G-C2G-O2G-C1B
25	F	303	MGE	C3G-C2G-O2G-C1B
25	G	204	MGE	C1G-C2G-O2G-C1B
25	G	204	MGE	C3G-C2G-O2G-C1B
29	J	104	DGD	C3G-C2G-O2G-C1B
20	A	833	CLA	C1A-C2A-CAA-CBA
20	A	849	CLA	C1A-C2A-CAA-CBA
20	B	803	CLA	C1A-C2A-CAA-CBA
20	B	816	CLA	C1A-C2A-CAA-CBA
20	B	826	CLA	C1A-C2A-CAA-CBA
20	B	847	CLA	C1A-C2A-CAA-CBA
19	2	302	CHL	C2C-C3C-CAC-CBC
20	A	808	CLA	C6-C7-C8-C10
20	A	826	CLA	C11-C10-C8-C7
20	A	826	CLA	C11-C12-C13-C15
20	A	849	CLA	C6-C7-C8-C10
20	B	822	CLA	C2-C3-C5-C6
20	B	829	CLA	C11-C10-C8-C7
20	B	831	CLA	C11-C10-C8-C7
20	O	206	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
20	A	853	CLA	C13-C15-C16-C17
24	1	314	LHG	C26-C27-C28-C29
24	1	314	LHG	C10-C11-C12-C13
20	3	320	CLA	CAA-CBA-CGA-O1A
20	3	320	CLA	CAA-CBA-CGA-O2A
20	A	811	CLA	C6-C7-C8-C9
20	A	832	CLA	C16-C17-C18-C20
20	A	829	CLA	C2A-CAA-CBA-CGA
20	A	830	CLA	C2A-CAA-CBA-CGA
20	B	849	CLA	C2A-CAA-CBA-CGA
24	I	101	LHG	C14-C15-C16-C17
29	B	840	DGD	C9B-CAB-CBB-CCB
20	B	807	CLA	C13-C15-C16-C17
20	A	856	CLA	CBA-CGA-O2A-C1
24	I	101	LHG	C15-C16-C17-C18
20	B	844	CLA	C16-C17-C18-C20
20	1	306	CLA	CAA-CBA-CGA-O2A
20	3	314	CLA	CAA-CBA-CGA-O1A
20	A	836	CLA	C4-C3-C5-C6
20	B	811	CLA	C4-C3-C5-C6
24	A	821	LHG	C17-C18-C19-C20
20	B	812	CLA	C8-C10-C11-C12
19	1	301	CHL	C2B-C3B-CAB-CBB
19	2	302	CHL	C2B-C3B-CAB-CBB
28	A	824	CL0	C2B-C3B-CAB-CBB
20	2	305	CLA	C3-C5-C6-C7
20	B	852	CLA	C3-C5-C6-C7
20	K	204	CLA	C3-C5-C6-C7
21	1	323	LUT	C32-C33-C34-C35
22	2	311	XAT	C32-C33-C34-C35
22	3	302	XAT	C28-C29-C30-C31
23	A	816	BCR	C12-C13-C14-C15
23	A	816	BCR	C16-C17-C18-C19
23	B	835	BCR	C11-C10-C9-C8
23	B	835	BCR	C20-C21-C22-C23
23	F	302	BCR	C12-C13-C14-C15
23	L	301	BCR	C11-C10-C9-C8
20	1	318	CLA	CAA-CBA-CGA-O1A
20	B	813	CLA	C8-C10-C11-C12
20	4	316	CLA	C16-C17-C18-C19
20	1	304	CLA	O1A-CGA-O2A-C1
20	B	825	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
20	B	812	CLA	C10-C11-C12-C13
20	A	826	CLA	C4-C3-C5-C6
20	A	855	CLA	C4-C3-C5-C6
20	N	202	CLA	C4-C3-C5-C6
20	1	319	CLA	C2-C1-O2A-CGA
20	A	811	CLA	C2-C1-O2A-CGA
20	A	850	CLA	C2-C1-O2A-CGA
28	A	824	CL0	C2-C1-O2A-CGA
20	B	803	CLA	C2-C3-C5-C6
20	B	813	CLA	O1A-CGA-O2A-C1
19	2	322	CHL	CAA-CBA-CGA-O1A
26	A	810	PQN	C16-C17-C18-C19
19	2	322	CHL	CAA-CBA-CGA-O2A
24	B	841	LHG	C9-C10-C11-C12
19	2	302	CHL	O1A-CGA-O2A-C1
29	G	202	DGD	O1B-C1B-O2G-C2G
20	B	808	CLA	C10-C11-C12-C13
20	A	812	CLA	C2A-CAA-CBA-CGA
25	1	324	MGE	C4B-C5B-C6B-C7B
23	A	815	BCR	C1-C6-C7-C8
23	A	818	BCR	C5-C6-C7-C8
23	B	836	BCR	C23-C24-C25-C30
23	G	201	BCR	C23-C24-C25-C30
23	I	102	BCR	C5-C6-C7-C8
23	J	101	BCR	C1-C6-C7-C8
23	L	301	BCR	C1-C6-C7-C8
23	L	301	BCR	C23-C24-C25-C26
23	O	202	BCR	C5-C6-C7-C8
24	2	315	LHG	C23-C24-C25-C26
20	B	813	CLA	CBA-CGA-O2A-C1
20	A	811	CLA	C4-C3-C5-C6
20	A	842	CLA	C4-C3-C5-C6
20	B	827	CLA	C2-C3-C5-C6
20	B	849	CLA	C2-C3-C5-C6
20	2	306	CLA	CAA-CBA-CGA-O2A
20	A	839	CLA	CAA-CBA-CGA-O2A
25	1	324	MGE	C2G-C3G-O3G-C1D
29	G	202	DGD	C2B-C1B-O2G-C2G
20	A	805	CLA	C6-C7-C8-C9
19	4	307	CHL	CAA-CBA-CGA-O2A
20	4	304	CLA	CAA-CBA-CGA-O2A
20	1	303	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
20	A	808	CLA	C8-C10-C11-C12
24	A	821	LHG	O6-C4-C5-O7
20	G	205	CLA	O1A-CGA-O2A-C1
20	2	323	CLA	CAA-CBA-CGA-O1A
19	4	306	CHL	CAA-CBA-CGA-O2A
20	A	809	CLA	C2A-CAA-CBA-CGA
20	B	825	CLA	CAA-CBA-CGA-O1A
19	1	301	CHL	C4B-C3B-CAB-CBB
20	4	309	CLA	C4-C3-C5-C6
20	O	207	CLA	C4-C3-C5-C6
19	2	318	CHL	C6-C7-C8-C10
20	A	811	CLA	C2-C3-C5-C6
20	A	826	CLA	C2-C3-C5-C6
20	A	836	CLA	C2-C3-C5-C6
20	A	854	CLA	C11-C12-C13-C15
20	B	823	CLA	C12-C13-C15-C16
20	B	829	CLA	C2-C3-C5-C6
20	A	838	CLA	CAA-CBA-CGA-O2A
20	1	304	CLA	CBA-CGA-O2A-C1
20	A	837	CLA	CAA-CBA-CGA-O2A
25	1	324	MGE	C4A-C5A-C6A-C7A
29	B	840	DGD	O6E-C5E-C6E-O5E
20	A	854	CLA	CAA-CBA-CGA-O2A
20	A	827	CLA	O1D-CGD-O2D-CED
23	A	818	BCR	C11-C10-C9-C34
23	B	834	BCR	C11-C10-C9-C34
23	F	302	BCR	C35-C13-C14-C15
23	G	203	BCR	C20-C21-C22-C37
23	L	304	BCR	C20-C21-C22-C37
20	A	804	CLA	CAA-CBA-CGA-O2A
20	A	844	CLA	CAA-CBA-CGA-O2A
20	A	830	CLA	C4-C3-C5-C6
20	B	815	CLA	C4-C3-C5-C6
20	B	848	CLA	C16-C17-C18-C20
20	2	307	CLA	C11-C10-C8-C9
20	2	319	CLA	C11-C12-C13-C14
20	A	832	CLA	C11-C10-C8-C9
20	A	833	CLA	C11-C12-C13-C14
20	O	206	CLA	C14-C13-C15-C16
20	B	816	CLA	C3A-C2A-CAA-CBA
20	B	826	CLA	C3A-C2A-CAA-CBA
20	1	305	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
20	4	309	CLA	CAA-CBA-CGA-O2A
20	4	312	CLA	CAA-CBA-CGA-O2A
20	A	851	CLA	CAA-CBA-CGA-O2A
24	B	842	LHG	C25-C26-C27-C28
19	3	313	CHL	CAD-CBD-CGD-O2D
20	1	304	CLA	CAD-CBD-CGD-O2D
20	1	322	CLA	CAD-CBD-CGD-O2D
20	2	304	CLA	CAD-CBD-CGD-O2D
20	2	308	CLA	CAD-CBD-CGD-O2D
20	2	317	CLA	CAD-CBD-CGD-O2D
20	2	320	CLA	CAD-CBD-CGD-O2D
20	4	314	CLA	CAD-CBD-CGD-O2D
20	A	801	CLA	CAD-CBD-CGD-O2D
20	A	805	CLA	CAD-CBD-CGD-O2D
20	A	829	CLA	CAD-CBD-CGD-O2D
20	A	838	CLA	CAD-CBD-CGD-O2D
20	A	839	CLA	CAD-CBD-CGD-O2D
20	A	844	CLA	CAD-CBD-CGD-O2D
20	A	846	CLA	CAD-CBD-CGD-O2D
20	B	812	CLA	CAD-CBD-CGD-O2D
20	B	821	CLA	CAD-CBD-CGD-O2D
20	B	846	CLA	CAD-CBD-CGD-O2D
20	F	304	CLA	CAD-CBD-CGD-O2D
20	G	205	CLA	CAD-CBD-CGD-O2D
20	G	206	CLA	CAD-CBD-CGD-O2D
20	H	201	CLA	CAD-CBD-CGD-O2D
20	J	103	CLA	CAD-CBD-CGD-O2D
20	O	208	CLA	CAD-CBD-CGD-O2D
24	1	314	LHG	C6-C5-O7-C7
24	2	314	LHG	C4-C5-O7-C7
25	3	305	MGE	C1G-C2G-O2G-C1B
24	A	819	LHG	C12-C13-C14-C15
20	3	317	CLA	C5-C6-C7-C8
26	B	832	PQN	C20-C21-C22-C23
19	4	315	CHL	CAA-CBA-CGA-O2A
20	A	849	CLA	CAA-CBA-CGA-O2A
20	A	840	CLA	C2C-C3C-CAC-CBC
20	A	832	CLA	C4-C3-C5-C6
20	A	845	CLA	C4-C3-C5-C6
20	A	853	CLA	C4-C3-C5-C6
20	2	306	CLA	CAA-CBA-CGA-O1A
20	4	304	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
20	F	304	CLA	C8-C10-C11-C12
20	N	202	CLA	C2-C3-C5-C6
20	3	309	CLA	CAA-CBA-CGA-O2A
20	B	847	CLA	CAA-CBA-CGA-O2A
23	J	101	BCR	C7-C8-C9-C10
22	2	311	XAT	O4-C6-C7-C8
19	4	306	CHL	CAA-CBA-CGA-O1A
19	4	307	CHL	CAA-CBA-CGA-O1A
20	1	320	CLA	O2A-C1-C2-C3
20	B	805	CLA	CAA-CBA-CGA-O2A
20	A	811	CLA	O2A-C1-C2-C3
20	A	812	CLA	O2A-C1-C2-C3
20	A	834	CLA	O2A-C1-C2-C3
20	A	850	CLA	O2A-C1-C2-C3
20	A	853	CLA	O2A-C1-C2-C3
20	A	854	CLA	O2A-C1-C2-C3
20	B	803	CLA	O2A-C1-C2-C3
20	B	807	CLA	O2A-C1-C2-C3
20	B	814	CLA	O2A-C1-C2-C3
20	B	822	CLA	O2A-C1-C2-C3
20	B	833	CLA	O2A-C1-C2-C3
20	B	845	CLA	O2A-C1-C2-C3
20	H	201	CLA	O2A-C1-C2-C3
20	H	201	CLA	C2A-CAA-CBA-CGA
20	B	806	CLA	C8-C10-C11-C12
20	B	804	CLA	C13-C15-C16-C17
20	2	307	CLA	CAA-CBA-CGA-O2A
20	A	839	CLA	CAA-CBA-CGA-O1A
20	1	307	CLA	CAA-CBA-CGA-O1A
24	A	819	LHG	O10-C23-C24-C25
19	1	301	CHL	CHA-CBD-CGD-O2D
20	1	309	CLA	CHA-CBD-CGD-O1D
20	1	309	CLA	CHA-CBD-CGD-O2D
20	2	307	CLA	CHA-CBD-CGD-O2D
20	2	321	CLA	CHA-CBD-CGD-O1D
20	2	321	CLA	CHA-CBD-CGD-O2D
20	3	308	CLA	CHA-CBD-CGD-O1D
20	3	309	CLA	CHA-CBD-CGD-O1D
20	3	309	CLA	CHA-CBD-CGD-O2D
20	3	317	CLA	CHA-CBD-CGD-O2D
20	4	304	CLA	CHA-CBD-CGD-O2D
20	A	804	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	A	828	CLA	CHA-CBD-CGD-O2D
20	A	837	CLA	CHA-CBD-CGD-O1D
20	A	848	CLA	CHA-CBD-CGD-O1D
20	A	848	CLA	CHA-CBD-CGD-O2D
20	B	806	CLA	CHA-CBD-CGD-O2D
20	B	809	CLA	CHA-CBD-CGD-O2D
20	B	826	CLA	CHA-CBD-CGD-O2D
20	B	848	CLA	CHA-CBD-CGD-O1D
20	B	851	CLA	CHA-CBD-CGD-O1D
20	B	851	CLA	CHA-CBD-CGD-O2D
20	1	319	CLA	CAA-CBA-CGA-O2A
20	A	806	CLA	CAA-CBA-CGA-O2A
20	B	850	CLA	CAA-CBA-CGA-O2A
20	A	830	CLA	C2-C3-C5-C6
20	B	845	CLA	C3-C5-C6-C7
24	A	822	LHG	C11-C12-C13-C14
23	A	818	BCR	C11-C10-C9-C8
23	B	834	BCR	C11-C10-C9-C8
23	L	304	BCR	C20-C21-C22-C23
20	B	812	CLA	CAA-CBA-CGA-O2A
20	B	830	CLA	CAA-CBA-CGA-O2A
24	2	316	LHG	C29-C30-C31-C32
20	A	838	CLA	CAA-CBA-CGA-O1A
20	2	320	CLA	O1A-CGA-O2A-C1
20	4	310	CLA	CAA-CBA-CGA-O2A
20	A	808	CLA	CAA-CBA-CGA-O2A
20	B	849	CLA	CAA-CBA-CGA-O2A
20	3	310	CLA	CAA-CBA-CGA-O1A
20	B	805	CLA	CAA-CBA-CGA-O1A
20	B	833	CLA	C5-C6-C7-C8
20	1	307	CLA	C4-C3-C5-C6
20	A	844	CLA	CAA-CBA-CGA-O1A
20	A	853	CLA	C2-C3-C5-C6
20	B	807	CLA	C11-C10-C8-C7
20	B	809	CLA	C11-C10-C8-C7
20	B	811	CLA	C2-C3-C5-C6
20	B	819	CLA	C11-C12-C13-C15
20	K	204	CLA	C2-C3-C5-C6
20	4	316	CLA	C16-C17-C18-C20
24	2	313	LHG	C24-C25-C26-C27
19	4	305	CHL	O1A-CGA-O2A-C1
20	A	811	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	B	845	CLA	CAA-CBA-CGA-O2A
20	A	826	CLA	C11-C12-C13-C14
20	B	809	CLA	C11-C10-C8-C9
20	B	829	CLA	C11-C12-C13-C14
20	F	304	CLA	C6-C7-C8-C9
20	K	204	CLA	C11-C10-C8-C9
22	1	311	XAT	C33-C34-C35-C15
20	1	304	CLA	C2B-C3B-CAB-CBB
20	2	304	CLA	C2B-C3B-CAB-CBB
20	4	302	CLA	C2B-C3B-CAB-CBB
20	B	803	CLA	C2B-C3B-CAB-CBB
20	B	812	CLA	C2B-C3B-CAB-CBB
19	3	313	CHL	O2A-C1-C2-C3
20	A	807	CLA	CAA-CBA-CGA-O2A
20	A	811	CLA	C6-C7-C8-C10
19	2	302	CHL	C4C-C3C-CAC-CBC
20	3	312	CLA	C2A-CAA-CBA-CGA
20	4	309	CLA	C2A-CAA-CBA-CGA
29	J	104	DGD	C8A-C9A-CAA-CBA
20	A	841	CLA	C2-C3-C5-C6
20	1	305	CLA	CAA-CBA-CGA-O1A
20	A	829	CLA	C5-C6-C7-C8
20	4	309	CLA	C2-C3-C5-C6
19	3	313	CHL	CAA-CBA-CGA-O2A
19	4	315	CHL	CAA-CBA-CGA-O1A
20	A	804	CLA	CAA-CBA-CGA-O1A
20	A	851	CLA	CAA-CBA-CGA-O1A
19	4	315	CHL	CHA-CBD-CGD-O2D
20	A	826	CLA	C1A-C2A-CAA-CBA
20	B	845	CLA	CAA-CBA-CGA-O1A
20	B	847	CLA	CAA-CBA-CGA-O1A
20	2	320	CLA	CBA-CGA-O2A-C1
20	B	806	CLA	CBA-CGA-O2A-C1
20	A	854	CLA	CAA-CBA-CGA-O1A
29	B	840	DGD	O1G-C1G-C2G-C3G
19	2	301	CHL	O1A-CGA-O2A-C1
20	A	825	CLA	CAA-CBA-CGA-O2A
20	B	827	CLA	CAA-CBA-CGA-O2A
25	N	201	MGE	O1G-C1A-C2A-C3A
20	A	826	CLA	C2A-CAA-CBA-CGA
20	A	839	CLA	C2A-CAA-CBA-CGA
20	A	837	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
24	1	314	LHG	O9-C7-C8-C9
20	B	830	CLA	C10-C11-C12-C13
20	O	208	CLA	CAA-CBA-CGA-O2A
20	B	806	CLA	O1A-CGA-O2A-C1
20	A	829	CLA	CAA-CBA-CGA-O2A
24	B	841	LHG	O7-C7-C8-C9
24	1	314	LHG	C11-C12-C13-C14
20	3	309	CLA	CAA-CBA-CGA-O1A
20	B	815	CLA	C2-C3-C5-C6
23	B	838	BCR	C22-C23-C24-C25
24	O	205	LHG	C28-C29-C30-C31
24	2	313	LHG	C4-O6-P-O5
24	2	315	LHG	C3-O3-P-O5
28	A	824	CL0	C4B-C3B-CAB-CBB
20	B	829	CLA	O1D-CGD-O2D-CED
20	L	305	CLA	CBA-CGA-O2A-C1
20	1	319	CLA	CAA-CBA-CGA-O1A
20	2	307	CLA	CAA-CBA-CGA-O1A
20	4	312	CLA	CAA-CBA-CGA-O1A
20	A	806	CLA	CAA-CBA-CGA-O1A
20	B	850	CLA	CAA-CBA-CGA-O1A
24	2	314	LHG	O10-C23-C24-C25
20	A	809	CLA	CAA-CBA-CGA-O2A
24	A	822	LHG	C24-C25-C26-C27
21	1	323	LUT	C5-C6-C7-C8
23	3	303	BCR	C5-C6-C7-C8
23	4	320	BCR	C5-C6-C7-C8
23	A	857	BCR	C5-C6-C7-C8
23	F	302	BCR	C1-C6-C7-C8
20	B	808	CLA	C5-C6-C7-C8
24	2	314	LHG	O8-C23-C24-C25
20	B	820	CLA	C5-C6-C7-C8
20	A	842	CLA	CAA-CBA-CGA-O2A
24	A	821	LHG	C32-C33-C34-C35
19	2	309	CHL	CAD-CBD-CGD-O1D
19	4	306	CHL	CAD-CBD-CGD-O1D
20	2	321	CLA	CAD-CBD-CGD-O1D
20	4	314	CLA	CAD-CBD-CGD-O1D
20	B	803	CLA	CAD-CBD-CGD-O1D
20	B	810	CLA	CAD-CBD-CGD-O1D
20	B	850	CLA	CAD-CBD-CGD-O1D
20	K	205	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
20	O	206	CLA	CAD-CBD-CGD-O1D
24	2	314	LHG	C6-C5-O7-C7
25	1	315	MGE	C1G-C2G-O2G-C1B
25	3	305	MGE	C3G-C2G-O2G-C1B
25	F	303	MGE	C1G-C2G-O2G-C1B
20	F	304	CLA	C10-C11-C12-C13
19	2	318	CHL	C6-C7-C8-C9
20	A	843	CLA	C14-C13-C15-C16
20	B	809	CLA	C14-C13-C15-C16
20	B	819	CLA	C11-C12-C13-C14
20	B	831	CLA	C11-C10-C8-C9
20	B	851	CLA	C13-C15-C16-C17
20	1	318	CLA	C3-C5-C6-C7
20	B	811	CLA	C3-C5-C6-C7
24	2	313	LHG	O7-C7-C8-C9
29	B	840	DGD	O2G-C1B-C2B-C3B
20	A	809	CLA	C10-C11-C12-C13
20	B	849	CLA	CAA-CBA-CGA-O1A
20	3	319	CLA	CAA-CBA-CGA-O2A
20	4	303	CLA	CAA-CBA-CGA-O2A
20	4	314	CLA	CAA-CBA-CGA-O2A
20	A	836	CLA	CAA-CBA-CGA-O2A
20	F	304	CLA	CAA-CBA-CGA-O2A
20	F	306	CLA	CAA-CBA-CGA-O2A
20	H	201	CLA	CAA-CBA-CGA-O2A
25	3	304	MGE	O1G-C1A-C2A-C3A
25	4	322	MGE	O1G-C1A-C2A-C3A
20	B	827	CLA	O1A-CGA-O2A-C1
20	A	801	CLA	C5-C6-C7-C8
20	B	817	CLA	C10-C11-C12-C13
29	B	840	DGD	CBB-CCB-CDB-CEB
28	A	824	CL0	C3-C5-C6-C7
20	B	812	CLA	CAA-CBA-CGA-O1A
20	B	808	CLA	C4-C3-C5-C6
20	B	853	CLA	C4-C3-C5-C6
23	B	838	BCR	C7-C8-C9-C34
19	4	315	CHL	CAD-CBD-CGD-O2D
20	3	308	CLA	C11-C10-C8-C7
20	A	809	CLA	C11-C10-C8-C7
20	A	855	CLA	C2-C3-C5-C6
20	B	829	CLA	C11-C12-C13-C15
26	A	810	PQN	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
19	3	313	CHL	CAA-CBA-CGA-O1A
20	A	829	CLA	CAA-CBA-CGA-O1A
20	B	827	CLA	CAA-CBA-CGA-O1A
20	2	305	CLA	CAA-CBA-CGA-O2A
20	B	828	CLA	CAA-CBA-CGA-O2A
20	L	307	CLA	CAA-CBA-CGA-O2A
24	2	314	LHG	O7-C7-C8-C9
24	B	841	LHG	O8-C23-C24-C25
25	1	324	MGE	O1G-C1A-C2A-C3A
20	B	815	CLA	O1A-CGA-O2A-C1
20	A	825	CLA	CAA-CBA-CGA-O1A
20	B	828	CLA	CAA-CBA-CGA-O1A
25	N	201	MGE	O1A-C1A-C2A-C3A
29	B	840	DGD	O1B-C1B-C2B-C3B
20	O	208	CLA	CAA-CBA-CGA-O1A
22	4	318	XAT	C29-C30-C31-C32
25	3	306	MGE	O1G-C1A-C2A-C3A
25	N	201	MGE	C9B-CAB-CBB-CCB
20	B	809	CLA	C8-C10-C11-C12
20	K	204	CLA	C8-C10-C11-C12
20	4	314	CLA	CAA-CBA-CGA-O1A
20	A	825	CLA	C5-C6-C7-C8
20	B	852	CLA	CAA-CBA-CGA-O2A
24	4	301	LHG	O7-C7-C8-C9
24	O	205	LHG	O7-C7-C8-C9
20	A	808	CLA	CAA-CBA-CGA-O1A
20	A	809	CLA	CAA-CBA-CGA-O1A
24	B	841	LHG	O9-C7-C8-C9
20	A	849	CLA	C2A-CAA-CBA-CGA
20	2	303	CLA	CAA-CBA-CGA-O2A
20	A	807	CLA	CAA-CBA-CGA-O1A
20	A	836	CLA	CAA-CBA-CGA-O1A
20	F	304	CLA	CAA-CBA-CGA-O1A
20	H	201	CLA	CAA-CBA-CGA-O1A
25	1	324	MGE	O1A-C1A-C2A-C3A
19	4	305	CHL	CAA-CBA-CGA-O2A
20	B	804	CLA	CAA-CBA-CGA-O2A
25	J	102	MGE	O2G-C1B-C2B-C3B
20	B	802	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

199 monomers are involved in 678 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	4	302	CLA	3	0
20	K	204	CLA	2	0
20	B	816	CLA	6	0
19	2	302	CHL	7	0
20	B	814	CLA	12	0
20	A	801	CLA	5	0
20	G	206	CLA	1	0
19	2	322	CHL	3	0
23	G	203	BCR	4	0
20	A	838	CLA	2	0
19	4	315	CHL	5	0
22	3	302	XAT	12	0
23	L	301	BCR	3	0
26	A	810	PQN	11	0
20	A	840	CLA	2	0
20	L	305	CLA	2	0
20	1	319	CLA	5	0
20	B	815	CLA	3	0
20	G	205	CLA	6	0
21	3	301	LUT	15	0
20	B	809	CLA	5	0
20	A	806	CLA	6	0
20	4	316	CLA	1	0
23	4	320	BCR	6	0
19	1	301	CHL	6	0
21	1	323	LUT	15	0
20	G	207	CLA	1	0
20	A	805	CLA	4	0
19	4	306	CHL	7	0
20	B	817	CLA	4	0
20	4	314	CLA	2	0
20	B	813	CLA	1	0
20	B	823	CLA	2	0
24	A	819	LHG	3	0
20	4	312	CLA	2	0
20	O	207	CLA	1	0
19	2	309	CHL	4	0
20	A	855	CLA	2	0
20	4	304	CLA	4	0
19	4	307	CHL	5	0
24	1	313	LHG	2	0
23	1	312	BCR	4	0
20	4	308	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	L	306	CLA	2	0
20	2	306	CLA	1	0
23	L	303	BCR	4	0
20	2	303	CLA	3	0
20	B	805	CLA	4	0
20	A	839	CLA	2	0
20	L	307	CLA	1	0
20	1	302	CLA	2	0
25	1	315	MGE	12	0
20	A	848	CLA	2	0
20	1	322	CLA	4	0
20	B	851	CLA	1	0
19	4	305	CHL	12	0
20	A	826	CLA	5	0
20	1	321	CLA	1	0
20	1	303	CLA	6	0
20	F	306	CLA	5	0
20	A	852	CLA	4	0
23	L	304	BCR	3	0
25	N	201	MGE	15	0
20	A	842	CLA	1	0
23	A	857	BCR	6	0
20	3	315	CLA	1	0
20	3	317	CLA	3	0
20	1	304	CLA	2	0
20	A	841	CLA	1	0
20	F	304	CLA	4	0
23	F	301	BCR	7	0
23	K	201	BCR	4	0
20	3	311	CLA	4	0
20	B	801	CLA	3	0
20	B	825	CLA	4	0
22	1	311	XAT	25	0
25	J	102	MGE	13	0
20	4	309	CLA	2	0
20	B	827	CLA	3	0
20	A	827	CLA	1	0
20	1	309	CLA	2	0
20	3	312	CLA	2	0
20	A	809	CLA	4	0
20	1	320	CLA	2	0
20	B	830	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	837	CLA	1	0
20	A	846	CLA	3	0
20	A	847	CLA	3	0
20	A	825	CLA	4	0
20	B	812	CLA	7	0
20	2	308	CLA	2	0
23	A	817	BCR	3	0
20	A	802	CLA	3	0
20	A	836	CLA	2	0
23	G	201	BCR	6	0
23	A	818	BCR	2	0
20	A	833	CLA	5	0
20	A	829	CLA	1	0
20	B	846	CLA	3	0
23	B	837	BCR	6	0
23	B	838	BCR	10	0
20	2	307	CLA	6	0
20	4	303	CLA	1	0
20	B	810	CLA	3	0
20	B	802	CLA	1	0
23	O	202	BCR	3	0
20	B	829	CLA	6	0
29	G	202	DGD	13	0
20	A	845	CLA	4	0
23	A	814	BCR	4	0
20	A	854	CLA	3	0
20	B	828	CLA	7	0
23	L	302	BCR	6	0
24	A	820	LHG	4	0
20	1	308	CLA	3	0
23	A	815	BCR	3	0
21	1	310	LUT	12	0
19	1	317	CHL	10	0
20	K	205	CLA	3	0
20	A	850	CLA	1	0
23	3	303	BCR	2	0
23	K	202	BCR	2	0
26	B	832	PQN	16	0
20	B	822	CLA	2	0
28	A	824	CL0	13	0
20	1	318	CLA	8	0
23	B	834	BCR	4	0

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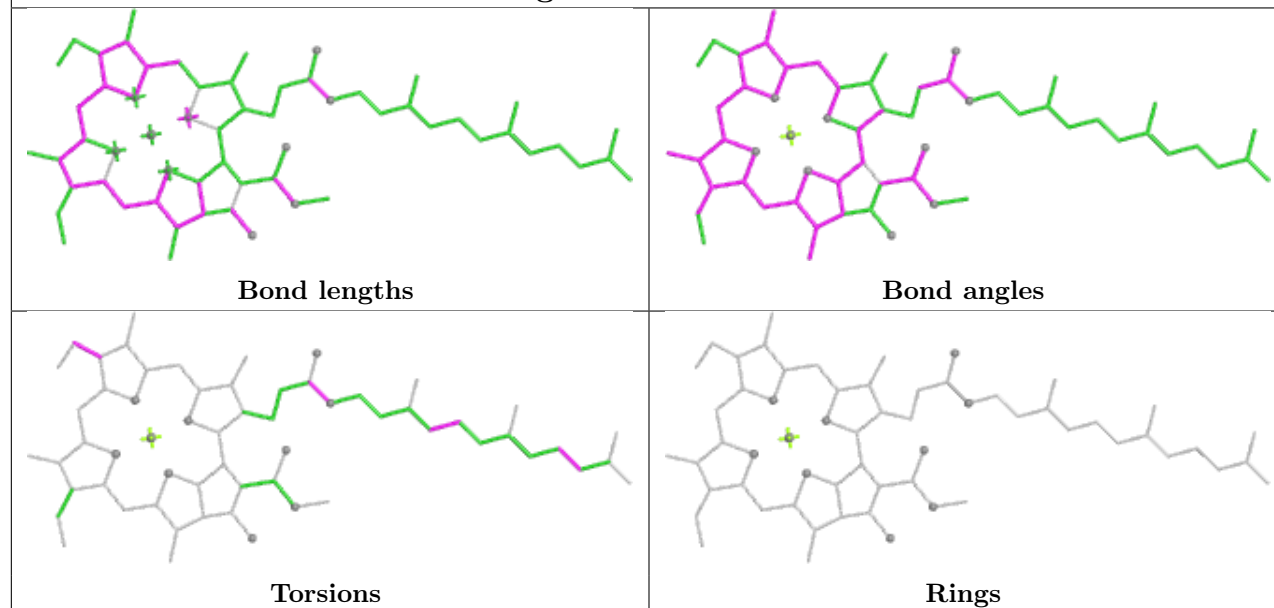
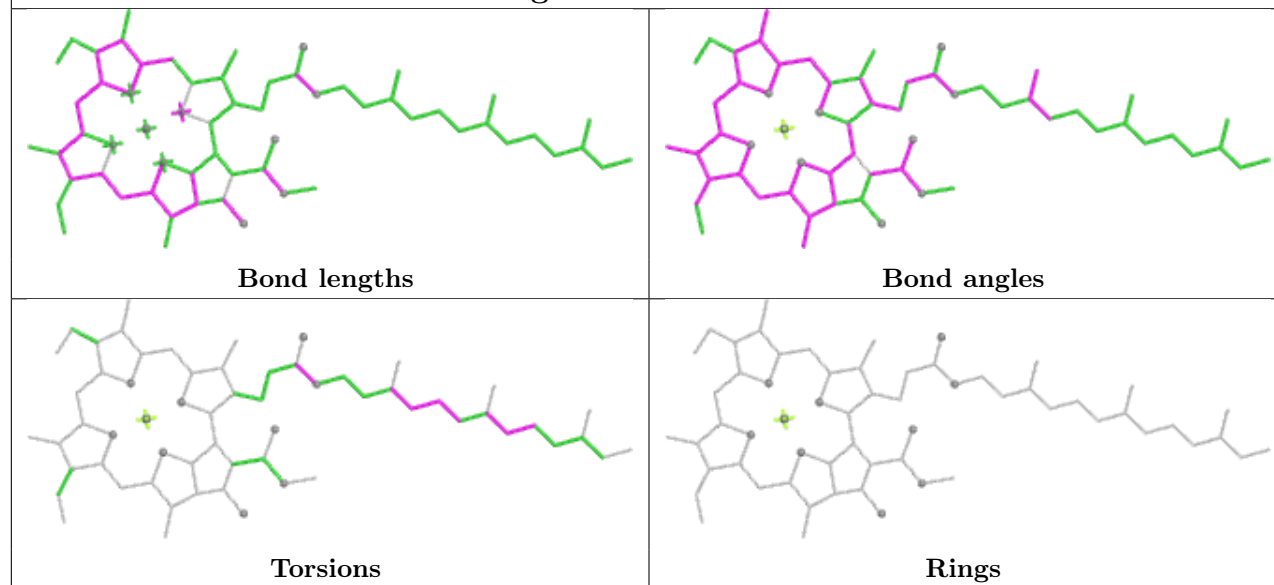
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	2	318	CHL	12	0
23	4	319	BCR	6	0
22	2	311	XAT	8	0
20	B	821	CLA	5	0
20	3	309	CLA	2	0
23	J	101	BCR	6	0
20	B	850	CLA	1	0
25	4	322	MGE	6	0
25	A	823	MGE	15	0
19	2	301	CHL	4	0
20	H	201	CLA	2	0
20	N	202	CLA	4	0
20	B	826	CLA	1	0
23	B	835	BCR	3	0
20	B	852	CLA	1	0
20	3	310	CLA	3	0
25	1	316	MGE	11	0
20	A	831	CLA	6	0
20	A	849	CLA	4	0
25	G	204	MGE	9	0
20	B	845	CLA	6	0
20	A	812	CLA	11	0
20	B	847	CLA	2	0
23	2	312	BCR	6	0
21	2	310	LUT	19	0
20	1	307	CLA	4	0
20	2	321	CLA	2	0
25	1	324	MGE	9	0
25	3	304	MGE	10	0
20	2	304	CLA	2	0
24	O	205	LHG	2	0
20	A	853	CLA	5	0
20	B	818	CLA	2	0
20	B	844	CLA	9	0
20	B	819	CLA	1	0
20	A	843	CLA	3	0
25	3	305	MGE	8	0
24	1	314	LHG	1	0
20	B	833	CLA	1	0
20	3	308	CLA	1	0
23	B	839	BCR	3	0
20	B	824	CLA	1	0

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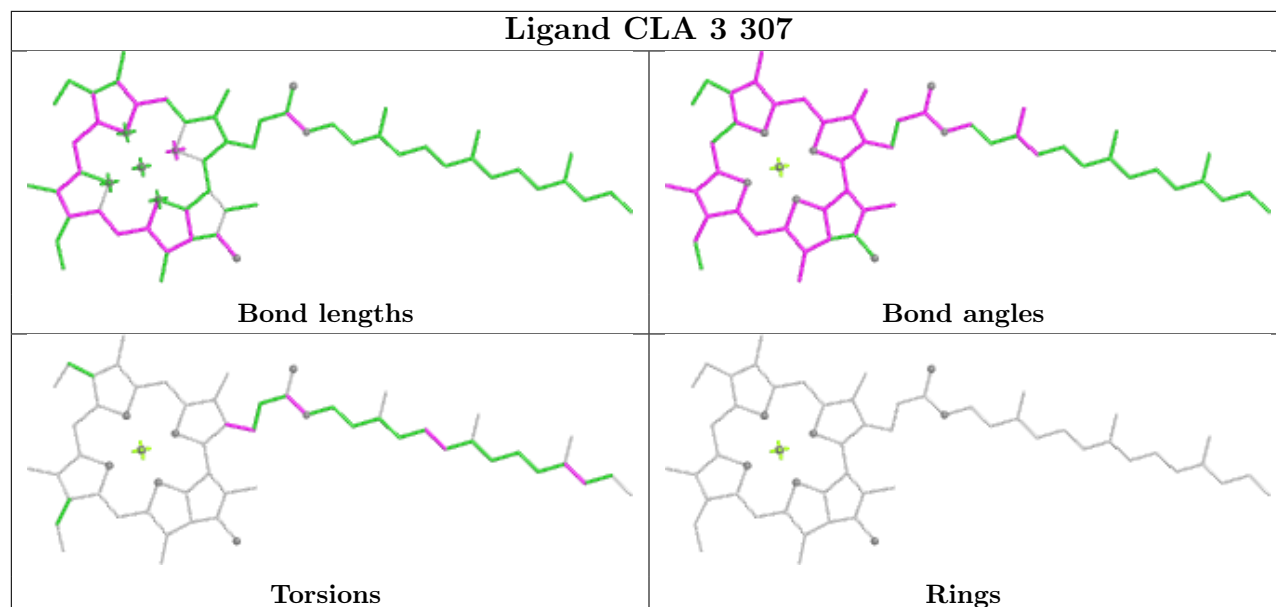
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	803	CLA	4	0
25	F	303	MGE	5	0
20	2	319	CLA	4	0
20	B	853	CLA	1	0
20	B	807	CLA	6	0
20	B	820	CLA	1	0
20	B	804	CLA	1	0
20	3	320	CLA	1	0
20	4	310	CLA	1	0
19	3	313	CHL	11	0
20	3	314	CLA	1	0
23	A	816	BCR	6	0
23	I	102	BCR	2	0
23	O	203	BCR	5	0
23	B	836	BCR	5	0
20	O	206	CLA	1	0
25	3	306	MGE	10	0
20	A	832	CLA	2	0
24	4	321	LHG	1	0
20	A	834	CLA	2	0
29	B	840	DGD	1	0
20	2	323	CLA	1	0
20	4	313	CLA	1	0
21	4	317	LUT	17	0
22	4	318	XAT	11	0
23	F	302	BCR	3	0
20	A	830	CLA	2	0
20	A	844	CLA	1	0
20	2	305	CLA	1	0
20	B	808	CLA	5	0

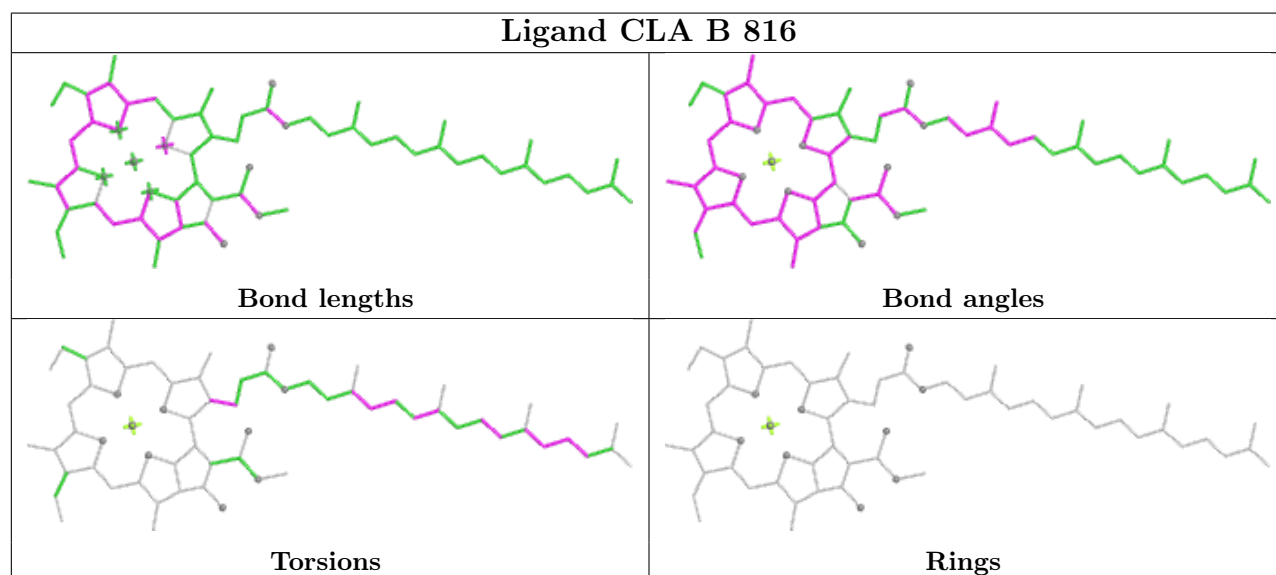
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand CLA 4 302**Ligand CLA K 204**

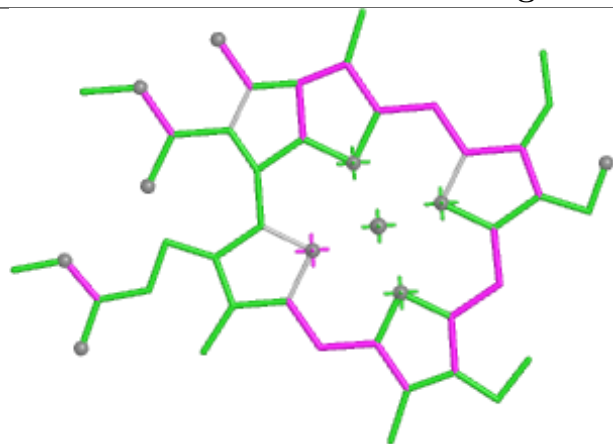
Ligand CLA 3 307



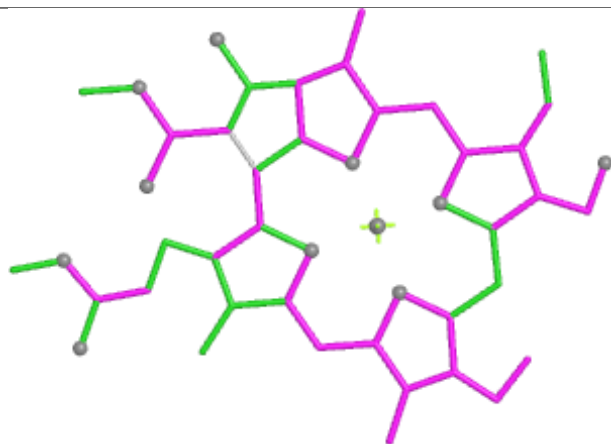
Ligand CLA B 816



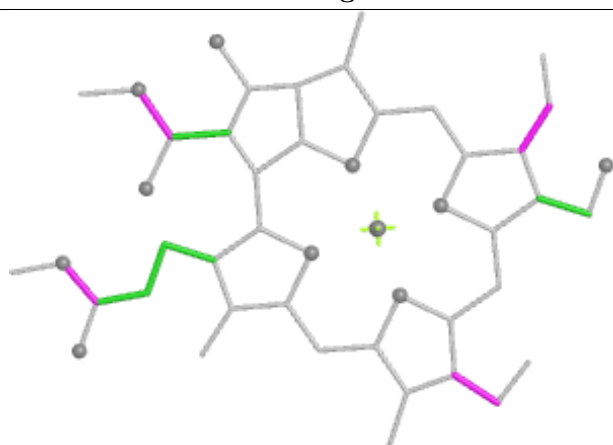
Ligand CHL 2 302



Bond lengths



Bond angles

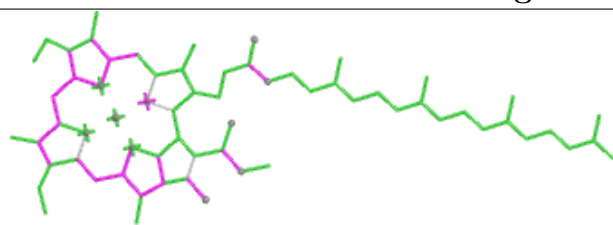


Torsions

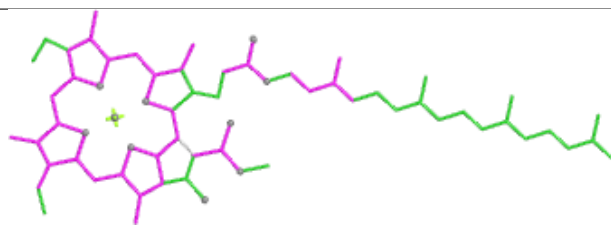


Rings

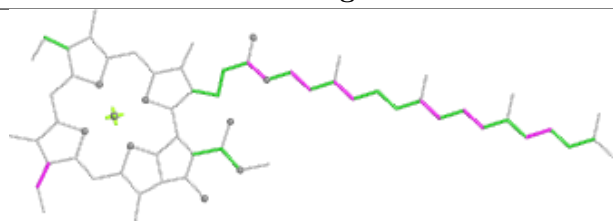
Ligand CLA B 814



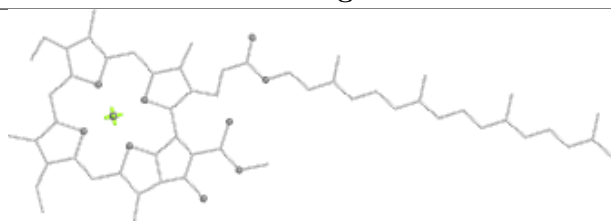
Bond lengths



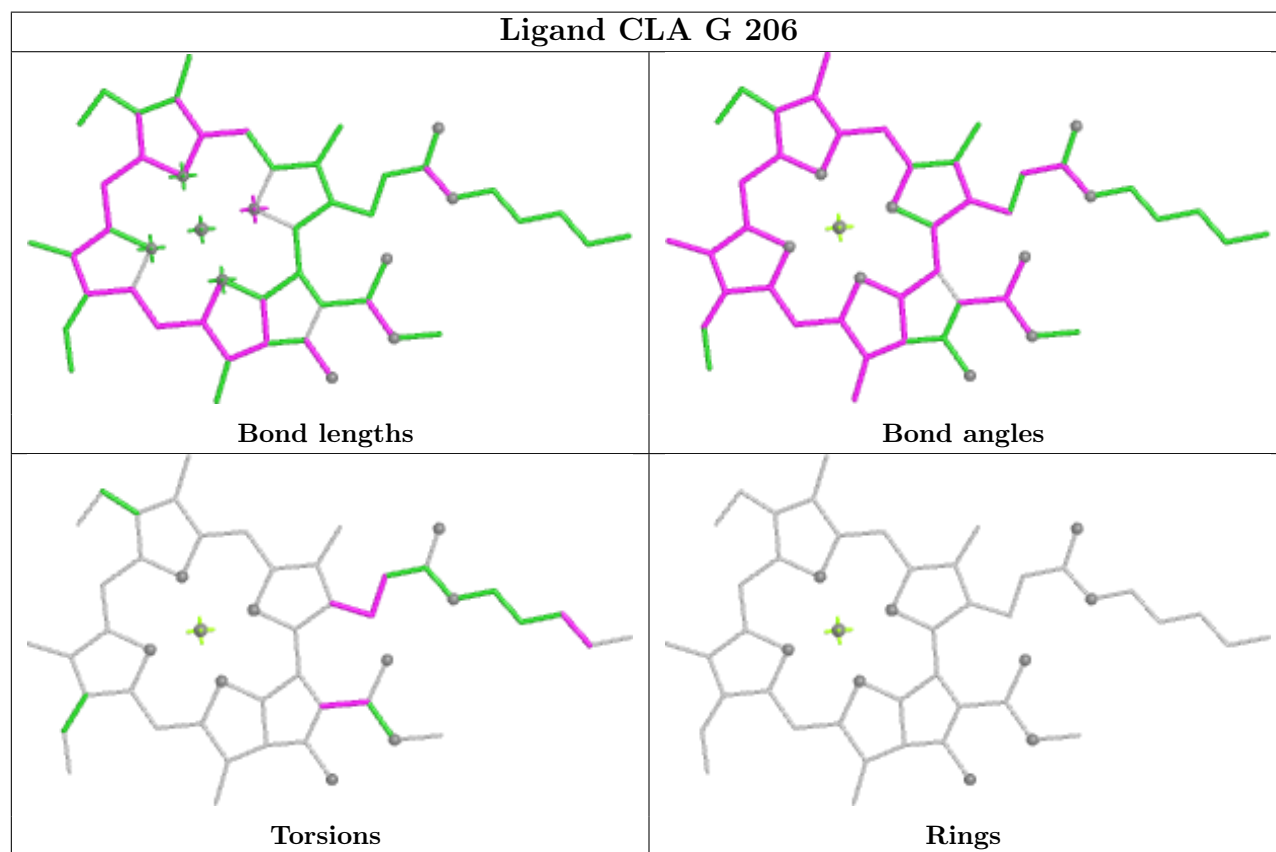
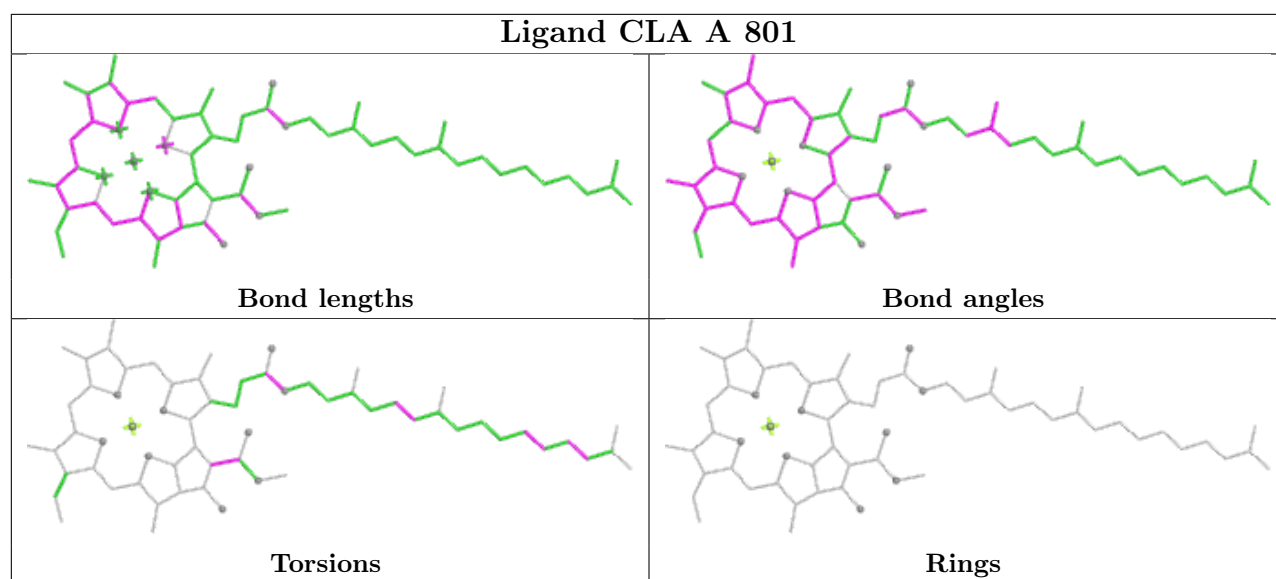
Bond angles



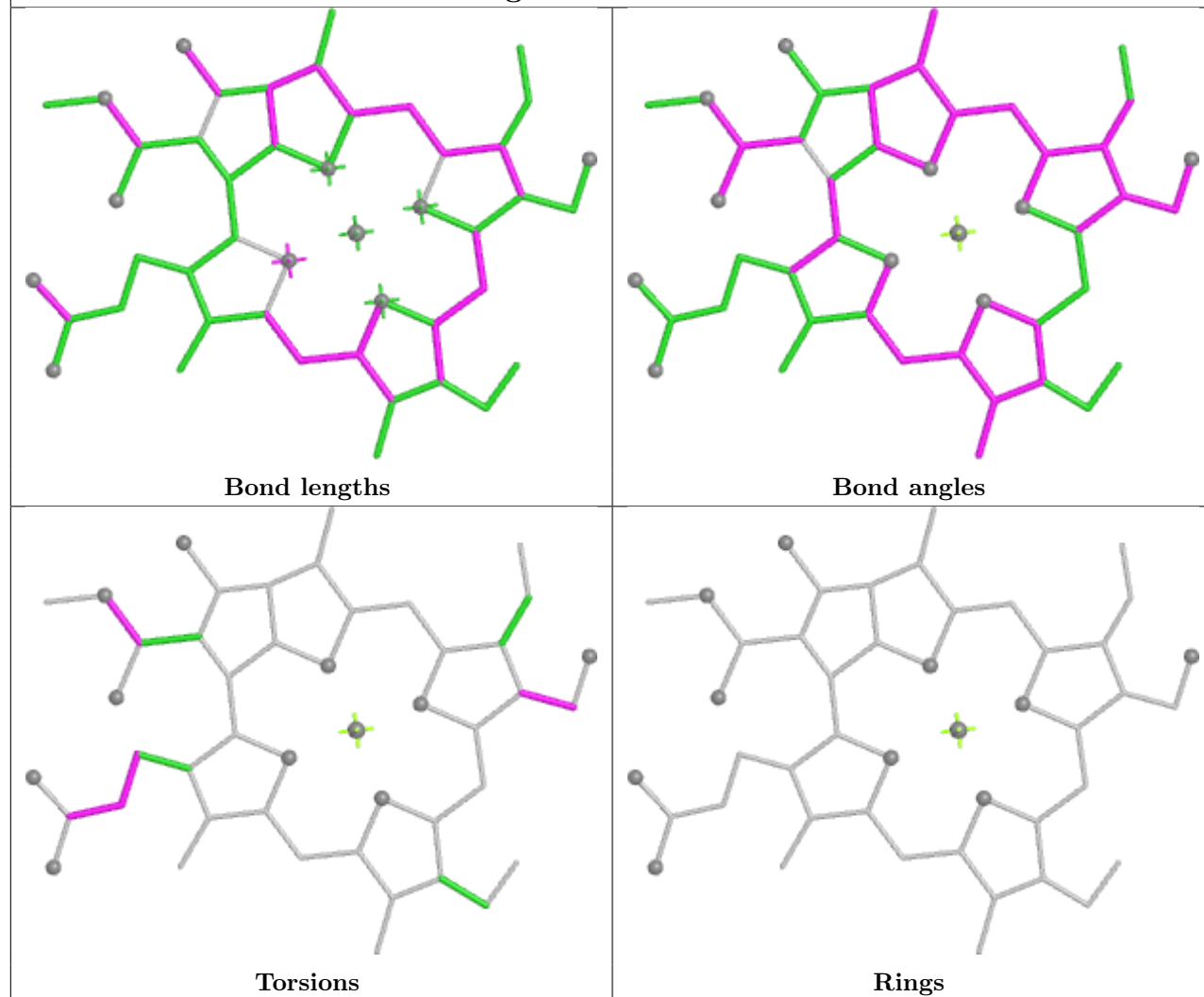
Torsions



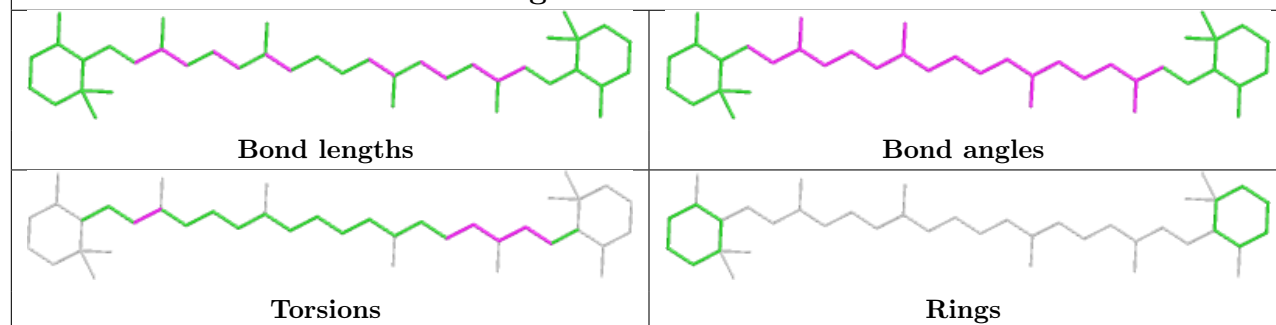
Rings



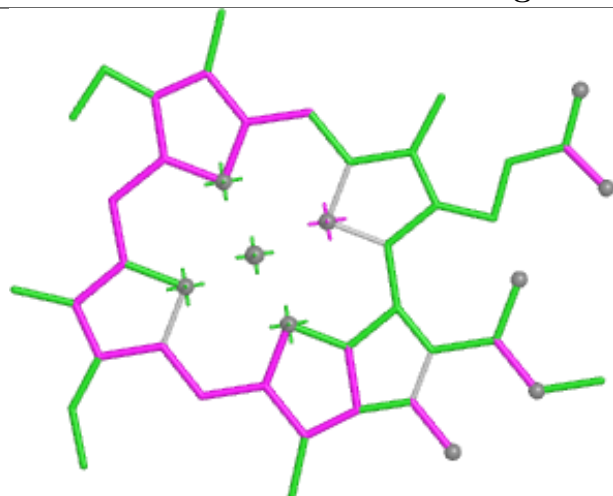
Ligand CHL 2 322



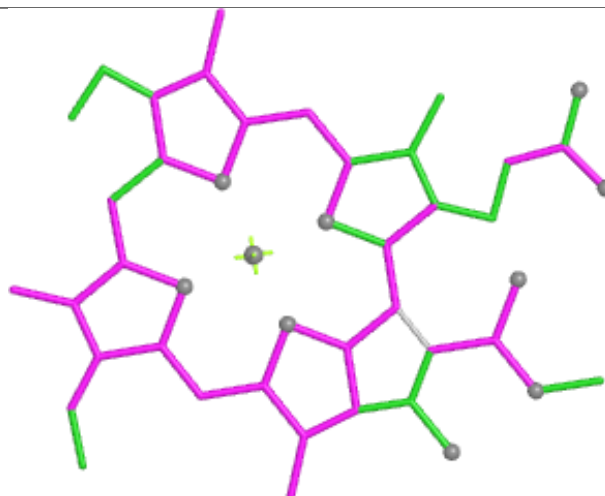
Ligand BCR G 203



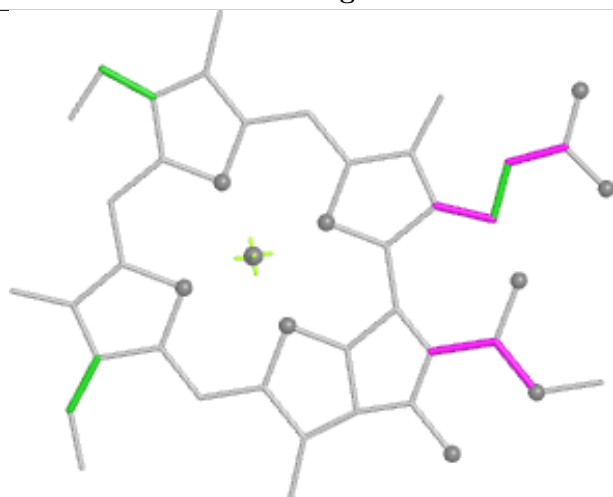
Ligand CLA A 838



Bond lengths



Bond angles

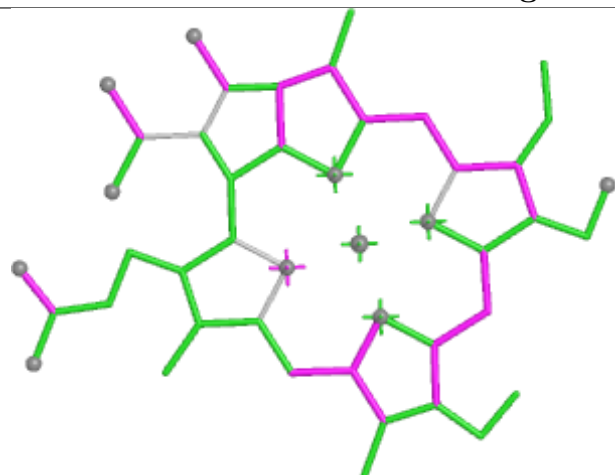


Torsions

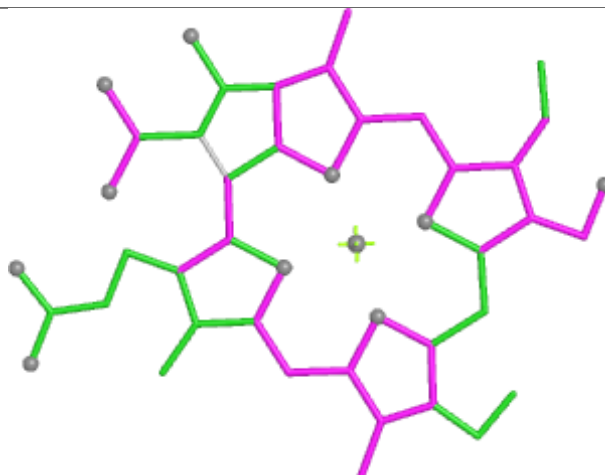


Rings

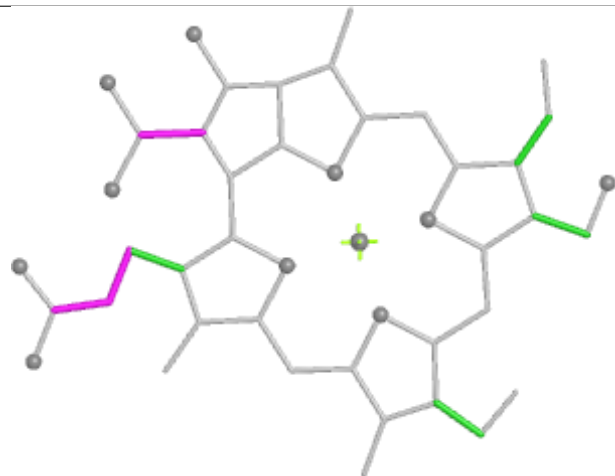
Ligand CHL 4 315



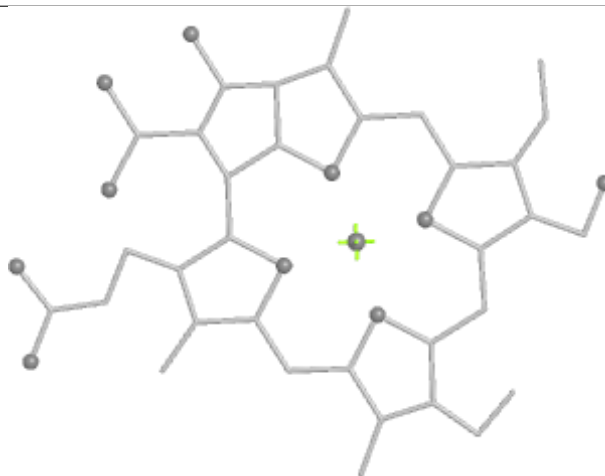
Bond lengths



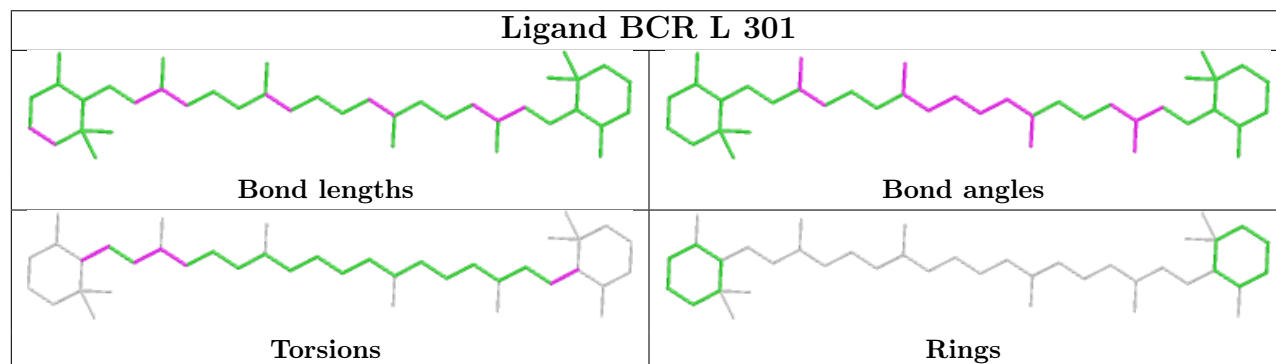
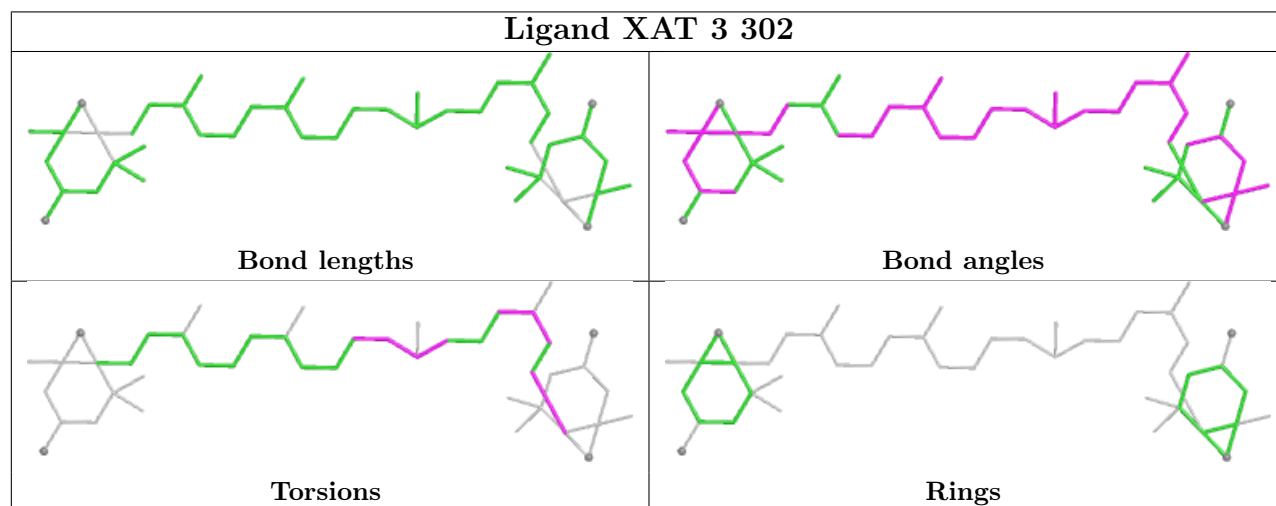
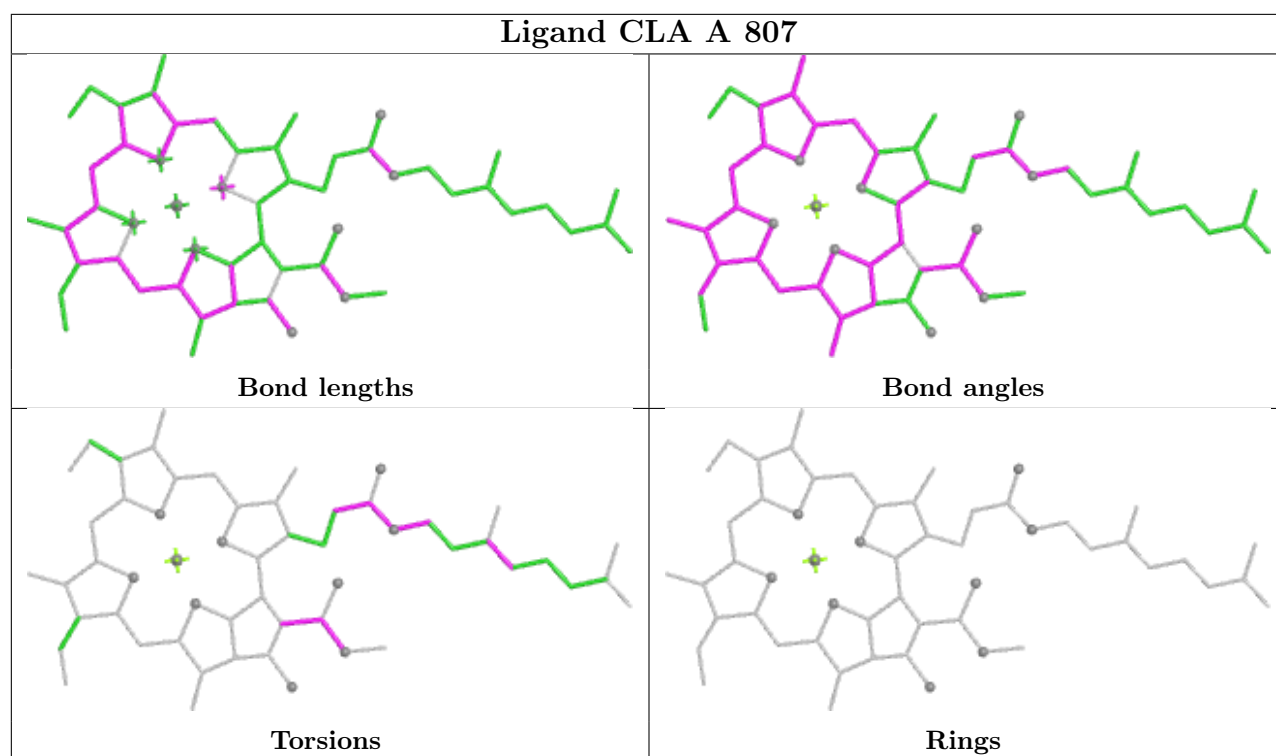
Bond angles

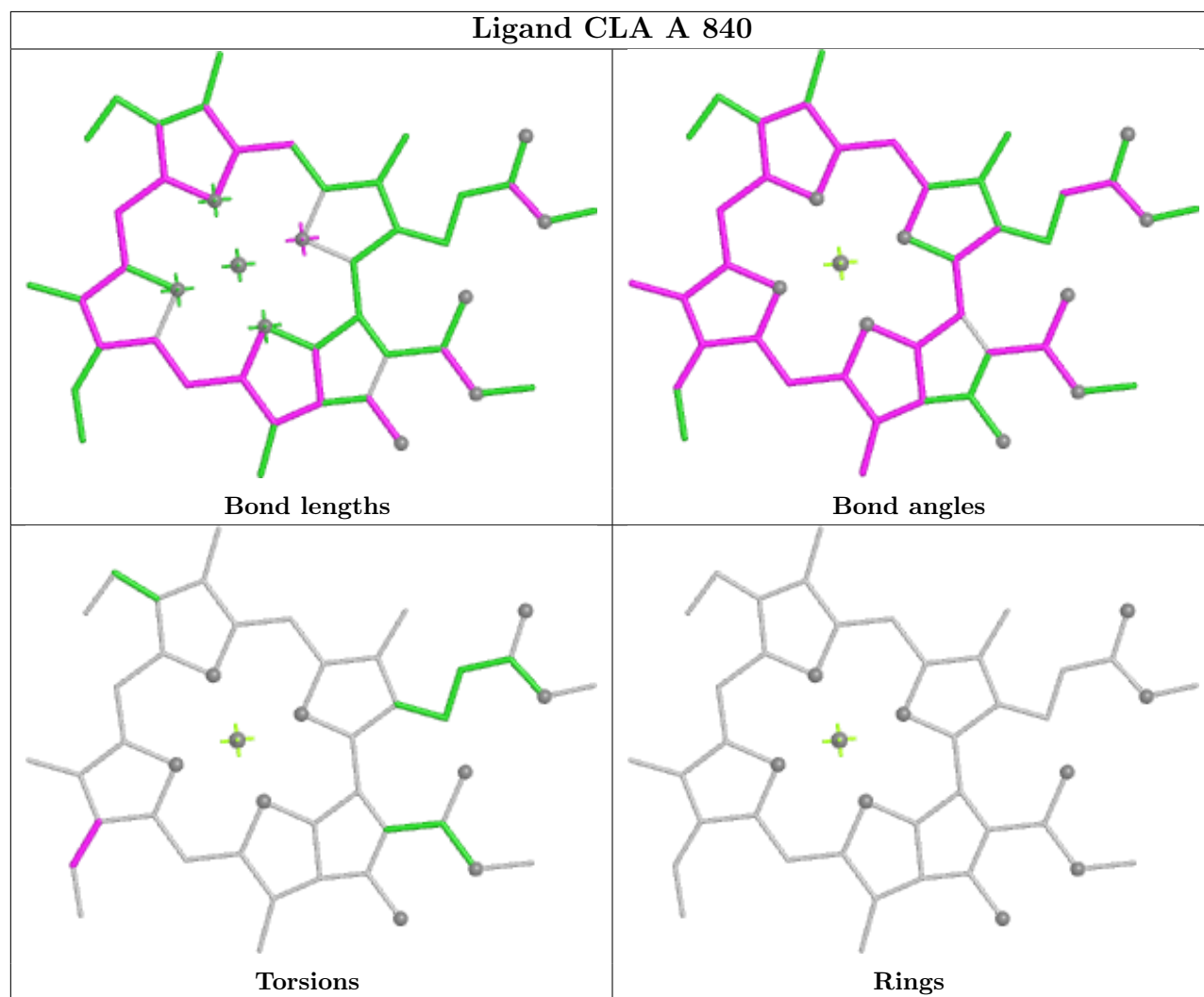
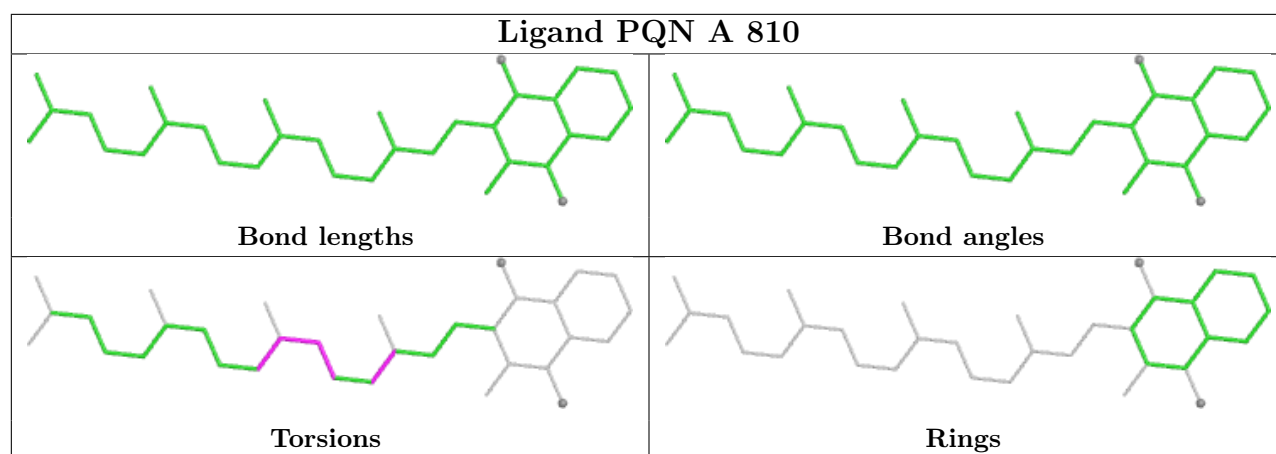


Torsions

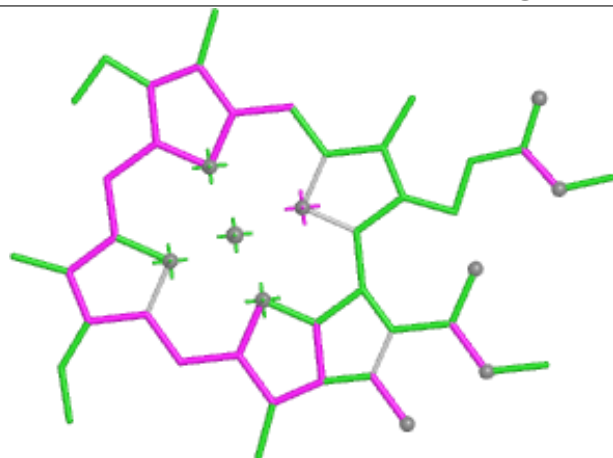


Rings

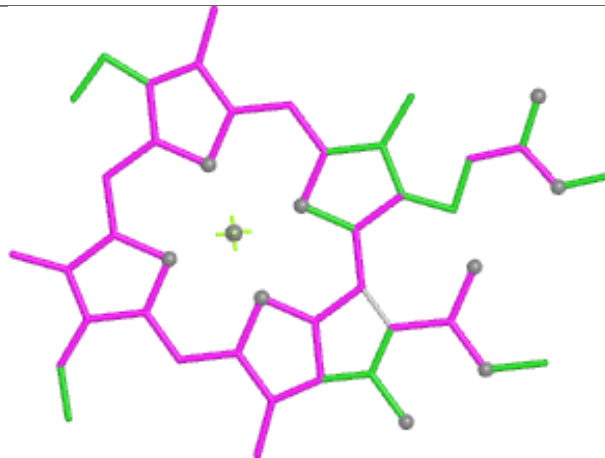




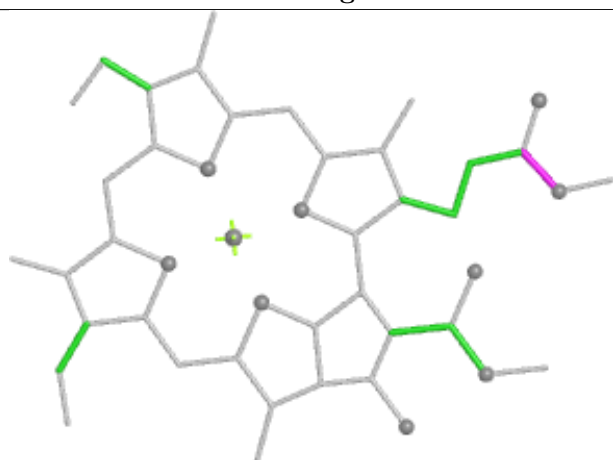
Ligand CLA L 305



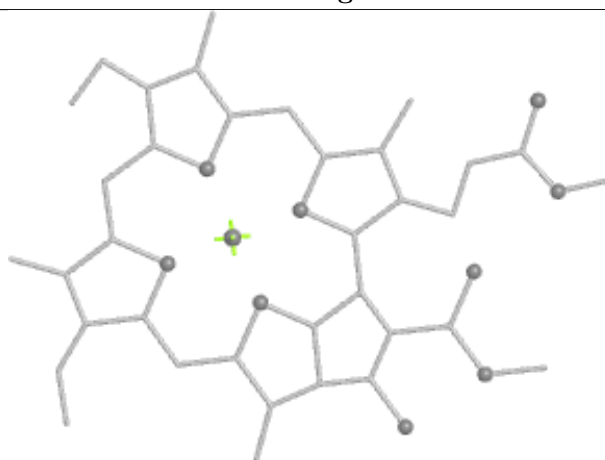
Bond lengths



Bond angles

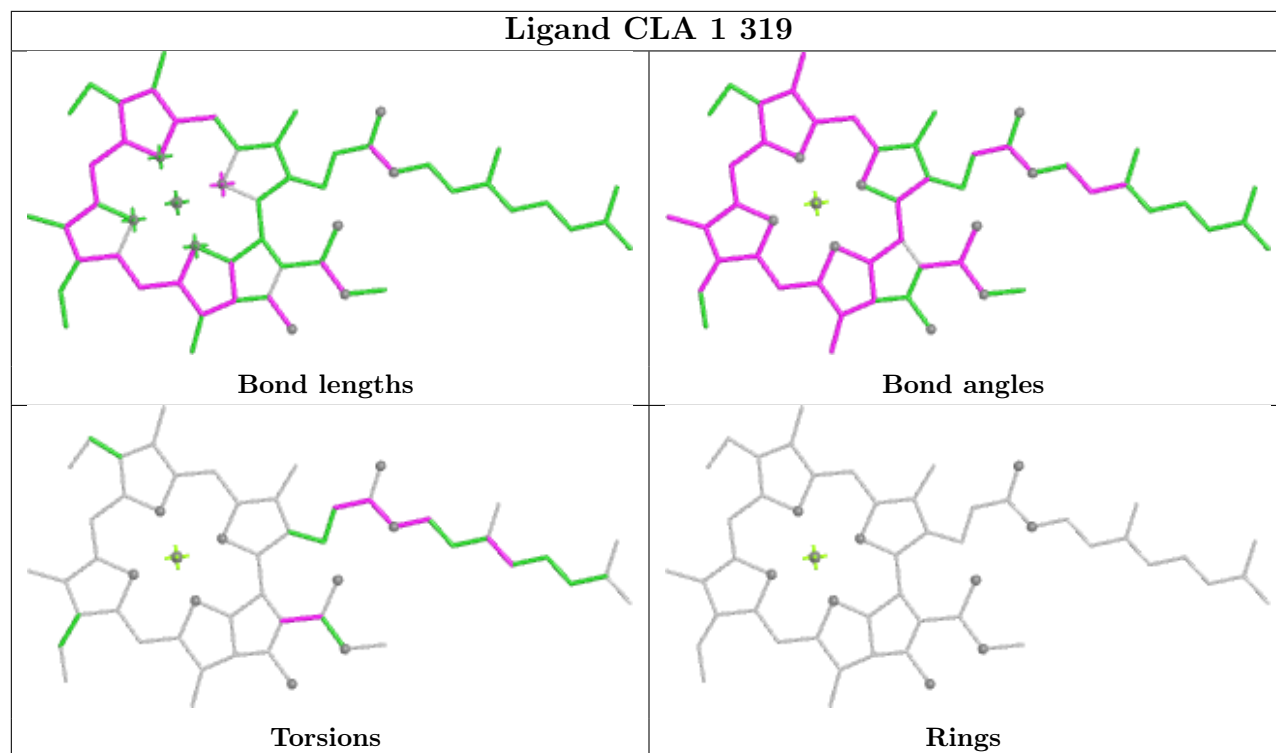


Torsions

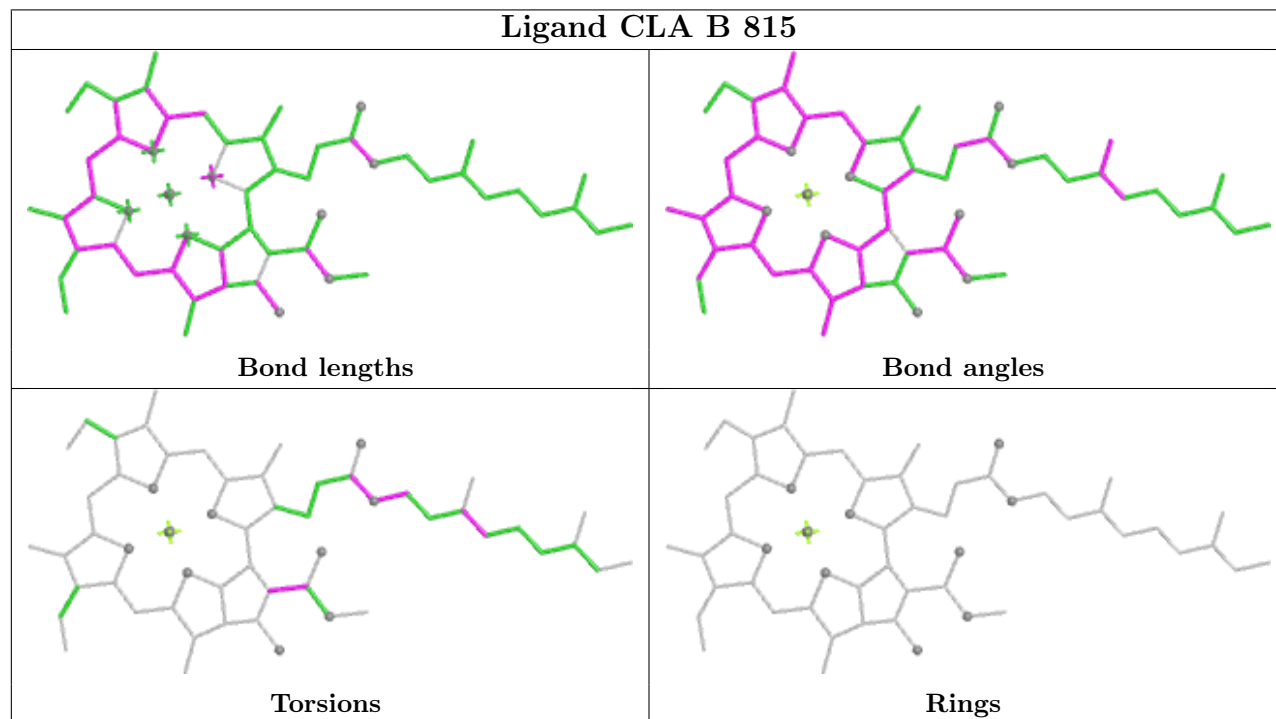


Rings

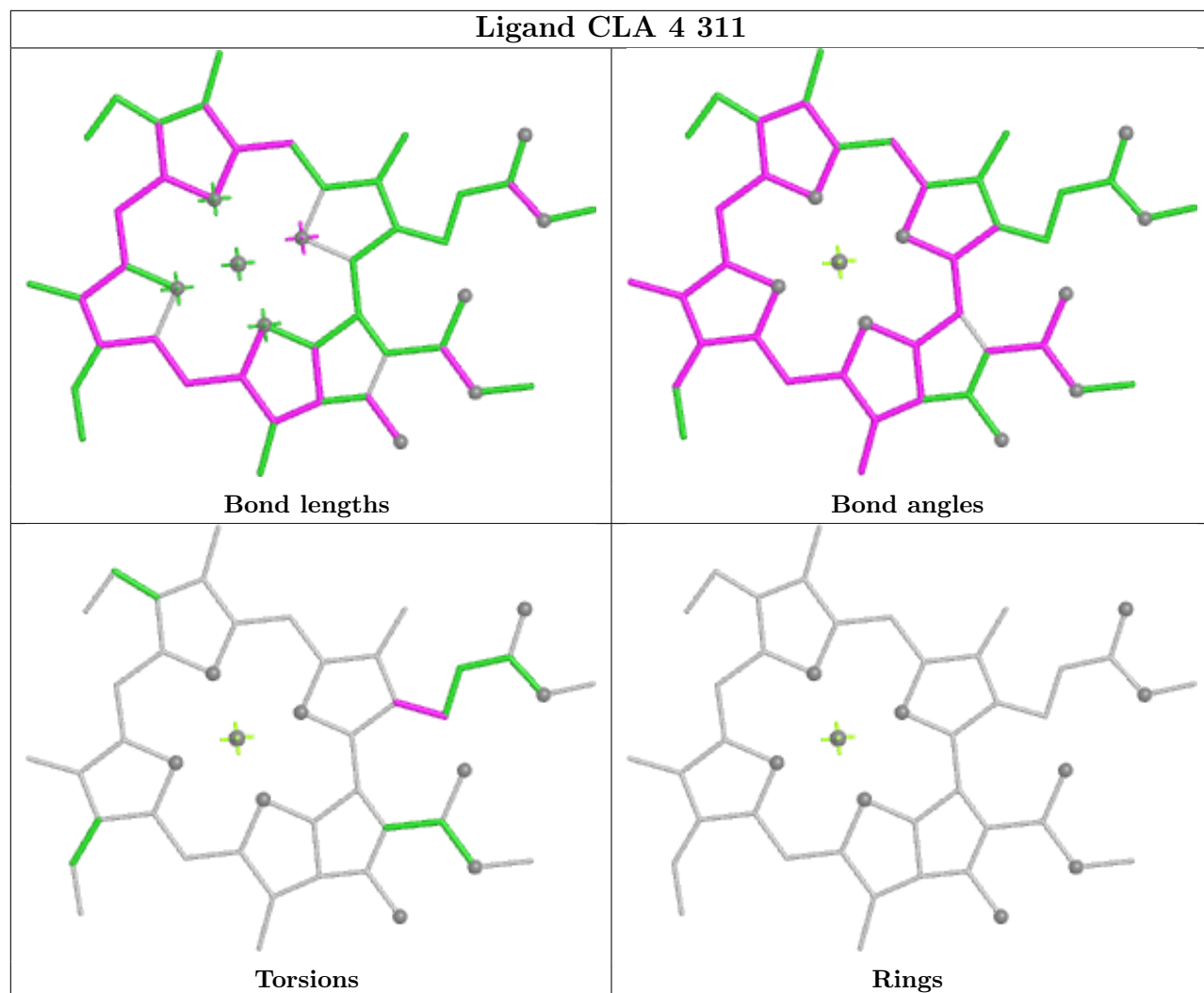
Ligand CLA 1 319

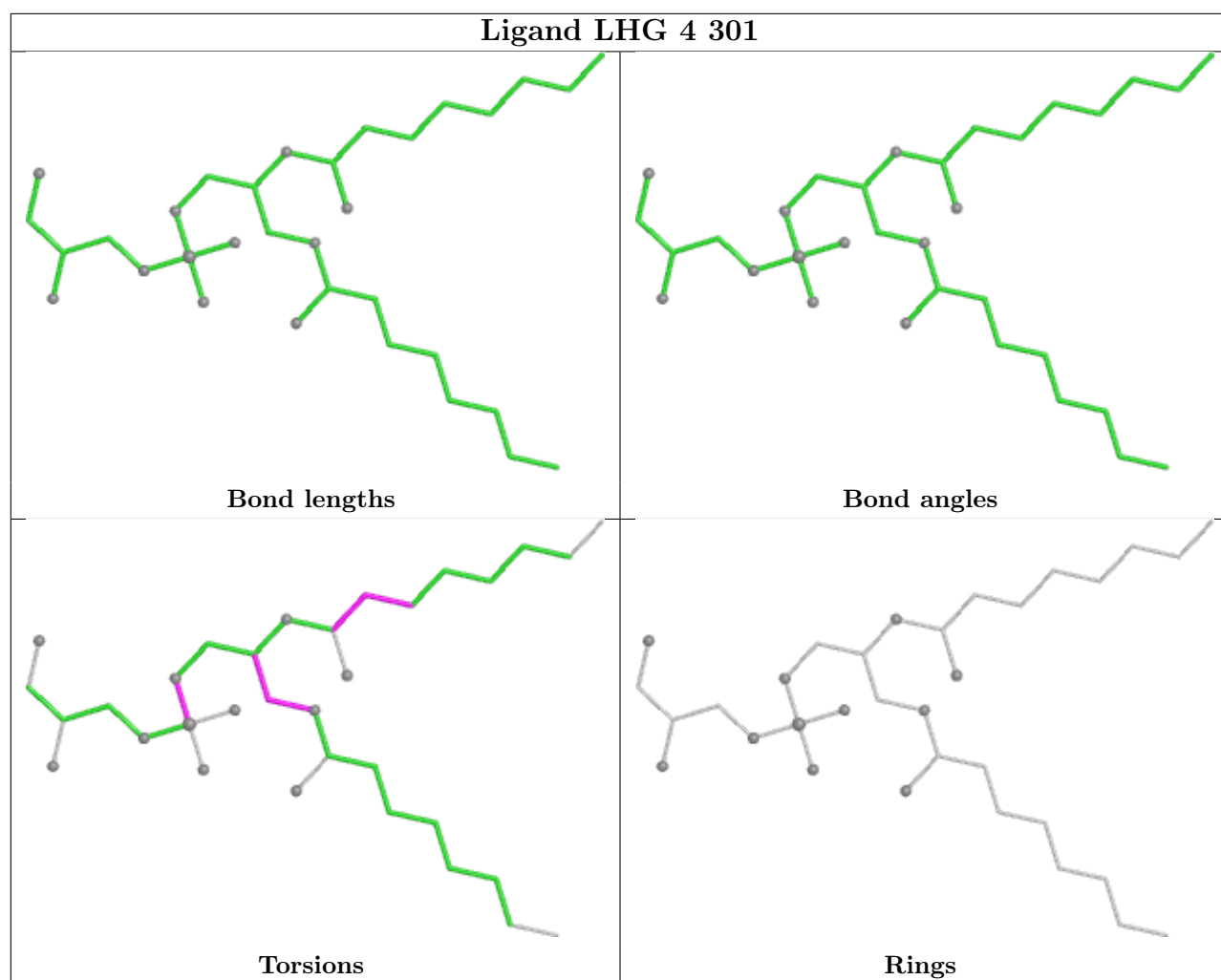


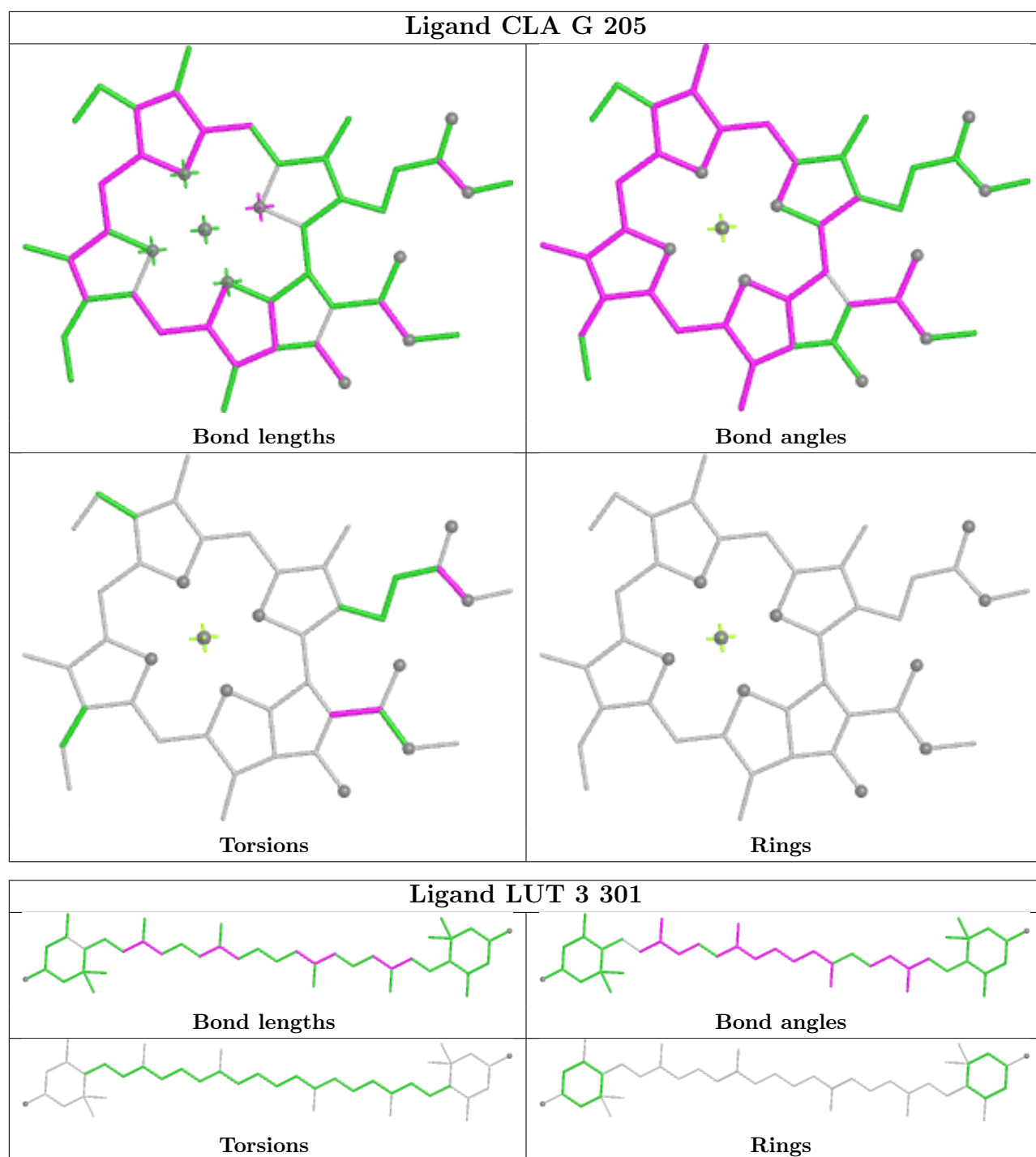
Ligand CLA B 815

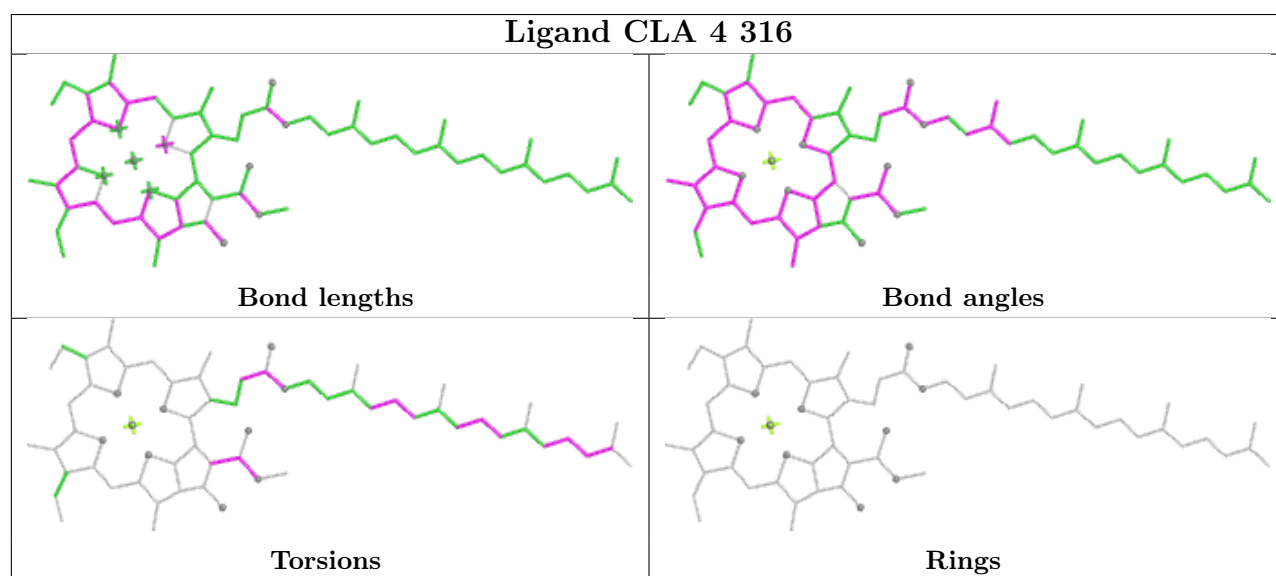
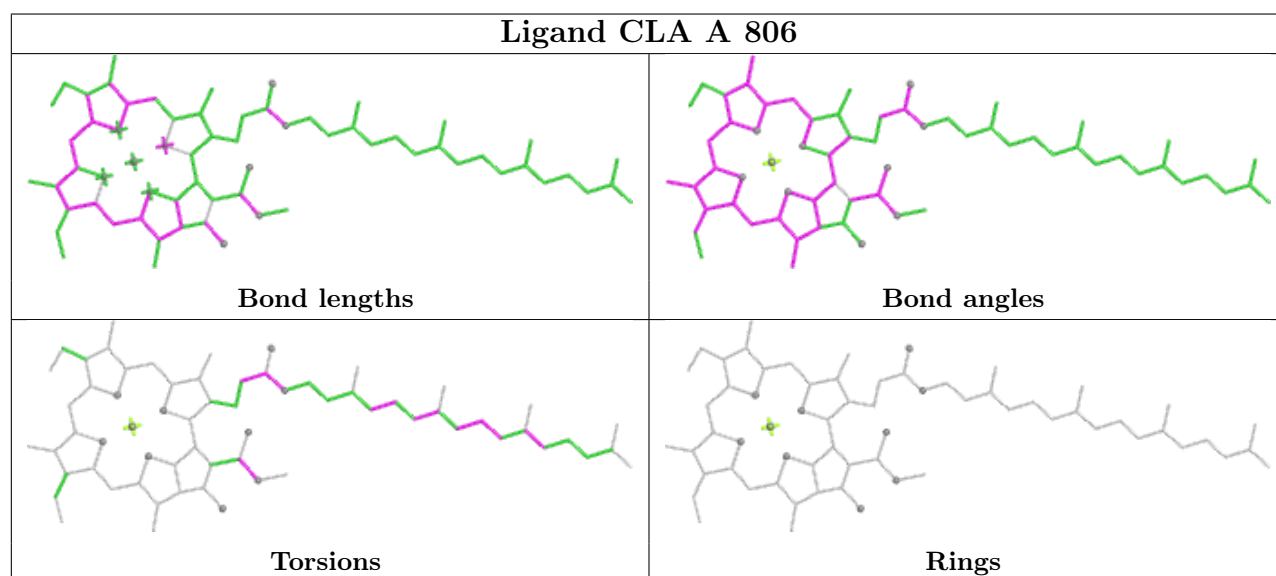
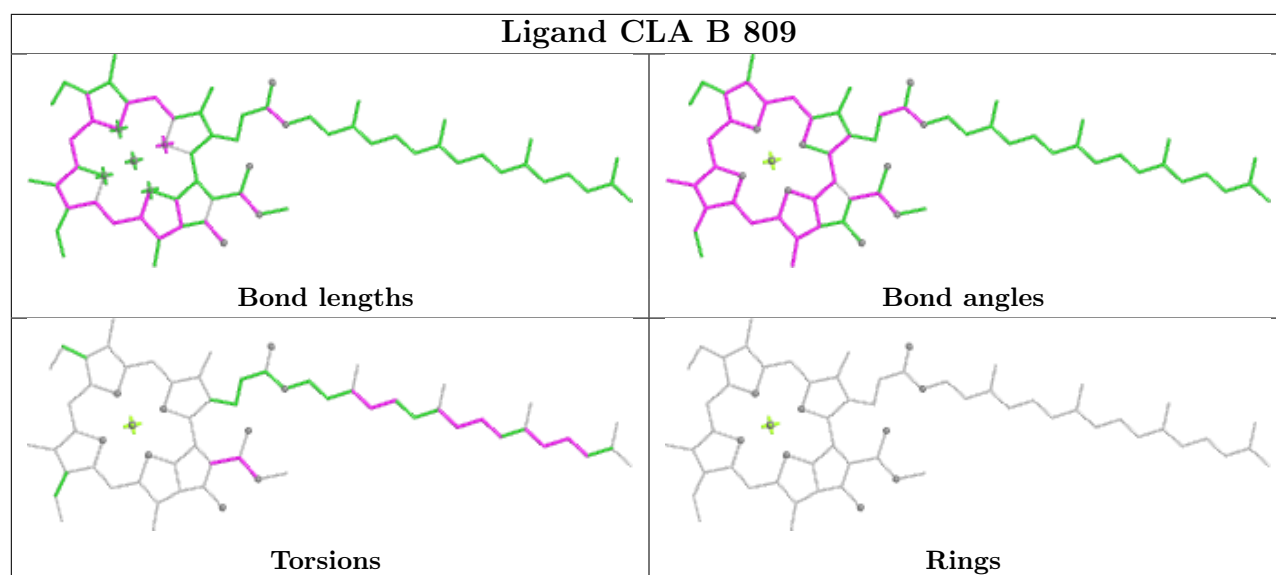


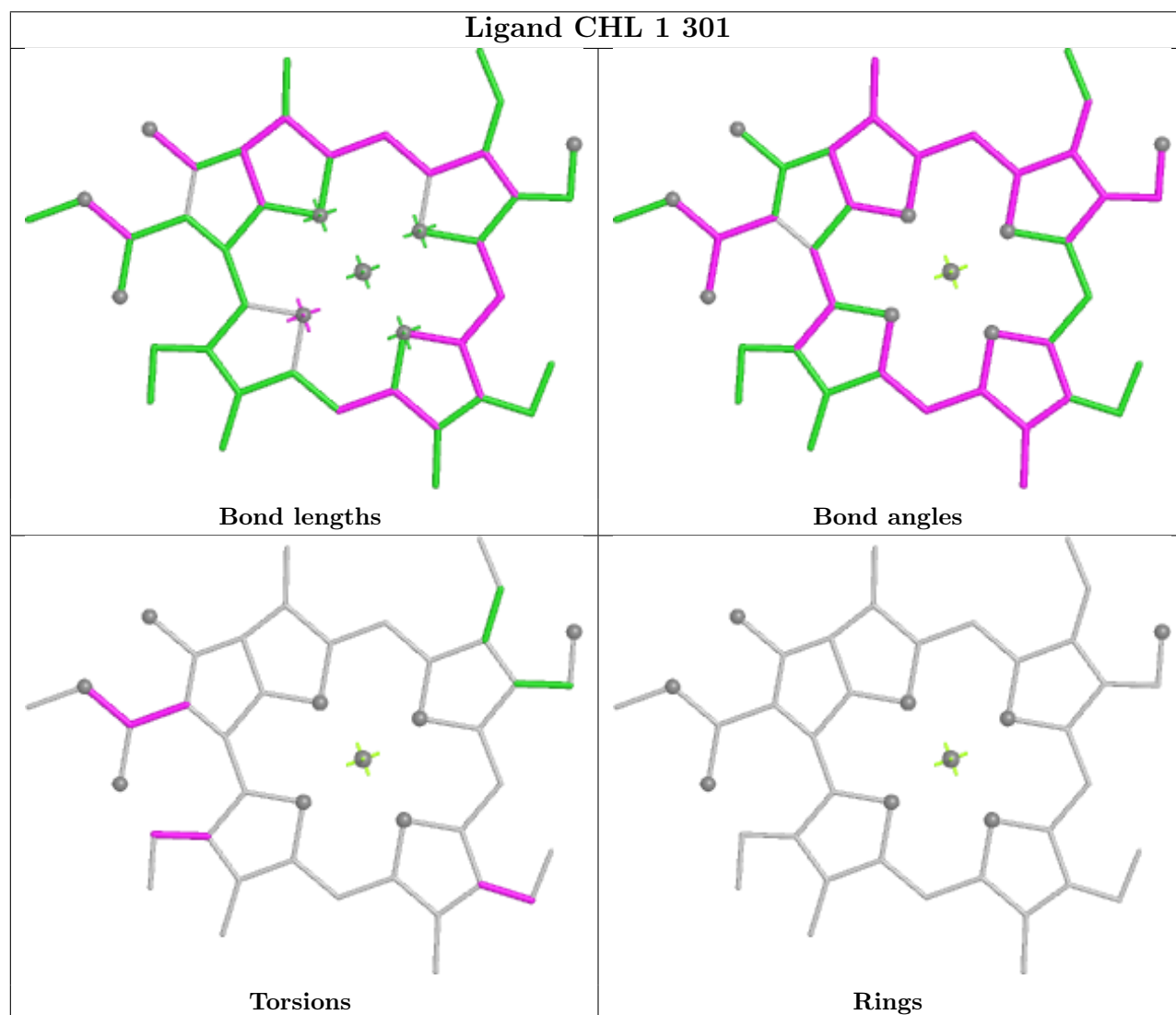
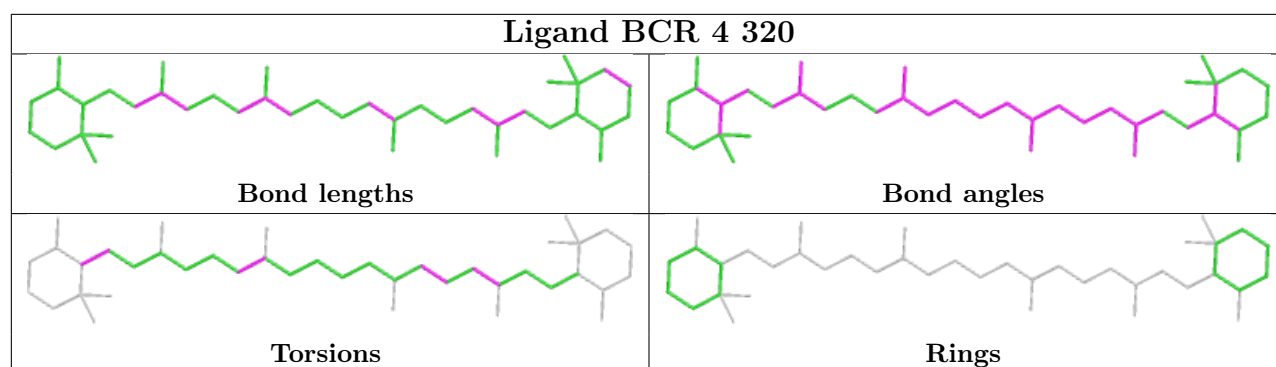
Ligand CLA 4 311

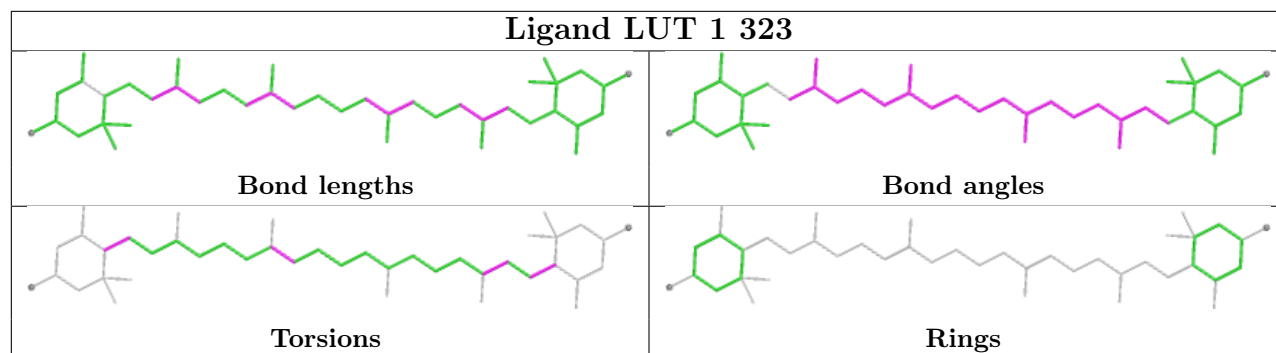
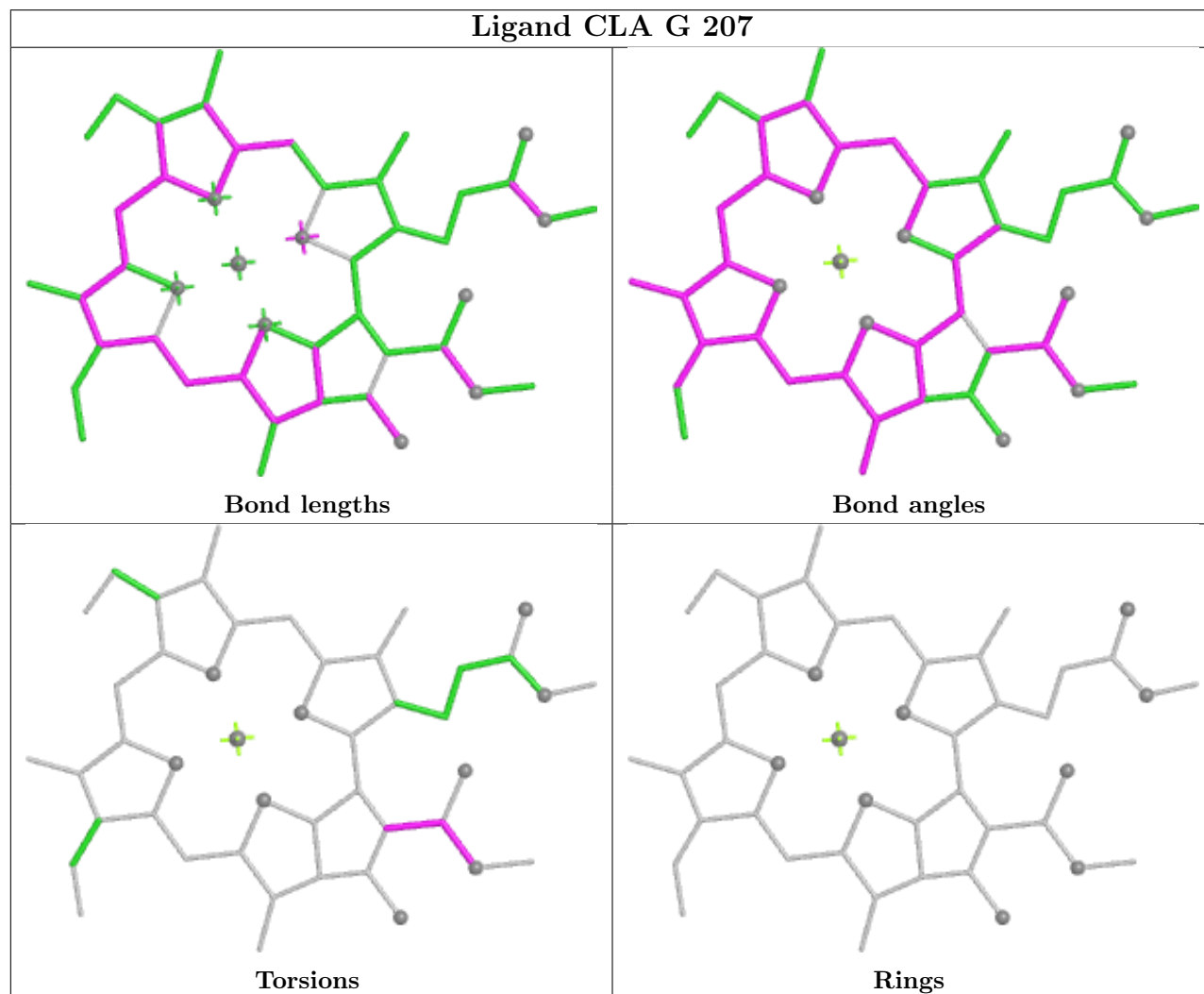


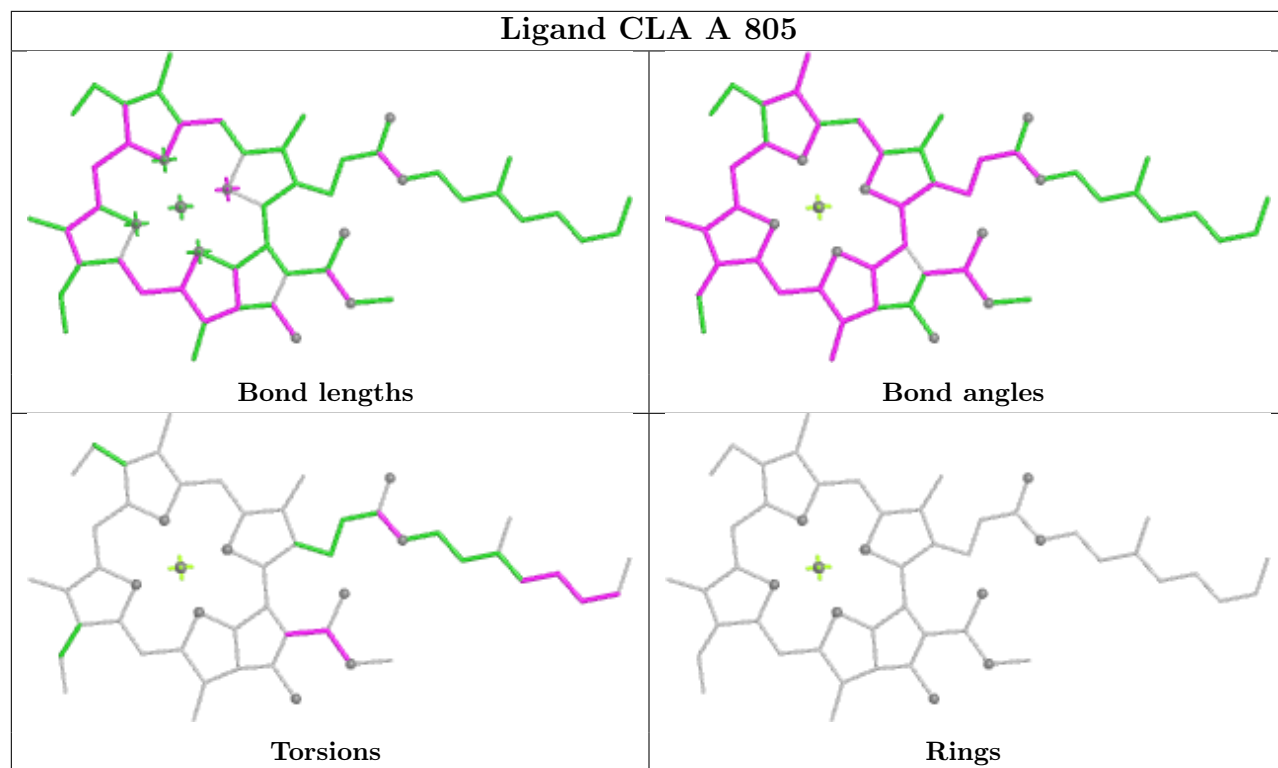




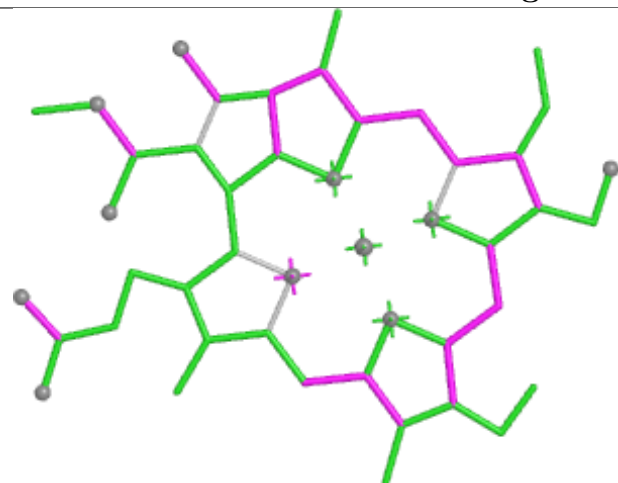




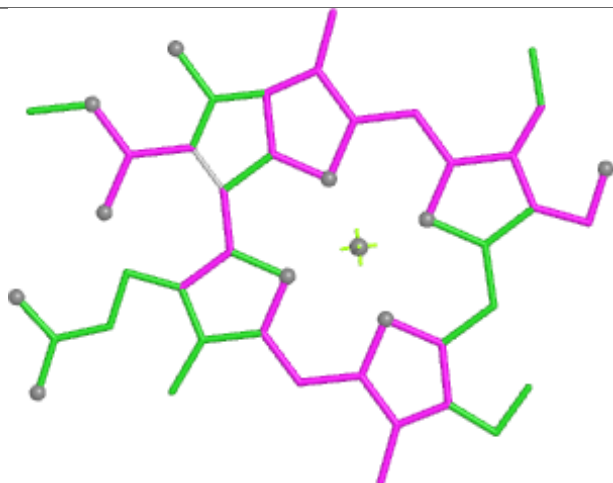
Ligand LUT 1 323**Ligand CLA G 207**



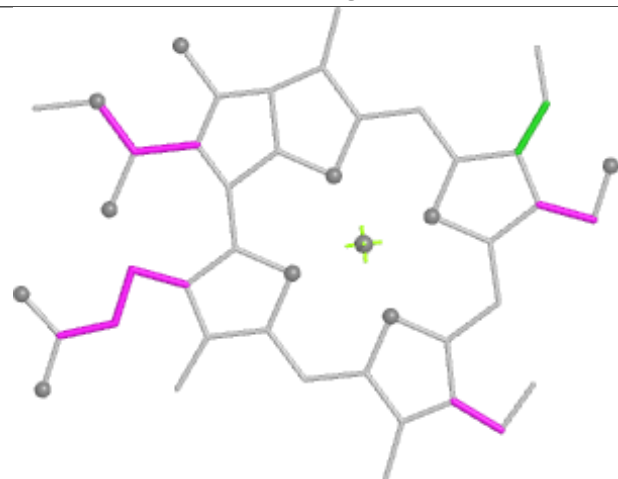
Ligand CHL 4 306



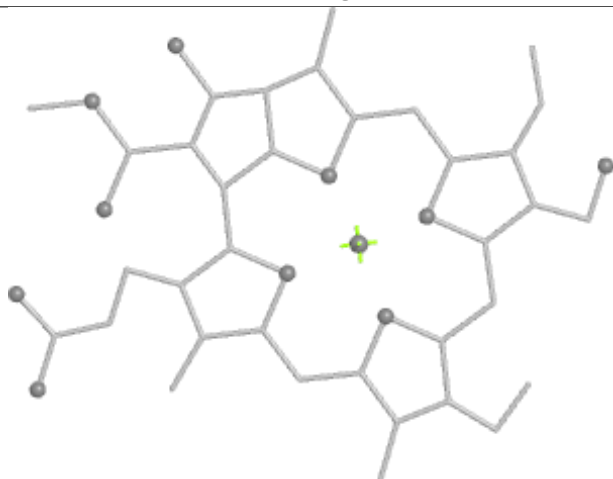
Bond lengths



Bond angles

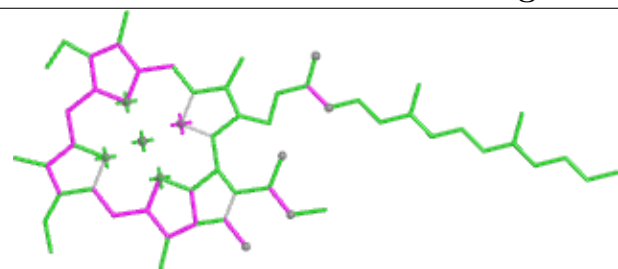


Torsions

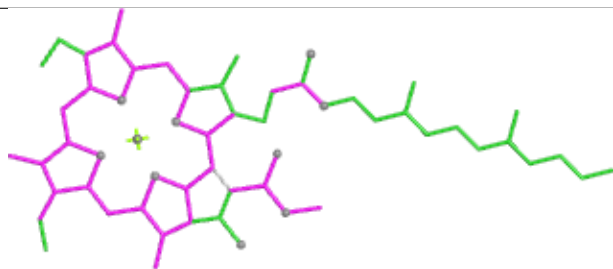


Rings

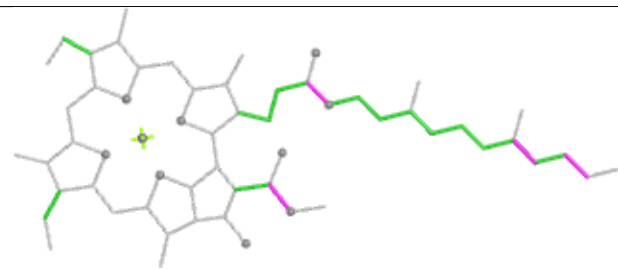
Ligand CLA B 817



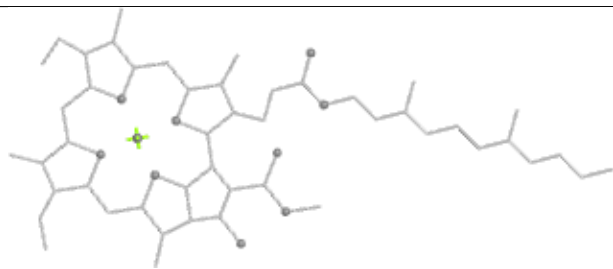
Bond lengths



Bond angles

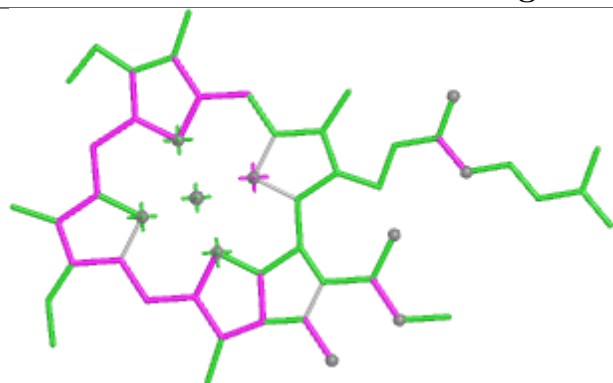


Torsions

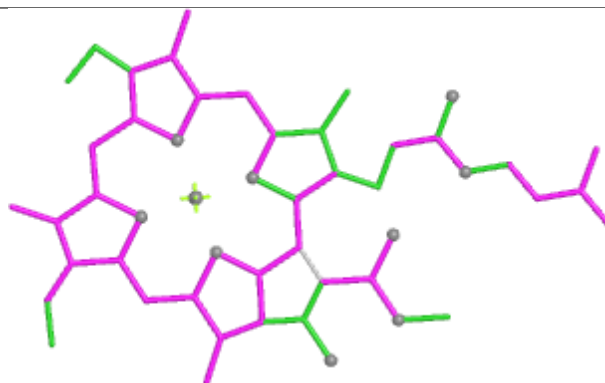


Rings

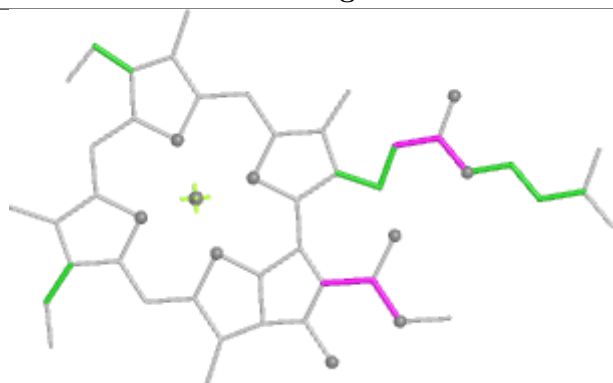
Ligand CLA 4 314



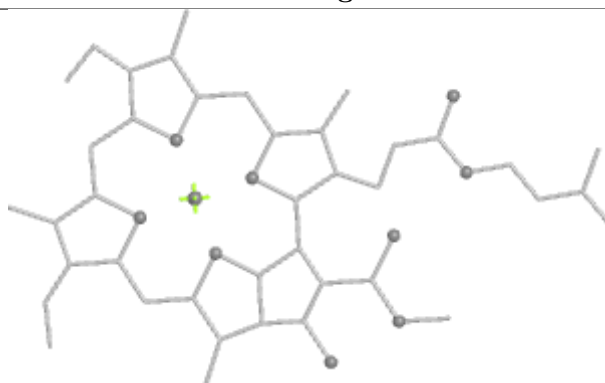
Bond lengths



Bond angles

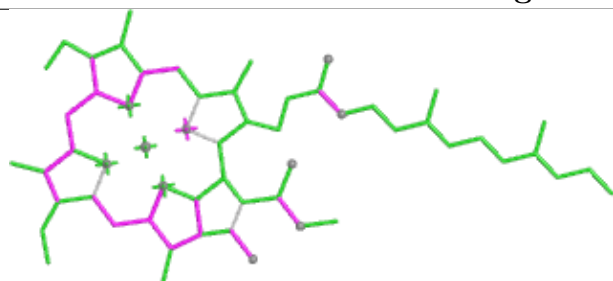


Torsions

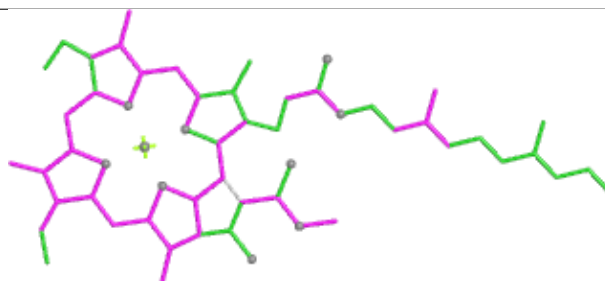


Rings

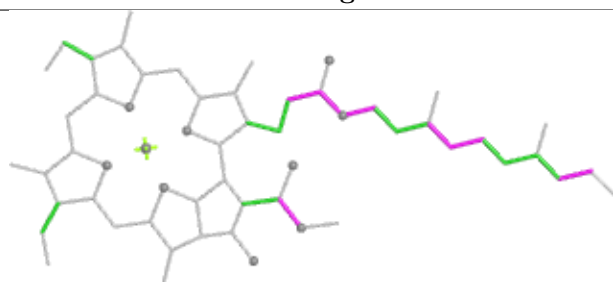
Ligand CLA B 813



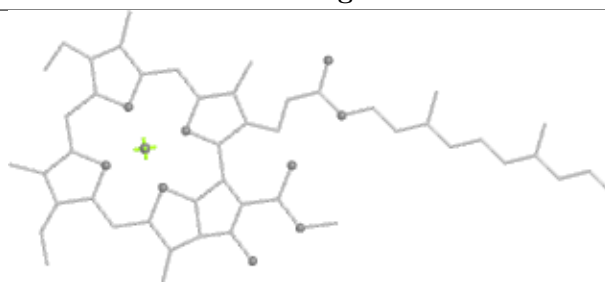
Bond lengths



Bond angles

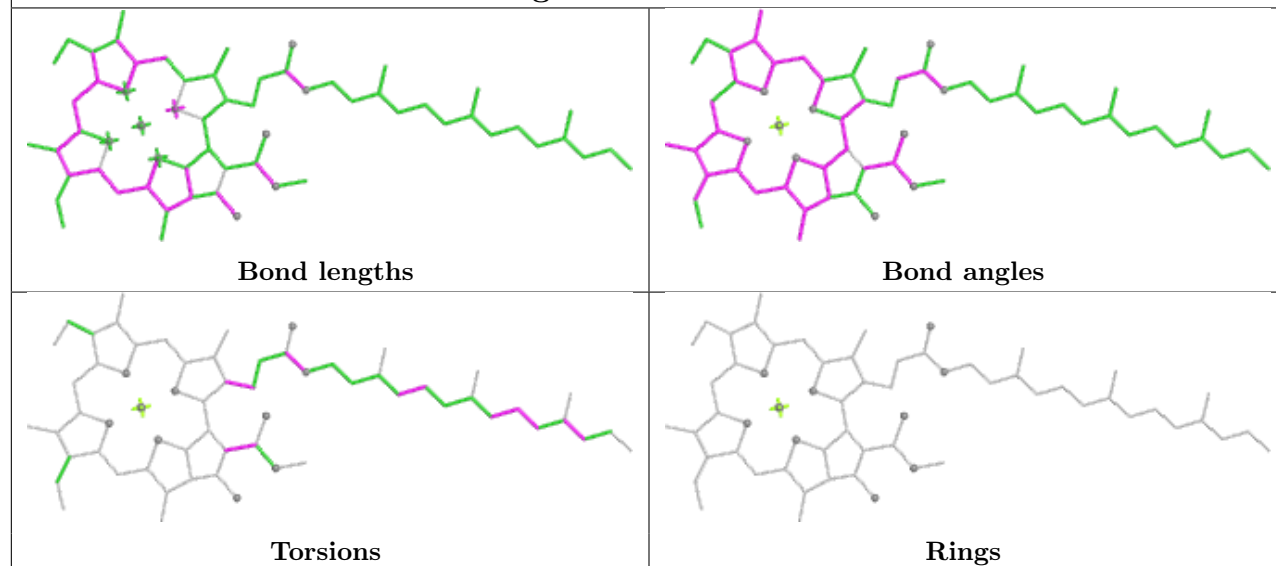


Torsions

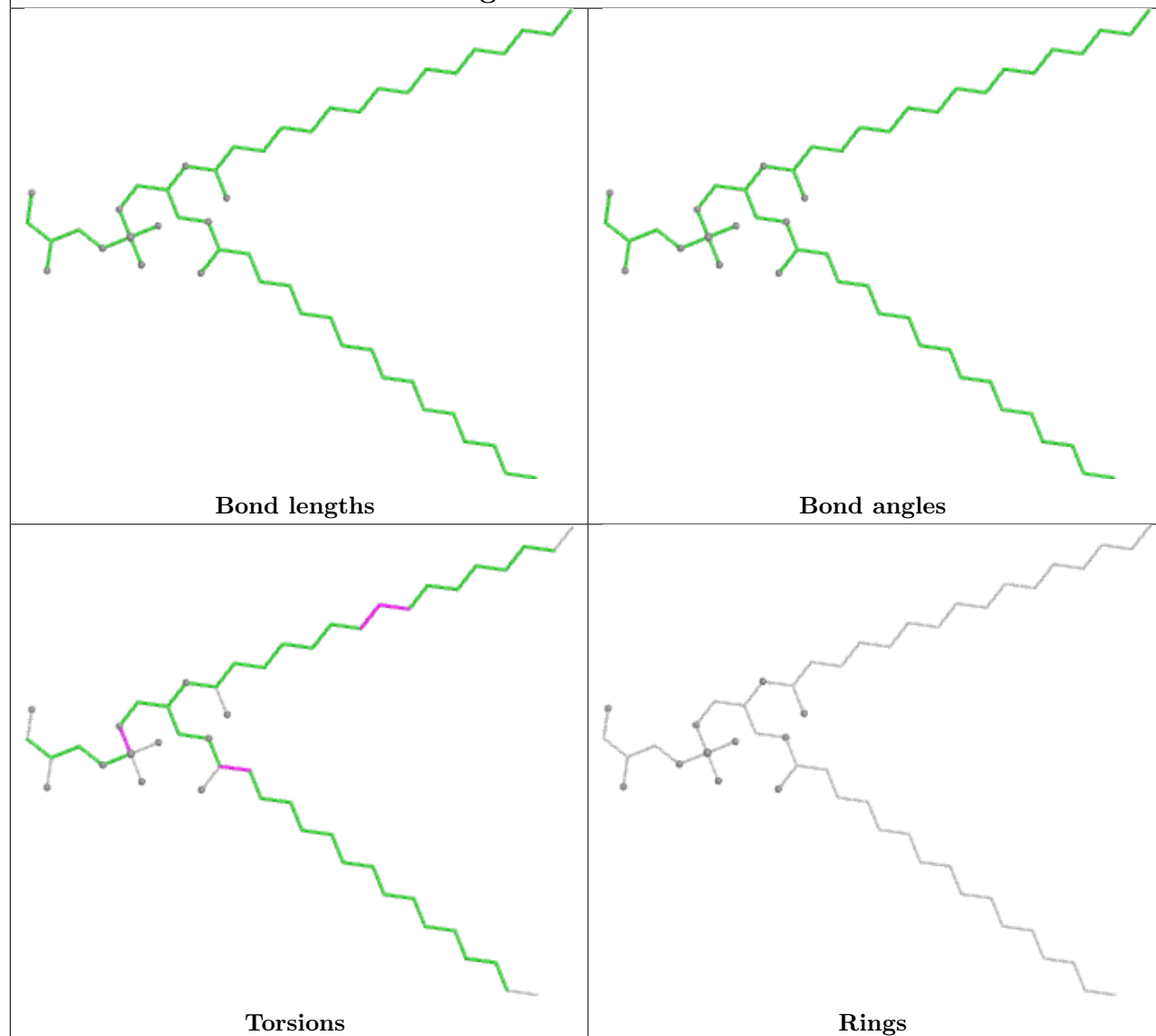


Rings

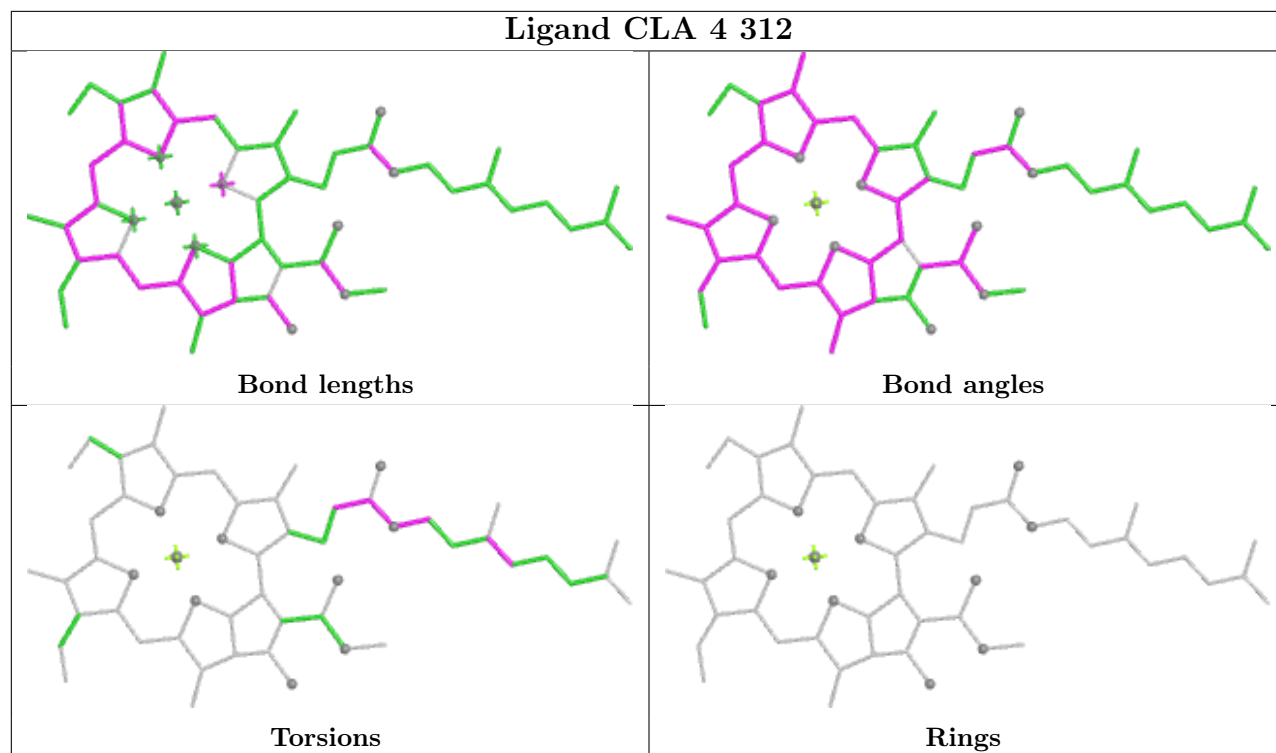
Ligand CLA B 823



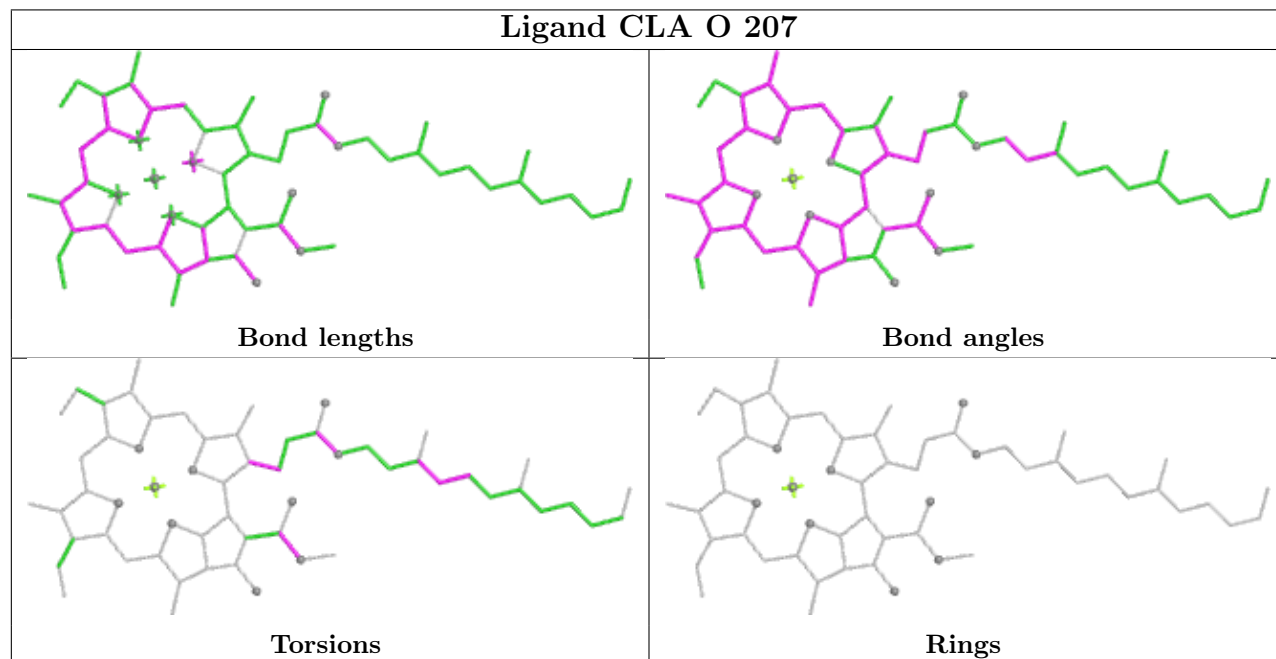
Ligand LHG A 819



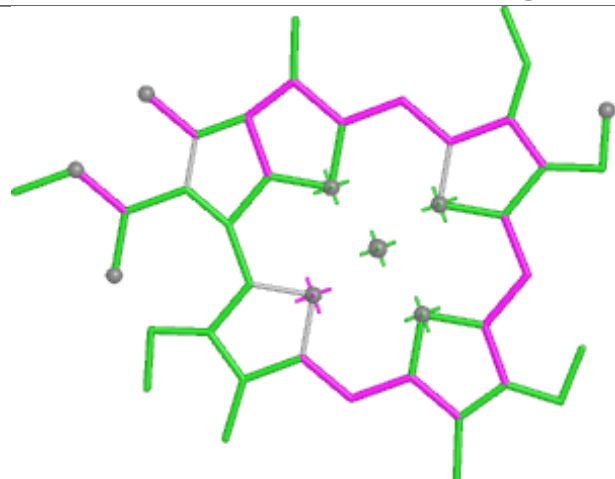
Ligand CLA 4 312



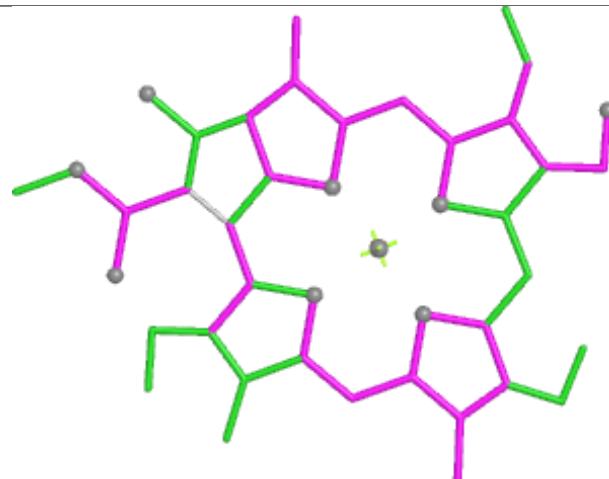
Ligand CLA O 207



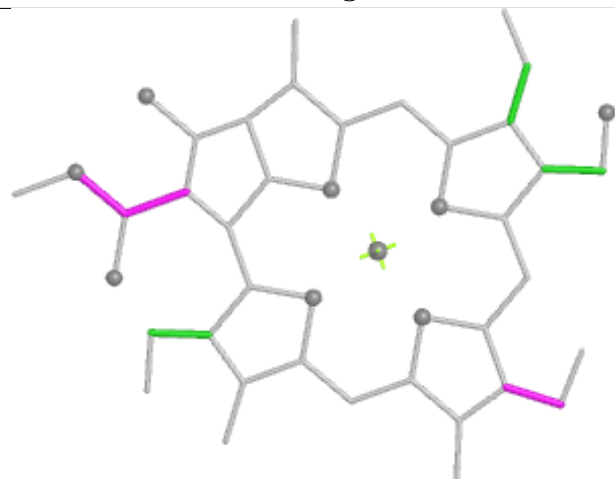
Ligand CHL 2 309



Bond lengths



Bond angles

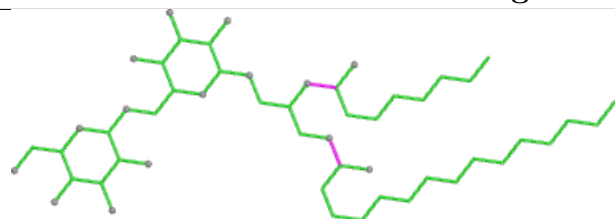


Torsions

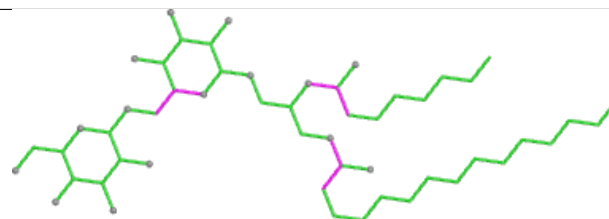


Rings

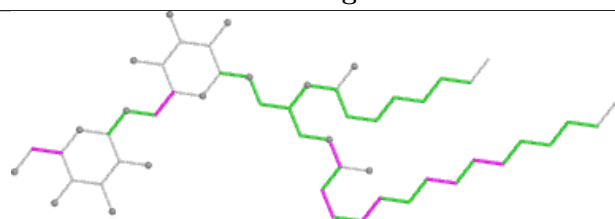
Ligand DGD O 201



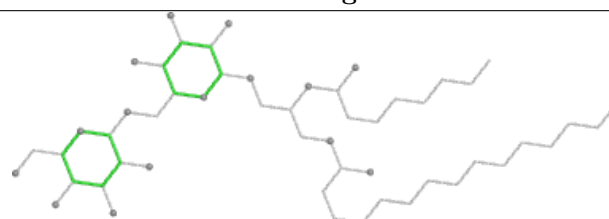
Bond lengths



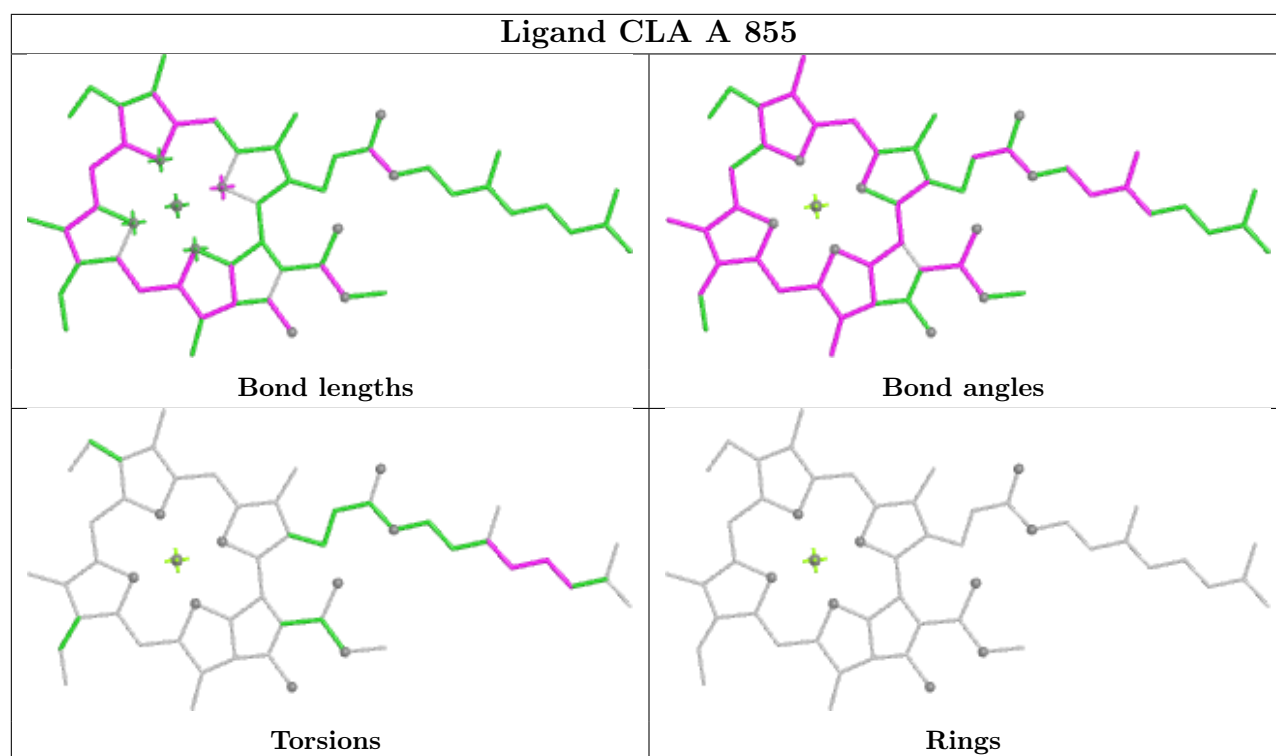
Bond angles



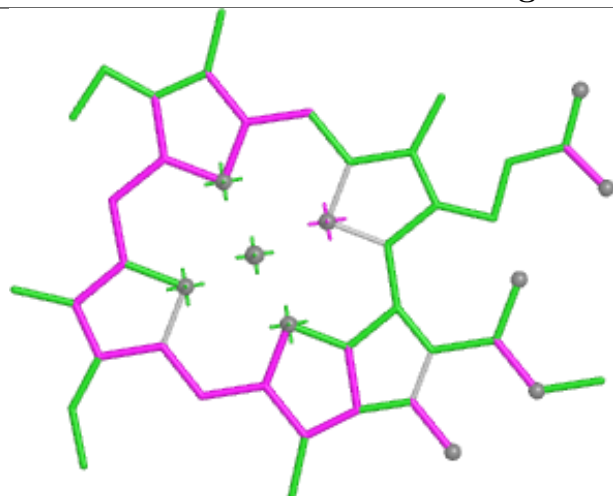
Torsions



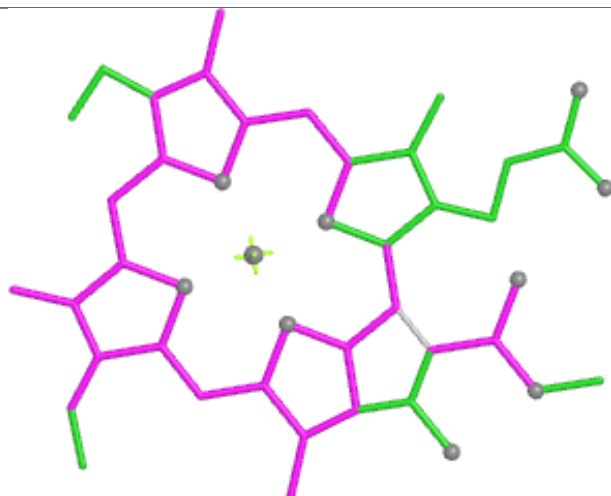
Rings



Ligand CLA 4 304



Bond lengths



Bond angles

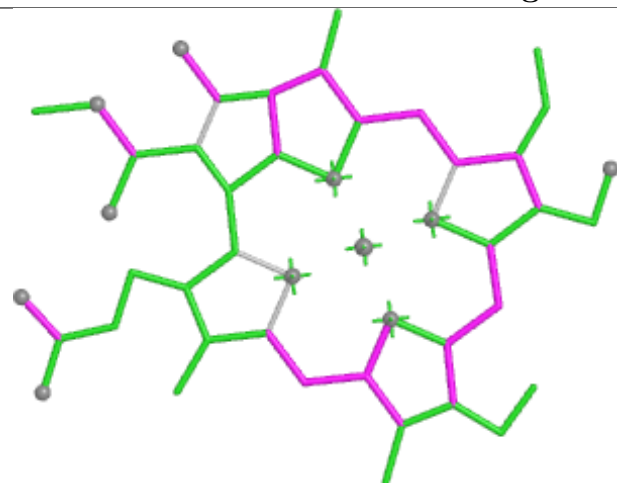


Torsions

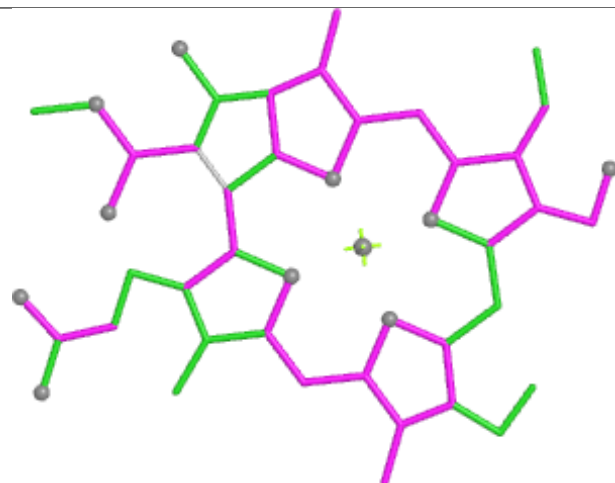


Rings

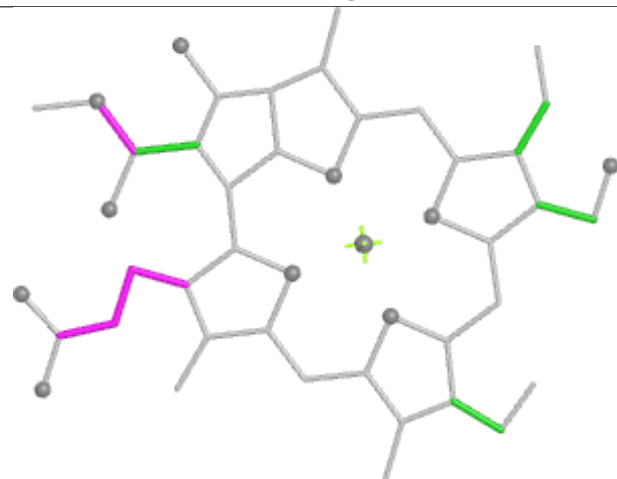
Ligand CHL 4 307



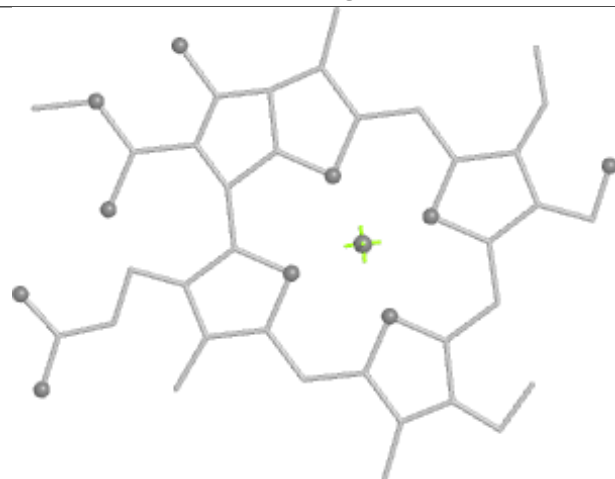
Bond lengths



Bond angles

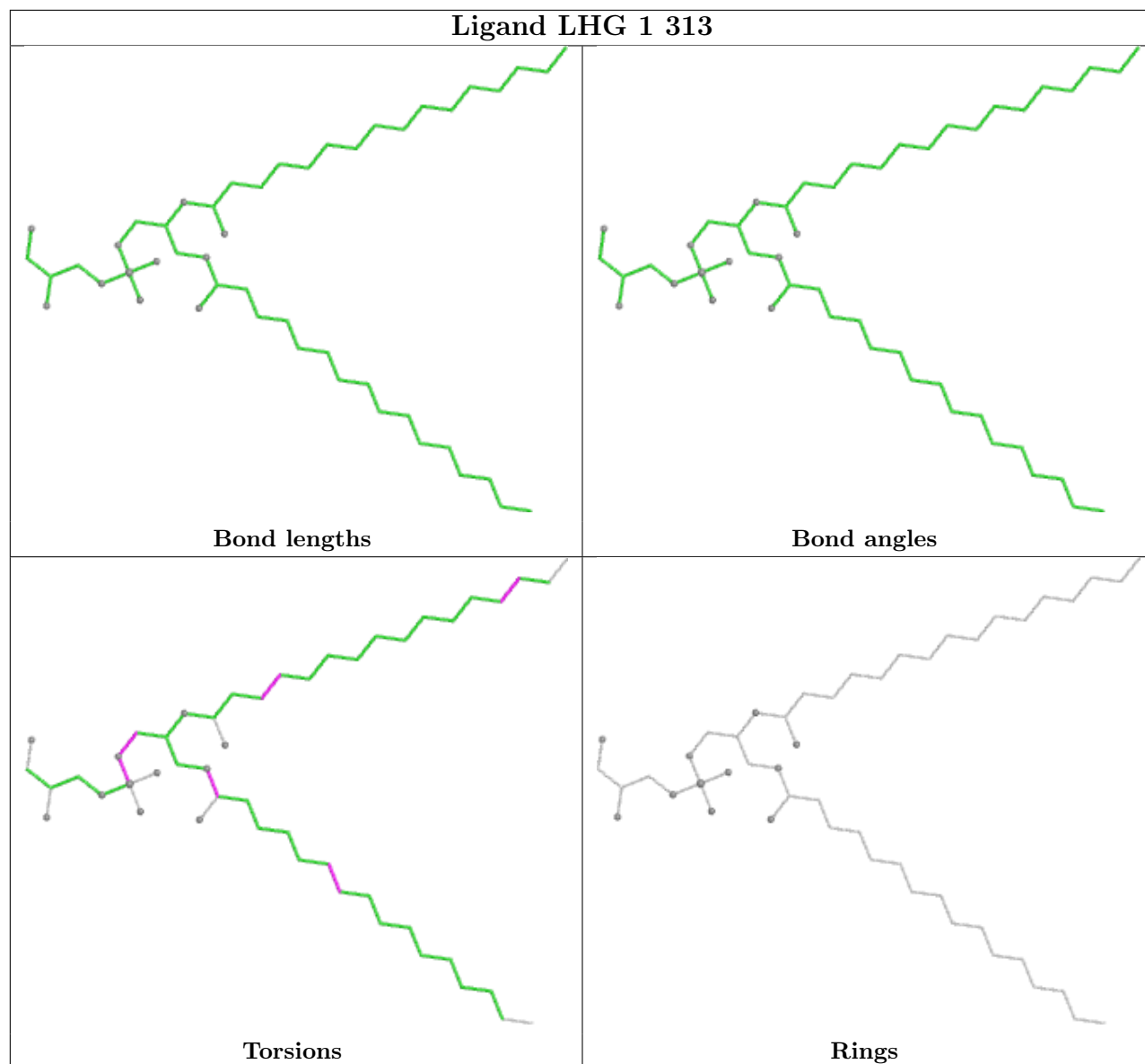


Torsions

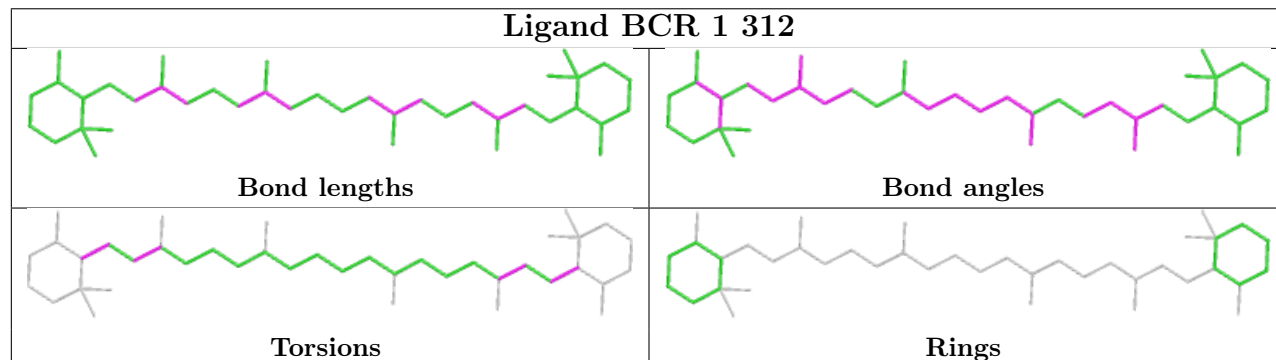


Rings

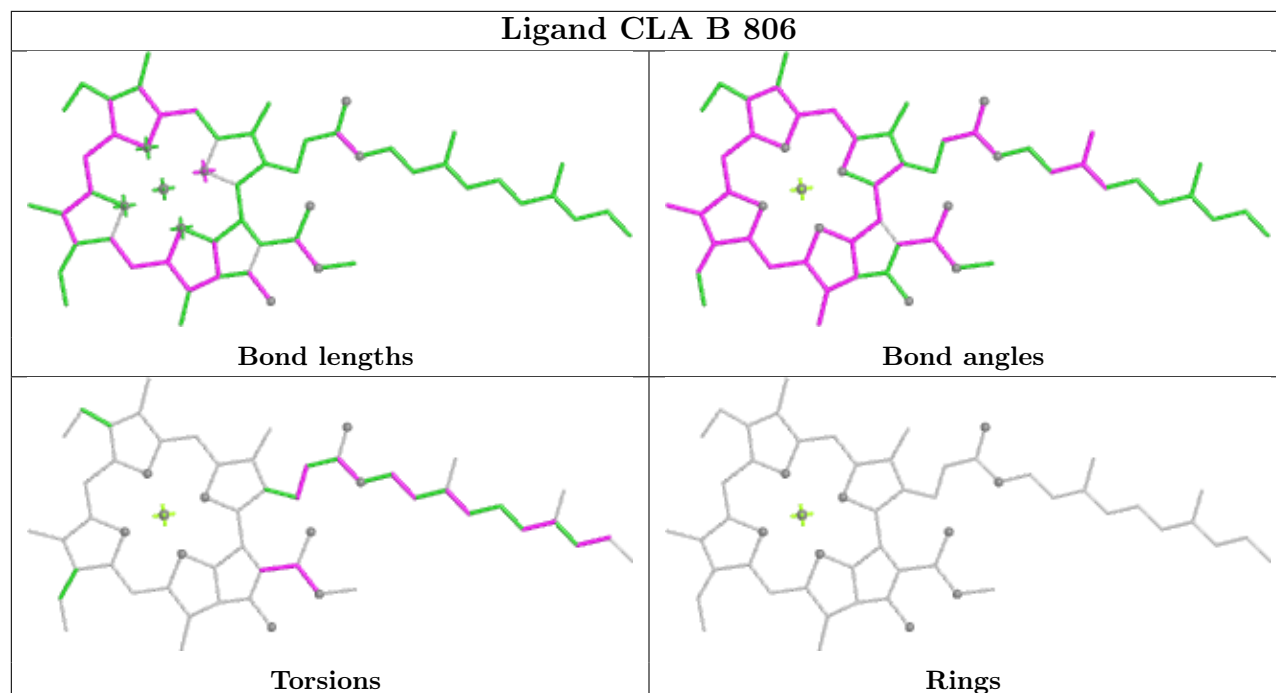
Ligand LHG 1 313



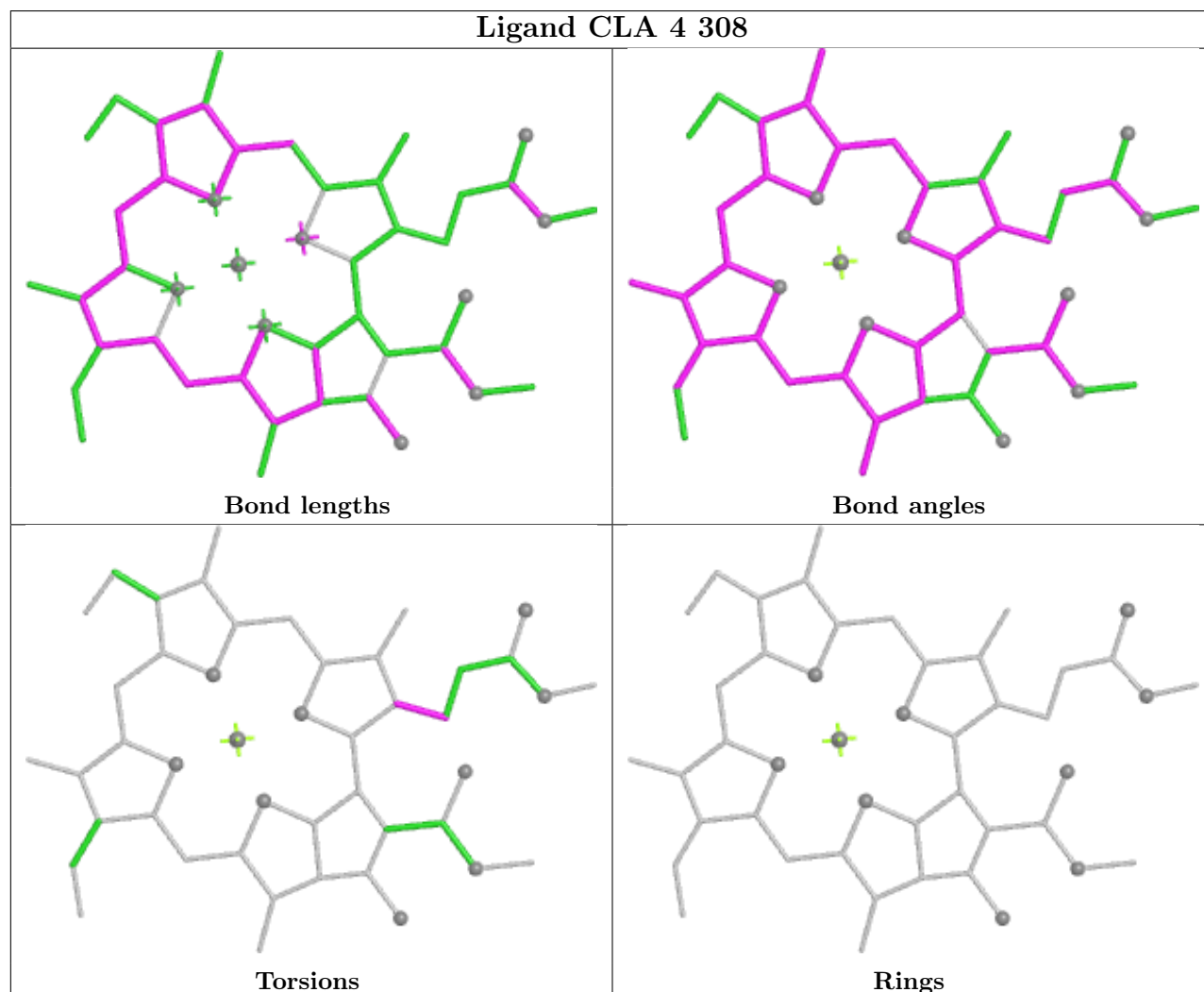
Ligand BCR 1 312

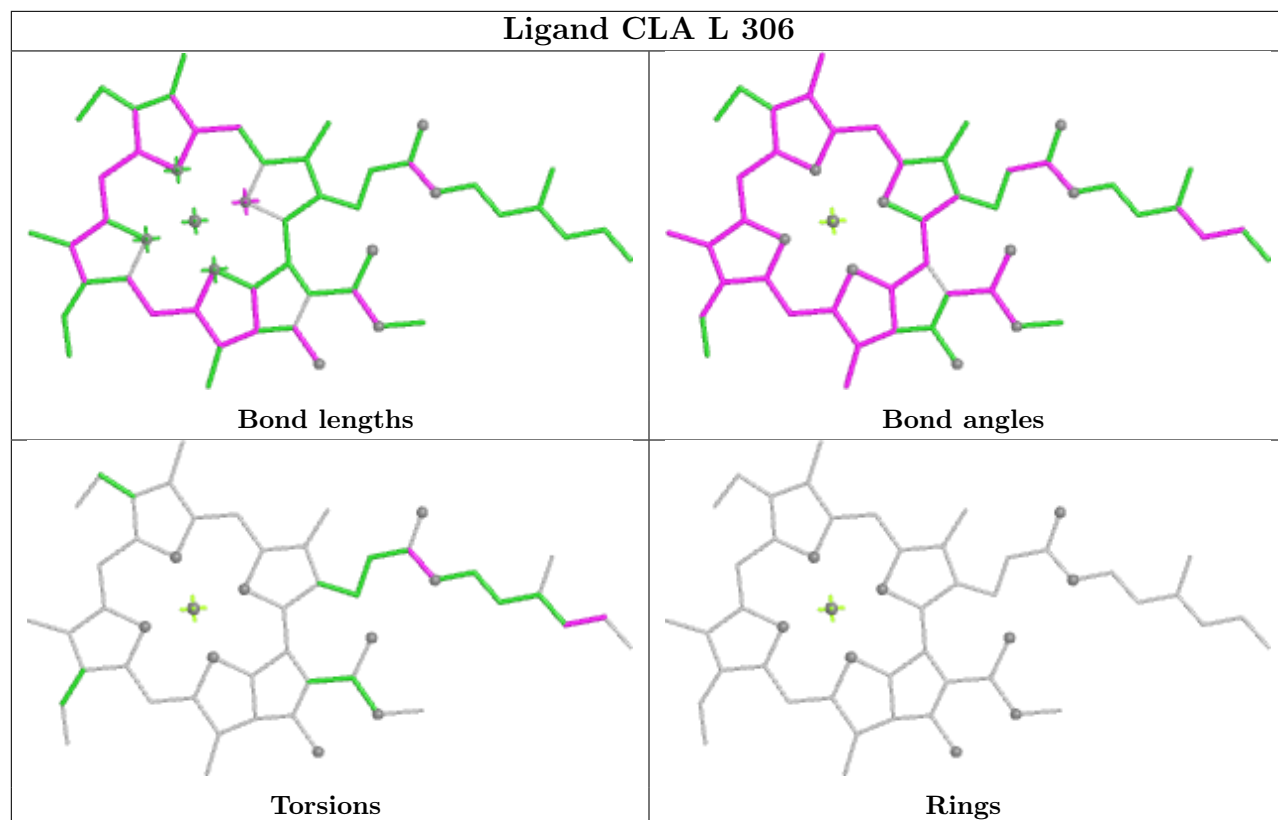


Ligand CLA B 806

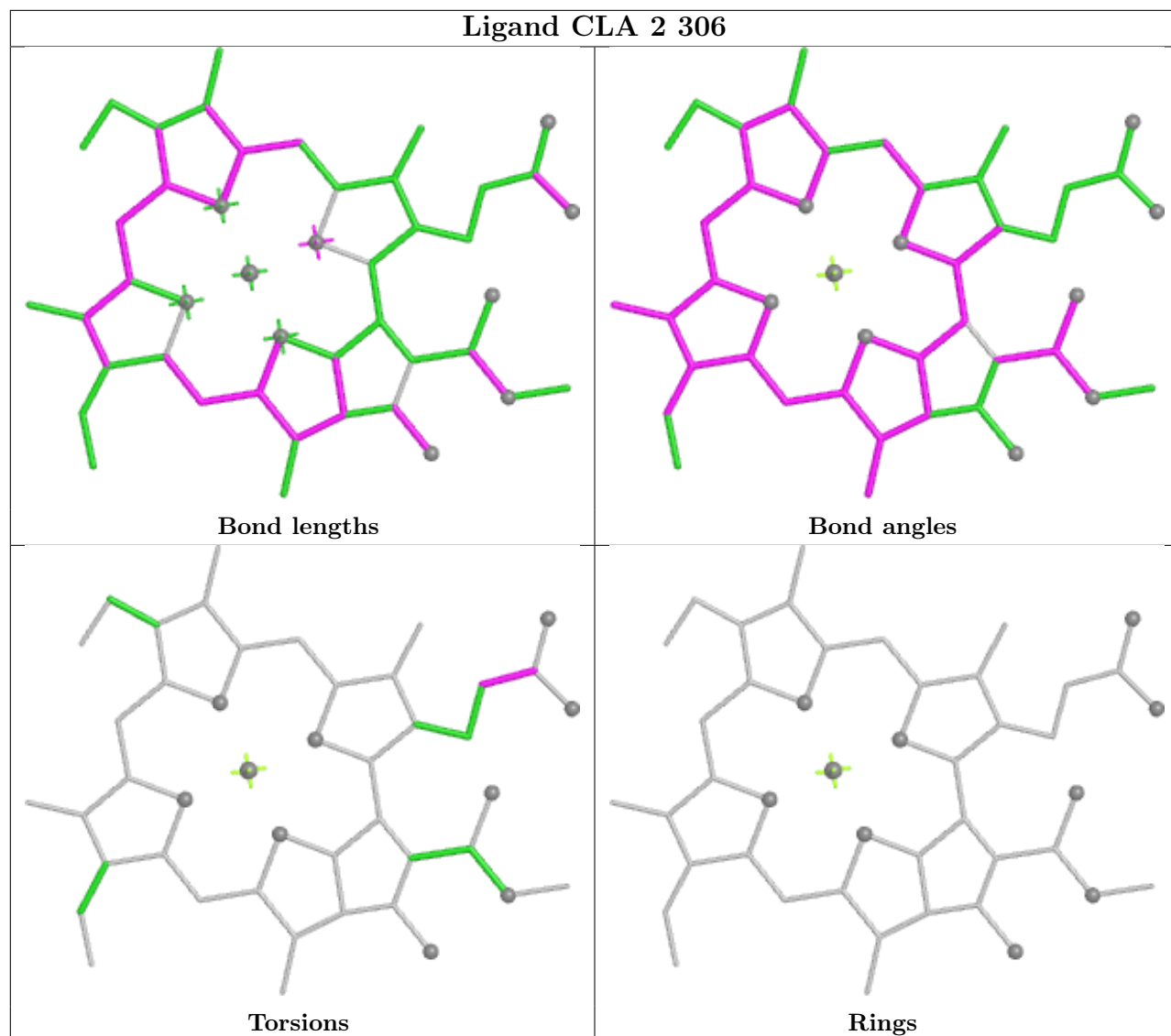


Ligand CLA 4 308

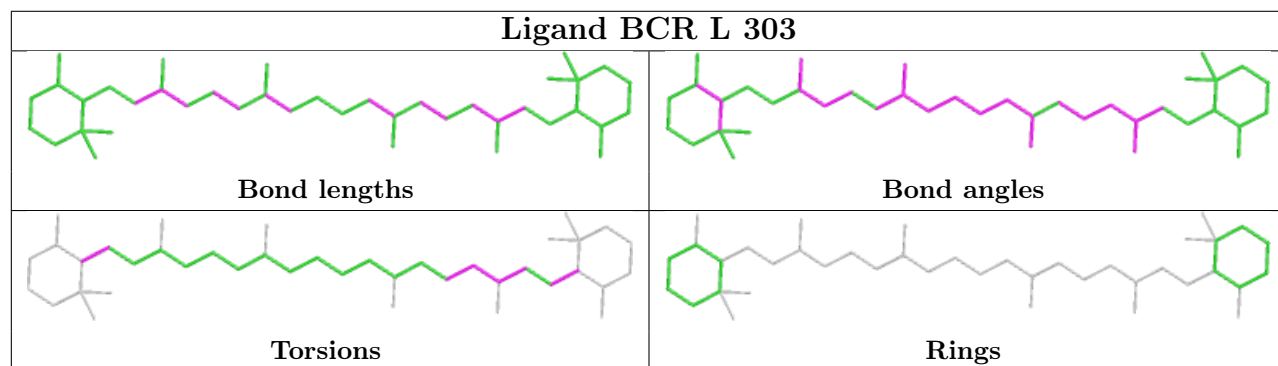




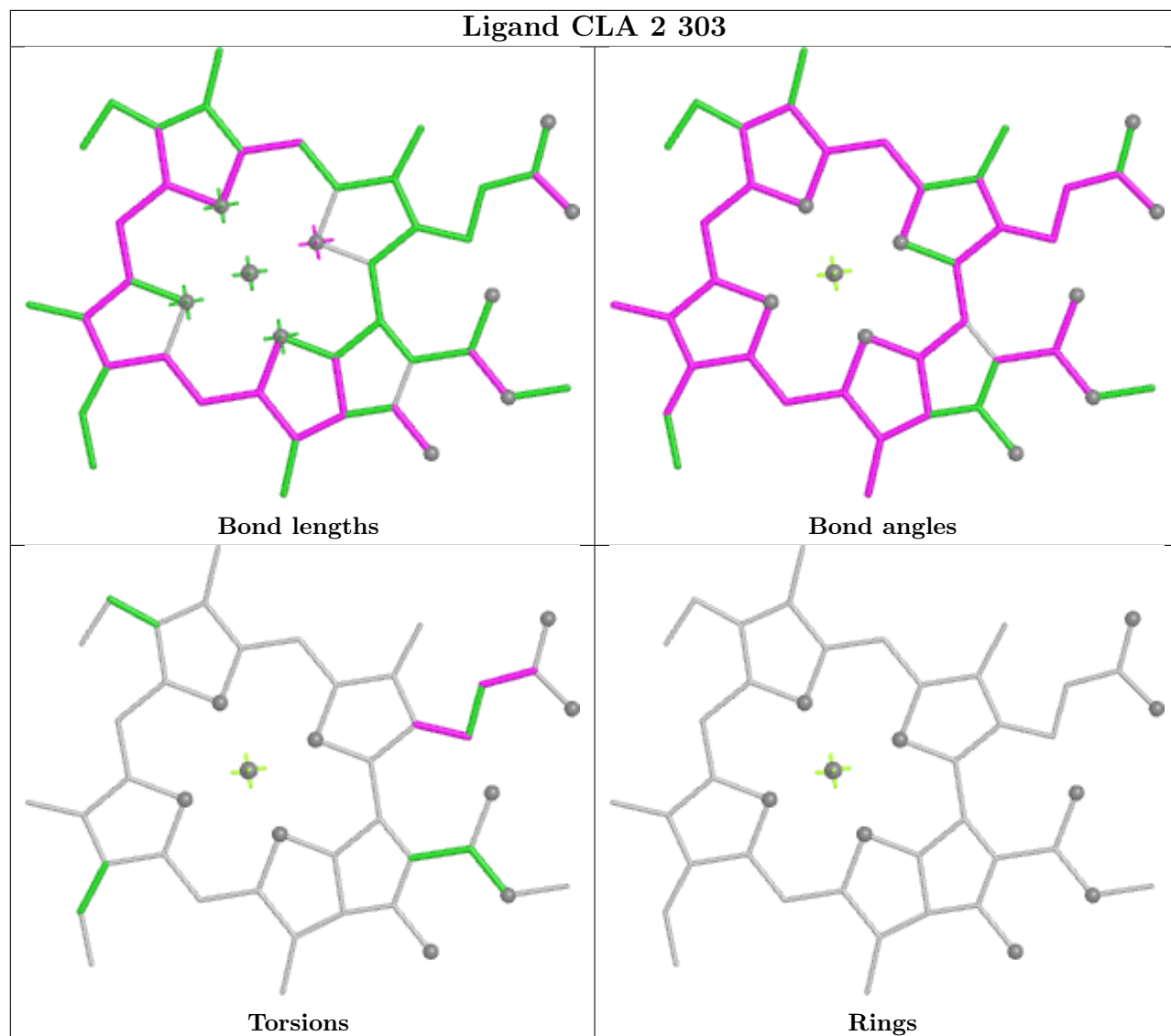
Ligand CLA 2 306

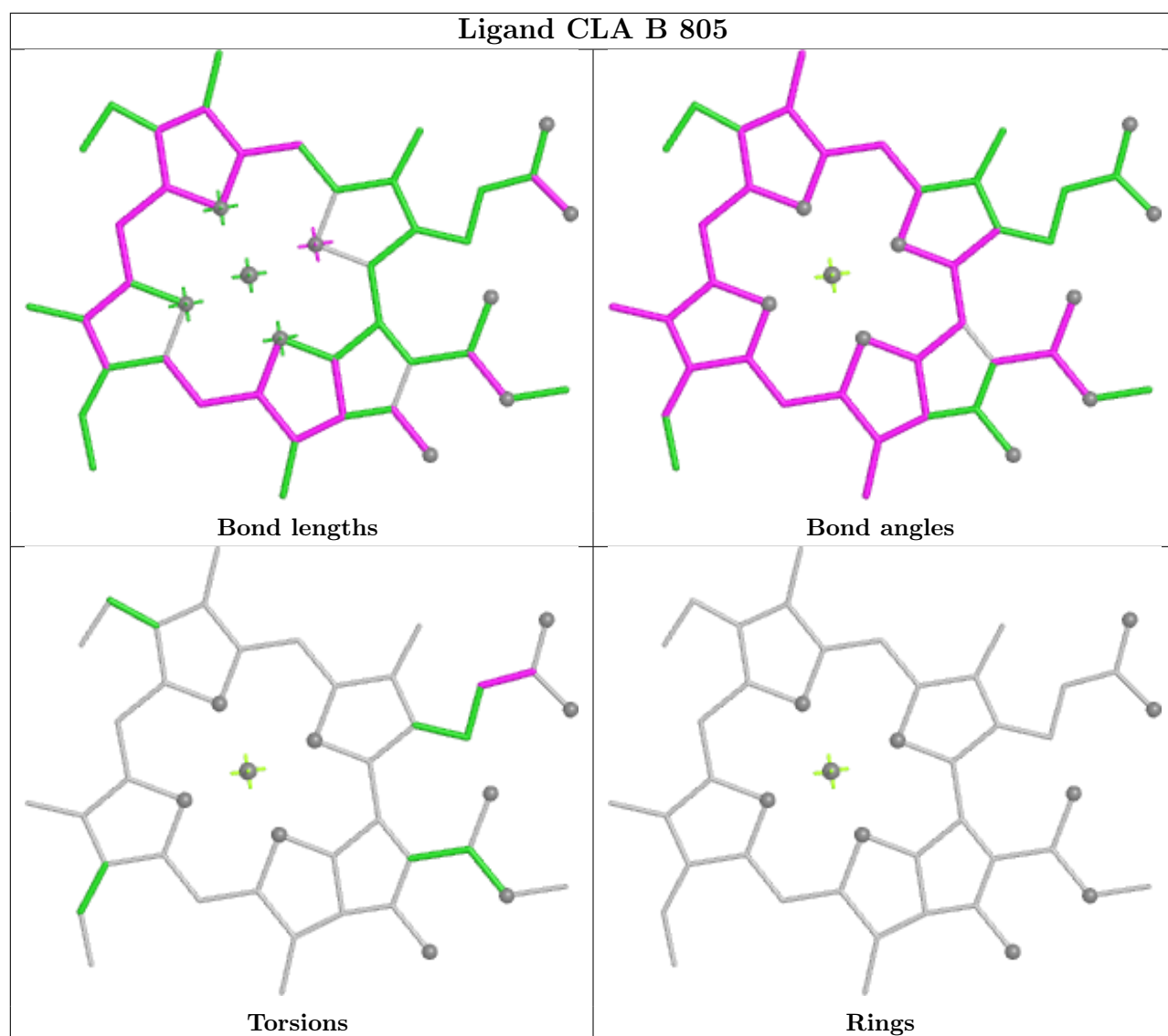


Ligand BCR L 303

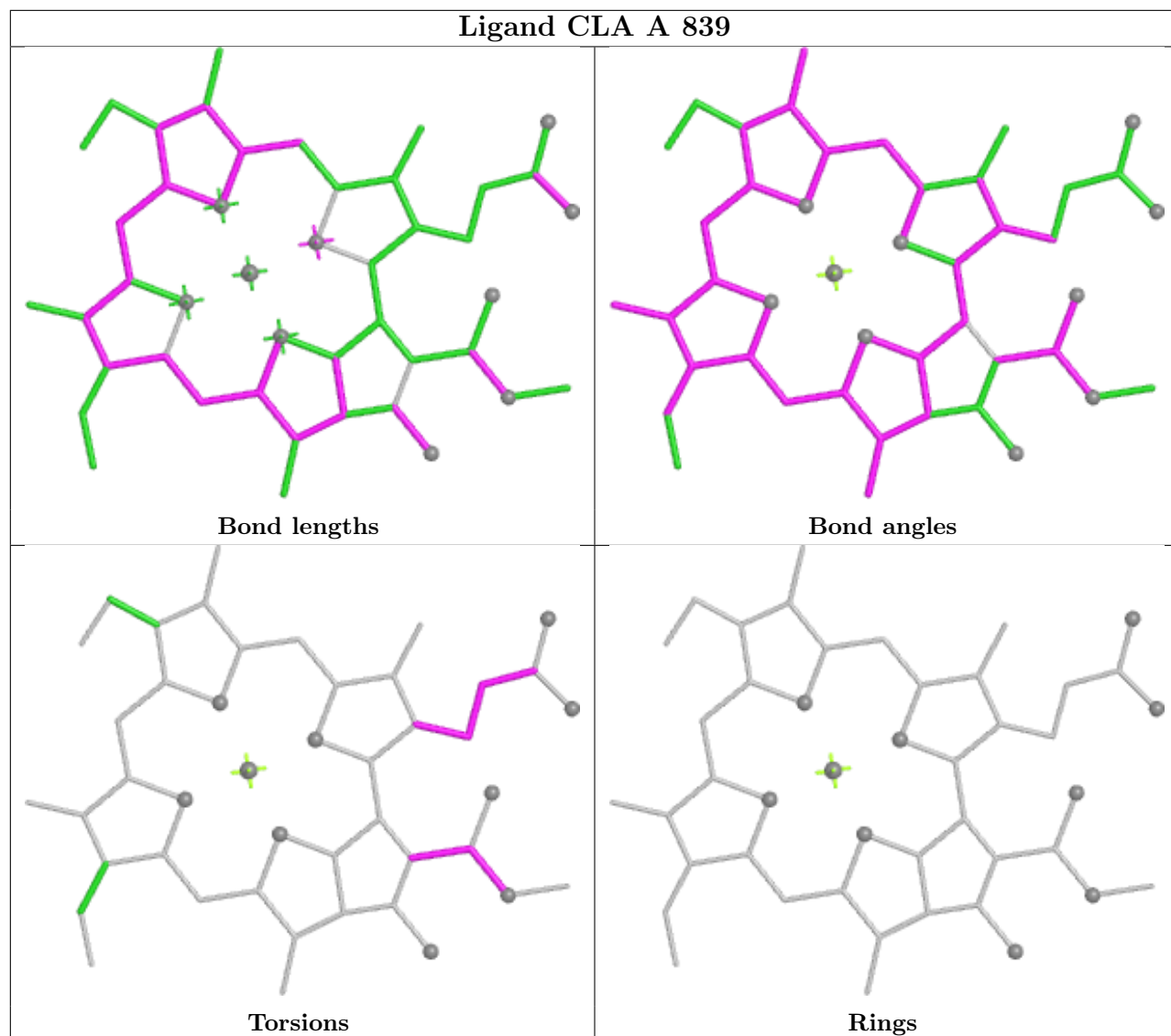


Ligand CLA 2 303

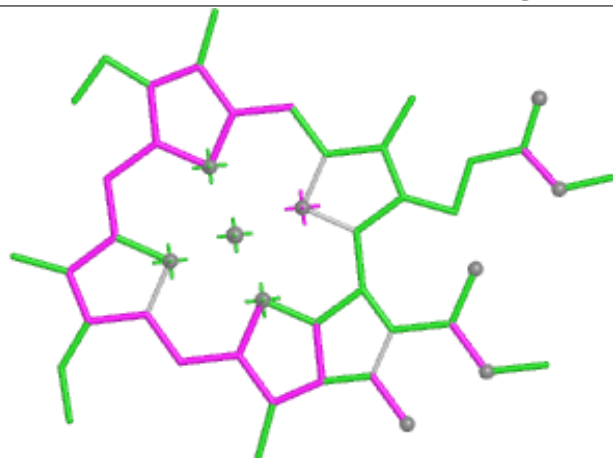




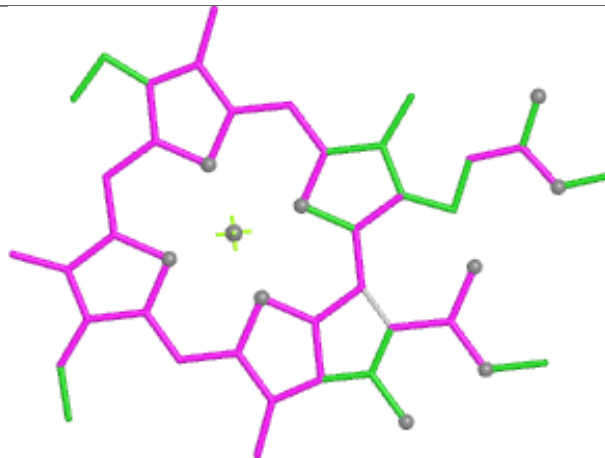
Ligand CLA A 839



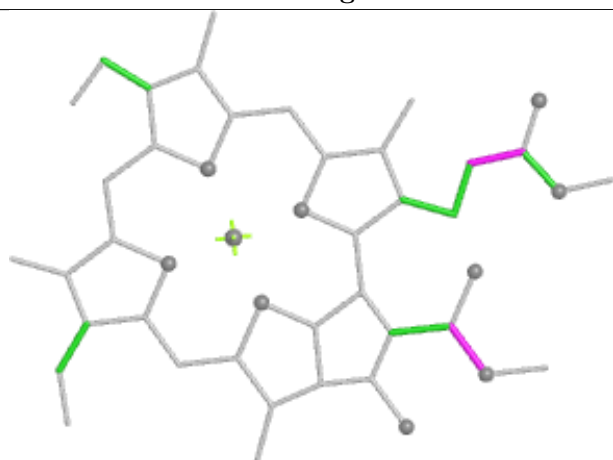
Ligand CLA L 307



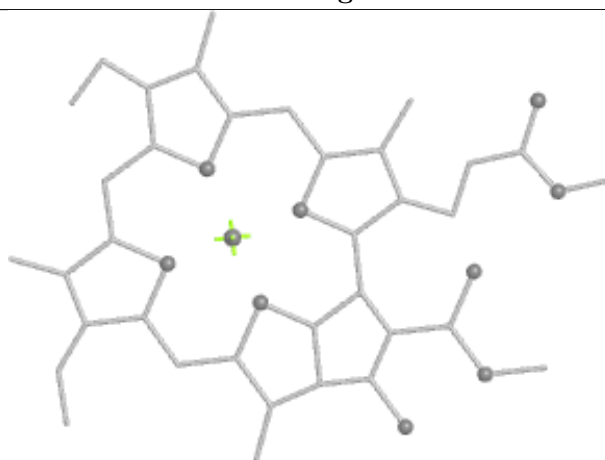
Bond lengths



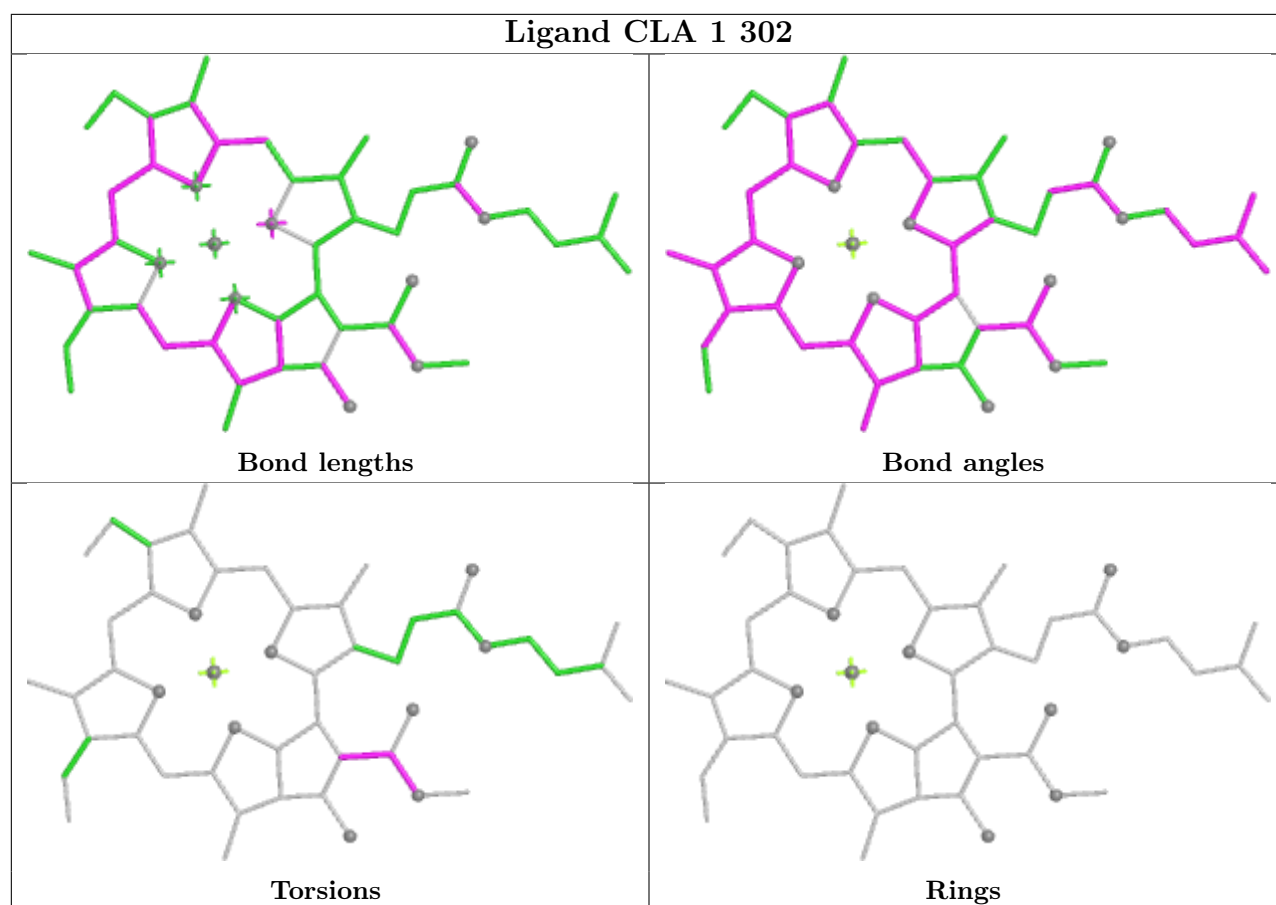
Bond angles

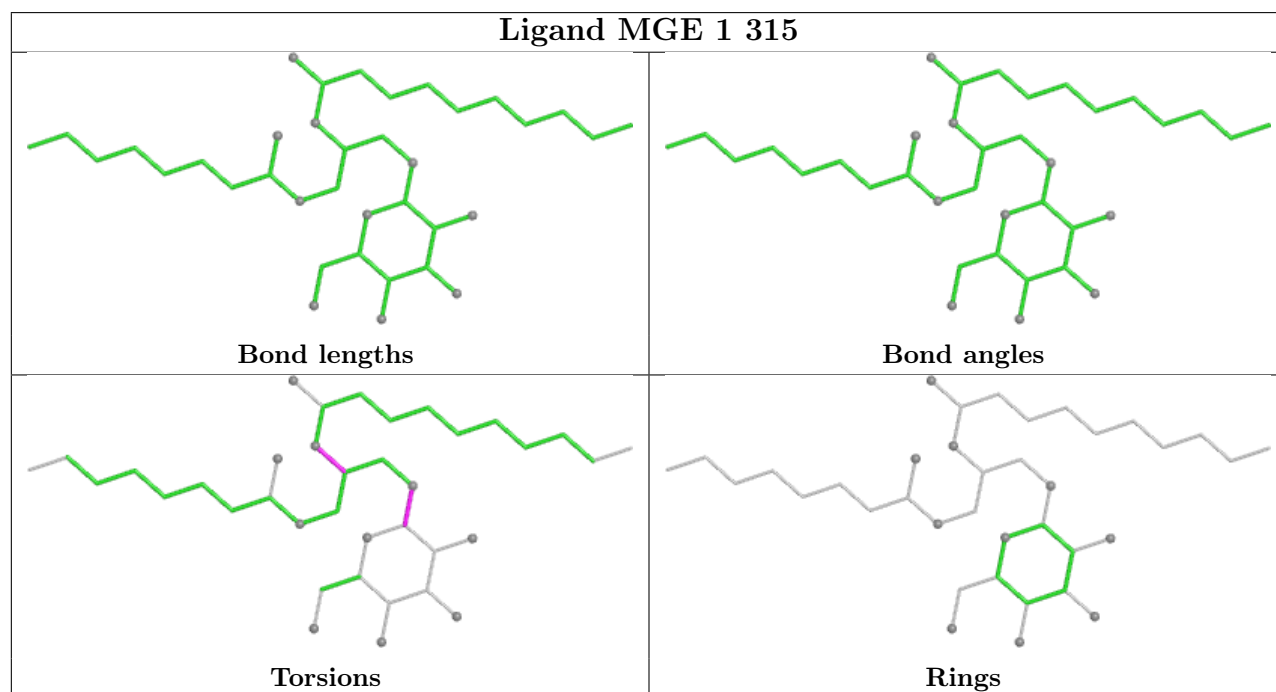
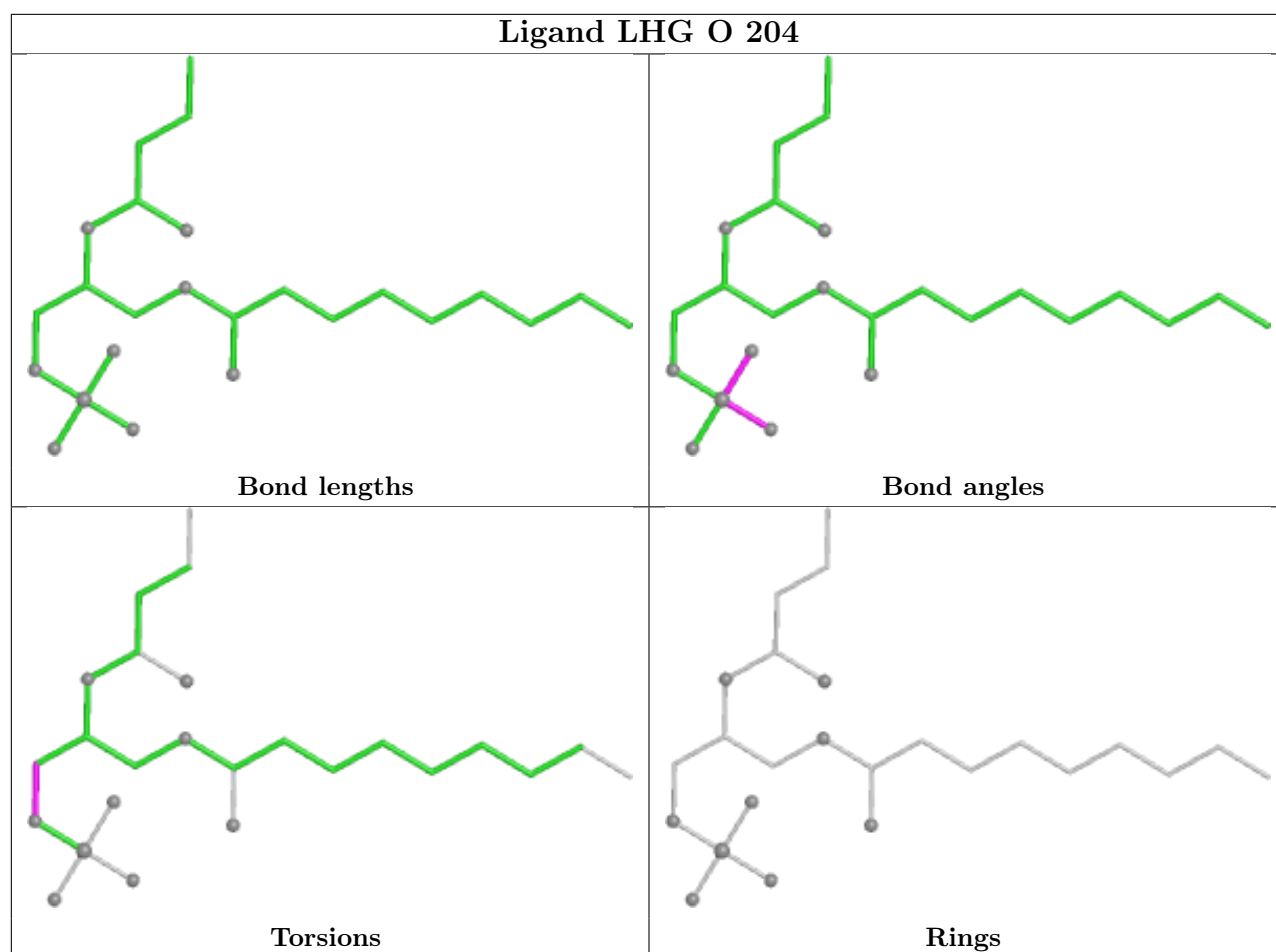


Torsions

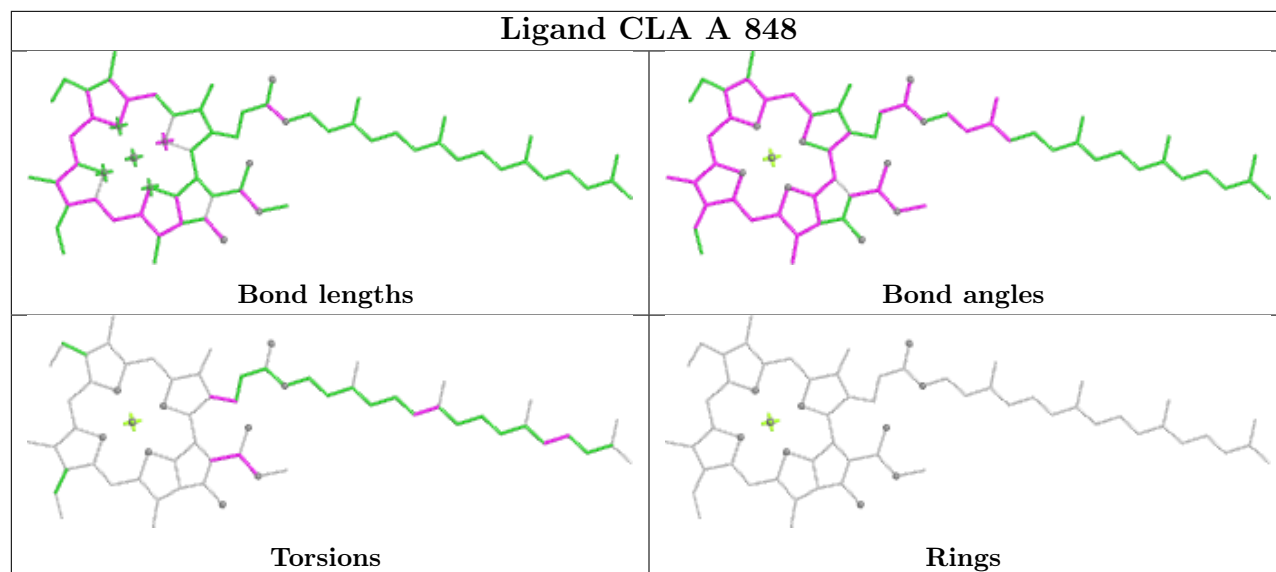


Rings

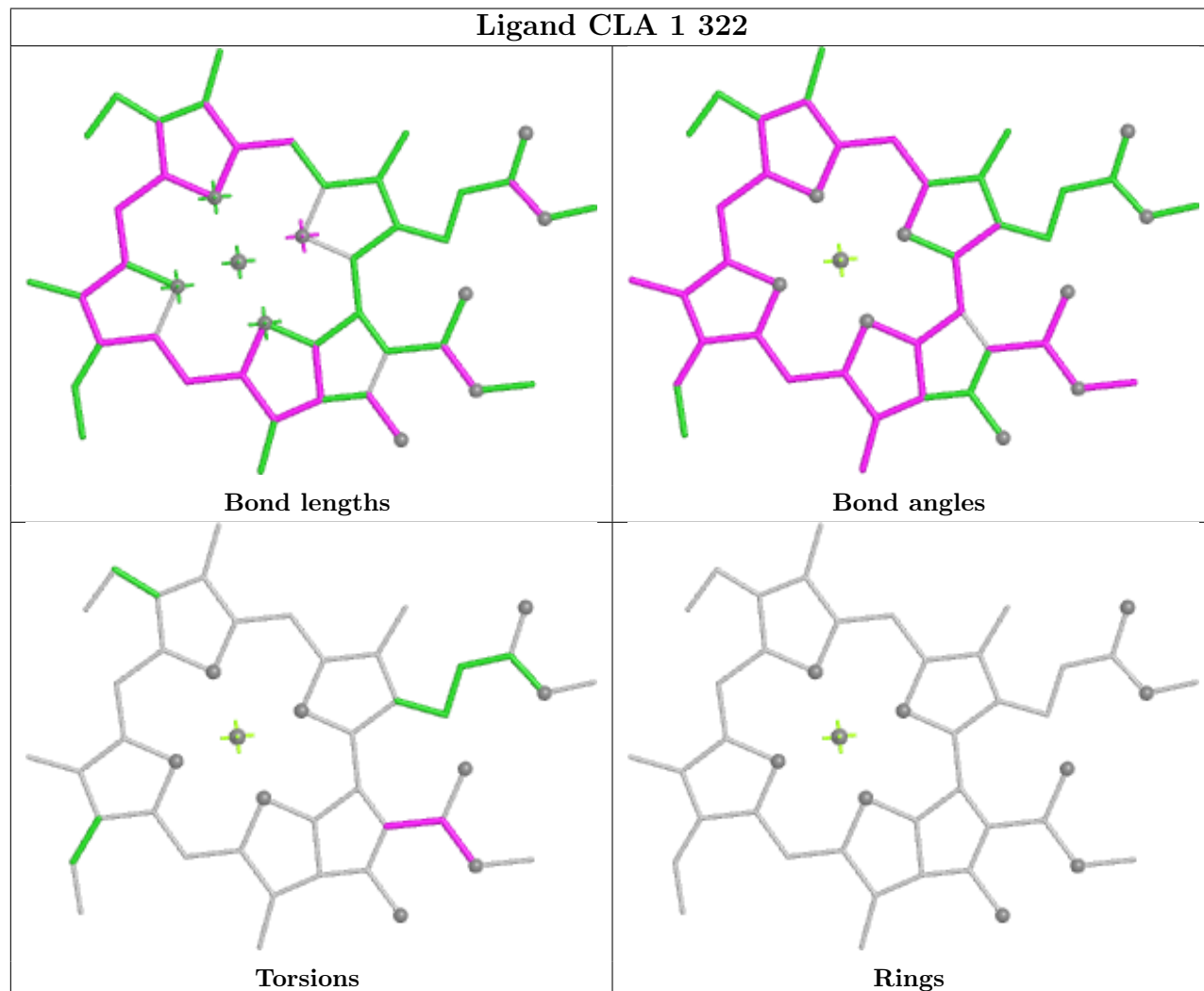


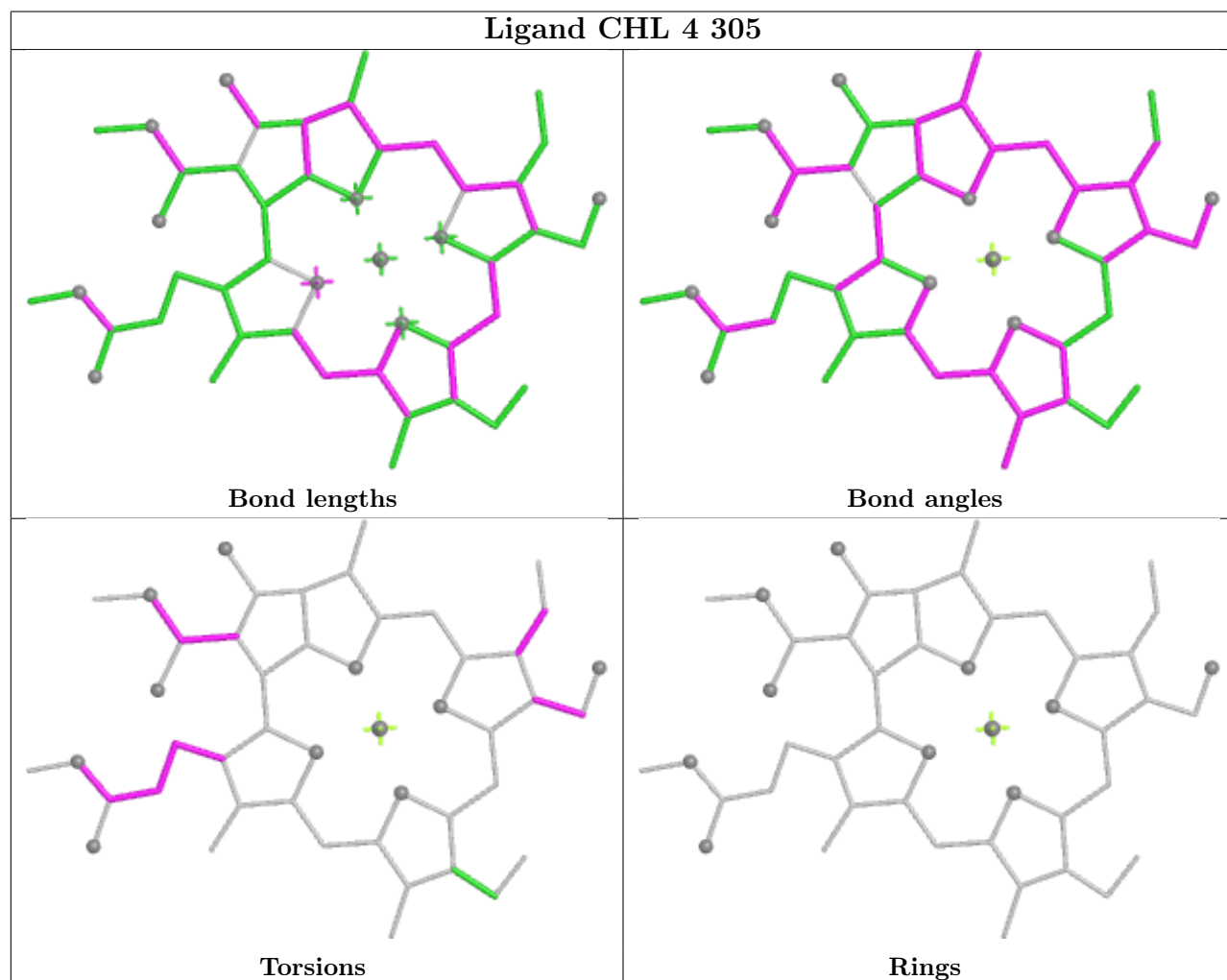
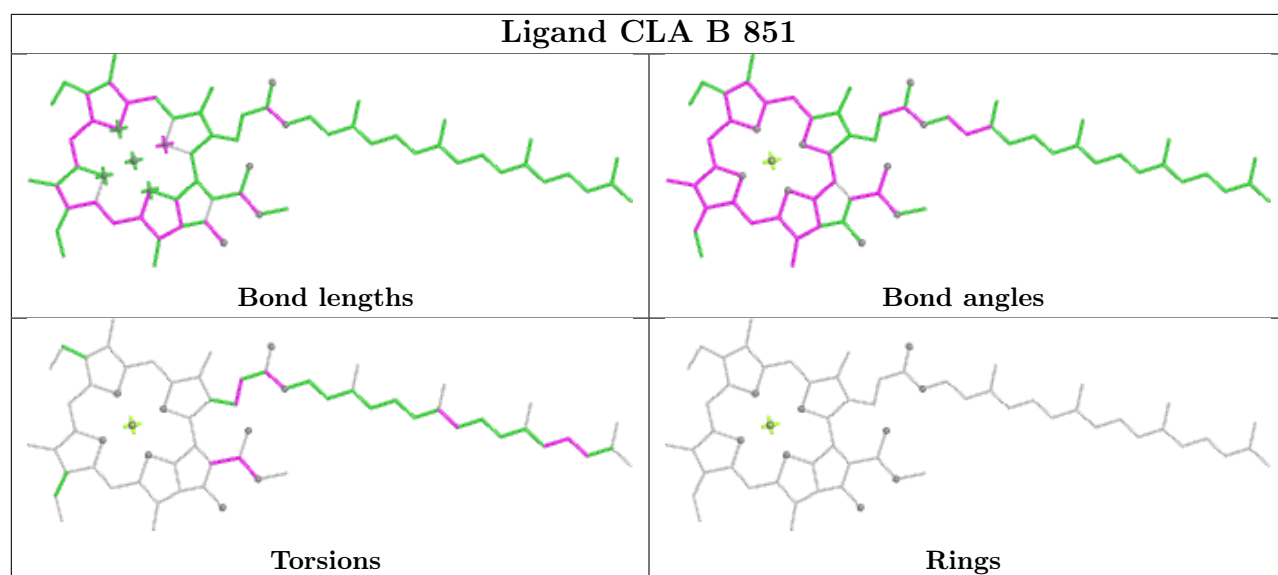


Ligand CLA A 848

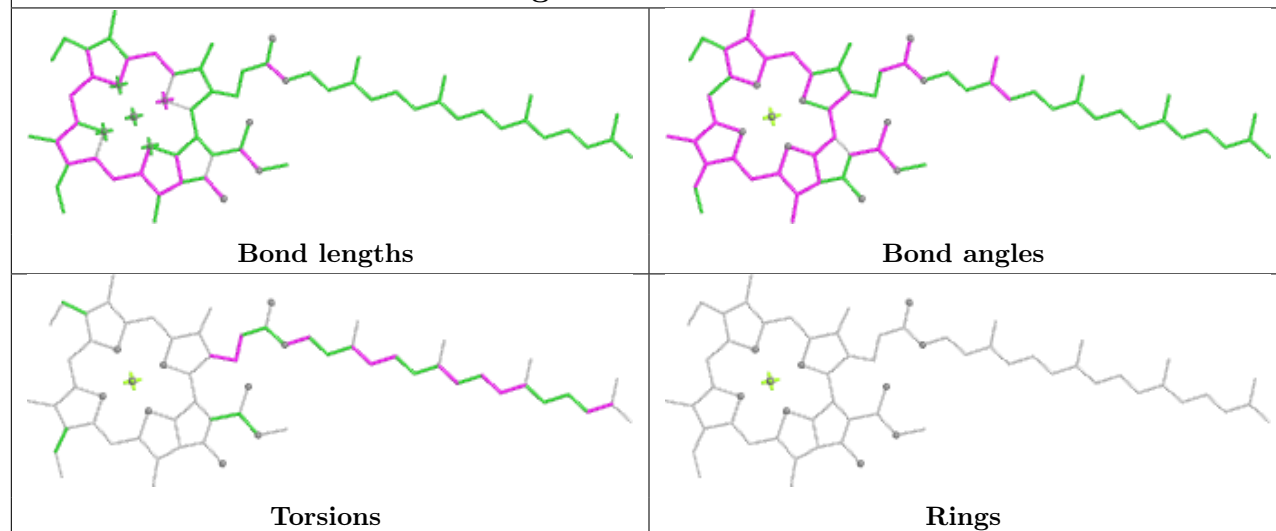


Ligand CLA 1 322

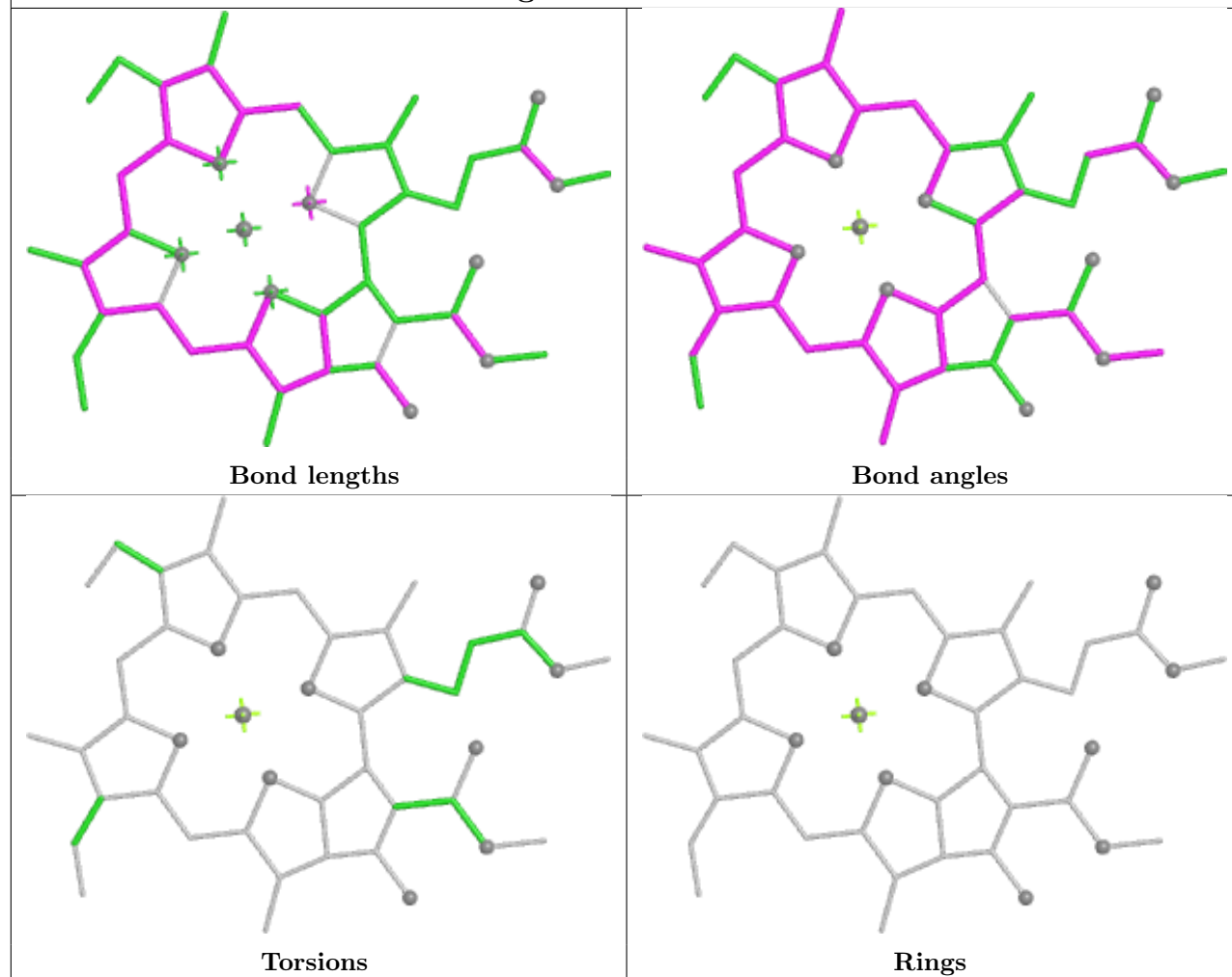


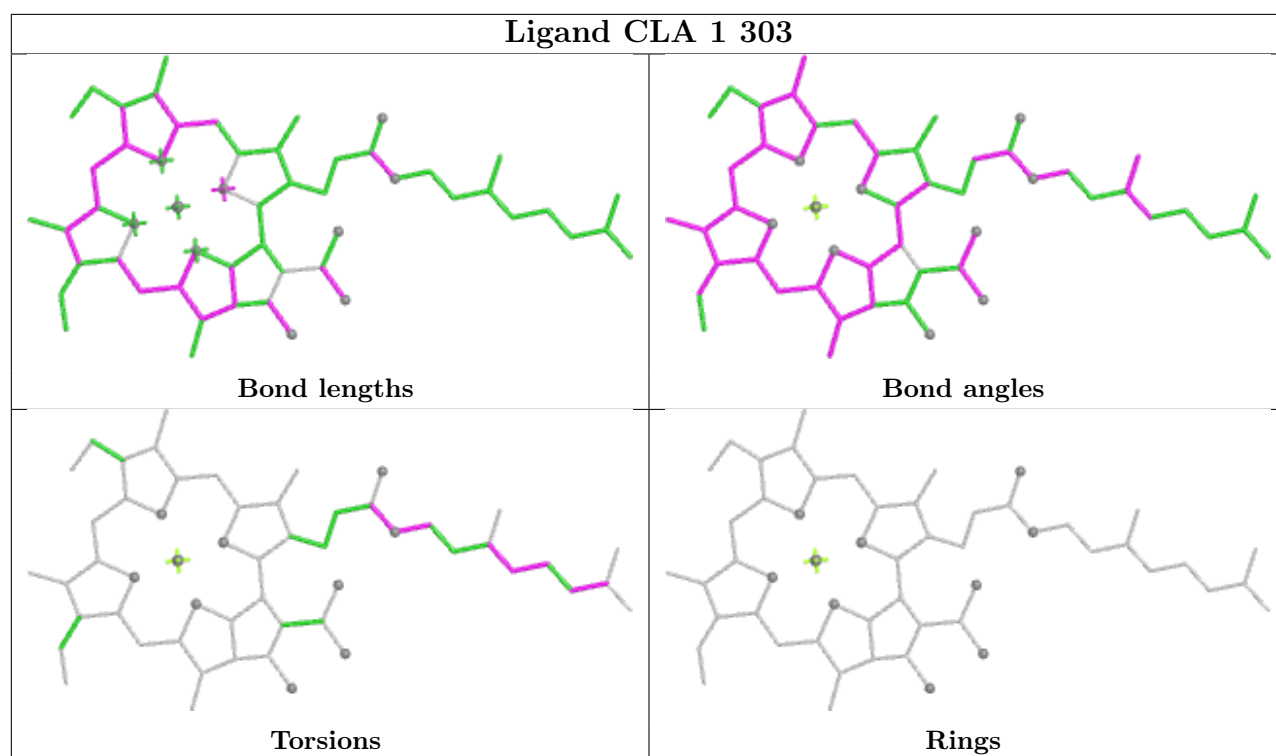


Ligand CLA A 826

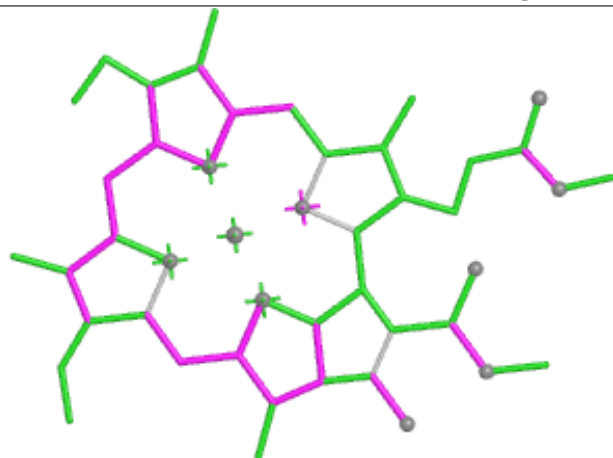


Ligand CLA 1 321

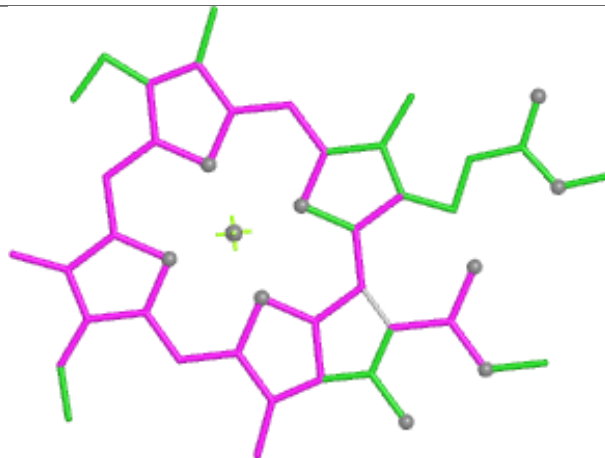




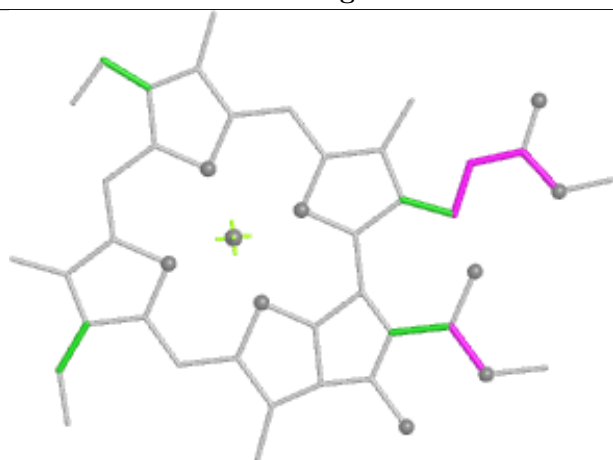
Ligand CLA F 306



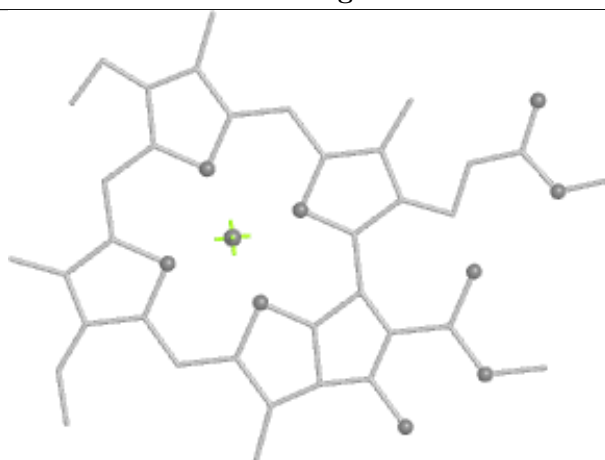
Bond lengths



Bond angles

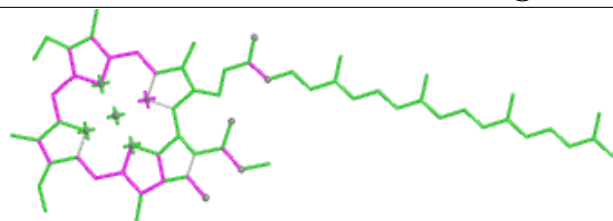


Torsions

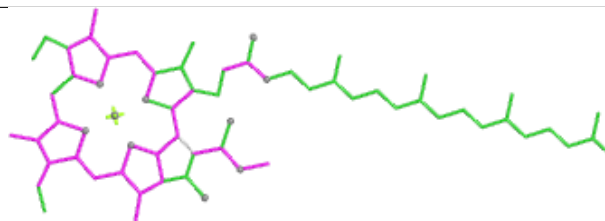


Rings

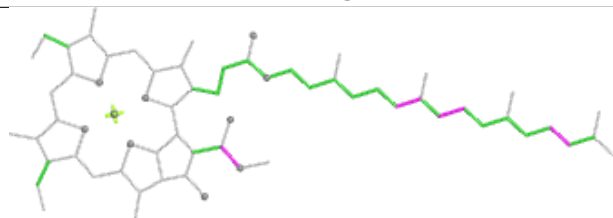
Ligand CLA A 852



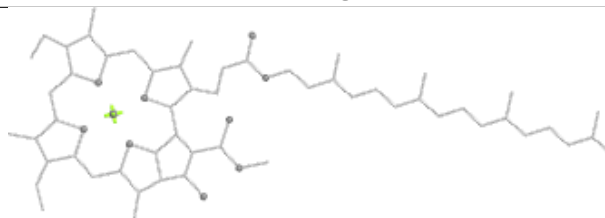
Bond lengths



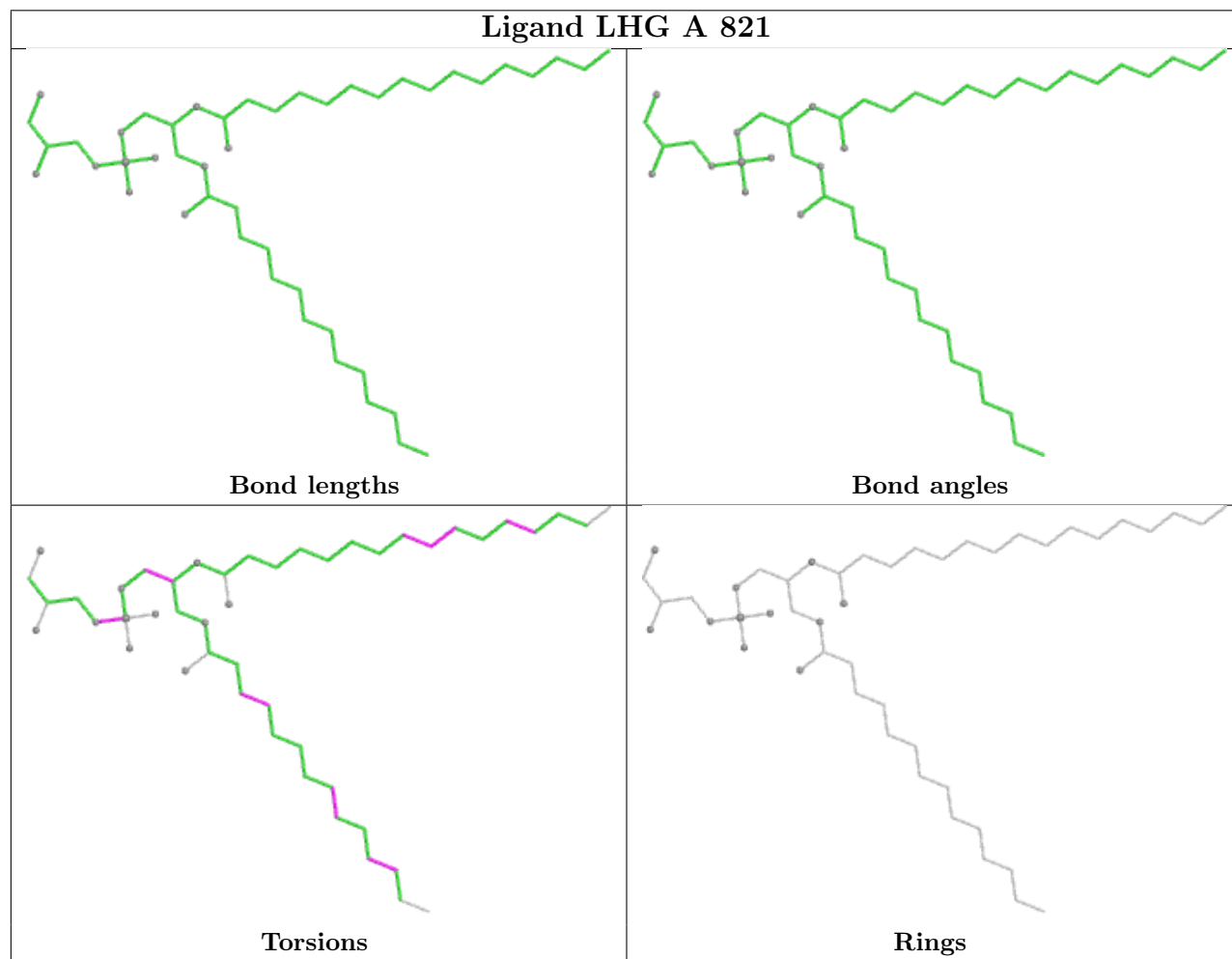
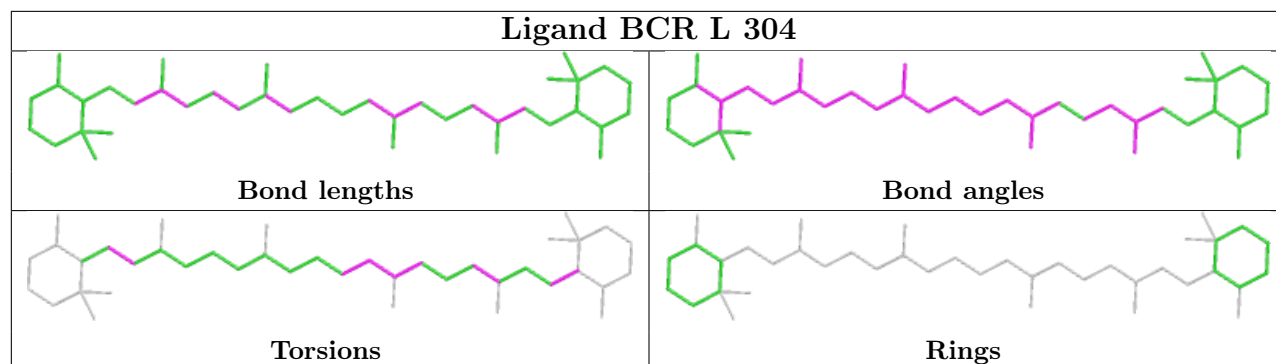
Bond angles

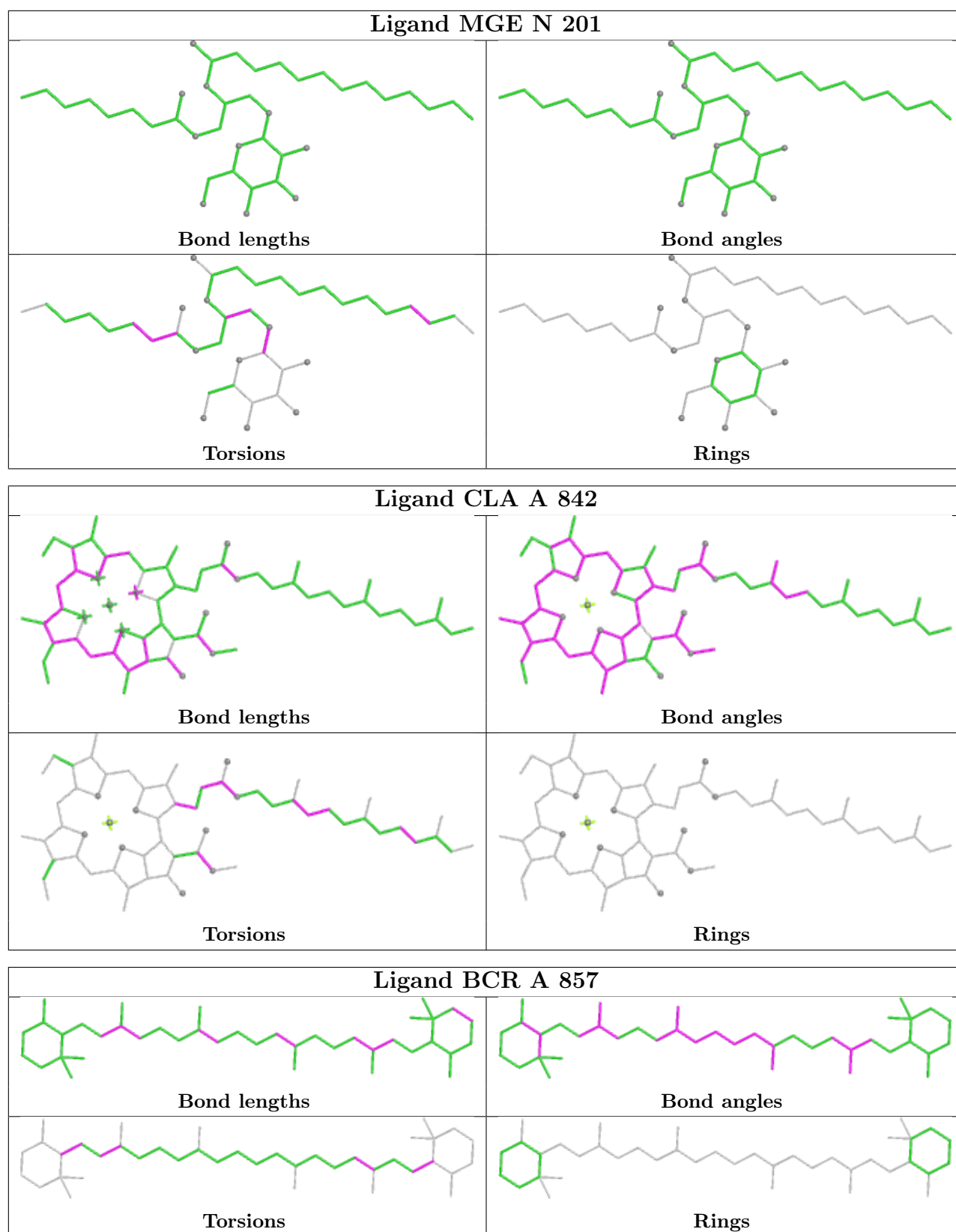


Torsions

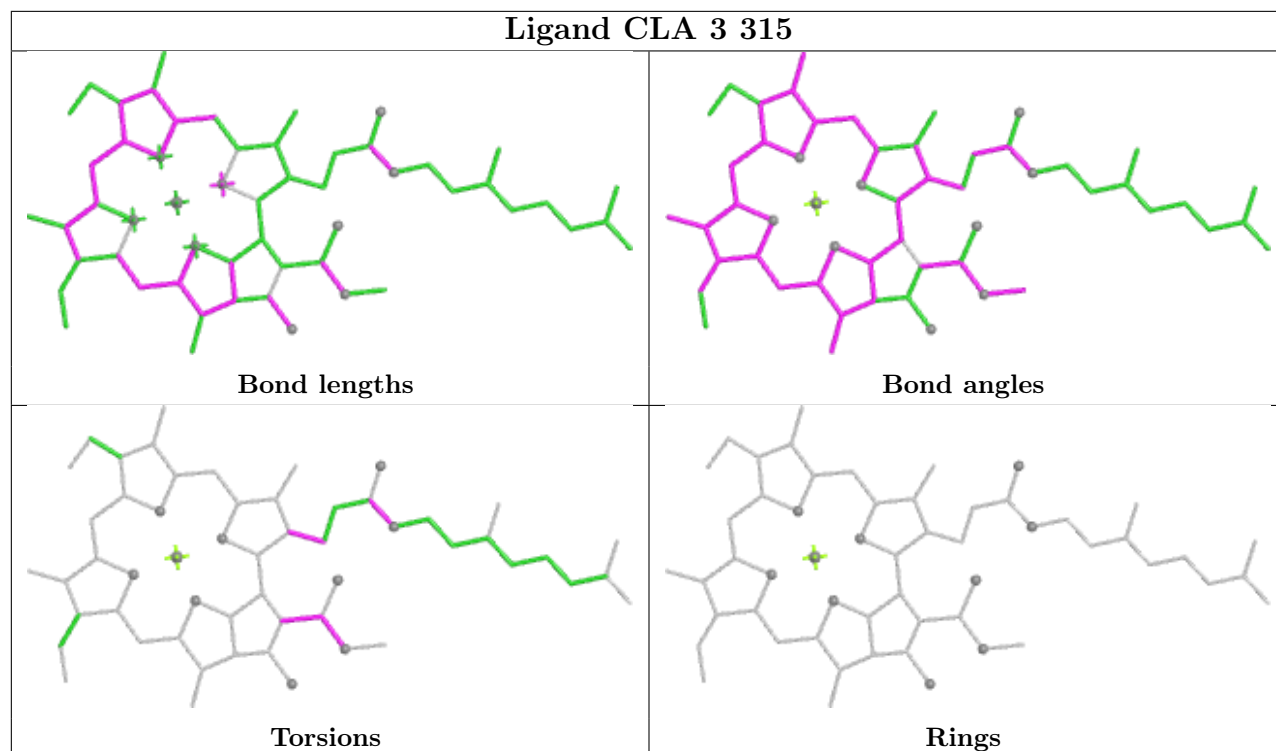


Rings

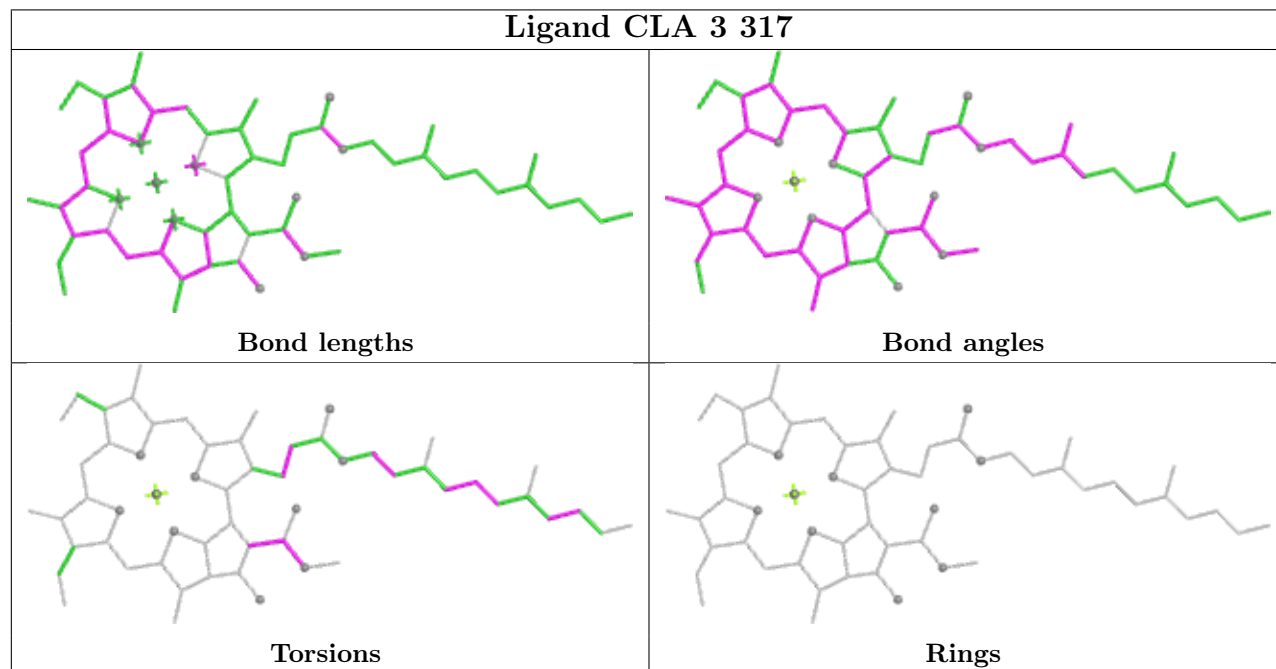




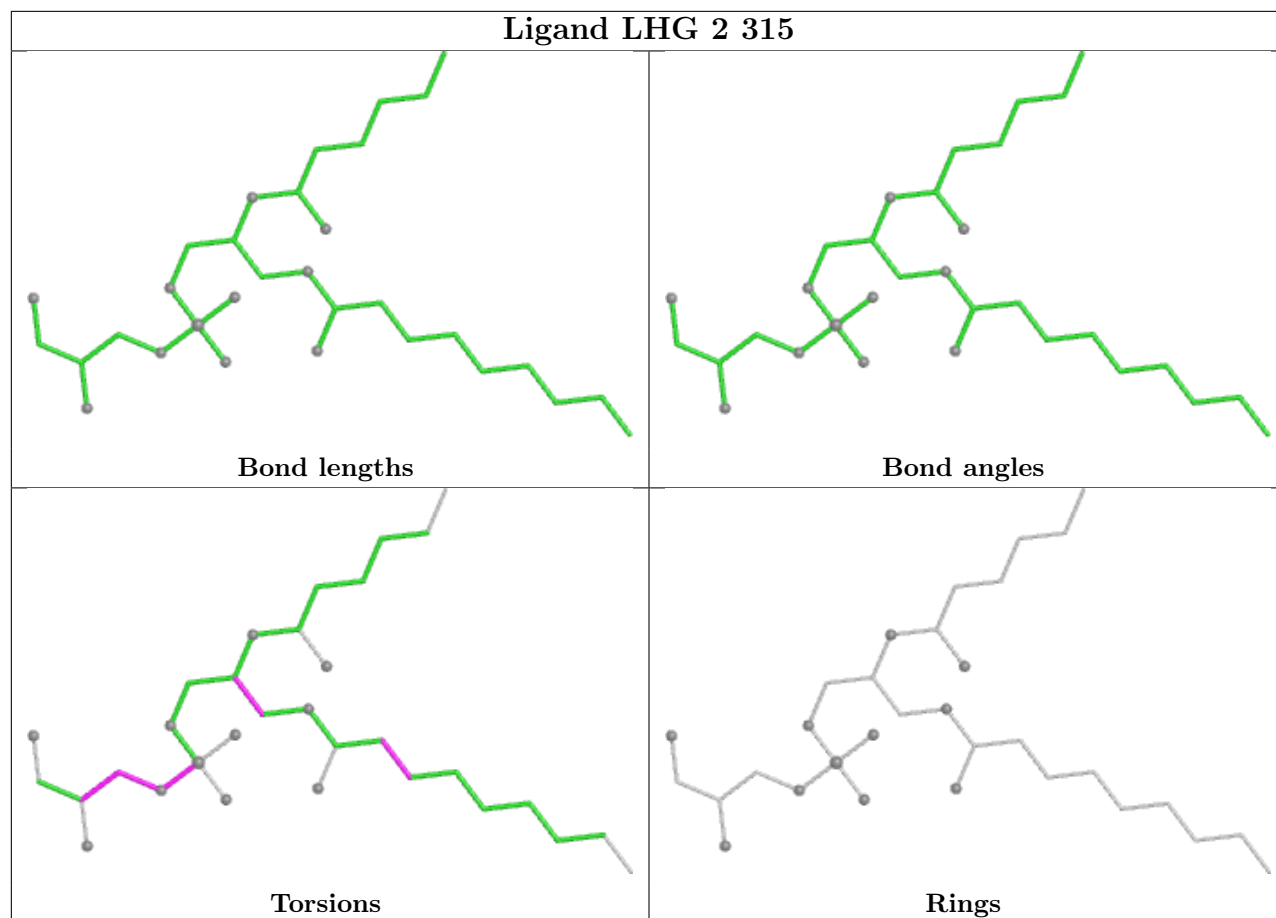
Ligand CLA 3 315



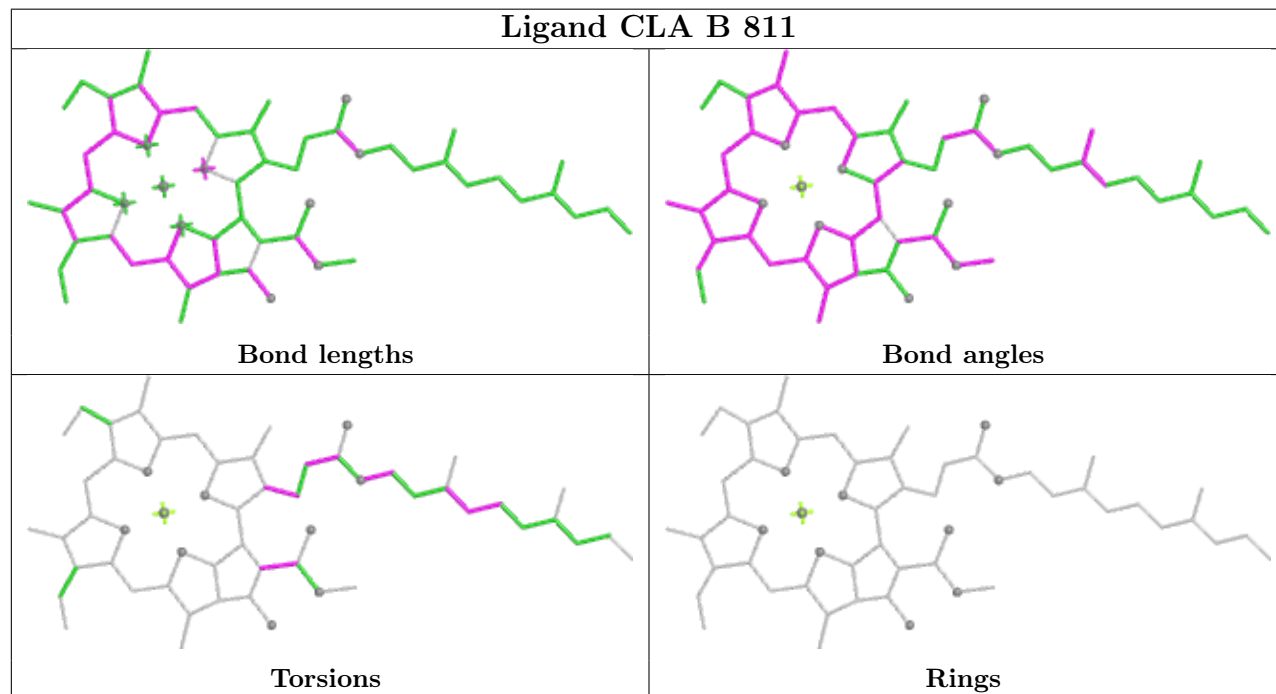
Ligand CLA 3 317



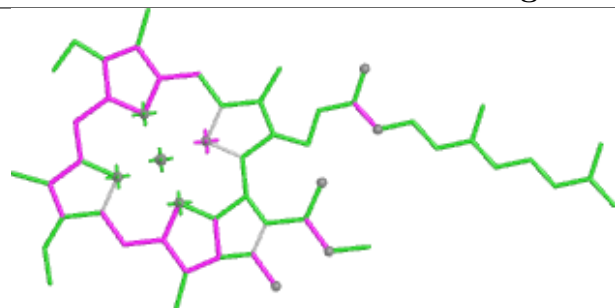
Ligand LHG 2 315



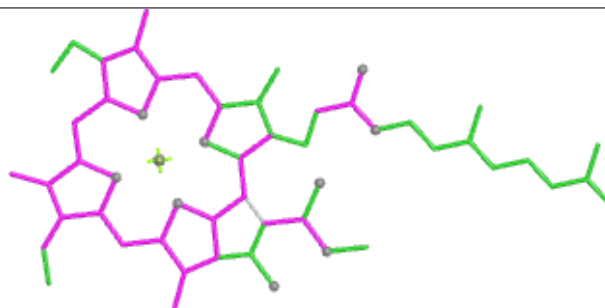
Ligand CLA B 811



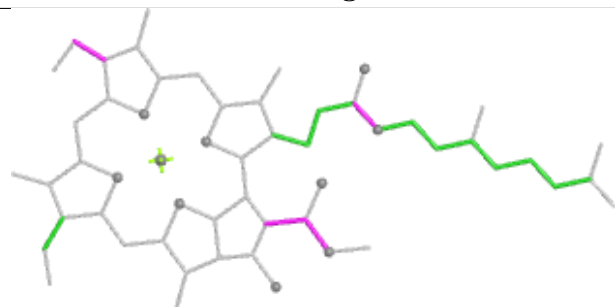
Ligand CLA 1 304



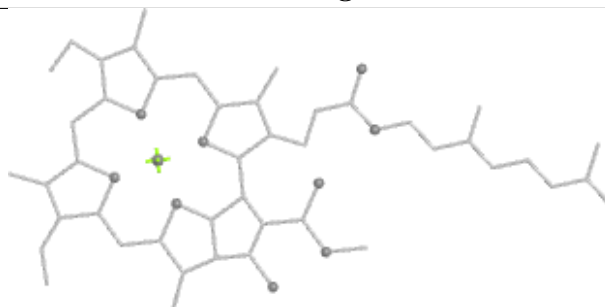
Bond lengths



Bond angles

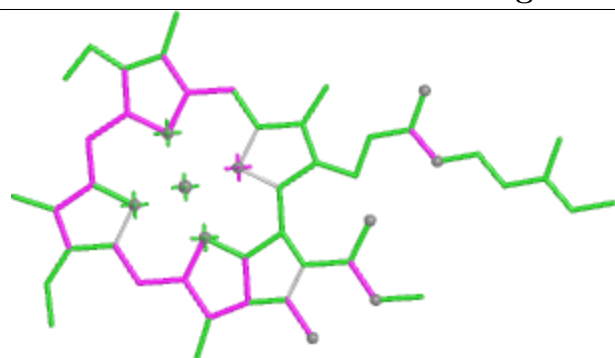


Torsions

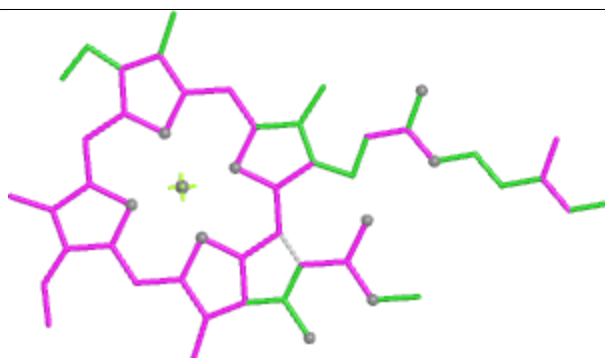


Rings

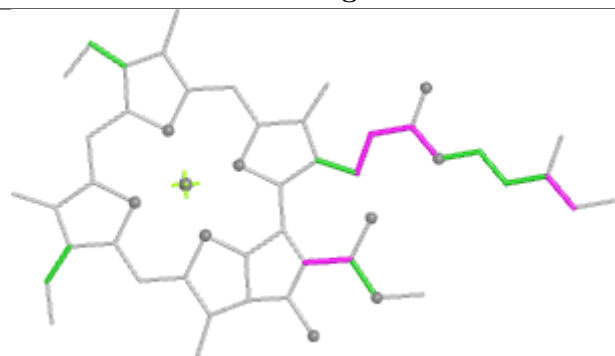
Ligand CLA A 804



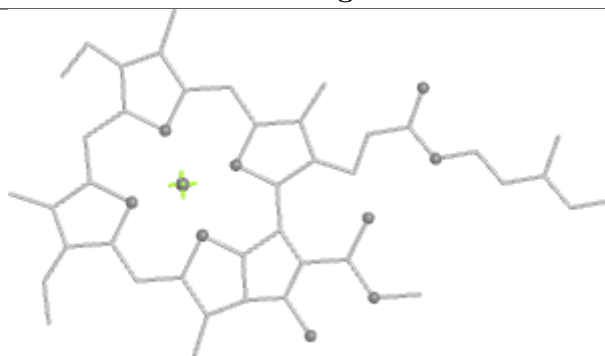
Bond lengths



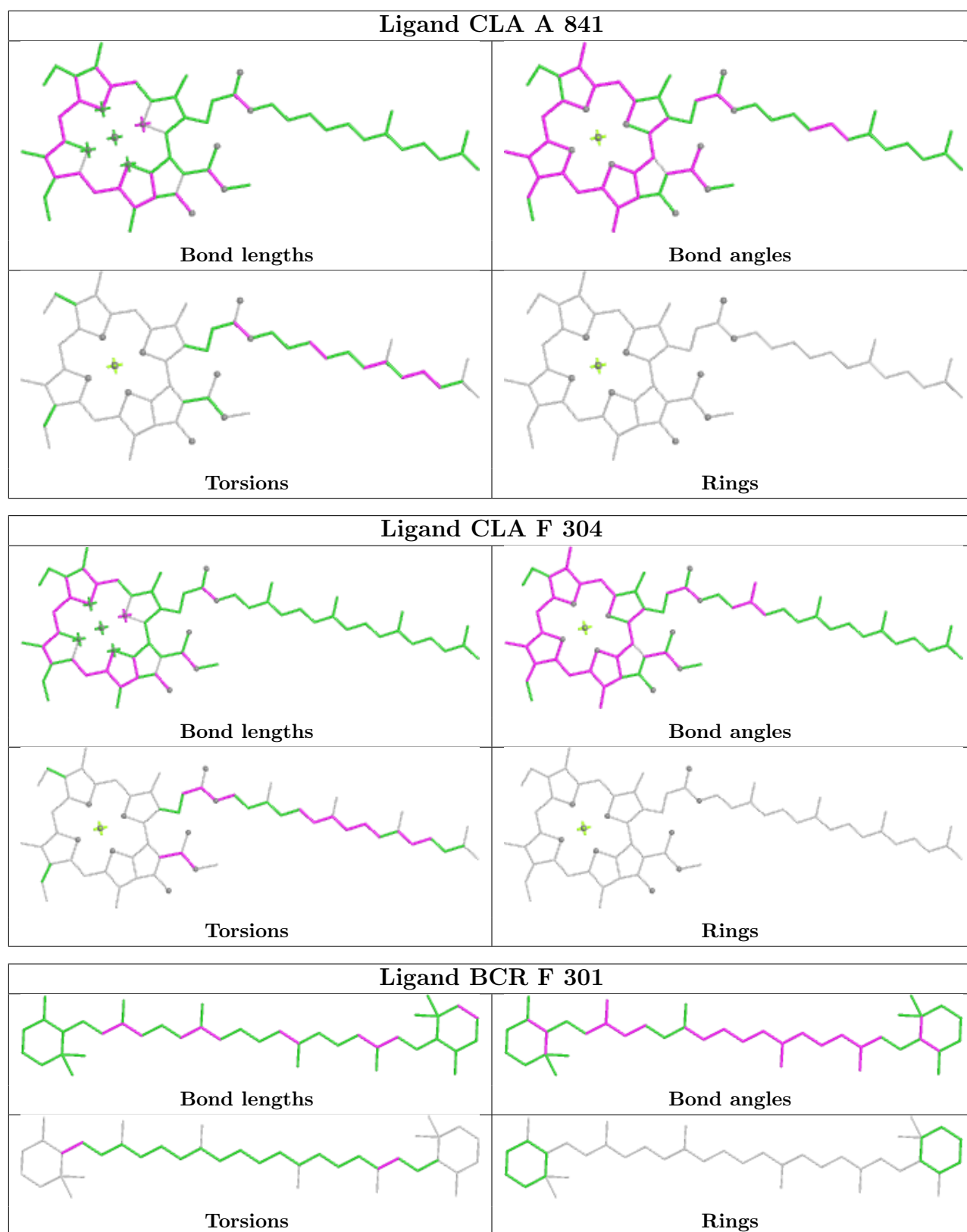
Bond angles

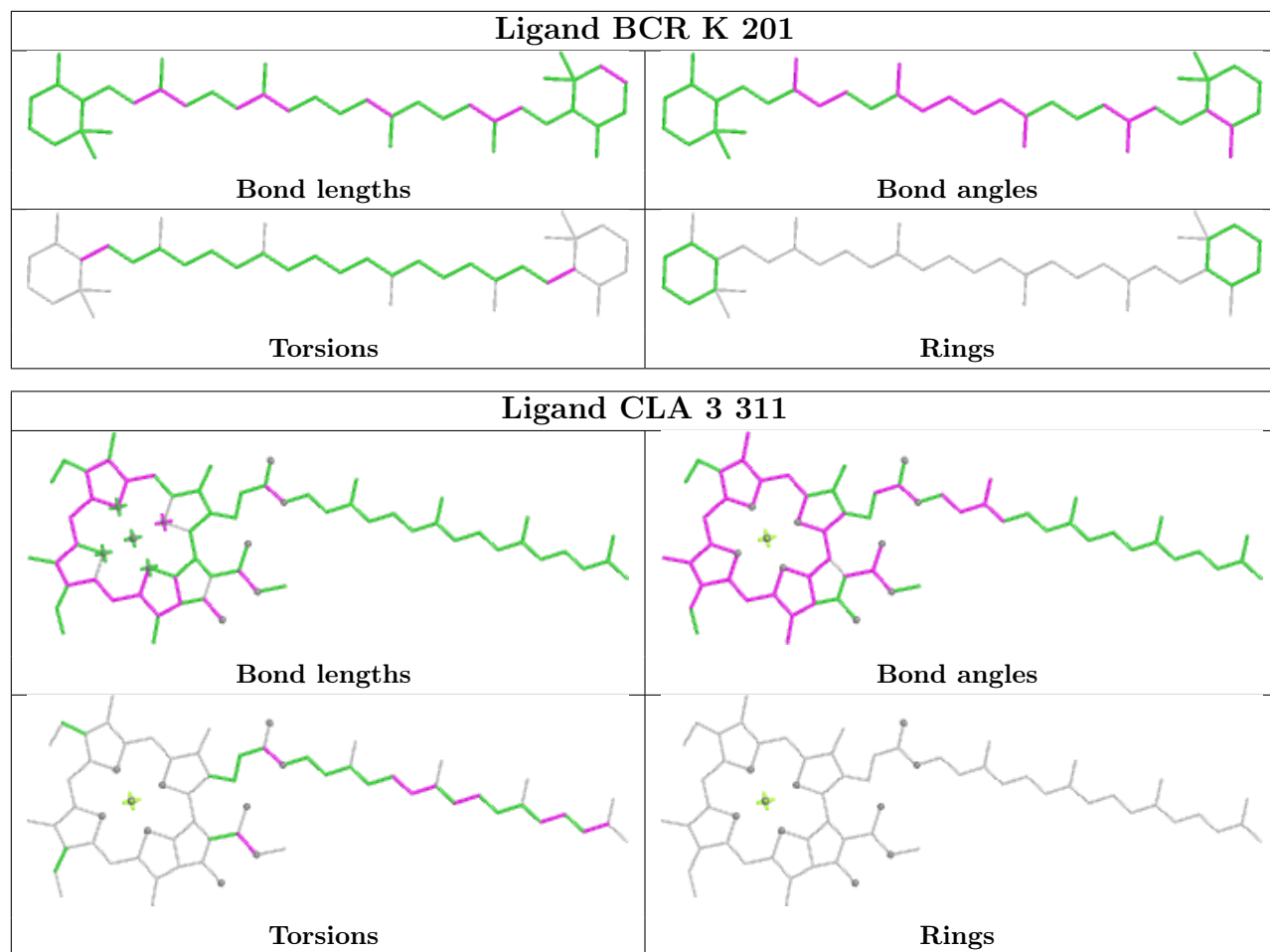


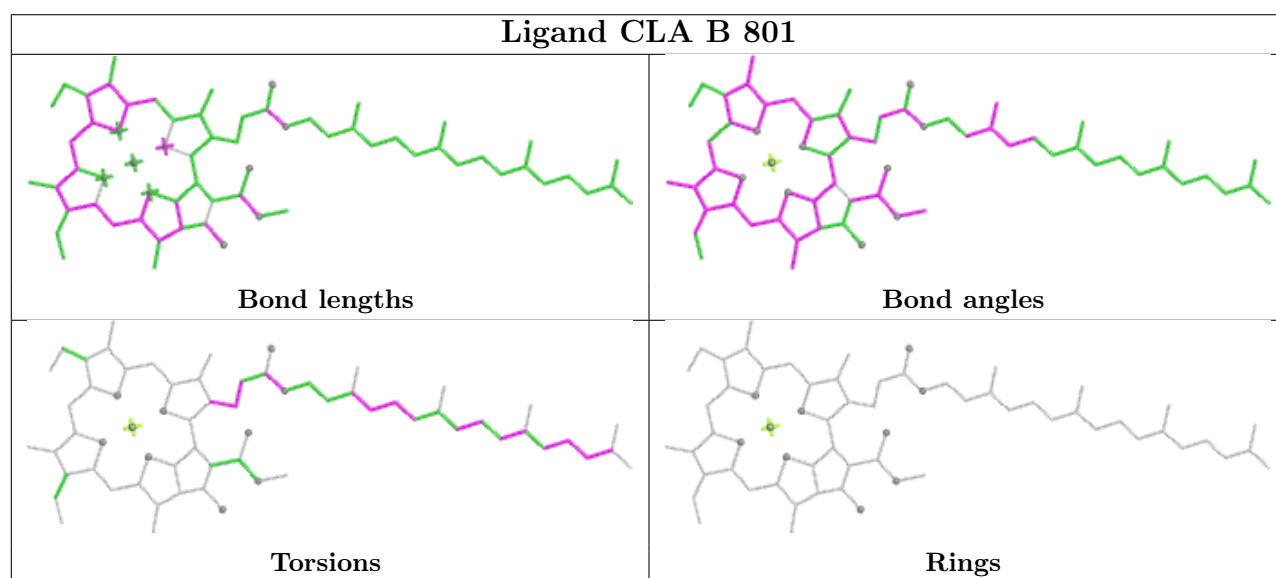
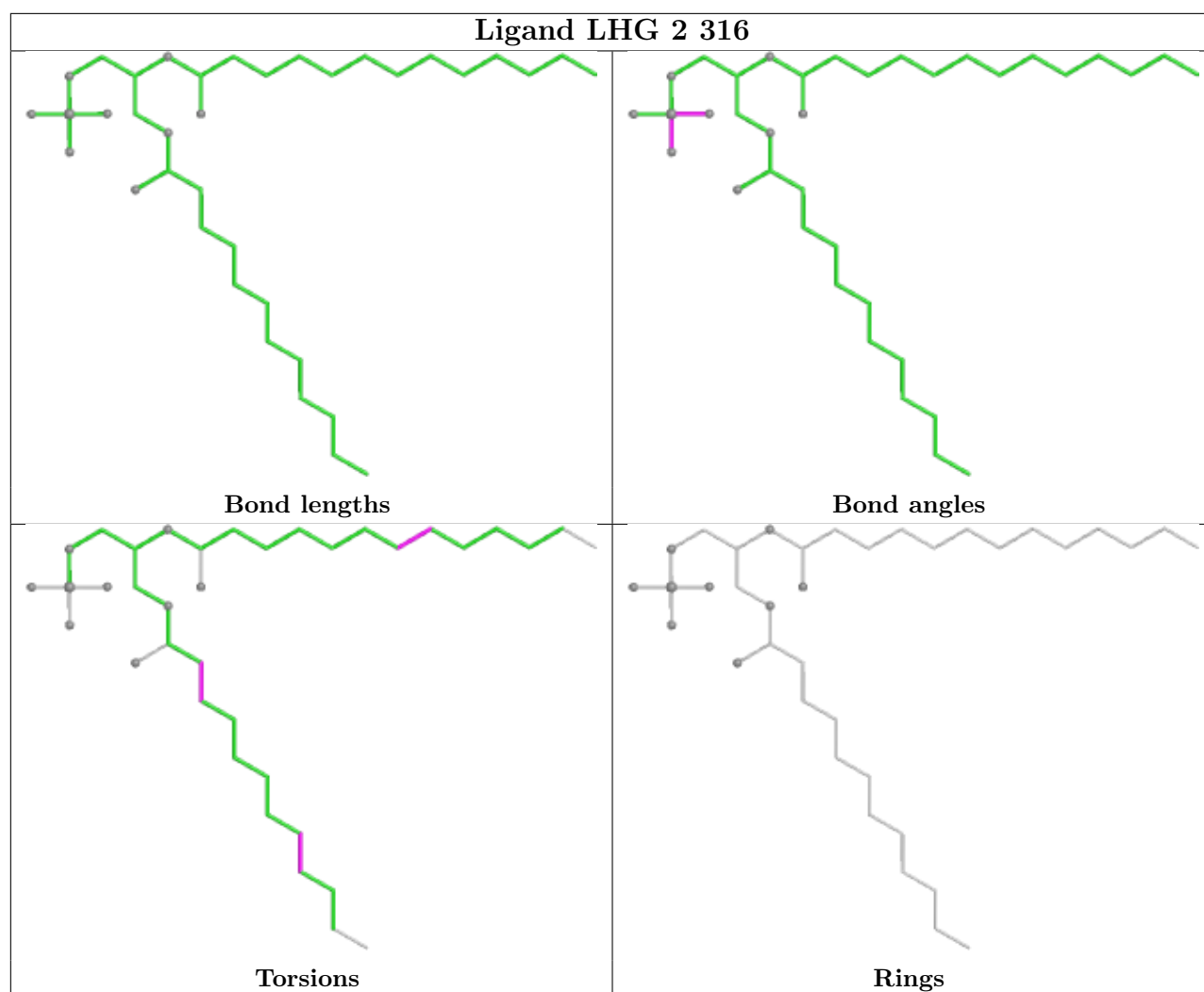
Torsions



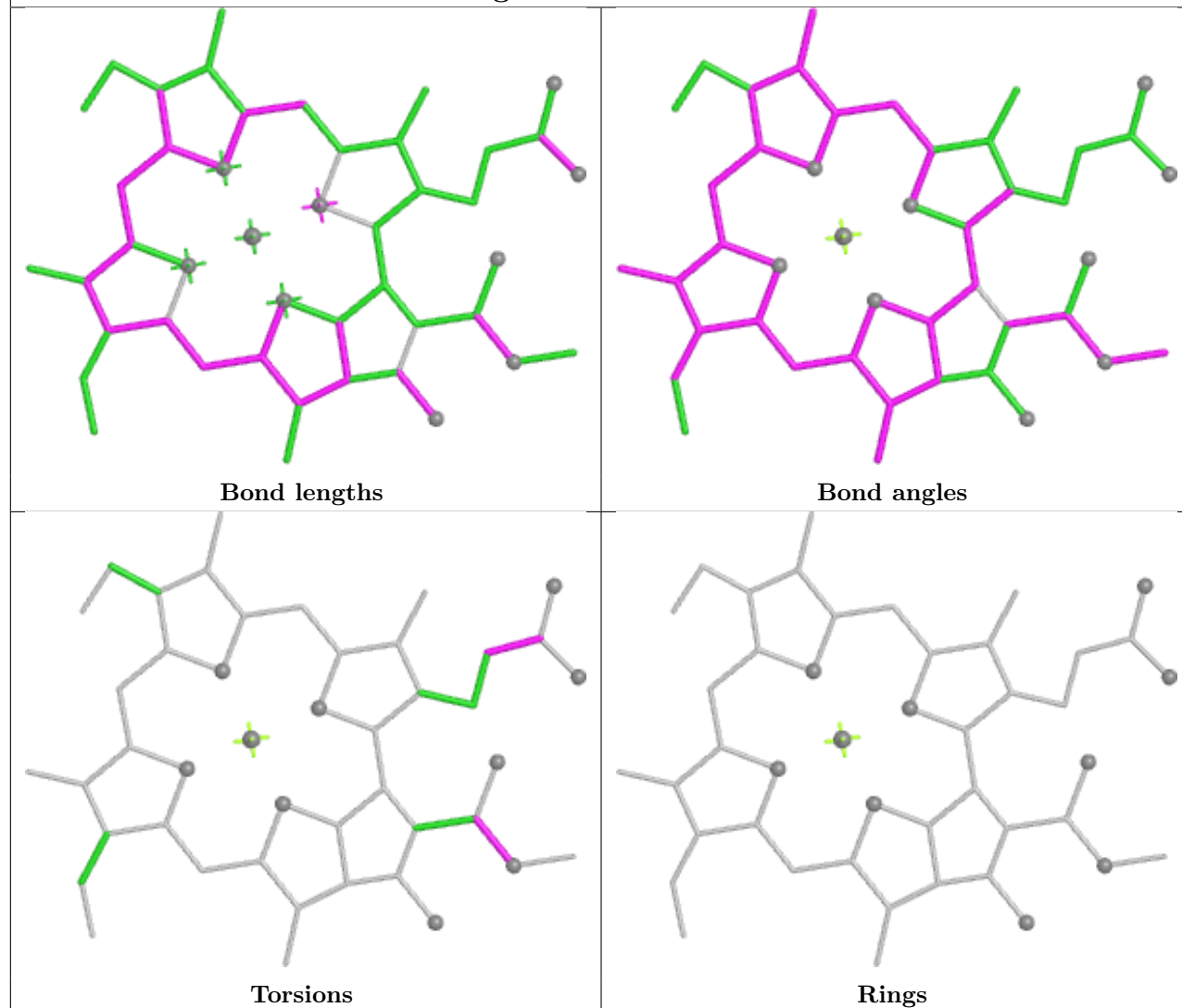
Rings



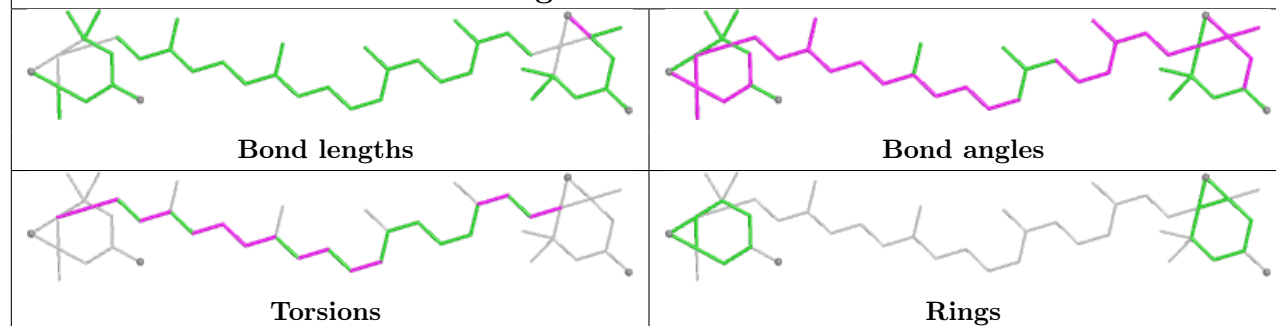




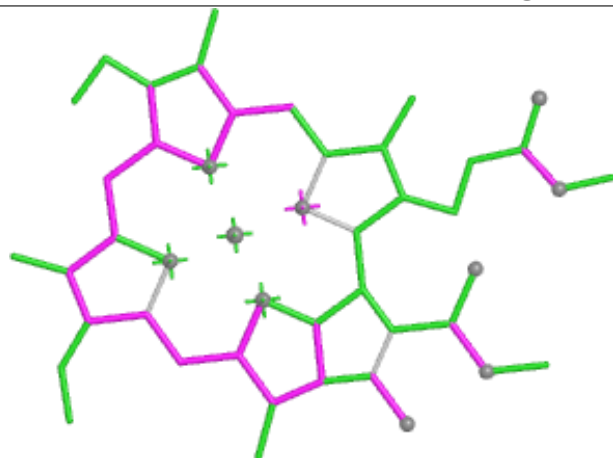
Ligand CLA B 825



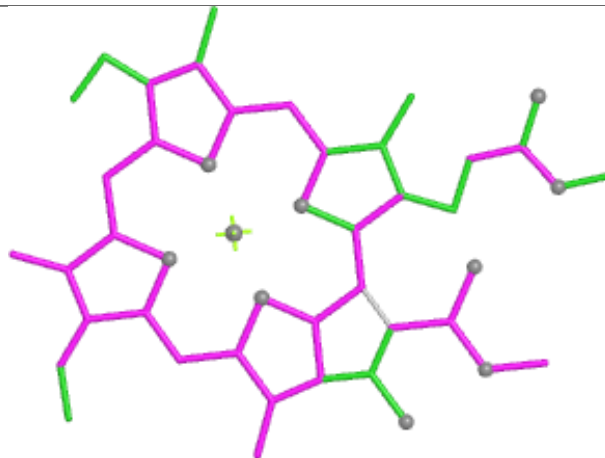
Ligand XAT 1 311



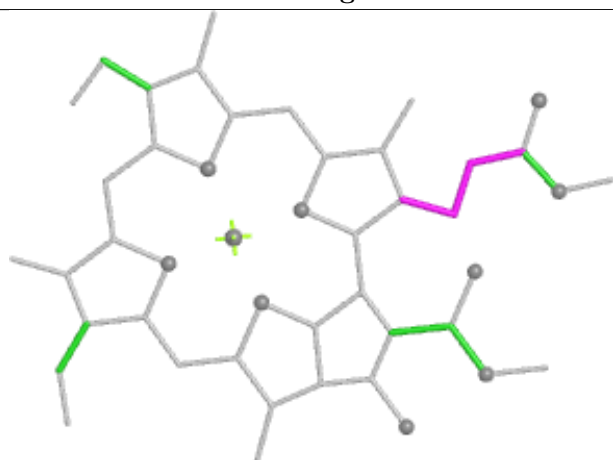
Ligand CLA 1 305



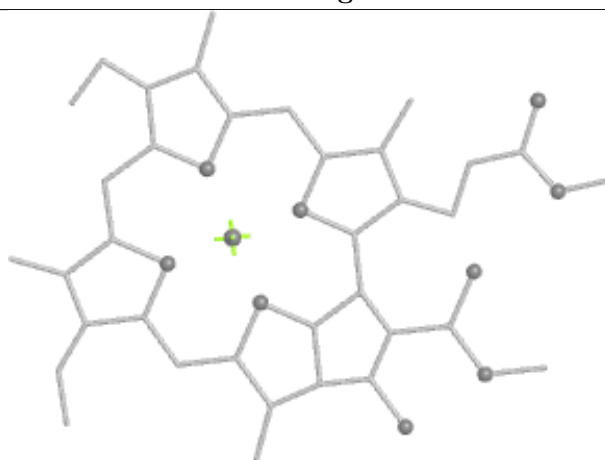
Bond lengths



Bond angles

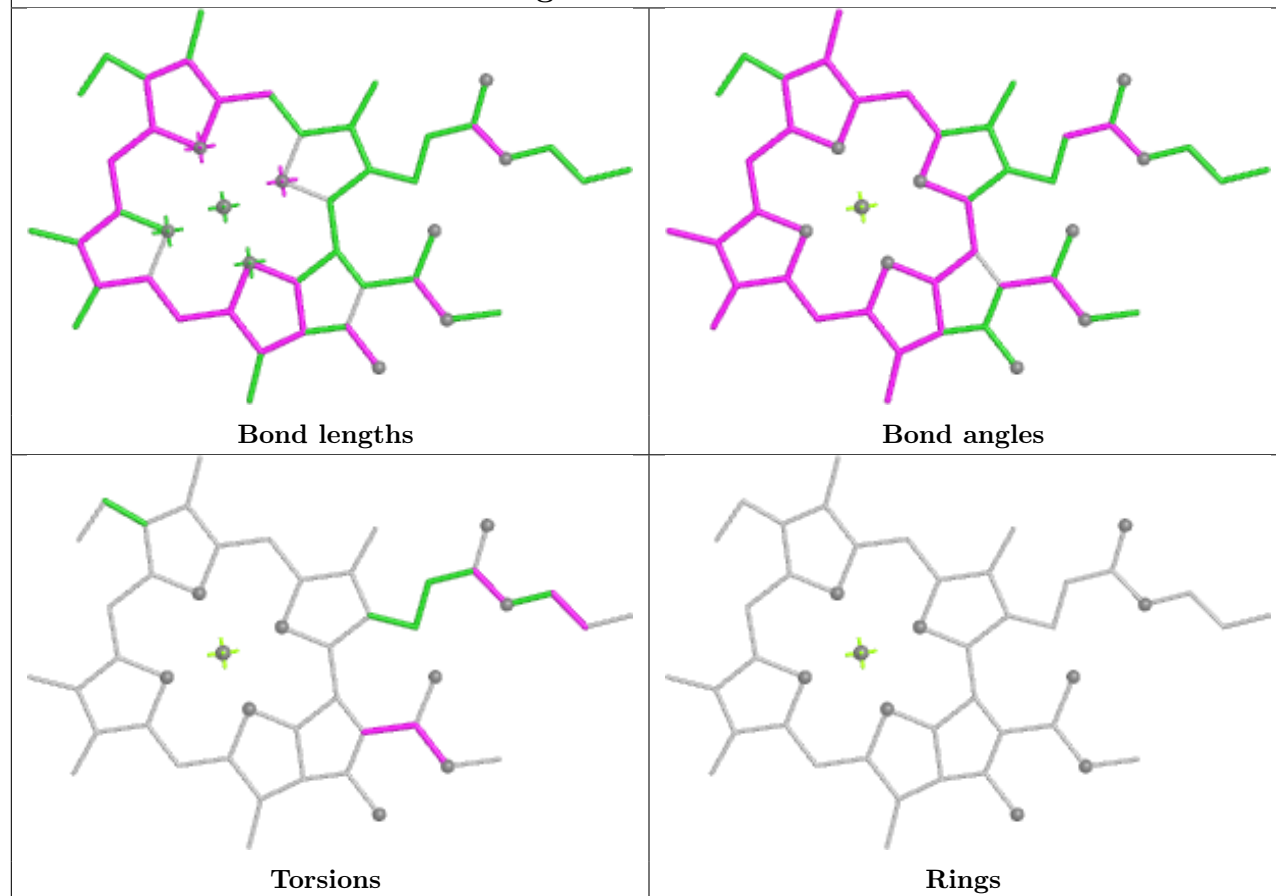


Torsions

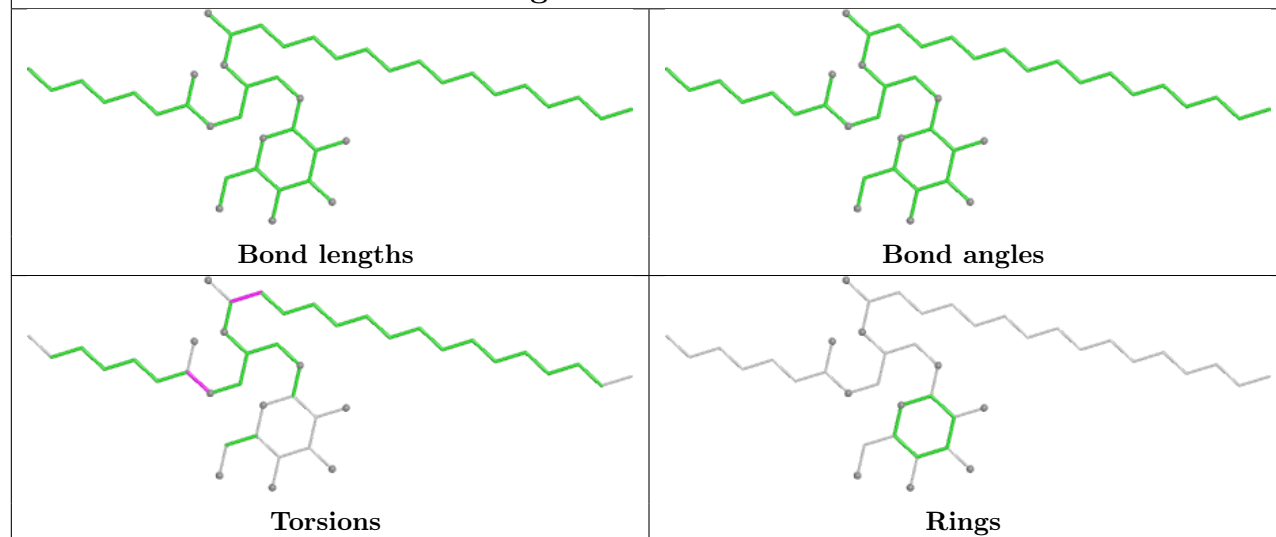


Rings

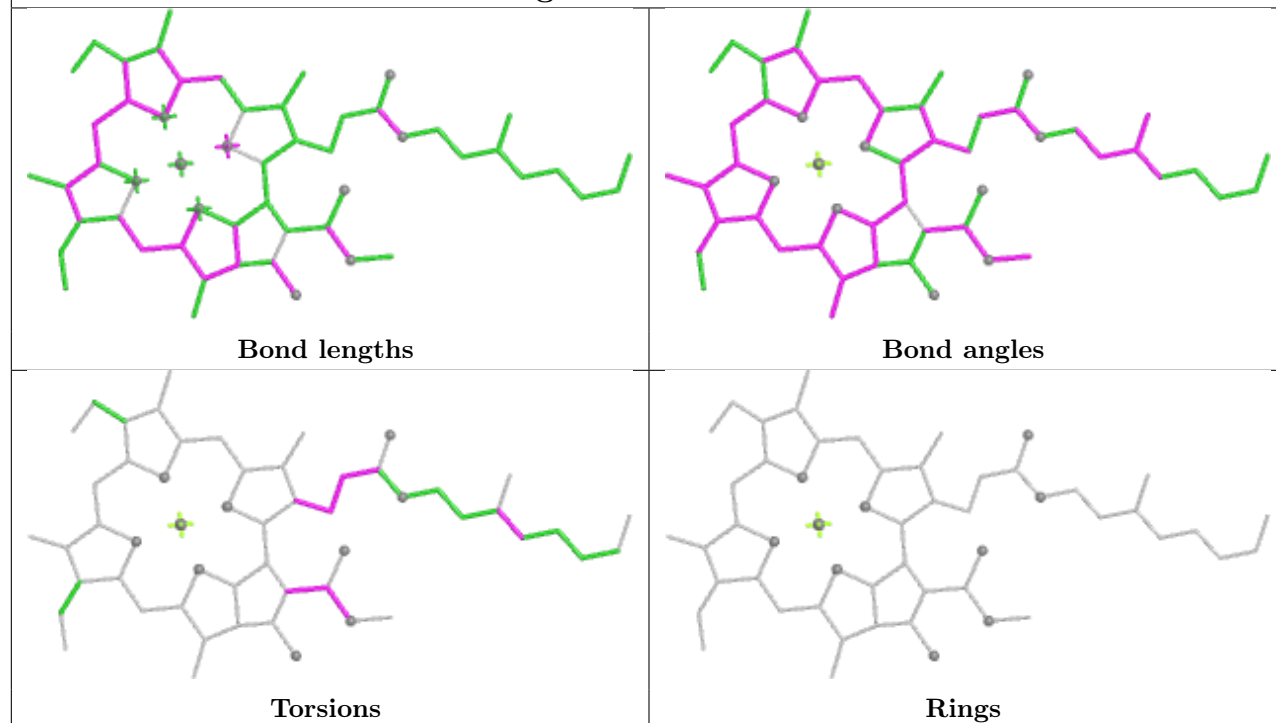
Ligand CLA 2 320



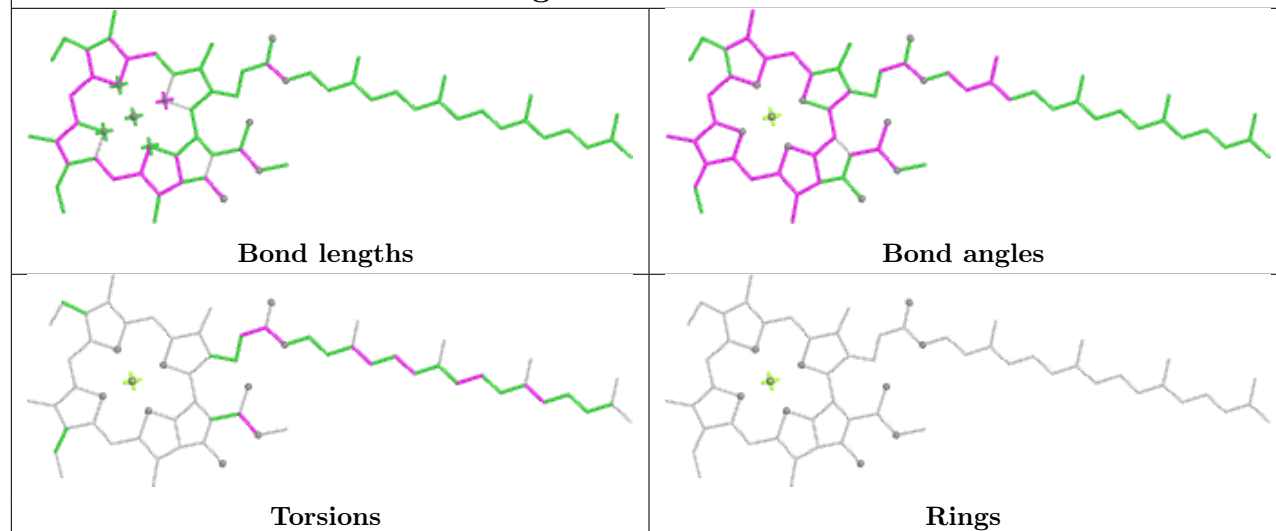
Ligand MGE J 102



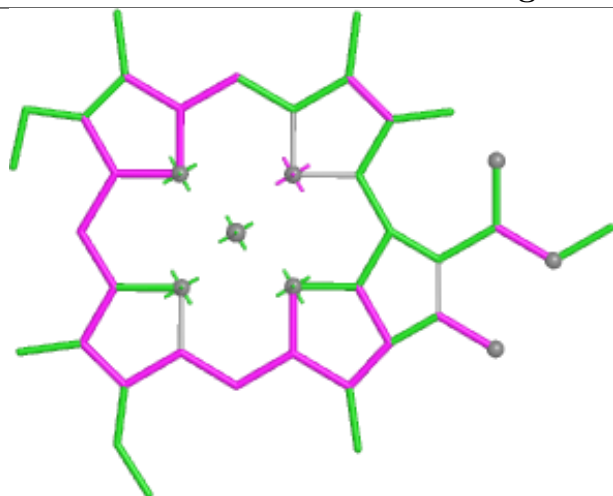
Ligand CLA 4 309



Ligand CLA B 827



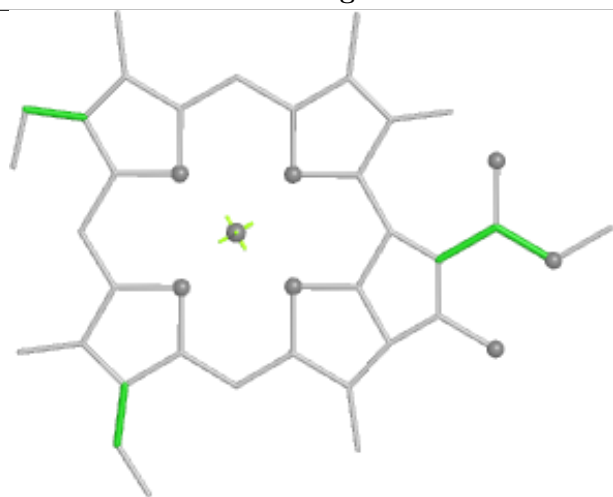
Ligand CLA 3 318



Bond lengths



Bond angles

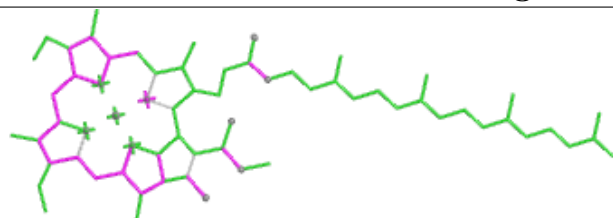


Torsions

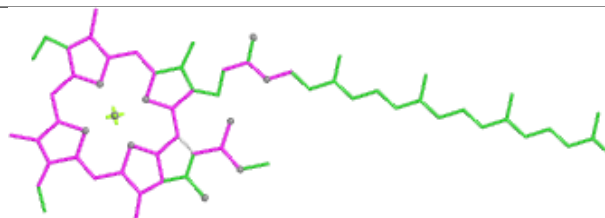


Rings

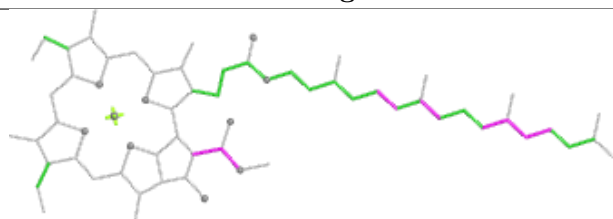
Ligand CLA A 827



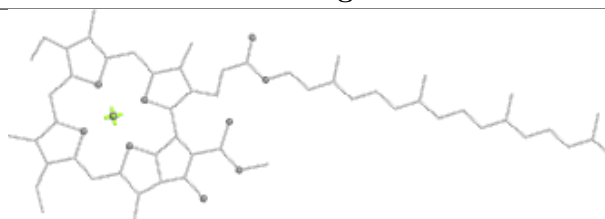
Bond lengths



Bond angles

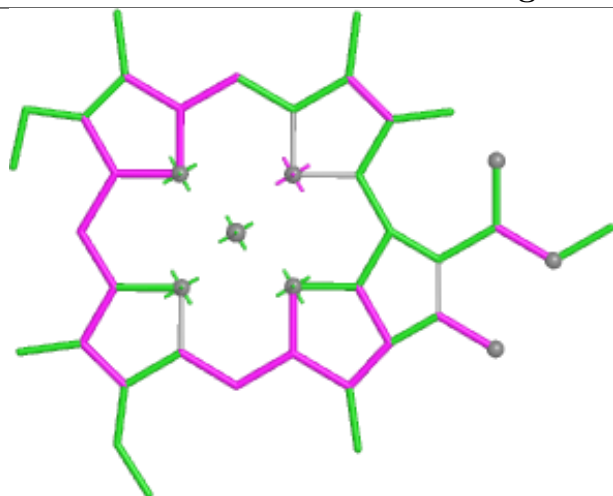


Torsions



Rings

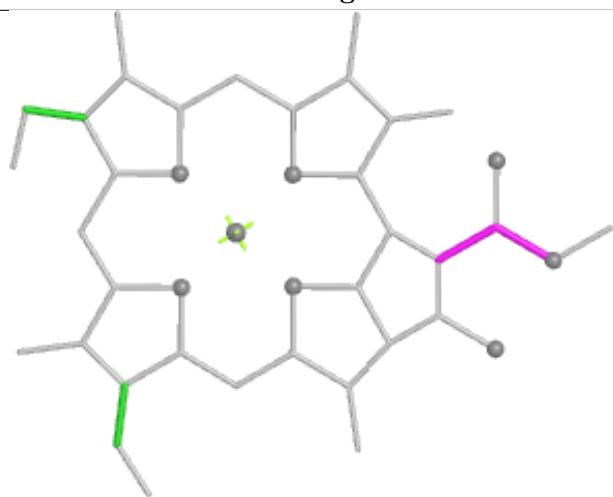
Ligand CLA 1 309



Bond lengths



Bond angles

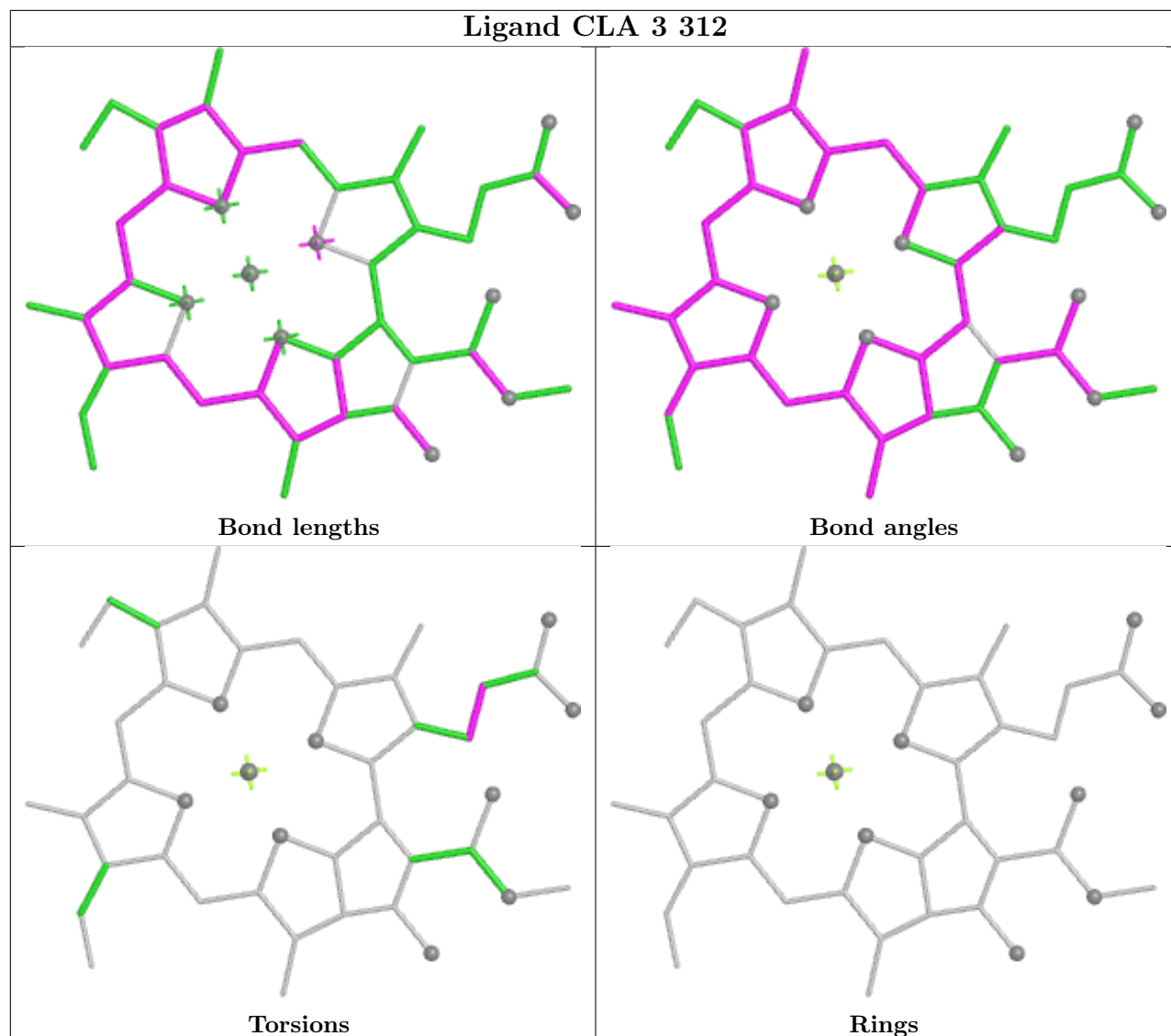


Torsions

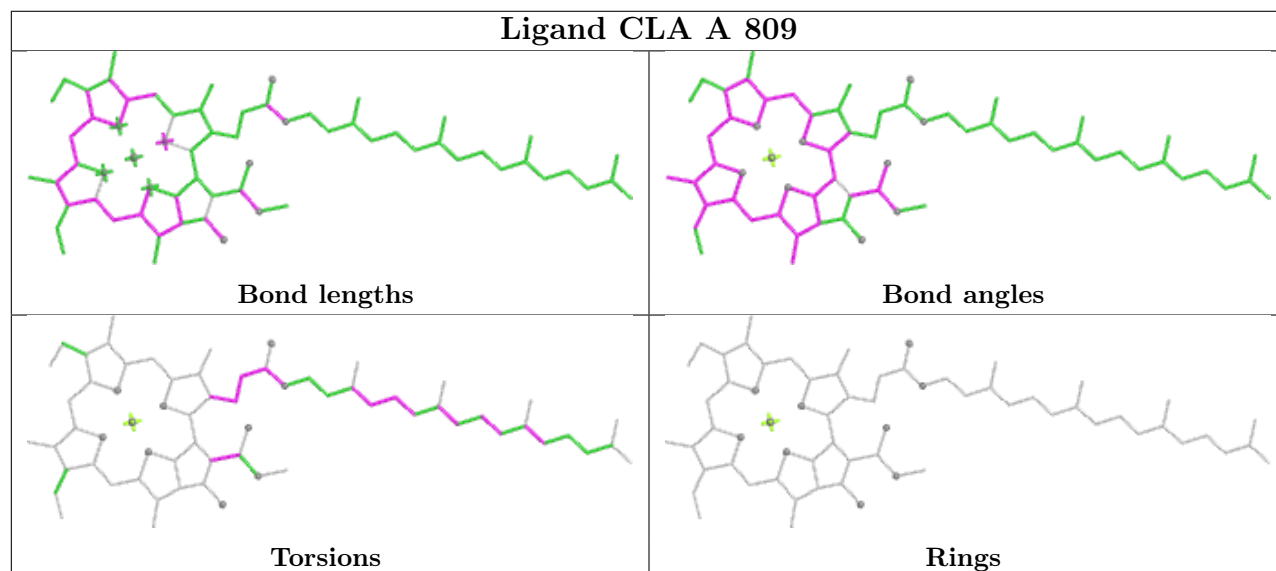


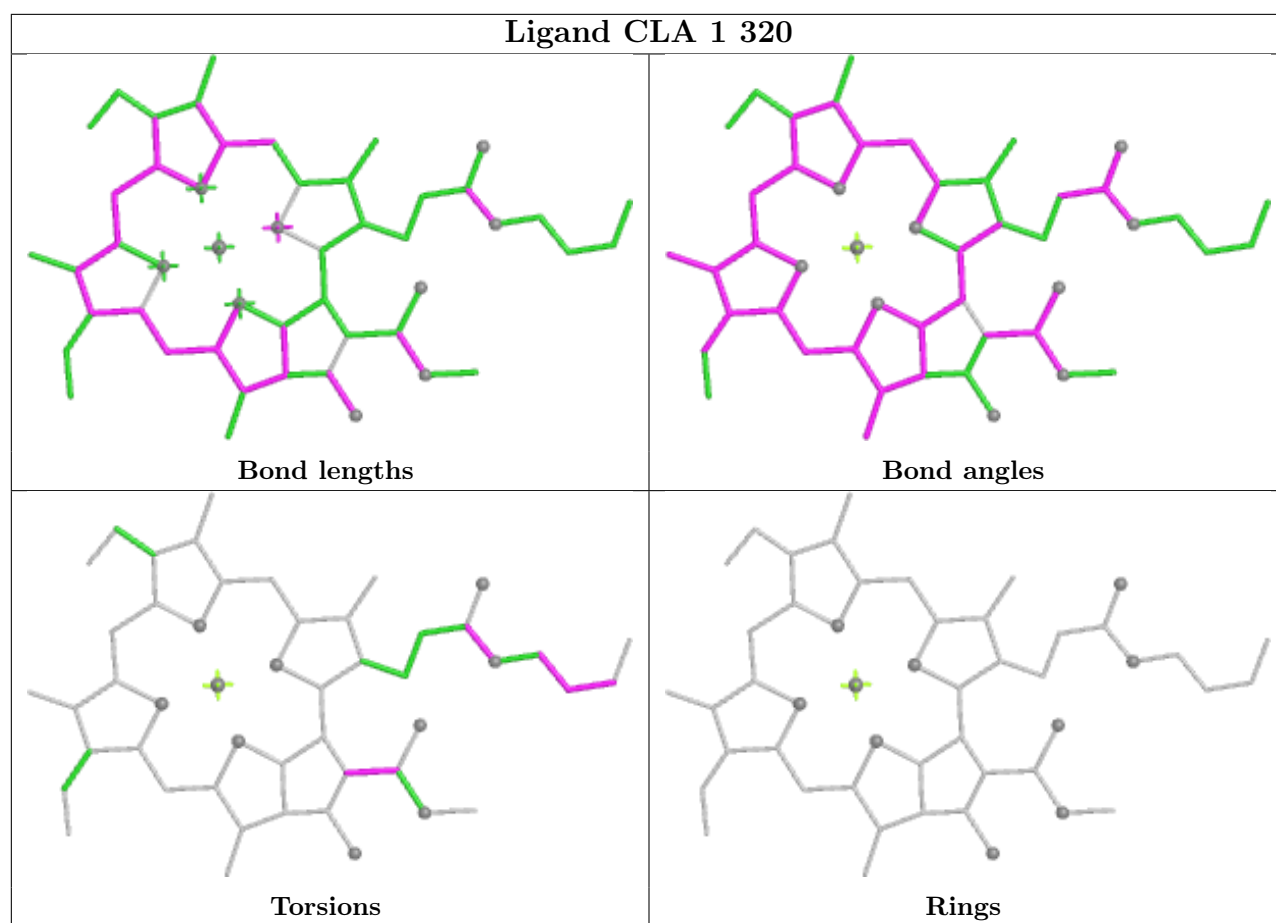
Rings

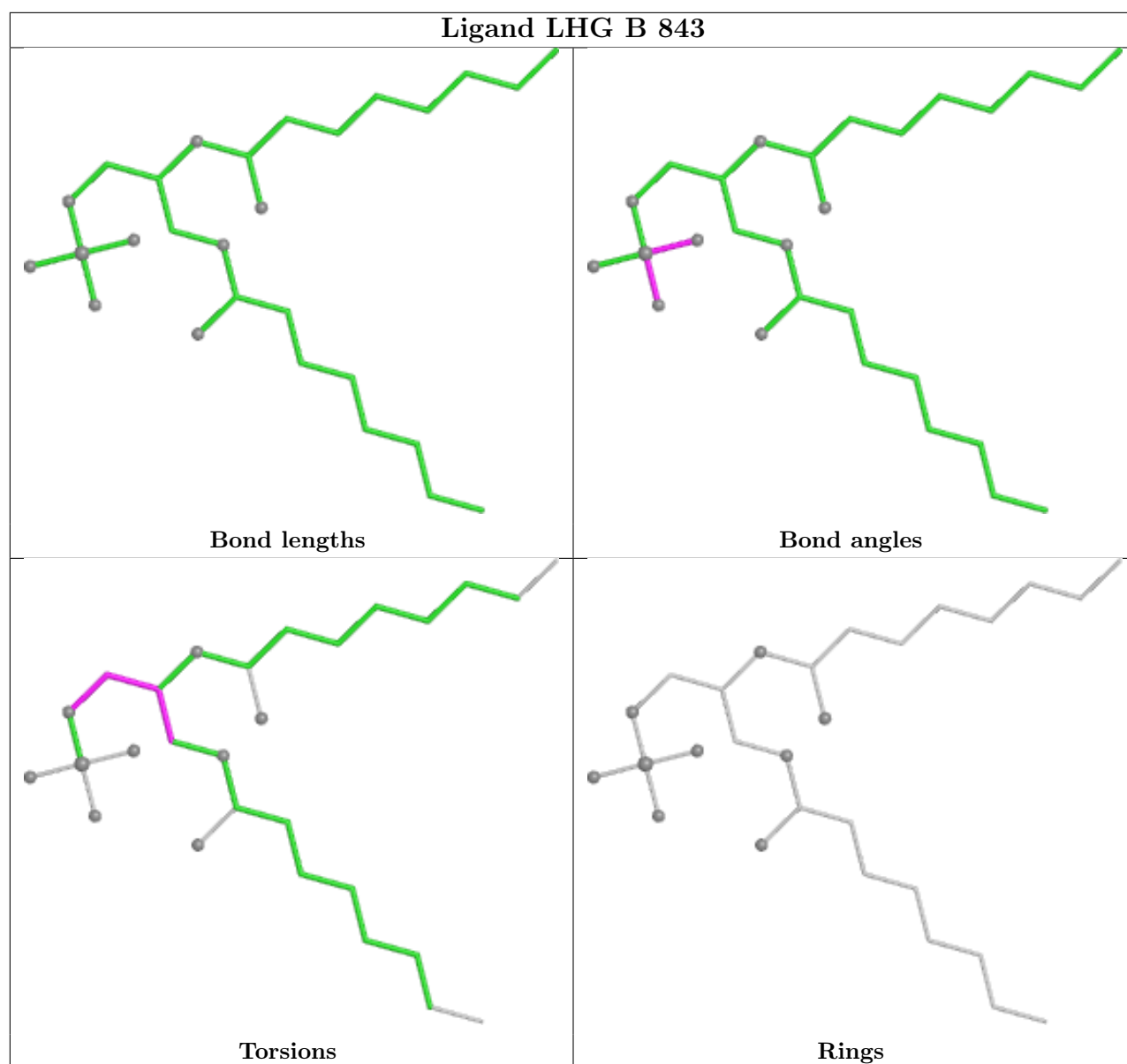
Ligand CLA 3 312

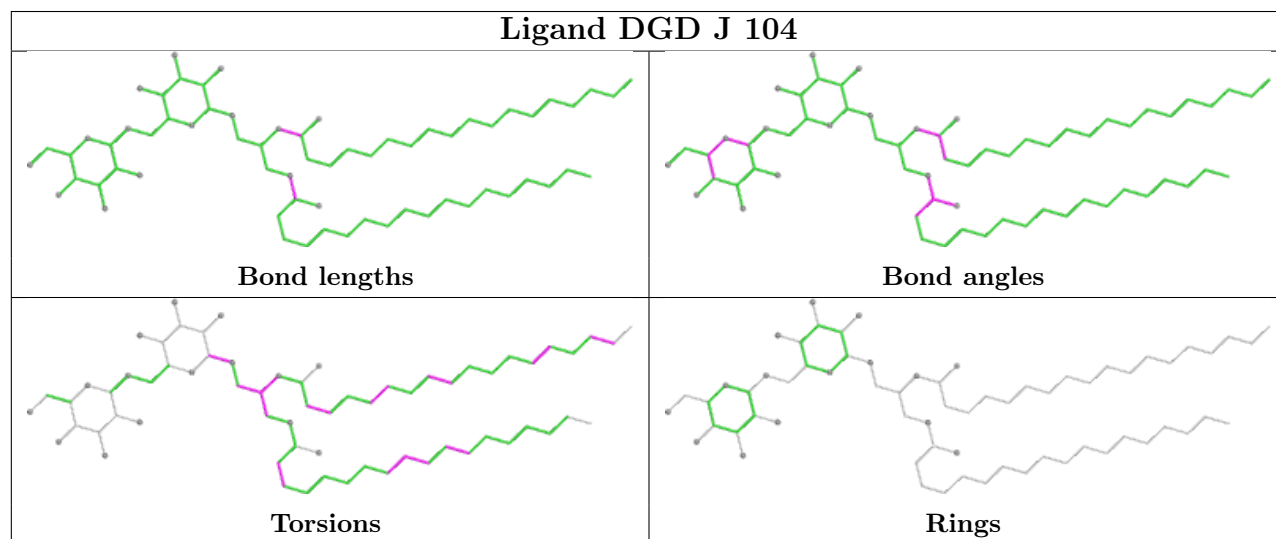
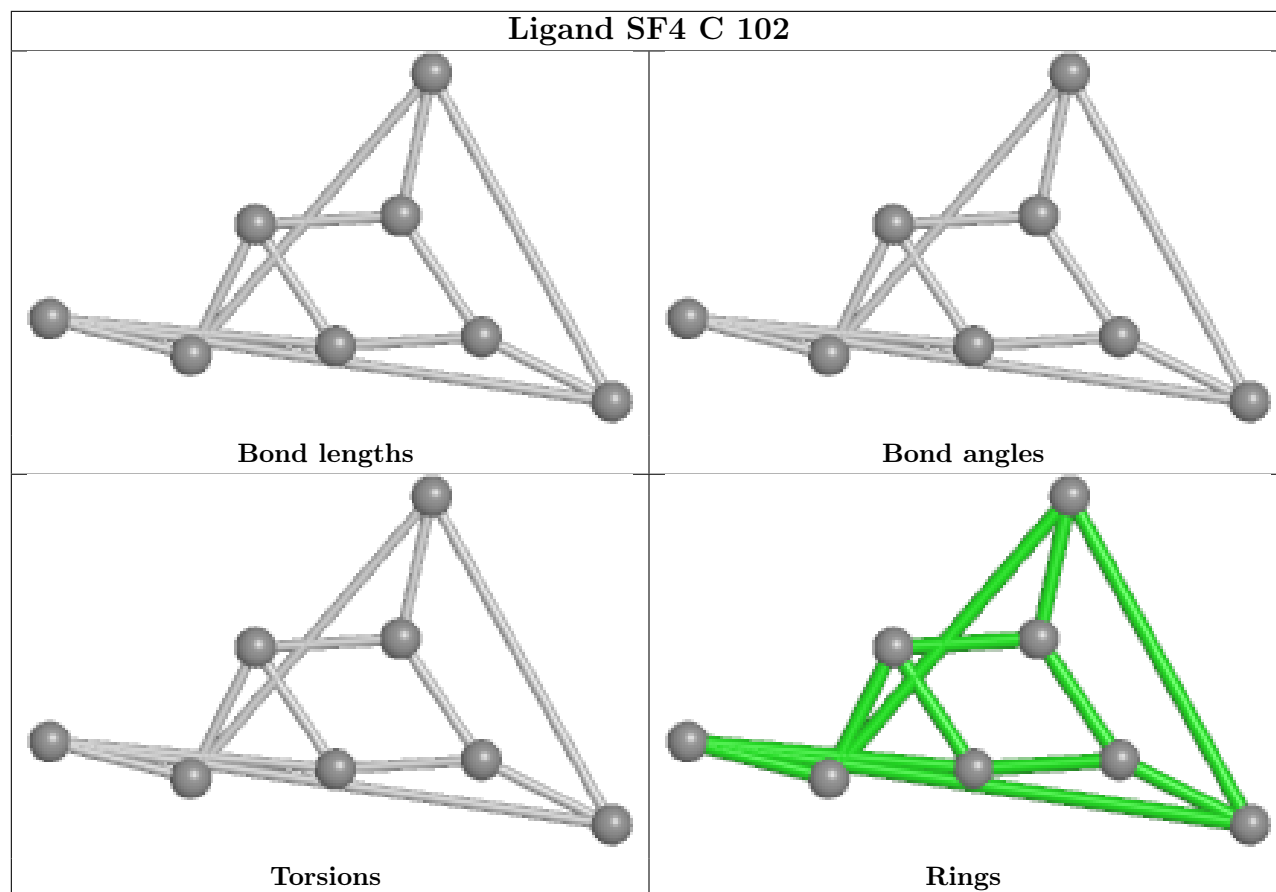


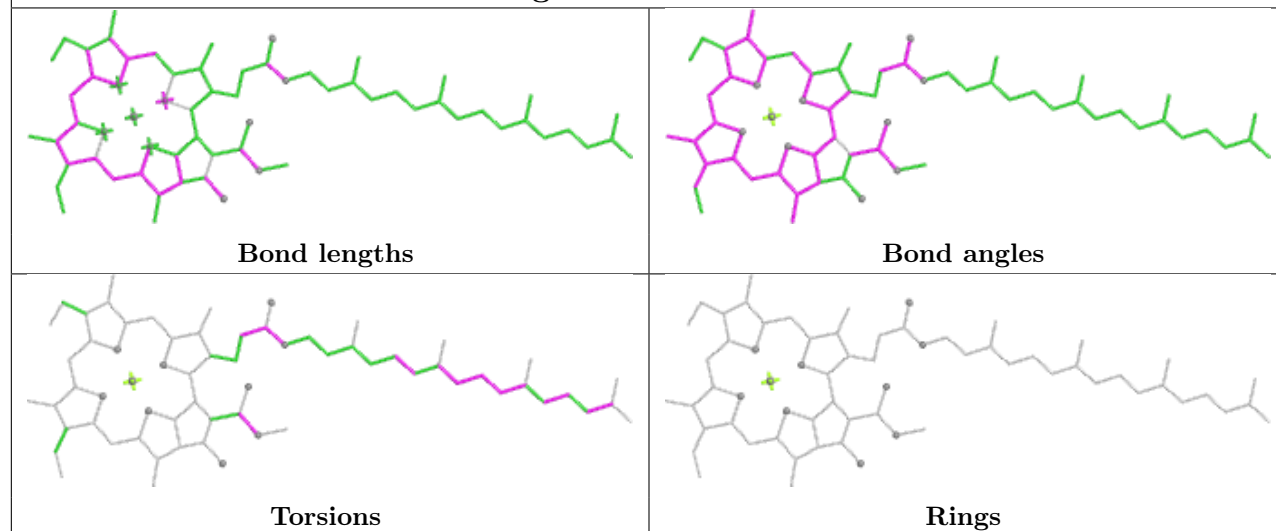
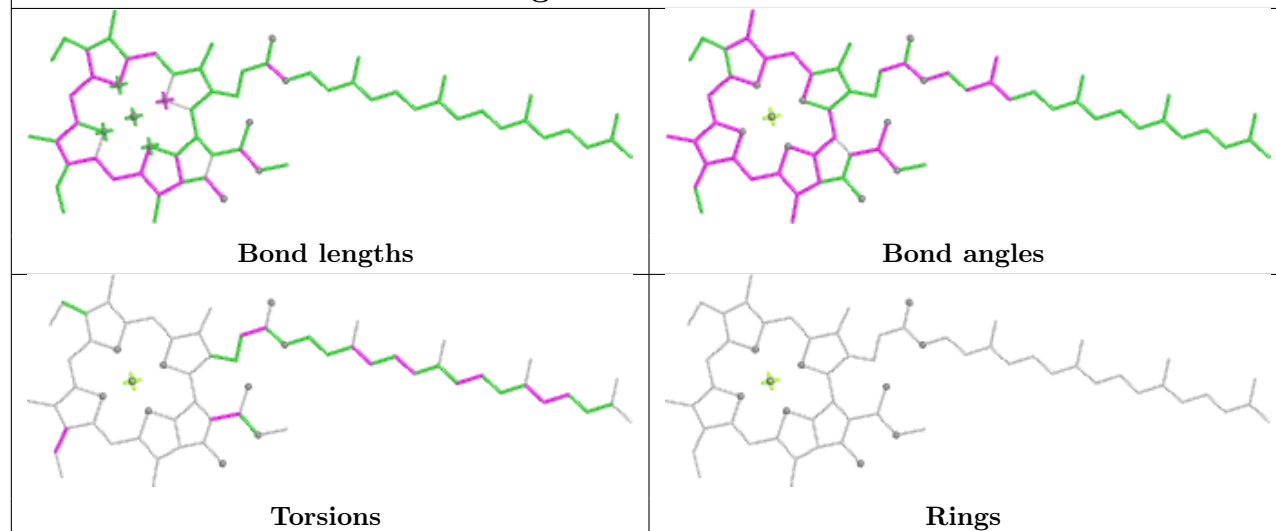
Ligand CLA A 809



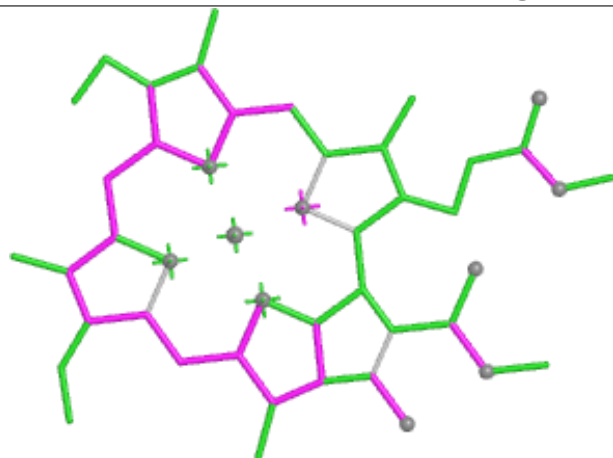




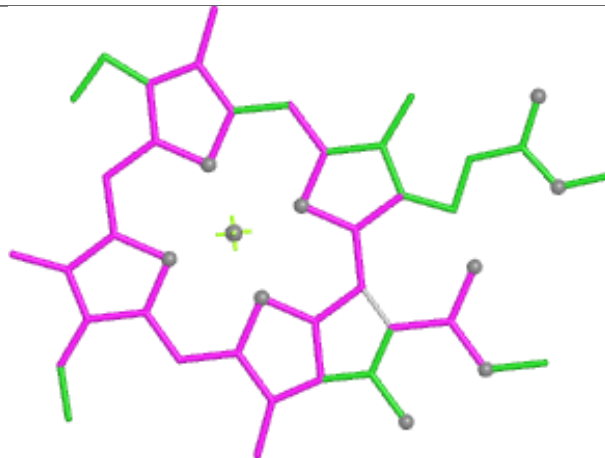


Ligand CLA B 830**Ligand CLA A 837**

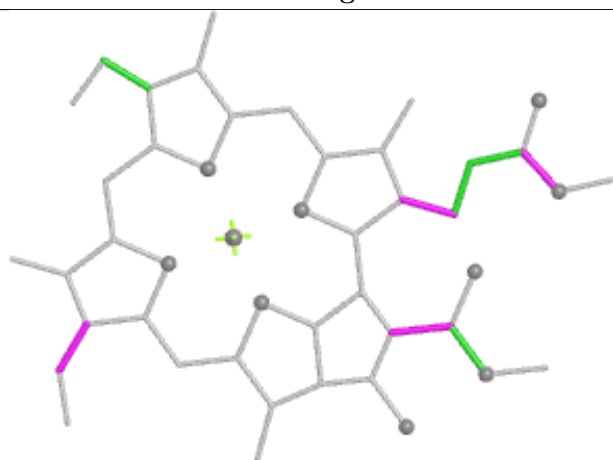
Ligand CLA A 846



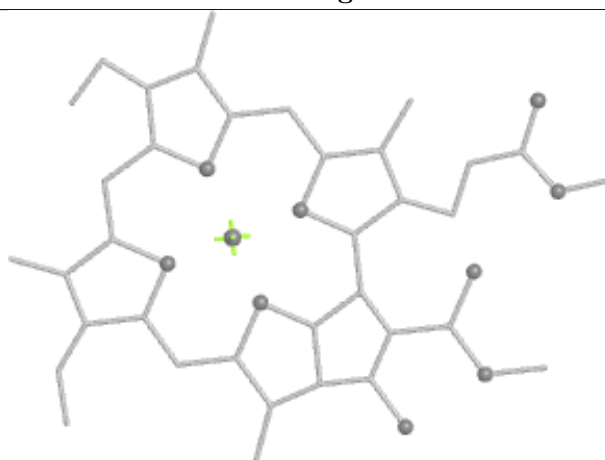
Bond lengths



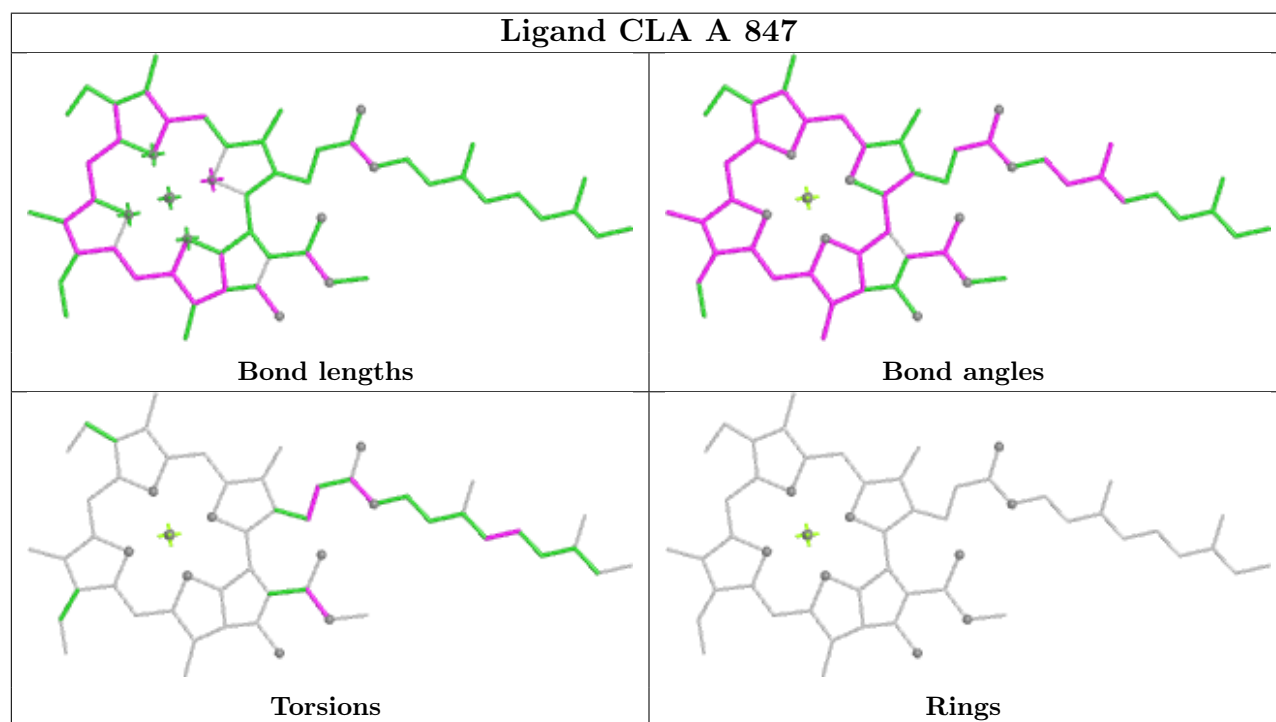
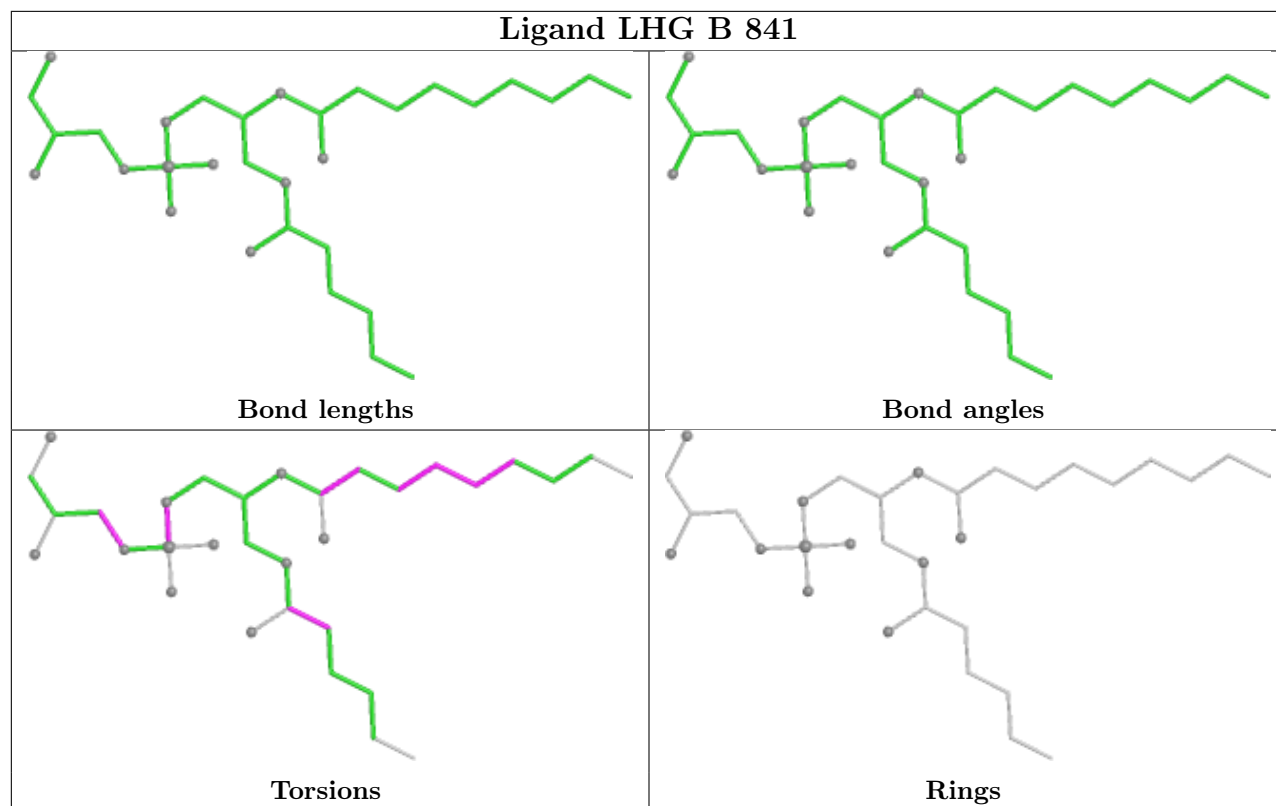
Bond angles



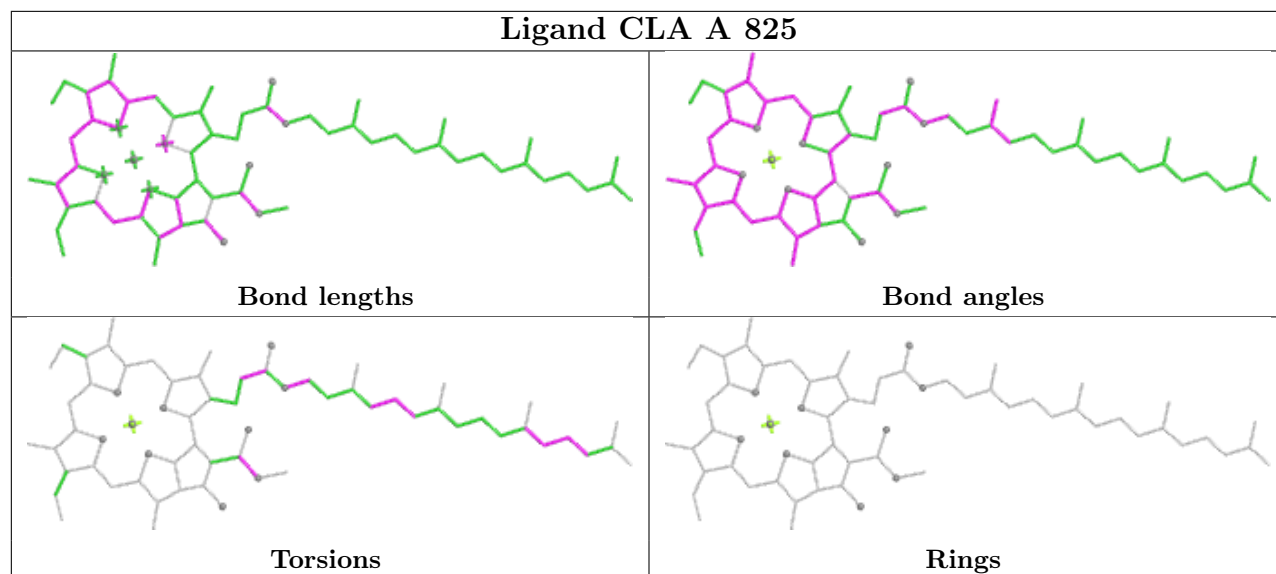
Torsions



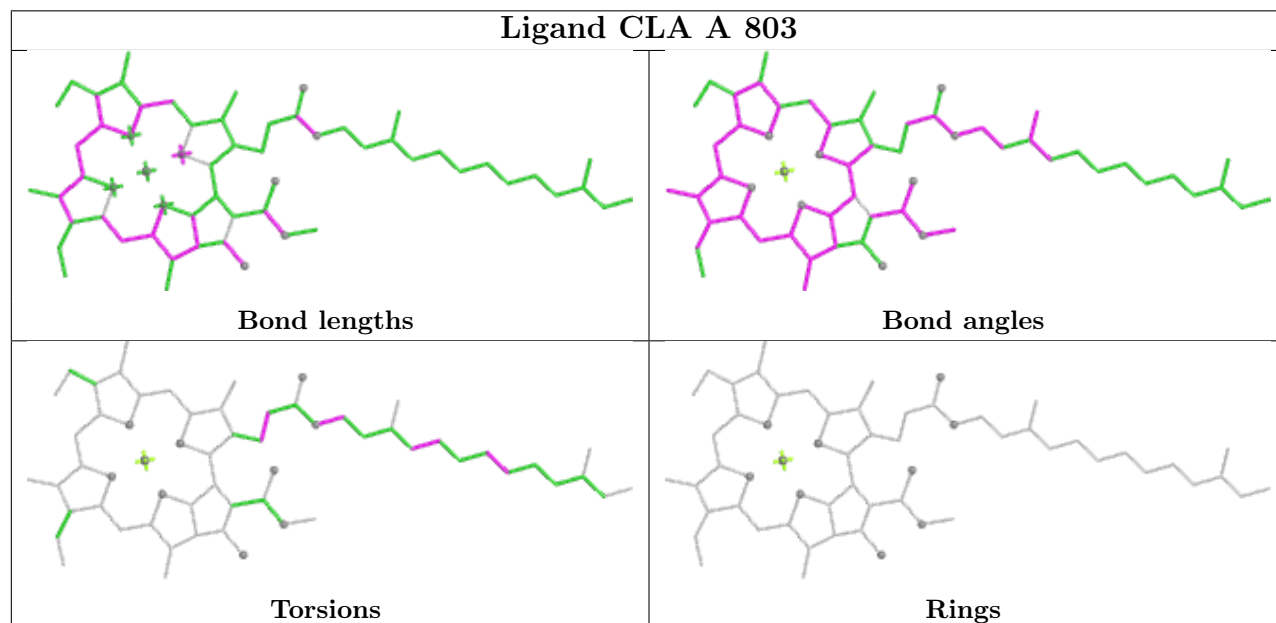
Rings



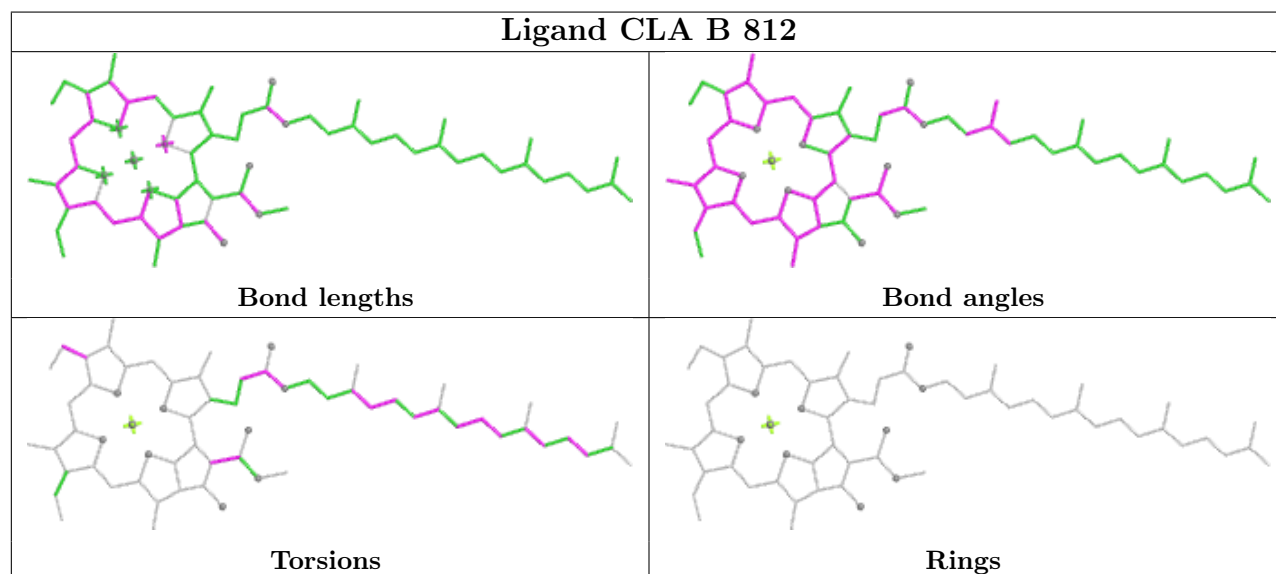
Ligand CLA A 825

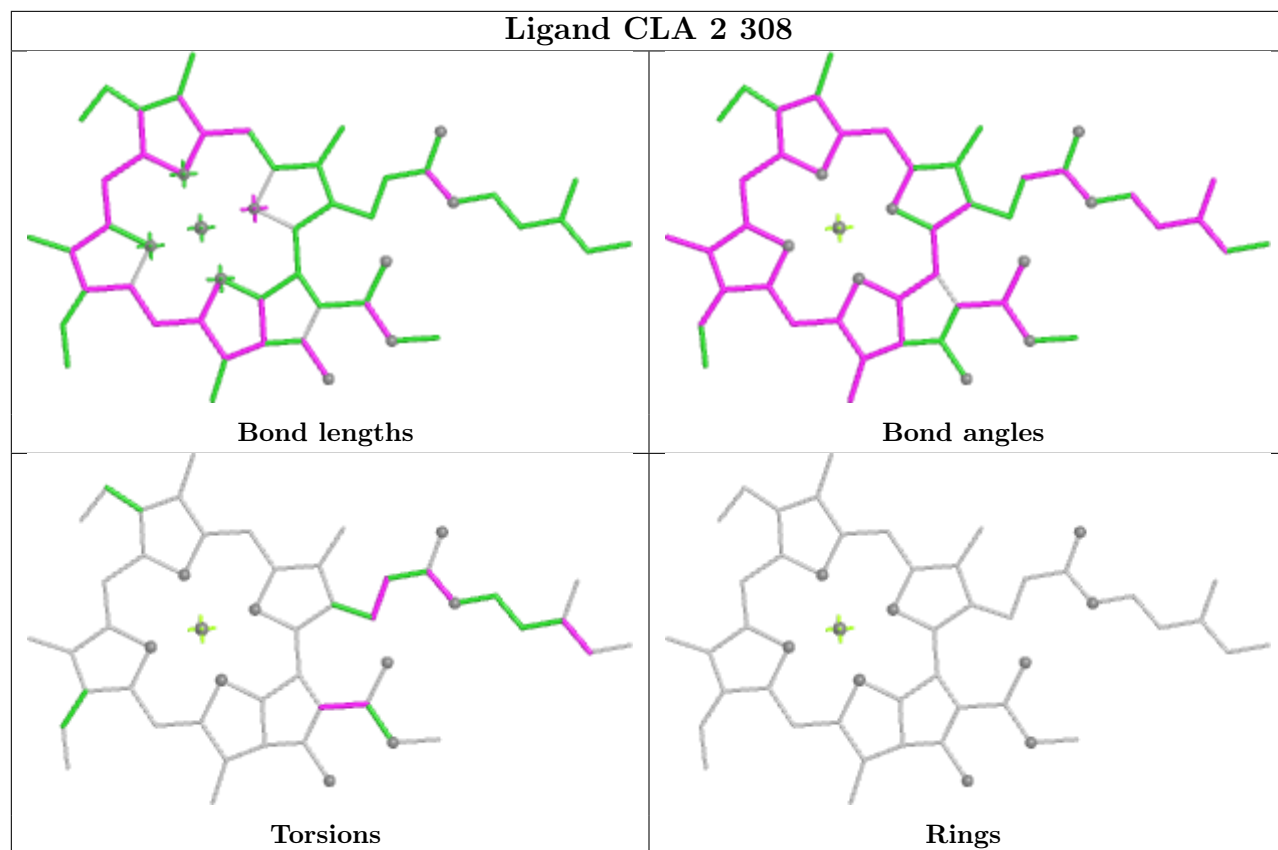


Ligand CLA A 803

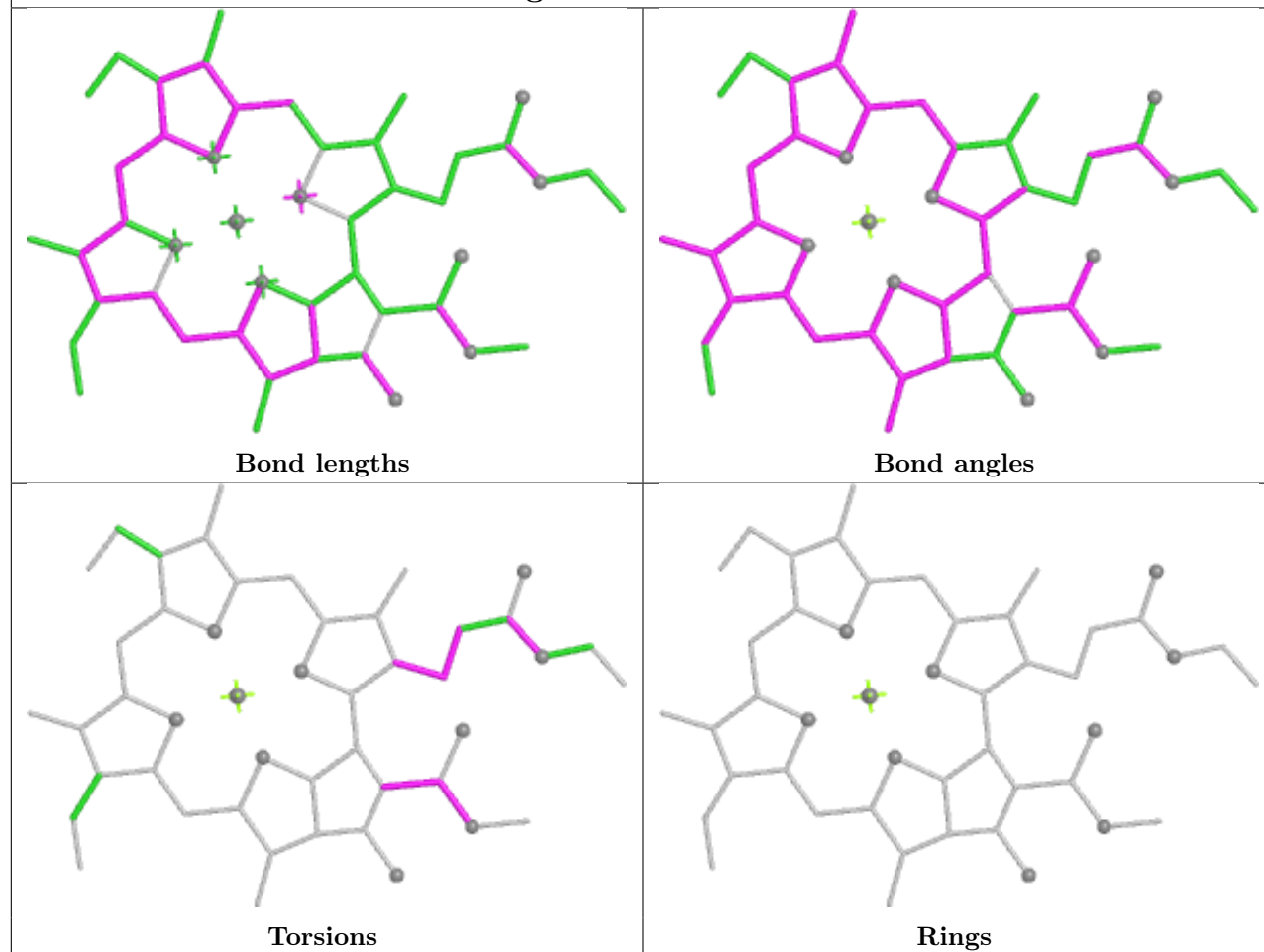


Ligand CLA B 812

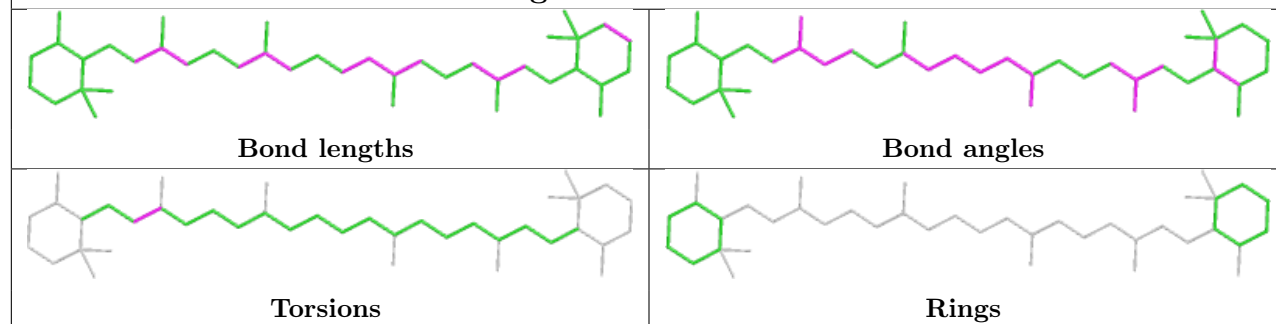


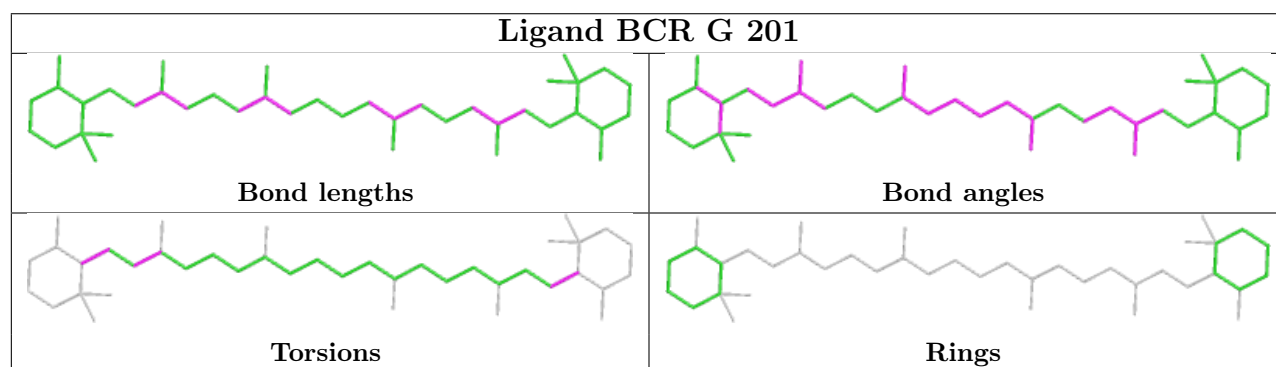
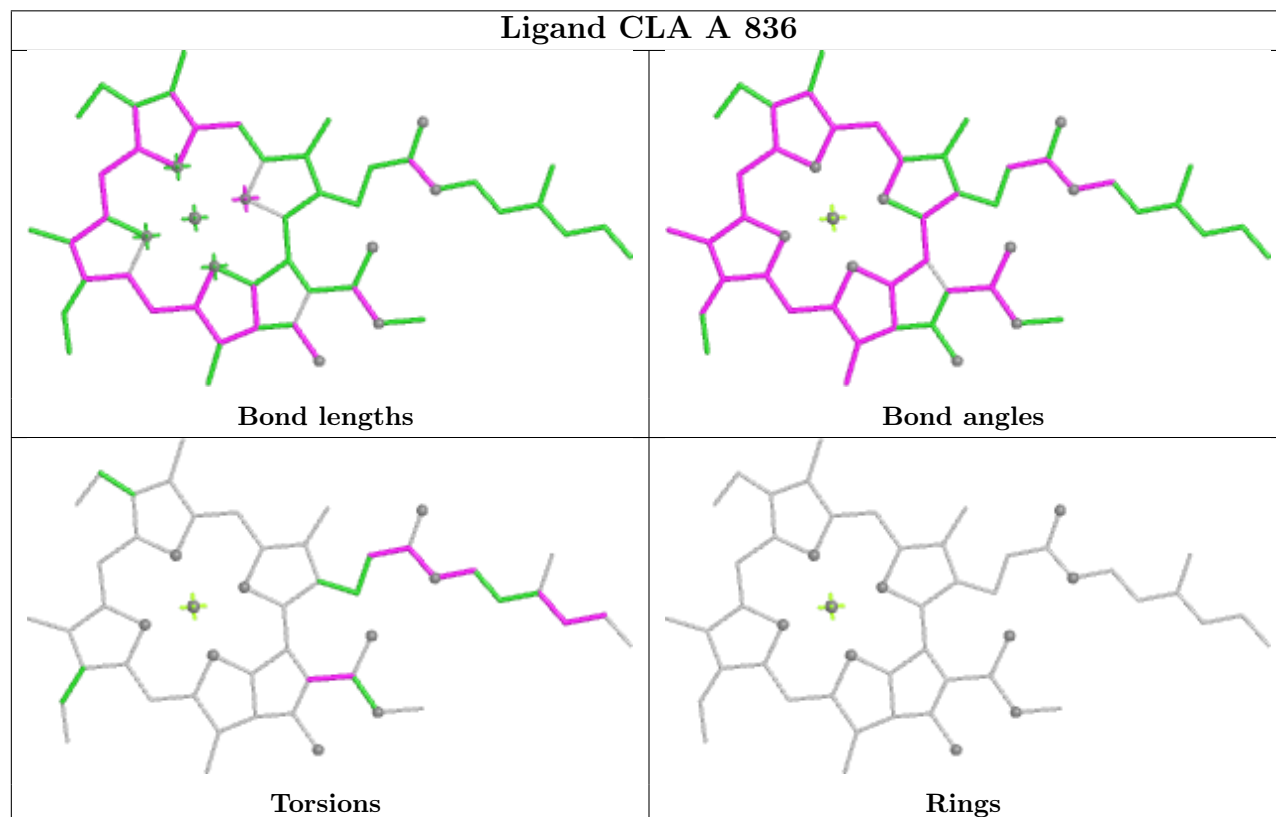
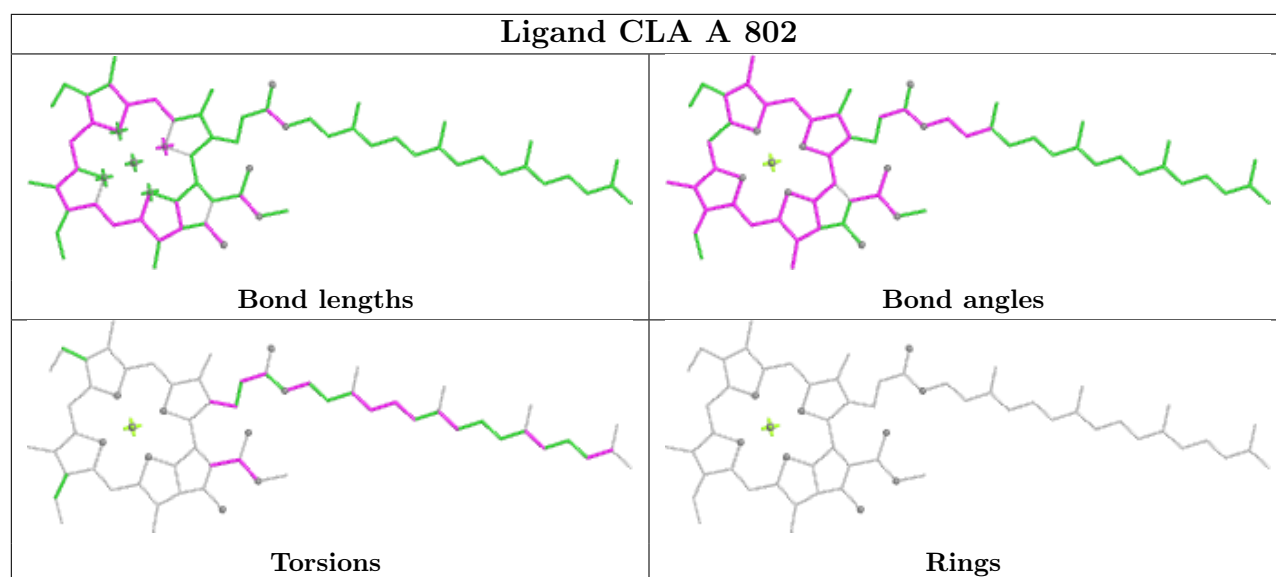


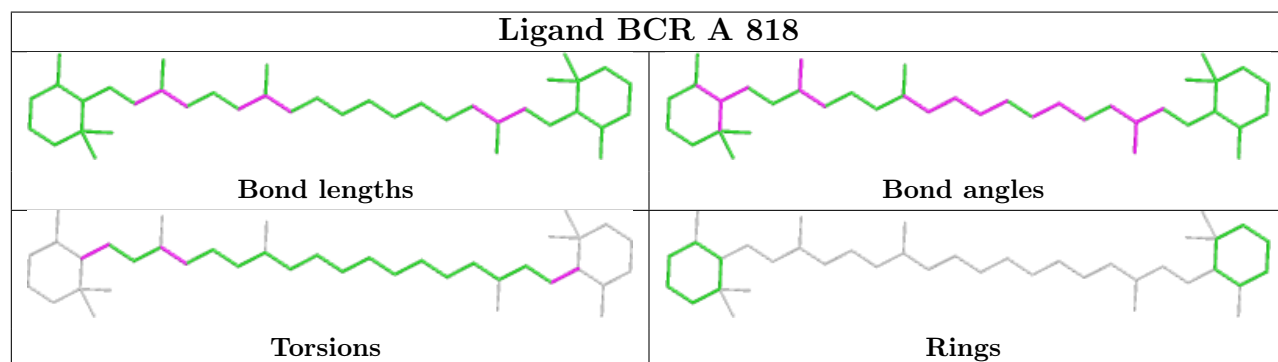
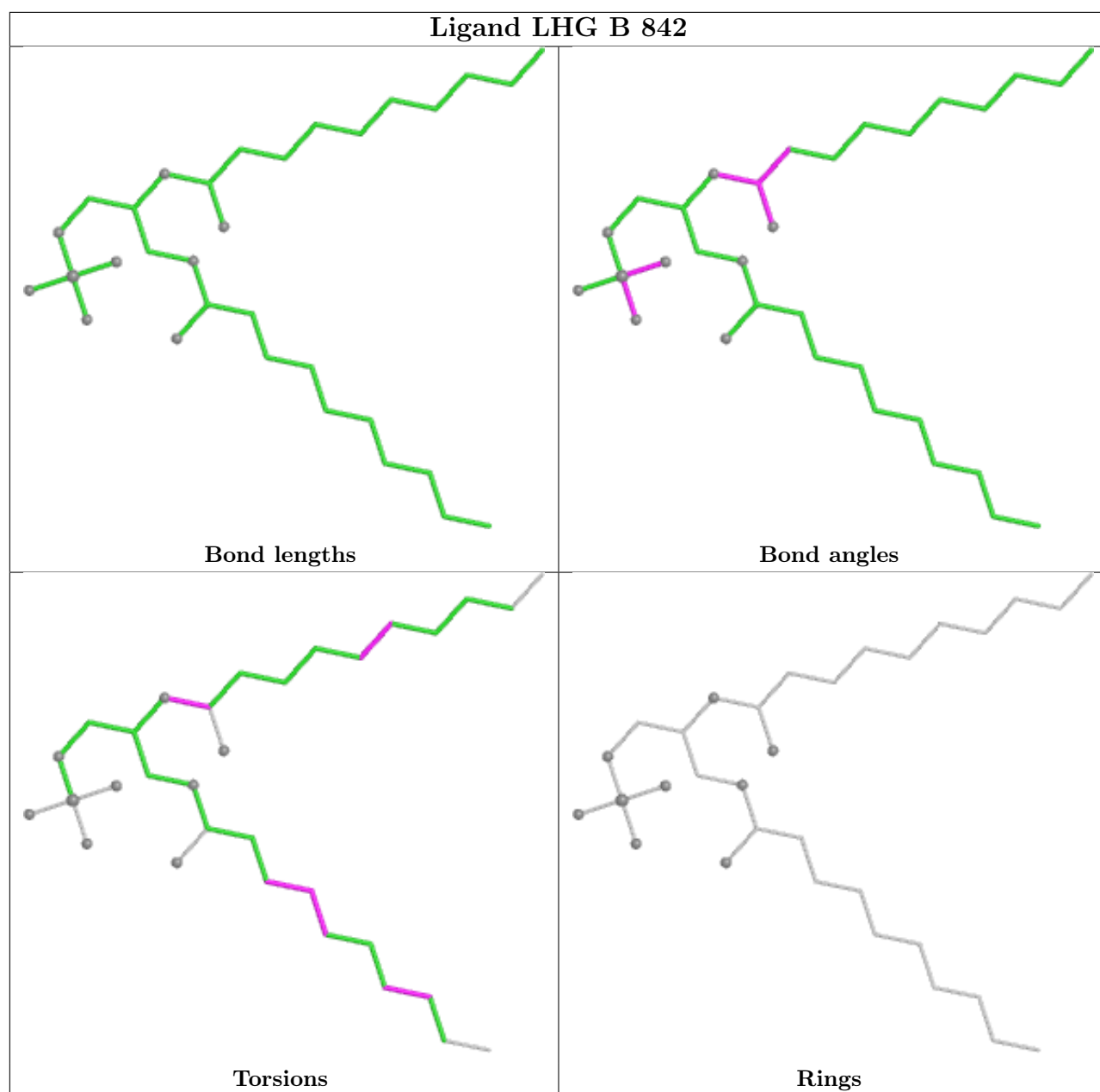
Ligand CLA K 203



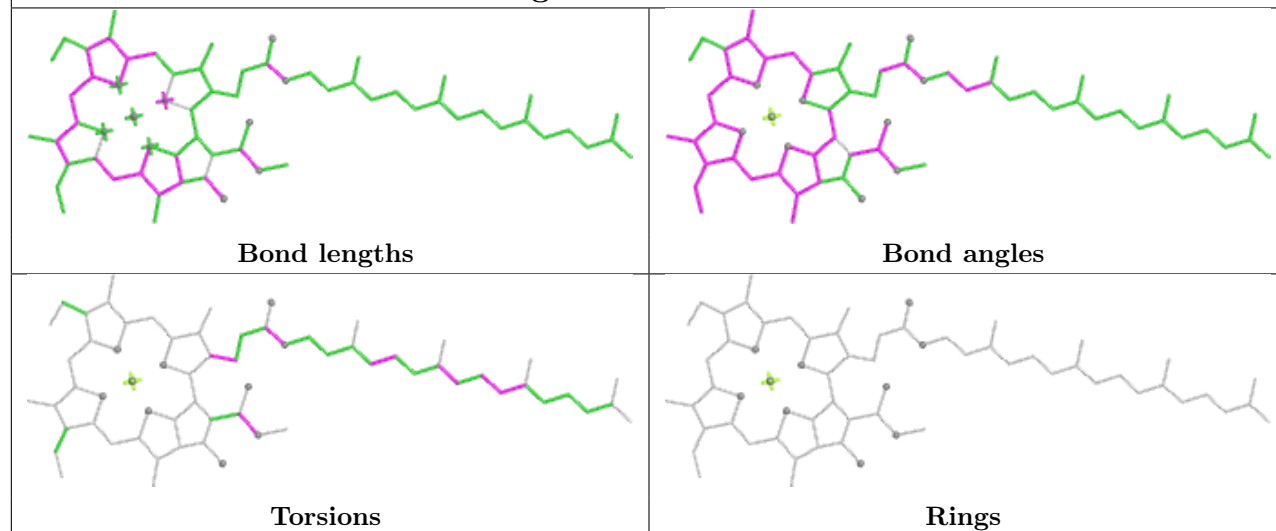
Ligand BCR A 817



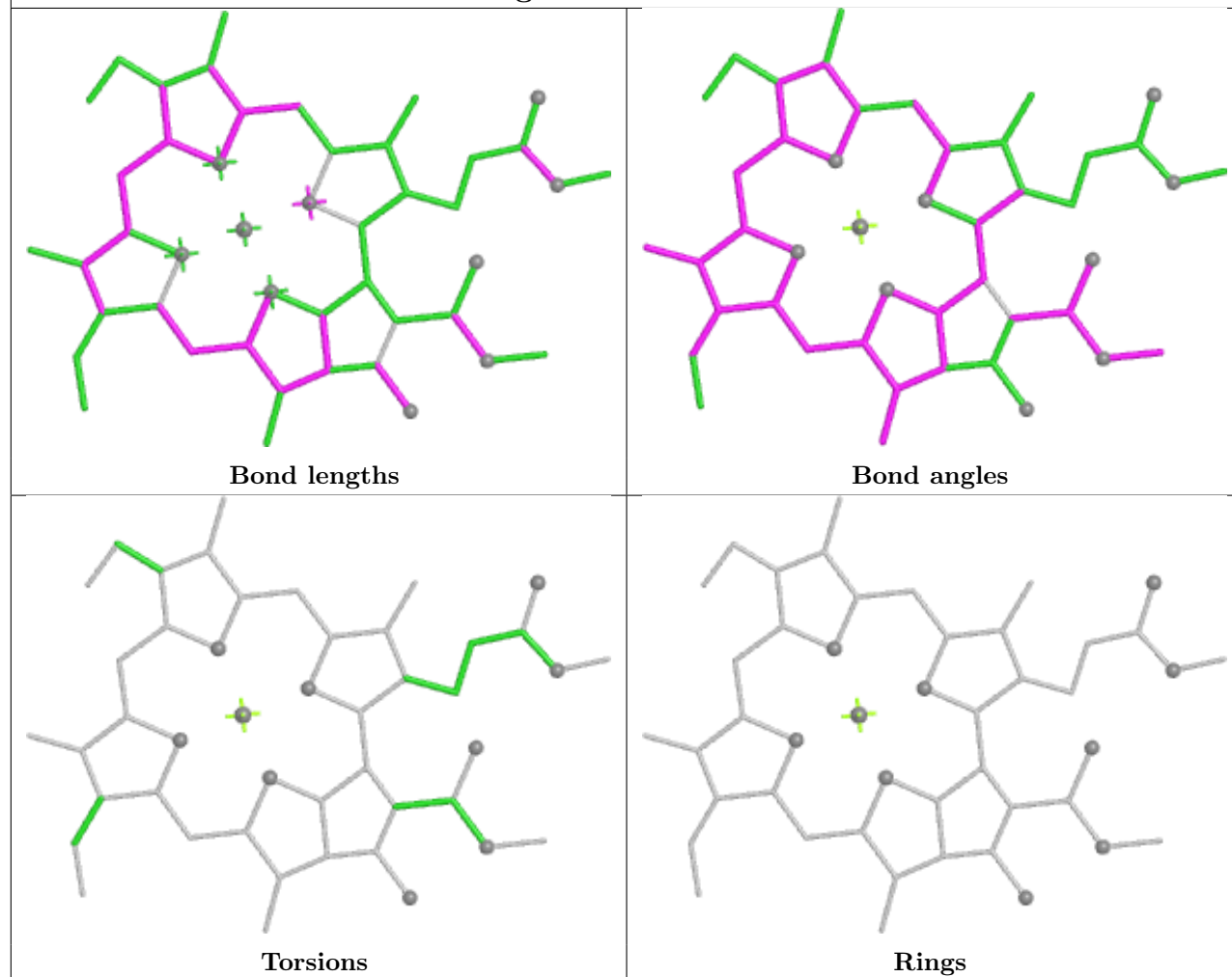




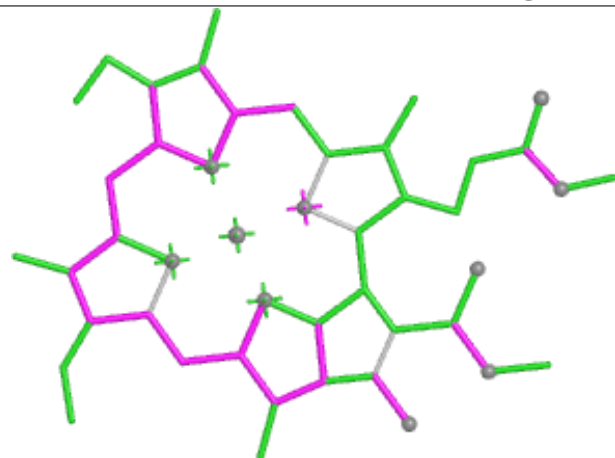
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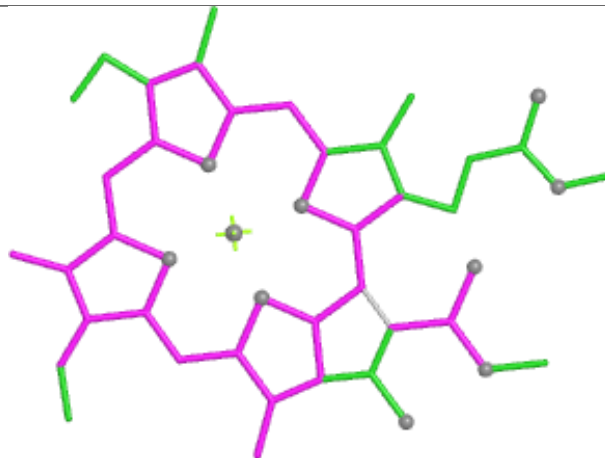
Ligand CLA F 305



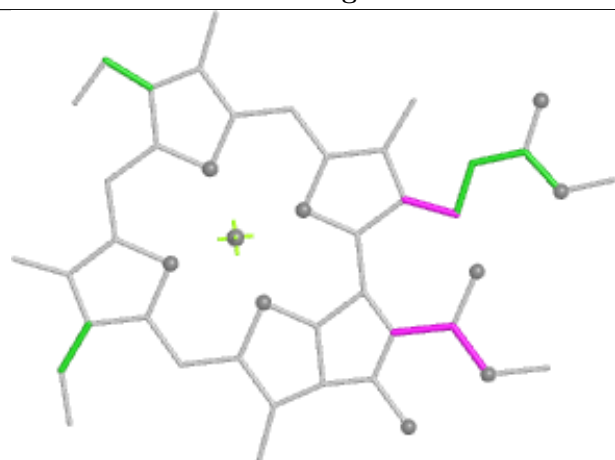
Ligand CLA J 103



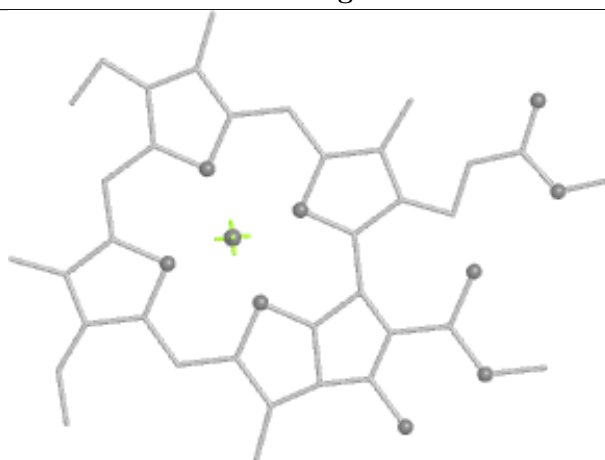
Bond lengths



Bond angles

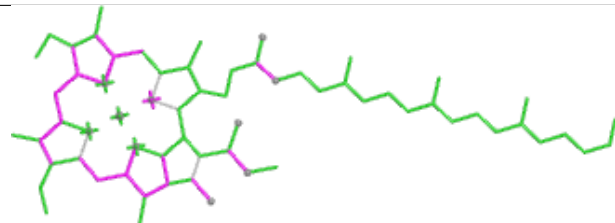


Torsions

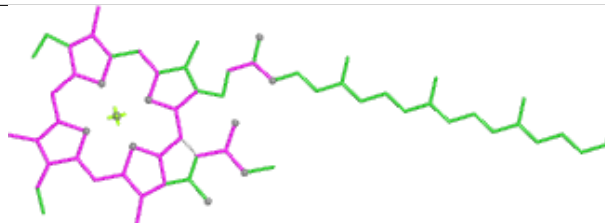


Rings

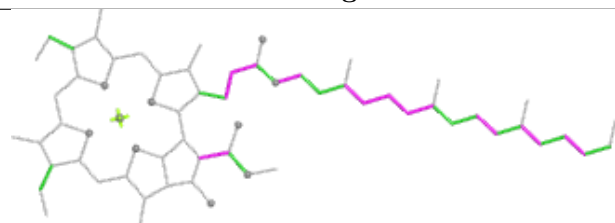
Ligand CLA A 829



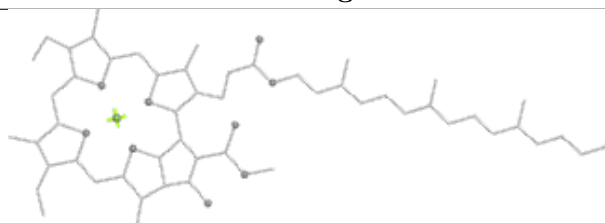
Bond lengths



Bond angles

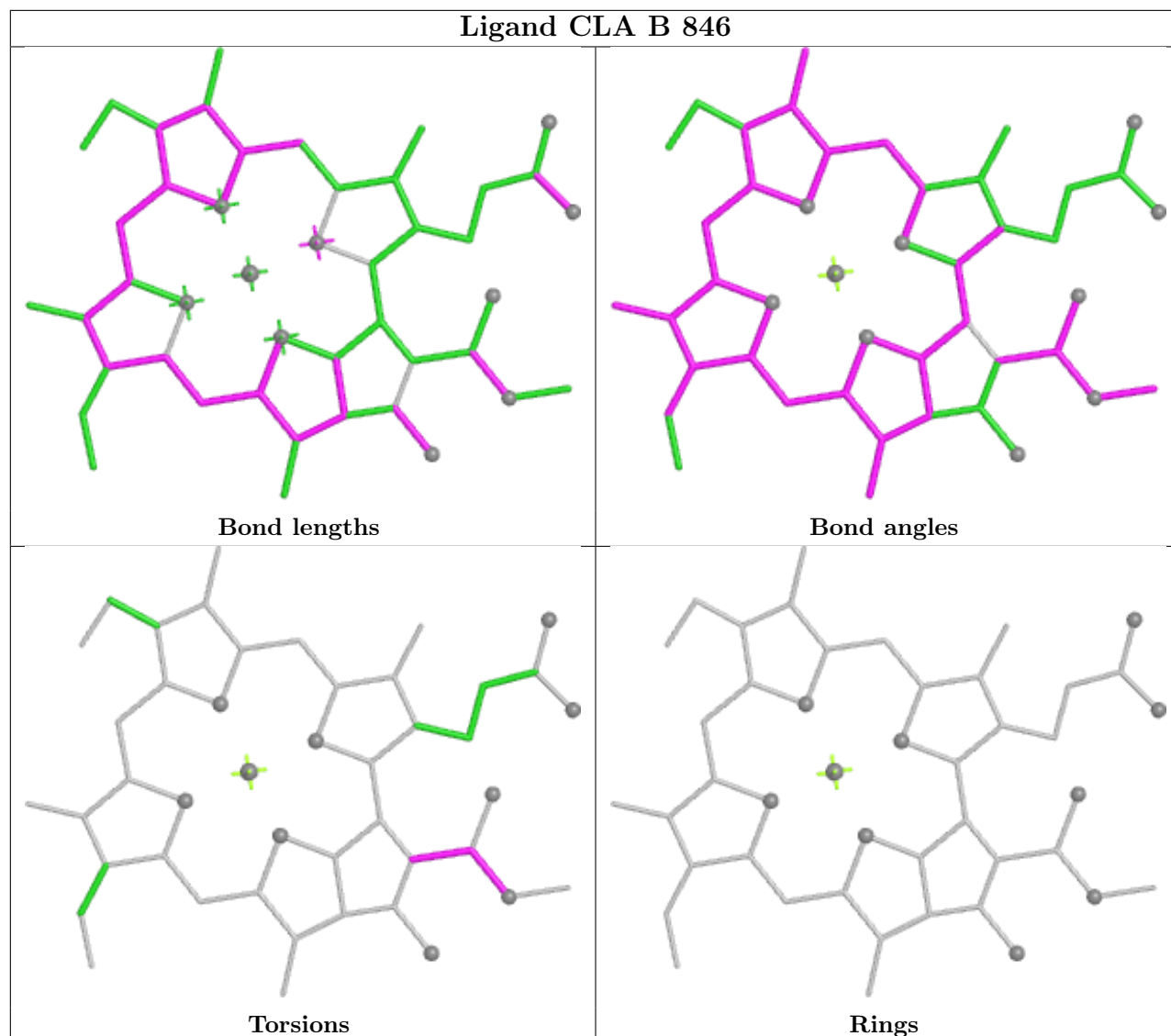


Torsions

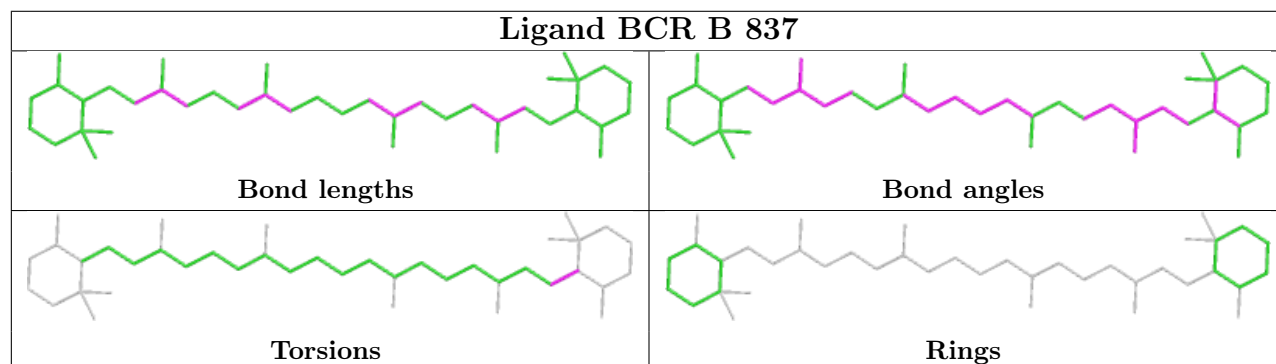


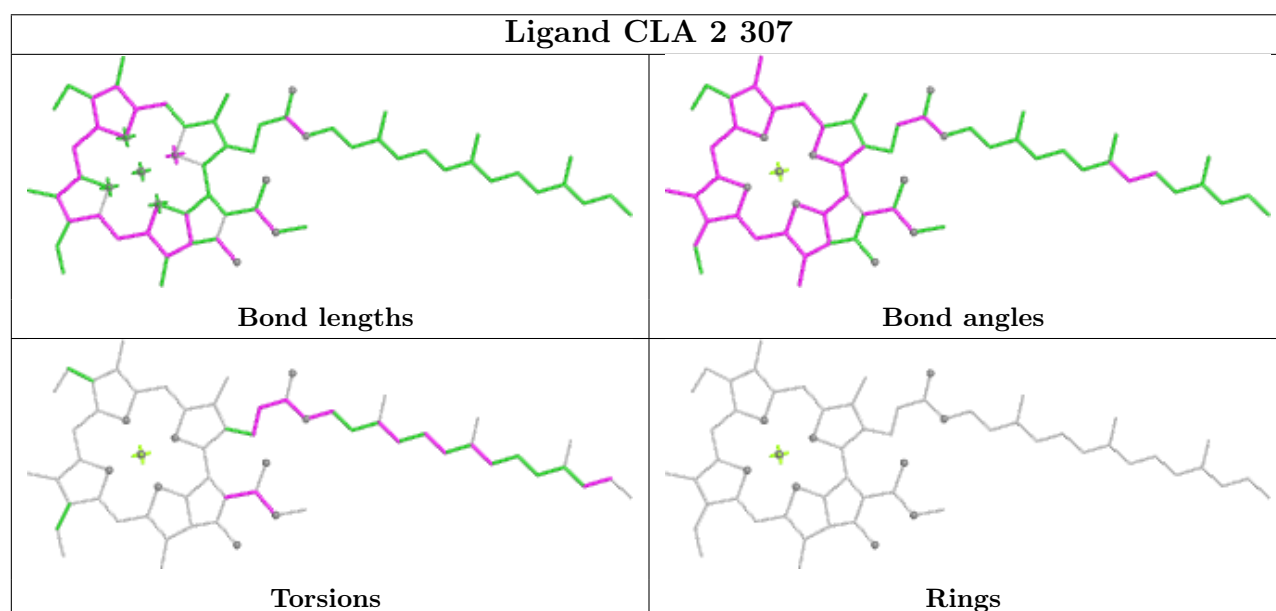
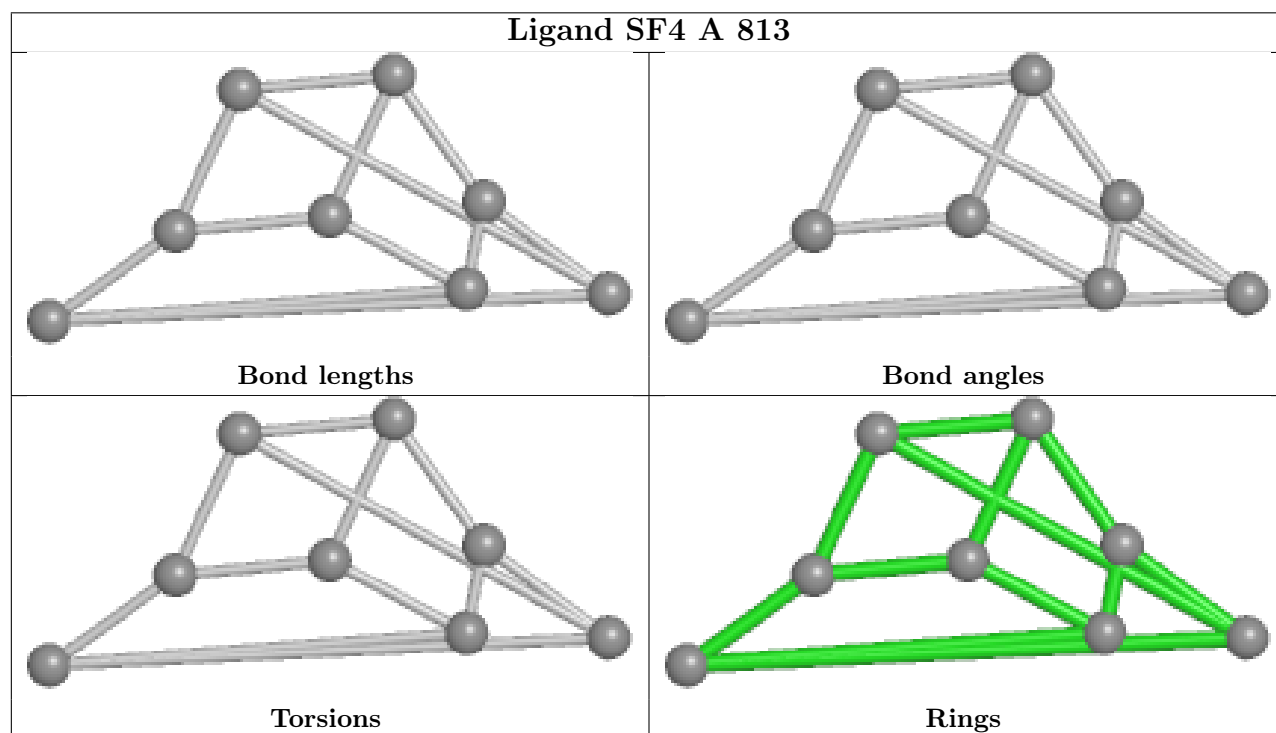
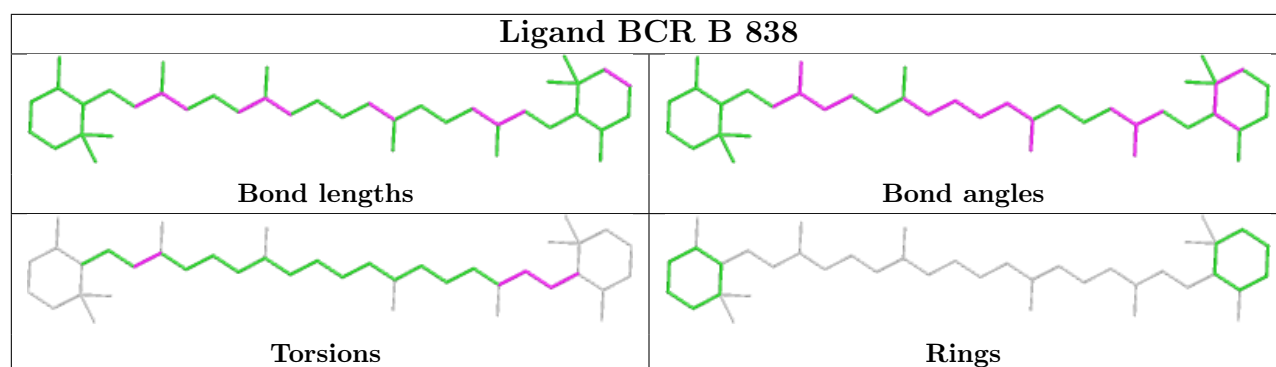
Rings

Ligand CLA B 846

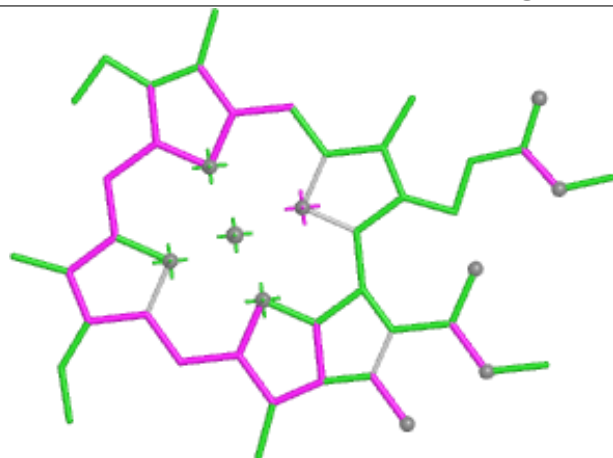


Ligand BCR B 837

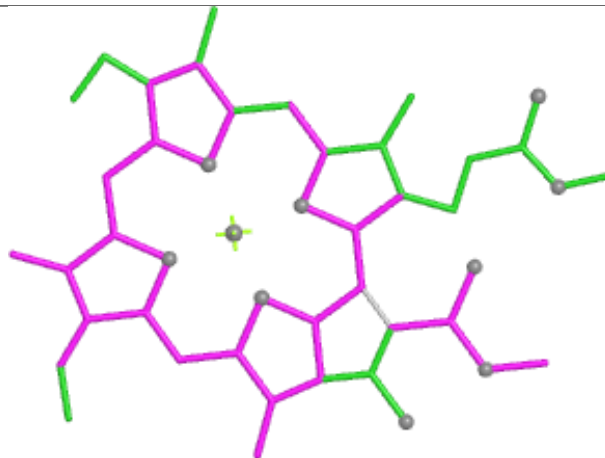




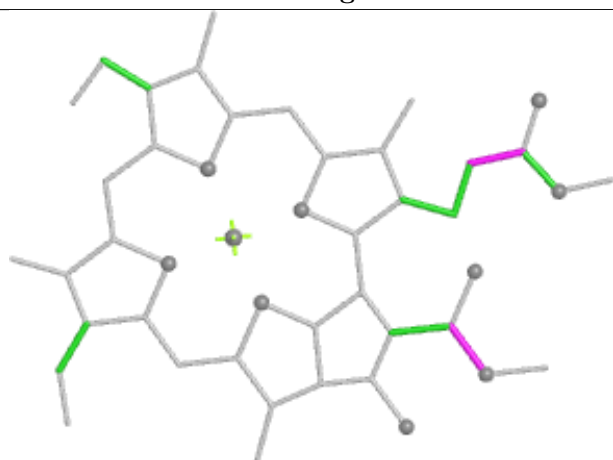
Ligand CLA 4 303



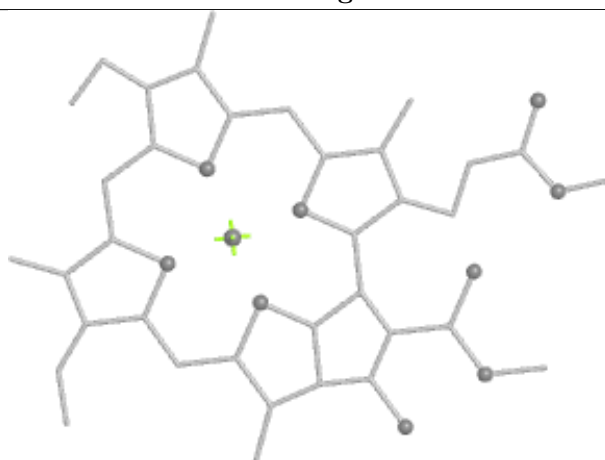
Bond lengths



Bond angles

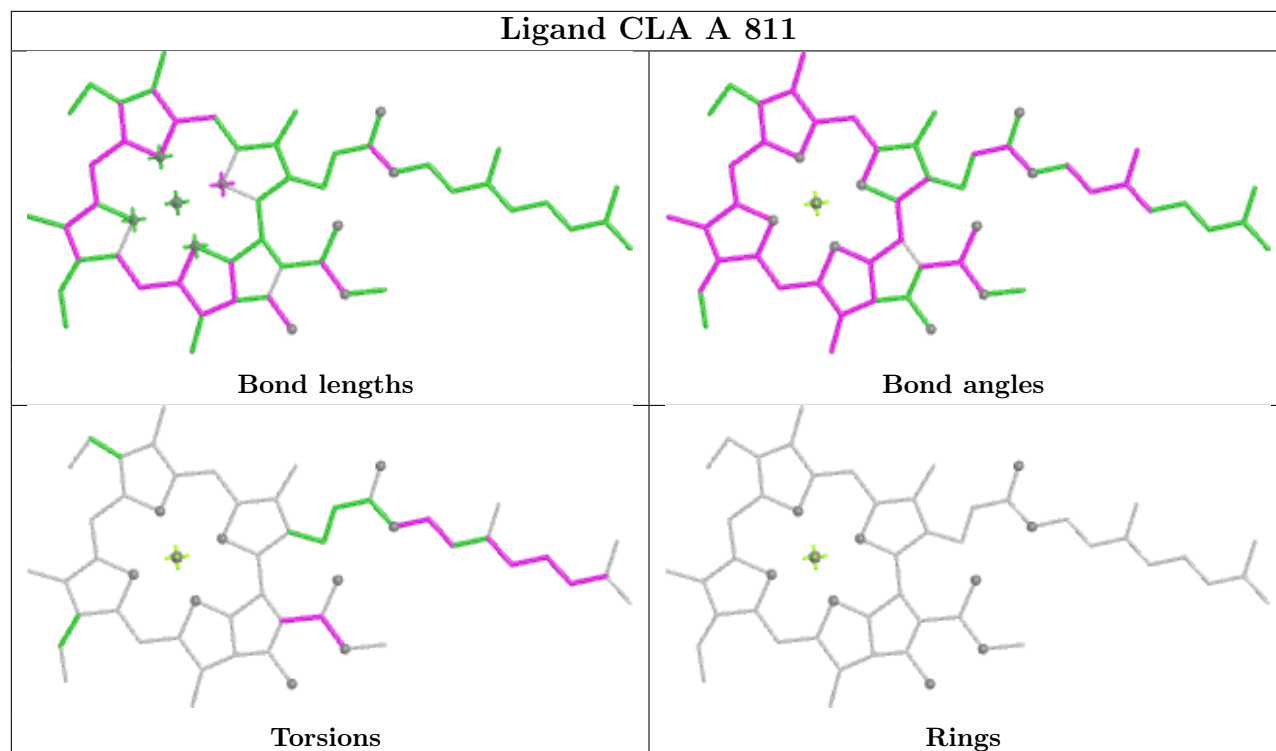


Torsions

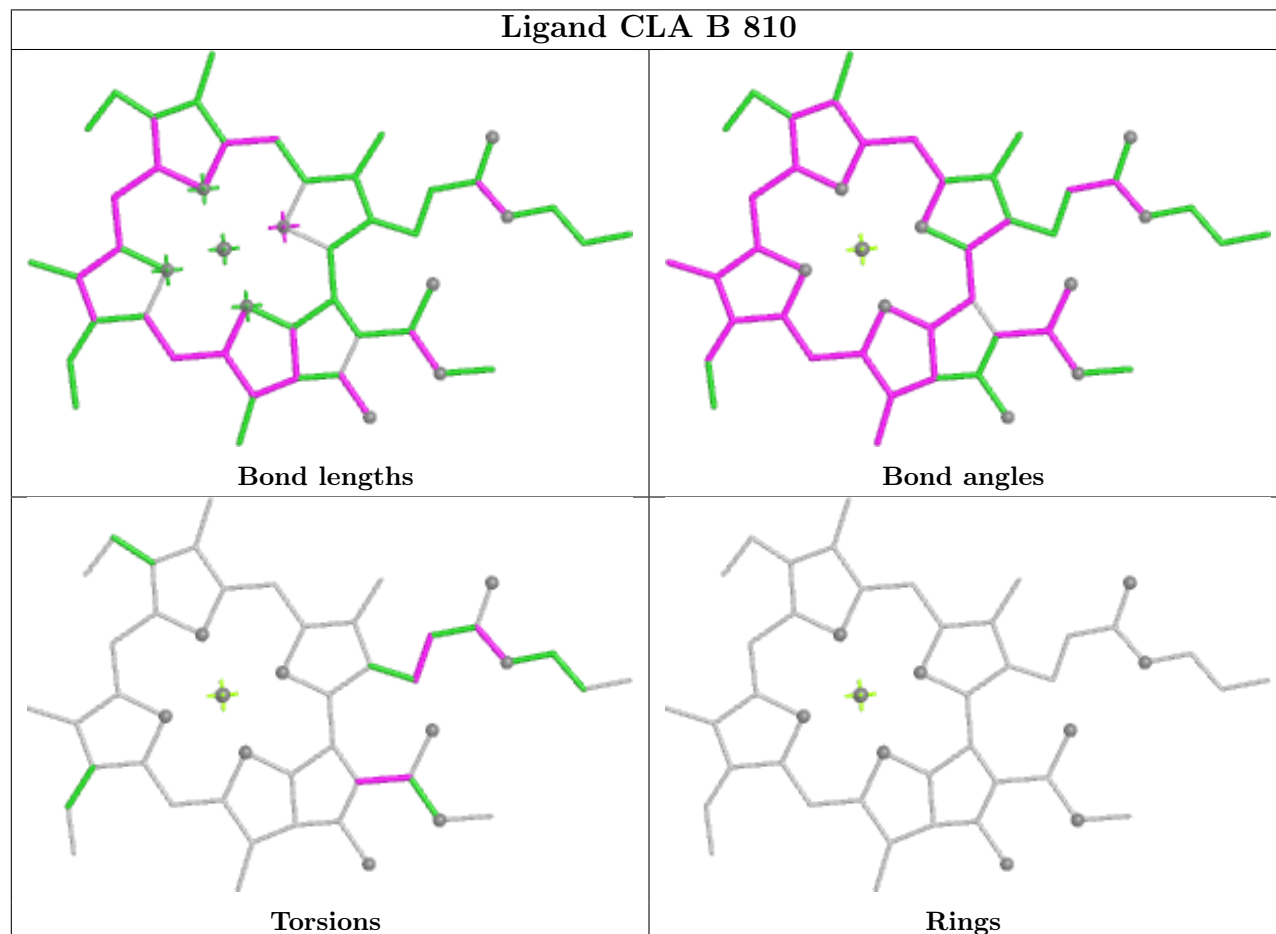


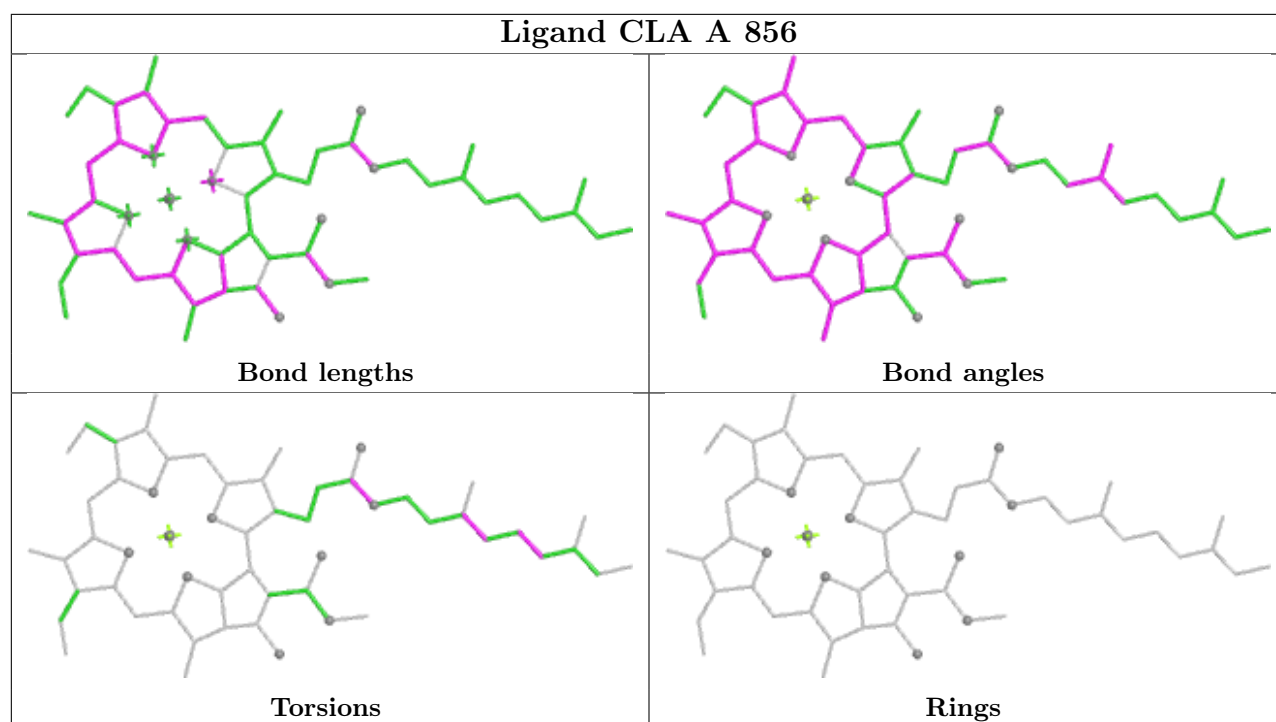
Rings

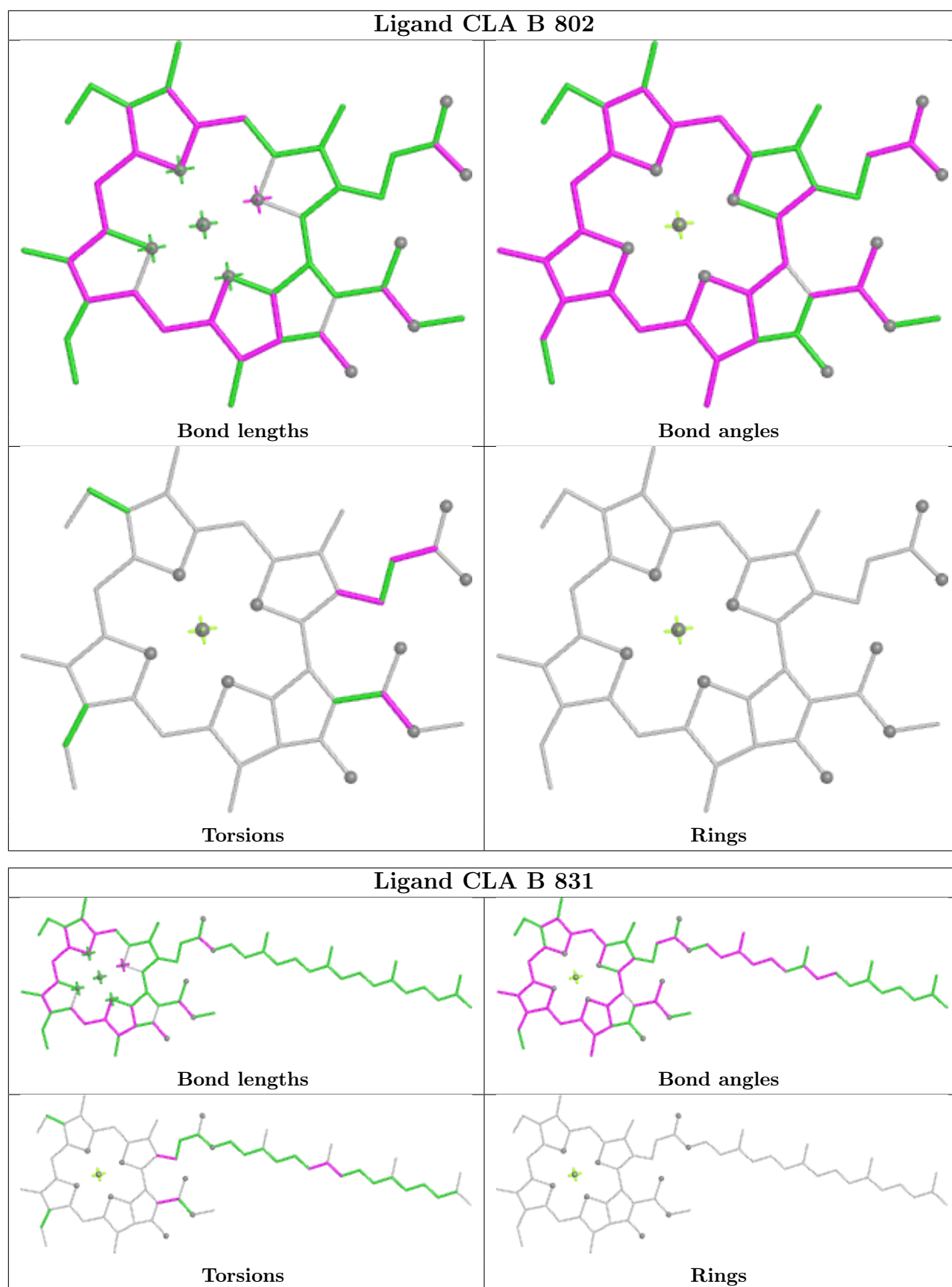
Ligand CLA A 811

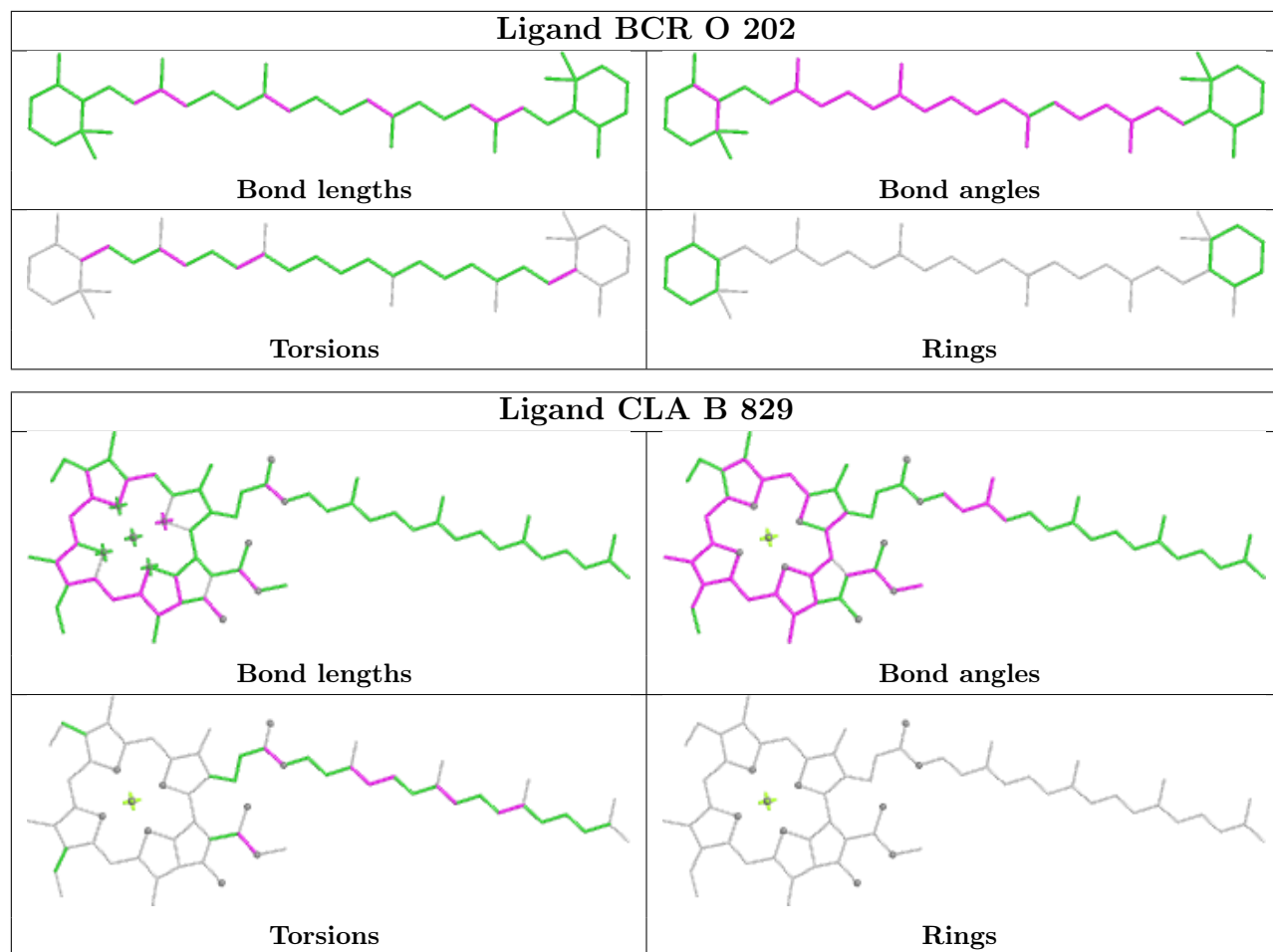


Ligand CLA B 810

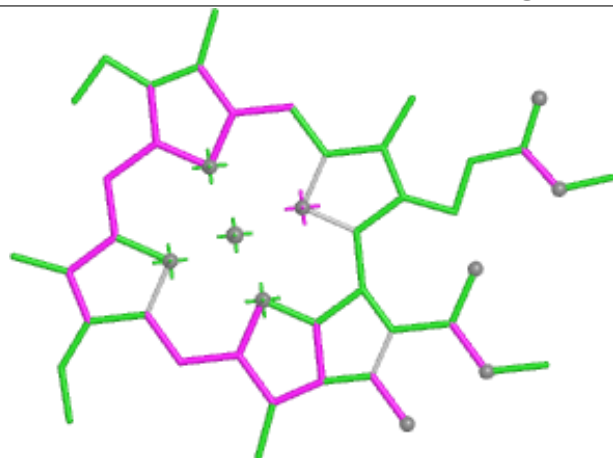




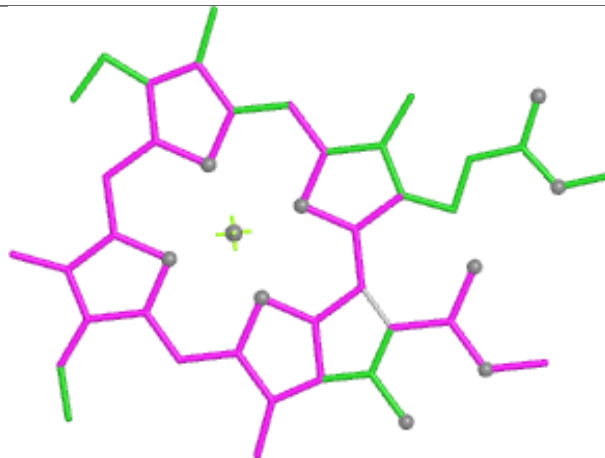




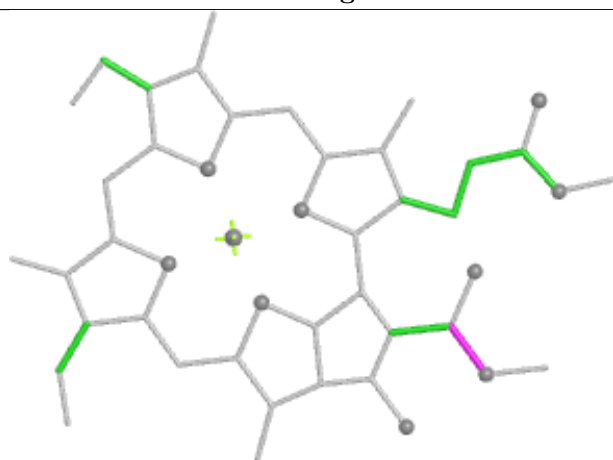
Ligand CLA 3 316



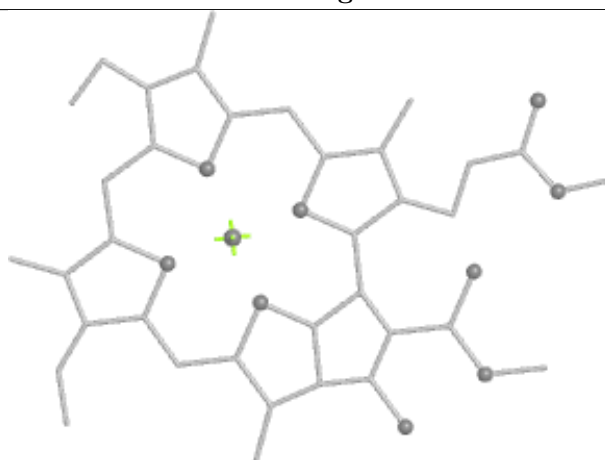
Bond lengths



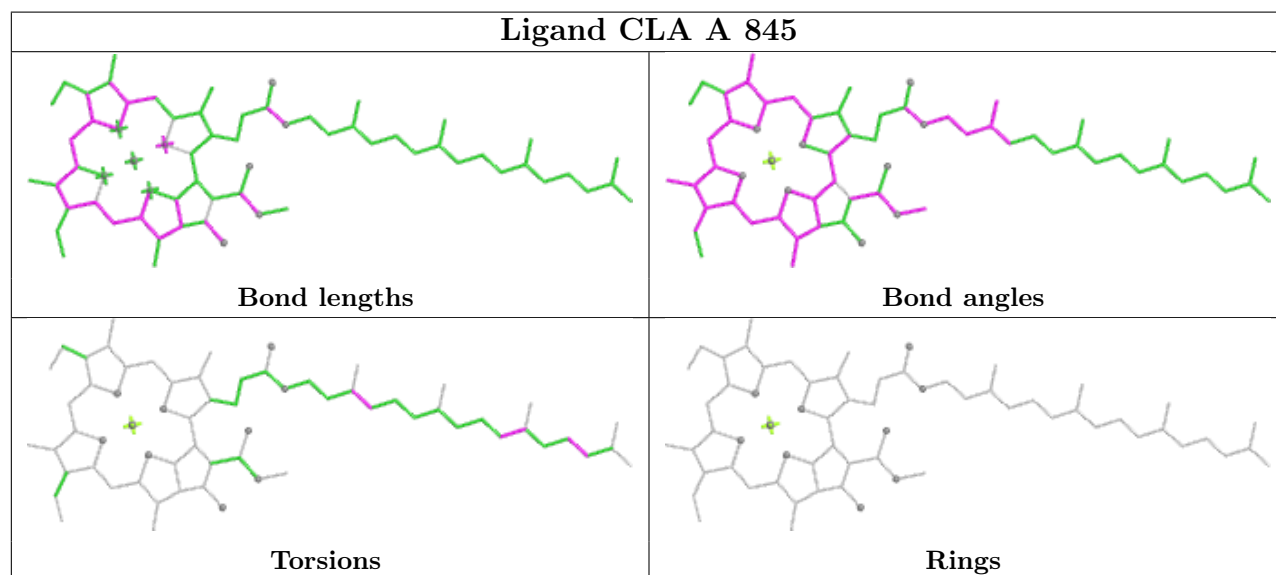
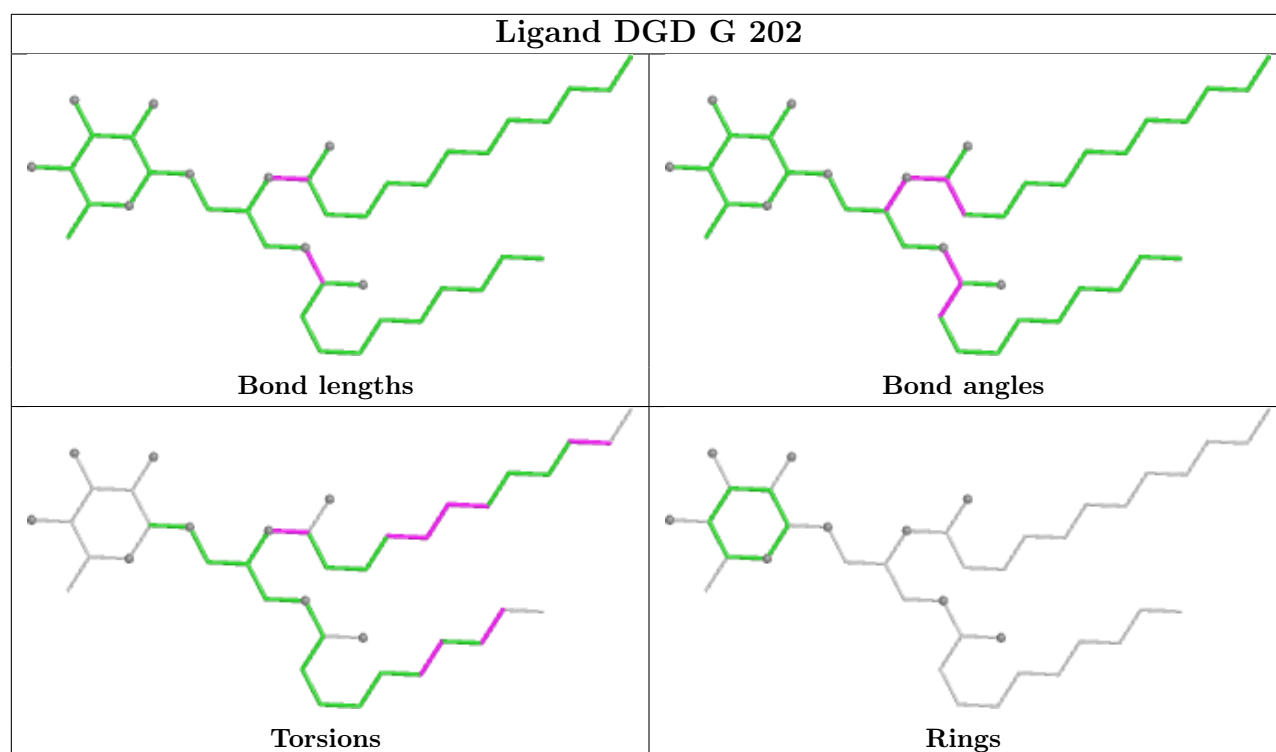
Bond angles

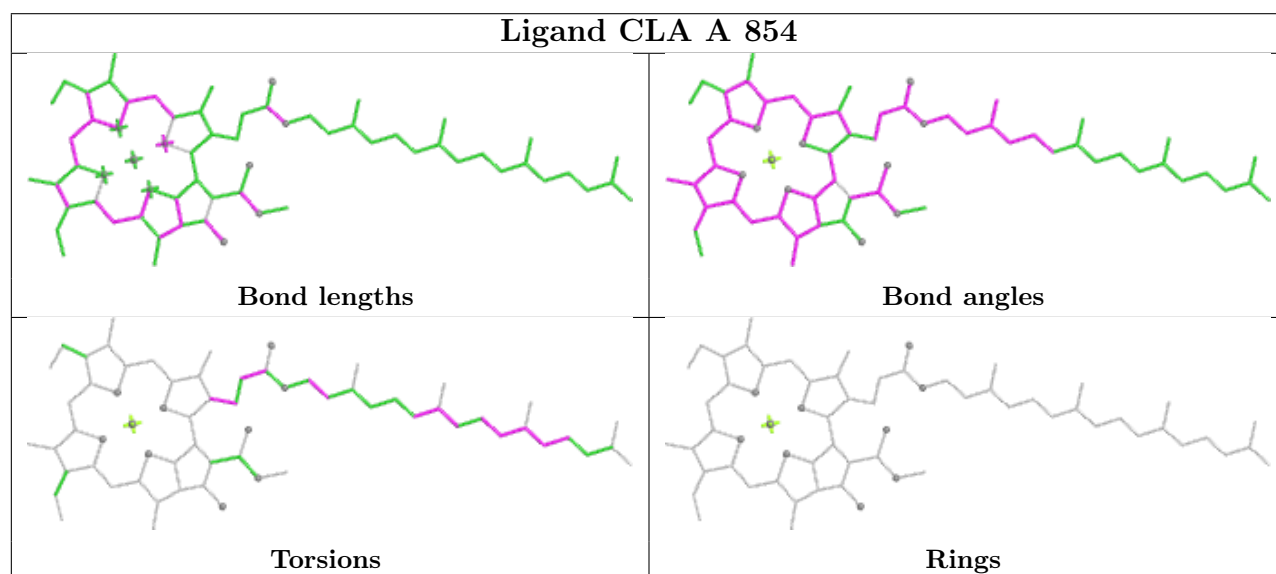
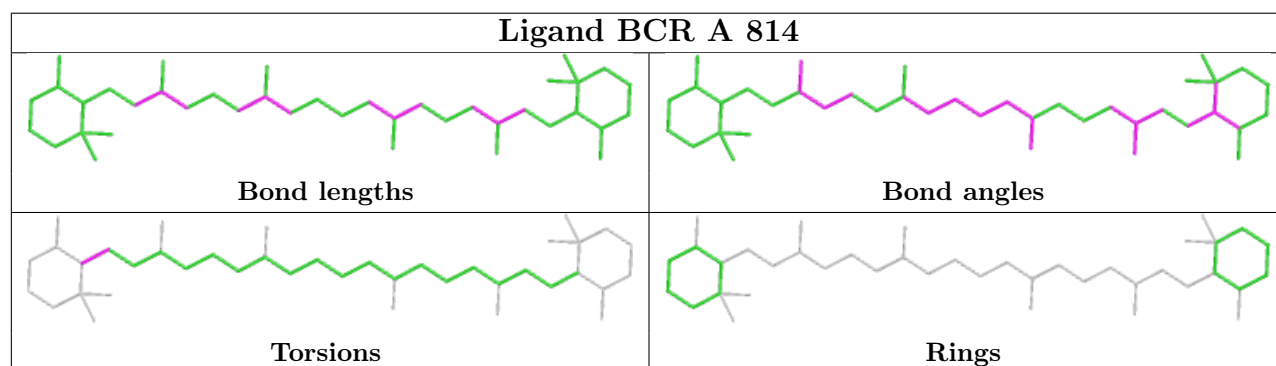
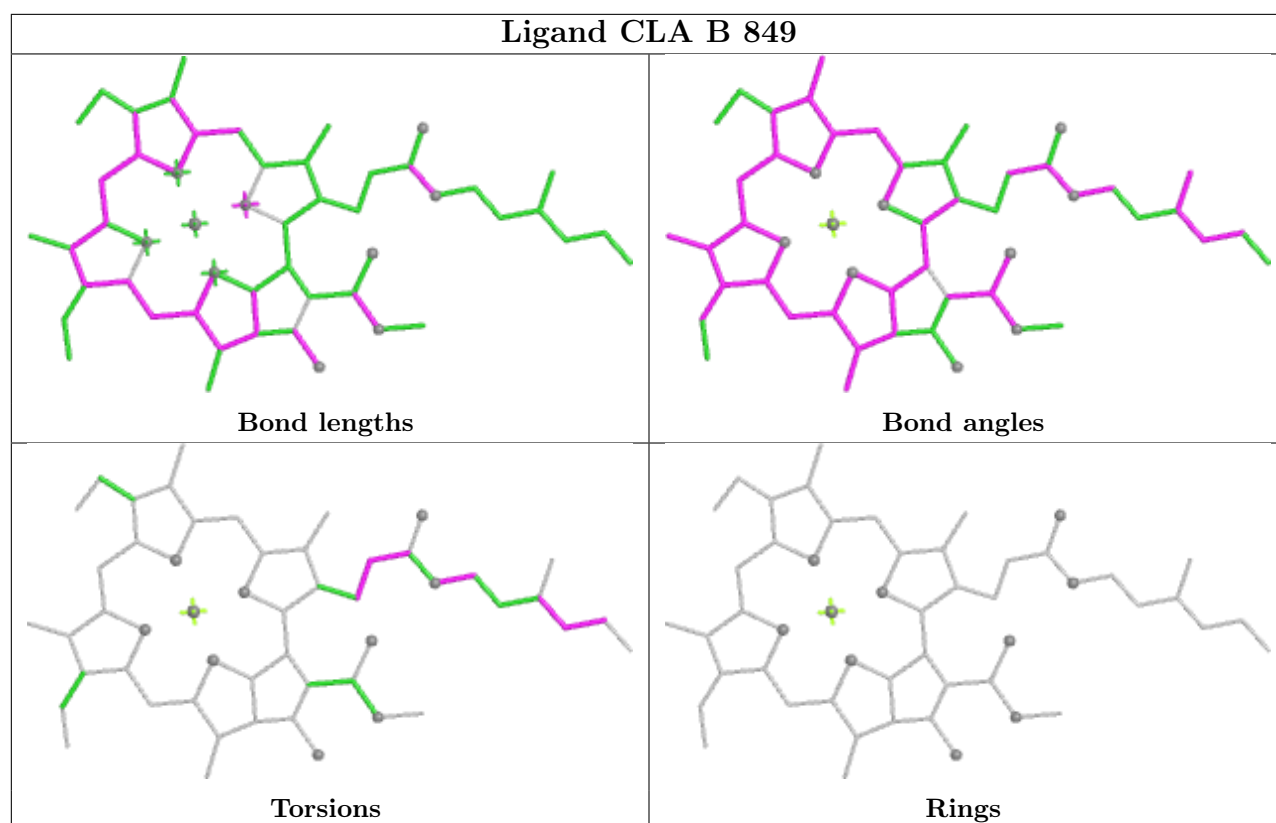


Torsions

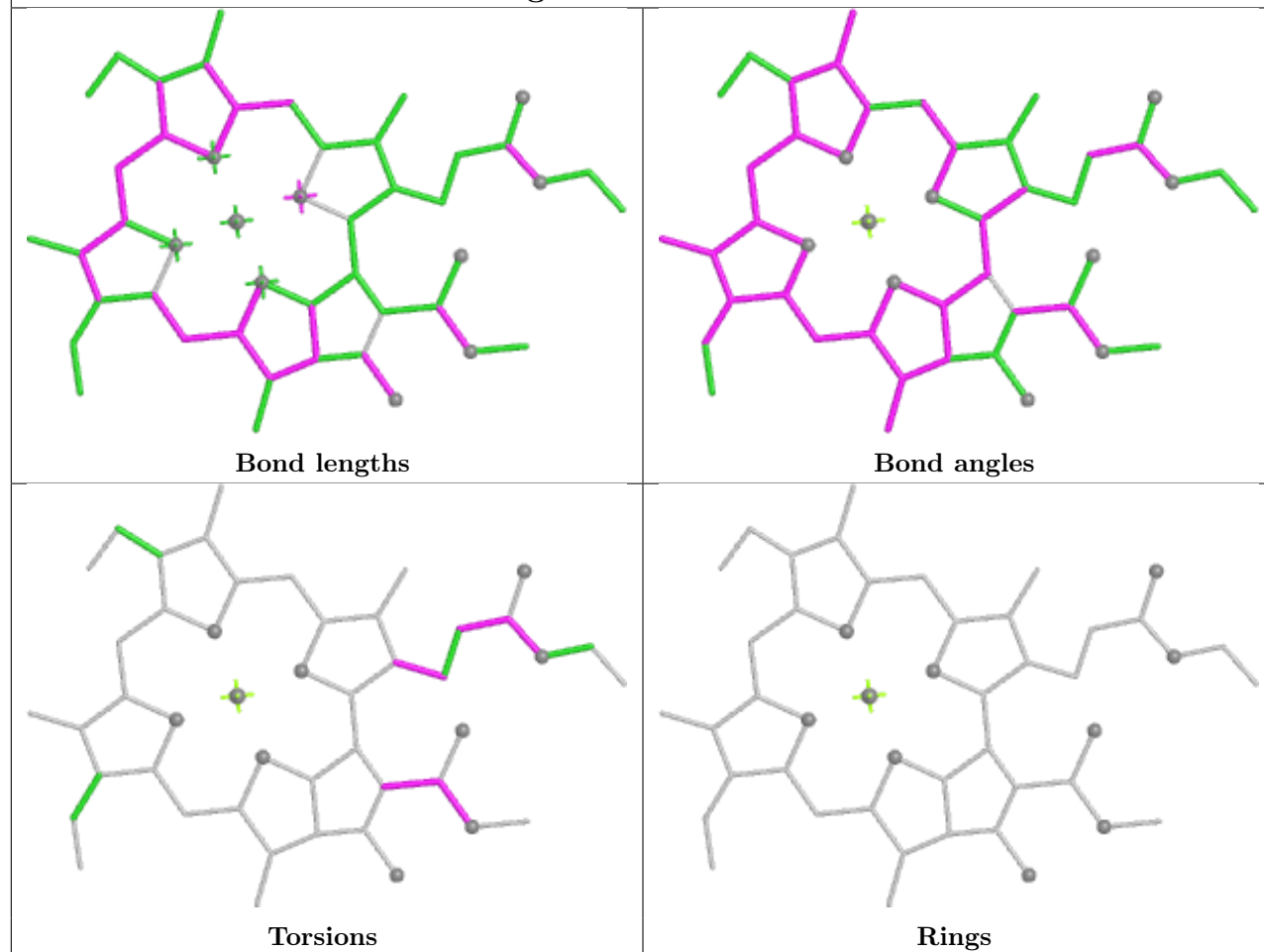


Rings

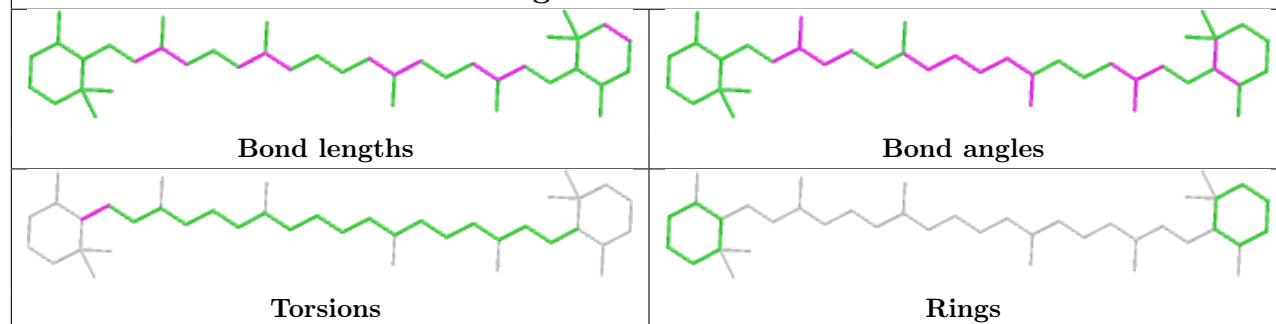


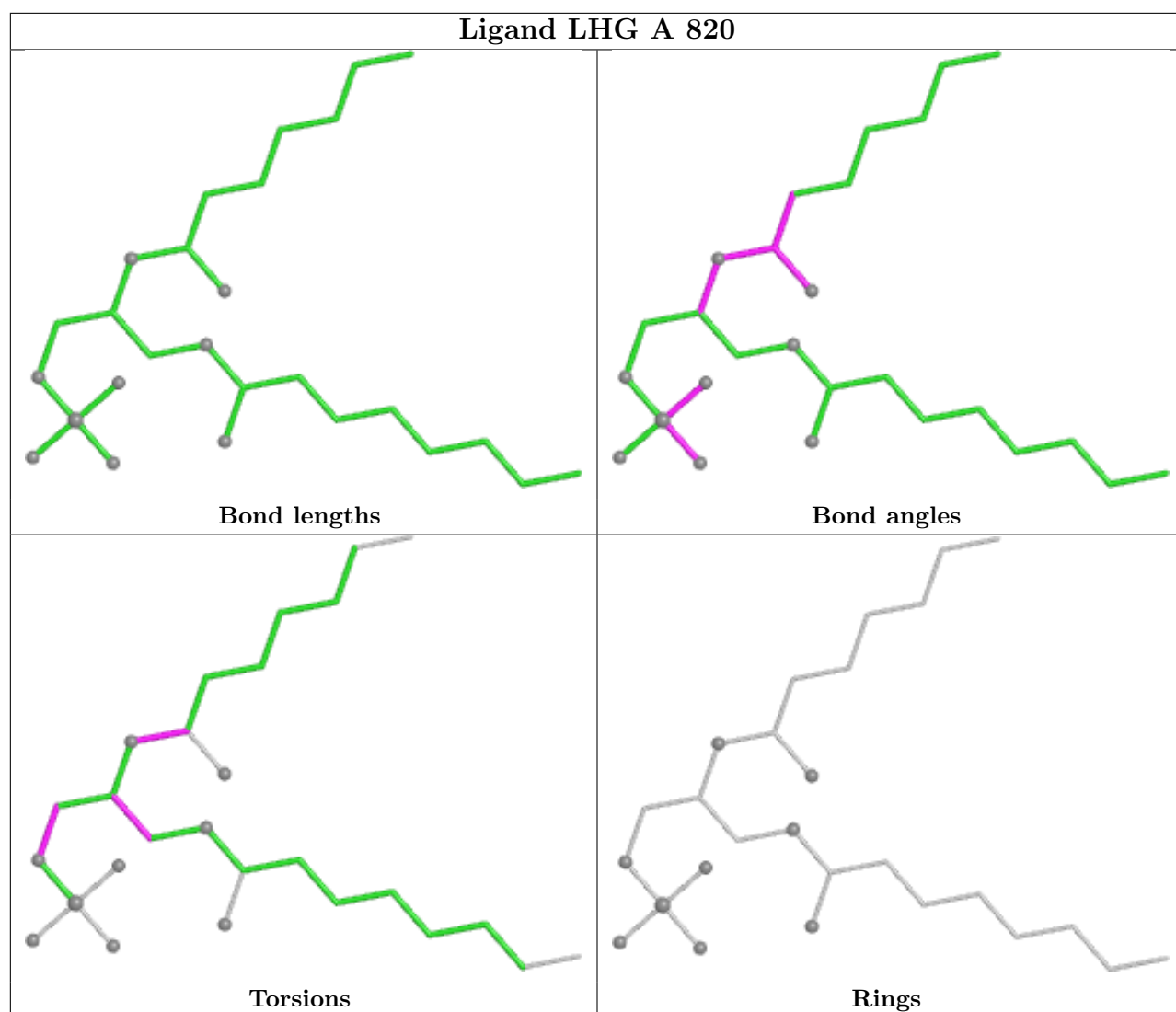


Ligand CLA B 828

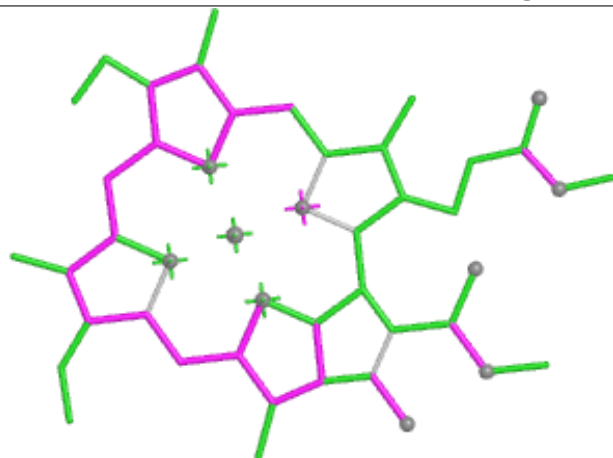


Ligand BCR L 302

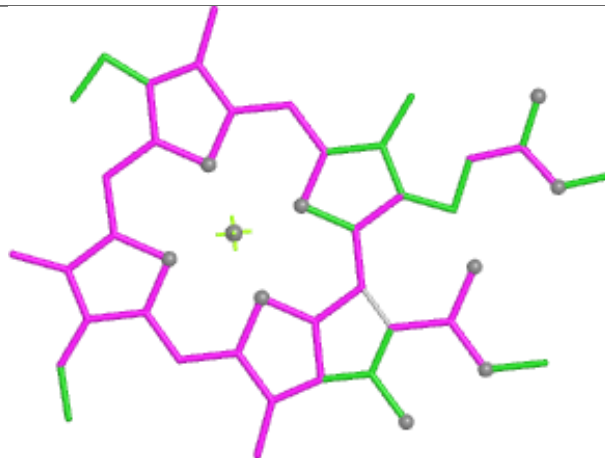




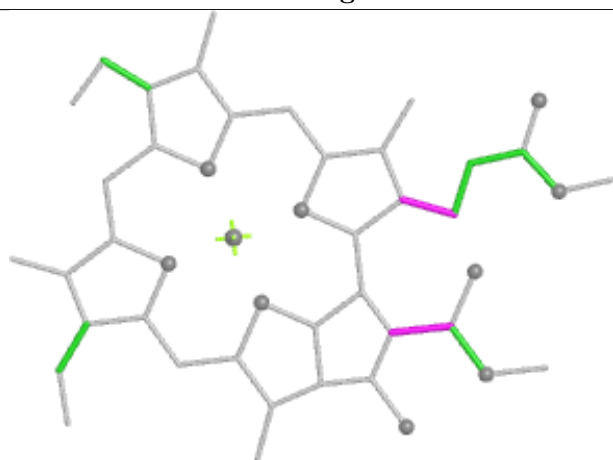
Ligand CLA 1 308



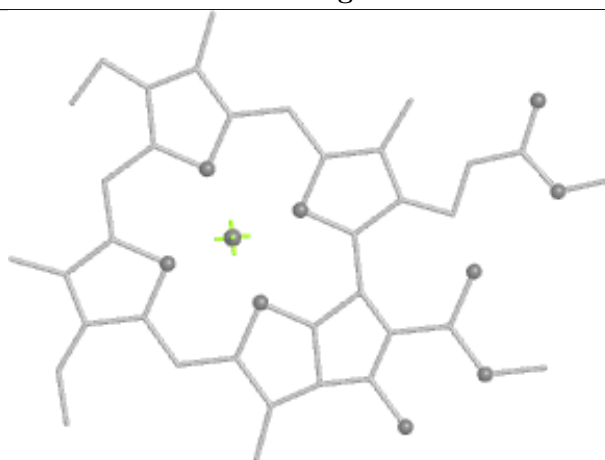
Bond lengths



Bond angles

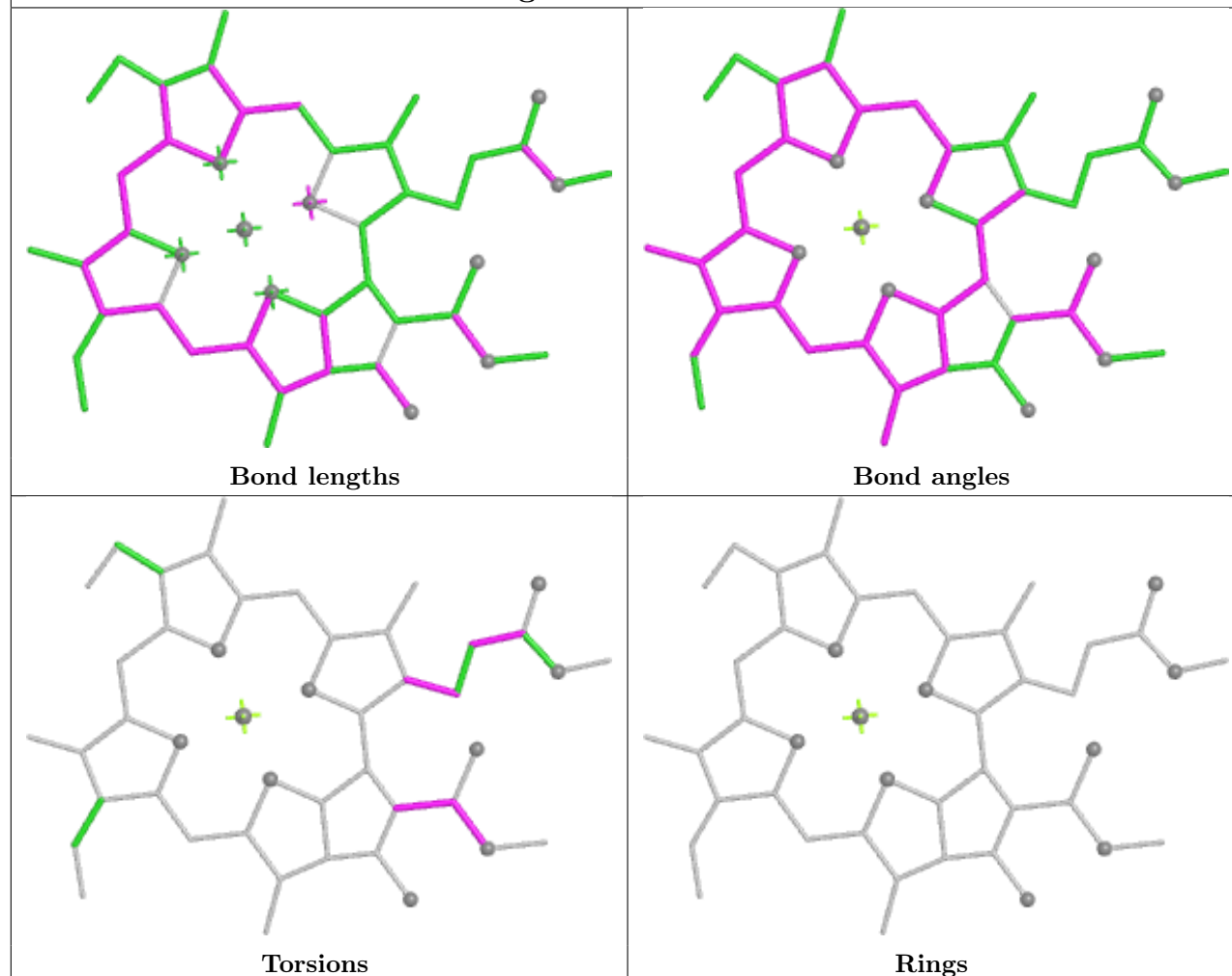


Torsions

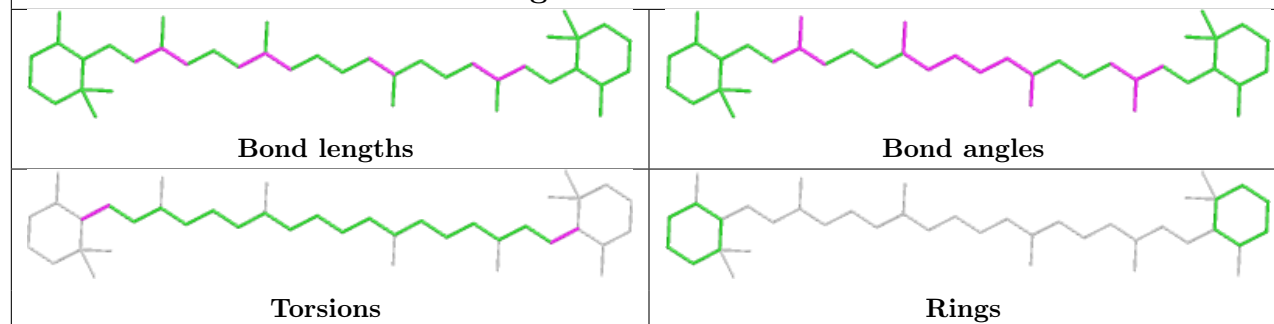


Rings

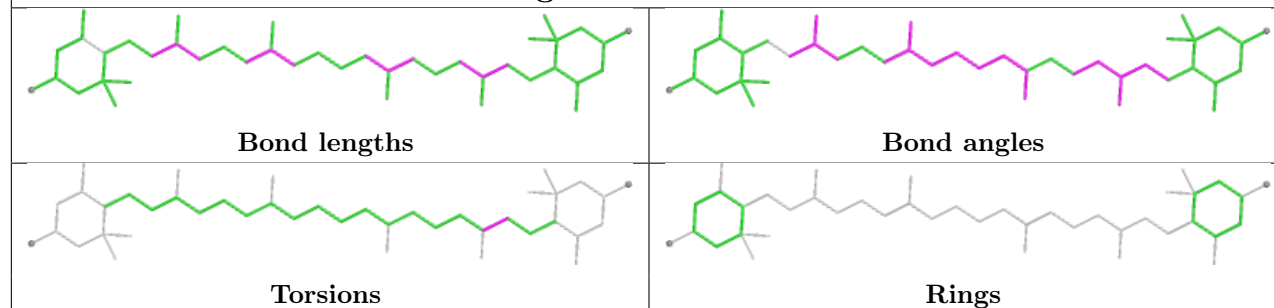
Ligand CLA 3 319

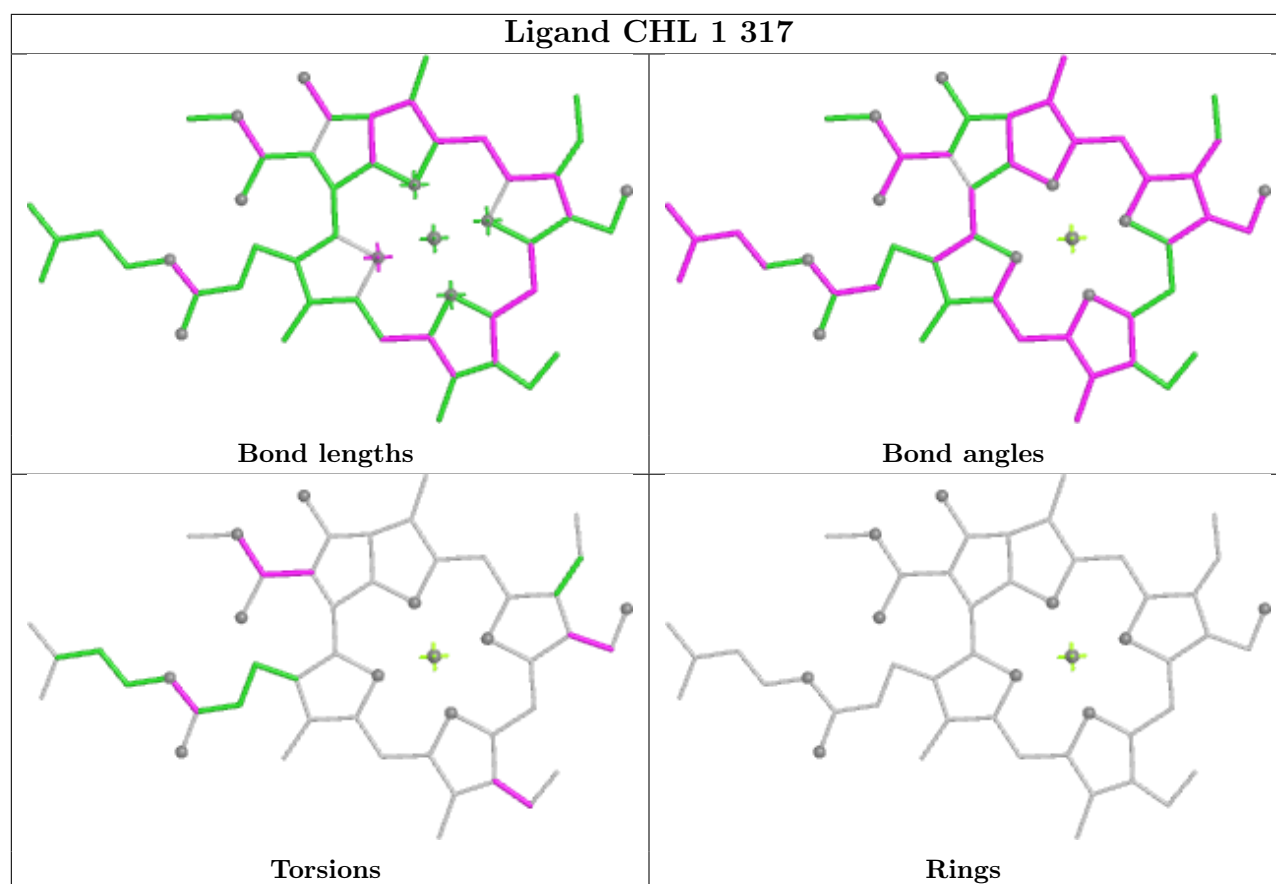


Ligand BCR A 815

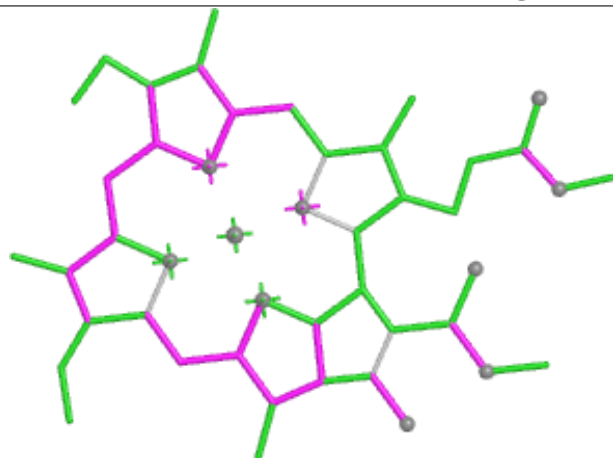


Ligand LUT 1 310

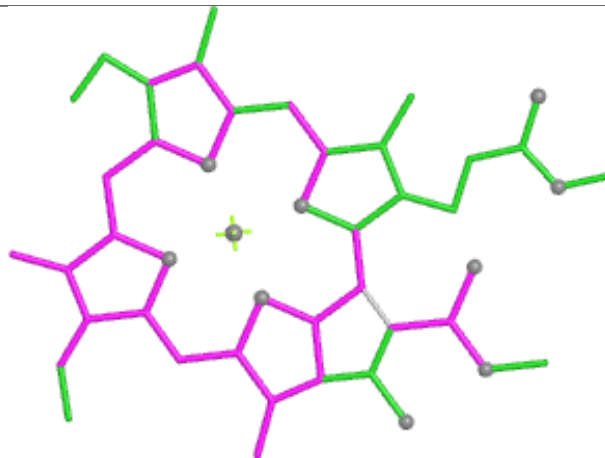




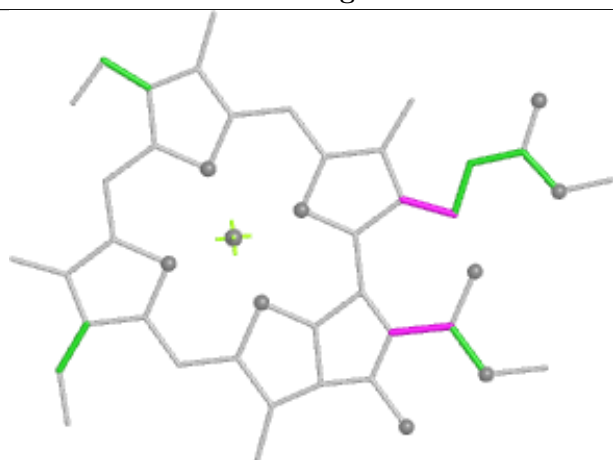
Ligand CLA K 205



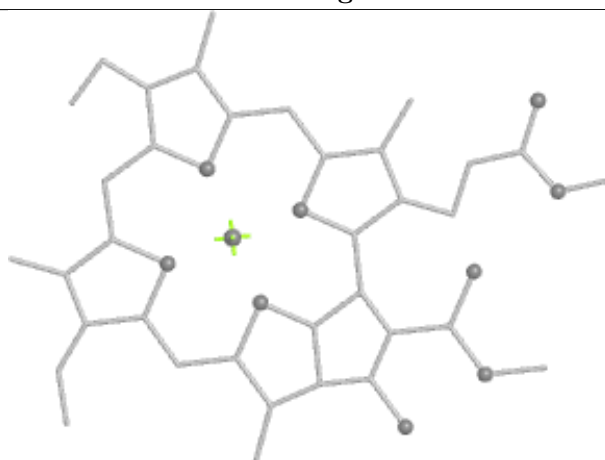
Bond lengths



Bond angles

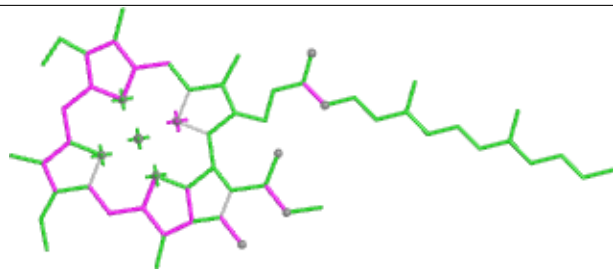


Torsions

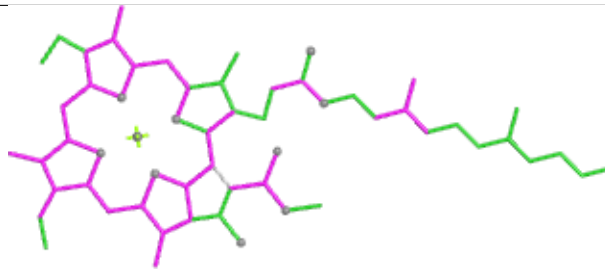


Rings

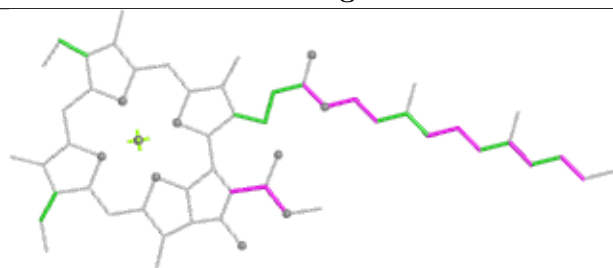
Ligand CLA A 850



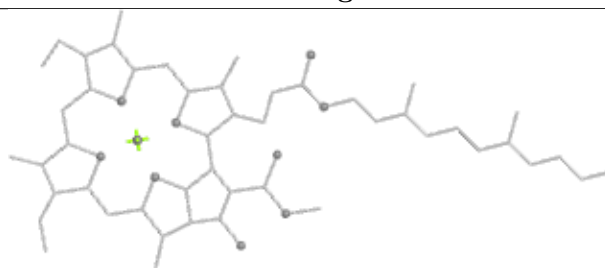
Bond lengths



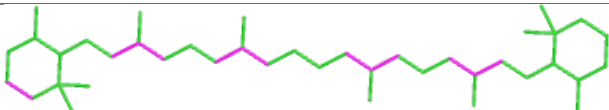
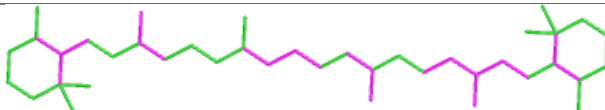
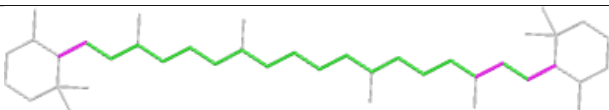
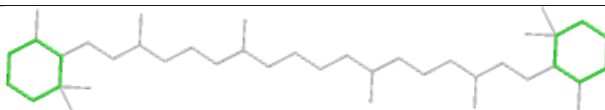
Bond angles

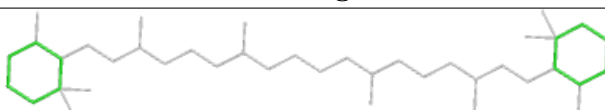


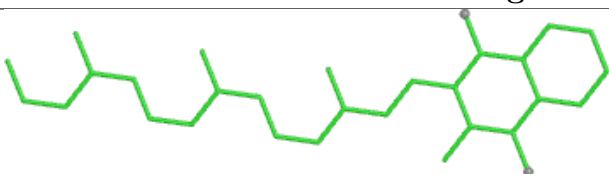
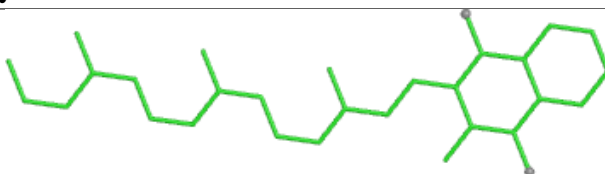
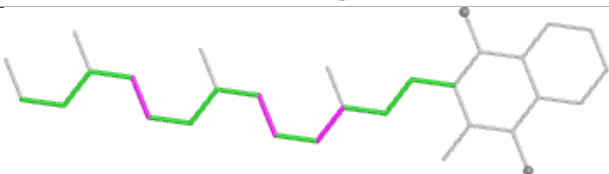
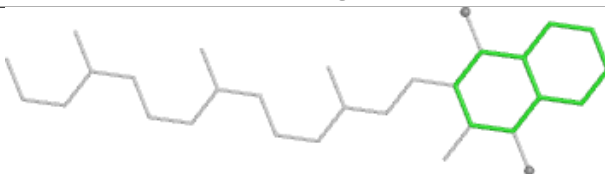
Torsions



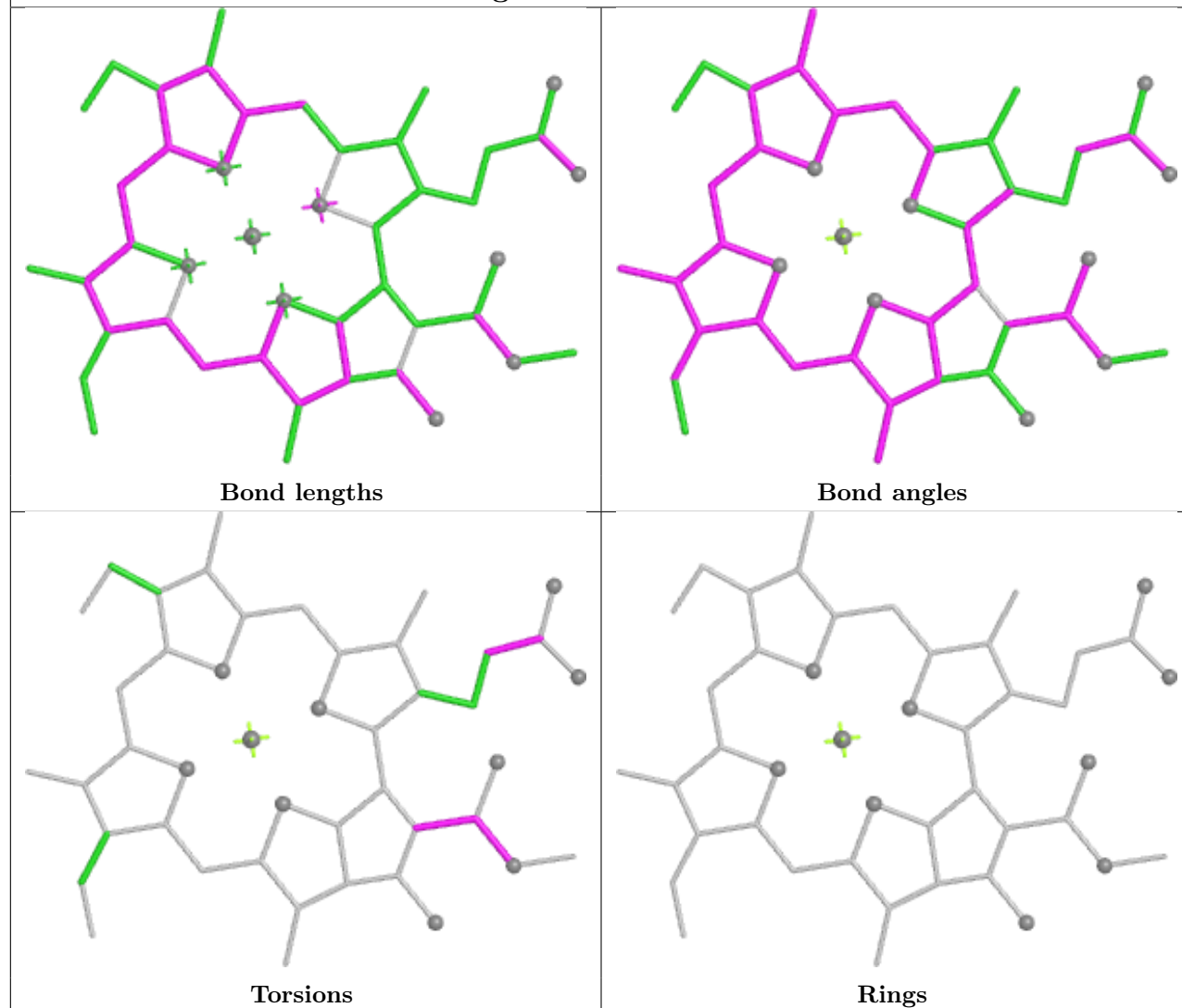
Rings

Ligand BCR 3 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

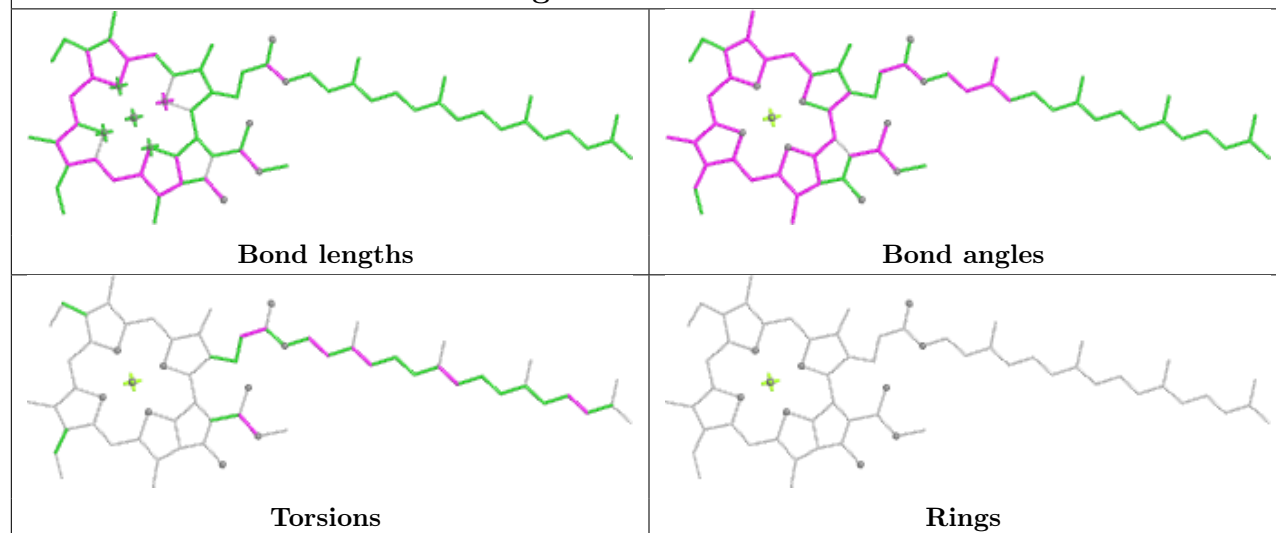
Ligand BCR K 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

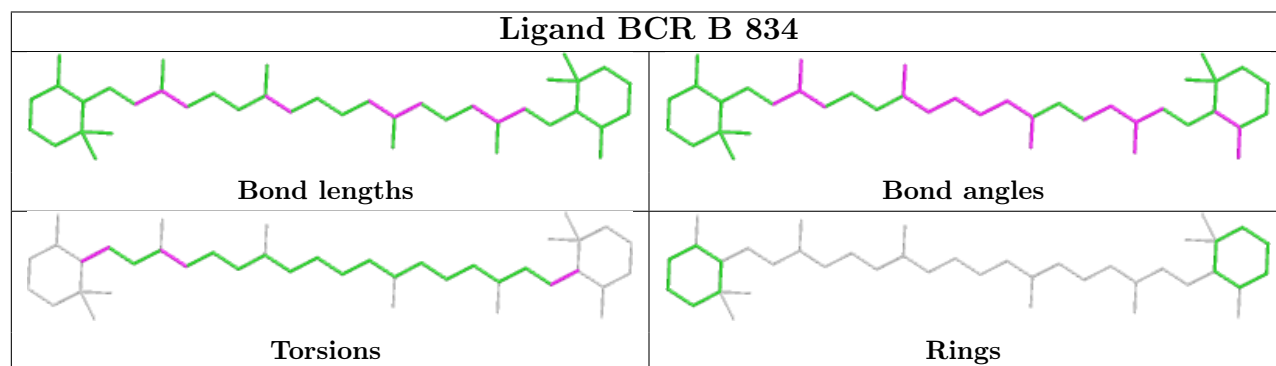
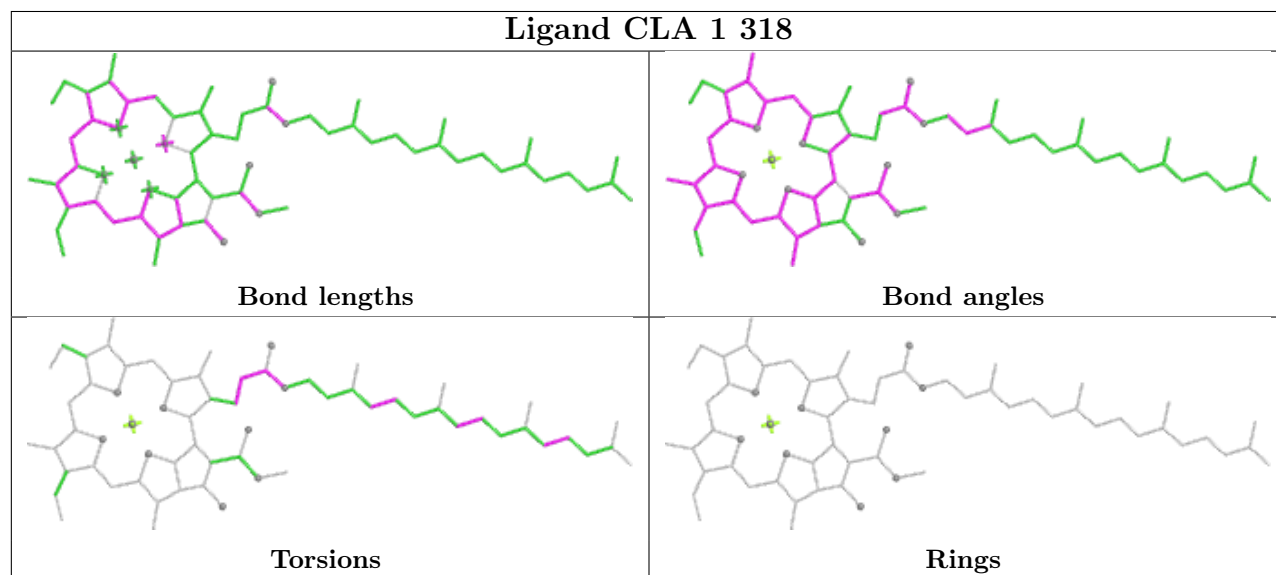
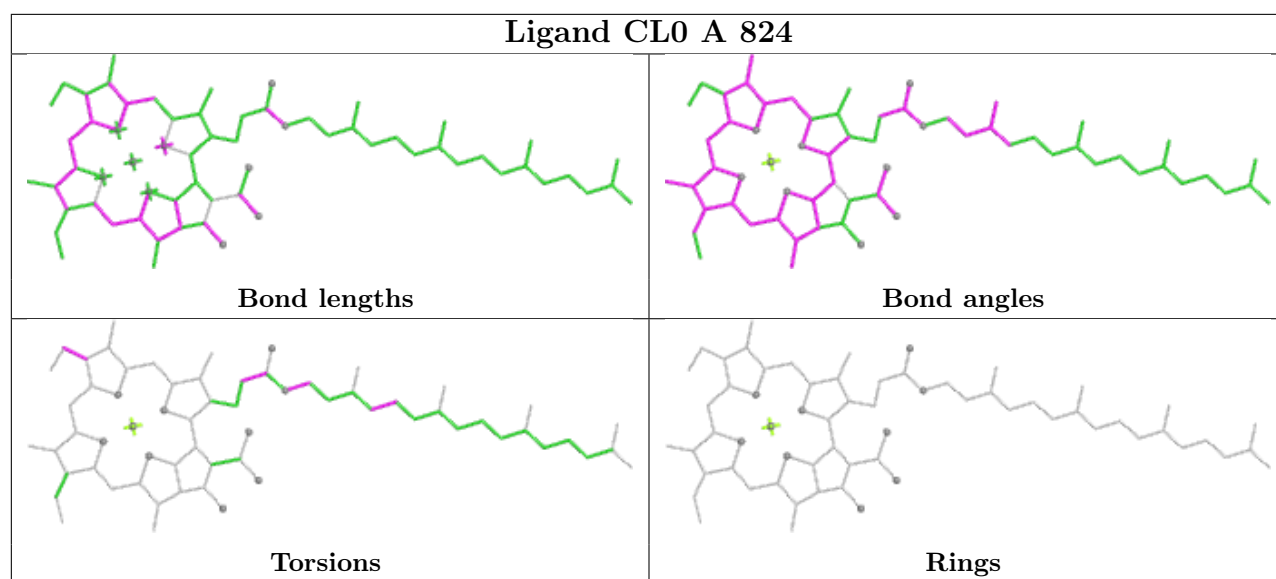
Ligand PQN B 832	
	
Bond lengths	Bond angles
	
Torsions	Rings

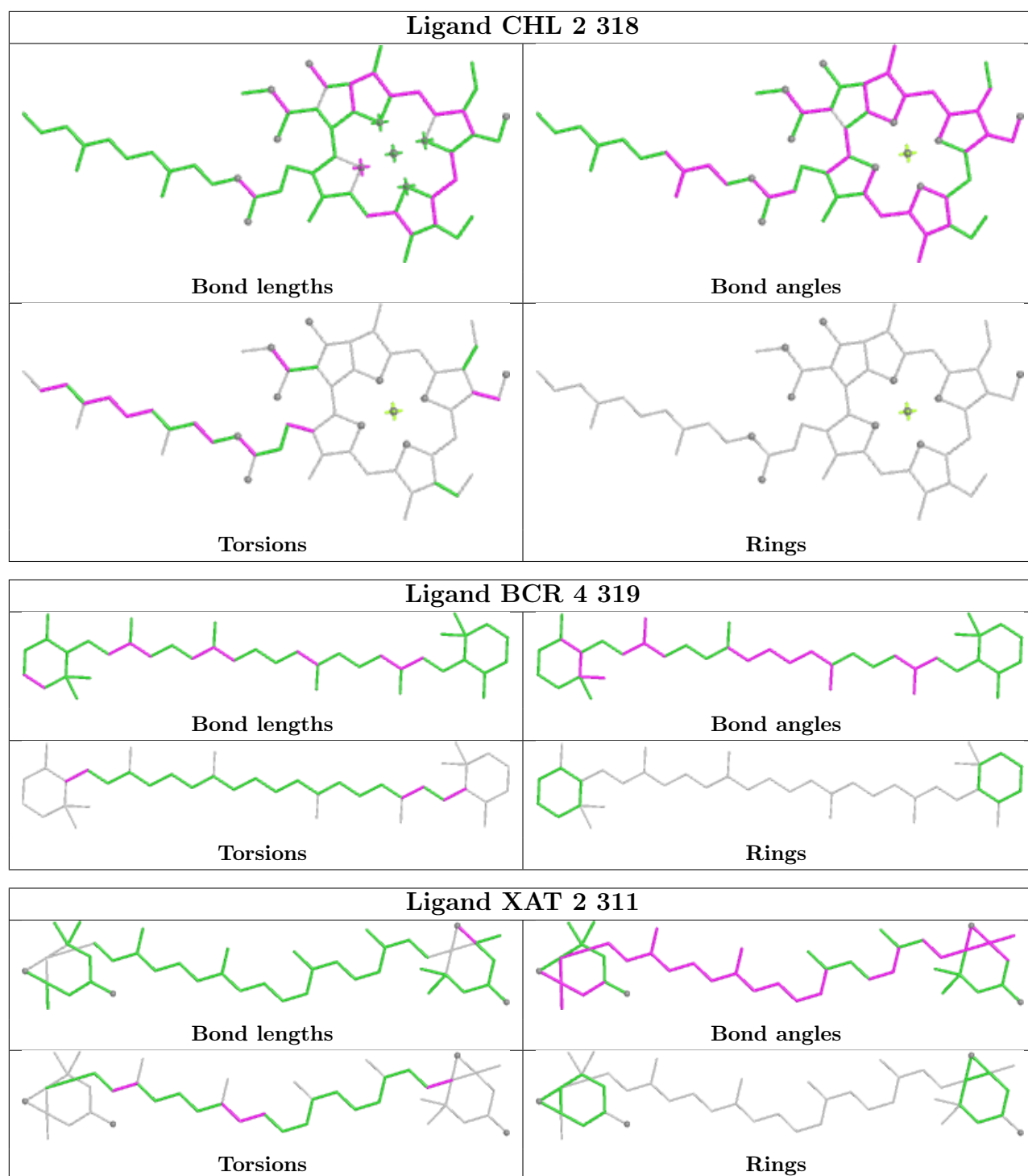
Ligand CLA O 208



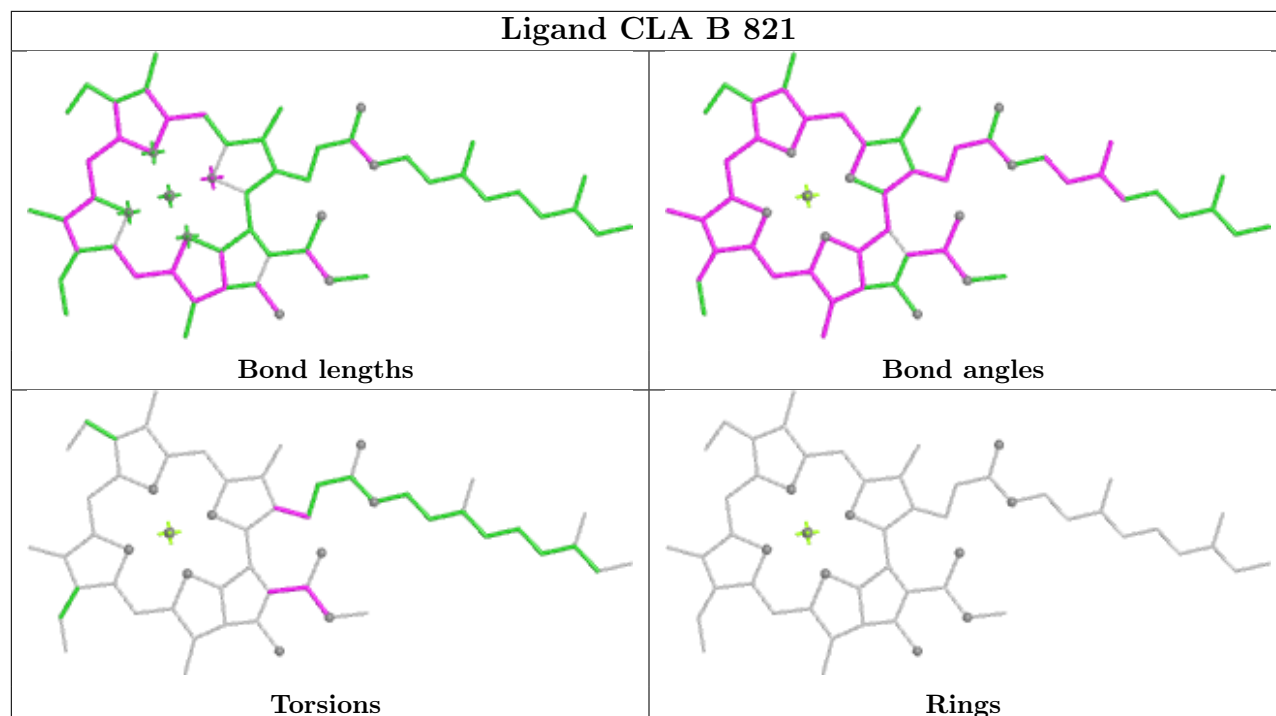
Ligand CLA B 822



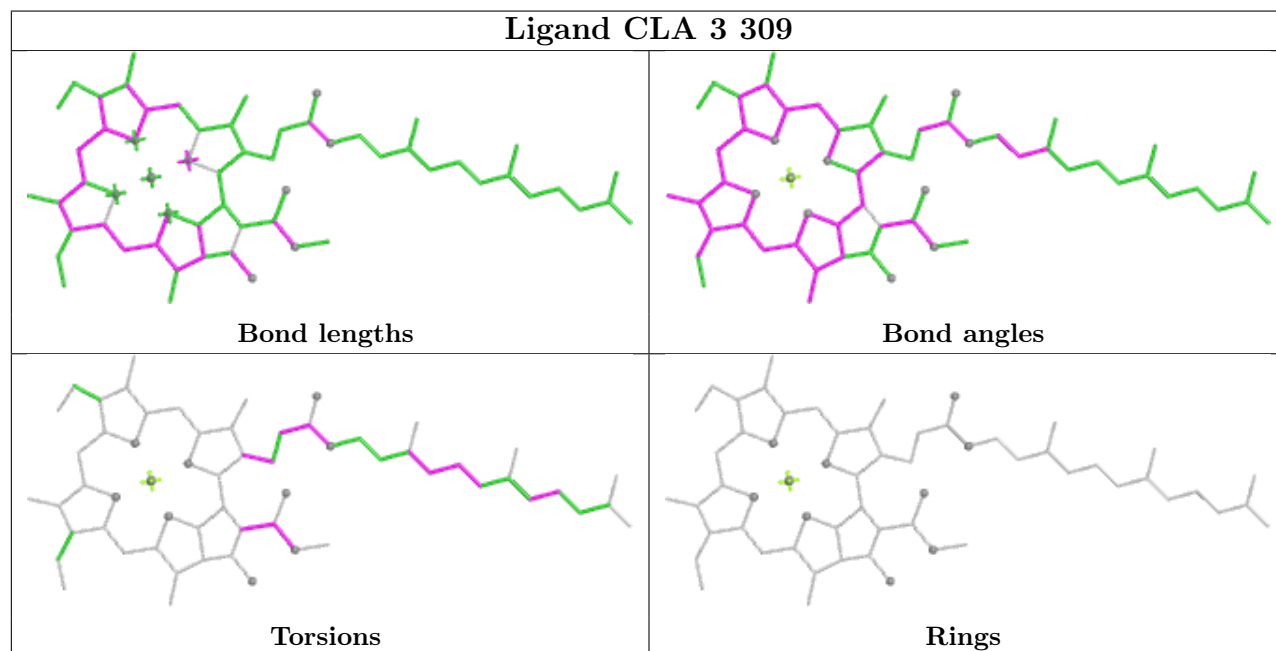




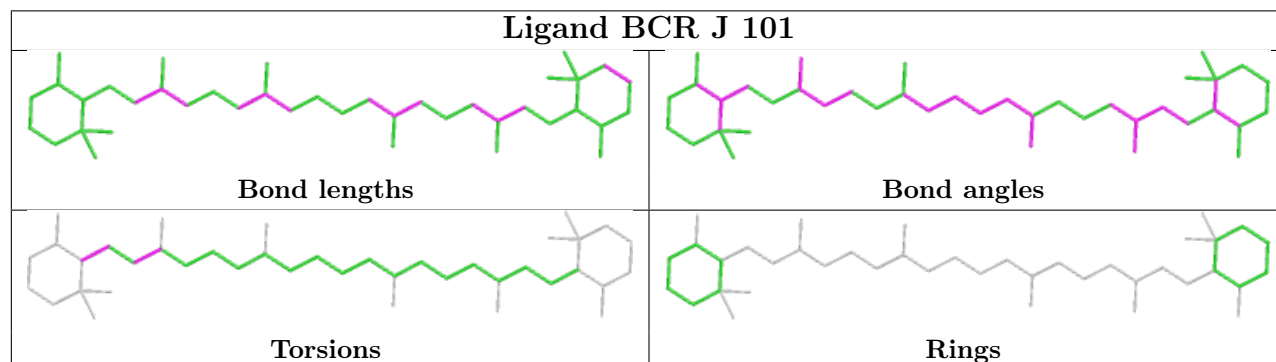
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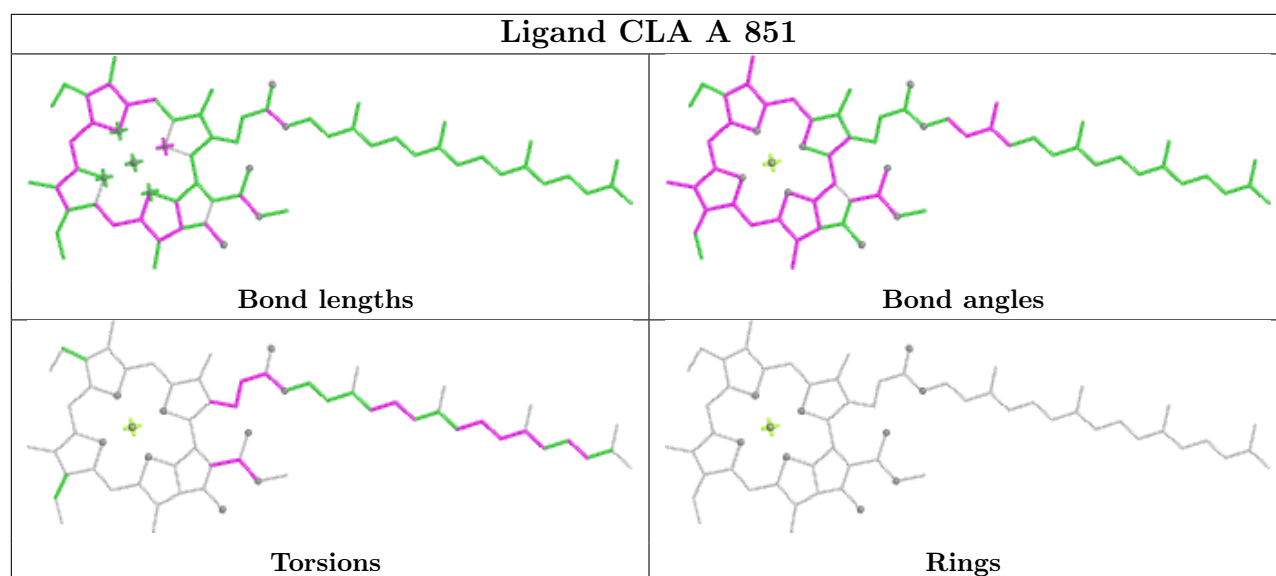
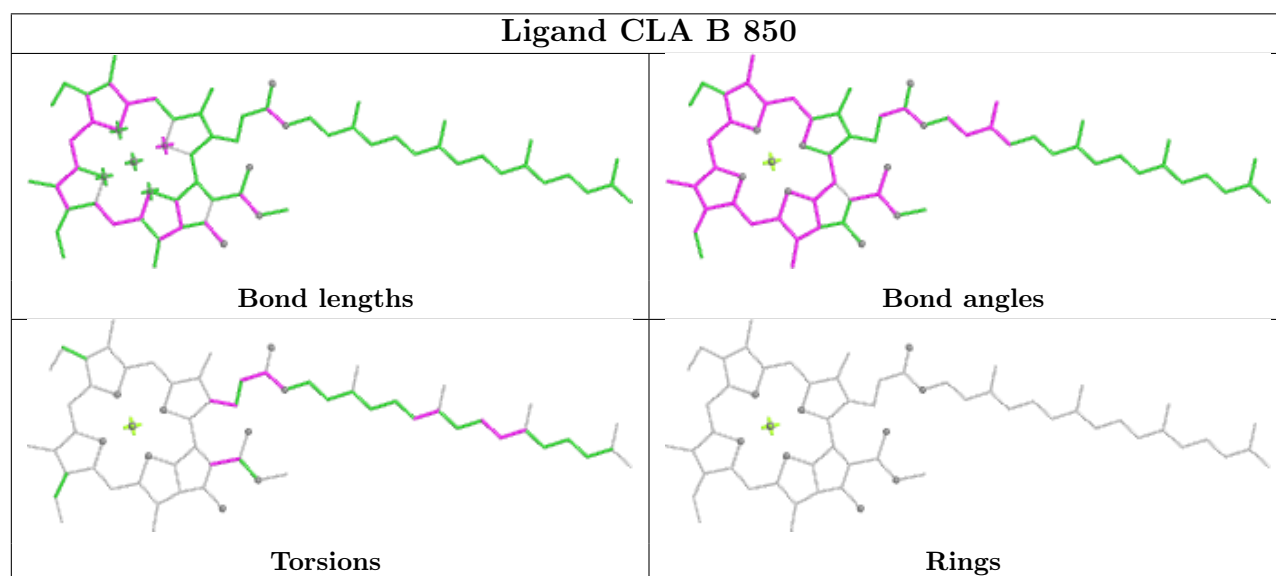
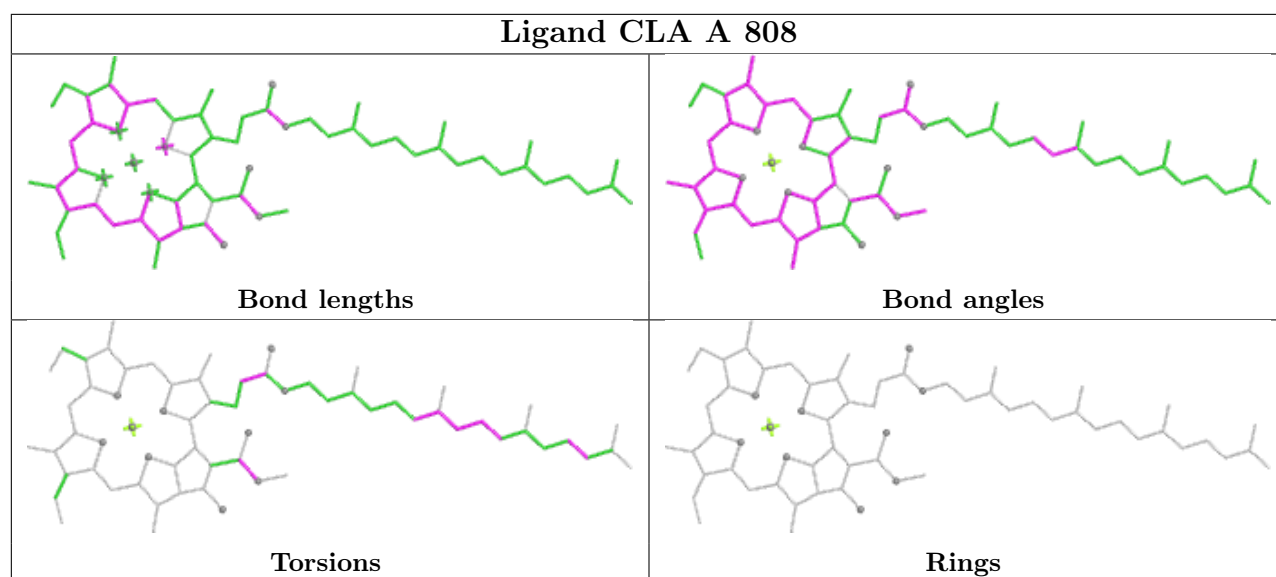


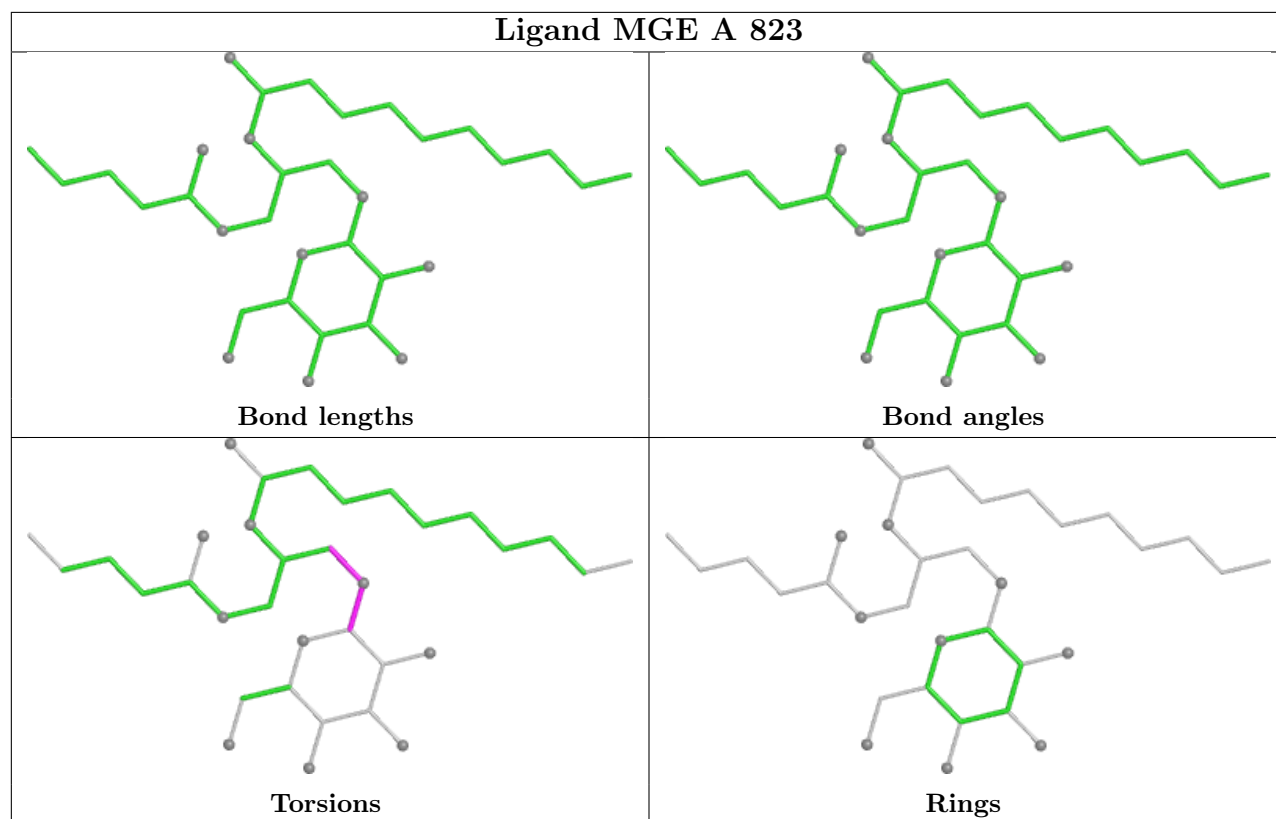
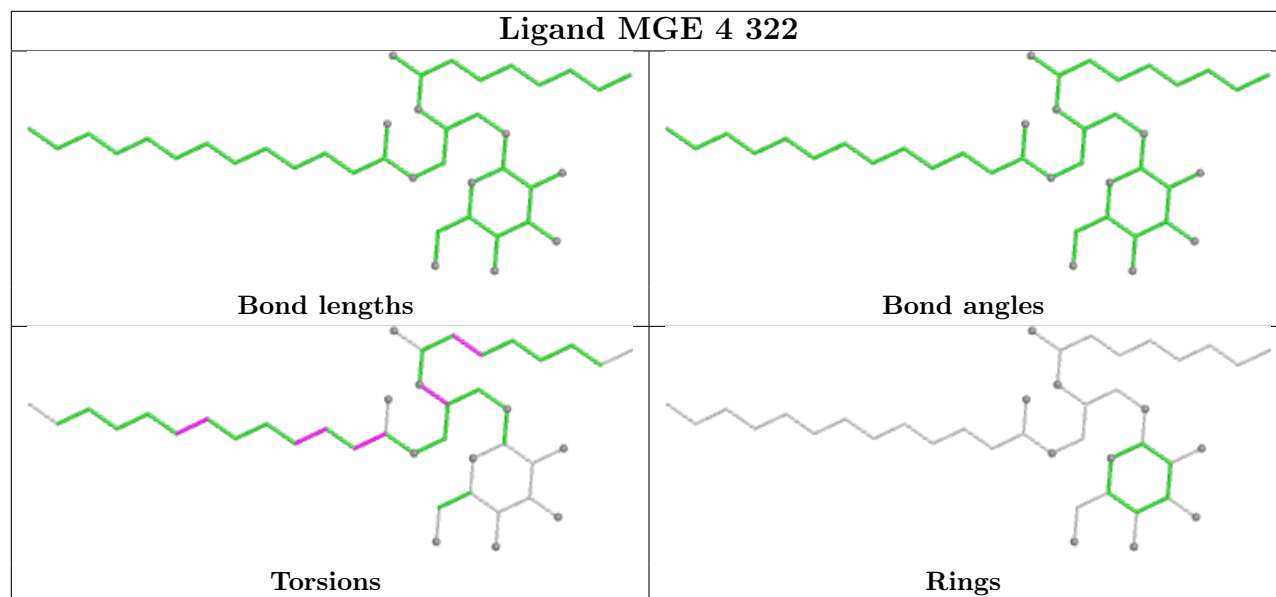
Ligand CLA 3 309



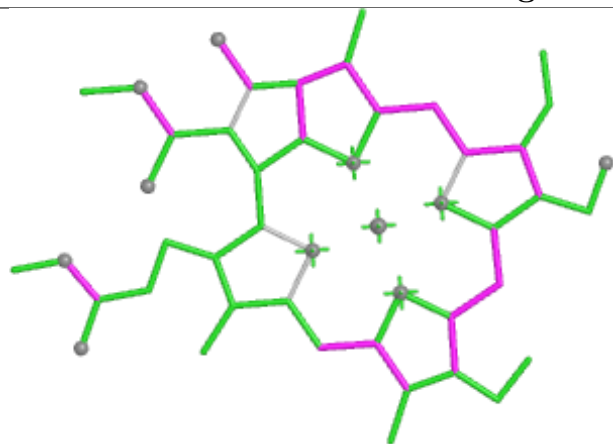
Ligand BCR J 101



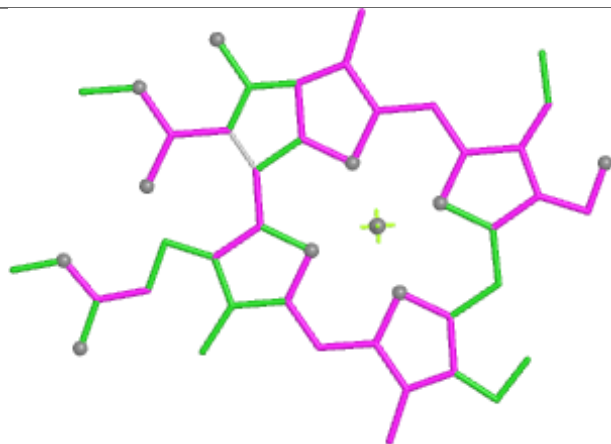




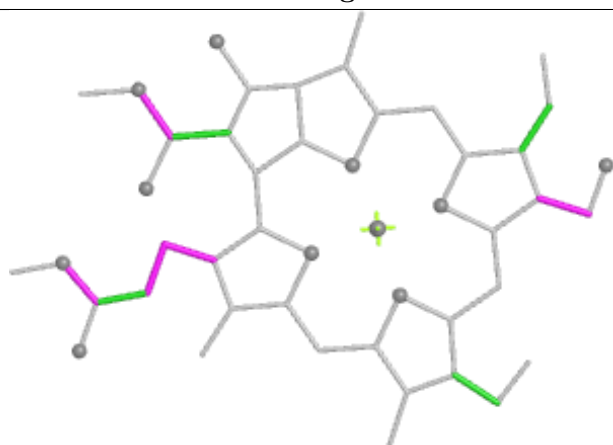
Ligand CHL 2 301



Bond lengths



Bond angles

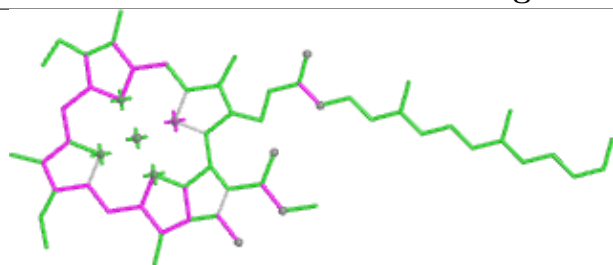


Torsions

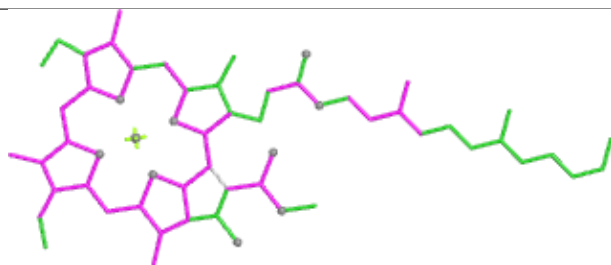


Rings

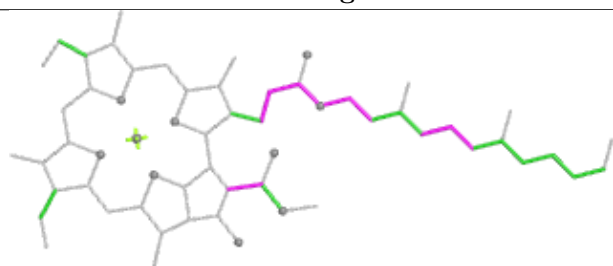
Ligand CLA H 201



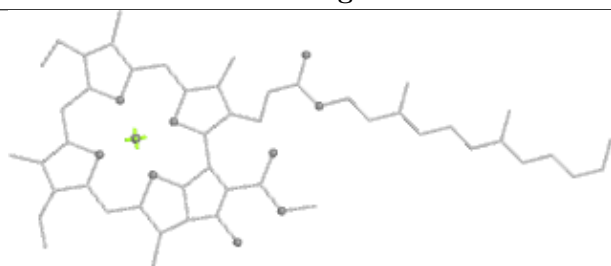
Bond lengths



Bond angles

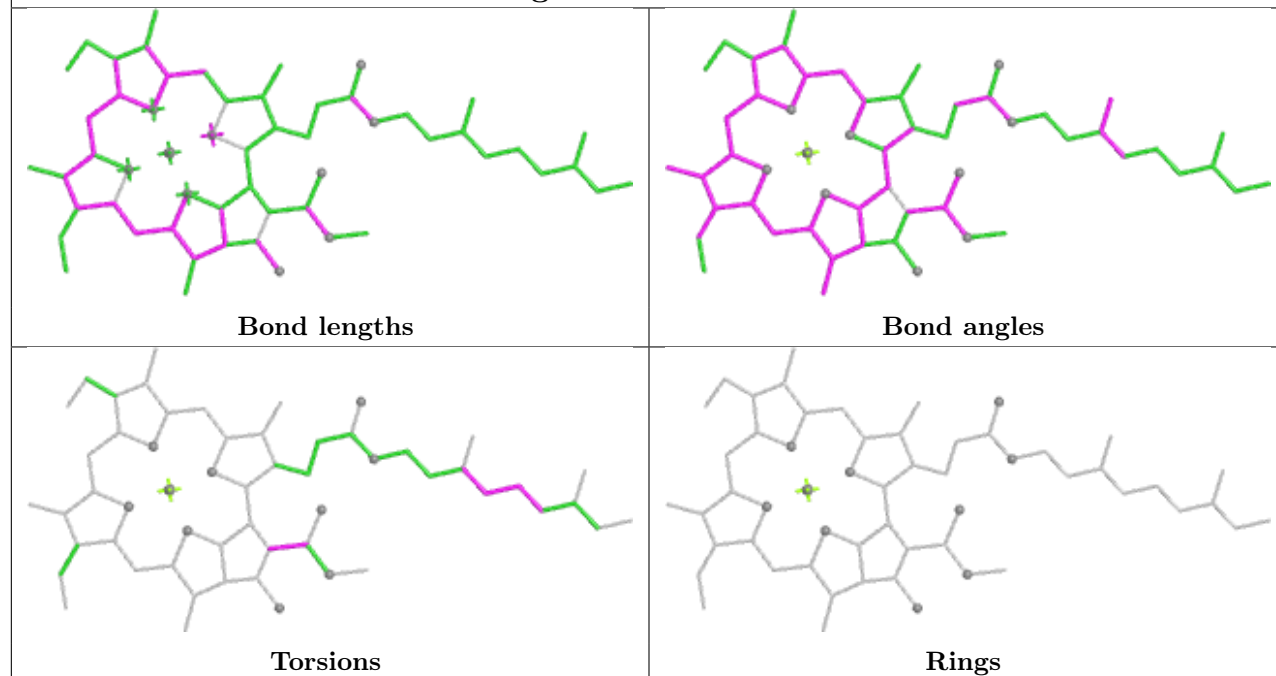


Torsions

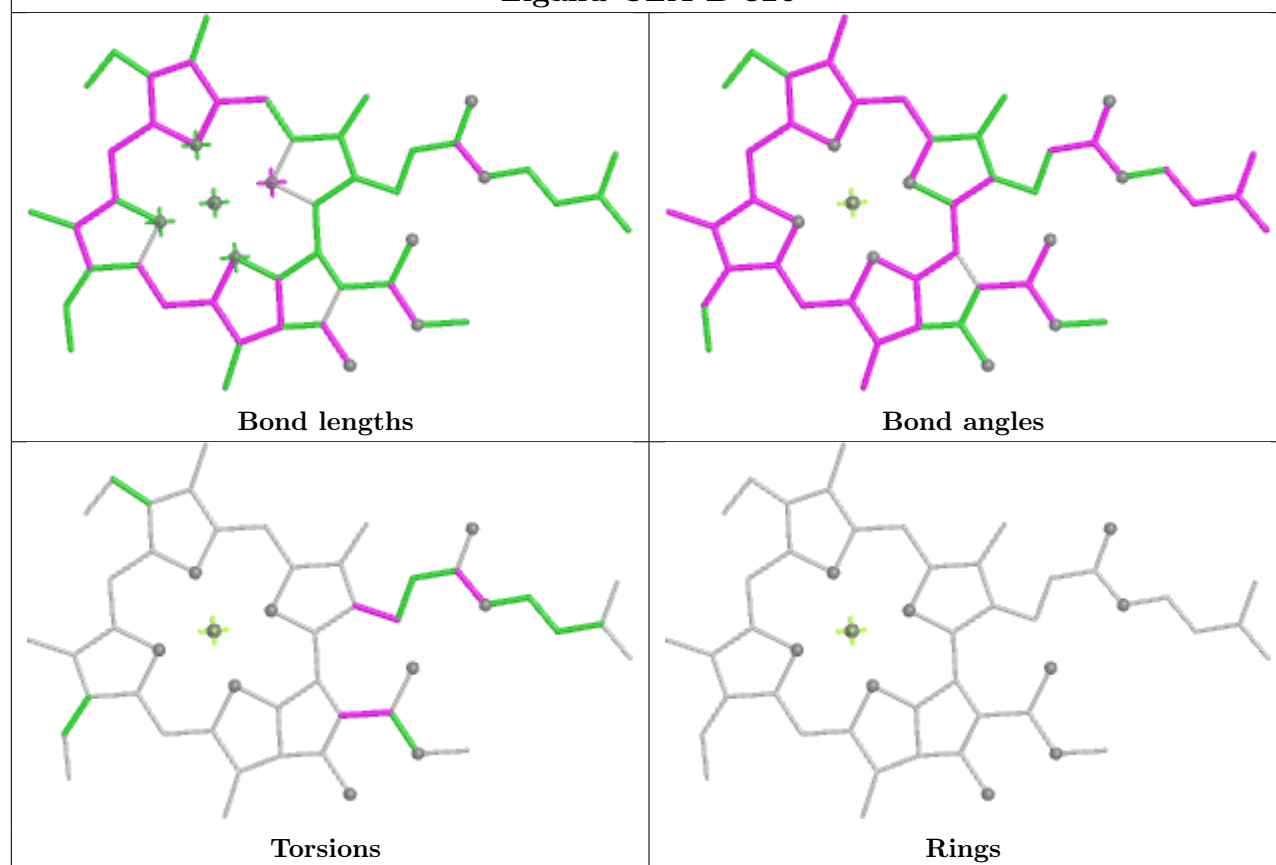


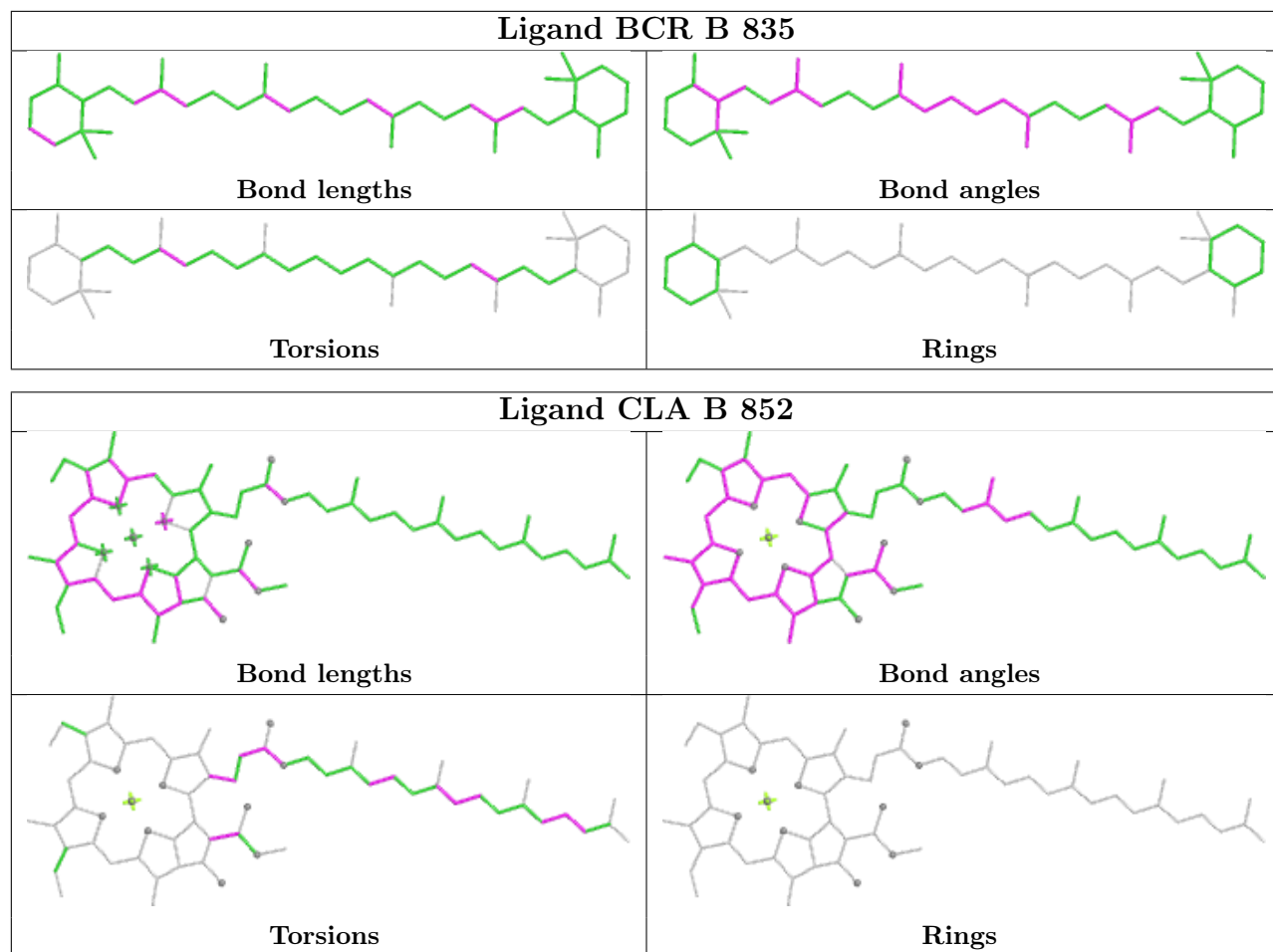
Rings

Ligand CLA N 202

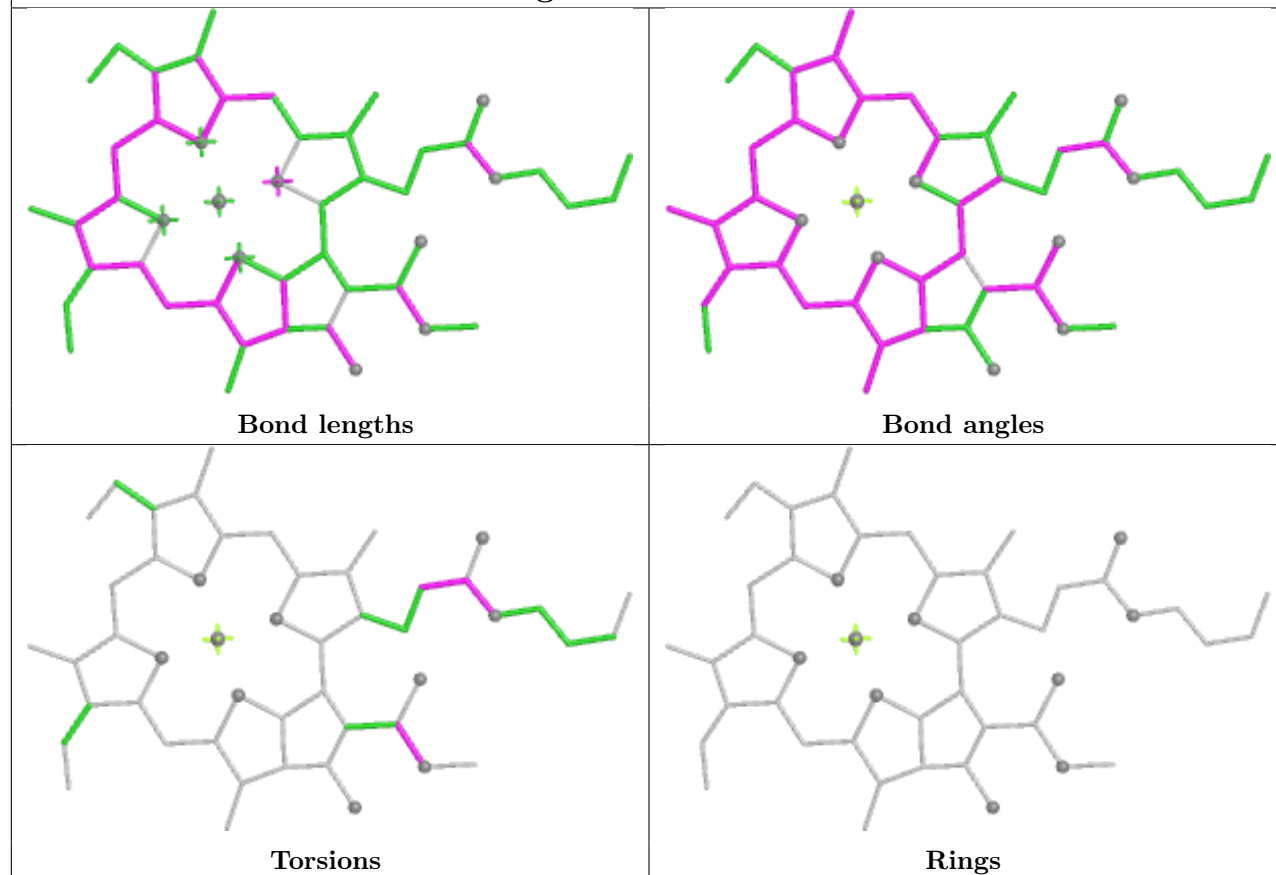


Ligand CLA B 826

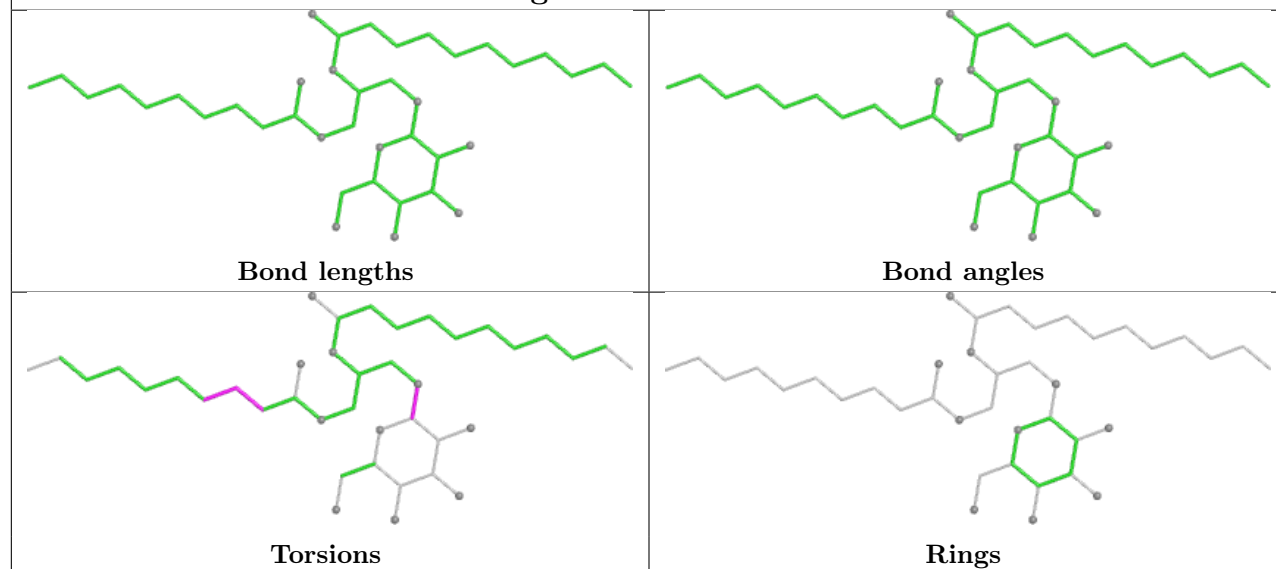




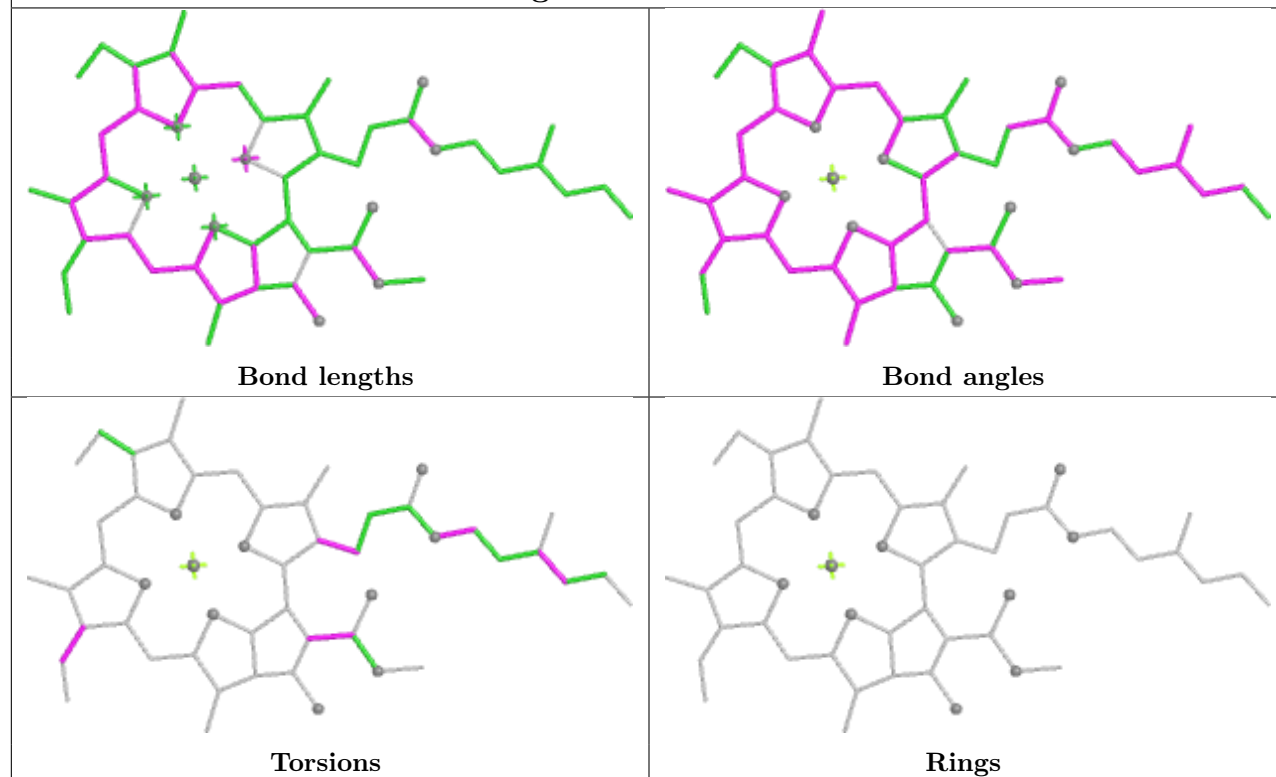
Ligand CLA 3 310



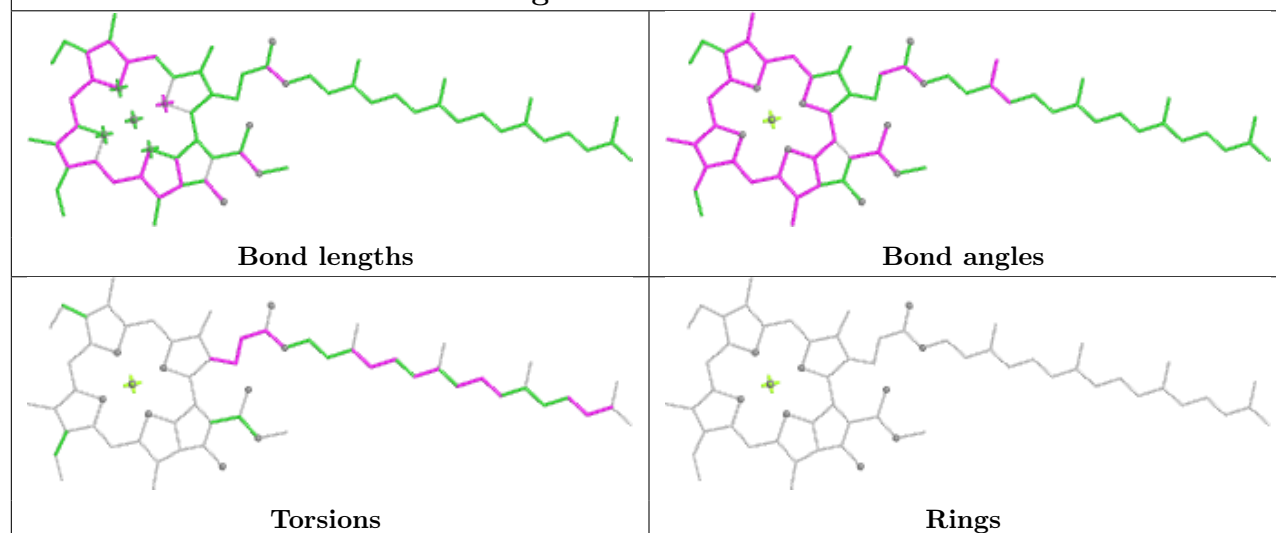
Ligand MGE 1 316

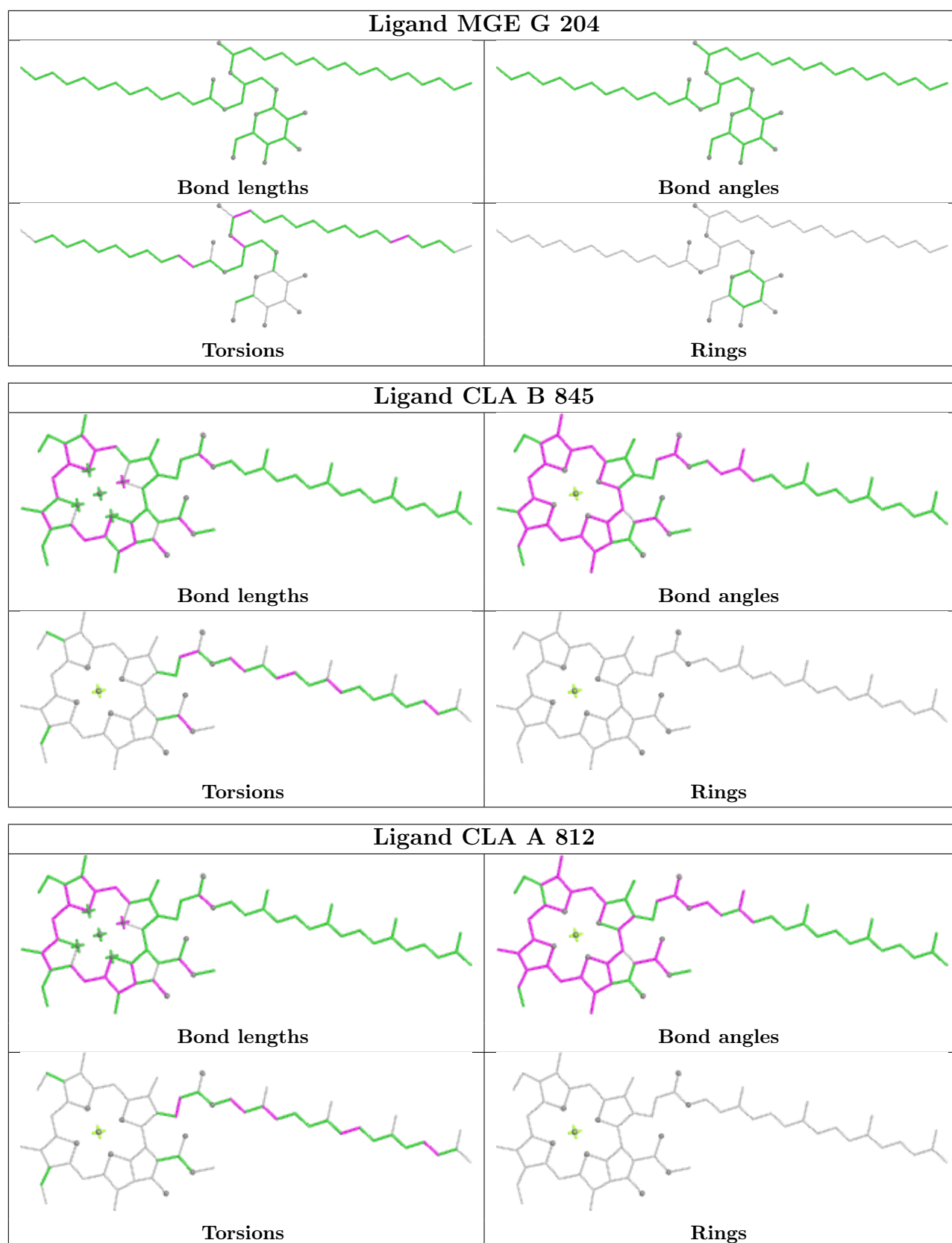


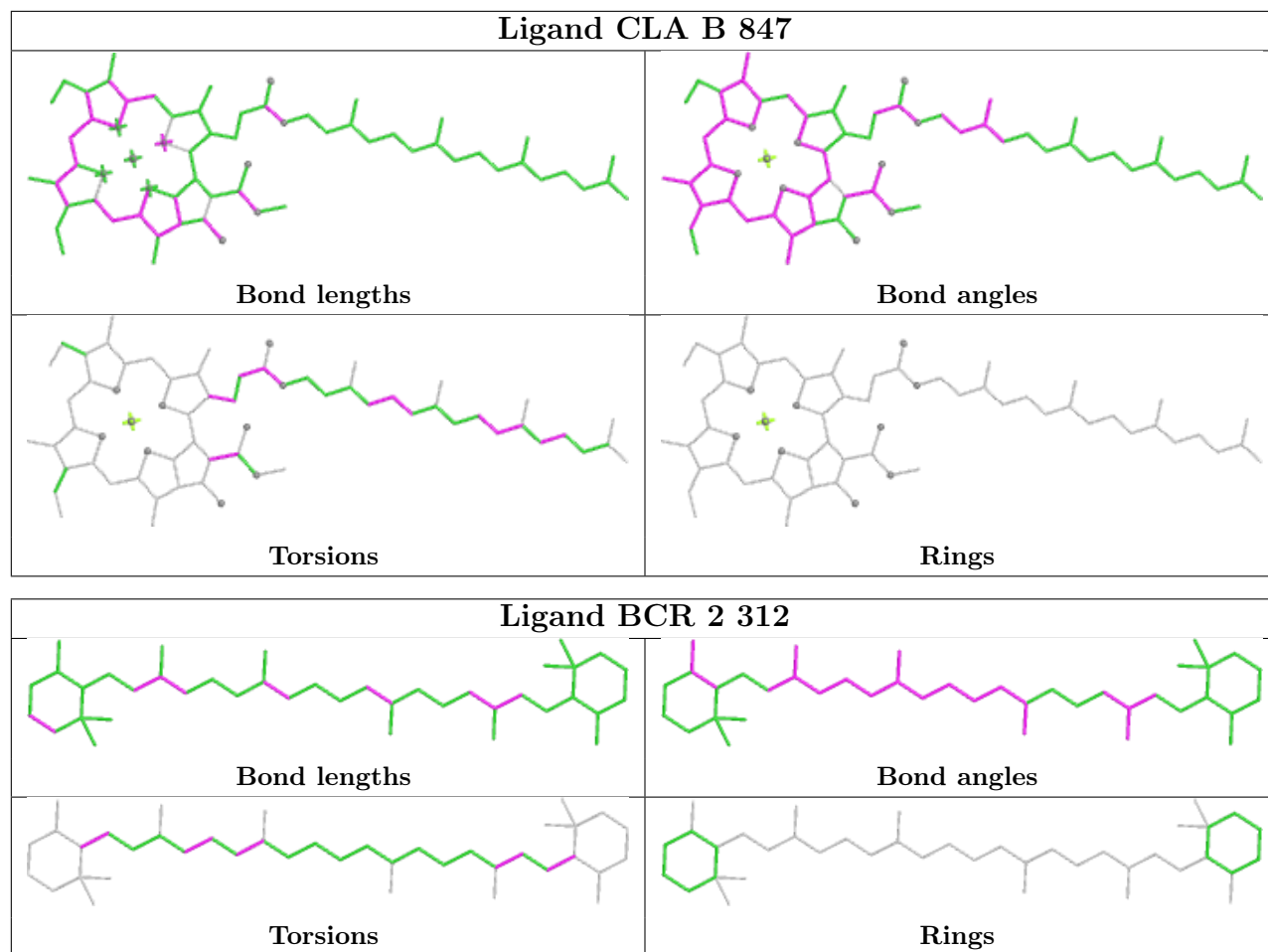
Ligand CLA A 831

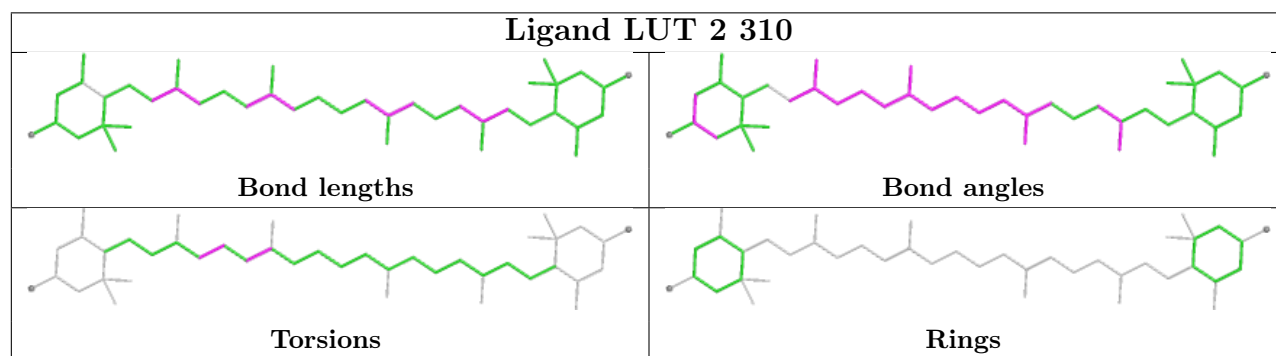
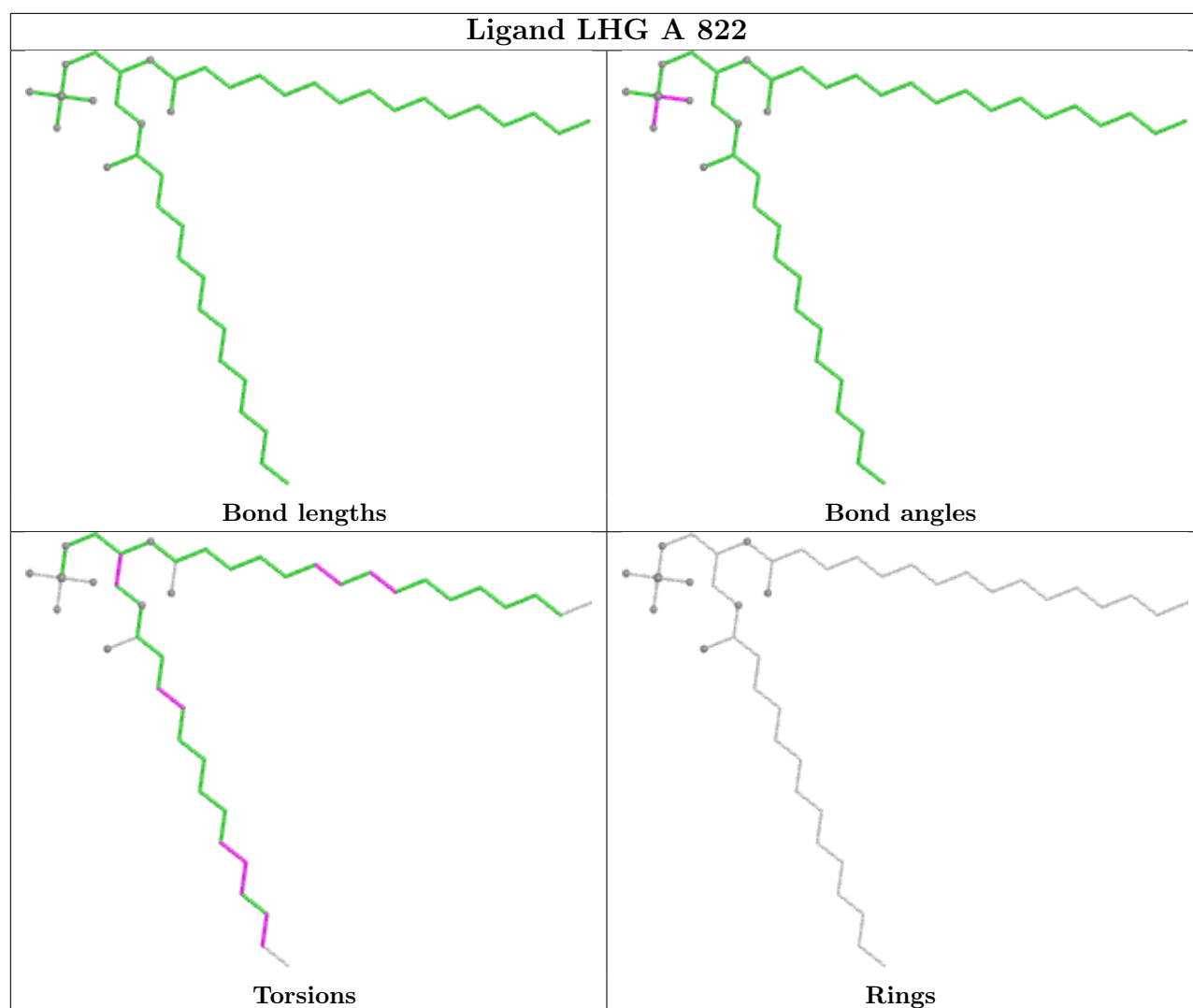


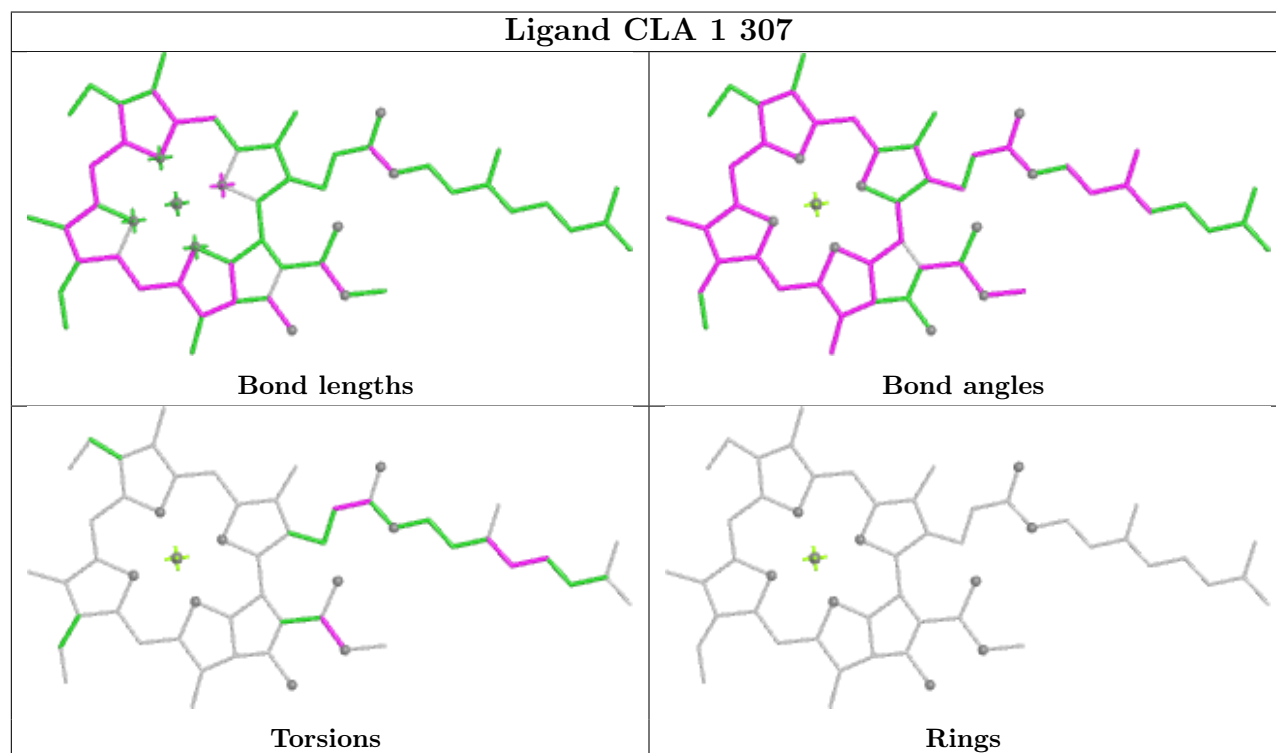
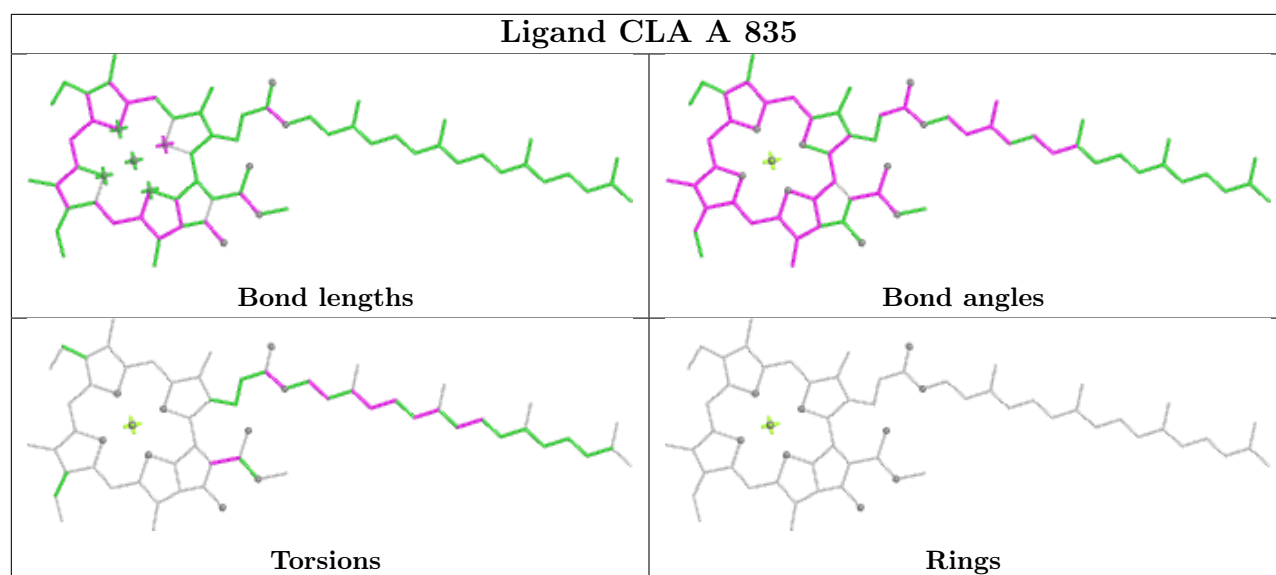
Ligand CLA A 849



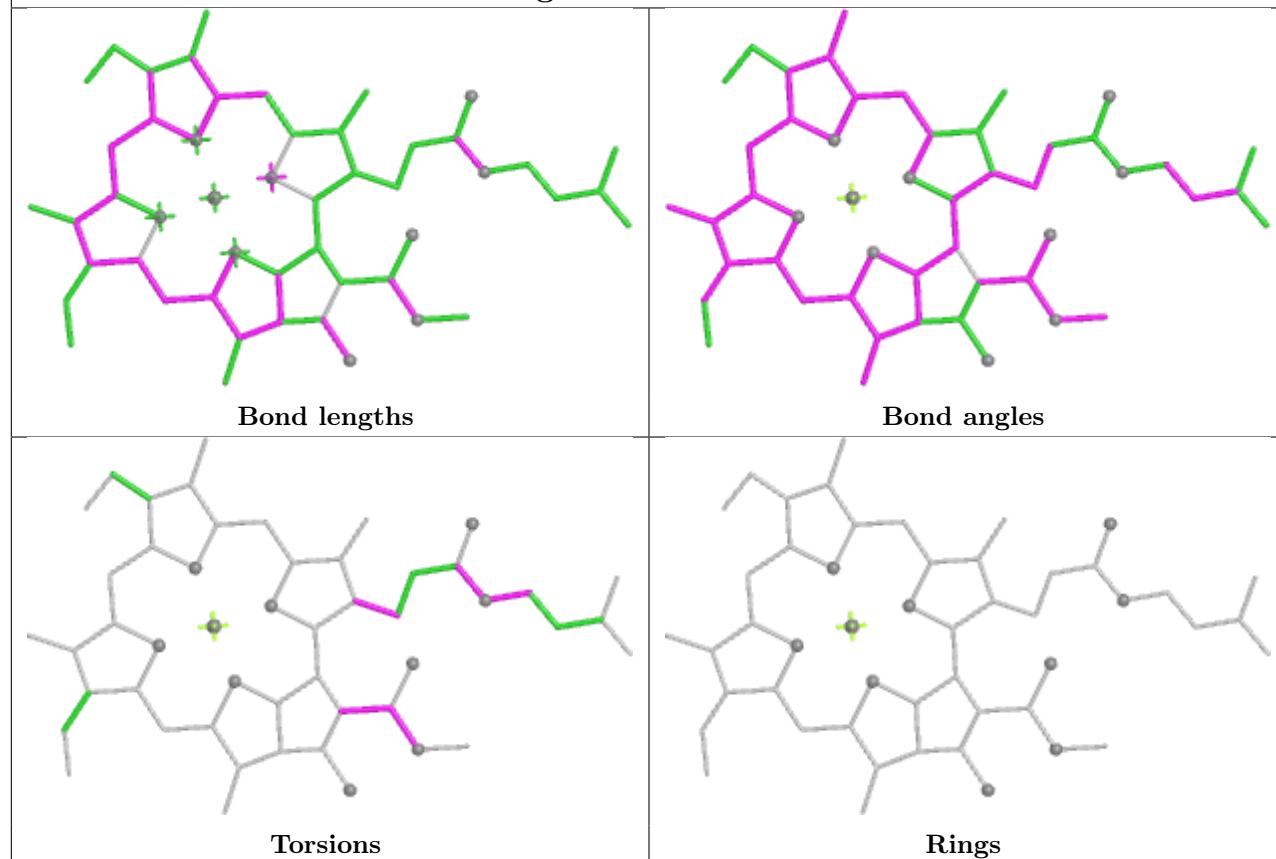




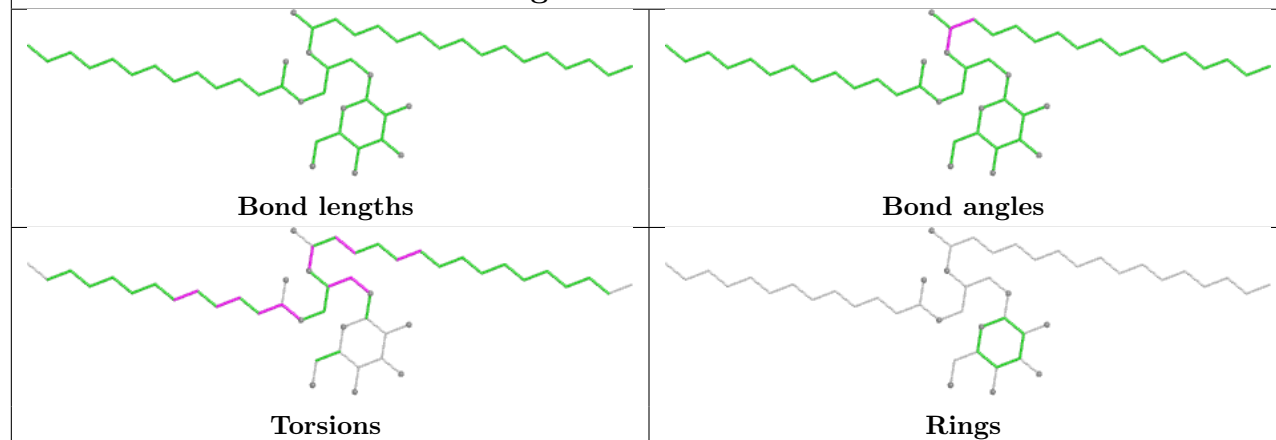


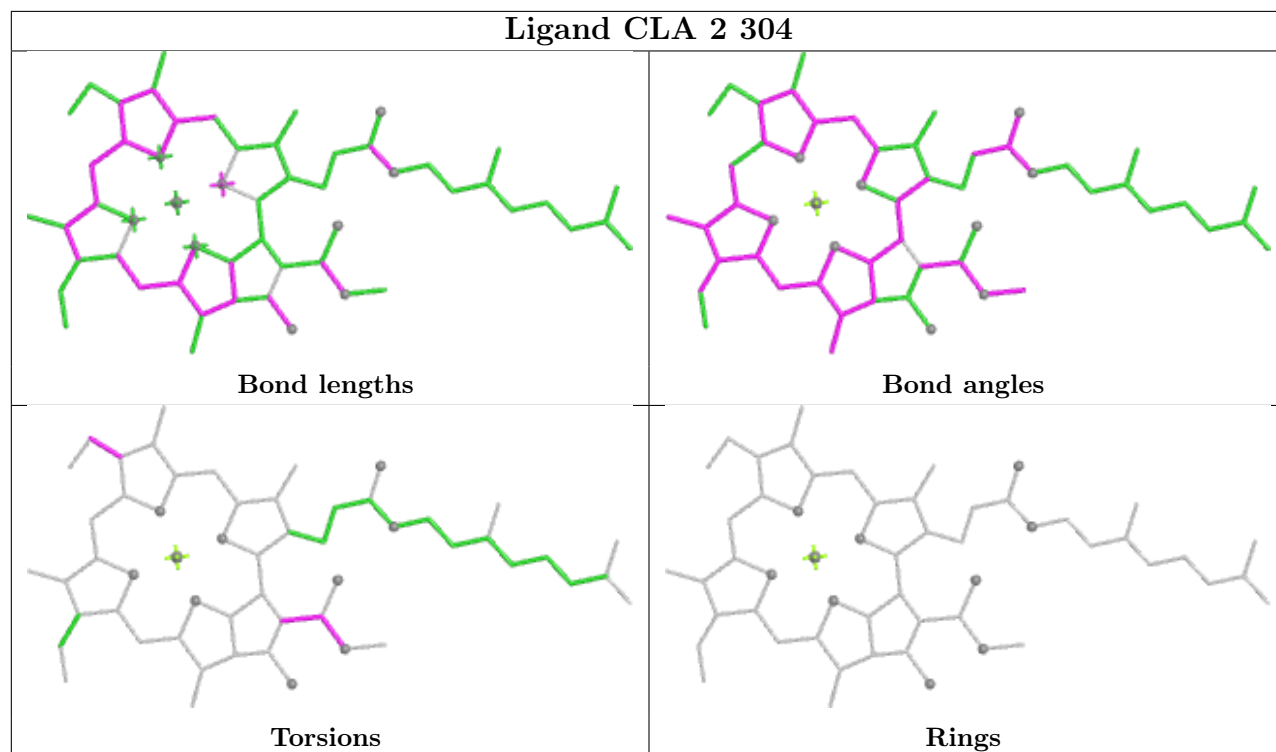
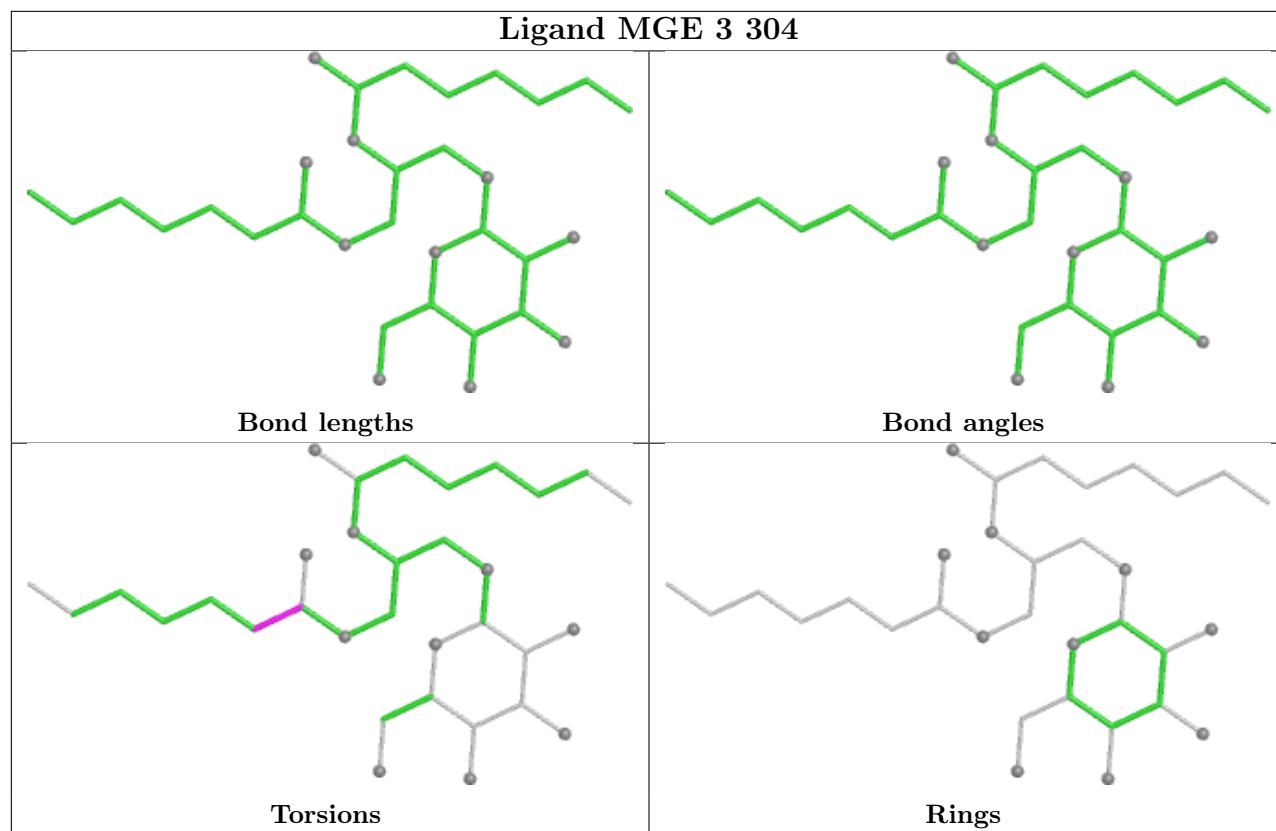


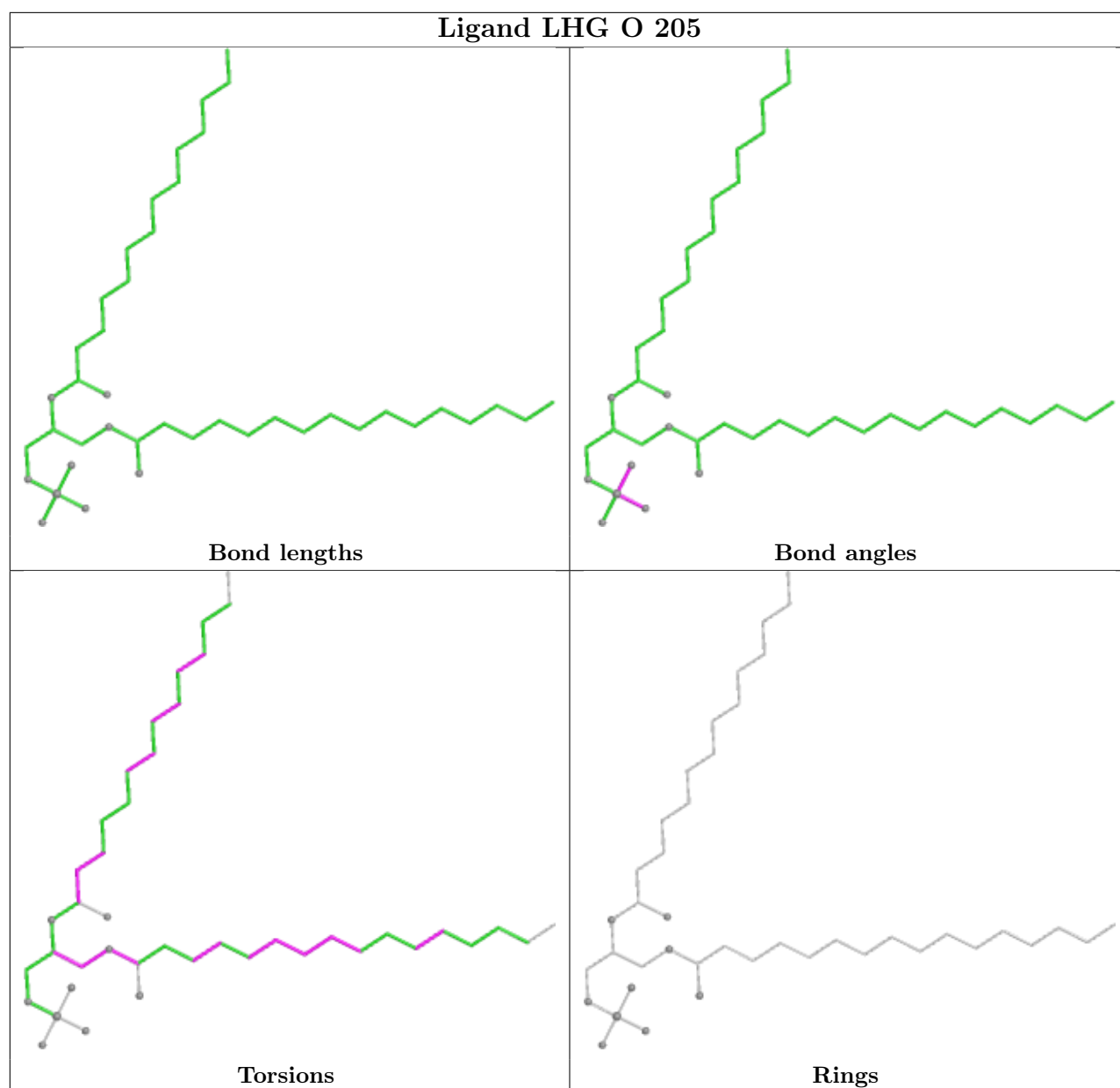
Ligand CLA 2 321



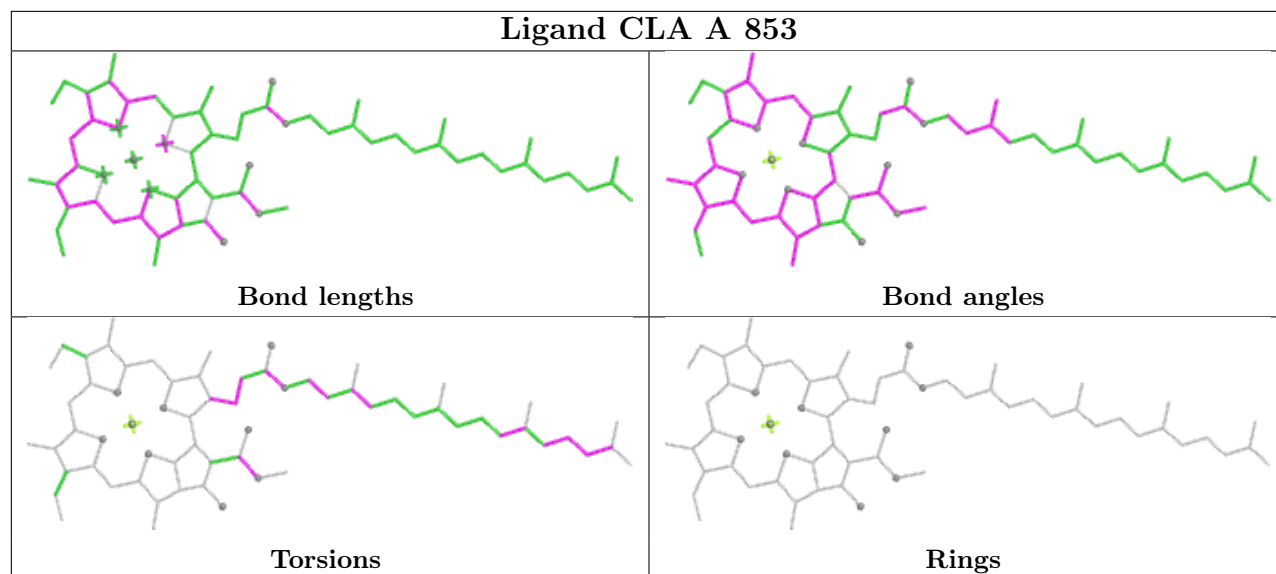
Ligand MGE 1 324



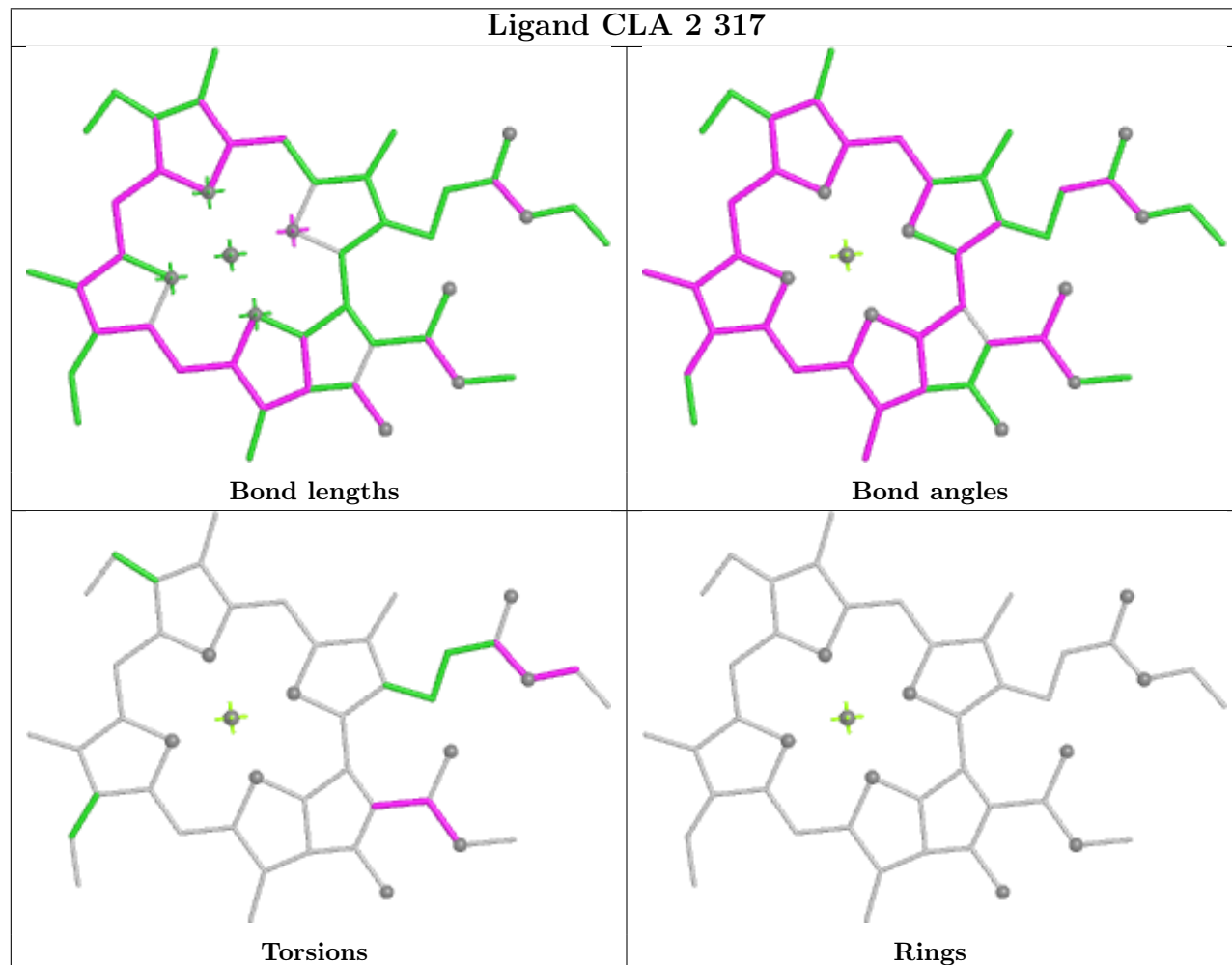


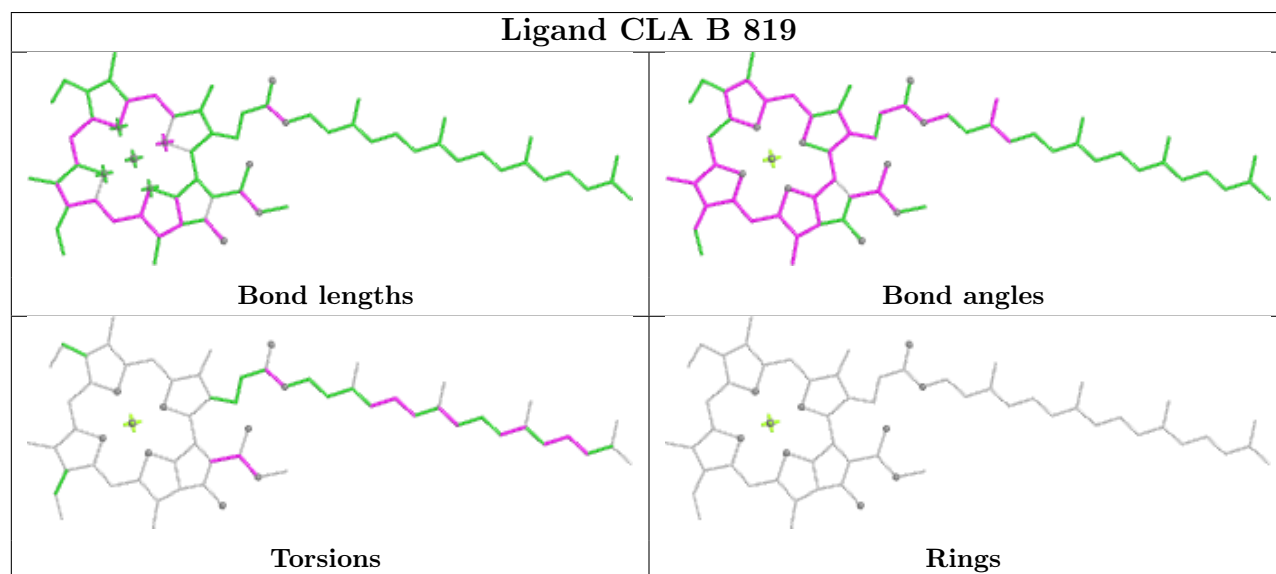
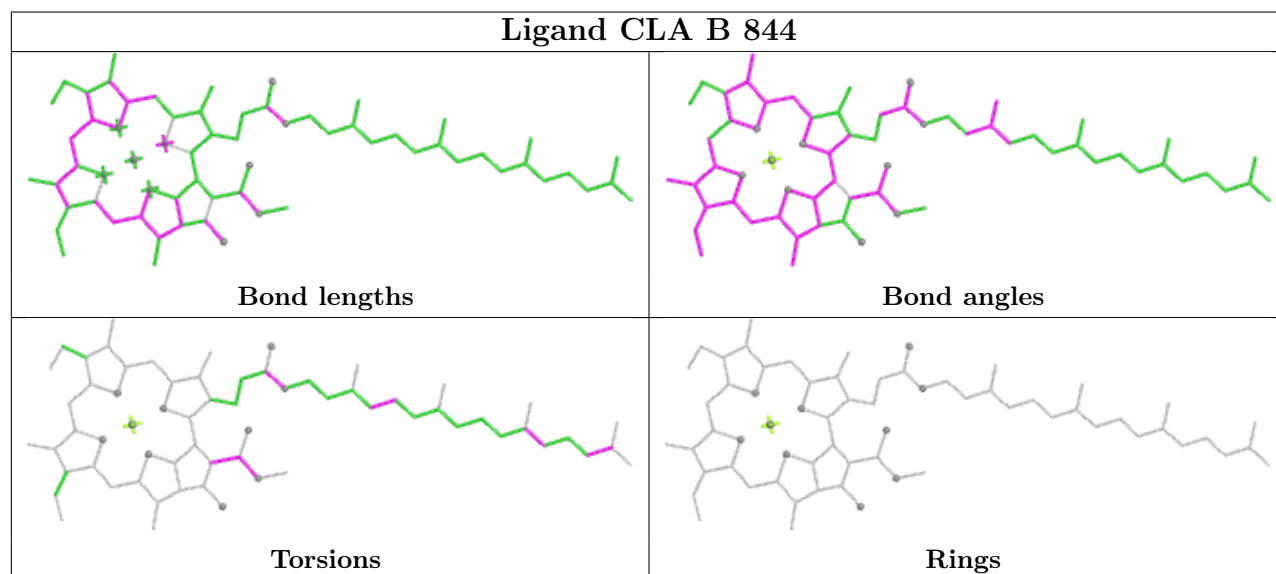
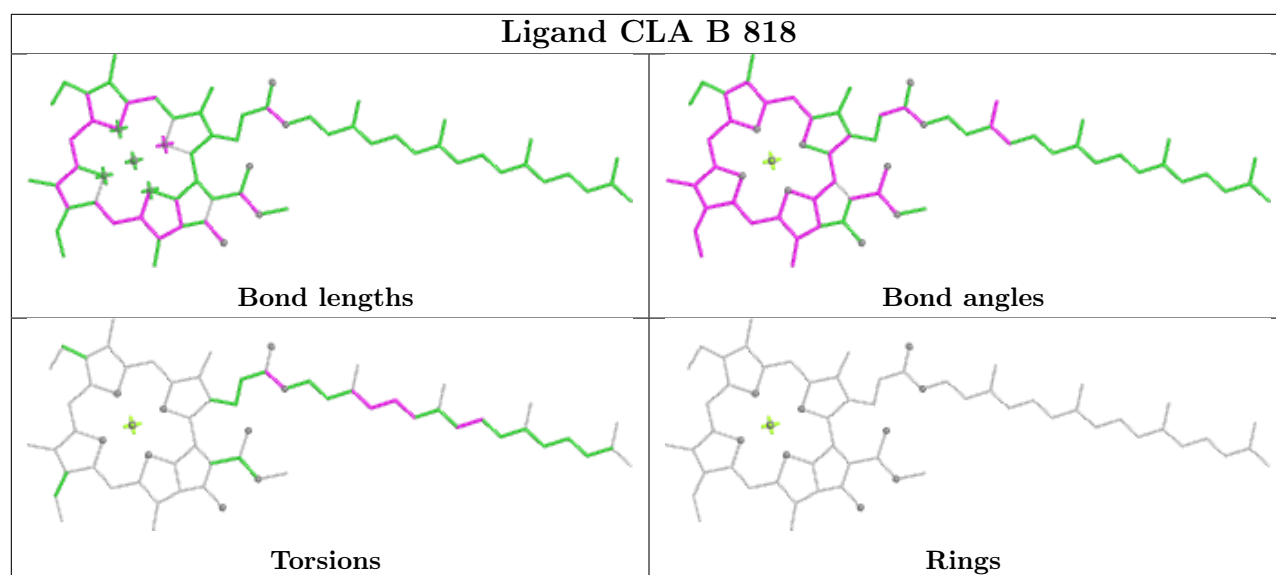


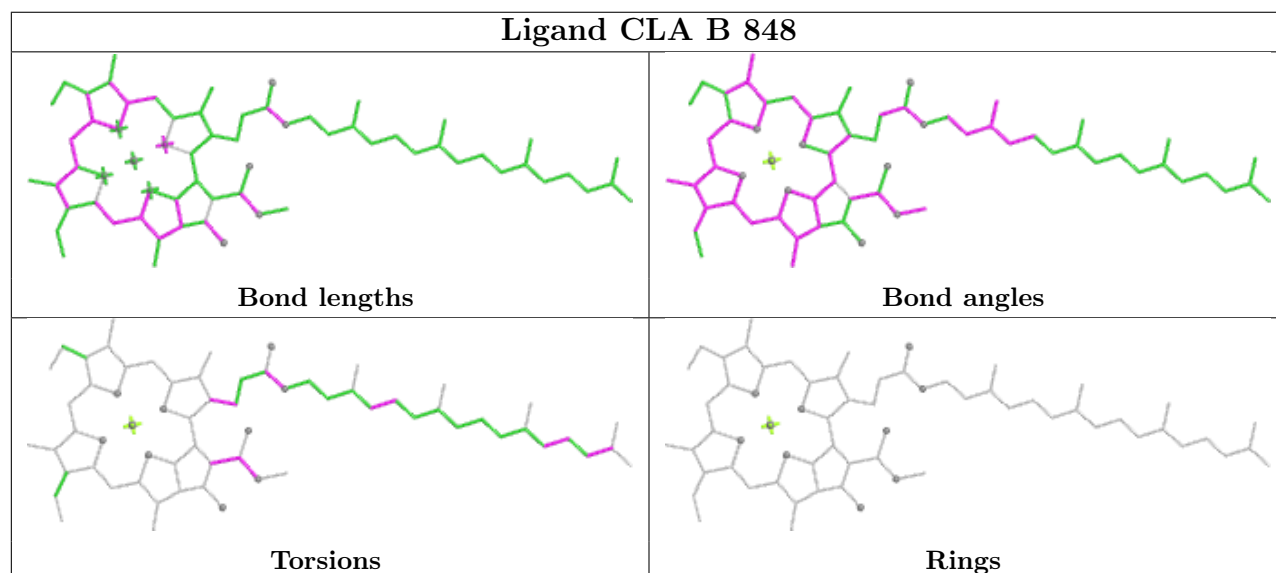
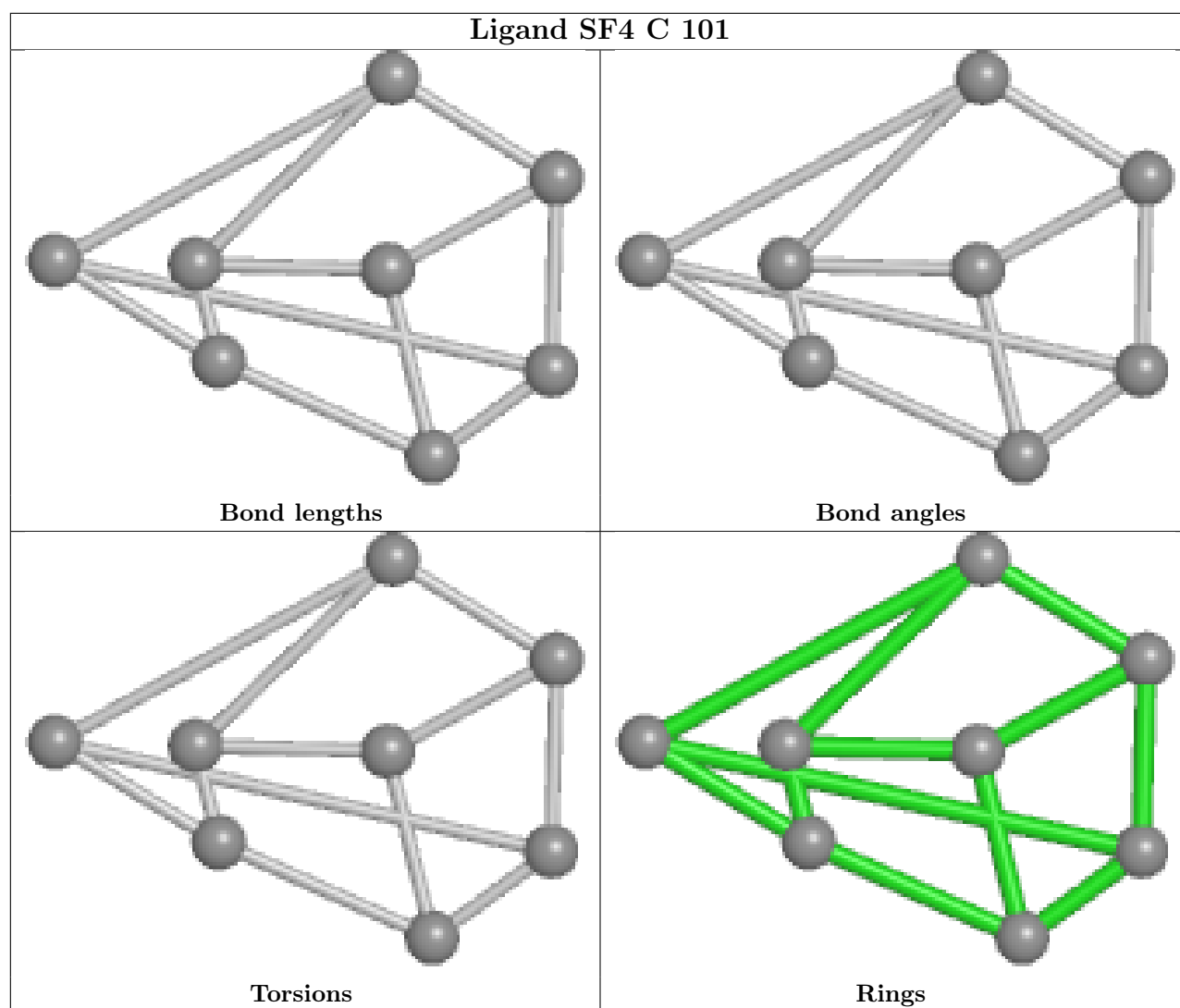
Ligand CLA A 853

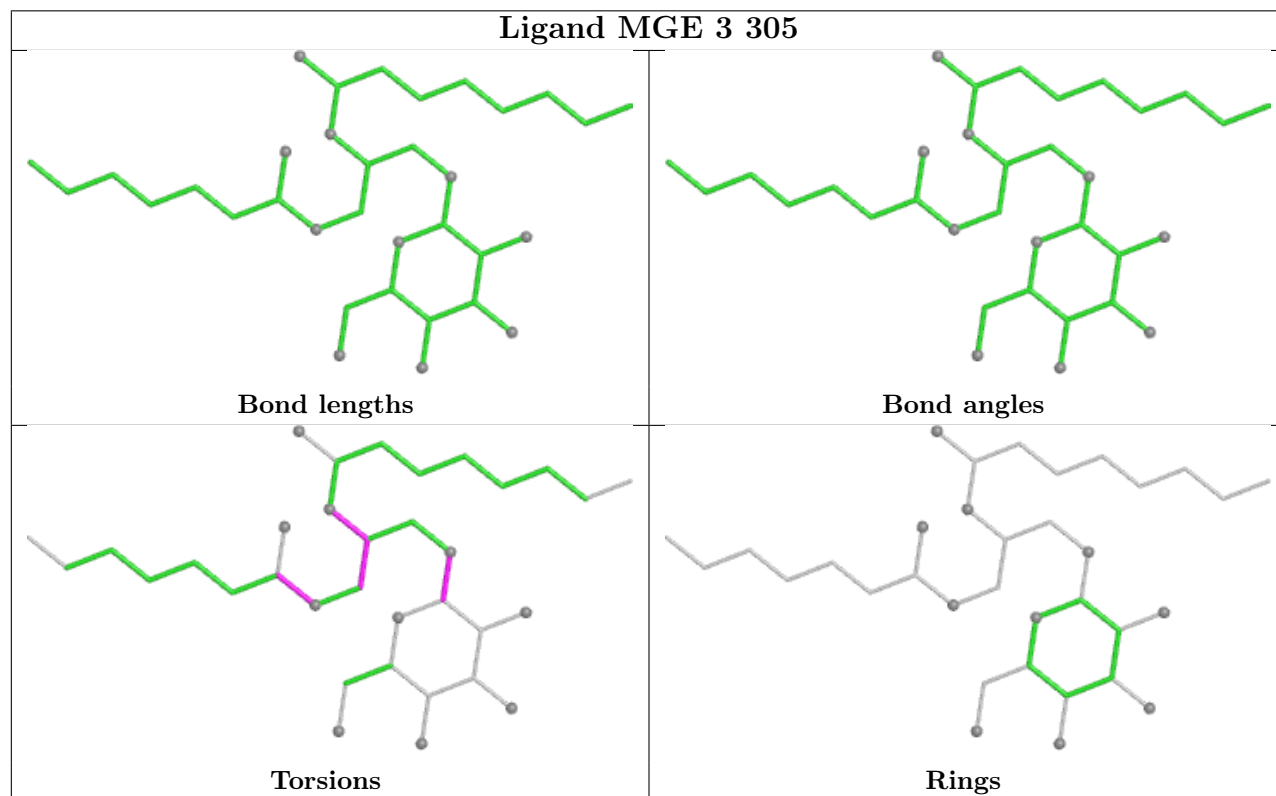
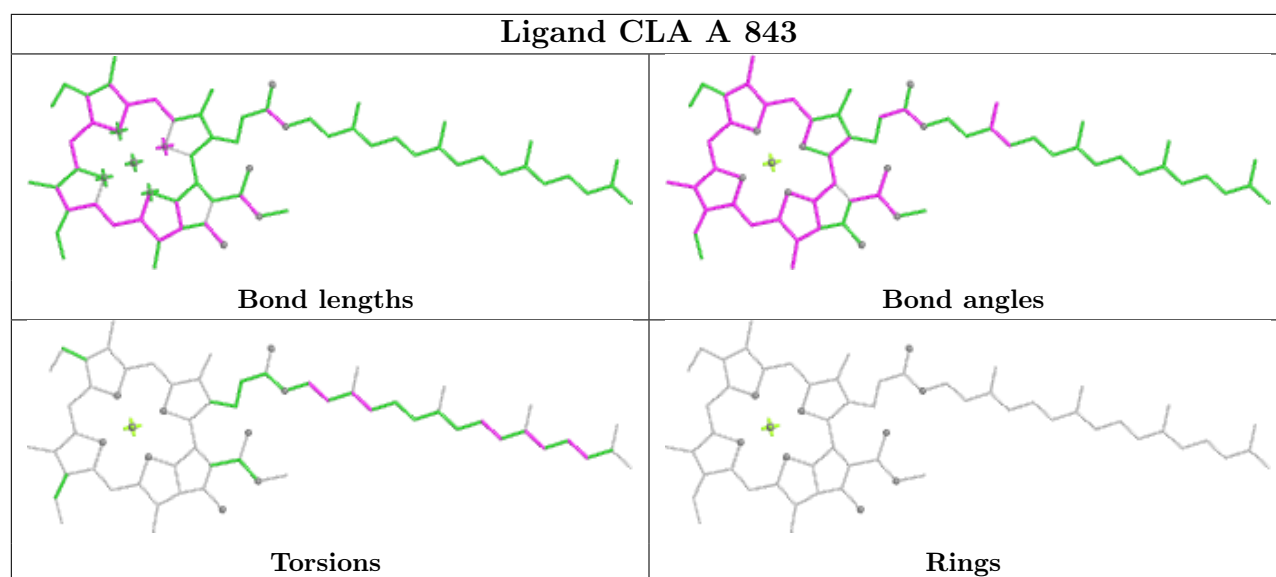


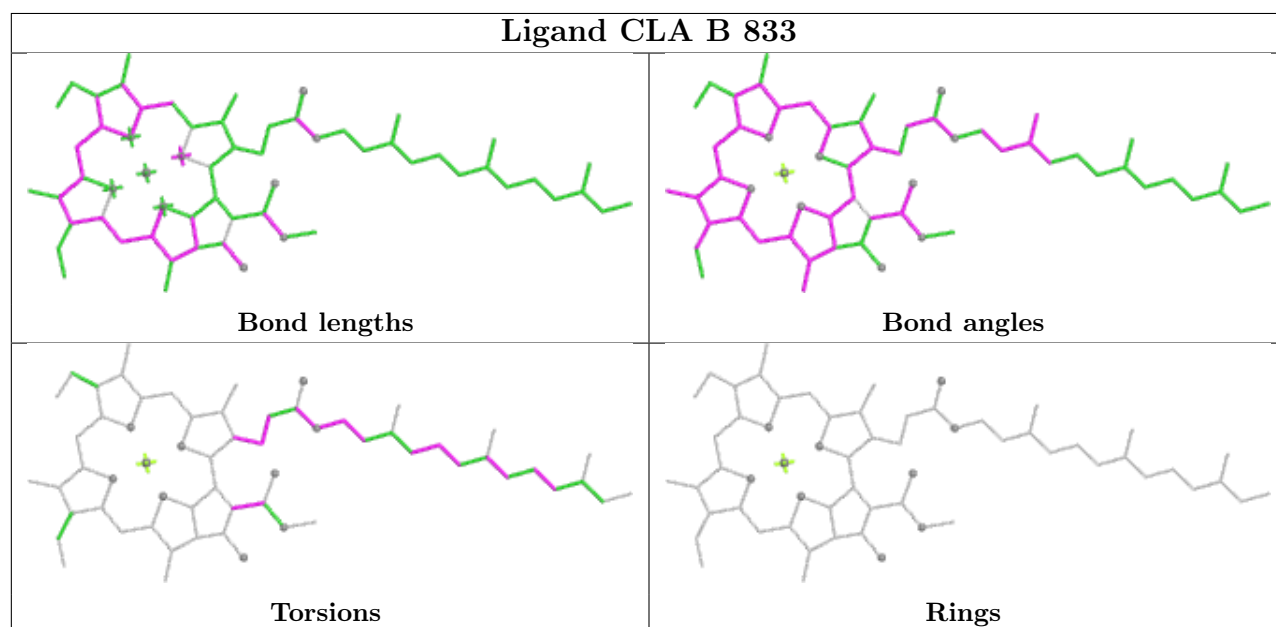
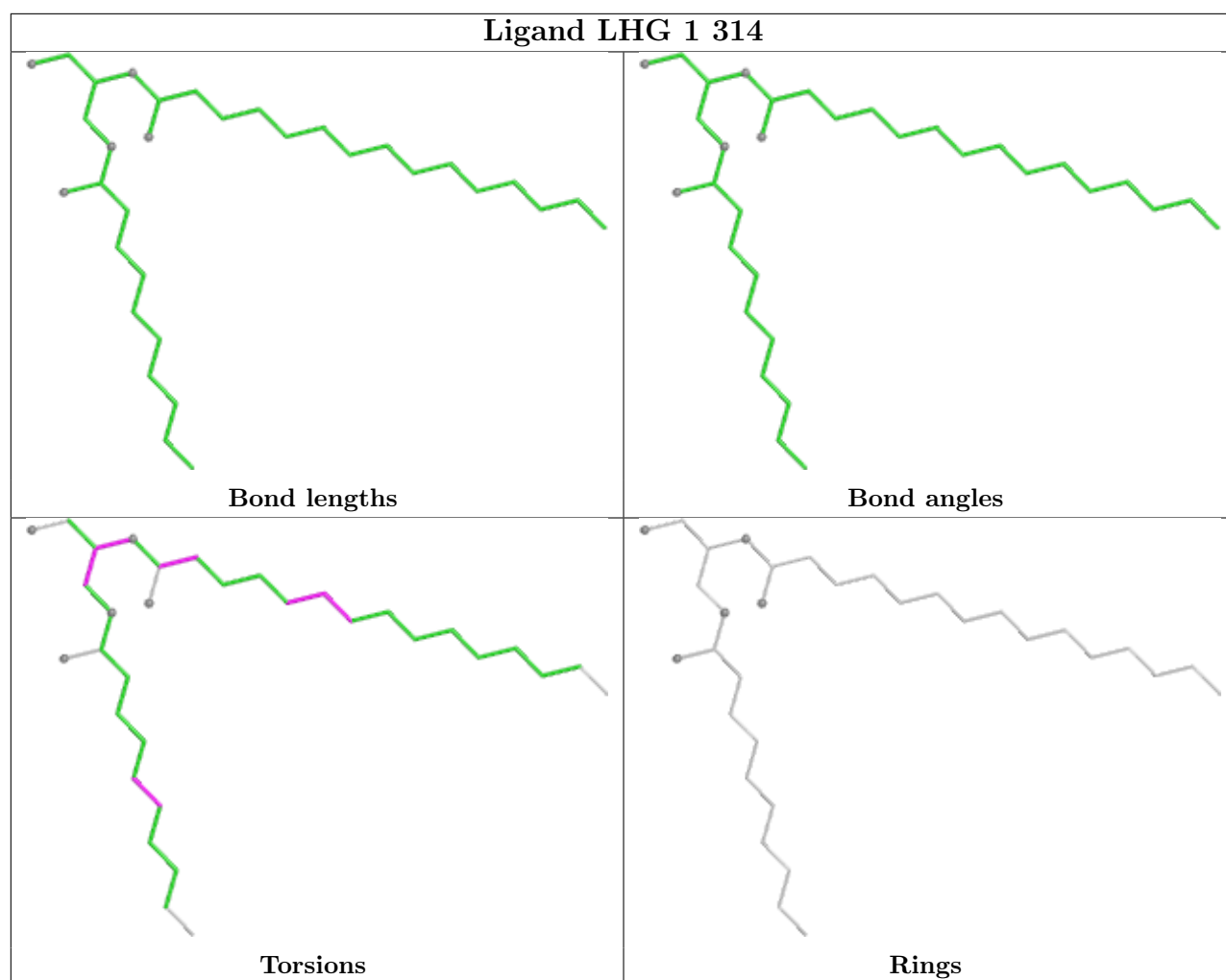
Ligand CLA 2 317

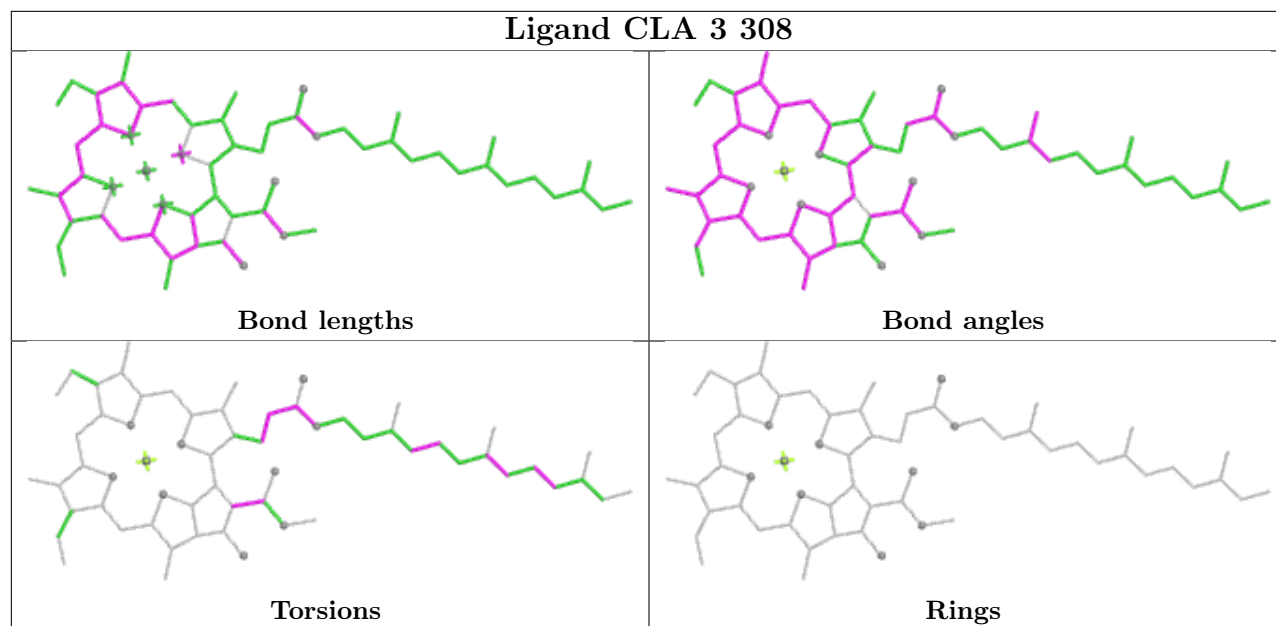


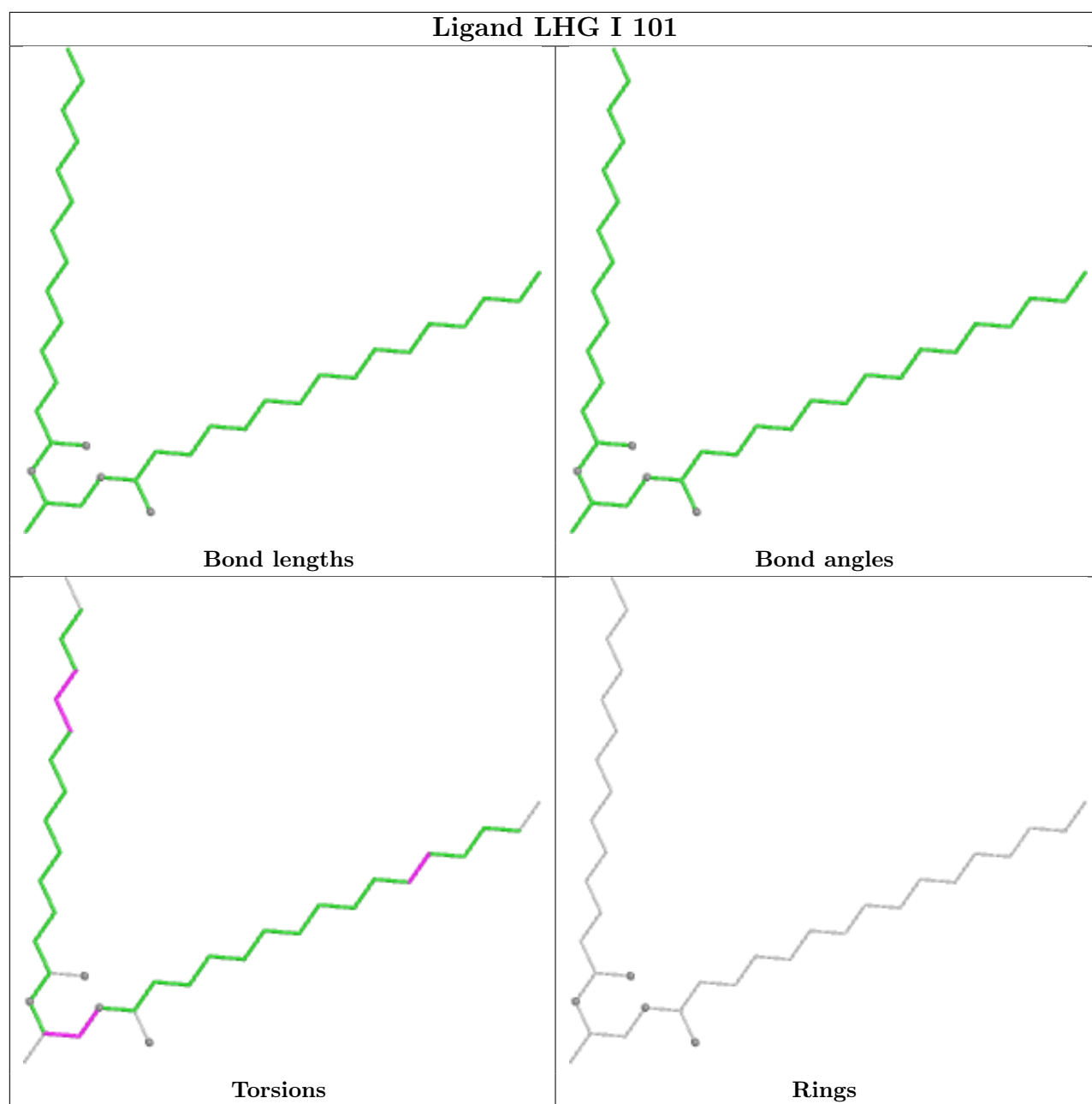


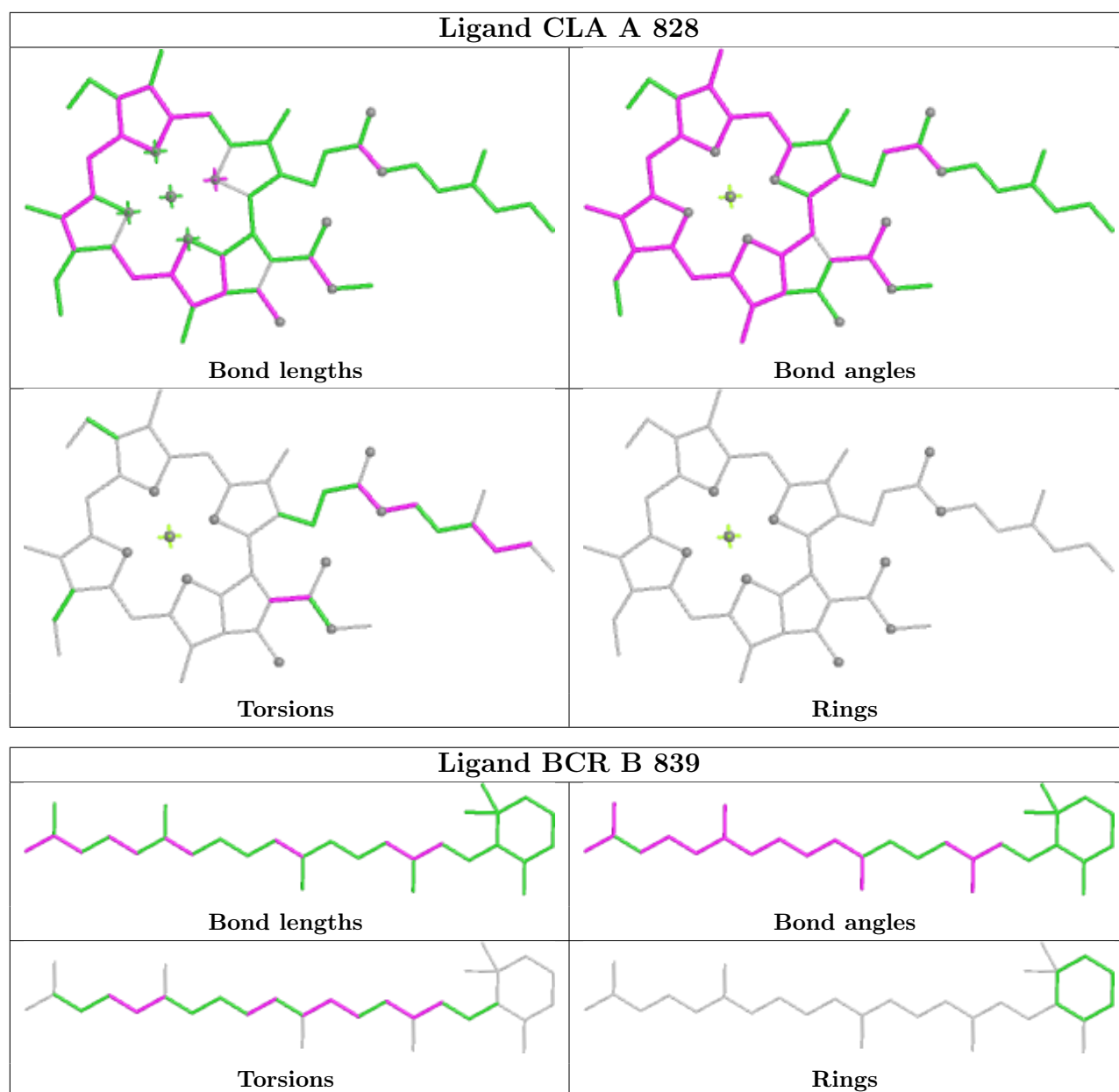


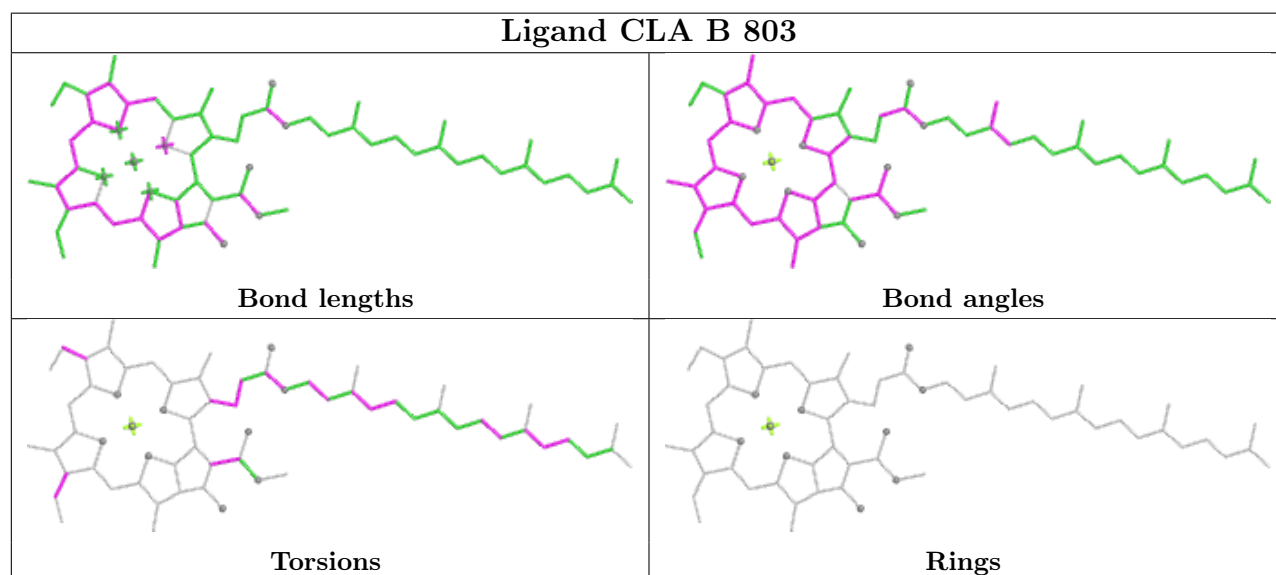
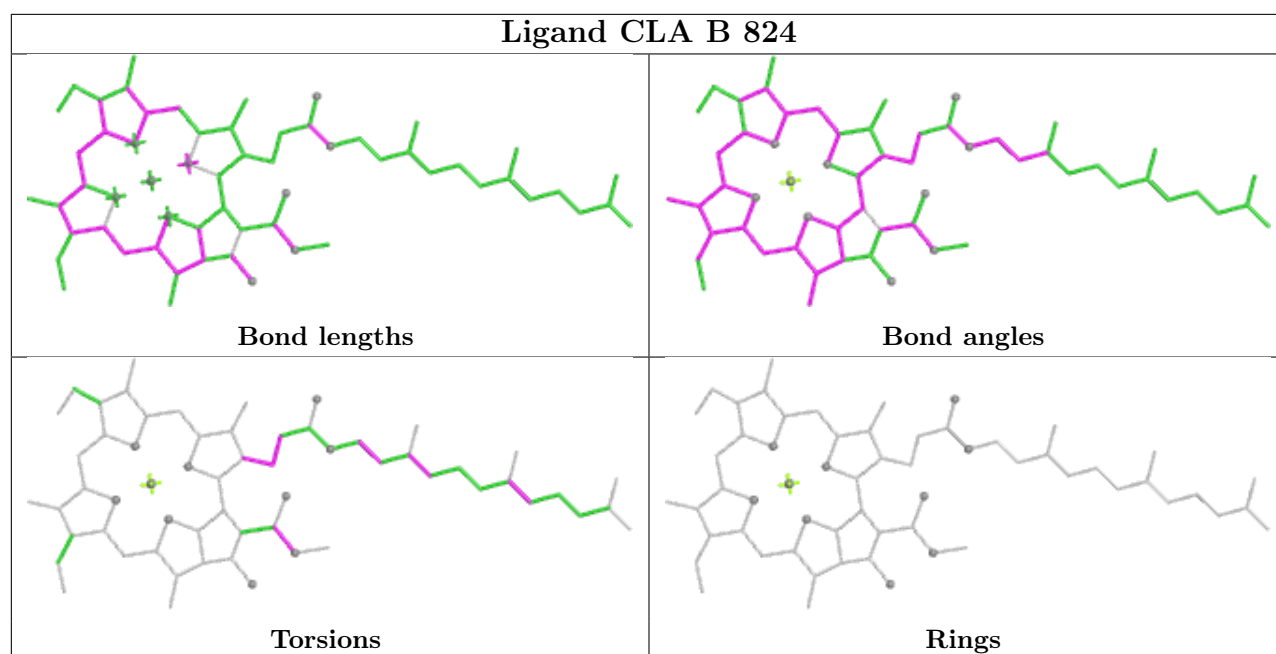


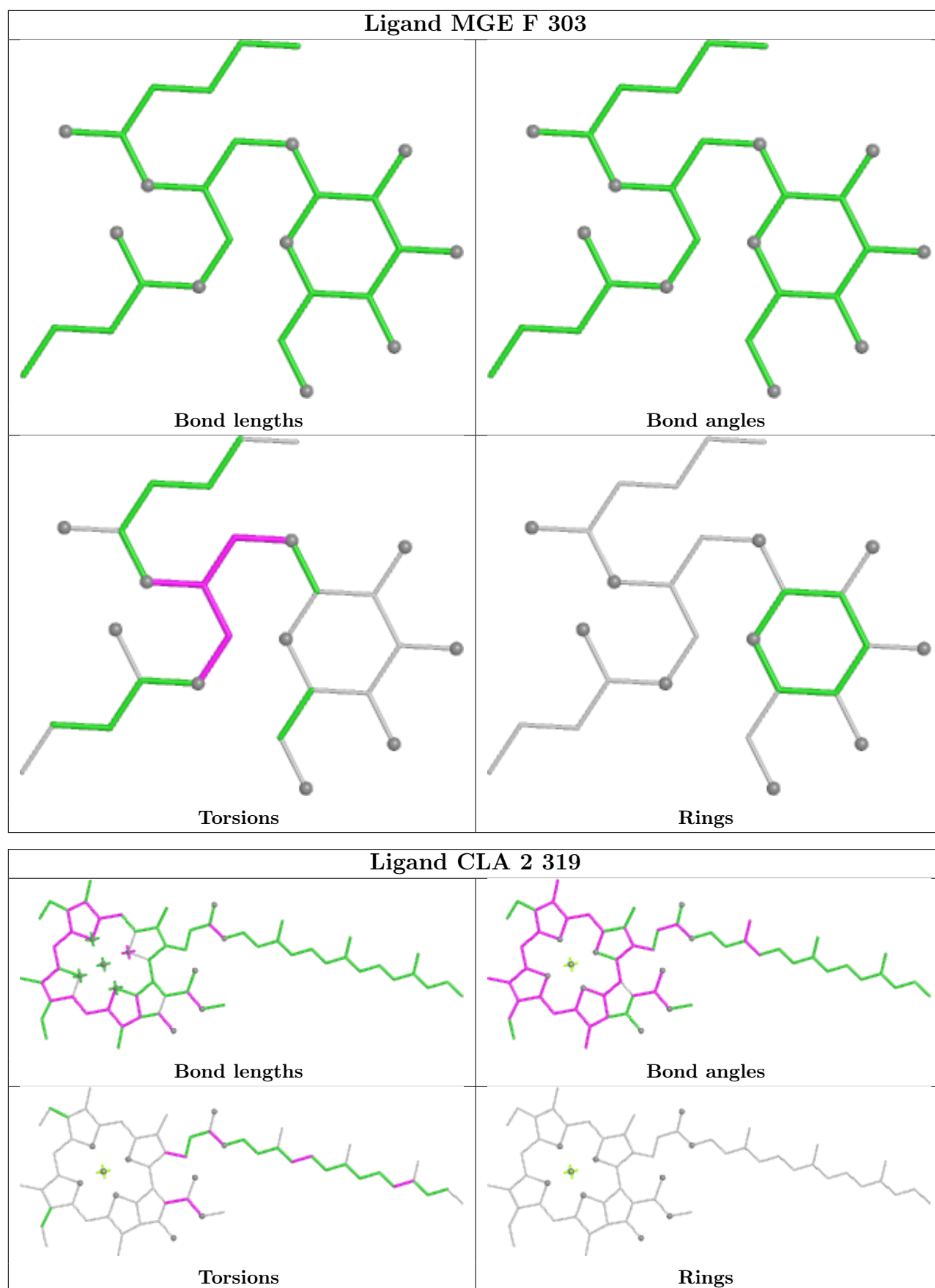




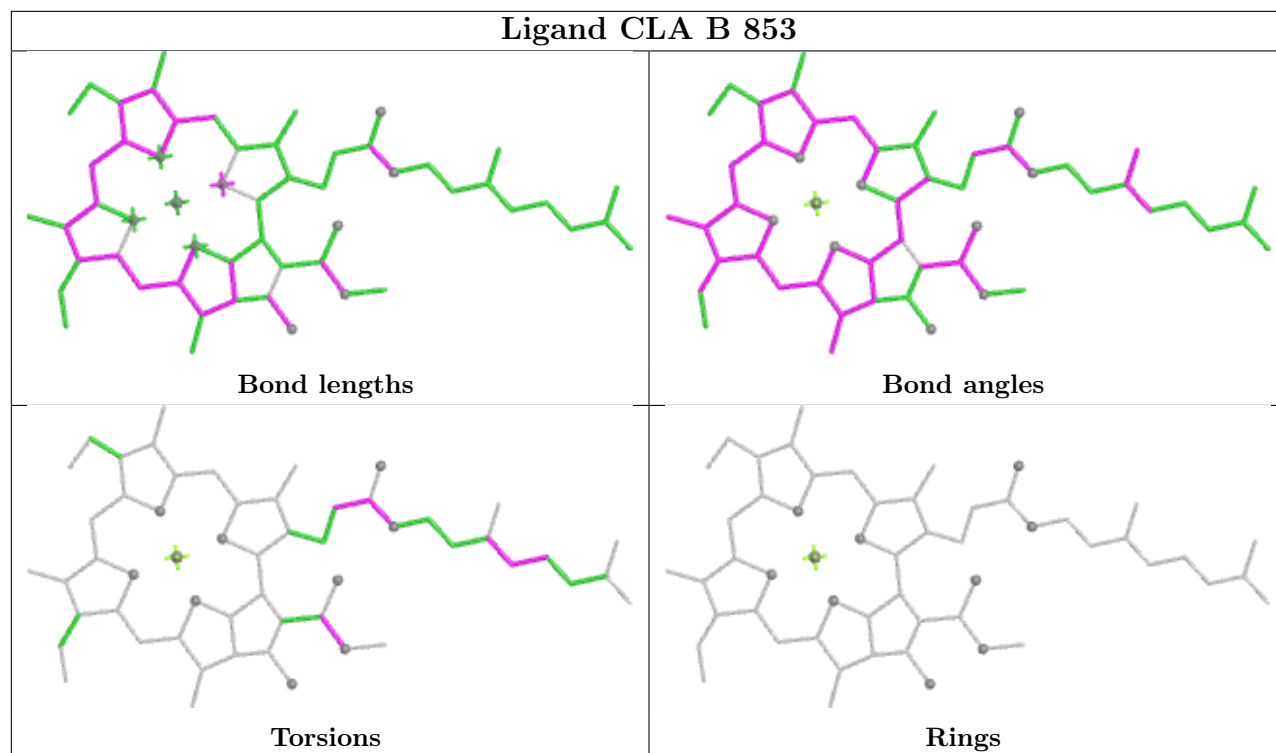




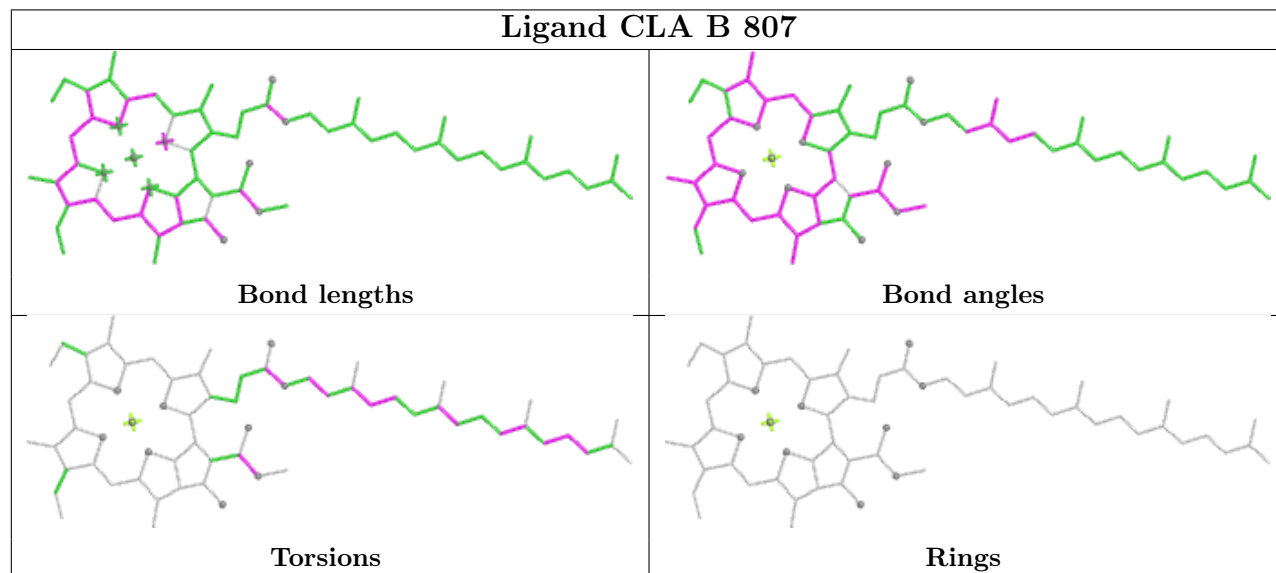




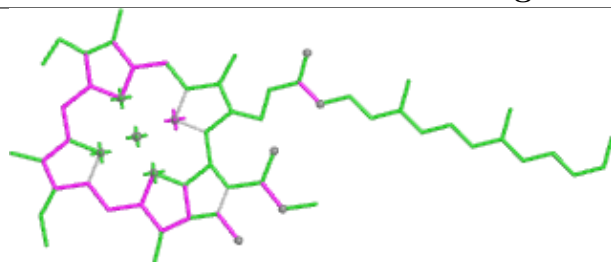
Ligand CLA B 853



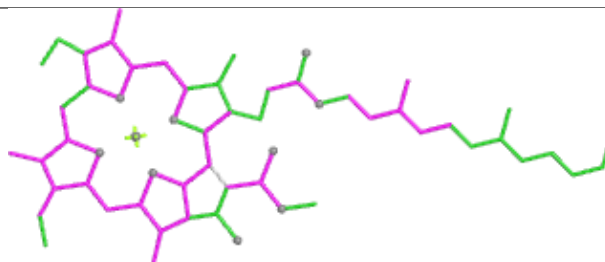
Ligand CLA B 807



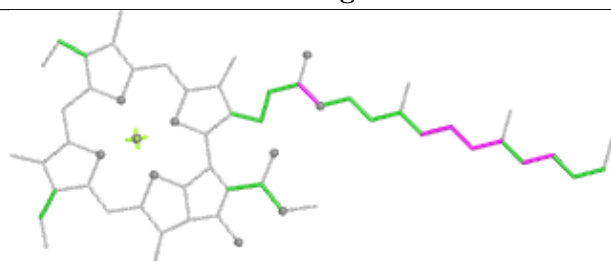
Ligand CLA B 820



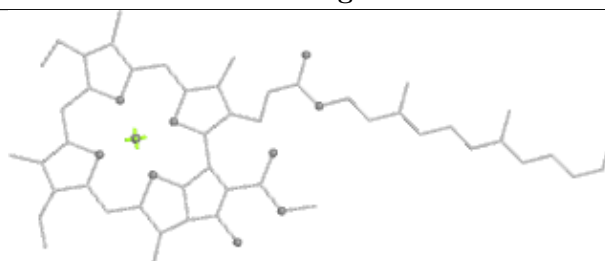
Bond lengths



Bond angles

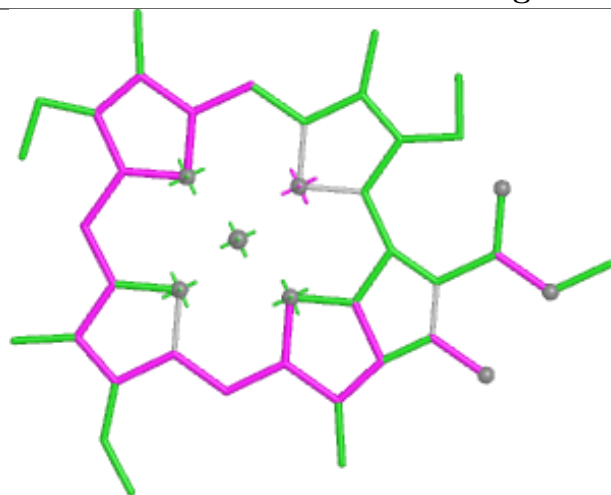


Torsions



Rings

Ligand CLA K 206



Bond lengths



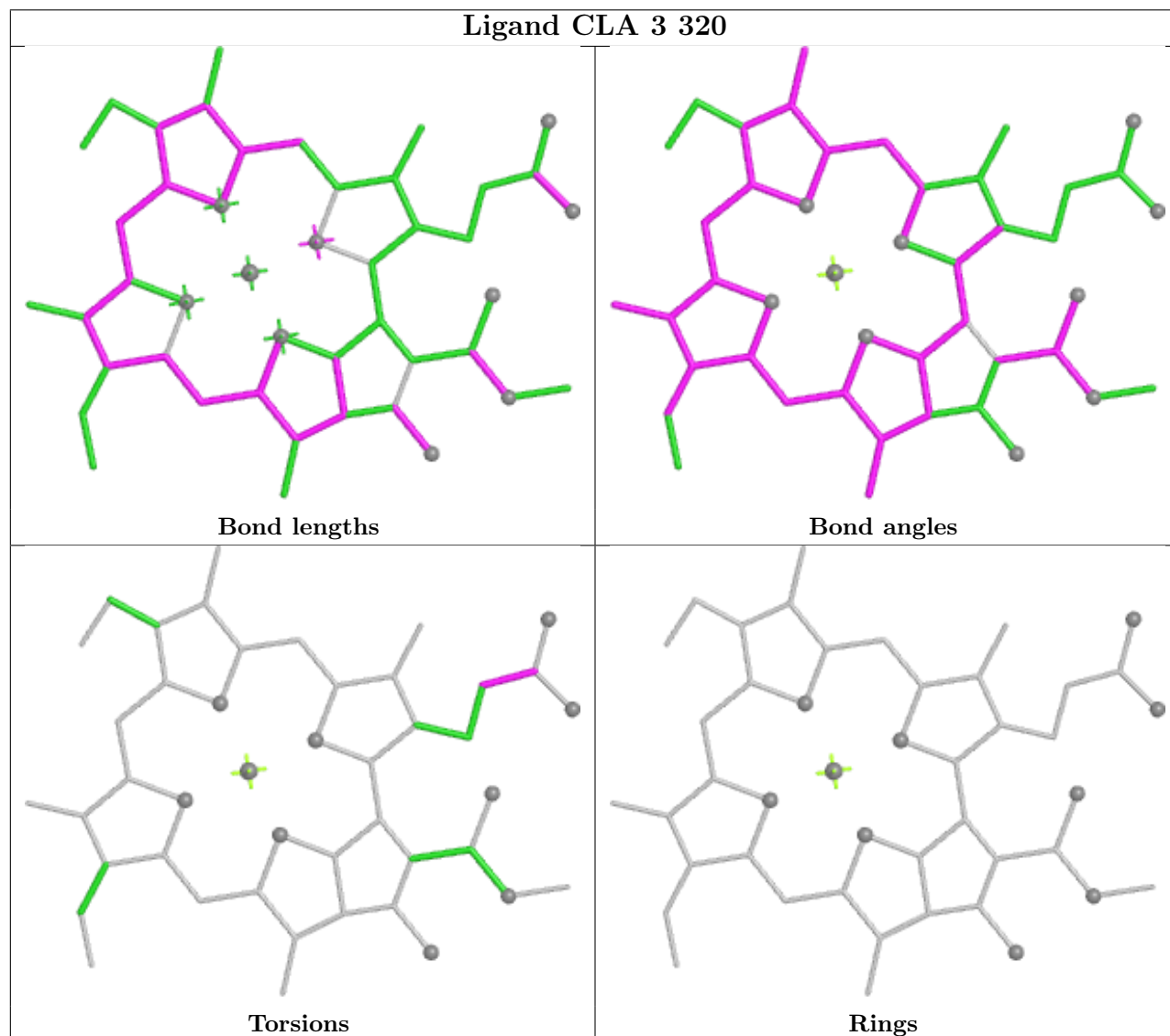
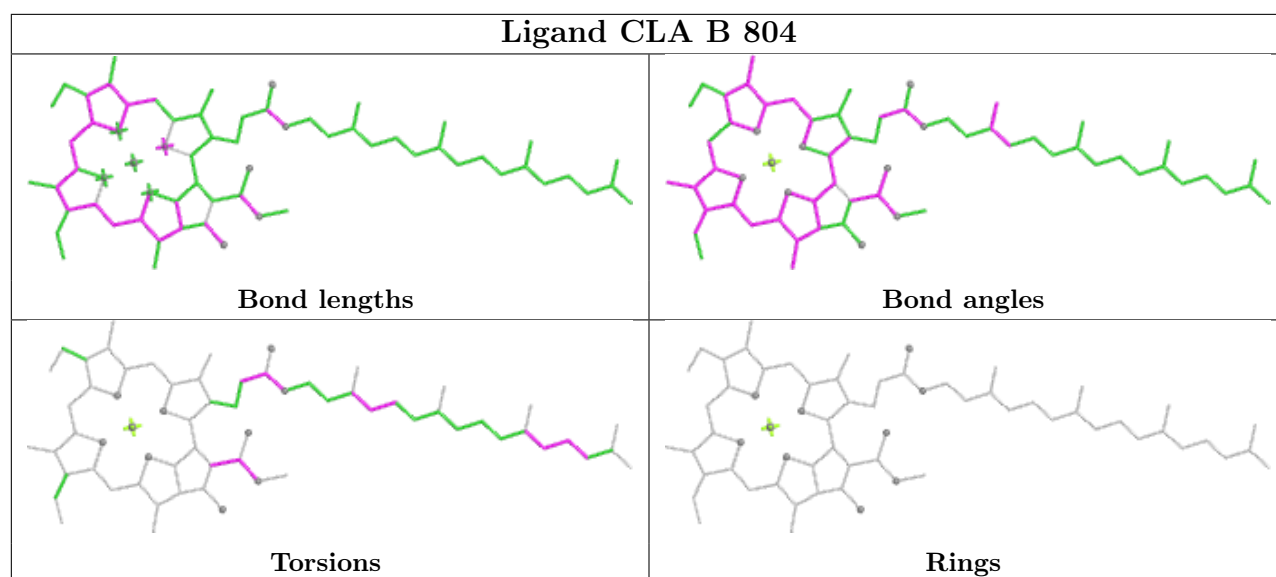
Bond angles



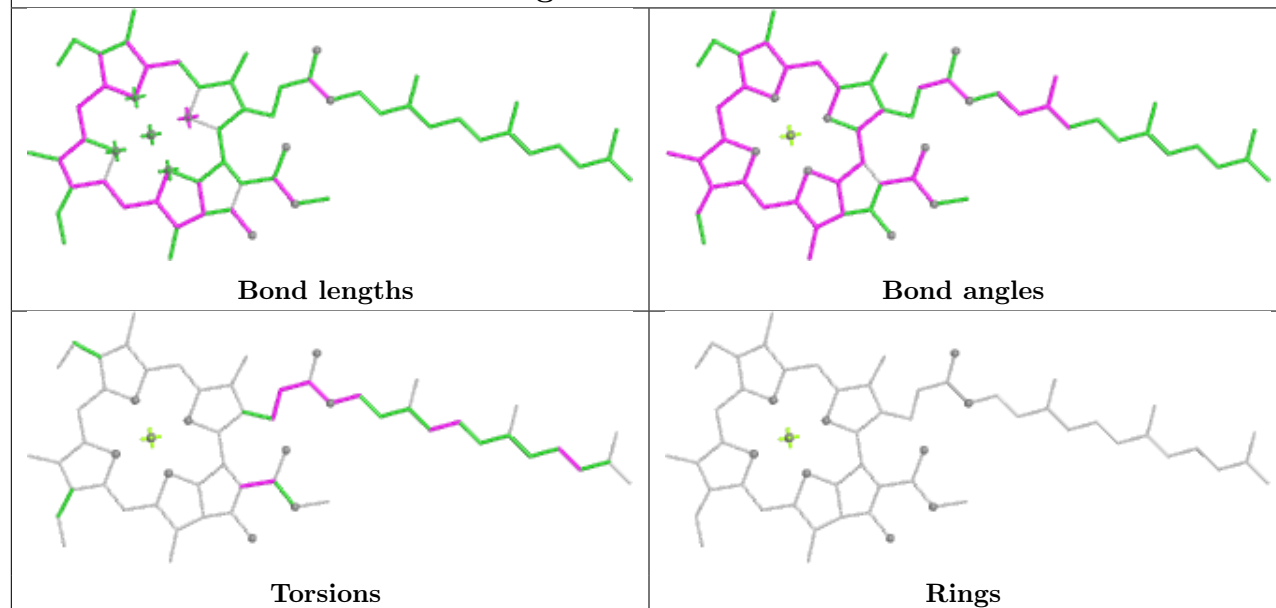
Torsions



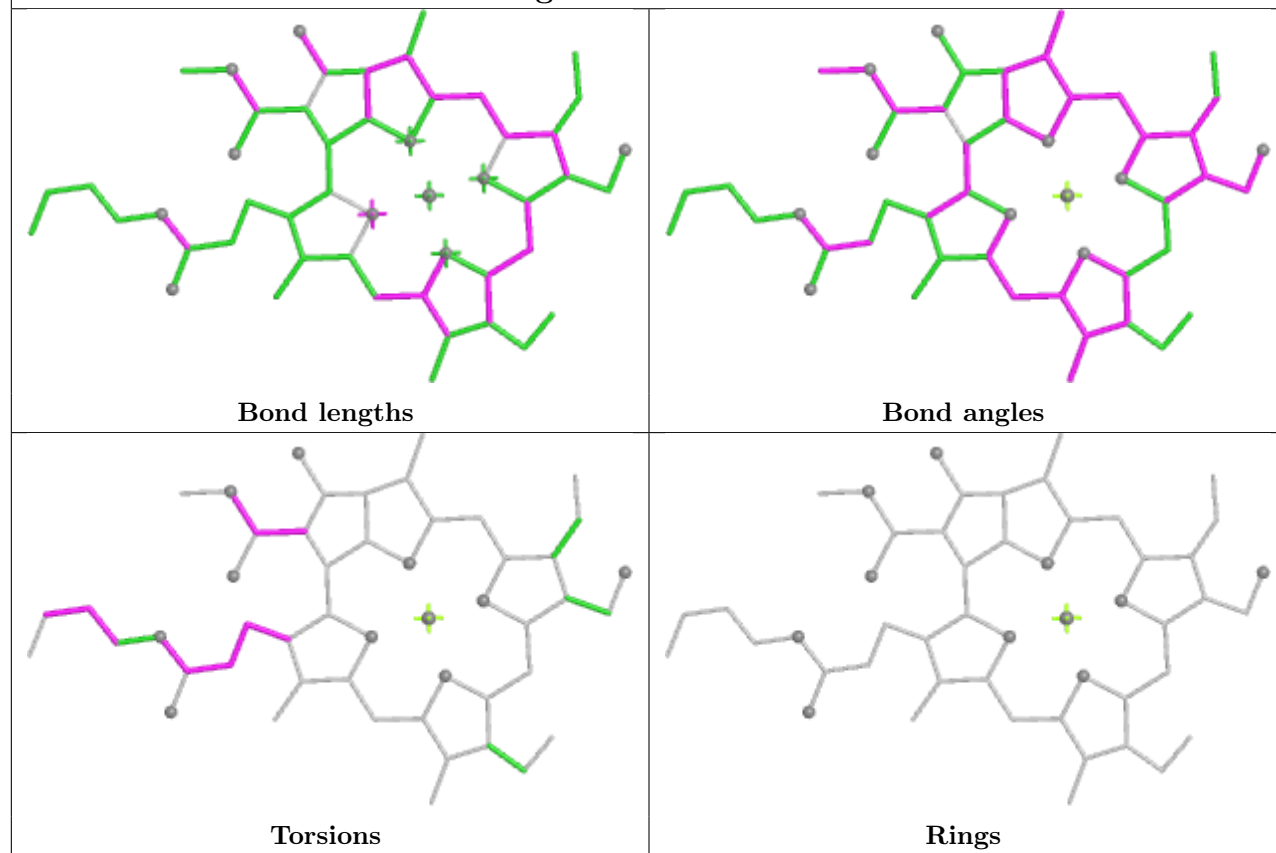
Rings



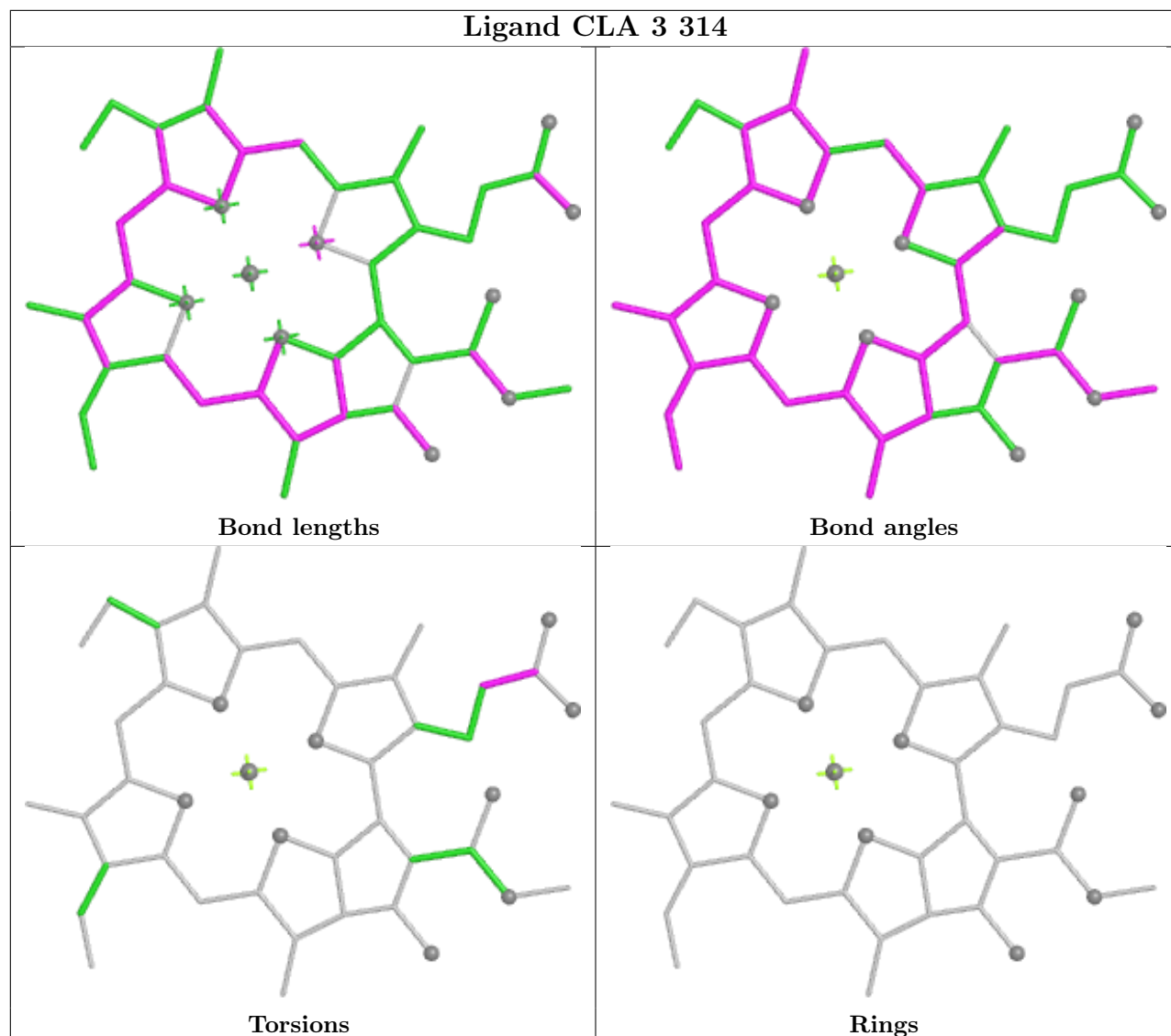
Ligand CLA 4 310



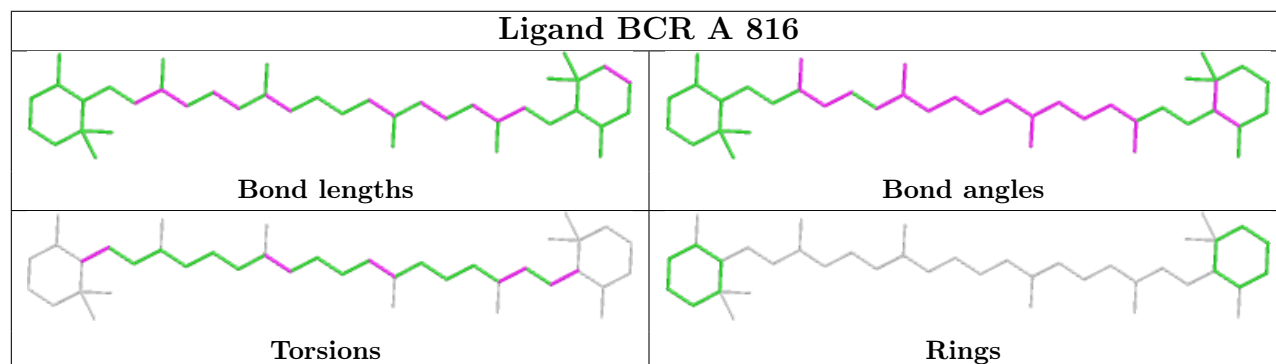
Ligand CHL 3 313

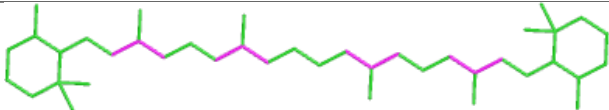
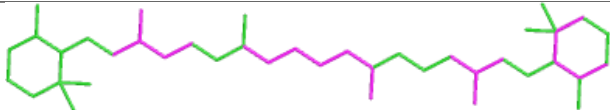
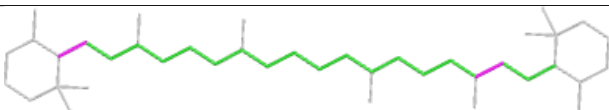
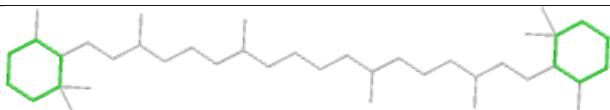


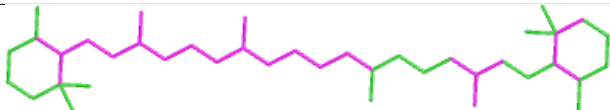
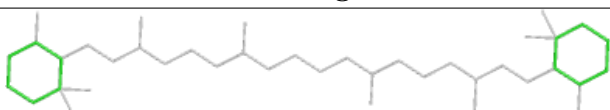
Ligand CLA 3 314

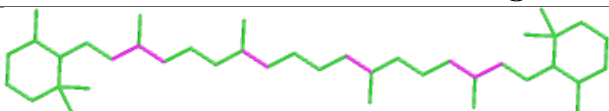
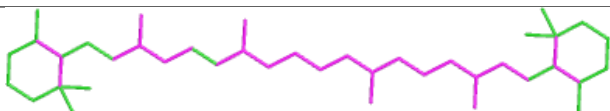
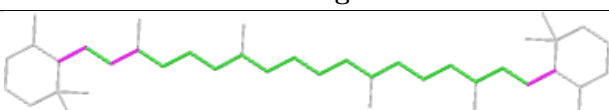
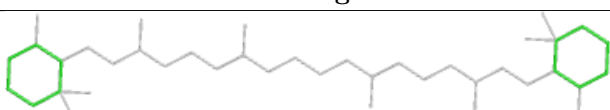


Ligand BCR A 816

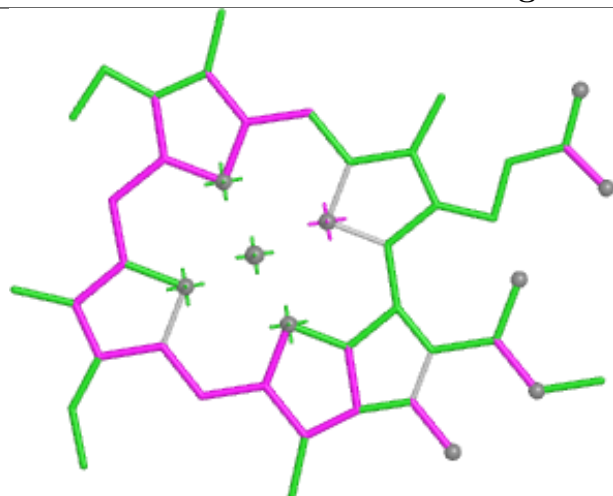


Ligand BCR I 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

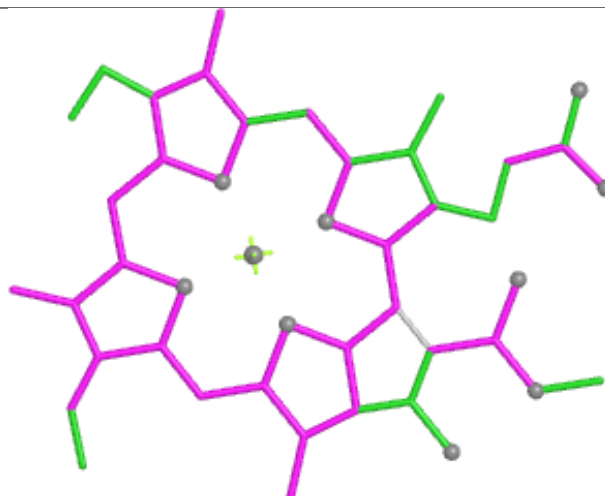
Ligand BCR O 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 836	
	
Bond lengths	Bond angles
	
Torsions	Rings

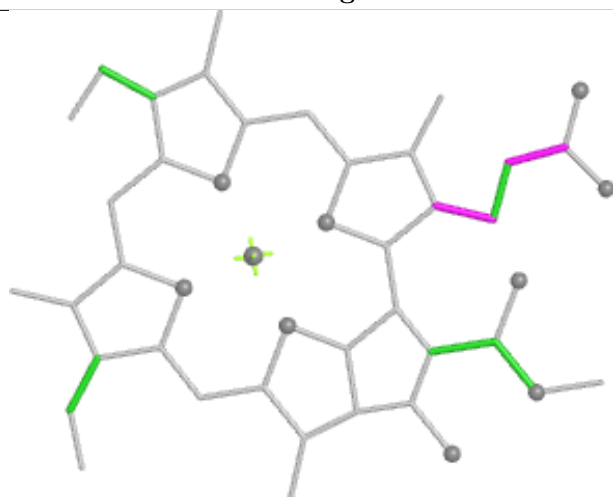
Ligand CLA 1 306



Bond lengths



Bond angles

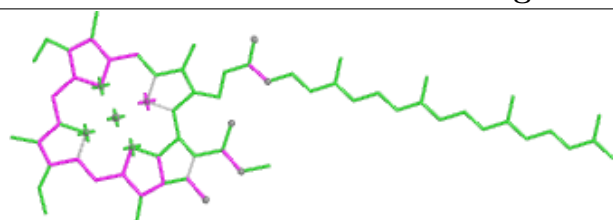


Torsions

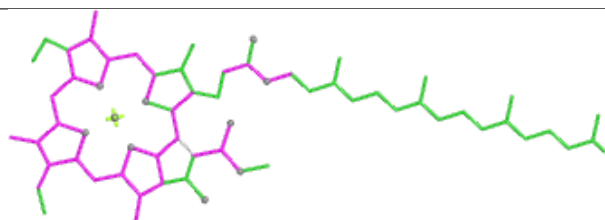


Rings

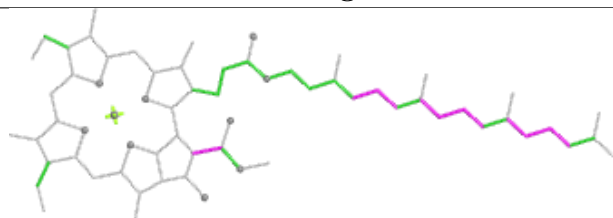
Ligand CLA O 206



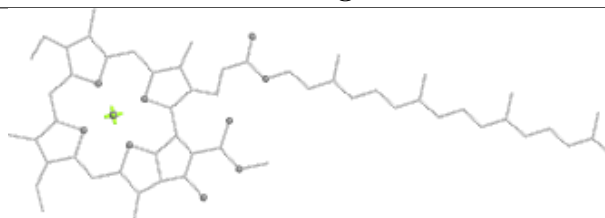
Bond lengths



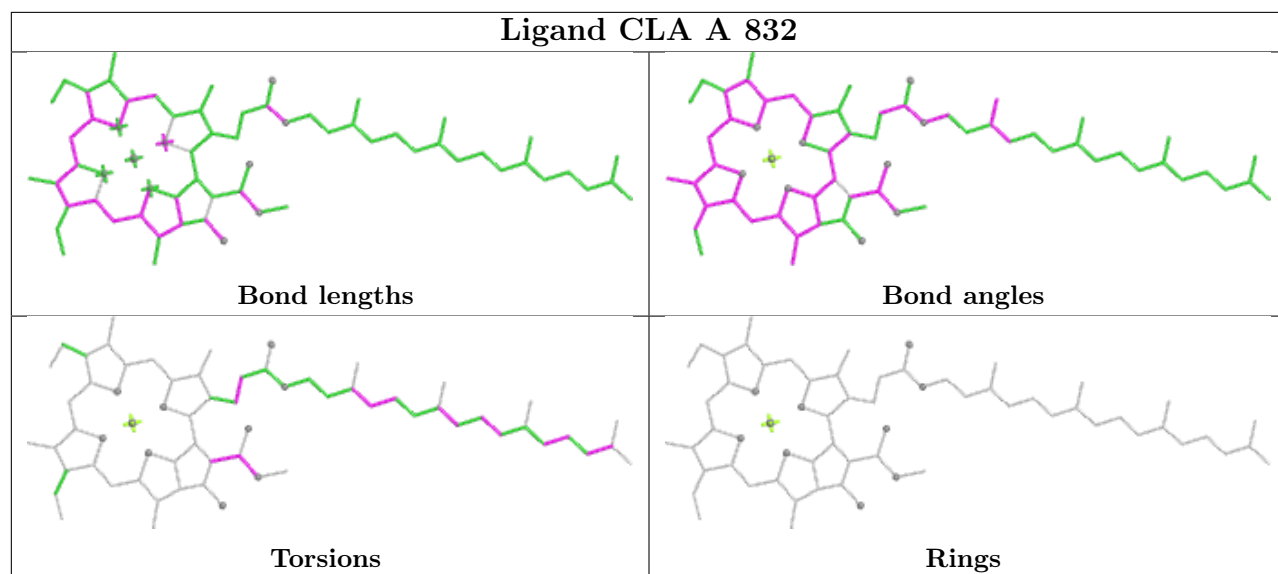
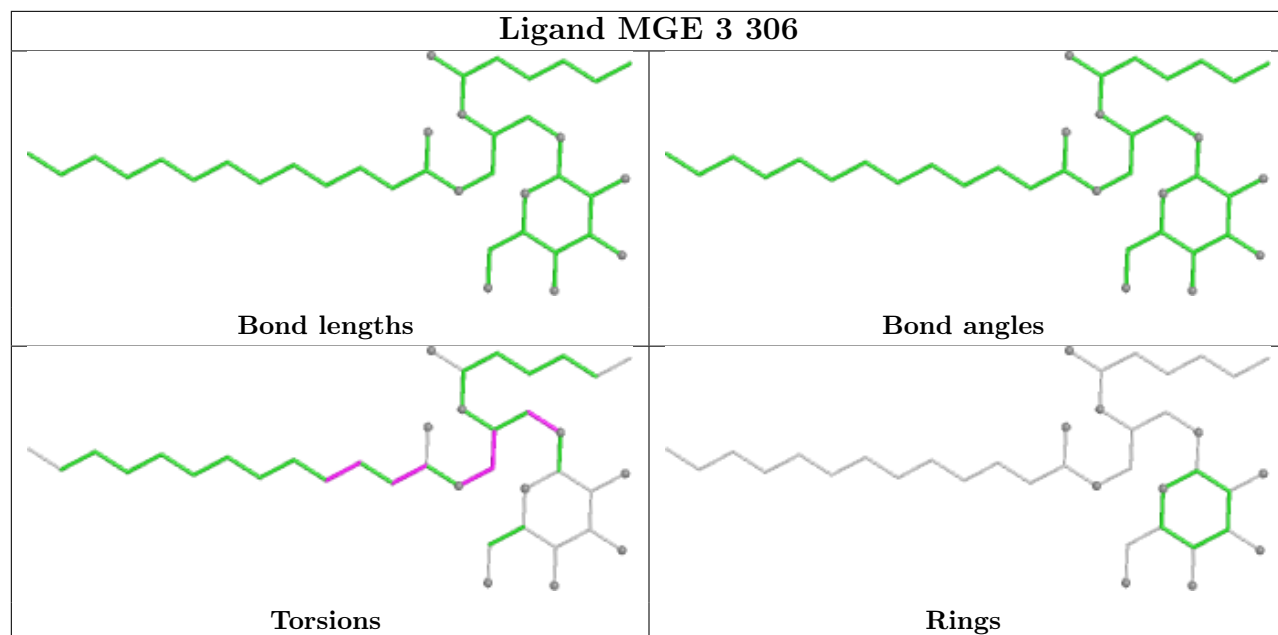
Bond angles

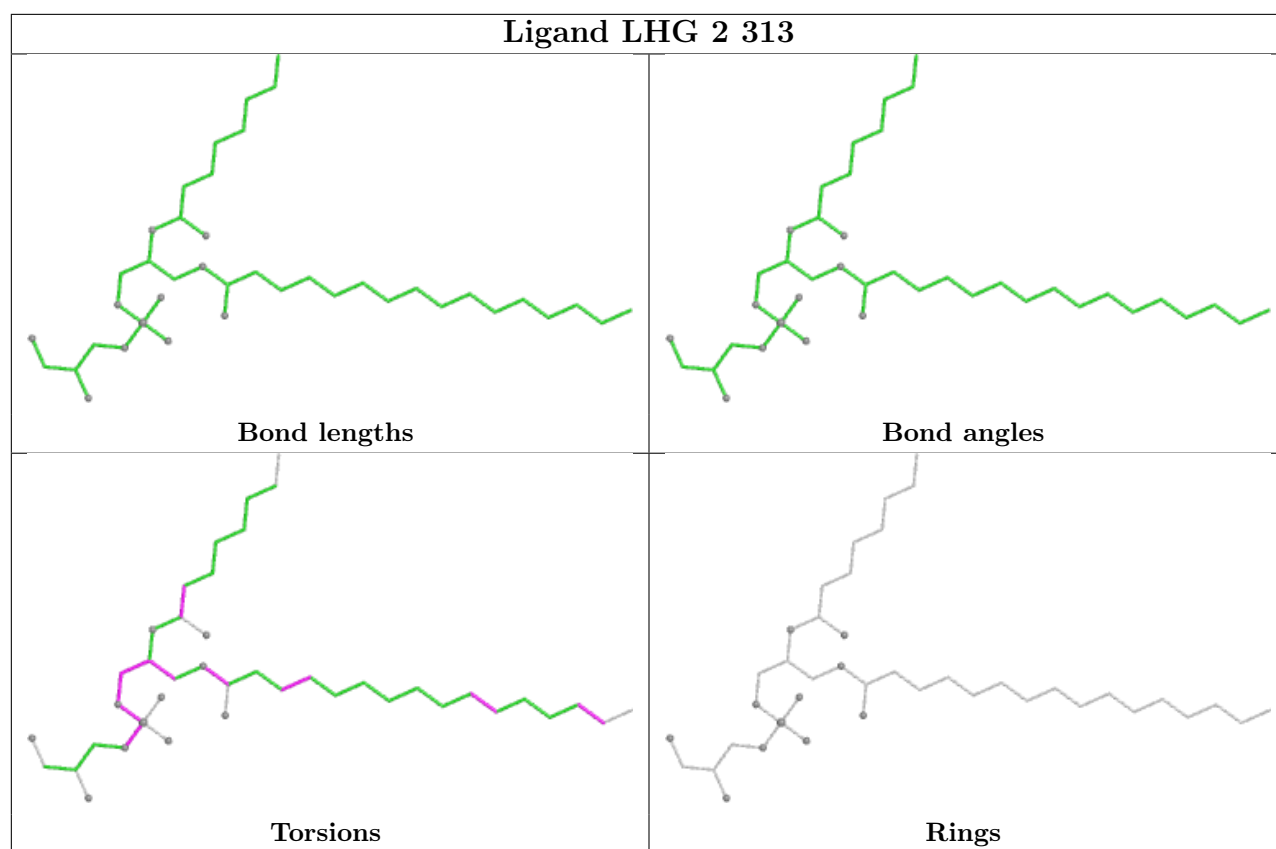


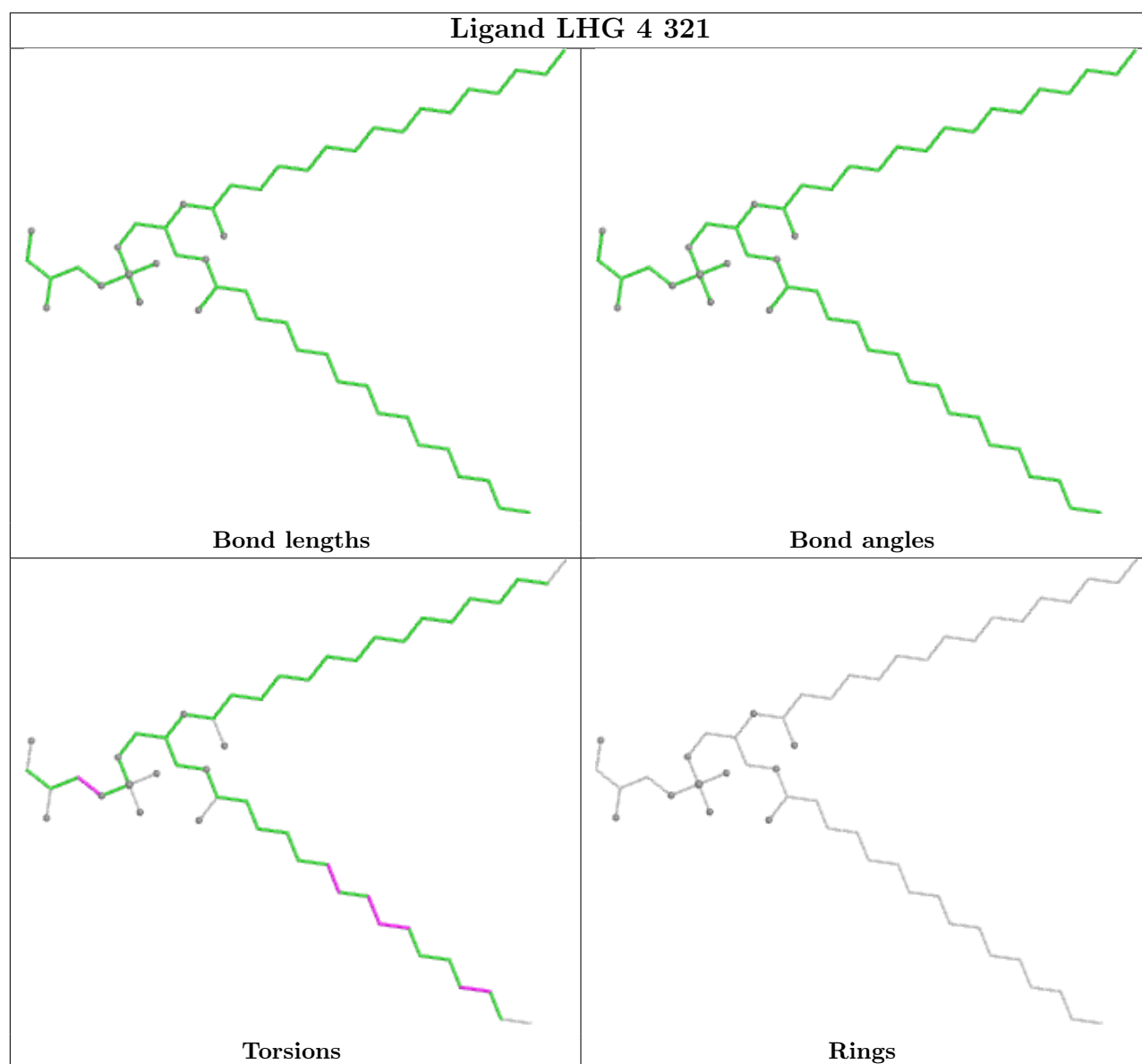
Torsions

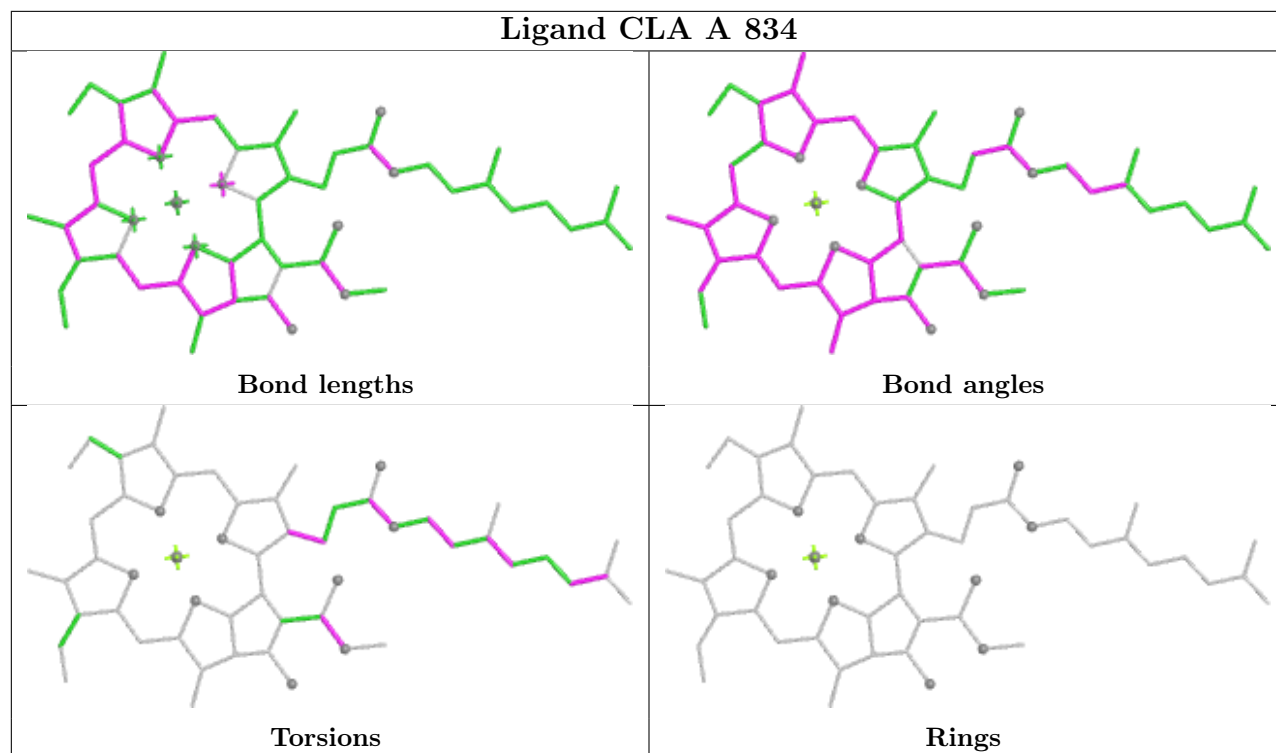
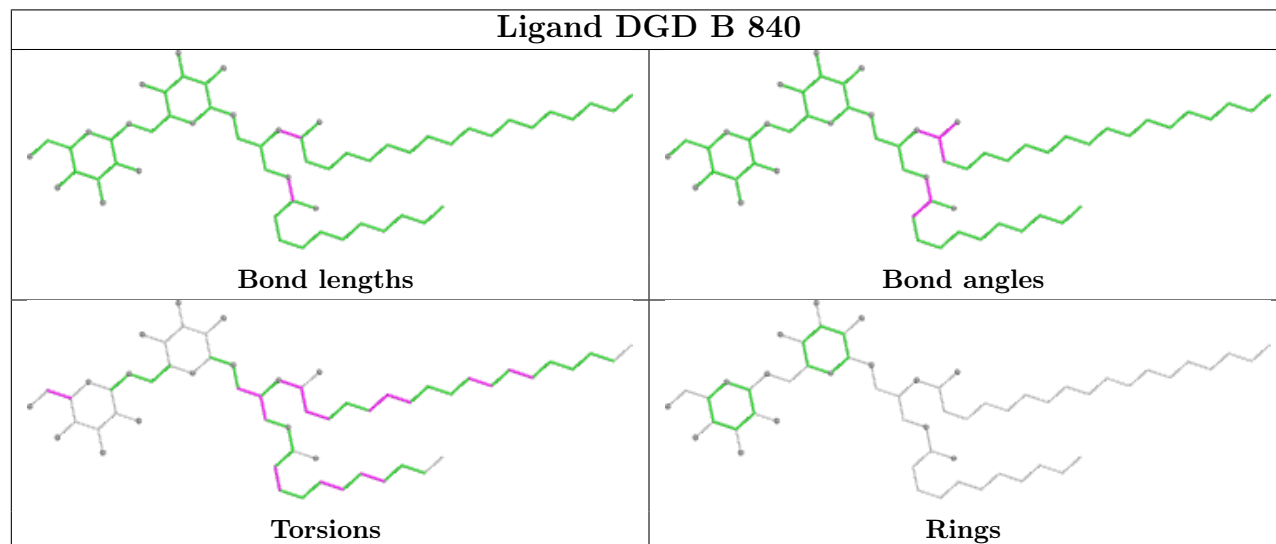


Rings

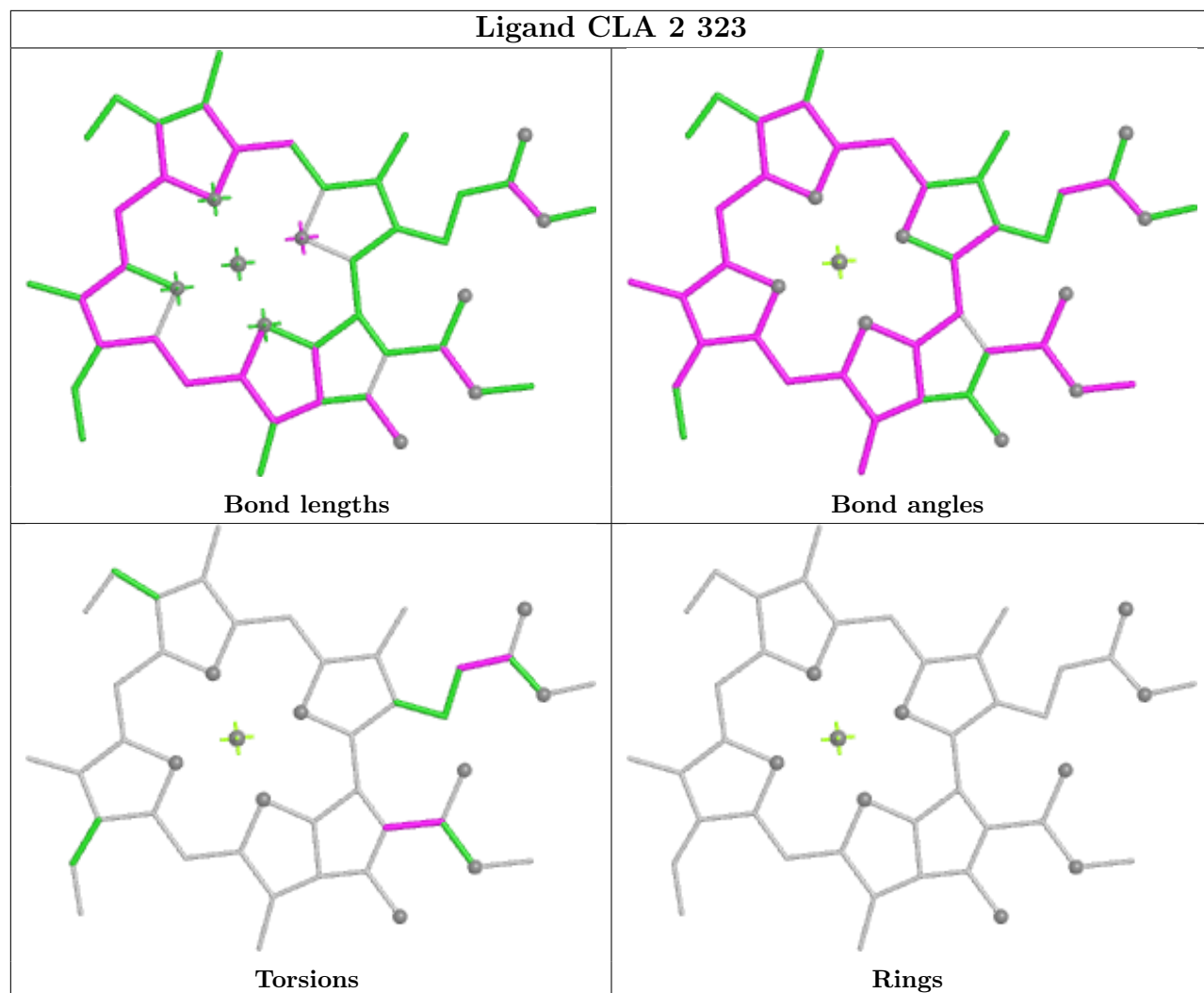




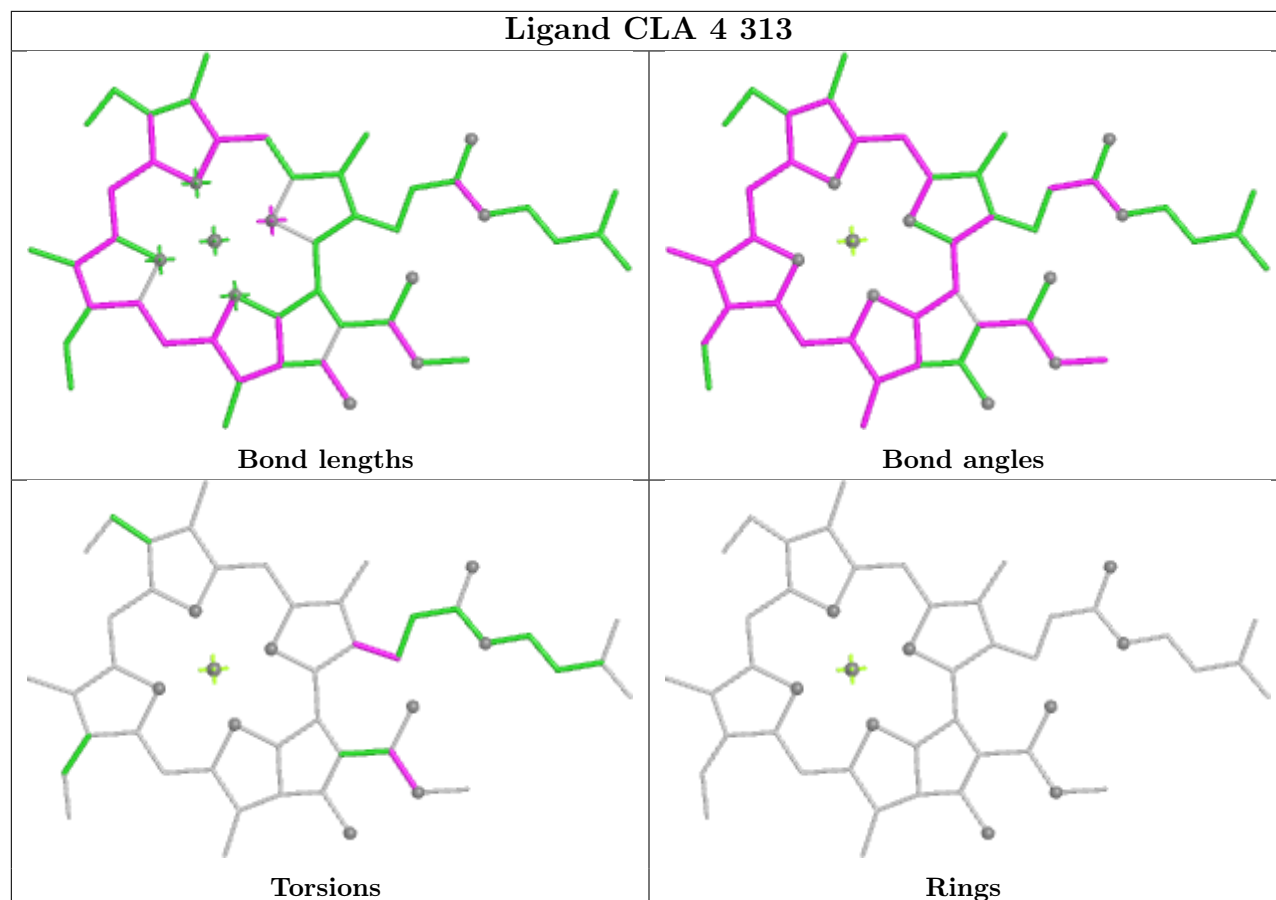


Ligand CLA A 834**Ligand DGD B 840**

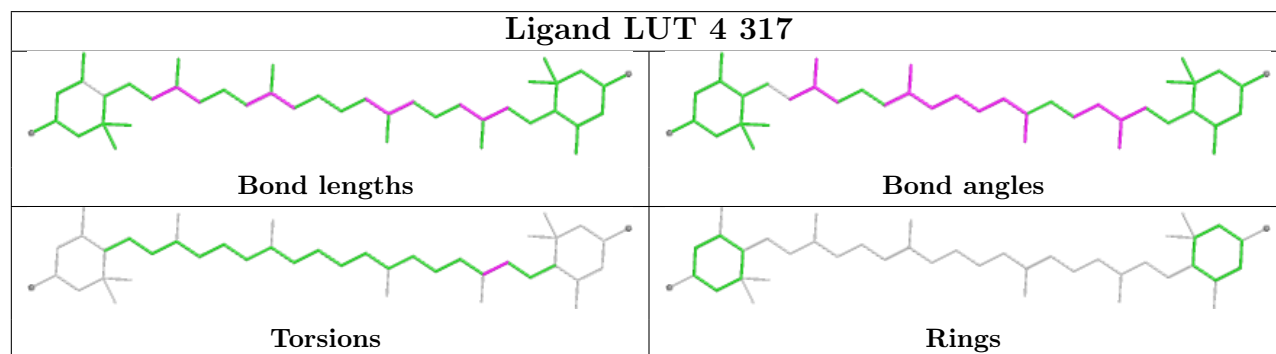
Ligand CLA 2 323



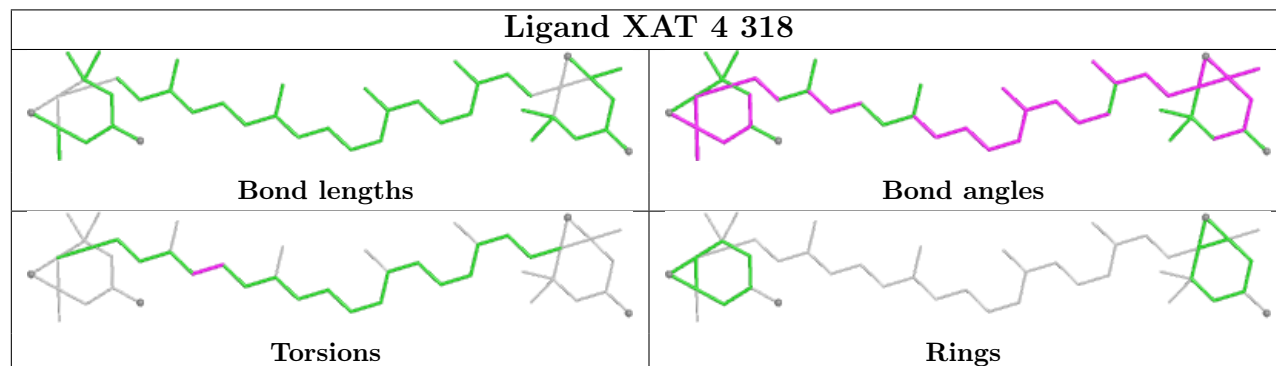
Ligand CLA 4 313

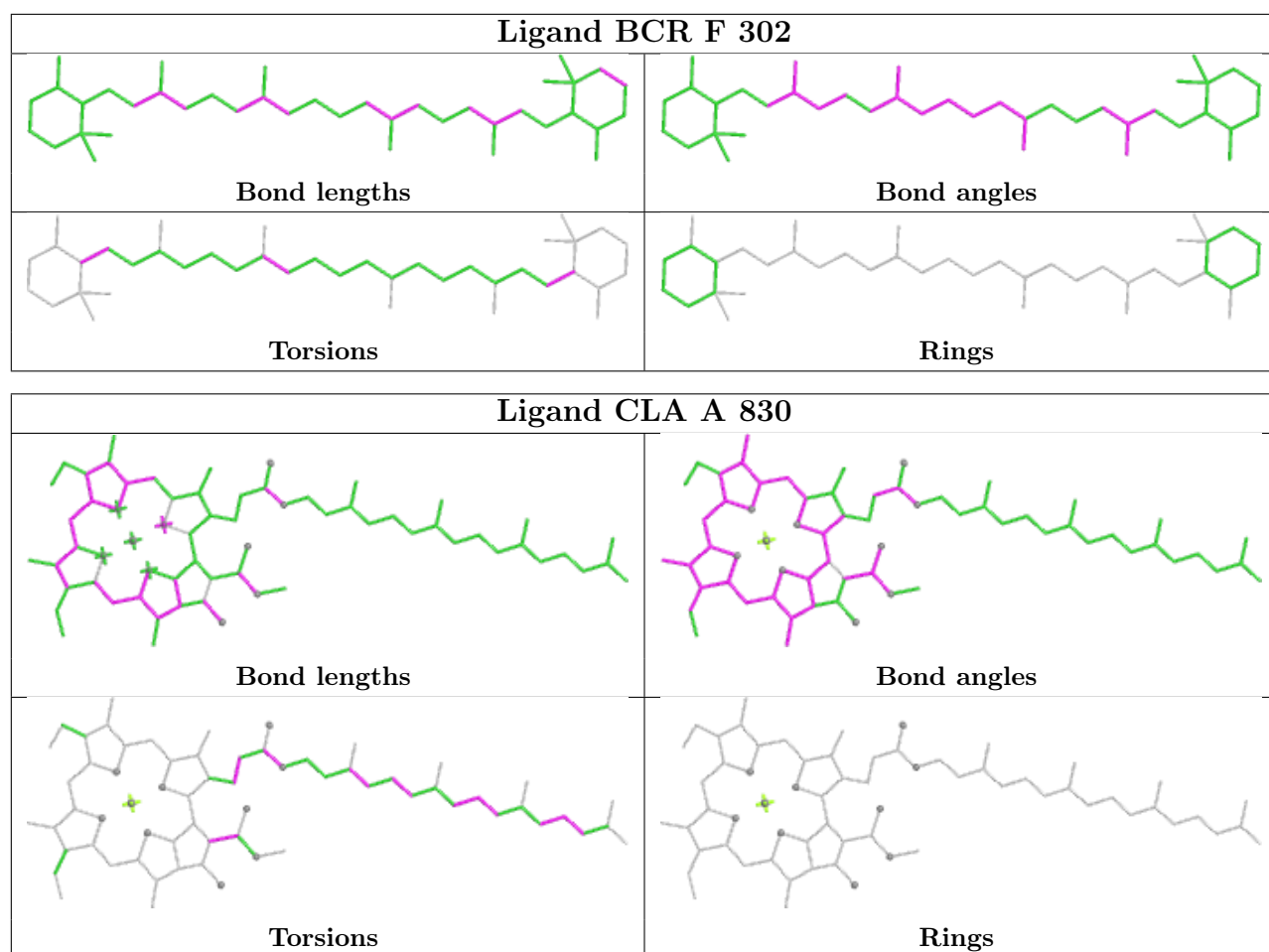


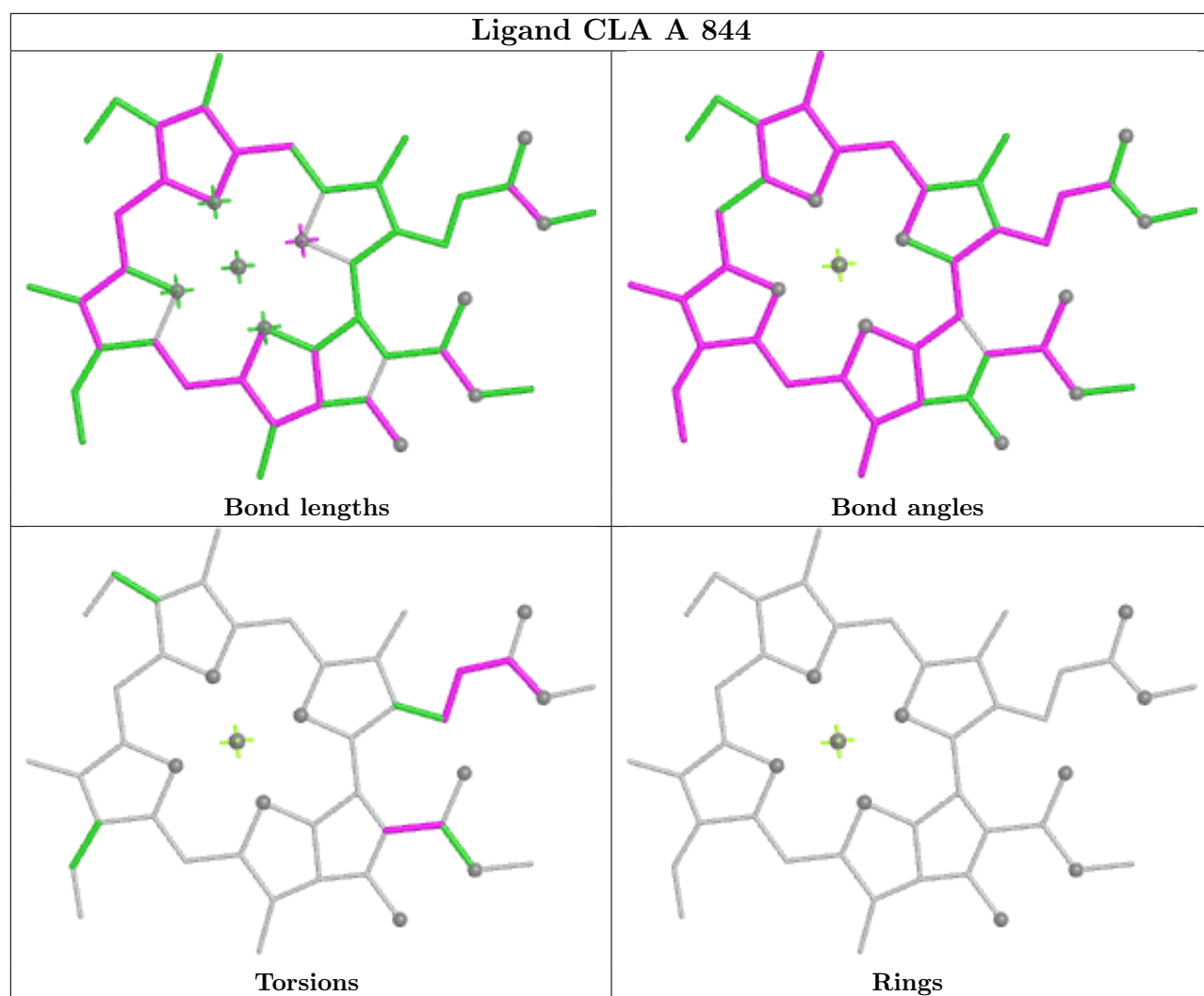
Ligand LUT 4 317



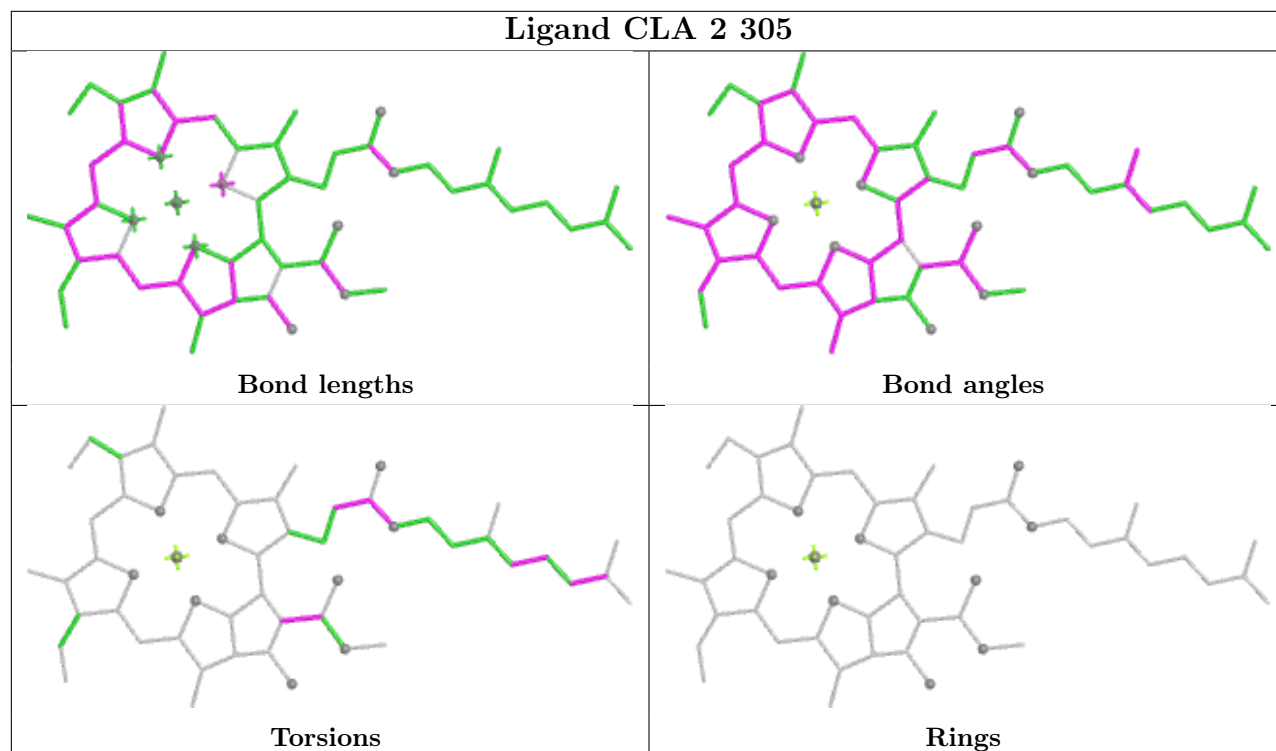
Ligand XAT 4 318



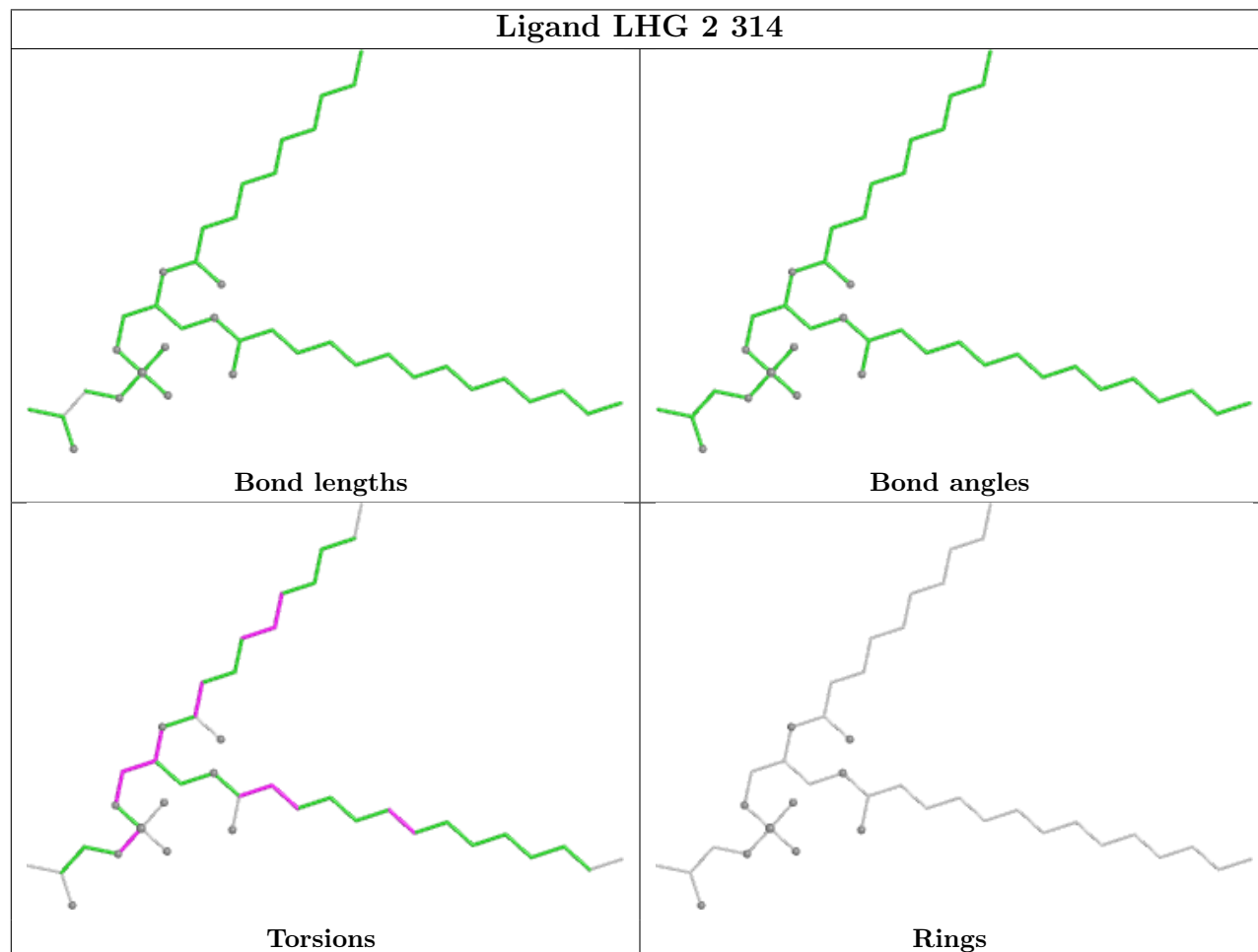


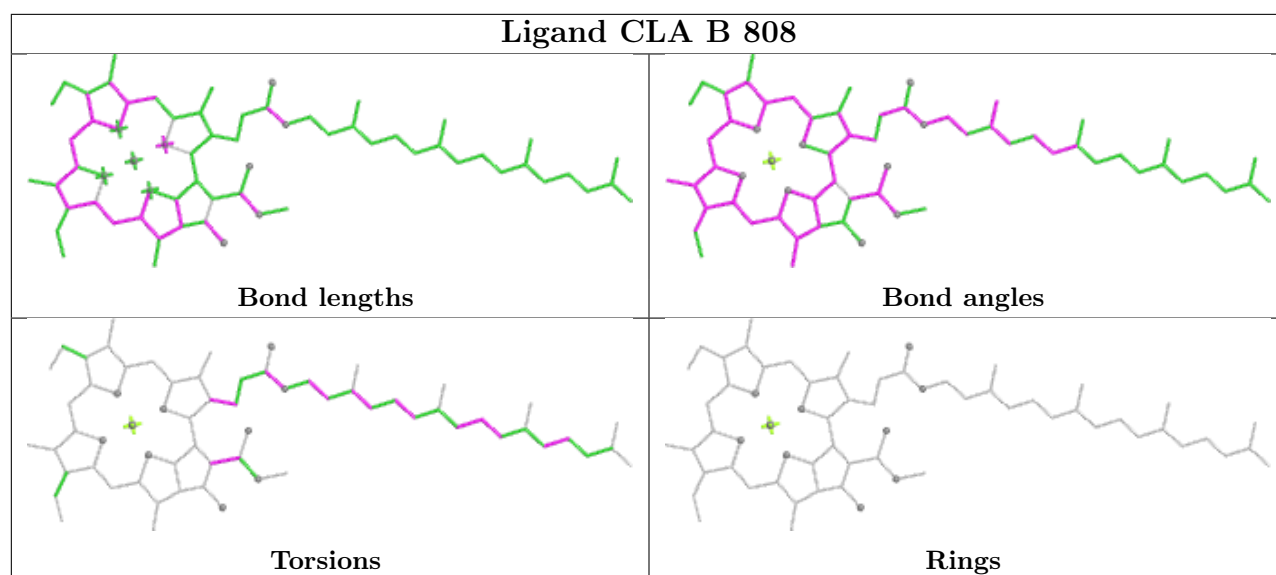


Ligand CLA 2 305



Ligand LHG 2 314





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

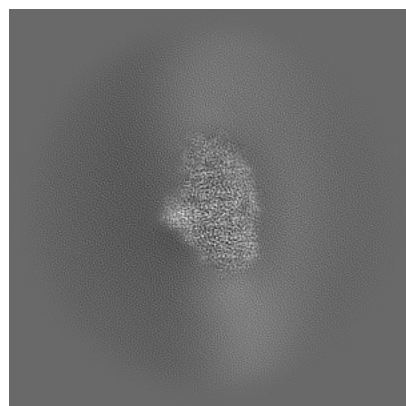
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66925. These allow visual inspection of the internal detail of the map and identification of artifacts.

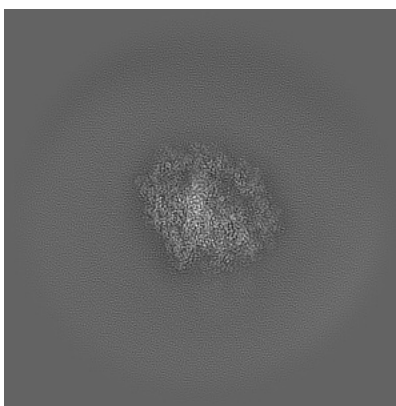
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

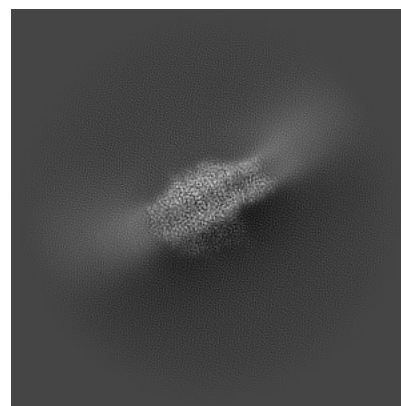
6.1.1 Primary map



X



Y

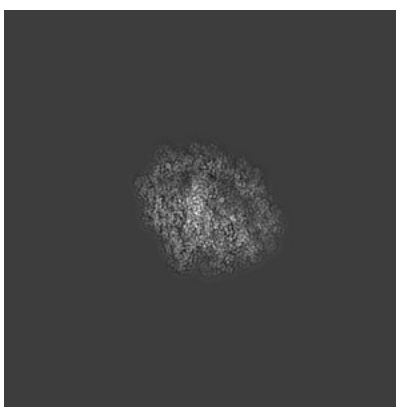


Z

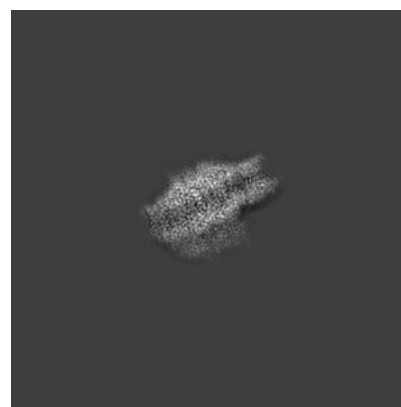
6.1.2 Raw map



X



Y

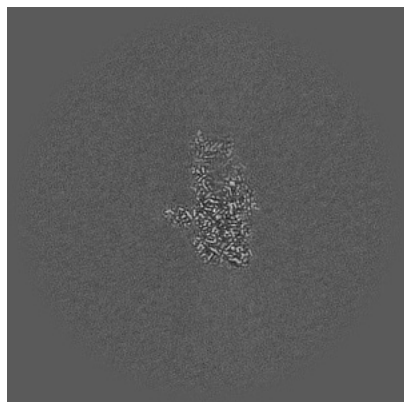


Z

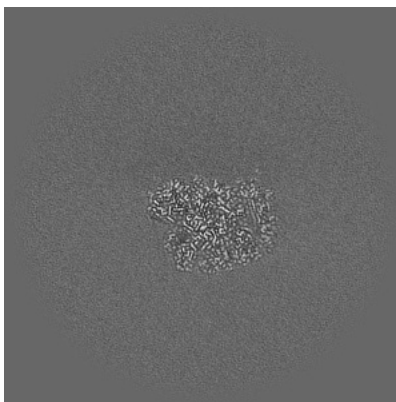
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

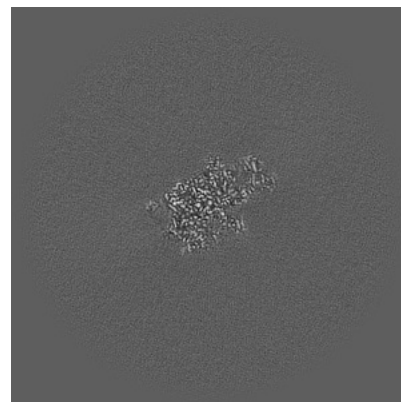
6.2.1 Primary map



X Index: 256

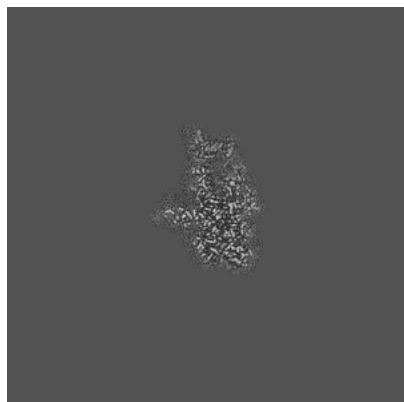


Y Index: 256

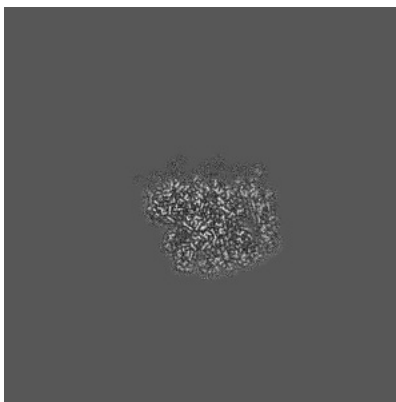


Z Index: 256

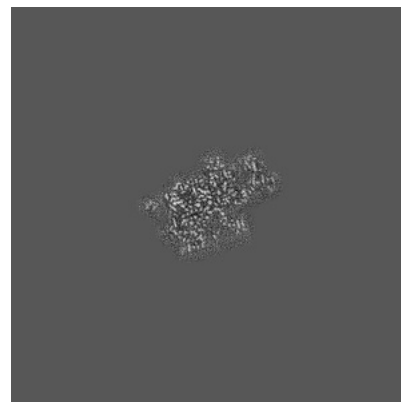
6.2.2 Raw map



X Index: 256



Y Index: 256

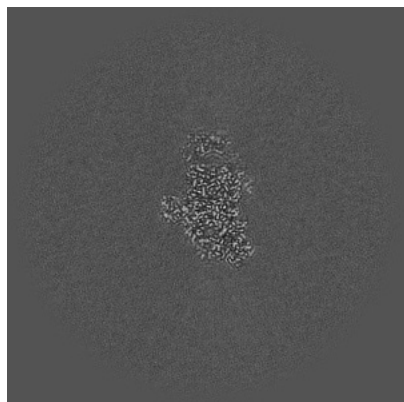


Z Index: 256

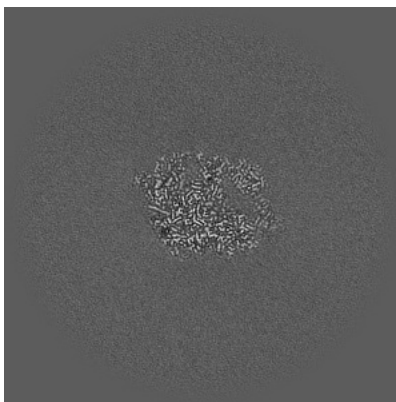
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

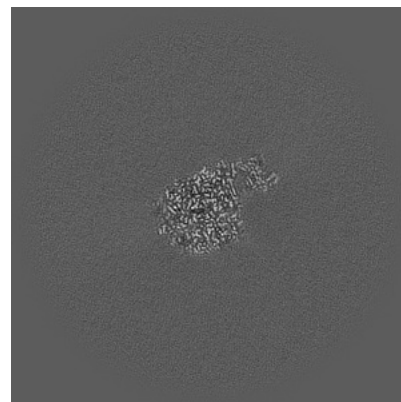
6.3.1 Primary map



X Index: 240

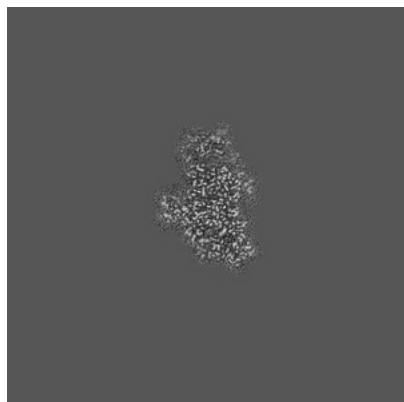


Y Index: 274

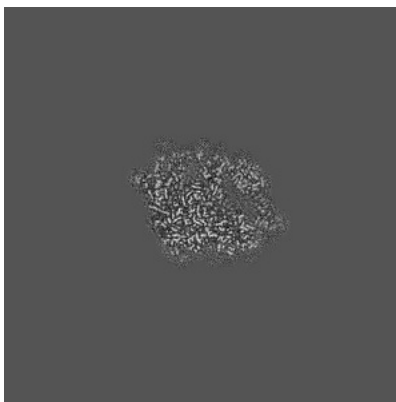


Z Index: 245

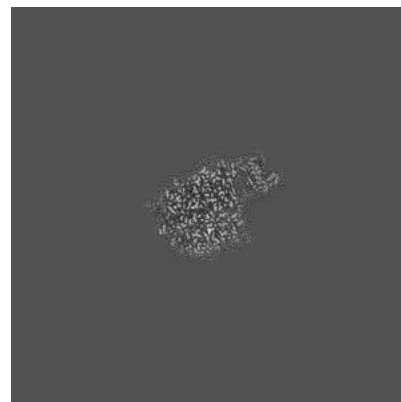
6.3.2 Raw map



X Index: 240



Y Index: 274

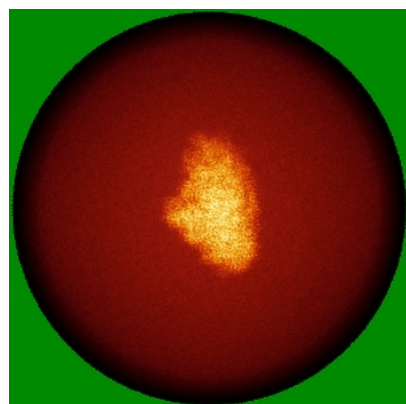


Z Index: 245

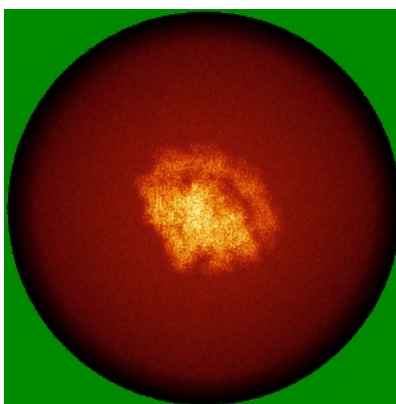
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

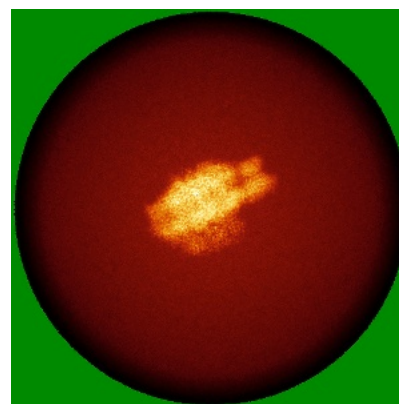
6.4.1 Primary map



X

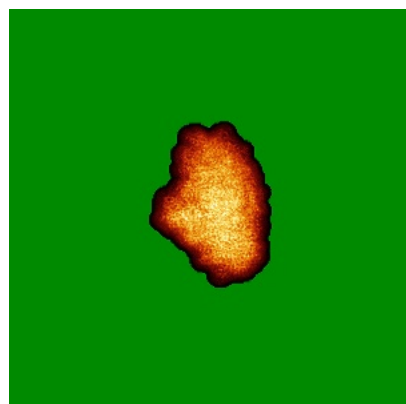


Y

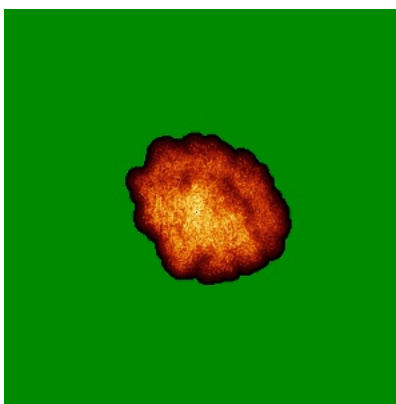


Z

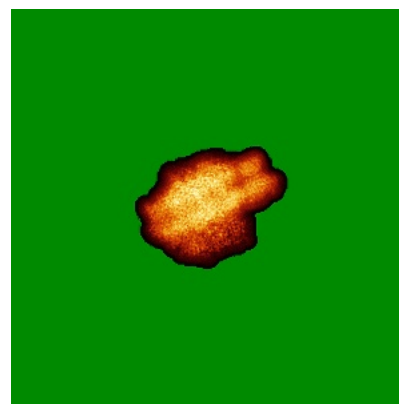
6.4.2 Raw map



X



Y

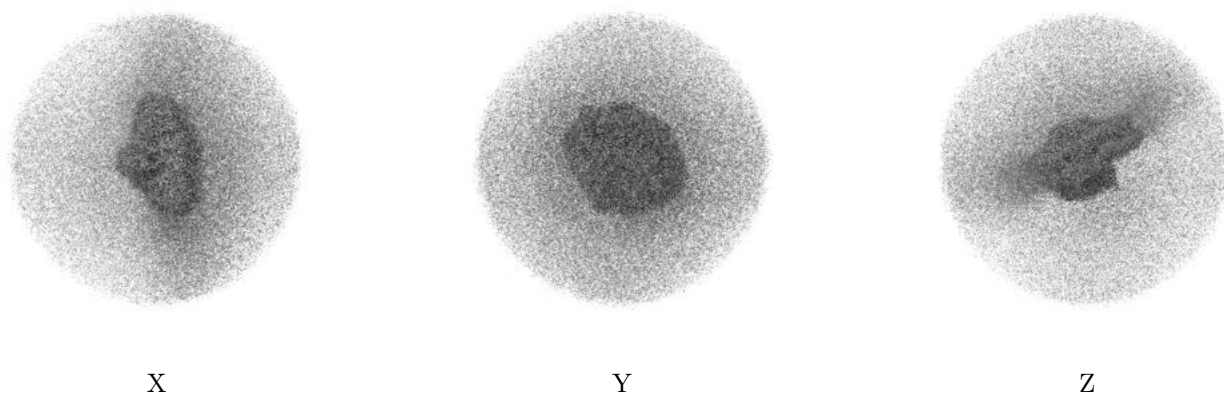


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

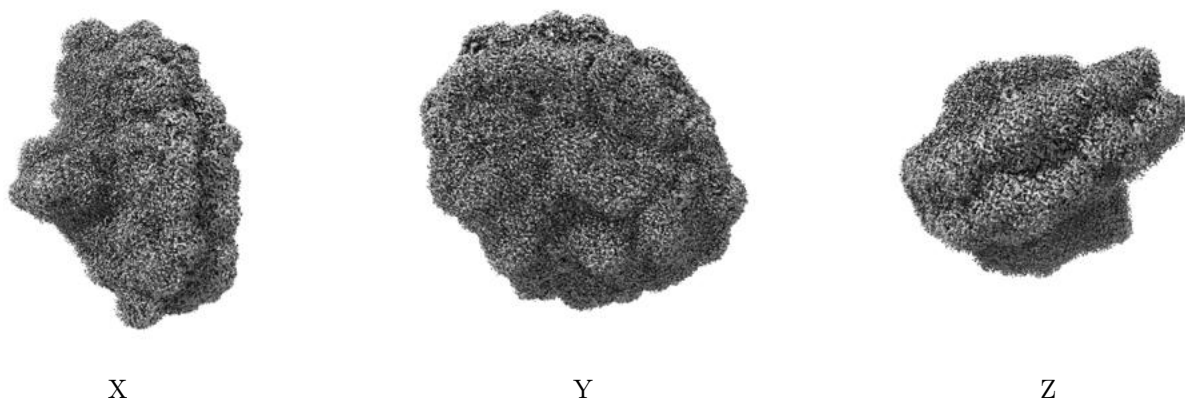
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

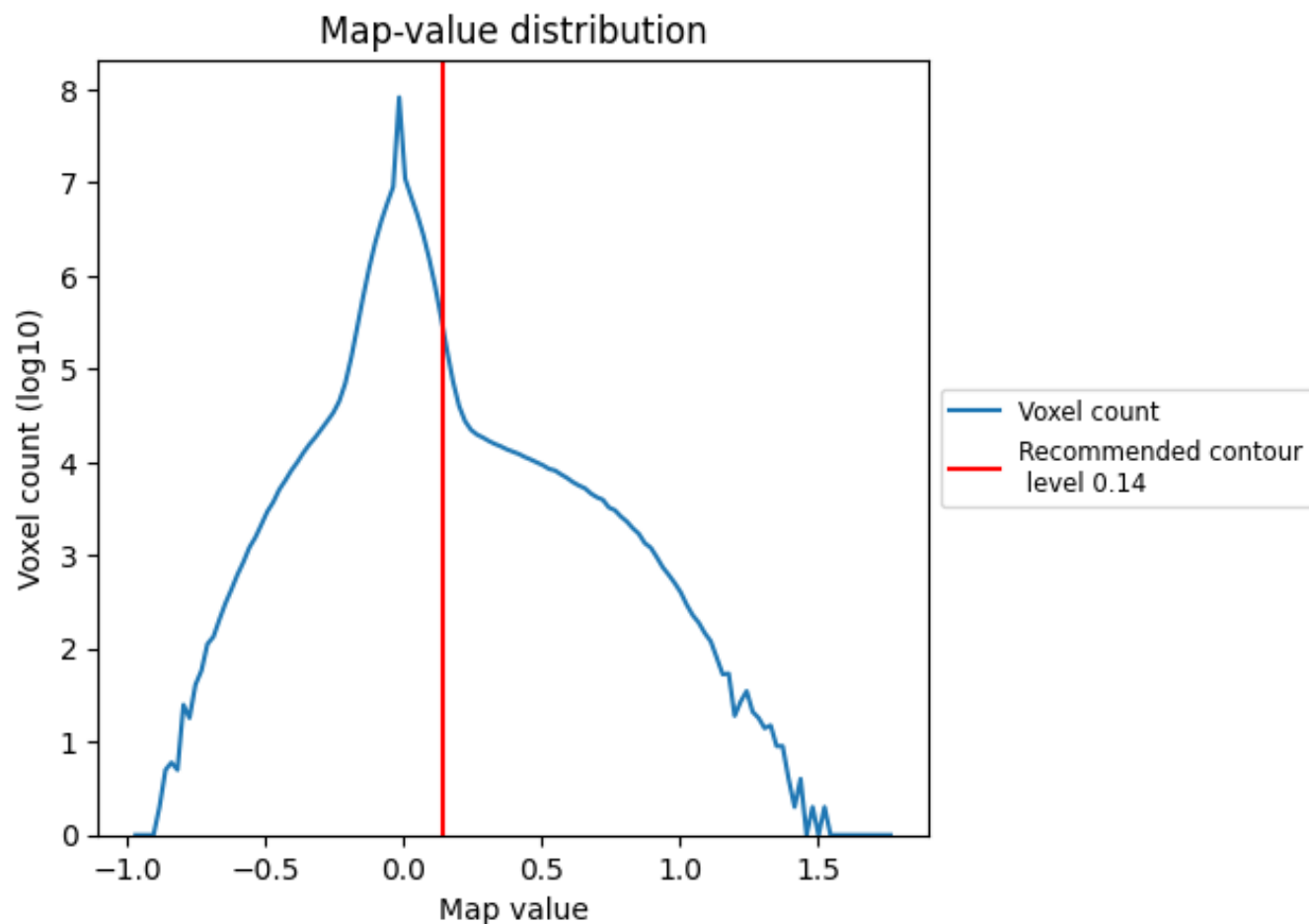
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

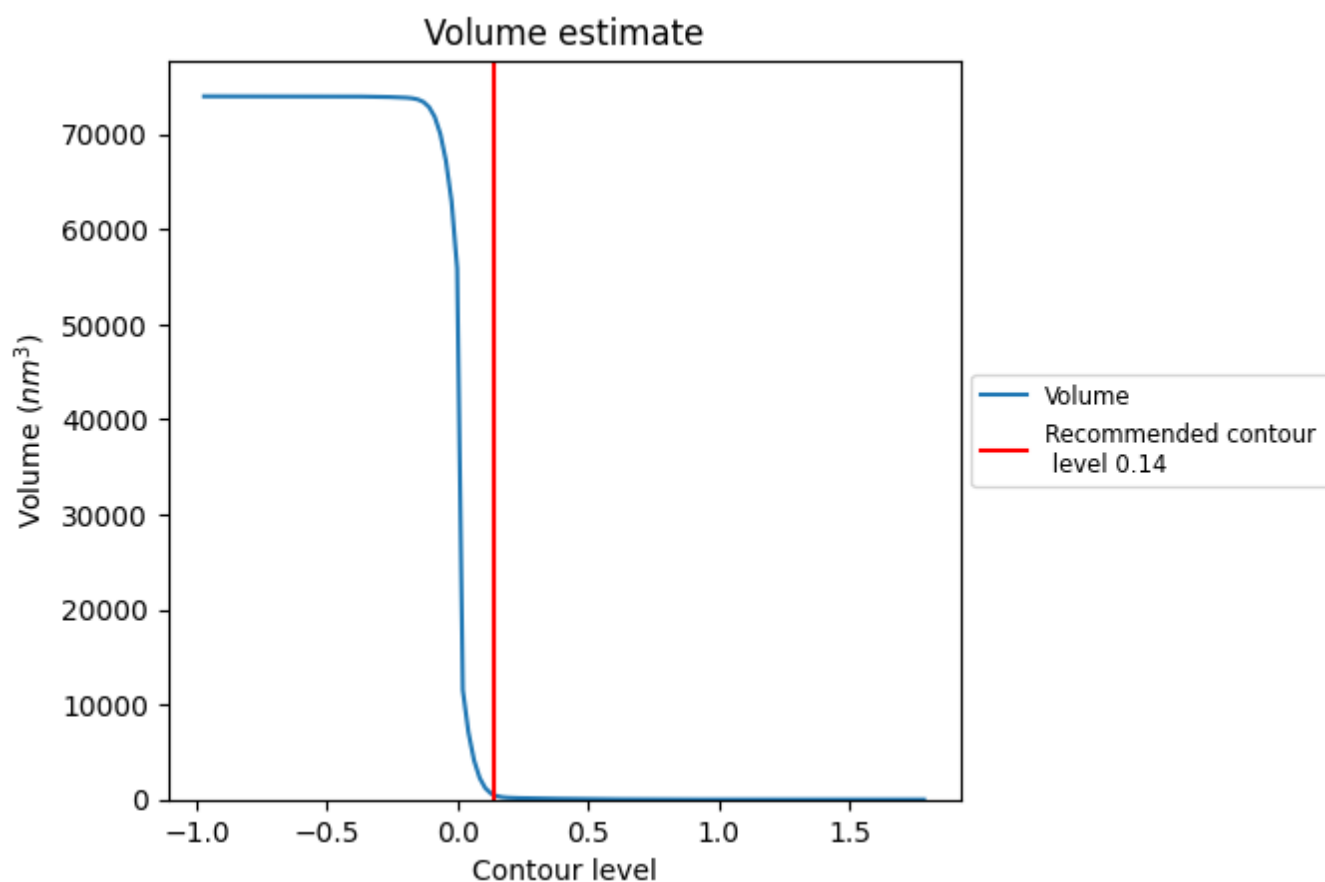
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

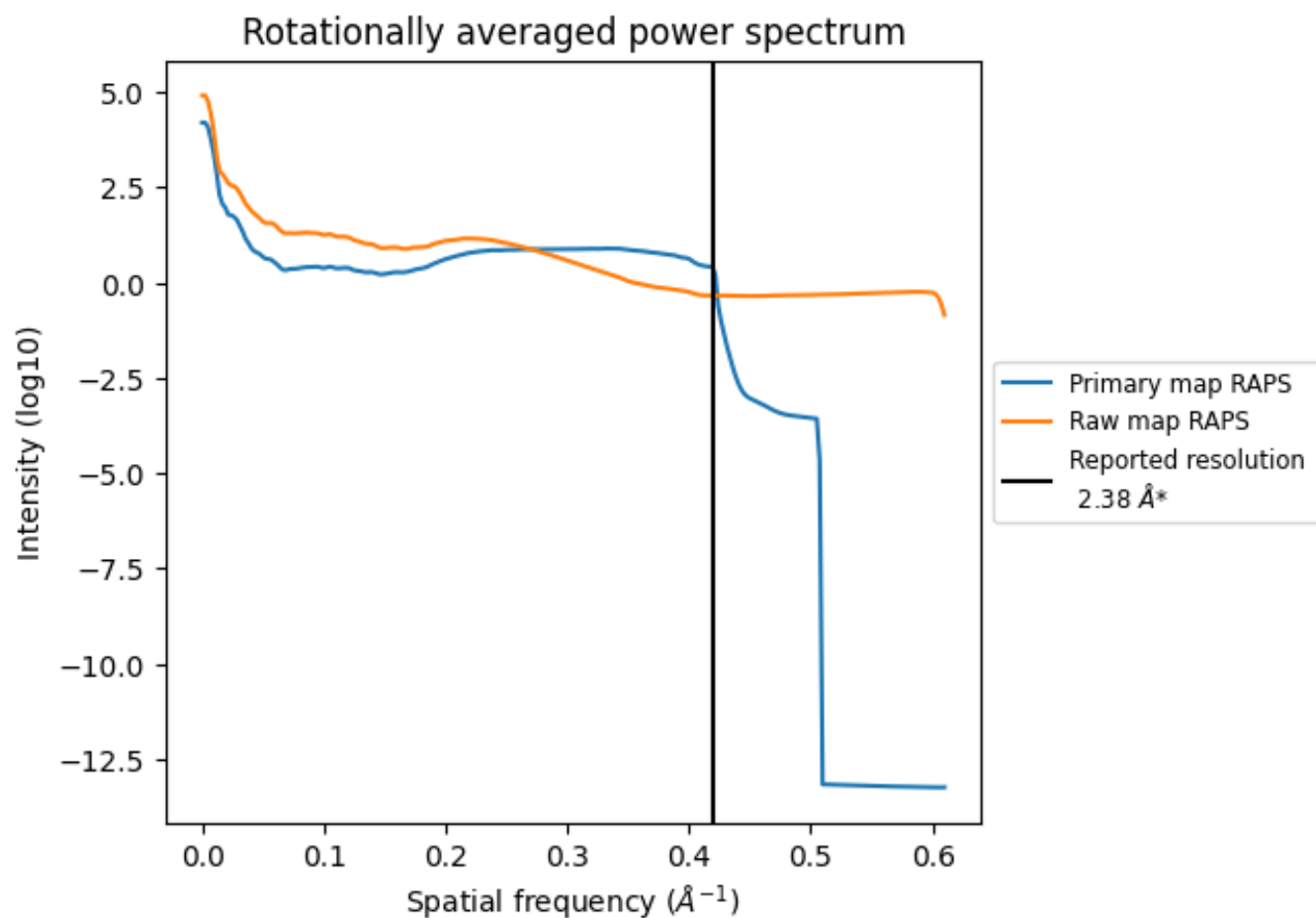
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 489 nm³; this corresponds to an approximate mass of 442 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

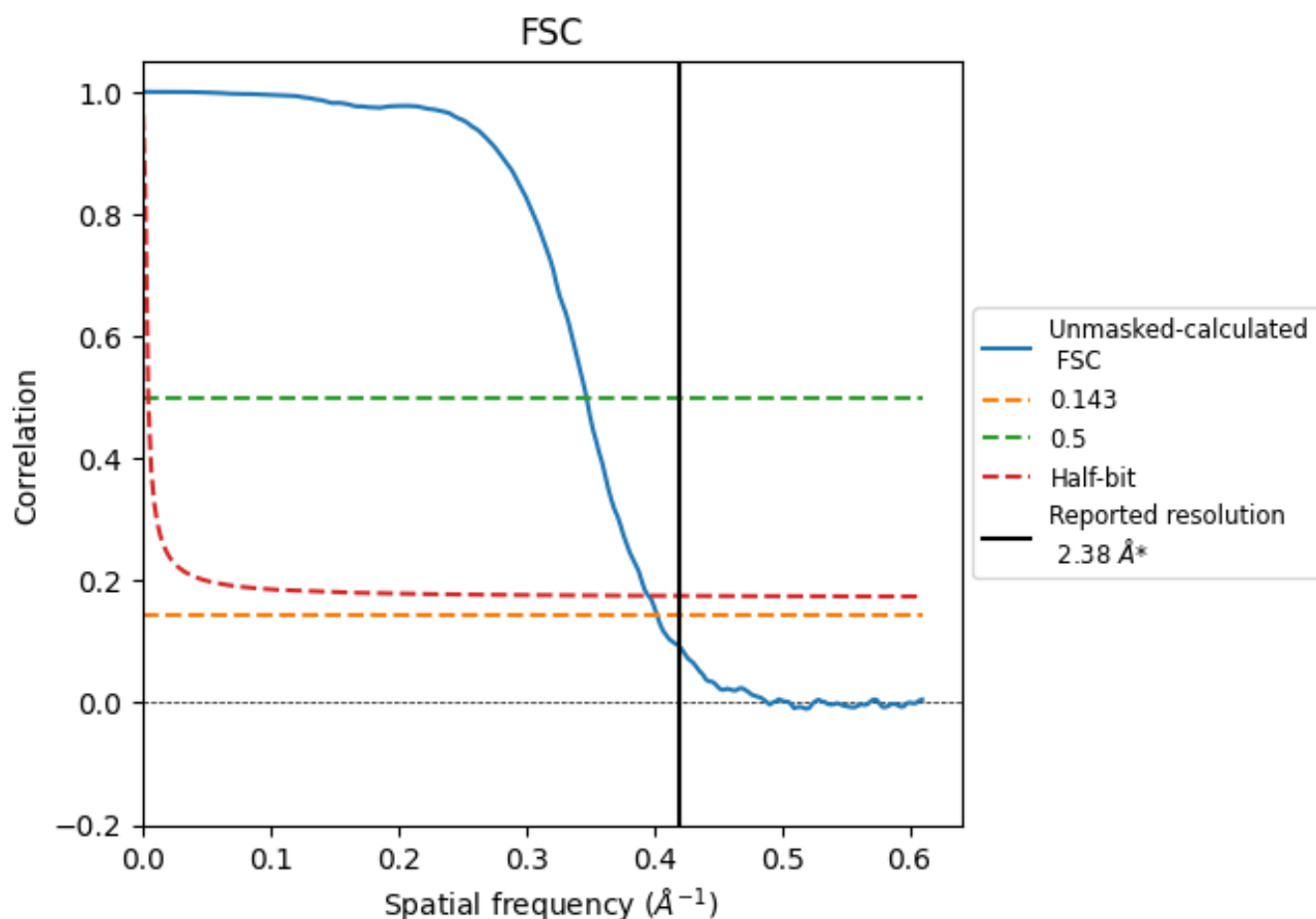


*Reported resolution corresponds to spatial frequency of 0.420 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.420 Å⁻¹

8.2 Resolution estimates [i](#)

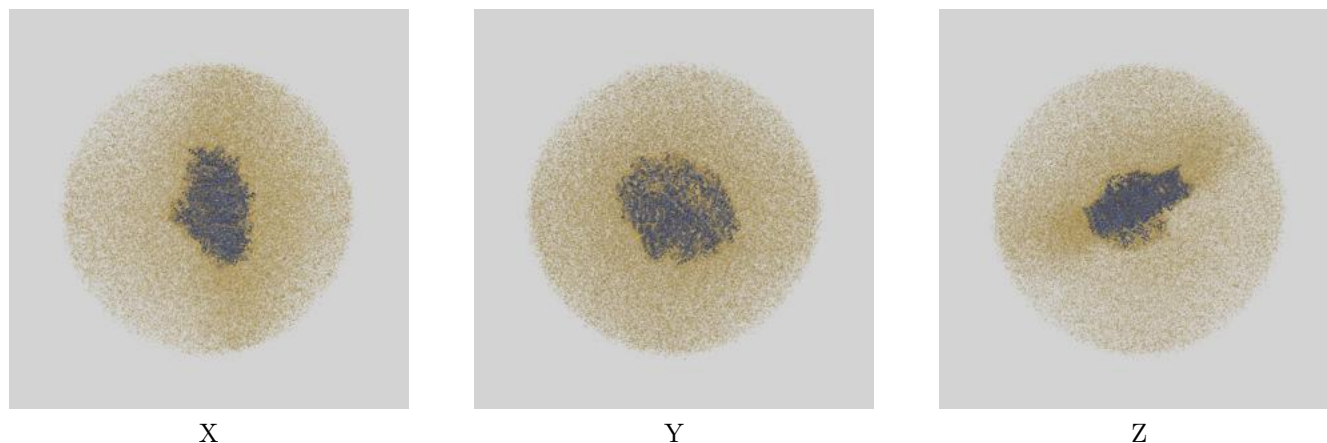
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.38	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.48	2.88	2.53

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

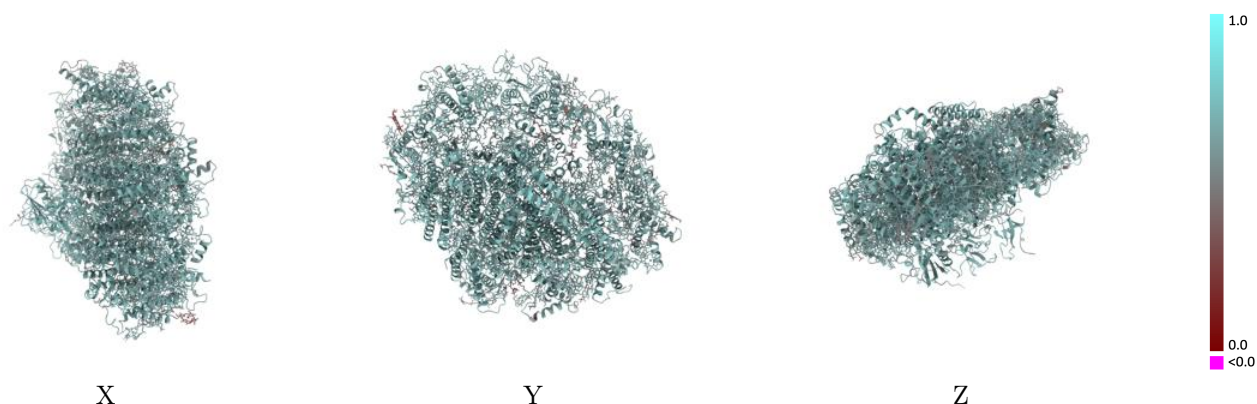
This section contains information regarding the fit between EMDB map EMD-66925 and PDB model 9XJ1. Per-residue inclusion information can be found in section [3](#) on page [27](#).

9.1 Map-model overlay [i](#)



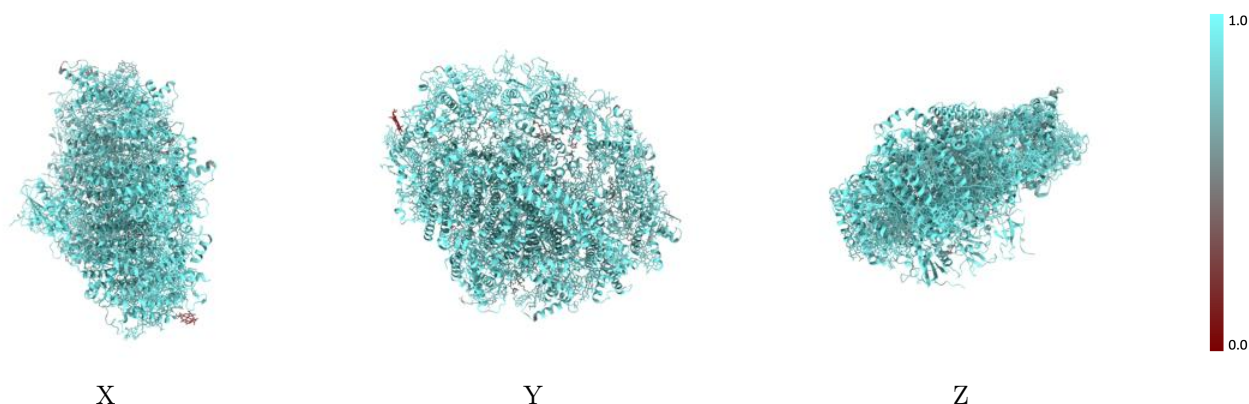
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



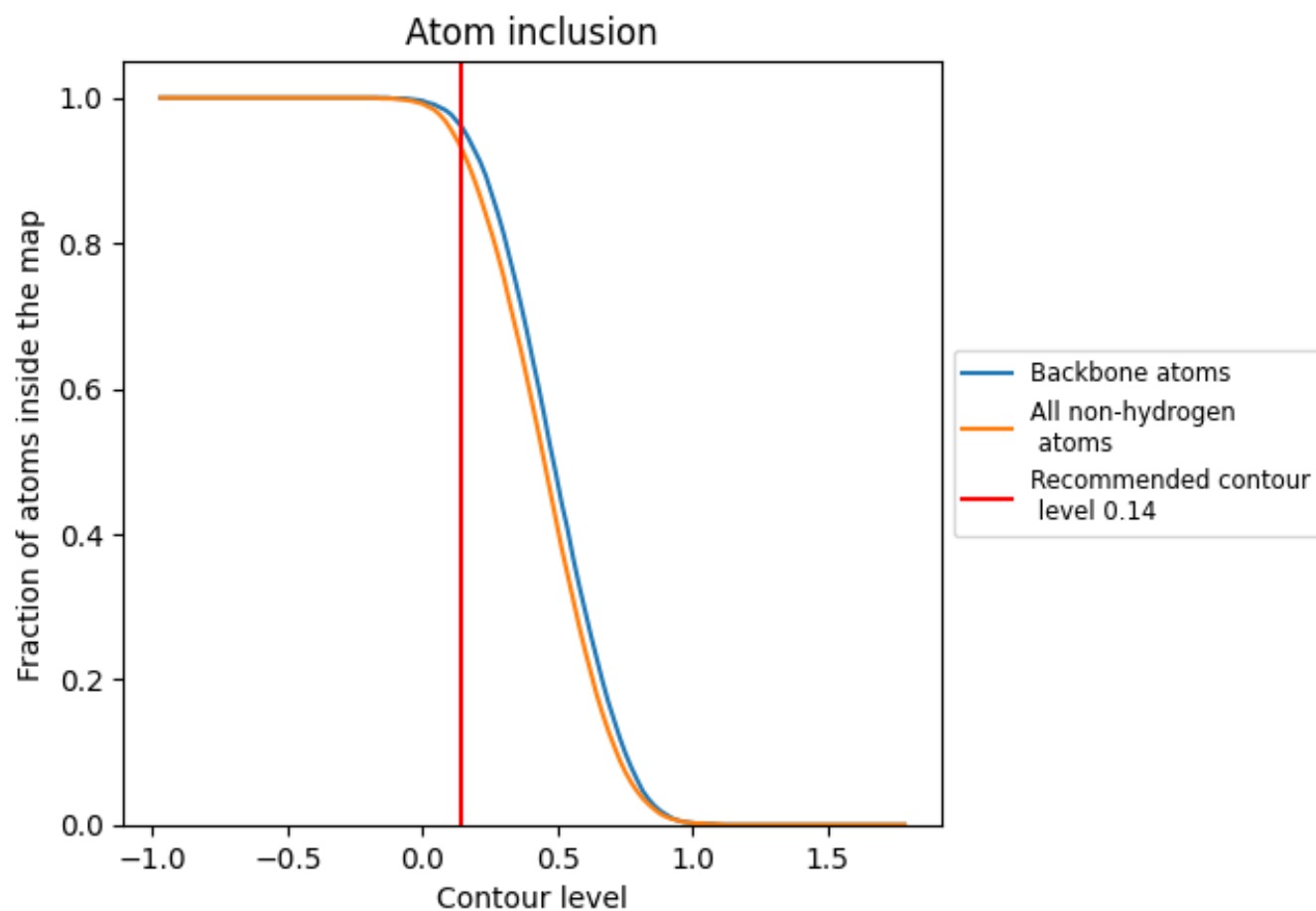
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.14).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9340	0.6460
1	0.8930	0.6190
2	0.8810	0.6200
3	0.8790	0.6140
4	0.8840	0.6100
A	0.9710	0.6700
B	0.9650	0.6670
C	0.9800	0.6720
D	0.9630	0.6590
E	0.9480	0.6500
F	0.9590	0.6630
G	0.9080	0.6330
H	0.9100	0.6240
I	0.9250	0.6310
J	0.9270	0.6330
K	0.9070	0.6240
L	0.9570	0.6550
N	0.8210	0.6040
O	0.8780	0.6070

