



## Full wwPDB EM Validation Report ⓘ

Jun 22, 2026 – 03:28 PM JST

PDB ID : 9M5A / pdb\_00009m5a  
EMDB ID : EMD-63639  
Title : cryo-EM structure of PSII D1-V185T from *Thermosynechococcus vestitus* BP-1  
Authors : Jiang, H.W.; Nakajima, Y.; Akita, F.; Li, H.J.; Kato, K.; Sugiura, M.; Shen, J.R.  
Deposited on : 2025-03-05  
Resolution : 1.88 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](mailto: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:

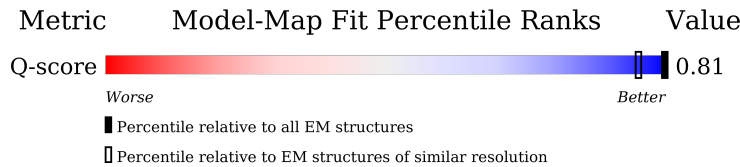
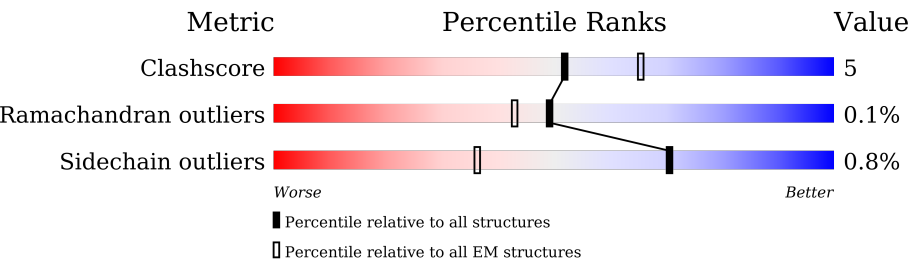
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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) : 2.49

# 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 1.88 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.






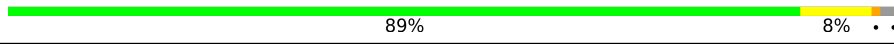


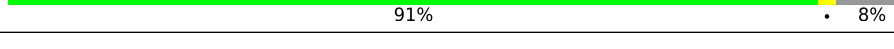
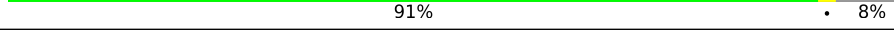
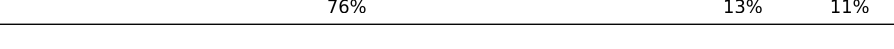
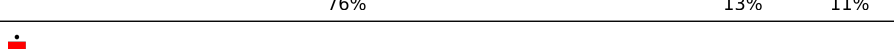
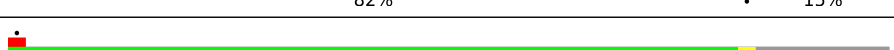

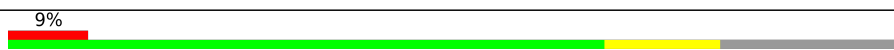

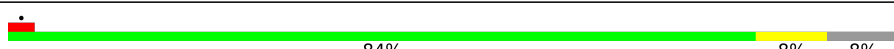





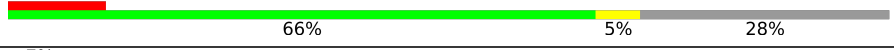
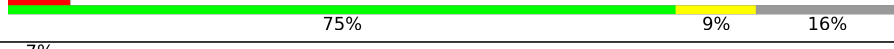



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1004 ( 1.39 - 2.38 )

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  $\geq 3$ , 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	A	360	<div><div></div><div>83%</div><div>9%</div><div>7%</div></div>
1	a	360	<div><div></div><div>84%</div><div>9%</div><div>7%</div></div>
2	B	510	<div><div></div><div>87%</div><div>12%</div><div>.</div></div>
2	b	510	<div><div></div><div>87%</div><div>12%</div><div>.</div></div>

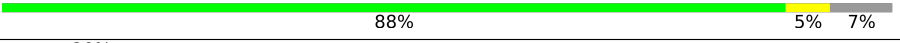








Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	F	45	
5	f	45	
6	H	66	
6	h	66	
7	I	38	
7	i	38	
8	J	40	
8	j	40	
9	K	46	
9	k	46	
10	L	37	
10	l	37	
11	M	36	
11	m	36	
12	T	32	
12	t	32	
13	U	134	
13	u	134	
14	V	163	
14	v	163	
15	X	41	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	x	41	
16	Y	46	
16	y	46	
17	E	84	
17	e	84	
18	O	272	
18	o	272	
19	Z	62	
19	z	62	

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
29	UNL	d	413	-	-	X	-

## 2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 50208 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 Photosystem II protein D1 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	5	1
			2625	1723	431	457	14		
1	a	334	Total	C	N	O	S	5	1
			2625	1723	431	457	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	185	THR	VAL	conflict	UNP Q8DIV4
a	185	THR	VAL	conflict	UNP Q8DIV4

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	504	Total	C	N	O	S	1	0
			3896	2571	646	666	13		
2	b	504	Total	C	N	O	S	1	0
			3896	2571	646	666	13		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	450	Total	C	N	O	S	2	1
			3451	2264	576	598	13		
3	c	450	Total	C	N	O	S	2	1
			3451	2264	576	598	13		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	2	1
			2700	1793	439	456	12		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	341	Total	C	N	O	S	2	1
			2700	1793	439	456	12		

- Molecule 5 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	33	Total	C	N	O	S	0	0
			269	184	44	40	1		
5	f	33	Total	C	N	O	S	0	0
			269	184	44	40	1		

- Molecule 6 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	61	Total	C	N	O	S	0	0
			474	319	73	80	2		
6	h	61	Total	C	N	O	S	0	0
			474	319	73	80	2		

- Molecule 7 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	34	Total	C	N	O	S	0	0
			265	182	39	43	1		
7	i	34	Total	C	N	O	S	0	0
			265	182	39	43	1		

- Molecule 8 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	34	Total	C	N	O	S	0	0
			243	167	35	40	1		
8	j	34	Total	C	N	O	S	0	0
			243	167	35	40	1		

- Molecule 9 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	K	37	Total	C	N	O	0	0
			285	199	42	44		
9	k	37	Total	C	N	O	0	0
			285	199	42	44		

- Molecule 10 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	34	Total	C	N	O	1	0
			278	189	42	47		
10	l	34	Total	C	N	O	1	0
			278	189	42	47		

- Molecule 11 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	33	Total	C	N	O	S	0	0
			249	168	36	44	1		
11	m	33	Total	C	N	O	S	0	0
			249	168	36	44	1		

- Molecule 12 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	29	Total	C	N	O	S	0	0
			241	172	32	35	2		
12	t	29	Total	C	N	O	S	0	0
			241	172	32	35	2		

- Molecule 13 is a protein called Photosystem II extrinsic protein U.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	U	96	Total	C	N	O	0	0
			718	463	123	132		
13	u	96	Total	C	N	O	0	0
			718	463	123	132		

- Molecule 14 is a protein called Photosystem II extrinsic protein V.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	137	Total	C	N	O	S	1	0
			1024	654	169	197	4		
14	v	137	Total	C	N	O	S	1	0
			1024	654	169	197	4		

- Molecule 15 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	X	38	Total	C	N	O	0	1
			269	180	43	46		
15	x	38	Total	C	N	O	0	1
			269	180	43	46		

- Molecule 16 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	29	Total	C	N	O	S	0	0
			199	132	31	33	3		
16	y	29	Total	C	N	O	S	0	0
			199	132	31	33	3		

- Molecule 17 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	E	78	Total	C	N	O	1	0
			610	404	97	109		
17	e	78	Total	C	N	O	1	0
			610	404	97	109		

- Molecule 18 is a protein called Photosystem II extrinsic protein O.

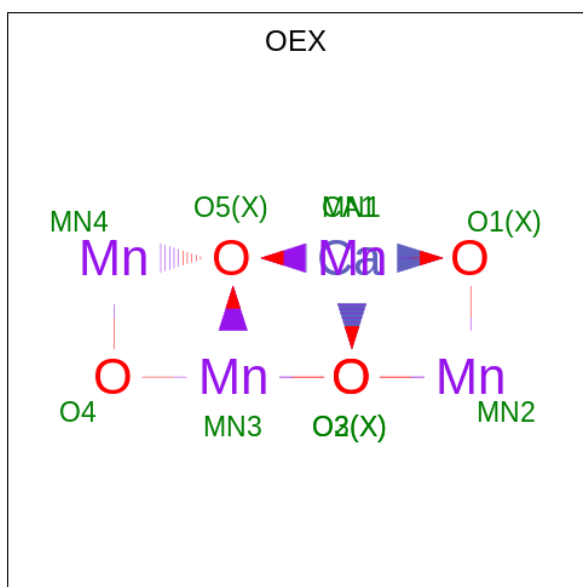
Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	233	Total	C	N	O	S	3	0
			1676	1066	283	322	5		
18	o	233	Total	C	N	O	S	3	0
			1676	1066	283	322	5		

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	55	Total 393	C 270	N 58	O 63	S 2	0	0
19	z	55	Total 393	C 270	N 58	O 63	S 2	0	0

- Molecule 20 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).





Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
20	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

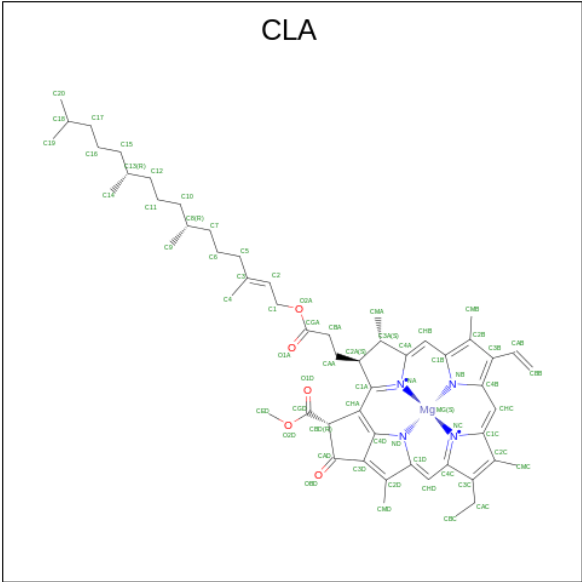
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	Fe	0
			1	1	
21	a	1	Total	Fe	0
			1	1	

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
22	A	2	Total	Cl	0
			2	2	
22	a	2	Total	Cl	0
			2	2	

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					AltConf
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			58	49	1	4	4	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 46	C 36	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 52	C 42	Mg 1	N 4	O 5	0
23	C	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	D	1	Total 48	C 38	Mg 1	N 4	O 5	0

*Continued on next page...*

*Continued from previous page...*

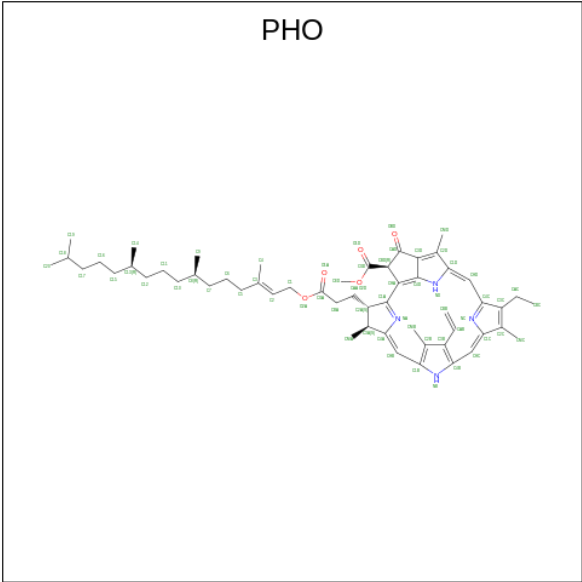
Mol	Chain	Residues	Atoms					AltConf
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
23	a	1	Total 52	C 42	Mg 1	N 4	O 5	0
23	b	1	Total 58	C 49	Mg 1	N 4	O 4	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

*Continued on next page...*

*Continued from previous page...*

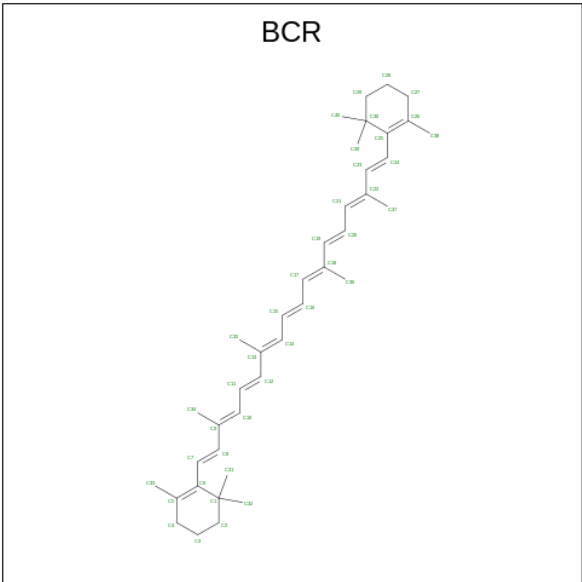
Mol	Chain	Residues	Atoms					AltConf
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	d	1	Total	C	Mg	N	O	0
			48	38	1	4	5	

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



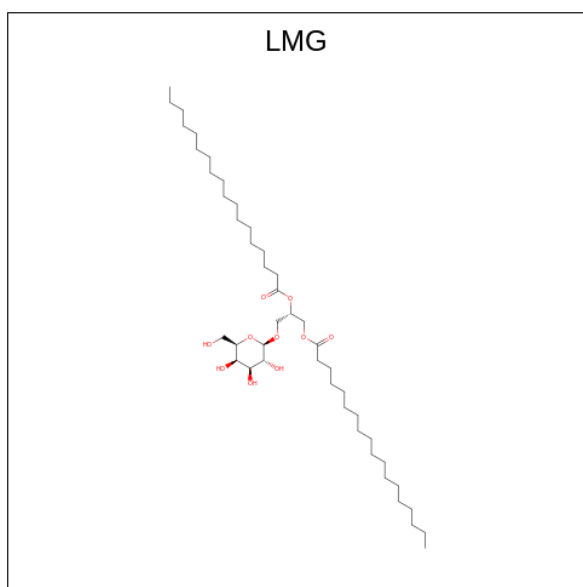
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	N	O	0
			64	55	4	5	
24	D	1	Total	C	N	O	0
			64	55	4	5	
24	a	1	Total	C	N	O	0
			64	55	4	5	
24	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ).



Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 37 37	0
25	B	1	Total C 40 40	0
25	C	1	Total C 38 38	0
25	C	1	Total C 40 40	0
25	D	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	T	1	Total C 39 39	0
25	Y	1	Total C 40 40	0
25	a	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	b	1	Total C 37 37	0
25	b	1	Total C 40 40	0
25	c	1	Total C 38 38	0
25	c	1	Total C 40 40	0
25	d	1	Total C 40 40	0
25	k	1	Total C 40 40	0
25	t	1	Total C 39 39	0
25	y	1	Total C 40 40	0

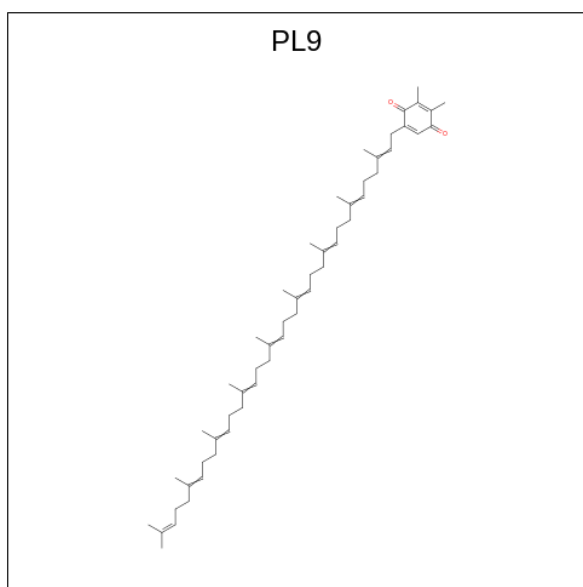
- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			51	41	10	
26	B	1	Total	C	O	0
			47	37	10	
26	C	1	Total	C	O	0
			51	41	10	
26	C	1	Total	C		0
			16	16		
26	D	1	Total	C	O	0
			43	33	10	
26	a	1	Total	C	O	0
			51	41	10	
26	b	1	Total	C	O	0
			47	37	10	
26	c	1	Total	C	O	0
			51	41	10	
26	c	1	Total	C		0
			16	16		
26	d	1	Total	C	O	0
			43	33	10	

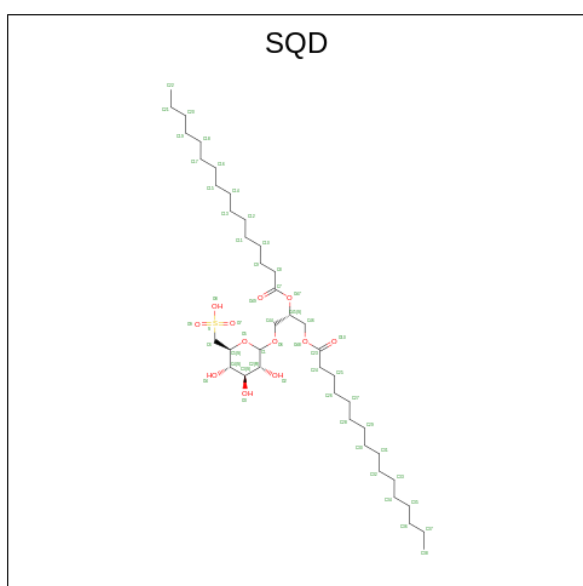
- Molecule 27 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).





Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			42	40	2	
27	D	1	Total	C	O	0
			55	53	2	
27	a	1	Total	C	O	0
			42	40	2	
27	d	1	Total	C	O	0
			55	53	2	

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O	S	0
			39	26	12	1	
28	C	1	Total	C	O	S	0
			32	19	12	1	
28	D	1	Total	C	O	S	0
			27	15	11	1	
28	T	1	Total	C	O		0
			27	25	2		
28	a	1	Total	C	O	S	0
			39	26	12	1	
28	c	1	Total	C	O	S	0
			32	19	12	1	
28	d	1	Total	C	O	S	0
			27	15	11	1	
28	t	1	Total	C	O		0
			27	25	2		

- Molecule 29 is UNKNOWN LIGAND (CCD ID: UNL) (formula: ).

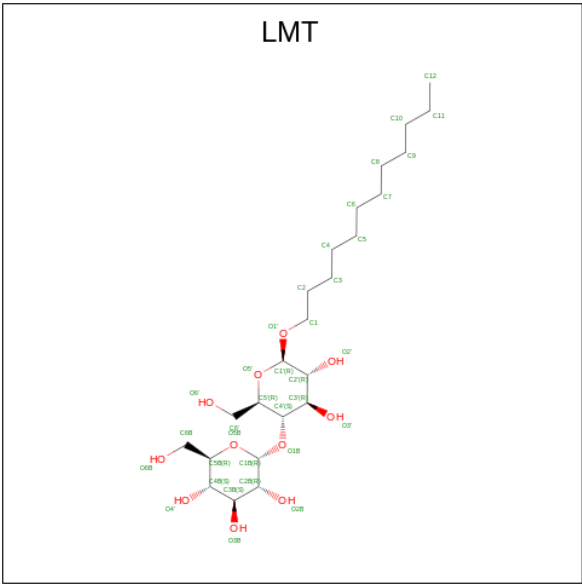
Mol	Chain	Residues	Atoms		AltConf
29	A	1	Total	C	0
			6	6	
29	B	1	Total	C	0
			14	14	
29	D	3	Total	C	0
			42	42	
29	I	2	Total	C	0
			12	12	
29	K	1	Total	C	0
			15	15	
29	T	1	Total	C	0
			7	7	
29	X	1	Total	C	0
			15	15	
29	a	1	Total	C	0
			6	6	
29	b	1	Total	C	0
			14	14	
29	d	3	Total	C	0
			42	42	
29	i	2	Total	C	0
			12	12	
29	k	1	Total	C	0
			15	15	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
29	t	1	Total	C	0
			7	7	
29	x	1	Total	C	0
			15	15	
29	E	1	Total	C	0
			10	10	
29	e	1	Total	C	0
			10	10	

- Molecule 30 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



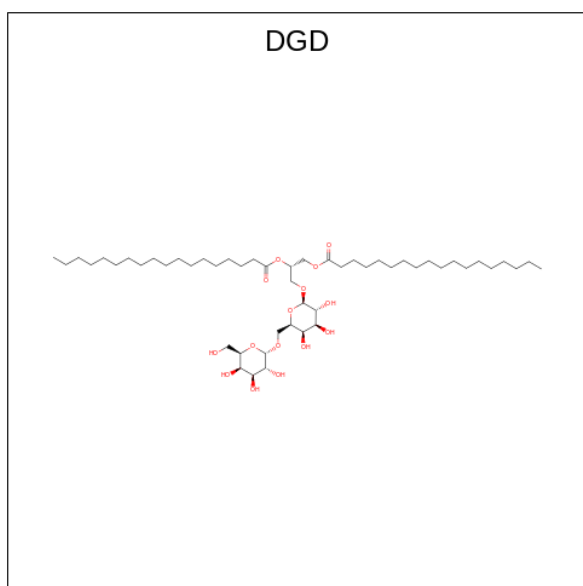
Mol	Chain	Residues	Atoms			AltConf
30	B	1	Total	C	O	0
			35	24	11	
30	B	1	Total	C	O	0
			17	16	1	
30	J	1	Total	C	O	0
			24	18	6	
30	M	1	Total	C	O	0
			35	24	11	
30	T	1	Total	C	O	0
			17	16	1	
30	T	1	Total	C	O	0
			13	12	1	
30	b	1	Total	C	O	0
			35	24	11	

Continued on next page...

*Continued from previous page...*

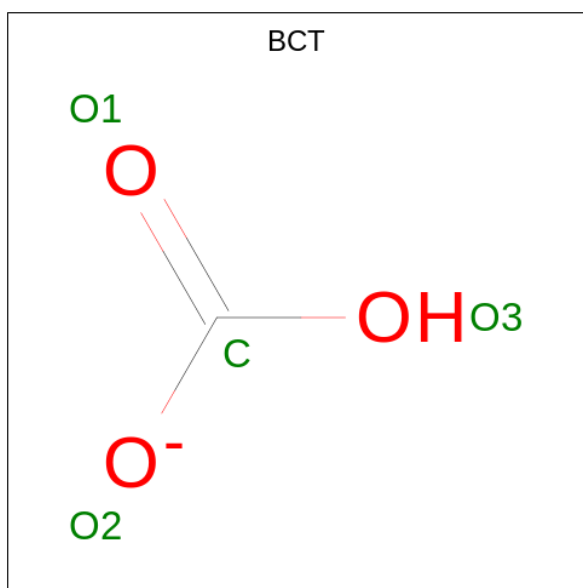
Mol	Chain	Residues	Atoms			AltConf
30	j	1	Total	C	O	0
			24	18	6	
30	m	1	Total	C	O	0
			35	24	11	
30	t	1	Total	C	O	0
			13	12	1	

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



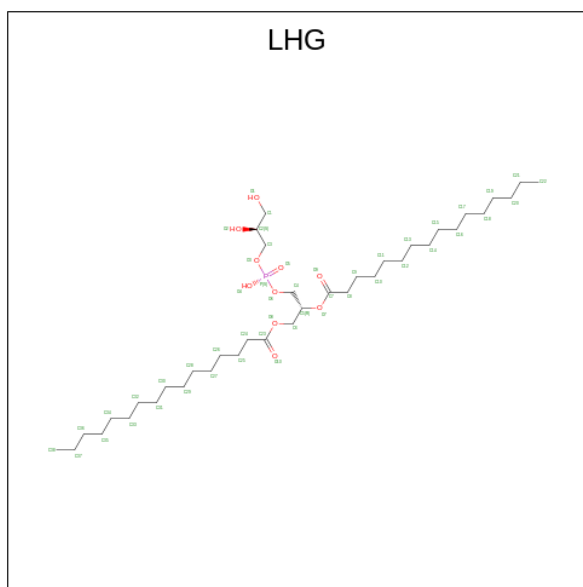
Mol	Chain	Residues	Atoms			AltConf
31	C	1	Total	C	O	0
			53	38	15	
31	C	1	Total	C	O	0
			52	37	15	
31	C	1	Total	C	O	0
			60	45	15	
31	H	1	Total	C	O	0
			62	47	15	
31	c	1	Total	C	O	0
			53	38	15	
31	c	1	Total	C	O	0
			52	37	15	
31	c	1	Total	C	O	0
			60	45	15	
31	h	1	Total	C	O	0
			62	47	15	

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3^-$ ).



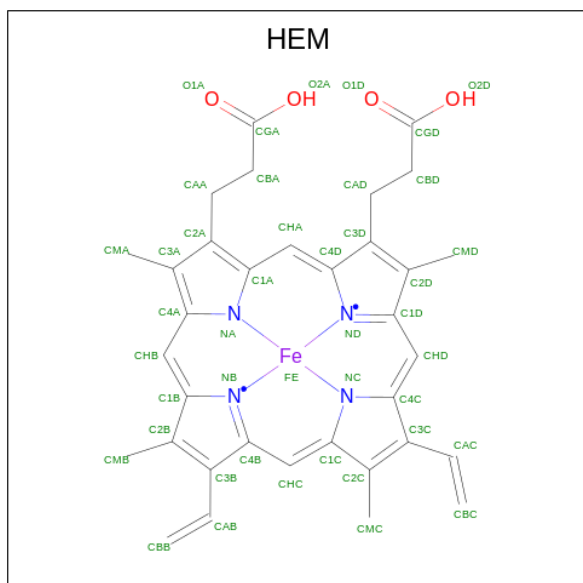
Mol	Chain	Residues	Atoms			AltConf
32	D	1	Total	C	O	1
			4	1	3	
32	d	1	Total	C	O	1
			4	1	3	

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula:  $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$ ).



Mol	Chain	Residues	Atoms				AltConf
33	D	1	Total 43	C 32	O 10	P 1	0
33	D	1	Total 49	C 38	O 10	P 1	0
33	D	1	Total 45	C 34	O 10	P 1	0
33	L	1	Total 49	C 38	O 10	P 1	0
33	d	1	Total 43	C 32	O 10	P 1	0
33	d	1	Total 49	C 38	O 10	P 1	0
33	d	1	Total 45	C 34	O 10	P 1	0
33	l	1	Total 49	C 38	O 10	P 1	0
33	E	1	Total 35	C 24	O 10	P 1	0
33	e	1	Total 35	C 24	O 10	P 1	0

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



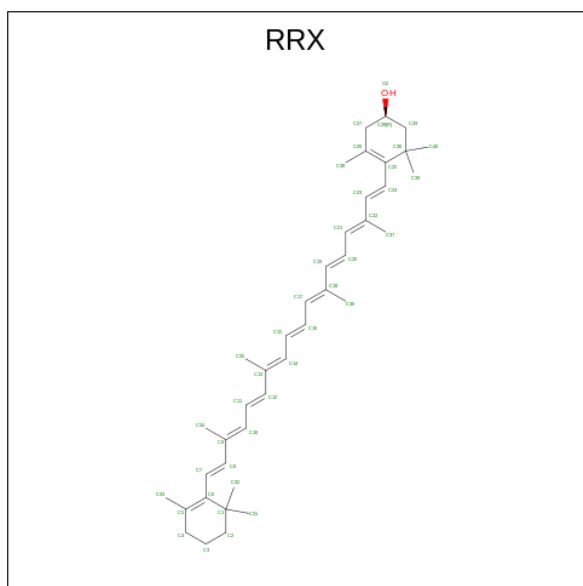
Mol	Chain	Residues	Atoms					AltConf
34	F	1	Total 43	C 34	Fe 1	N 4	O 4	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
34	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 35 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula:  $C_{40}H_{56}O$ ).

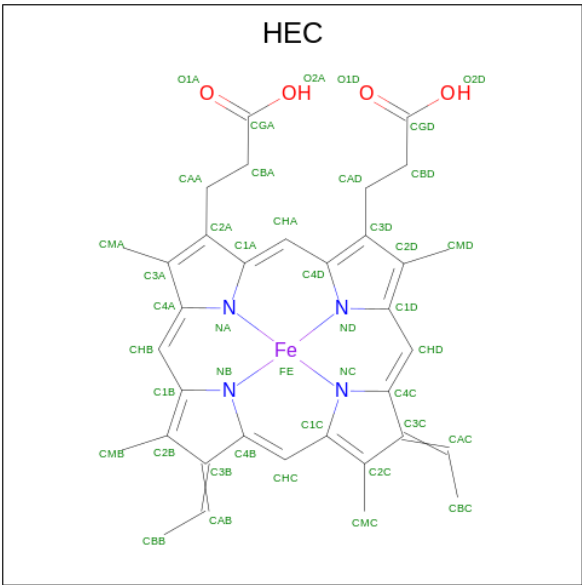


Mol	Chain	Residues	Atoms			AltConf
35	H	1	Total	C	O	0
			41	40	1	
35	h	1	Total	C	O	0
			41	40	1	

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	J	1	Total	Mg	0
			1	1	
36	j	1	Total	Mg	0
			1	1	

- Molecule 37 is HEME C (CCD ID: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					AltConf
37	V	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
37	v	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 38 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
38	O	1	Total	Ca	0
			1	1	
38	o	1	Total	Ca	0
			1	1	

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		AltConf
39	A	156	Total	O	5
			159	159	
39	B	317	Total	O	5
			322	322	
39	C	239	Total	O	1
			240	240	
39	D	150	Total	O	6
			156	156	
39	F	12	Total	O	0
			12	12	

Continued on next page...



*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
39	H	42	Total 43	O 43	1
39	I	21	Total 21	O 21	0
39	J	10	Total 10	O 10	0
39	K	3	Total 3	O 3	0
39	L	21	Total 21	O 21	1
39	M	11	Total 11	O 11	0
39	T	16	Total 16	O 16	0
39	U	52	Total 52	O 52	1
39	V	92	Total 93	O 93	1
39	X	10	Total 10	O 10	0
39	Y	3	Total 3	O 3	0
39	a	155	Total 158	O 158	5
39	b	316	Total 321	O 321	5
39	c	239	Total 240	O 240	1
39	d	150	Total 157	O 157	7
39	f	12	Total 12	O 12	0
39	h	42	Total 43	O 43	1
39	i	22	Total 22	O 22	0
39	j	10	Total 10	O 10	0
39	k	4	Total 4	O 4	0
39	l	21	Total 21	O 21	1

*Continued on next page...*


*Continued from previous page...*

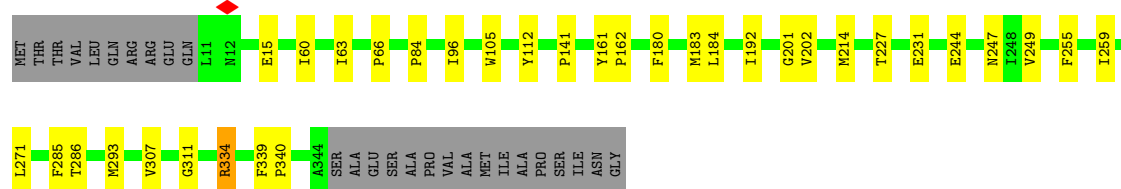
Mol	Chain	Residues	Atoms		AltConf
39	m	11	Total 11	O 11	0
39	t	16	Total 16	O 16	0
39	u	51	Total 51	O 51	1
39	v	92	Total 93	O 93	1
39	x	10	Total 10	O 10	0
39	y	3	Total 3	O 3	0
39	E	20	Total 20	O 20	0
39	O	107	Total 107	O 107	1
39	Z	2	Total 2	O 2	0
39	e	20	Total 20	O 20	0
39	o	106	Total 106	O 106	1
39	z	1	Total 1	O 1	0

### 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.

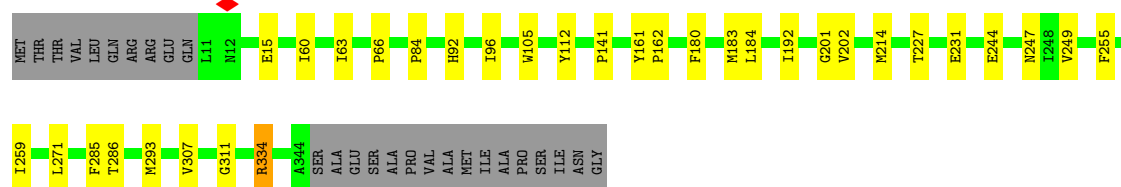
#### • Molecule 1: Photosystem II protein D1 3

Chain A: 




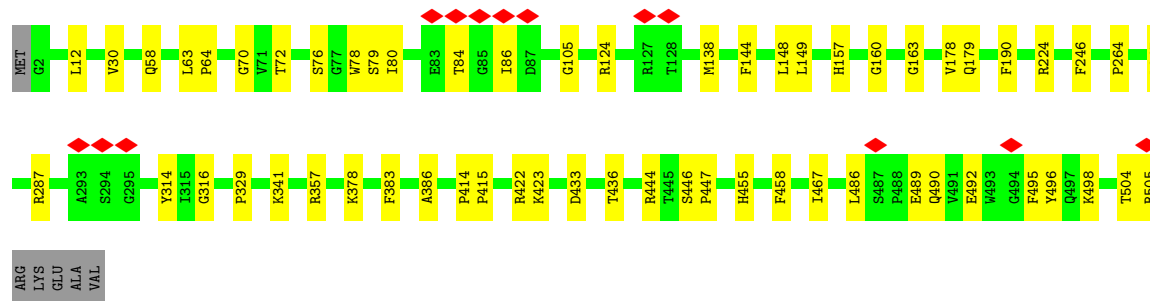
#### • Molecule 1: Photosystem II protein D1 3

Chain a: 




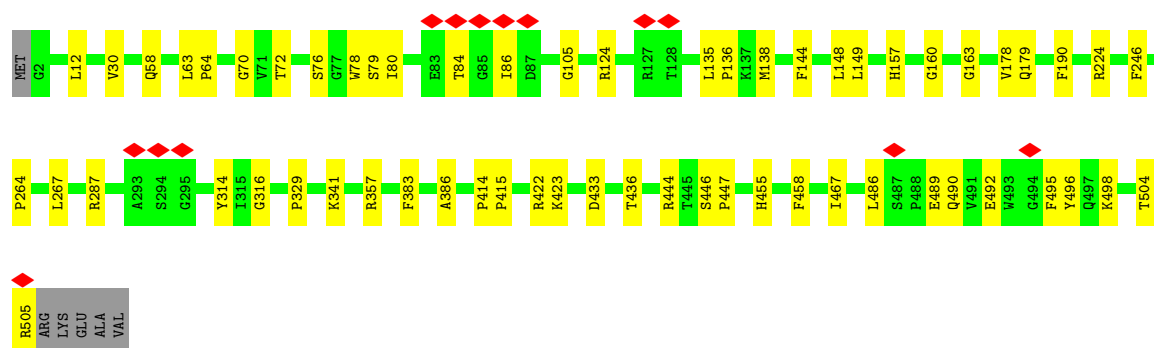
#### • Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 




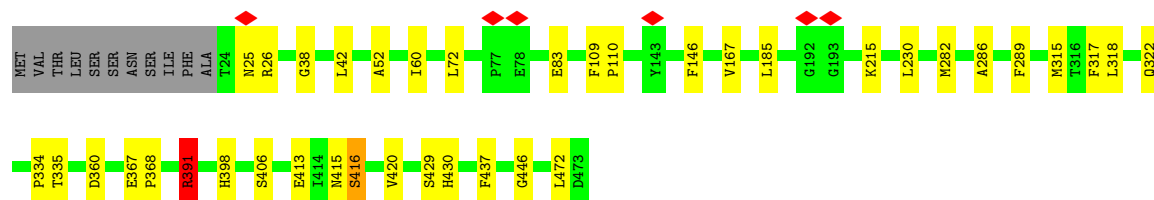
#### • Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  87% 12%




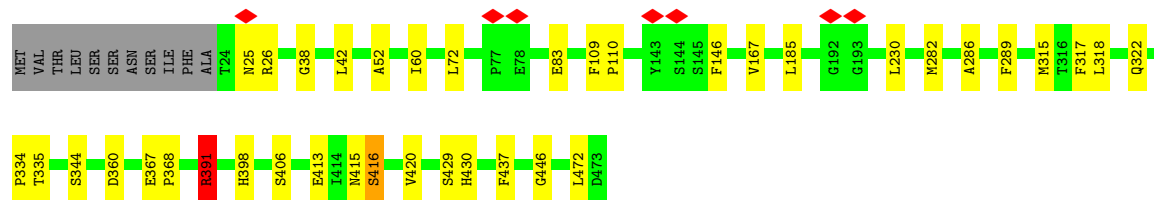
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  89% 8%



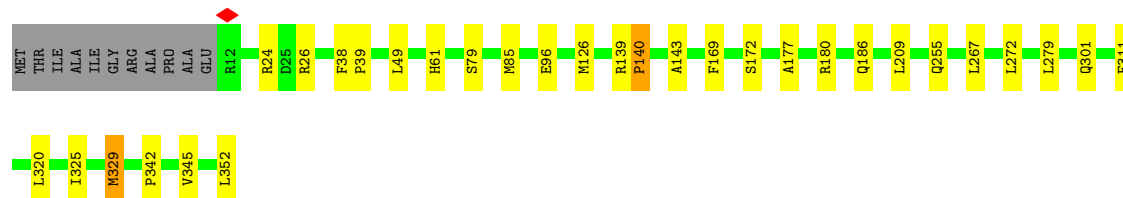
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  89% 8%




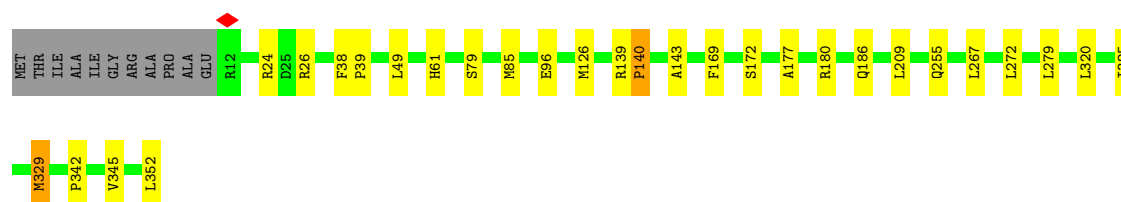
- Molecule 4: Photosystem II D2 protein

Chain D:  88% 8%

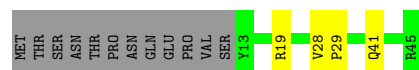


- Molecule 4: Photosystem II D2 protein

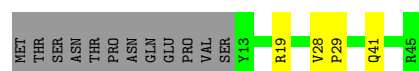
Chain d:  89% 8%



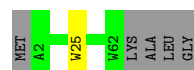
- Molecule 5: Cytochrome b559 subunit beta



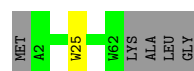
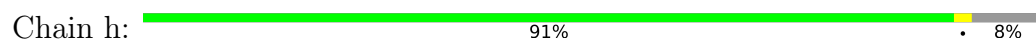
- Molecule 5: Cytochrome b559 subunit beta



- Molecule 6: Photosystem II reaction center protein H



- Molecule 6: Photosystem II reaction center protein H



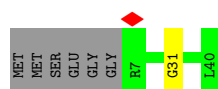
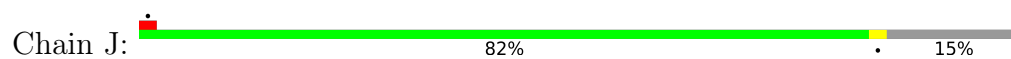
- Molecule 7: Photosystem II reaction center protein I



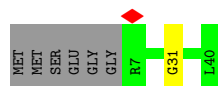
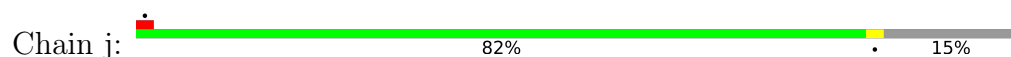
- Molecule 7: Photosystem II reaction center protein I



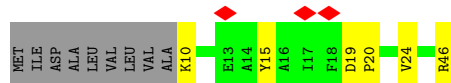
- Molecule 8: Photosystem II reaction center protein J



- Molecule 8: Photosystem II reaction center protein J



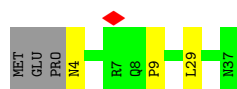
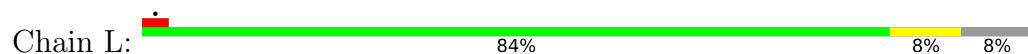
- Molecule 9: Photosystem II reaction center protein K



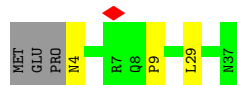
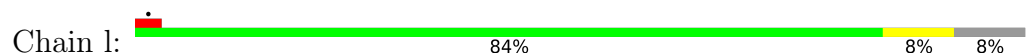
- Molecule 9: Photosystem II reaction center protein K



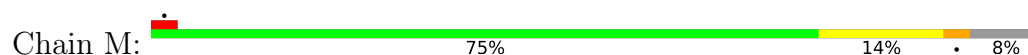
- Molecule 10: Photosystem II reaction center protein L



- Molecule 10: Photosystem II reaction center protein L

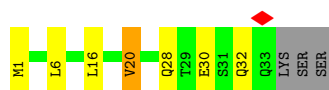


- Molecule 11: Photosystem II reaction center protein M




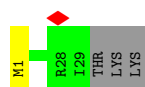
- Molecule 11: Photosystem II reaction center protein M

Chain m:  72% 17% 8%




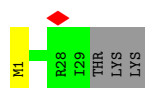
- Molecule 12: Photosystem II reaction center protein T

Chain T:  88% 9%



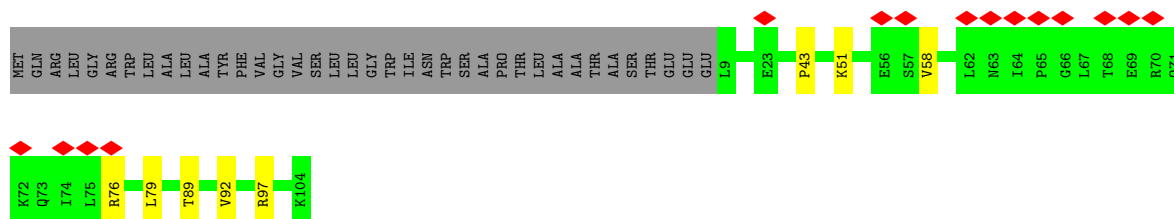
- Molecule 12: Photosystem II reaction center protein T

Chain t:  88% 9%



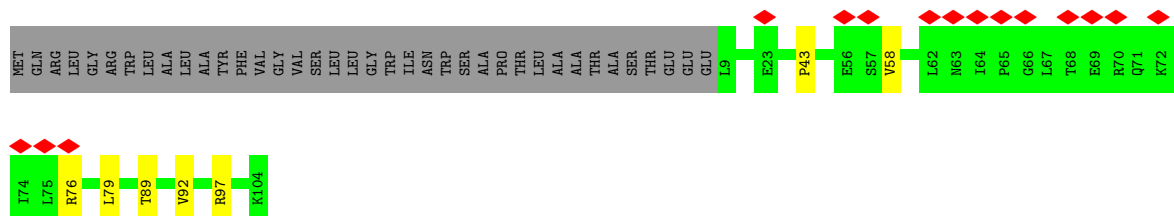
- Molecule 13: Photosystem II extrinsic protein U

Chain U:  11% 66% 6% 28%




- Molecule 13: Photosystem II extrinsic protein U

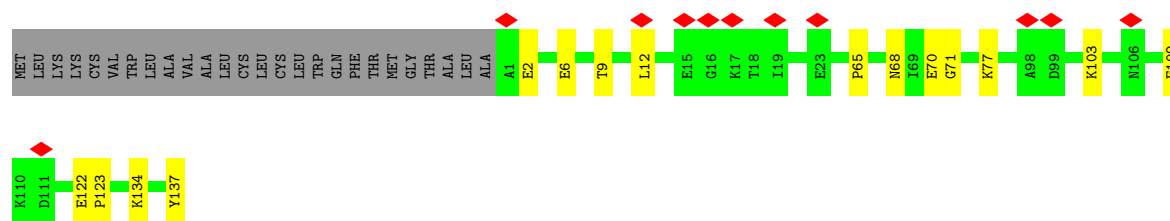
Chain u:  11% 66% 5% 28%



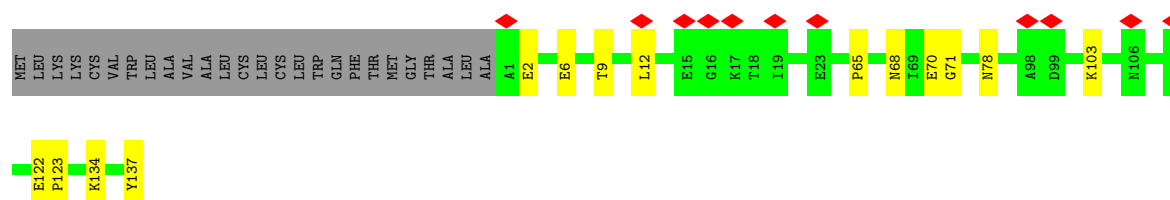
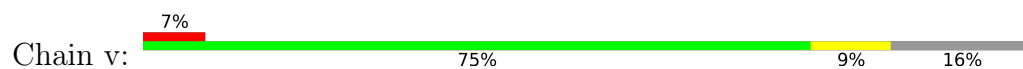
- Molecule 14: Photosystem II extrinsic protein V

Chain V:  7% 75% 9% 16%

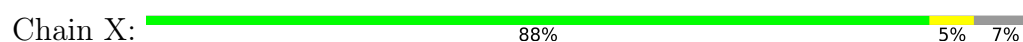




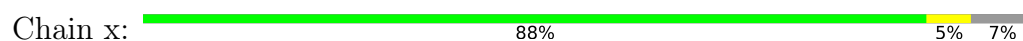
- Molecule 14: Photosystem II extrinsic protein V



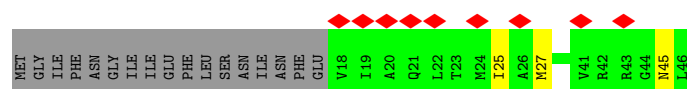
- Molecule 15: Photosystem II reaction center protein X



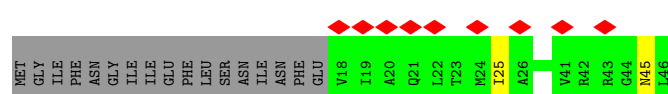
- Molecule 15: Photosystem II reaction center protein X



- Molecule 16: Photosystem II reaction center protein Psb30

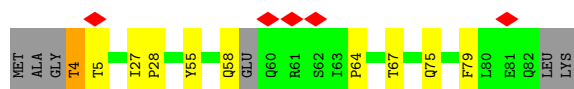
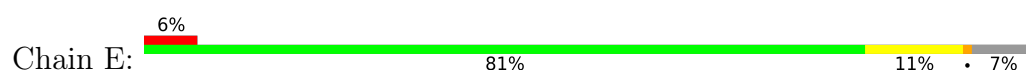


- Molecule 16: Photosystem II reaction center protein Psb30

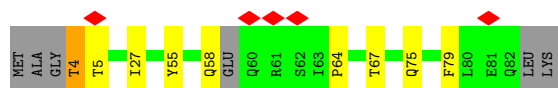
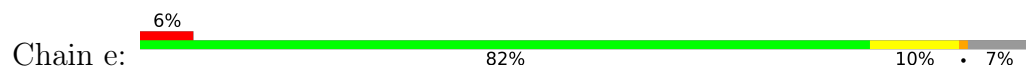


- Molecule 17: Cytochrome b559 subunit alpha

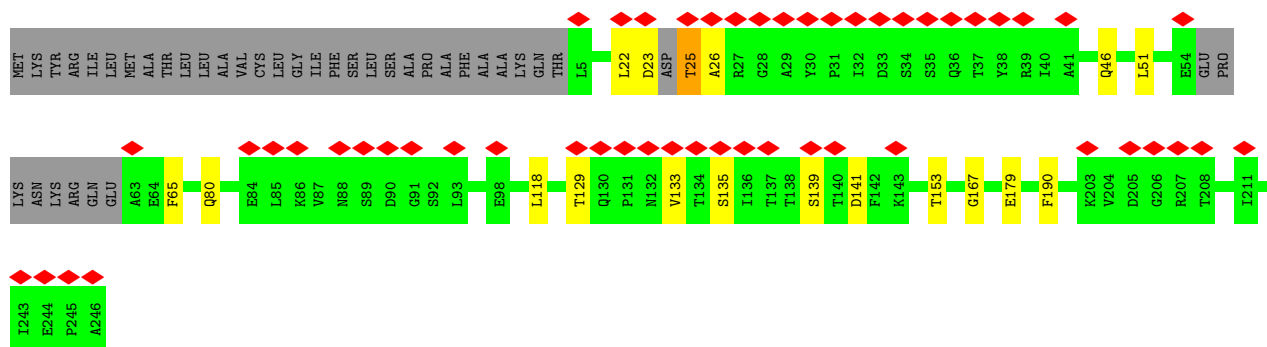
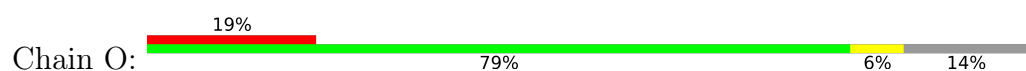




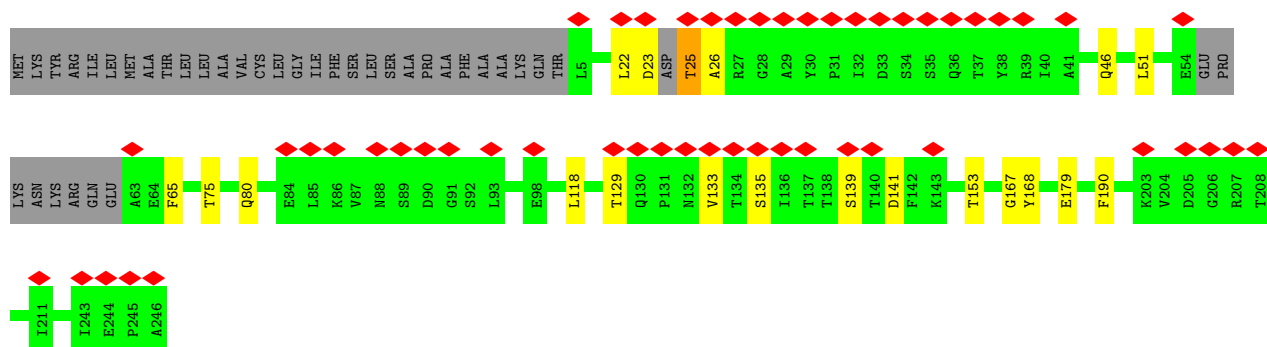
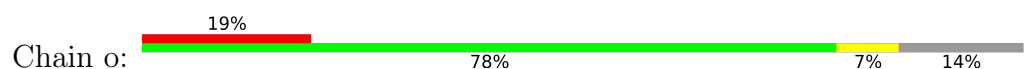
- Molecule 17: Cytochrome b559 subunit alpha



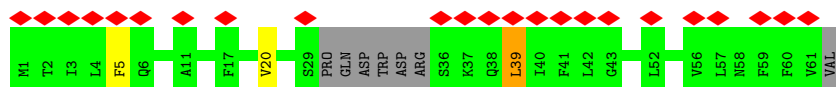
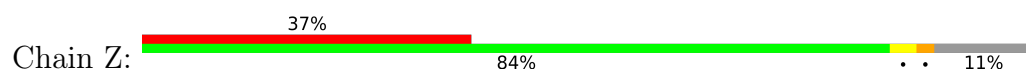
- Molecule 18: Photosystem II extrinsic protein O



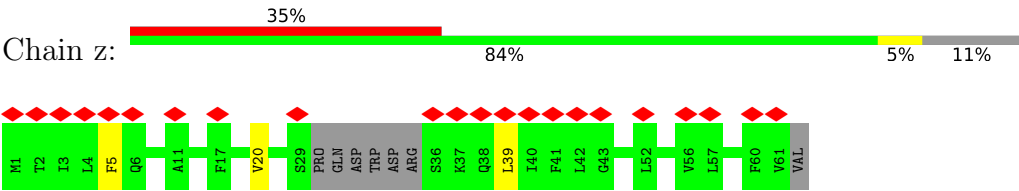
- Molecule 18: Photosystem II extrinsic protein O



- Molecule 19: Photosystem II reaction center protein Z



● Molecule 19: Photosystem II reaction center protein Z



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171514	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	290.56, 290.56, 290.56	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.454, 0.454, 0.454	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, PHO, RRX, FME, MG, LMT, BCR, BCT, CL, DGD, PL9, CA, FE2, UNL, OEX, LMG, LHG, SQD, HEM, HEC

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	A	0.58	0/2710	0.91	1/3703 (0.0%)
1	a	0.58	0/2710	0.91	1/3703 (0.0%)
2	B	0.58	0/4036	0.89	3/5511 (0.1%)
2	b	0.58	0/4036	0.89	3/5511 (0.1%)
3	C	0.56	0/3568	0.91	3/4858 (0.1%)
3	c	0.56	0/3568	0.91	3/4858 (0.1%)
4	D	0.58	0/2798	0.91	4/3814 (0.1%)
4	d	0.58	0/2798	0.91	4/3814 (0.1%)
5	F	0.53	0/278	0.87	0/379
5	f	0.53	0/278	0.87	0/379
6	H	0.55	0/487	0.85	0/667
6	h	0.55	0/487	0.85	0/667
7	I	0.53	0/262	0.87	0/358
7	i	0.52	0/262	0.87	0/358
8	J	0.56	0/249	0.84	0/339
8	j	0.56	0/249	0.84	0/339
9	K	0.56	0/295	0.81	0/407
9	k	0.56	0/295	0.81	0/407
10	L	0.58	0/287	0.88	0/390
10	l	0.58	0/287	0.88	0/390
11	M	0.56	0/242	0.79	0/332
11	m	0.56	0/242	0.79	0/332
12	T	0.55	0/240	0.83	0/327
12	t	0.55	0/240	0.83	0/327
13	U	0.46	0/729	0.86	0/992
13	u	0.46	0/729	0.86	0/992
14	V	0.50	0/1045	0.87	0/1427
14	v	0.50	0/1045	0.87	0/1427
15	X	0.52	0/272	0.86	0/367
15	x	0.52	0/272	0.86	0/367
16	Y	0.53	0/200	0.94	0/269

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	y	0.53	0/200	0.94	0/269
17	E	0.54	0/631	0.89	0/864
17	e	0.54	0/631	0.89	0/864
18	O	0.54	0/1712	0.86	0/2327
18	o	0.54	0/1712	0.86	0/2327
19	Z	0.48	0/399	0.87	0/544
19	z	0.48	0/399	0.87	0/544
All	All	0.56	0/40880	0.89	22/55750 (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
1	A	0	1
1	a	0	1
2	B	0	3
2	b	0	3
3	C	0	1
3	c	0	1
4	D	0	1
4	d	0	1
All	All	0	12

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	317	PHE	CA-CB-CG	-6.99	106.81	113.80
3	c	317	PHE	CA-CB-CG	-6.99	106.81	113.80
3	C	430	HIS	CA-CB-CG	-6.58	107.22	113.80
3	c	430	HIS	CA-CB-CG	-6.58	107.22	113.80
4	D	140	PRO	N-CA-CB	-6.10	96.85	103.25
4	d	140	PRO	N-CA-CB	-6.10	96.85	103.25
2	B	455	HIS	CA-CB-CG	-6.08	107.72	113.80
2	b	455	HIS	CA-CB-CG	-6.08	107.72	113.80
4	D	38	PHE	CA-CB-CG	-5.82	107.98	113.80
4	d	38	PHE	CA-CB-CG	-5.82	107.98	113.80
2	B	246	PHE	CA-CB-CG	5.46	119.26	113.80
3	C	437	PHE	CA-CB-CG	-5.46	108.34	113.80
2	b	246	PHE	CA-CB-CG	5.46	119.26	113.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	437	PHE	CA-CB-CG	-5.46	108.34	113.80
4	D	169	PHE	CA-CB-CG	-5.31	108.49	113.80
4	d	169	PHE	CA-CB-CG	-5.31	108.49	113.80
4	D	329	MET	CG-SD-CE	-5.28	89.28	100.90
4	d	329	MET	CG-SD-CE	-5.28	89.28	100.90
1	A	285	PHE	CA-CB-CG	-5.26	108.54	113.80
1	a	285	PHE	CA-CB-CG	-5.26	108.54	113.80
2	B	190	PHE	CA-CB-CG	-5.22	108.58	113.80
2	b	190	PHE	CA-CB-CG	-5.22	108.58	113.80

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	334	ARG	Sidechain
2	B	124	ARG	Sidechain
2	B	357	ARG	Sidechain
2	B	444	ARG	Sidechain
3	C	391	ARG	Sidechain
4	D	139	ARG	Sidechain
1	a	334	ARG	Sidechain
2	b	124	ARG	Sidechain
2	b	357	ARG	Sidechain
2	b	444	ARG	Sidechain
3	c	391	ARG	Sidechain
4	d	139	ARG	Sidechain

## 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	A	2625	0	2506	24	0
1	a	2625	0	2506	24	0
2	B	3896	0	3711	40	0
2	b	3896	0	3711	40	0
3	C	3451	0	3355	30	0
3	c	3451	0	3355	30	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2700	0	2602	25	0
4	d	2700	0	2602	24	0
5	F	269	0	277	3	0
5	f	269	0	277	3	0
6	H	474	0	480	2	0
6	h	474	0	480	2	0
7	I	265	0	268	4	0
7	i	265	0	268	4	0
8	J	243	0	251	1	0
8	j	243	0	251	1	0
9	K	285	0	287	7	0
9	k	285	0	287	7	0
10	L	278	0	289	4	0
10	l	278	0	289	3	0
11	M	249	0	261	11	0
11	m	249	0	261	12	0
12	T	241	0	236	1	0
12	t	241	0	236	1	0
13	U	718	0	706	6	0
13	u	718	0	706	5	0
14	V	1024	0	997	9	0
14	v	1024	0	997	9	0
15	X	269	0	291	1	0
15	x	269	0	291	1	0
16	Y	199	0	211	4	0
16	y	199	0	211	3	0
17	E	610	0	585	9	0
17	e	610	0	585	8	0
18	O	1676	0	1588	14	0
18	o	1676	0	1588	16	0
19	Z	393	0	418	3	0
19	z	393	0	418	2	0
20	A	10	0	0	0	0
20	a	10	0	0	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	1	0
22	a	2	0	0	1	0
23	A	173	0	166	6	0
23	B	1012	0	1087	23	0
23	C	785	0	814	24	0
23	D	178	0	180	7	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	a	173	0	166	6	0
23	b	1012	0	1087	22	0
23	c	785	0	814	21	0
23	d	178	0	180	6	0
24	A	64	0	74	2	0
24	D	64	0	74	3	0
24	a	64	0	74	3	0
24	d	64	0	74	3	0
25	A	40	0	56	1	0
25	B	117	0	159	14	0
25	C	78	0	106	9	0
25	D	40	0	56	3	0
25	K	40	0	56	2	0
25	T	39	0	54	6	0
25	Y	40	0	56	3	0
25	a	40	0	56	1	0
25	b	117	0	159	12	0
25	c	78	0	106	11	0
25	d	40	0	56	2	0
25	k	40	0	56	2	0
25	t	39	0	54	5	0
25	y	40	0	56	4	0
26	A	51	0	72	1	0
26	B	47	0	64	0	0
26	C	67	0	100	0	0
26	D	43	0	56	0	0
26	a	51	0	72	1	0
26	b	47	0	64	0	0
26	c	67	0	100	0	0
26	d	43	0	56	0	0
27	A	42	0	56	2	0
27	D	55	0	80	1	0
27	a	42	0	56	2	0
27	d	55	0	80	1	0
28	A	39	0	47	0	0
28	C	32	0	28	0	0
28	D	27	0	19	0	0
28	T	27	0	40	1	0
28	a	39	0	47	0	0
28	c	32	0	28	0	0
28	d	27	0	19	1	0
28	t	27	0	40	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	A	6	0	0	0	0
29	B	14	0	0	0	0
29	D	42	0	0	2	0
29	E	10	0	0	0	0
29	I	12	0	0	0	0
29	K	15	0	0	0	0
29	T	7	0	0	0	0
29	X	15	0	0	0	0
29	a	6	0	0	0	0
29	b	14	0	0	0	0
29	d	42	0	0	2	0
29	e	10	0	0	0	0
29	i	12	0	0	0	0
29	k	15	0	0	0	0
29	t	7	0	0	0	0
29	x	15	0	0	0	0
30	B	52	0	71	1	0
30	J	24	0	35	1	0
30	M	35	0	46	1	0
30	T	30	0	50	2	0
30	b	35	0	46	0	0
30	j	24	0	35	1	0
30	m	35	0	46	1	0
30	t	13	0	25	0	0
31	C	165	0	204	1	0
31	H	62	0	82	0	0
31	c	165	0	204	1	0
31	h	62	0	82	0	0
32	D	4	0	0	0	0
32	d	4	0	0	0	0
33	D	137	0	191	1	0
33	E	35	0	43	1	0
33	L	49	0	74	0	0
33	d	137	0	191	1	0
33	e	35	0	43	1	0
33	l	49	0	74	0	0
34	F	43	0	30	3	0
34	f	43	0	30	3	0
35	H	41	0	56	1	0
35	h	41	0	56	2	0
36	J	1	0	0	0	0
36	j	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	V	43	0	30	0	0
37	v	43	0	30	0	0
38	O	1	0	0	0	0
38	o	1	0	0	0	0
39	A	159	0	0	5	0
39	B	322	0	0	11	0
39	C	240	0	0	5	0
39	D	156	0	0	9	0
39	E	20	0	0	2	0
39	F	12	0	0	0	0
39	H	43	0	0	0	0
39	I	21	0	0	1	0
39	J	10	0	0	1	0
39	K	3	0	0	1	0
39	L	21	0	0	2	0
39	M	11	0	0	1	0
39	O	107	0	0	7	0
39	T	16	0	0	0	0
39	U	52	0	0	3	0
39	V	93	0	0	1	0
39	X	10	0	0	0	0
39	Y	3	0	0	0	0
39	Z	2	0	0	0	0
39	a	158	0	0	5	0
39	b	321	0	0	11	0
39	c	240	0	0	5	0
39	d	157	0	0	10	0
39	e	20	0	0	2	0
39	f	12	0	0	0	0
39	h	43	0	0	0	0
39	i	22	0	0	1	0
39	j	10	0	0	1	0
39	k	4	0	0	1	0
39	l	21	0	0	1	0
39	m	11	0	0	1	0
39	o	106	0	0	7	0
39	t	16	0	0	0	0
39	u	51	0	0	2	0
39	v	93	0	0	2	0
39	x	10	0	0	0	0
39	y	3	0	0	0	0
39	z	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	50208	0	47412	509	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 5.

All (509) 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)
1:A:15:GLU:CG	39:A:645:HOH:O	1.82	1.21
1:a:15:GLU:CG	39:a:644:HOH:O	1.84	1.20
25:T:101:BCR:C25	25:T:101:BCR:C23	2.21	1.19
25:t:103:BCR:C25	25:t:103:BCR:C23	2.21	1.18
4:D:352:LEU:HB2	39:D:505:HOH:O	1.50	1.11
4:d:352:LEU:HB2	39:d:504:HOH:O	1.50	1.08
18:o:179:GLU:N	39:o:401:HOH:O	1.81	1.02
18:O:179:GLU:N	39:O:401:HOH:O	1.86	1.01
1:a:244:GLU:OE1	39:a:571[B]:HOH:O	1.76	1.00
11:M:16:LEU:HD23	11:m:16:LEU:HD23	1.50	0.92
17:e:67:THR:H	17:e:75:GLN:HE22	1.21	0.89
17:E:67:THR:H	17:E:75:GLN:HE22	1.21	0.87
1:A:244:GLU:OE1	39:A:573[B]:HOH:O	1.97	0.82
1:A:249[B]:VAL:HG21	39:B:996:HOH:O	1.88	0.72
14:v:6:GLU:O	14:v:9:THR:HG22	1.90	0.72
25:B:619:BCR:H331	25:B:619:BCR:HC8	1.72	0.71
14:V:6:GLU:O	14:V:9:THR:HG22	1.90	0.71
1:a:249[B]:VAL:HG21	39:b:996:HOH:O	1.88	0.71
25:b:619:BCR:H331	25:b:619:BCR:HC8	1.72	0.70
23:c:506:CLA:HHC	23:c:506:CLA:HBB1	1.74	0.70
4:D:352:LEU:CA	39:D:505:HOH:O	2.41	0.69
23:b:605:CLA:HHC	23:b:605:CLA:HBB1	1.75	0.69
23:C:506:CLA:HHC	23:C:506:CLA:HBB1	1.74	0.68
22:A:403:CL:CL	39:A:545:HOH:O	2.47	0.68
22:a:403:CL:CL	39:a:544:HOH:O	2.47	0.68
4:D:352:LEU:CB	39:D:505:HOH:O	2.23	0.68
4:d:352:LEU:CA	39:d:504:HOH:O	2.41	0.68
3:C:282:MET:HE3	23:C:504:CLA:H91	1.76	0.68
23:B:605:CLA:HHC	23:B:605:CLA:HBB1	1.75	0.67
23:c:503:CLA:H61	23:c:513:CLA:H42	1.77	0.67
3:c:282:MET:HE3	23:c:504:CLA:H91	1.76	0.66
25:T:101:BCR:H311	25:T:101:BCR:HC8	1.77	0.66
29:D:413:UNL:C11	39:D:608:HOH:O	2.44	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:t:103:BCR:H311	25:t:103:BCR:HC8	1.77	0.66
2:b:386:ALA:O	39:b:701:HOH:O	2.13	0.65
25:d:407:BCR:H331	25:d:407:BCR:C8	2.27	0.65
23:C:503:CLA:H61	23:C:513:CLA:H42	1.77	0.65
23:C:514:CLA:HHC	23:C:514:CLA:HBB1	1.79	0.64
25:D:407:BCR:H331	25:D:407:BCR:C8	2.27	0.64
3:C:282:MET:HE2	23:C:504:CLA:H142	1.80	0.64
23:c:514:CLA:HHC	23:c:514:CLA:HBB1	1.79	0.64
25:B:619:BCR:H331	25:B:619:BCR:C8	2.28	0.64
18:o:139:SER:HA	39:o:494:HOH:O	1.97	0.63
11:M:16:LEU:CD2	11:m:16:LEU:HD23	2.27	0.63
18:O:139:SER:HA	39:O:496:HOH:O	1.97	0.63
3:c:282:MET:HE2	23:c:504:CLA:H142	1.80	0.63
23:d:406:CLA:HHC	23:d:406:CLA:HBB1	1.82	0.62
25:B:618:BCR:H331	25:B:618:BCR:C8	2.30	0.62
25:b:618:BCR:H331	25:b:618:BCR:C8	2.30	0.62
25:b:619:BCR:H331	25:b:619:BCR:C8	2.28	0.61
13:u:92:VAL:CG2	39:u:238:HOH:O	2.48	0.61
23:D:406:CLA:HBB1	23:D:406:CLA:HHC	1.82	0.60
25:c:515:BCR:H382	25:c:515:BCR:H23C	1.83	0.60
4:D:126:MET:HE3	4:D:143:ALA:O	2.02	0.60
11:M:20:VAL:HG11	11:m:20:VAL:CG2	2.31	0.60
25:b:617:BCR:H23C	25:b:617:BCR:H382	1.84	0.60
25:C:515:BCR:H382	25:C:515:BCR:H23C	1.83	0.60
11:M:20:VAL:CG2	11:m:20:VAL:HG11	2.31	0.60
13:U:92:VAL:CG2	39:U:239:HOH:O	2.49	0.60
25:B:618:BCR:H331	25:B:618:BCR:HC8	1.84	0.60
23:b:613:CLA:HBB1	23:b:613:CLA:HMB1	1.84	0.60
23:C:504:CLA:HHC	23:C:504:CLA:HBB1	1.84	0.59
2:B:386:ALA:O	39:B:701:HOH:O	2.16	0.59
25:B:617:BCR:H382	25:B:617:BCR:H23C	1.84	0.59
23:b:606:CLA:HHC	23:b:606:CLA:HBB1	1.84	0.59
2:B:287:ARG:NH1	39:B:706:HOH:O	2.34	0.59
25:b:618:BCR:H331	25:b:618:BCR:HC8	1.84	0.59
23:B:615:CLA:HHC	23:B:615:CLA:HBB1	1.85	0.59
1:A:227:THR:HB	1:A:231:GLU:HG3	1.84	0.59
4:d:126:MET:HE3	4:d:143:ALA:O	2.02	0.59
9:K:46:ARG:NH2	39:K:202:HOH:O	2.31	0.59
11:M:16:LEU:HD23	11:m:16:LEU:CD2	2.27	0.59
23:c:504:CLA:HHC	23:c:504:CLA:HBB1	1.84	0.59
9:k:24:VAL:HG13	16:y:25:ILE:HD13	1.84	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:613:CLA:HBB1	23:B:613:CLA:HMB1	1.84	0.58
9:K:24:VAL:HG13	16:Y:25:ILE:HD13	1.84	0.58
1:a:227:THR:HB	1:a:231:GLU:HG3	1.83	0.58
23:b:615:CLA:HHC	23:b:615:CLA:HBB1	1.85	0.58
23:B:610:CLA:HHC	23:B:610:CLA:HBB1	1.85	0.58
9:k:46:ARG:NH2	39:k:202:HOH:O	2.33	0.58
4:d:352:LEU:N	39:d:504:HOH:O	2.37	0.58
23:B:606:CLA:HHC	23:B:606:CLA:HBB1	1.84	0.58
2:B:224:ARG:HD3	6:H:25:TRP:CE2	2.39	0.58
23:b:610:CLA:HHC	23:b:610:CLA:HBB1	1.85	0.58
24:A:407:PHO:HBB1	24:A:407:PHO:HMB3	1.86	0.58
2:b:287:ARG:NH1	39:b:706:HOH:O	2.34	0.58
3:c:406:SER:HA	3:c:420:VAL:HG23	1.86	0.57
10:L:9:PRO:HA	30:m:101:LMT:H6D	1.86	0.57
3:C:406:SER:HA	3:C:420:VAL:HG23	1.86	0.57
4:D:24:ARG:NE	39:D:504:HOH:O	2.37	0.57
11:M:20:VAL:HG11	11:m:20:VAL:HG22	1.86	0.57
11:M:20:VAL:HG22	11:m:20:VAL:HG11	1.86	0.57
30:M:101:LMT:H6D	10:l:9:PRO:HA	1.86	0.57
3:c:360:ASP:OD1	39:c:601:HOH:O	2.18	0.57
29:d:413:UNL:C11	39:d:609:HOH:O	2.52	0.57
4:D:352:LEU:N	39:D:505:HOH:O	2.37	0.56
24:a:407:PHO:HBB1	24:a:407:PHO:HMB3	1.85	0.56
2:B:224:ARG:HD3	6:H:25:TRP:CD2	2.40	0.56
25:K:102:BCR:C8	25:K:102:BCR:H331	2.36	0.56
2:b:224:ARG:HD3	6:h:25:TRP:CD2	2.40	0.56
14:V:12:LEU:O	14:V:70:GLU:HG3	2.06	0.56
18:O:179:GLU:CB	39:O:401:HOH:O	2.52	0.56
2:B:498:LYS:HE2	39:B:850:HOH:O	2.06	0.56
1:a:184[B]:LEU:HD21	4:d:186:GLN:HG2	1.87	0.56
2:b:224:ARG:HD3	6:h:25:TRP:CE2	2.39	0.56
23:C:502:CLA:HHC	23:C:502:CLA:HBB1	1.88	0.55
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.41	0.55
23:c:502:CLA:HHC	23:c:502:CLA:HBB1	1.88	0.55
2:b:498:LYS:HE2	39:b:850:HOH:O	2.06	0.55
10:l:4:ASN:N	39:l:201:HOH:O	2.39	0.55
30:B:623:LMT:H12	12:t:1:FME:HCN	1.88	0.55
2:B:489:GLU:HB3	2:B:495:PHE:CD2	2.42	0.55
3:C:282:MET:CE	23:C:504:CLA:H142	2.37	0.55
10:L:4:ASN:N	39:L:201:HOH:O	2.39	0.55
17:e:4:THR:CB	39:e:201:HOH:O	2.51	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.41	0.55
2:b:489:GLU:HB3	2:b:495:PHE:CD2	2.42	0.55
24:A:407:PHO:ND	24:A:407:PHO:NC	2.53	0.55
3:C:360:ASP:OD1	39:C:601:HOH:O	2.18	0.55
25:c:516:BCR:H382	25:c:516:BCR:H23C	1.89	0.55
25:C:516:BCR:H23C	25:C:516:BCR:H382	1.89	0.54
10:L:4:ASN:N	39:L:202:HOH:O	2.40	0.54
12:T:1:FME:HCN	30:T:104:LMT:H12	1.88	0.54
1:A:271:LEU:HD11	27:A:411:PL9:HC71	1.90	0.54
1:a:271:LEU:HD11	27:a:411:PL9:HC71	1.90	0.54
14:v:12:LEU:O	14:v:70:GLU:HG3	2.06	0.54
1:A:183:MET:HA	23:A:405:CLA:HMD1	1.90	0.54
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.90	0.54
23:B:607:CLA:HMB1	23:B:607:CLA:HBB1	1.90	0.54
5:F:19:ARG:NH1	33:E:101:LHG:O2	2.41	0.54
24:a:407:PHO:ND	24:a:407:PHO:NC	2.53	0.54
17:E:4:THR:CB	39:E:201:HOH:O	2.52	0.54
1:A:184[B]:LEU:HD21	4:D:186:GLN:HG2	1.87	0.54
25:k:102:BCR:H331	25:k:102:BCR:C8	2.36	0.54
3:c:282:MET:CE	23:c:504:CLA:H142	2.37	0.54
25:c:516:BCR:HC31	7:i:23:PHE:HB3	1.89	0.54
5:f:19:ARG:NH1	33:e:101:LHG:O2	2.41	0.54
25:C:516:BCR:C3	7:I:23:PHE:HB3	2.38	0.54
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.90	0.53
25:C:516:BCR:HC31	7:I:23:PHE:HB3	1.89	0.53
11:M:30:GLU:OE2	39:M:201:HOH:O	2.19	0.53
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.90	0.53
25:c:516:BCR:C3	7:i:23:PHE:HB3	2.38	0.53
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.90	0.53
23:c:513:CLA:O2D	23:c:514:CLA:HBB2	2.09	0.53
11:m:30:GLU:OE2	39:m:201:HOH:O	2.19	0.53
25:a:409:BCR:H331	25:a:409:BCR:C8	2.38	0.53
23:d:402:CLA:HHC	23:d:402:CLA:HBB1	1.90	0.53
1:a:183:MET:HA	23:a:405:CLA:HMD1	1.90	0.53
18:o:179:GLU:CB	39:o:401:HOH:O	2.57	0.53
23:D:402:CLA:HHC	23:D:402:CLA:HBB1	1.90	0.53
18:O:22:LEU:O	18:O:23:ASP:C	2.51	0.53
3:C:83:GLU:OE2	3:C:398:HIS:NE2	2.42	0.53
17:e:4:THR:HG21	39:e:201:HOH:O	2.08	0.53
18:o:22:LEU:O	18:o:23:ASP:C	2.51	0.53
23:b:607:CLA:HMB1	23:b:607:CLA:HBB1	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:513:CLA:O2D	23:C:514:CLA:HBB2	2.09	0.52
4:d:180:ARG:HD3	4:d:180:ARG:C	2.35	0.52
4:D:180:ARG:HD3	4:D:180:ARG:C	2.35	0.52
25:A:409:BCR:H331	25:A:409:BCR:C8	2.38	0.52
17:E:4:THR:HG21	39:E:201:HOH:O	2.09	0.52
1:A:247:ASN:OD1	1:A:249[B]:VAL:HG22	2.10	0.52
1:a:247:ASN:OD1	1:a:249[B]:VAL:HG22	2.10	0.52
28:d:415:SQD:O4	39:d:501:HOH:O	2.19	0.52
3:c:83:GLU:OE2	3:c:398:HIS:NE2	2.42	0.51
2:b:383:PHE:CZ	18:o:167:GLY:HA2	2.46	0.51
2:B:378:LYS:NZ	39:B:715:HOH:O	2.43	0.51
25:b:619:BCR:H383	25:b:619:BCR:H23C	1.93	0.51
2:B:383:PHE:CZ	18:O:167:GLY:HA2	2.46	0.51
25:B:619:BCR:H383	25:B:619:BCR:H23C	1.93	0.51
11:M:16:LEU:CD2	11:m:16:LEU:CD2	2.89	0.51
24:d:401:PHO:NC	24:d:401:PHO:ND	2.57	0.51
13:u:89:THR:HG22	18:o:190:PHE:CE1	2.46	0.51
23:A:406:CLA:HHC	23:A:406:CLA:HBB1	1.93	0.51
39:A:563:HOH:O	17:E:55:TYR:HB2	2.11	0.51
13:U:89:THR:HG22	18:O:190:PHE:CE1	2.46	0.51
23:a:406:CLA:HHC	23:a:406:CLA:HBB1	1.93	0.51
24:D:401:PHO:NC	24:D:401:PHO:ND	2.57	0.50
13:U:92:VAL:HG23	39:U:239:HOH:O	2.10	0.50
18:o:25:THR:OG1	18:o:26:ALA:N	2.43	0.50
30:j:102:LMT:H3'	39:j:201:HOH:O	2.11	0.50
13:u:92:VAL:HG23	39:u:238:HOH:O	2.09	0.50
18:O:25:THR:OG1	18:O:26:ALA:N	2.43	0.50
27:A:411:PL9:H502	4:D:39:PRO:HG3	1.94	0.50
27:a:411:PL9:H502	4:d:39:PRO:HG3	1.94	0.50
4:d:325:ILE:O	4:d:329:MET:HB3	2.12	0.50
30:J:102:LMT:H3'	39:J:201:HOH:O	2.11	0.50
2:b:138:MET:HE3	23:b:615:CLA:CHD	2.42	0.50
34:F:101:HEM:HBB2	34:F:101:HEM:HMB2	1.94	0.49
13:U:76:ARG:HA	13:U:79:LEU:HG	1.94	0.49
5:f:41:GLN:OE1	8:j:31:GLY:HA3	2.12	0.49
2:B:138:MET:HE3	23:B:615:CLA:CHD	2.42	0.49
13:u:76:ARG:HA	13:u:79:LEU:HG	1.94	0.49
4:D:26:ARG:HA	17:E:5:THR:HB	1.94	0.49
5:F:41:GLN:OE1	8:J:31:GLY:HA3	2.12	0.49
2:b:492:GLU:CG	2:b:495:PHE:HB2	2.42	0.49
2:B:423:LYS:HE3	39:B:844:HOH:O	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:V:77:LYS:NZ	14:V:109:GLU:OE2	2.34	0.49
39:a:561:HOH:O	17:e:55:TYR:HB2	2.11	0.49
33:d:411:LHG:H151	33:d:411:LHG:H331	1.94	0.49
2:b:179:GLN:NE2	39:b:708:HOH:O	2.37	0.49
4:D:325:ILE:O	4:D:329:MET:HB3	2.12	0.49
23:b:615:CLA:H2	23:b:616:CLA:HBB2	1.94	0.49
3:C:38:GLY:HA3	23:C:512:CLA:HMD2	1.95	0.49
2:b:504:THR:O	2:b:505:ARG:HB3	2.13	0.49
23:d:406:CLA:H2	15:x:17:GLY:HA3	1.95	0.49
2:B:492:GLU:CG	2:B:495:PHE:HB2	2.42	0.49
3:C:318:LEU:C	3:C:318:LEU:HD23	2.38	0.49
33:D:411:LHG:H151	33:D:411:LHG:H331	1.94	0.49
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.95	0.49
3:c:318:LEU:C	3:c:318:LEU:HD23	2.38	0.49
2:b:72:THR:HG22	2:b:80:ILE:HD11	1.95	0.48
3:c:38:GLY:HA3	23:c:512:CLA:HMD2	1.95	0.48
4:d:24:ARG:NE	39:d:501:HOH:O	2.46	0.48
3:C:429:SER:HB3	31:C:518:DGD:HBT2	1.94	0.48
23:b:605:CLA:C14	23:b:610:CLA:HED2	2.43	0.48
34:f:101:HEM:HBB2	34:f:101:HEM:HMB2	1.94	0.48
3:C:367:GLU:N	3:C:368:PRO:CD	2.76	0.48
3:c:367:GLU:N	3:c:368:PRO:CD	2.76	0.48
23:B:605:CLA:C14	23:B:610:CLA:HED2	2.43	0.48
3:c:429:SER:HB3	31:c:518:DGD:HBT2	1.94	0.48
2:b:423:LYS:HE3	39:b:843:HOH:O	2.12	0.48
4:D:272:LEU:C	4:D:272:LEU:HD23	2.38	0.48
3:c:334:PRO:HA	18:o:153:THR:OG1	2.14	0.48
4:d:26:ARG:HA	17:e:5:THR:HB	1.94	0.48
14:v:122:GLU:N	14:v:123:PRO:HD2	2.29	0.48
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.95	0.48
23:D:406:CLA:H2	15:X:17:GLY:HA3	1.95	0.48
1:A:249[B]:VAL:HG13	39:A:621:HOH:O	2.14	0.48
2:B:504:THR:O	2:B:505:ARG:HB3	2.13	0.48
2:B:72:THR:HG22	2:B:80:ILE:HD11	1.95	0.47
23:b:603:CLA:CMD	23:b:606:CLA:HMB2	2.44	0.47
1:A:84:PRO:HA	1:A:112:TYR:CG	2.50	0.47
23:B:615:CLA:H2	23:B:616:CLA:HBB2	1.94	0.47
4:d:61:HIS:HD2	39:d:637:HOH:O	1.97	0.47
4:d:272:LEU:C	4:d:272:LEU:HD23	2.38	0.47
18:o:133:VAL:O	18:o:135:SER:N	2.46	0.47
23:B:601:CLA:HAA1	23:B:601:CLA:HBD	1.97	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:215:LYS:NZ	39:C:607:HOH:O	2.37	0.47
3:C:334:PRO:HA	18:O:153:THR:OG1	2.14	0.47
23:B:603:CLA:CMD	23:B:606:CLA:HMB2	2.44	0.47
23:B:606:CLA:H111	23:B:606:CLA:H61	1.96	0.47
3:C:185:LEU:HB2	3:C:230:LEU:HD13	1.96	0.47
1:a:249[B]:VAL:HG13	39:a:624:HOH:O	2.14	0.47
3:c:167:VAL:HG11	23:c:513:CLA:HBA1	1.96	0.47
3:c:185:LEU:HB2	3:c:230:LEU:HD13	1.96	0.47
23:b:606:CLA:H111	23:b:606:CLA:H61	1.96	0.47
25:b:618:BCR:HC8	25:b:618:BCR:C33	2.45	0.47
14:V:122:GLU:N	14:V:123:PRO:HD2	2.29	0.47
2:b:486:LEU:HD13	39:d:645:HOH:O	2.15	0.47
25:C:516:BCR:H382	25:C:516:BCR:C23	2.45	0.47
25:Y:101:BCR:H311	25:Y:101:BCR:HC8	1.96	0.47
1:a:84:PRO:HA	1:a:112:TYR:CG	2.50	0.47
25:y:101:BCR:C8	25:y:101:BCR:H311	2.45	0.47
18:o:139:SER:CB	39:o:485:HOH:O	2.63	0.46
25:b:619:BCR:H383	25:b:619:BCR:C23	2.45	0.46
25:B:619:BCR:H383	25:B:619:BCR:C23	2.45	0.46
23:c:510:CLA:HMB1	23:c:510:CLA:HBB1	1.97	0.46
3:C:167:VAL:HG11	23:C:513:CLA:HBA1	1.96	0.46
25:Y:101:BCR:H311	25:Y:101:BCR:C8	2.45	0.46
2:b:76:SER:OG	2:b:78:TRP:CD1	2.69	0.46
1:A:66:PRO:HG2	39:O:452:HOH:O	2.15	0.46
2:B:486:LEU:HD13	39:D:645:HOH:O	2.15	0.46
2:B:492:GLU:HG3	2:B:495:PHE:HB2	1.97	0.46
23:B:601:CLA:HHC	23:B:601:CLA:HBB1	1.98	0.46
4:D:61:HIS:HD2	39:D:637:HOH:O	1.97	0.46
23:b:601:CLA:HAA1	23:b:601:CLA:HBD	1.97	0.46
23:b:601:CLA:HHC	23:b:601:CLA:HBB1	1.98	0.46
1:a:66:PRO:HG2	39:o:452:HOH:O	2.15	0.46
25:y:101:BCR:H311	25:y:101:BCR:HC8	1.96	0.46
23:C:505:CLA:HBB1	23:C:505:CLA:HMB1	1.98	0.46
2:B:422:ARG:NH2	39:B:710:HOH:O	2.40	0.45
23:B:611:CLA:HMB1	23:B:612:CLA:NB	2.31	0.45
34:F:101:HEM:HBB2	34:F:101:HEM:CMB	2.46	0.45
2:b:144:PHE:CE2	2:b:148:LEU:HD11	2.51	0.45
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.52	0.45
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.52	0.45
2:b:63:LEU:N	2:b:64:PRO:HD2	2.31	0.45
25:c:516:BCR:H382	25:c:516:BCR:C23	2.45	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:d:413:UNL:C24	39:d:650:HOH:O	2.63	0.45
2:B:63:LEU:N	2:B:64:PRO:HD2	2.31	0.45
23:C:510:CLA:HMB1	23:C:510:CLA:HBB1	1.97	0.45
35:H:101:RRX:H55	35:H:101:RRX:H46	1.99	0.45
25:T:101:BCR:H311	25:T:101:BCR:C8	2.45	0.45
1:a:184[B]:LEU:HD23	23:a:405:CLA:HBC1	1.99	0.45
23:b:611:CLA:HMB1	23:b:612:CLA:NB	2.31	0.45
23:c:505:CLA:HBB1	23:c:505:CLA:HMB1	1.98	0.45
18:O:80:GLN:HA	39:O:475:HOH:O	2.16	0.45
2:B:179:GLN:NE2	39:B:708:HOH:O	2.37	0.45
29:D:413:UNL:C24	39:D:650:HOH:O	2.64	0.45
23:b:609:CLA:HHC	23:b:609:CLA:HBB1	1.99	0.45
2:B:76:SER:OG	2:B:78:TRP:CD1	2.69	0.45
18:O:133:VAL:O	18:O:135:SER:N	2.46	0.45
4:D:85:MET:CE	4:D:96:GLU:HG2	2.47	0.45
2:B:144:PHE:CE2	2:B:148:LEU:HD11	2.51	0.45
23:B:609:CLA:HHC	23:B:609:CLA:HBB1	1.99	0.45
5:F:28:VAL:HB	5:F:29:PRO:HD3	1.99	0.45
34:f:101:HEM:HBB2	34:f:101:HEM:CMB	2.46	0.45
2:B:414:PRO:HB2	2:B:415:PRO:HD3	1.99	0.45
23:B:613:CLA:HBB1	23:B:613:CLA:CMB	2.46	0.45
3:C:472:LEU:HD11	4:D:255:GLN:HG3	1.98	0.45
2:b:492:GLU:HG3	2:b:495:PHE:HB2	1.97	0.45
27:D:408:PL9:H411	10:L:29:LEU:HD23	1.98	0.45
7:I:27:ASP:N	7:I:28:PRO:CD	2.81	0.45
4:d:85:MET:CE	4:d:96:GLU:HG2	2.47	0.45
18:o:80:GLN:HA	39:o:474:HOH:O	2.17	0.45
25:T:101:BCR:C23	25:T:101:BCR:C26	2.91	0.44
23:b:613:CLA:HBB1	23:b:613:CLA:CMB	2.46	0.44
13:U:92:VAL:HG12	13:U:97:ARG:HD2	1.99	0.44
39:b:773[B]:HOH:O	18:o:168:TYR:HA	2.17	0.44
3:c:472:LEU:HD11	4:d:255:GLN:HG3	1.98	0.44
25:c:515:BCR:H11C	25:c:515:BCR:H341	1.82	0.44
18:O:139:SER:CB	39:O:483:HOH:O	2.65	0.44
2:b:149:LEU:HG	23:b:606:CLA:HBB2	1.99	0.44
2:b:414:PRO:HB2	2:b:415:PRO:HD3	1.99	0.44
4:d:342:PRO:O	4:d:345:VAL:HG22	2.18	0.44
18:o:51:LEU:HB3	18:o:65:PHE:HB3	2.00	0.44
16:Y:27:MET:HE2	16:Y:27:MET:HB3	1.93	0.44
5:f:28:VAL:HB	5:f:29:PRO:HD3	1.99	0.44
2:B:433:ASP:OD2	2:B:436:THR:OG1	2.35	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:618:BCR:HC8	25:B:618:BCR:C33	2.45	0.44
25:B:618:BCR:H24C	25:B:618:BCR:H371	1.74	0.44
3:C:391:ARG:HA	3:C:391:ARG:HD3	1.59	0.44
23:C:513:CLA:HBA1	23:C:513:CLA:H3A	1.77	0.44
9:k:24:VAL:CG1	16:y:25:ILE:HD13	2.48	0.44
1:A:202:VAL:HG11	23:A:406:CLA:C3D	2.48	0.44
25:T:101:BCR:HC7	25:T:101:BCR:H331	1.75	0.44
2:b:79:SER:HB3	2:b:86:ILE:HG12	2.00	0.44
3:c:391:ARG:HA	3:c:391:ARG:HD3	1.59	0.44
27:d:408:PL9:H411	10:l:29:LEU:HD23	1.98	0.44
2:B:149:LEU:HG	23:B:606:CLA:HBB2	1.99	0.44
3:c:109:PHE:N	3:c:110:PRO:CD	2.81	0.44
23:B:611:CLA:HHC	23:B:611:CLA:HBB1	2.00	0.44
2:b:314:TYR:CE2	2:b:316:GLY:HA3	2.53	0.44
23:b:611:CLA:HHC	23:b:611:CLA:HBB1	2.00	0.44
35:h:101:RRX:H55	35:h:101:RRX:H46	1.99	0.44
14:v:65:PRO:HB3	39:v:306:HOH:O	2.17	0.44
1:A:184[B]:LEU:HD23	23:A:405:CLA:HBC1	1.99	0.44
23:A:405:CLA:CBD	23:D:402:CLA:HAC2	2.48	0.44
23:B:616:CLA:H171	25:B:619:BCR:H331	2.00	0.44
13:u:92:VAL:HG12	13:u:97:ARG:HD2	1.99	0.44
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.53	0.43
14:V:65:PRO:HB3	39:V:306:HOH:O	2.17	0.43
1:a:161:TYR:HB3	1:a:162:PRO:HD3	2.00	0.43
2:b:433:ASP:OD2	2:b:436:THR:OG1	2.35	0.43
23:b:616:CLA:H171	25:b:619:BCR:H331	2.00	0.43
25:t:103:BCR:H311	25:t:103:BCR:C8	2.45	0.43
23:a:405:CLA:CBD	23:d:402:CLA:HAC2	2.48	0.43
4:d:49:LEU:HD13	25:d:407:BCR:C15	2.49	0.43
25:t:103:BCR:HC7	25:t:103:BCR:H331	1.75	0.43
2:B:492:GLU:HB3	39:B:842:HOH:O	2.18	0.43
3:C:109:PHE:N	3:C:110:PRO:CD	2.81	0.43
3:C:413:GLU:CD	39:C:618:HOH:O	2.60	0.43
9:K:24:VAL:CG1	16:Y:25:ILE:HD13	2.48	0.43
4:D:342:PRO:O	4:D:345:VAL:HG22	2.18	0.43
25:b:619:BCR:C23	25:b:619:BCR:C38	2.97	0.43
25:c:516:BCR:H11C	25:c:516:BCR:H341	1.87	0.43
2:B:79:SER:HB3	2:B:86:ILE:HG12	2.00	0.43
9:K:15:TYR:CE2	19:Z:5:PHE:HZ	2.37	0.43
1:a:63:ILE:HB	3:c:335:THR:HG21	2.00	0.43
1:a:202:VAL:HG11	23:a:406:CLA:C3D	2.48	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:58:GLN:C	2:b:329:PRO:HB3	2.44	0.43
7:i:27:ASP:N	7:i:28:PRO:CD	2.80	0.43
11:M:28:GLN:O	11:M:32:GLN:HG3	2.19	0.43
14:V:134:LYS:HA	14:V:137:TYR:CG	2.54	0.43
1:a:180:PHE:O	1:a:184[A]:LEU:HD13	2.18	0.43
3:c:446:GLY:HA3	39:c:677:HOH:O	2.19	0.43
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.00	0.43
1:A:180:PHE:O	1:A:184[A]:LEU:HD13	2.18	0.43
23:A:406:CLA:HMB2	23:D:405:CLA:H122	2.01	0.43
1:a:307:VAL:CG1	1:a:311:GLY:HA2	2.49	0.43
23:a:406:CLA:HMB2	23:d:405:CLA:H122	2.01	0.43
3:c:146:PHE:HZ	23:c:513:CLA:HBB2	1.84	0.43
2:B:58:GLN:C	2:B:329:PRO:HB3	2.44	0.43
3:C:322:GLN:HG2	39:C:801:HOH:O	2.18	0.43
3:c:322:GLN:HG2	39:c:802:HOH:O	2.18	0.43
4:d:79:SER:HA	4:d:172:SER:HB3	2.01	0.43
2:B:160:GLY:HA2	2:B:163:GLY:O	2.19	0.42
2:B:458:PHE:HB3	23:B:604:CLA:HBC2	2.01	0.42
3:C:42:LEU:HD21	23:C:512:CLA:H2A	2.01	0.42
4:D:49:LEU:HD13	25:D:407:BCR:C15	2.49	0.42
4:D:267:LEU:C	4:D:267:LEU:HD23	2.44	0.42
4:d:267:LEU:C	4:d:267:LEU:HD23	2.44	0.42
18:O:51:LEU:HB3	18:O:65:PHE:HB3	2.00	0.42
1:A:60:ILE:HD12	1:A:84:PRO:HD2	2.01	0.42
1:A:307:VAL:CG1	1:A:311:GLY:HA2	2.49	0.42
2:B:446:SER:HB2	2:B:447:PRO:HD2	2.01	0.42
3:C:60:ILE:HG22	23:C:504:CLA:HHD	2.00	0.42
25:C:515:BCR:H24C	25:C:515:BCR:H371	1.85	0.42
3:c:413:GLU:CD	39:c:622:HOH:O	2.61	0.42
7:i:30:ARG:NH2	39:i:202:HOH:O	2.51	0.42
34:F:101:HEM:HMC3	17:E:27:ILE:HG12	2.01	0.42
1:a:201:GLY:HA3	1:a:286:THR:HB	2.01	0.42
25:B:619:BCR:C23	25:B:619:BCR:C38	2.97	0.42
7:I:30:ARG:NH2	39:I:202:HOH:O	2.53	0.42
2:b:30:VAL:HG12	23:b:605:CLA:HHD	2.02	0.42
2:b:160:GLY:HA2	2:b:163:GLY:O	2.19	0.42
23:d:402:CLA:H203	23:d:402:CLA:H162	1.76	0.42
14:v:78:ASN:ND2	39:v:310:HOH:O	2.49	0.42
1:A:201:GLY:HA3	1:A:286:THR:HB	2.01	0.42
2:B:467:ILE:HG21	4:D:126:MET:CE	2.50	0.42
25:B:619:BCR:H24C	25:B:619:BCR:H371	1.90	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:446:SER:HB2	2:b:447:PRO:HD2	2.01	0.42
2:b:458:PHE:HB3	23:b:604:CLA:HBC2	2.01	0.42
25:c:516:BCR:C23	25:c:516:BCR:C38	2.97	0.42
1:A:63:ILE:HB	3:C:335:THR:HG21	2.00	0.42
3:C:146:PHE:HZ	23:C:513:CLA:HBB2	1.84	0.42
4:D:79:SER:HA	4:D:172:SER:HB3	2.01	0.42
24:d:401:PHO:HBB1	24:d:401:PHO:CMB	2.50	0.42
2:B:157:HIS:C	2:B:157:HIS:CD2	2.98	0.42
3:C:26:ARG:HH22	16:Y:45:ASN:ND2	2.17	0.42
2:b:157:HIS:C	2:b:157:HIS:CD2	2.98	0.42
2:b:264:PRO:HG2	2:b:267:LEU:HD12	2.02	0.42
25:b:617:BCR:H24C	25:b:617:BCR:H371	1.87	0.42
3:c:60:ILE:HG22	23:c:504:CLA:HHD	2.00	0.42
14:v:134:LYS:HA	14:v:137:TYR:CG	2.54	0.42
26:A:410:LMG:H191	26:A:410:LMG:H152	2.02	0.42
2:B:264:PRO:HG2	2:B:267:LEU:HD12	2.02	0.42
1:a:92:HIS:HE1	39:c:798:HOH:O	2.03	0.42
2:b:422:ARG:NH2	39:b:710:HOH:O	2.40	0.42
2:b:467:ILE:HG21	4:d:126:MET:CE	2.50	0.42
2:b:492:GLU:HB3	39:b:842:HOH:O	2.17	0.42
3:c:26:ARG:HH22	16:y:45:ASN:ND2	2.17	0.42
3:c:415:ASN:O	3:c:416[B]:SER:HB2	2.20	0.42
9:k:15:TYR:CE2	19:z:5:PHE:HZ	2.37	0.42
25:t:103:BCR:C23	25:t:103:BCR:C38	2.98	0.42
25:Y:101:BCR:HC8	25:Y:101:BCR:H321	2.02	0.42
4:D:209:LEU:HD23	4:D:209:LEU:C	2.45	0.41
2:b:105:GLY:HA3	25:b:618:BCR:C26	2.50	0.41
25:c:515:BCR:C23	25:c:515:BCR:C38	2.98	0.41
14:v:68:ASN:ND2	14:v:71:GLY:H	2.18	0.41
25:y:101:BCR:HC8	25:y:101:BCR:H321	2.02	0.41
14:V:2:GLU:H	17:E:58:GLN:HE22	1.67	0.41
14:V:68:ASN:ND2	14:V:71:GLY:H	2.18	0.41
2:b:287:ARG:HD3	39:b:706:HOH:O	2.20	0.41
3:c:42:LEU:HD21	23:c:512:CLA:H2A	2.01	0.41
18:o:46:GLN:HG2	39:o:410:HOH:O	2.20	0.41
1:A:334:ARG:HD3	4:D:320:LEU:HD13	2.03	0.41
2:B:30:VAL:HG12	23:B:605:CLA:HHD	2.02	0.41
2:B:490:GLN:HA	2:B:496:TYR:CE2	2.56	0.41
3:C:286:ALA:HB2	23:C:503:CLA:HMD2	2.02	0.41
3:C:415:ASN:O	3:C:416[B]:SER:HB2	2.20	0.41
3:C:446:GLY:HA3	39:C:677:HOH:O	2.19	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:D:401:PHO:CMB	24:D:401:PHO:HBB1	2.50	0.41
18:O:46:GLN:HG2	39:O:410:HOH:O	2.20	0.41
25:c:516:BCR:H24C	25:c:516:BCR:H371	1.82	0.41
35:h:101:RRX:H26	35:h:101:RRX:H22	1.95	0.41
11:m:28:GLN:O	11:m:32:GLN:HG3	2.19	0.41
13:U:51:LYS:HB2	39:U:221:HOH:O	2.21	0.41
1:a:60:ILE:HD12	1:a:84:PRO:HD2	2.01	0.41
3:c:83:GLU:OE1	14:v:103:LYS:HE2	2.21	0.41
17:E:64:PRO:HB2	17:E:79:PHE:CD2	2.55	0.41
17:e:64:PRO:HB2	17:e:79:PHE:CD2	2.55	0.41
23:B:606:CLA:H111	23:B:606:CLA:C6	2.48	0.41
2:b:490:GLN:HA	2:b:496:TYR:CE2	2.56	0.41
3:c:286:ALA:HB2	23:c:503:CLA:HMD2	2.02	0.41
4:d:209:LEU:HD23	4:d:209:LEU:C	2.45	0.41
34:f:101:HEM:HMC3	17:e:27:ILE:HG12	2.01	0.41
2:B:287:ARG:HD3	39:B:706:HOH:O	2.20	0.41
3:C:83:GLU:OE1	14:V:103:LYS:HE2	2.21	0.41
23:c:510:CLA:HBD	23:c:510:CLA:HAA2	2.03	0.41
14:v:2:GLU:H	17:e:58:GLN:HE22	1.67	0.41
3:C:52:ALA:HB2	23:C:512:CLA:HMA2	2.03	0.41
25:T:101:BCR:C23	25:T:101:BCR:C38	2.98	0.41
2:b:12:LEU:HB2	23:b:612:CLA:HMC2	2.02	0.41
23:c:506:CLA:HBC2	25:c:516:BCR:H341	2.03	0.41
25:C:516:BCR:C23	25:C:516:BCR:C38	2.97	0.41
26:a:410:LMG:H191	26:a:410:LMG:H152	2.02	0.41
2:b:135:LEU:N	2:b:136:PRO:CD	2.84	0.41
3:c:52:ALA:HB2	23:c:512:CLA:HMA2	2.03	0.41
4:d:279:LEU:HD22	24:d:401:PHO:HBC3	2.01	0.41
3:C:72:LEU:O	9:K:10:LYS:N	2.54	0.41
23:C:511:CLA:HBB1	23:C:511:CLA:HMB3	2.03	0.41
23:C:512:CLA:HMB3	23:C:512:CLA:HBB1	2.02	0.41
30:T:105:LMT:H21	11:m:6:LEU:HD11	2.03	0.41
9:k:19:ASP:N	9:k:20:PRO:CD	2.85	0.41
23:C:506:CLA:HBC2	25:C:516:BCR:H341	2.03	0.40
23:C:507:CLA:HMC2	23:C:508:CLA:H101	2.02	0.40
23:D:402:CLA:H162	23:D:402:CLA:H203	1.76	0.40
9:K:15:TYR:CZ	19:Z:5:PHE:HZ	2.39	0.40
9:K:19:ASP:N	9:K:20:PRO:CD	2.85	0.40
11:M:20:VAL:HG11	11:m:20:VAL:HG21	2.02	0.40
4:d:352:LEU:CB	39:d:504:HOH:O	2.23	0.40
9:k:15:TYR:CZ	19:z:5:PHE:HZ	2.39	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:279:LEU:HD22	24:D:401:PHO:HBC3	2.01	0.40
23:D:405:CLA:HHD	23:D:405:CLA:HBC3	2.03	0.40
25:K:102:BCR:H23C	25:K:102:BCR:H383	2.03	0.40
2:b:341:LYS:NZ	39:b:739:HOH:O	2.54	0.40
19:Z:39:LEU:HD13	19:Z:39:LEU:HA	1.87	0.40
2:B:105:GLY:HA3	25:B:618:BCR:C26	2.50	0.40
25:B:619:BCR:HC8	25:B:619:BCR:C33	2.45	0.40
1:a:334:ARG:HD3	4:d:320:LEU:HD13	2.02	0.40
3:c:72:LEU:O	9:k:10:LYS:N	2.54	0.40
23:c:512:CLA:HMB3	23:c:512:CLA:HBB1	2.02	0.40
23:C:510:CLA:HAA2	23:C:510:CLA:HBD	2.03	0.40
4:D:301:GLN:HG3	4:D:311:PHE:HE2	1.87	0.40
28:T:103:SQD:H181	28:T:103:SQD:H152	1.92	0.40
18:O:129:THR:HA	18:O:141:ASP:O	2.21	0.40
18:o:129:THR:HA	18:o:141:ASP:O	2.21	0.40
1:A:339:PHE:HB3	1:A:340:PRO:HD2	2.04	0.40
2:B:12:LEU:HB2	23:B:612:CLA:HMC2	2.02	0.40
2:B:341:LYS:NZ	39:B:738:HOH:O	2.54	0.40
25:C:515:BCR:C23	25:C:515:BCR:C38	2.98	0.40
25:D:407:BCR:C8	25:D:407:BCR:C33	2.98	0.40
24:a:407:PHO:H61	24:a:407:PHO:H2	1.85	0.40
3:c:344:SER:O	18:o:75:THR:HG22	2.21	0.40
25:k:102:BCR:H24C	25:k:102:BCR:H371	1.87	0.40
25:y:101:BCR:C23	25:y:101:BCR:H382	2.52	0.40
17:E:27:ILE:HB	17:E:28:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	A	337/360 (94%)	334 (99%)	2 (1%)	1 (0%)	36 26

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	337/360 (94%)	334 (99%)	2 (1%)	1 (0%)	36	26
2	B	503/510 (99%)	498 (99%)	5 (1%)	0	100	100
2	b	503/510 (99%)	498 (99%)	5 (1%)	0	100	100
3	C	450/461 (98%)	442 (98%)	5 (1%)	3 (1%)	18	7
3	c	450/461 (98%)	442 (98%)	5 (1%)	3 (1%)	18	7
4	D	341/352 (97%)	334 (98%)	7 (2%)	0	100	100
4	d	341/352 (97%)	334 (98%)	7 (2%)	0	100	100
5	F	31/45 (69%)	31 (100%)	0	0	100	100
5	f	31/45 (69%)	31 (100%)	0	0	100	100
6	H	59/66 (89%)	57 (97%)	2 (3%)	0	100	100
6	h	59/66 (89%)	57 (97%)	2 (3%)	0	100	100
7	I	32/38 (84%)	31 (97%)	1 (3%)	0	100	100
7	i	32/38 (84%)	31 (97%)	1 (3%)	0	100	100
8	J	32/40 (80%)	31 (97%)	1 (3%)	0	100	100
8	j	32/40 (80%)	31 (97%)	1 (3%)	0	100	100
9	K	35/46 (76%)	35 (100%)	0	0	100	100
9	k	35/46 (76%)	35 (100%)	0	0	100	100
10	L	33/37 (89%)	33 (100%)	0	0	100	100
10	l	33/37 (89%)	33 (100%)	0	0	100	100
11	M	31/36 (86%)	31 (100%)	0	0	100	100
11	m	31/36 (86%)	31 (100%)	0	0	100	100
12	T	27/32 (84%)	27 (100%)	0	0	100	100
12	t	27/32 (84%)	27 (100%)	0	0	100	100
13	U	94/134 (70%)	90 (96%)	4 (4%)	0	100	100
13	u	94/134 (70%)	90 (96%)	4 (4%)	0	100	100
14	V	136/163 (83%)	134 (98%)	2 (2%)	0	100	100
14	v	136/163 (83%)	134 (98%)	2 (2%)	0	100	100
15	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
15	x	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
16	Y	27/46 (59%)	27 (100%)	0	0	100	100
16	y	27/46 (59%)	27 (100%)	0	0	100	100

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	E	75/84 (89%)	75 (100%)	0	0	100	100
17	e	75/84 (89%)	75 (100%)	0	0	100	100
18	O	230/272 (85%)	224 (97%)	6 (3%)	0	100	100
18	o	230/272 (85%)	224 (97%)	6 (3%)	0	100	100
19	Z	51/62 (82%)	51 (100%)	0	0	100	100
19	z	51/62 (82%)	51 (100%)	0	0	100	100
All	All	5120/5650 (91%)	5040 (98%)	72 (1%)	8 (0%)	49	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	25	ASN
3	C	416[A]	SER
3	C	416[B]	SER
3	c	25	ASN
3	c	416[A]	SER
3	c	416[B]	SER
1	A	259	ILE
1	a	259	ILE

### 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	A	266/291 (91%)	265 (100%)	1 (0%)	84	79
1	a	266/291 (91%)	265 (100%)	1 (0%)	84	79
2	B	380/407 (93%)	379 (100%)	1 (0%)	86	82
2	b	380/407 (93%)	379 (100%)	1 (0%)	86	82
3	C	345/362 (95%)	342 (99%)	3 (1%)	70	63
3	c	345/362 (95%)	342 (99%)	3 (1%)	70	63
4	D	273/283 (96%)	272 (100%)	1 (0%)	84	79

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	273/283 (96%)	272 (100%)	1 (0%)	84	79
5	F	27/39 (69%)	27 (100%)	0	100	100
5	f	27/39 (69%)	27 (100%)	0	100	100
6	H	50/55 (91%)	50 (100%)	0	100	100
6	h	50/55 (91%)	50 (100%)	0	100	100
7	I	27/34 (79%)	27 (100%)	0	100	100
7	i	27/34 (79%)	27 (100%)	0	100	100
8	J	23/28 (82%)	23 (100%)	0	100	100
8	j	23/28 (82%)	23 (100%)	0	100	100
9	K	27/37 (73%)	27 (100%)	0	100	100
9	k	27/37 (73%)	27 (100%)	0	100	100
10	L	31/35 (89%)	31 (100%)	0	100	100
10	l	31/35 (89%)	31 (100%)	0	100	100
11	M	26/32 (81%)	25 (96%)	1 (4%)	29	13
11	m	26/32 (81%)	25 (96%)	1 (4%)	29	13
12	T	22/28 (79%)	22 (100%)	0	100	100
12	t	22/28 (79%)	22 (100%)	0	100	100
13	U	71/112 (63%)	69 (97%)	2 (3%)	38	22
13	u	71/112 (63%)	69 (97%)	2 (3%)	38	22
14	V	105/138 (76%)	105 (100%)	0	100	100
14	v	105/138 (76%)	105 (100%)	0	100	100
15	X	28/34 (82%)	27 (96%)	1 (4%)	31	14
15	x	28/34 (82%)	27 (96%)	1 (4%)	31	14
16	Y	19/37 (51%)	19 (100%)	0	100	100
16	y	19/37 (51%)	19 (100%)	0	100	100
17	E	63/73 (86%)	62 (98%)	1 (2%)	55	43
17	e	63/73 (86%)	62 (98%)	1 (2%)	55	43
18	O	163/228 (72%)	161 (99%)	2 (1%)	63	53
18	o	163/228 (72%)	161 (99%)	2 (1%)	63	53
19	Z	40/52 (77%)	38 (95%)	2 (5%)	22	7
19	z	40/52 (77%)	38 (95%)	2 (5%)	22	7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3972/4610 (86%)	3942 (99%)	30 (1%)	70 68

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	PRO
2	B	84	THR
3	C	289	PHE
3	C	315	MET
3	C	391	ARG
4	D	140	PRO
11	M	20	VAL
13	U	43	PRO
13	U	58	VAL
15	X	3	ILE
1	a	141	PRO
2	b	84	THR
3	c	289	PHE
3	c	315	MET
3	c	391	ARG
4	d	140	PRO
11	m	20	VAL
13	u	43	PRO
13	u	58	VAL
15	x	3	ILE
17	E	4	THR
18	O	25	THR
18	O	118	LEU
19	Z	20	VAL
19	Z	39	LEU
17	e	4	THR
18	o	25	THR
18	o	118	LEU
19	z	20	VAL
19	z	39	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	310	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	312	ASN
2	B	14	ASN
2	B	179	GLN
3	C	28	GLN
3	C	332	GLN
3	C	388	GLN
4	D	61	HIS
4	D	186	GLN
4	D	255	GLN
6	H	59	ASN
13	U	37	GLN
13	U	52	ASN
14	V	78	ASN
15	X	33	GLN
16	Y	45	ASN
1	a	165	GLN
1	a	261	GLN
1	a	310	GLN
1	a	312	ASN
2	b	14	ASN
2	b	179	GLN
3	c	28	GLN
3	c	388	GLN
4	d	61	HIS
4	d	186	GLN
4	d	255	GLN
4	d	332	GLN
6	h	59	ASN
13	u	37	GLN
13	u	52	ASN
14	v	78	ASN
15	x	33	GLN
16	y	45	ASN
17	E	58	GLN
17	E	75	GLN
18	O	88	ASN
18	O	124	ASN
18	O	155	ASN
17	e	58	GLN
17	e	75	GLN
18	o	88	ASN
18	o	124	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
18	o	155	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
11	FME	m	1	11	8,9,10	0.70	0	7,9,11	1.49	1 (14%)
11	FME	M	1	11	8,9,10	0.69	0	7,9,11	1.49	1 (14%)
12	FME	T	1	12	8,9,10	0.55	0	7,9,11	1.62	0
12	FME	t	1	12	8,9,10	0.55	0	7,9,11	1.62	0
7	FME	i	1	7	8,9,10	0.89	0	7,9,11	1.52	2 (28%)
7	FME	I	1	7	8,9,10	0.89	0	7,9,11	1.53	2 (28%)

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
11	FME	m	1	11	-	2/7/9/11	-
11	FME	M	1	11	-	2/7/9/11	-
12	FME	T	1	12	-	4/7/9/11	-
12	FME	t	1	12	-	4/7/9/11	-
7	FME	i	1	7	-	1/7/9/11	-
7	FME	I	1	7	-	1/7/9/11	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	1	FME	CA-N-CN	-2.60	118.83	122.82
11	m	1	FME	CA-N-CN	-2.60	118.83	122.82
7	I	1	FME	CA-N-CN	-2.18	119.47	122.82
7	i	1	FME	CA-N-CN	-2.18	119.47	122.82
7	I	1	FME	O1-CN-N	-2.13	119.66	125.27
7	i	1	FME	O1-CN-N	-2.13	119.66	125.27

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	1	FME	O1-CN-N-CA
11	M	1	FME	O1-CN-N-CA
11	M	1	FME	CB-CA-N-CN
12	T	1	FME	O1-CN-N-CA
12	T	1	FME	N-CA-CB-CG
7	i	1	FME	O1-CN-N-CA
11	m	1	FME	O1-CN-N-CA
11	m	1	FME	CB-CA-N-CN
12	t	1	FME	O1-CN-N-CA
12	t	1	FME	N-CA-CB-CG
12	T	1	FME	C-CA-CB-CG
12	t	1	FME	C-CA-CB-CG
12	T	1	FME	CA-CB-CG-SD
12	t	1	FME	CA-CB-CG-SD

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	T	1	FME	1	0
12	t	1	FME	1	0

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 186 ligands modelled in this entry, 10 are monoatomic and 22 are unknown - leaving 154 for Mogul analysis.

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	$\# Z  > 2$
23	CLA	C	508	-	69,73,73	1.86	17 (24%)	83,113,113	2.68	27 (32%)
23	CLA	B	604	2	69,73,73	1.73	23 (33%)	83,113,113	2.77	25 (30%)
33	LHG	d	411	-	44,44,48	0.81	3 (6%)	47,50,54	0.95	2 (4%)
28	SQD	d	415	-	25,26,54	0.85	2 (8%)	32,35,65	2.44	9 (28%)
30	LMT	B	623	-	16,16,36	0.31	0	15,15,47	0.35	0
23	CLA	b	608	2	69,73,73	1.85	18 (26%)	83,113,113	2.65	30 (36%)
23	CLA	D	405	4	69,73,73	1.73	17 (24%)	83,113,113	2.59	25 (30%)
31	DGD	C	517	-	54,54,67	0.87	4 (7%)	68,68,81	0.96	3 (4%)
30	LMT	b	621	-	36,36,36	0.25	0	47,47,47	0.56	1 (2%)
23	CLA	c	506	3	69,73,73	1.74	18 (26%)	83,113,113	2.53	28 (33%)
33	LHG	D	410	-	48,48,48	0.82	3 (6%)	51,54,54	0.93	1 (1%)
28	SQD	a	412	-	38,39,54	1.09	3 (7%)	45,49,65	1.45	8 (17%)
30	LMT	B	621	-	36,36,36	0.25	0	47,47,47	0.56	1 (2%)
33	LHG	d	410	-	48,48,48	0.82	3 (6%)	51,54,54	0.93	1 (1%)
23	CLA	b	611	2	69,73,73	1.98	20 (28%)	83,113,113	3.46	32 (38%)
23	CLA	B	616	2	69,73,73	1.83	18 (26%)	83,113,113	2.78	26 (31%)
33	LHG	D	409	-	40,40,48	0.93	4 (10%)	41,44,54	0.95	2 (4%)
23	CLA	C	509	3	64,68,73	1.93	19 (29%)	77,107,113	2.76	29 (37%)
23	CLA	A	408	1	56,60,73	1.97	18 (32%)	67,97,113	3.08	31 (46%)
23	CLA	B	602	2	69,73,73	1.77	16 (23%)	83,113,113	2.90	32 (38%)
23	CLA	b	610	-	69,73,73	1.80	19 (27%)	83,113,113	2.62	29 (34%)
23	CLA	c	511	3	69,73,73	1.76	17 (24%)	83,113,113	2.82	31 (37%)
30	LMT	T	105	-	12,12,36	0.18	0	11,11,47	0.17	0
32	BCT	d	404[A]	21	2,3,3	0.96	0	2,3,3	0.38	0
33	LHG	e	101	-	34,34,48	0.89	2 (5%)	37,40,54	0.97	2 (5%)
23	CLA	B	611	2	69,73,73	1.98	20 (28%)	83,113,113	3.46	32 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	a	406	-	60,64,73	1.77	16 (26%)	72,102,113	2.84	27 (37%)
23	CLA	b	602	2	69,73,73	1.77	16 (23%)	83,113,113	2.90	32 (38%)
26	LMG	B	620	-	47,47,55	0.81	2 (4%)	55,55,63	1.33	6 (10%)
23	CLA	c	512	3	69,73,73	1.81	19 (27%)	83,113,113	2.66	28 (33%)
23	CLA	b	605	2	69,73,73	1.67	18 (26%)	83,113,113	2.90	29 (34%)
31	DGD	C	518	-	53,53,67	0.88	3 (5%)	67,67,81	0.95	2 (2%)
23	CLA	a	405	1	69,73,73	1.83	20 (28%)	83,113,113	2.52	31 (37%)
28	SQD	c	501	-	31,32,54	1.23	4 (12%)	40,43,65	2.30	12 (30%)
31	DGD	c	517	-	54,54,67	0.87	4 (7%)	68,68,81	0.95	3 (4%)
33	LHG	d	409	-	40,40,48	0.93	4 (10%)	41,44,54	0.95	2 (4%)
33	LHG	E	101	-	34,34,48	0.89	2 (5%)	37,40,54	0.97	2 (5%)
23	CLA	c	508	-	69,73,73	1.86	17 (24%)	83,113,113	2.68	27 (32%)
23	CLA	B	610	-	69,73,73	1.80	19 (27%)	83,113,113	2.62	29 (34%)
26	LMG	d	412	36	43,43,55	0.92	3 (6%)	51,51,63	0.94	4 (7%)
23	CLA	b	604	2	69,73,73	1.73	23 (33%)	83,113,113	2.77	25 (30%)
30	LMT	M	101	-	36,36,36	0.45	1 (2%)	47,47,47	0.64	2 (4%)
25	BCR	b	618	-	38,38,41	1.15	3 (7%)	47,49,56	1.59	12 (25%)
31	DGD	h	102	-	63,63,67	0.76	2 (3%)	77,77,81	1.06	6 (7%)
30	LMT	t	102	-	12,12,36	0.18	0	11,11,47	0.17	0
25	BCR	y	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.50	10 (17%)
23	CLA	B	601	-	61,65,73	1.86	17 (27%)	69,99,113	2.87	24 (34%)
34	HEM	F	101	5,17	50,50,50	1.50	6 (12%)	66,82,82	1.90	13 (19%)
23	CLA	b	613	2	59,63,73	1.86	16 (27%)	71,101,113	2.69	28 (39%)
25	BCR	D	407	-	41,41,41	1.13	3 (7%)	56,56,56	1.76	15 (26%)
23	CLA	c	502	3	69,73,73	1.66	17 (24%)	83,113,113	2.77	26 (31%)
34	HEM	f	101	5,17	50,50,50	1.50	6 (12%)	66,82,82	1.90	13 (19%)
23	CLA	C	511	3	69,73,73	1.76	17 (24%)	83,113,113	2.82	31 (37%)
30	LMT	T	104	-	16,16,36	0.31	0	15,15,47	0.35	0
23	CLA	b	601	-	61,65,73	1.86	17 (27%)	69,99,113	2.87	24 (34%)
23	CLA	c	509	3	64,68,73	1.93	19 (29%)	77,107,113	2.76	29 (37%)
31	DGD	C	519	-	61,61,67	0.79	3 (4%)	75,75,81	0.88	3 (4%)
23	CLA	B	609	2	69,73,73	1.78	17 (24%)	83,113,113	2.73	29 (34%)
23	CLA	d	405	4	69,73,73	1.73	17 (24%)	83,113,113	2.59	25 (30%)
23	CLA	C	513	3	56,60,73	2.01	16 (28%)	67,97,113	3.11	28 (41%)
23	CLA	B	613	2	59,63,73	1.86	16 (27%)	71,101,113	2.70	28 (39%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	B	617	-	41,41,41	1.05	3 (7%)	56,56,56	1.67	11 (19%)
23	CLA	A	406	39	60,64,73	1.77	16 (26%)	72,102,113	2.84	27 (37%)
25	BCR	k	102	-	41,41,41	0.97	2 (4%)	56,56,56	1.68	12 (21%)
35	RRX	h	101	-	42,42,42	1.60	10 (23%)	57,58,58	1.53	10 (17%)
35	RRX	H	101	-	42,42,42	1.60	10 (23%)	57,58,58	1.53	10 (17%)
23	CLA	c	504	3	69,73,73	1.80	17 (24%)	83,113,113	2.54	30 (36%)
24	PHO	A	407	-	58,69,69	2.22	16 (27%)	56,99,99	3.34	19 (33%)
26	LMG	b	620	-	47,47,55	0.81	2 (4%)	55,55,63	1.33	6 (10%)
23	CLA	b	615	2	69,73,73	1.72	15 (21%)	83,113,113	2.57	29 (34%)
23	CLA	b	606	2	69,73,73	1.70	18 (26%)	83,113,113	2.72	31 (37%)
33	LHG	l	101	-	48,48,48	0.88	3 (6%)	51,54,54	1.06	3 (5%)
27	PL9	D	408	-	55,55,55	0.78	2 (3%)	68,69,69	1.56	15 (22%)
33	LHG	D	411	-	44,44,48	0.81	3 (6%)	47,50,54	0.95	2 (4%)
23	CLA	b	616	2	69,73,73	1.83	18 (26%)	83,113,113	2.78	26 (31%)
28	SQD	T	103	-	25,25,54	0.84	1 (4%)	24,24,65	0.96	2 (8%)
23	CLA	B	605	2	69,73,73	1.67	18 (26%)	83,113,113	2.90	29 (34%)
30	LMT	J	102	-	24,24,36	0.23	0	29,29,47	0.49	0
25	BCR	c	516	-	41,41,41	1.09	2 (4%)	56,56,56	1.72	12 (21%)
23	CLA	B	608	2	69,73,73	1.85	18 (26%)	83,113,113	2.66	30 (36%)
23	CLA	C	504	3	69,73,73	1.80	17 (24%)	83,113,113	2.54	30 (36%)
25	BCR	t	103	-	39,39,41	1.05	3 (7%)	48,52,56	1.55	6 (12%)
23	CLA	C	507	3	50,54,73	2.10	19 (38%)	60,90,113	2.99	28 (46%)
23	CLA	B	603	2	69,73,73	1.67	17 (24%)	83,113,113	3.12	31 (37%)
23	CLA	d	402	39	69,73,73	1.58	15 (21%)	83,113,113	2.65	27 (32%)
23	CLA	b	607	-	69,73,73	1.84	17 (24%)	83,113,113	2.52	27 (32%)
31	DGD	H	102	-	63,63,67	0.76	2 (3%)	77,77,81	1.06	6 (7%)
23	CLA	C	514	3	46,50,73	2.24	17 (36%)	55,85,113	3.52	28 (50%)
31	DGD	c	519	-	61,61,67	0.79	3 (4%)	75,75,81	0.88	3 (4%)
23	CLA	B	606	2	69,73,73	1.70	18 (26%)	83,113,113	2.72	31 (37%)
23	CLA	B	607	-	69,73,73	1.85	17 (24%)	83,113,113	2.53	27 (32%)
23	CLA	C	505	-	69,73,73	1.79	18 (26%)	83,113,113	3.01	31 (37%)
23	CLA	c	513	3	56,60,73	2.01	16 (28%)	67,97,113	3.11	28 (41%)
25	BCR	d	407	-	41,41,41	1.13	3 (7%)	56,56,56	1.76	15 (26%)
25	BCR	b	617	-	41,41,41	1.05	3 (7%)	56,56,56	1.67	11 (19%)
25	BCR	C	516	-	41,41,41	1.09	2 (4%)	56,56,56	1.72	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	B	614	2	58,62,73	1.97	15 (25%)	69,99,113	3.09	30 (43%)
30	LMT	j	102	-	24,24,36	0.23	0	29,29,47	0.49	0
23	CLA	b	603	2	69,73,73	1.67	17 (24%)	83,113,113	3.12	31 (37%)
37	HEC	V	201	14	46,50,50	3.51	23 (50%)	60,82,82	2.62	25 (41%)
25	BCR	B	618	-	38,38,41	1.15	3 (7%)	47,49,56	1.59	12 (25%)
30	LMT	m	101	-	36,36,36	0.45	1 (2%)	47,47,47	0.64	2 (4%)
23	CLA	D	402	39	69,73,73	1.58	15 (21%)	83,113,113	2.65	27 (32%)
23	CLA	C	506	3	69,73,73	1.74	18 (26%)	83,113,113	2.53	28 (33%)
28	SQD	A	412	-	38,39,54	1.09	3 (7%)	45,49,65	1.45	8 (17%)
26	LMG	D	412	36	43,43,55	0.92	3 (6%)	51,51,63	0.94	4 (7%)
23	CLA	d	406	4	52,56,73	2.11	18 (34%)	62,92,113	3.18	29 (46%)
27	PL9	a	411	-	41,41,55	0.78	2 (4%)	49,51,69	1.71	10 (20%)
37	HEC	v	201	14	46,50,50	3.51	23 (50%)	60,82,82	2.62	25 (41%)
25	BCR	C	515	-	39,39,41	1.05	1 (2%)	50,51,56	2.17	17 (34%)
23	CLA	C	512	3	69,73,73	1.81	19 (27%)	83,113,113	2.66	28 (33%)
26	LMG	A	410	-	51,51,55	0.90	2 (3%)	59,59,63	0.99	3 (5%)
31	DGD	c	518	-	53,53,67	0.89	3 (5%)	67,67,81	0.95	2 (2%)
23	CLA	c	514	3	46,50,73	2.24	17 (36%)	55,85,113	3.52	28 (50%)
26	LMG	c	521	-	15,15,55	0.26	0	14,14,63	0.58	0
27	PL9	A	411	-	41,41,55	0.78	2 (4%)	49,51,69	1.71	10 (20%)
28	SQD	C	501	-	31,32,54	1.23	4 (12%)	40,43,65	2.30	12 (30%)
26	LMG	C	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.02	3 (5%)
23	CLA	C	503	3	69,73,73	1.64	19 (27%)	83,113,113	2.56	24 (28%)
23	CLA	b	609	2	69,73,73	1.78	17 (24%)	83,113,113	2.73	29 (34%)
24	PHO	a	407	-	58,69,69	2.22	16 (27%)	56,99,99	3.34	19 (33%)
23	CLA	A	405	1	69,73,73	1.83	20 (28%)	83,113,113	2.52	31 (37%)
32	BCT	D	404[A]	21	2,3,3	0.96	0	2,3,3	0.38	0
25	BCR	b	619	-	41,41,41	0.98	2 (4%)	56,56,56	1.49	14 (25%)
25	BCR	K	102	-	41,41,41	0.97	2 (4%)	56,56,56	1.68	12 (21%)
23	CLA	C	502	3	69,73,73	1.66	17 (24%)	83,113,113	2.77	26 (31%)
26	LMG	C	521	-	15,15,55	0.26	0	14,14,63	0.58	0
28	SQD	D	415	-	25,26,54	0.85	2 (8%)	32,35,65	2.44	9 (28%)
23	CLA	a	408	1	56,60,73	1.97	18 (32%)	67,97,113	3.08	31 (46%)
25	BCR	c	515	-	39,39,41	1.05	1 (2%)	50,51,56	2.17	17 (34%)
33	LHG	L	101	-	48,48,48	0.88	3 (6%)	51,54,54	1.06	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	B	615	2	69,73,73	1.72	15 (21%)	83,113,113	2.57	29 (34%)
24	PHO	D	401	-	58,69,69	2.38	16 (27%)	56,99,99	3.25	16 (28%)
25	BCR	T	101	-	39,39,41	1.05	3 (7%)	48,52,56	1.55	6 (12%)
24	PHO	d	401	-	58,69,69	2.38	16 (27%)	56,99,99	3.25	16 (28%)
23	CLA	b	614	2	58,62,73	1.97	15 (25%)	69,99,113	3.09	30 (43%)
23	CLA	b	612	2	69,73,73	1.73	15 (21%)	83,113,113	2.62	24 (28%)
25	BCR	B	619	-	41,41,41	0.98	2 (4%)	56,56,56	1.49	14 (25%)
25	BCR	A	409	-	41,41,41	0.90	2 (4%)	56,56,56	1.62	9 (16%)
26	LMG	c	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.01	3 (5%)
20	OEX	A	401	3,1	0,15,15	-	-	-	-	-
23	CLA	c	503	3	69,73,73	1.64	20 (28%)	83,113,113	2.56	24 (28%)
23	CLA	c	510	3	69,73,73	1.87	18 (26%)	83,113,113	2.73	26 (31%)
23	CLA	c	507	3	50,54,73	2.10	19 (38%)	60,90,113	3.00	28 (46%)
27	PL9	d	408	-	55,55,55	0.78	2 (3%)	68,69,69	1.56	15 (22%)
25	BCR	a	409	-	41,41,41	0.90	2 (4%)	56,56,56	1.62	9 (16%)
26	LMG	a	410	-	51,51,55	0.90	2 (3%)	59,59,63	0.99	3 (5%)
20	OEX	a	401	3,1	0,15,15	-	-	-	-	-
23	CLA	c	505	-	69,73,73	1.79	18 (26%)	83,113,113	3.01	31 (37%)
28	SQD	t	101	-	25,25,54	0.84	1 (4%)	24,24,65	0.96	2 (8%)
23	CLA	B	612	2	69,73,73	1.73	15 (21%)	83,113,113	2.62	24 (28%)
25	BCR	Y	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.50	10 (17%)
23	CLA	C	510	3	69,73,73	1.87	18 (26%)	83,113,113	2.73	26 (31%)
23	CLA	D	406	4	52,56,73	2.11	18 (34%)	62,92,113	3.18	29 (46%)

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
23	CLA	C	508	-	-	10/39/115/115	-
23	CLA	B	604	2	-	6/39/115/115	-
33	LHG	d	411	-	-	6/49/49/53	-
28	SQD	d	415	-	-	4/16/36/69	0/1/1/1
30	LMT	B	623	-	-	7/14/14/61	-
23	CLA	b	608	2	-	1/39/115/115	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	D	405	4	-	3/39/115/115	-
31	DGD	C	517	-	-	10/42/82/95	0/2/2/2
30	LMT	b	621	-	-	11/21/61/61	0/2/2/2
23	CLA	c	506	3	-	4/39/115/115	-
33	LHG	D	410	-	-	9/53/53/53	-
28	SQD	a	412	-	-	14/33/53/69	0/1/1/1
30	LMT	B	621	-	-	11/21/61/61	0/2/2/2
33	LHG	d	410	-	-	9/53/53/53	-
23	CLA	b	611	2	-	4/39/115/115	-
23	CLA	B	616	2	-	13/39/115/115	-
33	LHG	D	409	-	-	4/41/41/53	-
23	CLA	C	509	3	-	7/33/109/115	-
23	CLA	A	408	1	-	4/24/100/115	-
23	CLA	B	602	2	-	4/39/115/115	-
23	CLA	b	610	-	-	3/39/115/115	-
23	CLA	c	511	3	-	4/39/115/115	-
30	LMT	T	105	-	-	3/10/10/61	-
33	LHG	e	101	-	-	14/38/38/53	-
23	CLA	B	611	2	-	4/39/115/115	-
23	CLA	a	406	-	-	6/29/105/115	-
23	CLA	b	602	2	-	4/39/115/115	-
26	LMG	B	620	-	-	8/42/62/70	0/1/1/1
23	CLA	c	512	3	-	2/39/115/115	-
23	CLA	b	605	2	-	3/39/115/115	-
31	DGD	C	518	-	-	10/41/81/95	0/2/2/2
23	CLA	a	405	1	-	3/39/115/115	-
28	SQD	c	501	-	-	4/27/47/69	0/1/1/1
31	DGD	c	517	-	-	10/42/82/95	0/2/2/2
33	LHG	d	409	-	-	4/41/41/53	-
33	LHG	E	101	-	-	14/38/38/53	-
23	CLA	c	508	-	-	10/39/115/115	-
23	CLA	B	610	-	-	3/39/115/115	-
26	LMG	d	412	36	-	5/38/58/70	0/1/1/1
23	CLA	b	604	2	-	6/39/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMT	M	101	-	-	1/21/61/61	0/2/2/2
25	BCR	b	618	-	-	2/29/54/63	0/2/2/2
31	DGD	h	102	-	-	14/51/91/95	0/2/2/2
30	LMT	t	102	-	-	3/10/10/61	-
25	BCR	y	101	-	-	2/29/63/63	0/2/2/2
23	CLA	B	601	-	-	11/25/101/115	-
34	HEM	F	101	5,17	-	2/14/54/54	-
23	CLA	b	613	2	-	1/27/103/115	-
25	BCR	D	407	-	-	0/29/63/63	0/2/2/2
23	CLA	c	502	3	-	3/39/115/115	-
34	HEM	f	101	5,17	-	2/14/54/54	-
23	CLA	C	511	3	-	4/39/115/115	-
30	LMT	T	104	-	-	7/14/14/61	-
23	CLA	b	601	-	-	11/25/101/115	-
23	CLA	c	509	3	-	7/33/109/115	-
31	DGD	C	519	-	-	7/49/89/95	0/2/2/2
23	CLA	B	609	2	-	3/39/115/115	-
23	CLA	d	405	4	-	3/39/115/115	-
23	CLA	C	513	3	-	9/24/100/115	-
23	CLA	B	613	2	-	1/27/103/115	-
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
23	CLA	A	406	39	-	6/29/105/115	-
25	BCR	k	102	-	-	1/29/63/63	0/2/2/2
35	RRX	h	101	-	-	4/29/65/65	0/2/2/2
35	RRX	H	101	-	-	4/29/65/65	0/2/2/2
23	CLA	c	504	3	-	3/39/115/115	-
24	PHO	A	407	-	-	2/37/103/103	0/5/6/6
26	LMG	b	620	-	-	8/42/62/70	0/1/1/1
23	CLA	b	615	2	-	1/39/115/115	-
23	CLA	b	606	2	-	10/39/115/115	-
33	LHG	l	101	-	-	17/53/53/53	-
27	PL9	D	408	-	-	3/53/73/73	0/1/1/1
33	LHG	D	411	-	-	6/49/49/53	-
23	CLA	b	616	2	-	13/39/115/115	-
28	SQD	T	103	-	-	11/22/22/69	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	605	2	-	3/39/115/115	-
30	LMT	J	102	-	-	5/15/35/61	0/1/1/2
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
23	CLA	B	608	2	-	1/39/115/115	-
23	CLA	C	504	3	-	3/39/115/115	-
25	BCR	t	103	-	-	0/24/53/63	0/2/2/2
23	CLA	C	507	3	-	3/17/93/115	-
23	CLA	B	603	2	-	8/39/115/115	-
23	CLA	d	402	39	-	4/39/115/115	-
23	CLA	b	607	-	-	1/39/115/115	-
31	DGD	H	102	-	-	14/51/91/95	0/2/2/2
23	CLA	C	514	3	-	0/12/88/115	-
31	DGD	c	519	-	-	7/49/89/95	0/2/2/2
23	CLA	B	606	2	-	10/39/115/115	-
23	CLA	B	607	-	-	1/39/115/115	-
23	CLA	C	505	-	-	5/39/115/115	-
23	CLA	c	513	3	-	9/24/100/115	-
25	BCR	d	407	-	-	0/29/63/63	0/2/2/2
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
23	CLA	B	614	2	-	7/26/102/115	-
30	LMT	j	102	-	-	5/15/35/61	0/1/1/2
23	CLA	b	603	2	-	8/39/115/115	-
37	HEC	V	201	14	-	5/14/54/54	-
25	BCR	B	618	-	-	2/29/54/63	0/2/2/2
30	LMT	m	101	-	-	1/21/61/61	0/2/2/2
23	CLA	D	402	39	-	4/39/115/115	-
23	CLA	C	506	3	-	4/39/115/115	-
28	SQD	A	412	-	-	14/33/53/69	0/1/1/1
26	LMG	D	412	36	-	5/38/58/70	0/1/1/1
23	CLA	d	406	4	-	2/19/95/115	-
27	PL9	a	411	-	-	4/34/54/73	0/1/1/1
37	HEC	v	201	14	-	5/14/54/54	-
25	BCR	C	515	-	-	2/29/57/63	0/2/2/2
23	CLA	C	512	3	-	2/39/115/115	-
26	LMG	A	410	-	-	19/46/66/70	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DGD	c	518	-	-	10/41/81/95	0/2/2/2
23	CLA	c	514	3	-	0/12/88/115	-
26	LMG	c	521	-	-	1/13/13/70	-
27	PL9	A	411	-	-	4/34/54/73	0/1/1/1
28	SQD	C	501	-	-	4/27/47/69	0/1/1/1
26	LMG	C	520	-	-	15/46/66/70	0/1/1/1
23	CLA	C	503	3	-	3/39/115/115	-
23	CLA	b	609	2	-	3/39/115/115	-
24	PHO	a	407	-	-	2/37/103/103	0/5/6/6
23	CLA	A	405	1	-	3/39/115/115	-
25	BCR	b	619	-	-	0/29/63/63	0/2/2/2
25	BCR	K	102	-	-	1/29/63/63	0/2/2/2
23	CLA	C	502	3	-	3/39/115/115	-
26	LMG	C	521	-	-	1/13/13/70	-
28	SQD	D	415	-	-	4/16/36/69	0/1/1/1
23	CLA	a	408	1	-	4/24/100/115	-
25	BCR	c	515	-	-	2/29/57/63	0/2/2/2
33	LHG	L	101	-	-	17/53/53/53	-
23	CLA	B	615	2	-	1/39/115/115	-
24	PHO	D	401	-	-	1/37/103/103	0/5/6/6
25	BCR	T	101	-	-	0/24/53/63	0/2/2/2
24	PHO	d	401	-	-	1/37/103/103	0/5/6/6
23	CLA	b	614	2	-	7/26/102/115	-
23	CLA	b	612	2	-	5/39/115/115	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
25	BCR	A	409	-	-	1/29/63/63	0/2/2/2
26	LMG	c	520	-	-	15/46/66/70	0/1/1/1
23	CLA	c	503	3	-	3/39/115/115	-
23	CLA	c	510	3	-	5/39/115/115	-
23	CLA	c	507	3	-	3/17/93/115	-
27	PL9	d	408	-	-	3/53/73/73	0/1/1/1
25	BCR	a	409	-	-	1/29/63/63	0/2/2/2
26	LMG	a	410	-	-	19/46/66/70	0/1/1/1
23	CLA	c	505	-	-	5/39/115/115	-
28	SQD	t	101	-	-	11/22/22/69	-
23	CLA	B	612	2	-	5/39/115/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	Y	101	-	-	2/29/63/63	0/2/2/2
23	CLA	C	510	3	-	5/39/115/115	-
23	CLA	D	406	4	-	2/19/95/115	-

All (1517) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	V	201	HEC	CAB-C3B	13.12	1.51	1.34
37	v	201	HEC	CAB-C3B	13.12	1.51	1.34
37	V	201	HEC	CAC-C3C	12.63	1.50	1.34
37	v	201	HEC	CAC-C3C	12.63	1.50	1.34
24	D	401	PHO	C1B-C2B	8.02	1.48	1.39
24	d	401	PHO	C1B-C2B	8.02	1.48	1.39
24	A	407	PHO	C1D-C2D	7.88	1.48	1.39
24	a	407	PHO	C1D-C2D	7.88	1.48	1.39
24	D	401	PHO	C1D-C2D	7.54	1.47	1.39
24	d	401	PHO	C1D-C2D	7.54	1.47	1.39
24	A	407	PHO	C1B-C2B	6.51	1.46	1.39
24	a	407	PHO	C1B-C2B	6.42	1.46	1.39
23	B	611	CLA	CMB-C2B	5.99	1.63	1.50
23	b	611	CLA	CMB-C2B	5.99	1.63	1.50
23	B	607	CLA	C1B-NB	-5.97	1.30	1.37
23	b	607	CLA	C1B-NB	-5.97	1.30	1.37
23	D	406	CLA	C1B-NB	-5.56	1.30	1.37
23	d	406	CLA	C1B-NB	-5.56	1.30	1.37
23	C	511	CLA	C1B-NB	-5.50	1.31	1.37
23	c	511	CLA	C1B-NB	-5.50	1.31	1.37
23	C	514	CLA	C1D-ND	5.47	1.44	1.37
23	c	514	CLA	C1D-ND	5.47	1.44	1.37
23	C	508	CLA	C1B-NB	-5.45	1.31	1.37
23	c	508	CLA	C1B-NB	-5.45	1.31	1.37
23	B	616	CLA	C3C-C2C	5.36	1.48	1.36
23	b	616	CLA	C3C-C2C	5.36	1.48	1.36
24	D	401	PHO	C3B-C2B	5.18	1.47	1.40
24	d	401	PHO	C3B-C2B	5.18	1.47	1.40
23	B	608	CLA	C3C-C2C	5.18	1.47	1.36
23	b	608	CLA	C3C-C2C	5.18	1.47	1.36
23	A	405	CLA	C3C-C2C	5.16	1.47	1.36
23	a	405	CLA	C3C-C2C	5.16	1.47	1.36
23	C	512	CLA	C3C-C2C	5.12	1.47	1.36
23	c	512	CLA	C3C-C2C	5.12	1.47	1.36
24	A	407	PHO	C3C-C2C	5.07	1.47	1.36

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	407	PHO	C3C-C2C	5.07	1.47	1.36
23	B	614	CLA	C3C-C2C	5.05	1.47	1.36
23	b	614	CLA	C3C-C2C	5.05	1.47	1.36
23	B	612	CLA	C1B-NB	-4.97	1.31	1.37
23	b	612	CLA	C1B-NB	-4.97	1.31	1.37
37	V	201	HEC	CHB-C4A	4.91	1.47	1.38
37	v	201	HEC	CHB-C4A	4.91	1.47	1.38
23	B	611	CLA	C1B-C2B	4.87	1.54	1.43
23	b	611	CLA	C1B-C2B	4.87	1.54	1.43
24	D	401	PHO	C3C-C2C	4.81	1.47	1.36
24	d	401	PHO	C3C-C2C	4.81	1.47	1.36
23	B	603	CLA	C3C-C2C	4.80	1.46	1.36
23	b	603	CLA	C3C-C2C	4.79	1.46	1.36
23	C	504	CLA	C3C-C2C	4.78	1.46	1.36
23	c	504	CLA	C3C-C2C	4.78	1.46	1.36
23	B	602	CLA	CHD-C1D	4.75	1.47	1.38
23	b	602	CLA	CHD-C1D	4.75	1.47	1.38
23	B	605	CLA	C3C-C2C	4.74	1.46	1.36
23	b	605	CLA	C3C-C2C	4.74	1.46	1.36
23	C	504	CLA	C1D-ND	4.72	1.43	1.37
23	A	408	CLA	C3C-C2C	4.71	1.46	1.36
23	a	408	CLA	C3C-C2C	4.71	1.46	1.36
23	C	514	CLA	C3C-C2C	4.70	1.46	1.36
23	c	514	CLA	C3C-C2C	4.70	1.46	1.36
24	D	401	PHO	C3B-C4B	4.70	1.46	1.41
24	d	401	PHO	C3B-C4B	4.70	1.46	1.41
23	C	502	CLA	C3C-C2C	4.69	1.46	1.36
23	c	502	CLA	C3C-C2C	4.69	1.46	1.36
23	B	611	CLA	CHC-C1C	4.68	1.48	1.38
23	b	611	CLA	CHC-C1C	4.68	1.48	1.38
23	c	504	CLA	C1D-ND	4.68	1.43	1.37
23	A	405	CLA	C1D-ND	4.67	1.43	1.37
23	a	405	CLA	C1D-ND	4.67	1.43	1.37
23	D	405	CLA	C4B-NB	-4.66	1.32	1.37
23	d	405	CLA	C4B-NB	-4.66	1.32	1.37
23	C	513	CLA	C3C-C2C	4.66	1.46	1.36
23	c	513	CLA	C3C-C2C	4.66	1.46	1.36
23	B	608	CLA	C4B-NB	-4.66	1.32	1.37
23	b	608	CLA	C4B-NB	-4.66	1.32	1.37
23	C	513	CLA	CHC-C1C	4.64	1.48	1.38
23	c	513	CLA	CHC-C1C	4.64	1.48	1.38
35	H	101	RRX	C21-C22	4.64	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	h	101	RRX	C21-C22	4.64	1.41	1.35
23	B	610	CLA	C1B-NB	-4.62	1.32	1.37
23	b	610	CLA	C1B-NB	-4.62	1.32	1.37
23	C	513	CLA	O2A-CGA	4.61	1.46	1.33
23	c	513	CLA	O2A-CGA	4.61	1.46	1.33
23	C	504	CLA	CHC-C1C	4.61	1.47	1.38
23	c	504	CLA	CHC-C1C	4.61	1.47	1.38
23	D	406	CLA	O2A-CGA	4.59	1.46	1.33
23	d	406	CLA	O2A-CGA	4.59	1.46	1.33
23	B	608	CLA	C1B-NB	-4.58	1.32	1.37
23	b	608	CLA	C1B-NB	-4.58	1.32	1.37
23	C	510	CLA	C3C-C2C	4.56	1.46	1.36
23	c	510	CLA	C3C-C2C	4.56	1.46	1.36
23	C	513	CLA	C1B-NB	-4.53	1.32	1.37
23	c	513	CLA	C1B-NB	-4.53	1.32	1.37
23	C	510	CLA	C1D-ND	4.52	1.43	1.37
23	c	510	CLA	C1D-ND	4.52	1.43	1.37
23	B	601	CLA	C3C-C2C	4.50	1.46	1.36
23	C	508	CLA	C3C-C2C	4.50	1.46	1.36
23	b	601	CLA	C3C-C2C	4.50	1.46	1.36
23	c	508	CLA	C3C-C2C	4.50	1.46	1.36
25	C	515	BCR	C23-C22	-4.49	1.36	1.45
25	c	515	BCR	C23-C22	-4.49	1.36	1.45
23	A	406	CLA	CHC-C1C	4.48	1.47	1.38
23	a	406	CLA	CHC-C1C	4.48	1.47	1.38
23	B	602	CLA	C3C-C2C	4.47	1.46	1.36
23	b	602	CLA	C3C-C2C	4.47	1.46	1.36
23	B	615	CLA	O2A-CGA	4.47	1.46	1.33
23	b	615	CLA	O2A-CGA	4.47	1.46	1.33
23	B	606	CLA	C3C-C2C	4.47	1.46	1.36
23	b	606	CLA	C3C-C2C	4.47	1.46	1.36
23	B	615	CLA	C1B-NB	-4.45	1.32	1.37
23	b	615	CLA	C1B-NB	-4.45	1.32	1.37
23	C	506	CLA	C3C-C2C	4.44	1.46	1.36
23	c	506	CLA	C3C-C2C	4.44	1.46	1.36
23	C	507	CLA	O2D-CGD	4.41	1.44	1.33
23	c	507	CLA	O2D-CGD	4.41	1.44	1.33
23	C	510	CLA	O2A-CGA	4.41	1.46	1.33
23	c	510	CLA	O2A-CGA	4.41	1.46	1.33
23	B	614	CLA	O2A-CGA	4.41	1.46	1.33
23	b	614	CLA	O2A-CGA	4.41	1.46	1.33
37	V	201	HEC	C2A-C3A	4.39	1.46	1.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	v	201	HEC	C2A-C3A	4.39	1.46	1.36
23	B	615	CLA	C3C-C2C	4.39	1.46	1.36
23	b	615	CLA	C3C-C2C	4.39	1.46	1.36
23	B	616	CLA	O2A-CGA	4.38	1.46	1.33
23	b	616	CLA	O2A-CGA	4.38	1.46	1.33
26	C	520	LMG	O8-C28	4.38	1.46	1.33
26	c	520	LMG	O8-C28	4.38	1.46	1.33
28	A	412	SQD	O47-C7	4.35	1.46	1.34
28	a	412	SQD	O47-C7	4.35	1.46	1.34
24	D	401	PHO	C4D-CHA	4.35	1.46	1.39
24	d	401	PHO	C4D-CHA	4.35	1.46	1.39
23	B	612	CLA	CHC-C1C	4.34	1.47	1.38
23	b	612	CLA	CHC-C1C	4.34	1.47	1.38
23	D	402	CLA	C3C-C2C	4.33	1.45	1.36
23	d	402	CLA	C3C-C2C	4.33	1.45	1.36
23	B	609	CLA	CHC-C1C	4.33	1.47	1.38
23	b	609	CLA	CHC-C1C	4.33	1.47	1.38
23	A	406	CLA	C1B-NB	-4.32	1.32	1.37
23	a	406	CLA	C1B-NB	-4.32	1.32	1.37
23	B	607	CLA	C3C-C2C	4.32	1.45	1.36
23	b	607	CLA	C3C-C2C	4.32	1.45	1.36
23	C	506	CLA	C1B-NB	-4.32	1.32	1.37
23	C	504	CLA	O2D-CGD	4.31	1.43	1.33
23	c	504	CLA	O2D-CGD	4.31	1.43	1.33
24	a	407	PHO	C4D-CHA	4.30	1.46	1.39
24	A	407	PHO	C4D-CHA	4.30	1.46	1.39
23	B	601	CLA	CHC-C1C	4.29	1.47	1.38
23	b	601	CLA	CHC-C1C	4.29	1.47	1.38
25	Y	101	BCR	C23-C22	-4.29	1.36	1.45
25	y	101	BCR	C23-C22	-4.29	1.36	1.45
23	c	506	CLA	C1B-NB	-4.28	1.32	1.37
23	C	503	CLA	C1B-NB	-4.28	1.32	1.37
23	c	503	CLA	C1B-NB	-4.28	1.32	1.37
25	D	407	BCR	C23-C22	-4.28	1.36	1.45
25	d	407	BCR	C23-C22	-4.28	1.36	1.45
24	A	407	PHO	C3B-C2B	4.27	1.46	1.40
24	a	407	PHO	C3B-C2B	4.27	1.46	1.40
23	C	509	CLA	C3C-C2C	4.22	1.45	1.36
23	c	509	CLA	C3C-C2C	4.22	1.45	1.36
23	C	514	CLA	O2D-CGD	4.22	1.43	1.33
23	c	514	CLA	O2D-CGD	4.22	1.43	1.33
23	c	507	CLA	C3C-C2C	4.21	1.45	1.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	C4B-NB	-4.21	1.32	1.37
23	b	614	CLA	C4B-NB	-4.21	1.32	1.37
23	C	507	CLA	C3C-C2C	4.20	1.45	1.36
23	B	609	CLA	O2D-CGD	4.20	1.43	1.33
23	b	609	CLA	O2D-CGD	4.20	1.43	1.33
23	A	405	CLA	O2D-CGD	4.19	1.43	1.33
23	a	405	CLA	O2D-CGD	4.19	1.43	1.33
23	B	602	CLA	C1D-ND	4.19	1.42	1.37
23	b	602	CLA	C1D-ND	4.19	1.42	1.37
23	B	603	CLA	C1B-NB	-4.17	1.32	1.37
23	b	603	CLA	C1B-NB	-4.17	1.32	1.37
23	C	511	CLA	C3C-C2C	4.16	1.45	1.36
23	c	511	CLA	C3C-C2C	4.16	1.45	1.36
23	C	505	CLA	C3C-C2C	4.15	1.45	1.36
23	c	505	CLA	C3C-C2C	4.15	1.45	1.36
34	F	101	HEM	C4D-ND	-4.15	1.33	1.40
34	f	101	HEM	C4D-ND	-4.15	1.33	1.40
23	B	614	CLA	C1B-NB	-4.14	1.32	1.37
23	b	614	CLA	C1B-NB	-4.14	1.32	1.37
23	C	505	CLA	OBD-CAD	4.14	1.29	1.22
23	c	505	CLA	OBD-CAD	4.14	1.29	1.22
23	B	606	CLA	C1B-NB	-4.14	1.32	1.37
23	b	606	CLA	C1B-NB	-4.14	1.32	1.37
37	V	201	HEC	CHA-C1A	4.12	1.46	1.38
37	v	201	HEC	CHA-C1A	4.12	1.46	1.38
23	B	607	CLA	O2D-CGD	4.12	1.43	1.33
23	b	607	CLA	O2D-CGD	4.12	1.43	1.33
23	D	406	CLA	C3C-C2C	4.11	1.45	1.36
23	d	406	CLA	C3C-C2C	4.11	1.45	1.36
23	c	510	CLA	C1B-NB	-4.11	1.32	1.37
23	D	405	CLA	C3C-C2C	4.09	1.45	1.36
23	d	405	CLA	C3C-C2C	4.09	1.45	1.36
23	B	601	CLA	C1D-ND	4.08	1.42	1.37
23	b	601	CLA	C1D-ND	4.08	1.42	1.37
23	C	508	CLA	C1D-ND	4.08	1.42	1.37
23	c	508	CLA	C1D-ND	4.08	1.42	1.37
23	C	510	CLA	C1B-NB	-4.07	1.32	1.37
23	b	607	CLA	CHC-C1C	4.06	1.46	1.38
23	B	610	CLA	C3C-C2C	4.06	1.45	1.36
23	b	610	CLA	C3C-C2C	4.06	1.45	1.36
23	B	604	CLA	C1C-NC	-4.06	1.31	1.37
23	B	607	CLA	C4B-NB	-4.06	1.32	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	607	CLA	C4B-NB	-4.06	1.32	1.37
23	A	405	CLA	CHC-C1C	4.06	1.46	1.38
23	B	607	CLA	CHC-C1C	4.06	1.46	1.38
23	a	405	CLA	CHC-C1C	4.06	1.46	1.38
23	b	604	CLA	C1C-NC	-4.06	1.31	1.37
25	C	516	BCR	C23-C22	-4.04	1.37	1.45
25	c	516	BCR	C23-C22	-4.04	1.37	1.45
23	C	514	CLA	CHC-C1C	4.04	1.46	1.38
23	c	514	CLA	CHC-C1C	4.04	1.46	1.38
23	B	616	CLA	CHD-C1D	4.04	1.46	1.38
23	b	616	CLA	CHD-C1D	4.04	1.46	1.38
23	C	505	CLA	CHC-C1C	4.03	1.46	1.38
23	c	505	CLA	CHC-C1C	4.03	1.46	1.38
23	C	510	CLA	O2D-CGD	4.03	1.43	1.33
23	c	510	CLA	O2D-CGD	4.03	1.43	1.33
25	B	618	BCR	C23-C22	-4.02	1.37	1.45
25	b	618	BCR	C23-C22	-4.02	1.37	1.45
23	B	609	CLA	C3C-C2C	4.02	1.45	1.36
23	b	609	CLA	C3C-C2C	4.02	1.45	1.36
26	A	410	LMG	O8-C28	4.01	1.45	1.33
26	a	410	LMG	O8-C28	4.01	1.45	1.33
23	B	609	CLA	C1B-NB	-4.00	1.32	1.37
23	b	609	CLA	C1B-NB	-4.00	1.32	1.37
23	C	509	CLA	CHD-C1D	3.99	1.46	1.38
23	c	509	CLA	CHD-C1D	3.99	1.46	1.38
23	B	605	CLA	C1B-NB	-3.99	1.32	1.37
23	b	605	CLA	C1B-NB	-3.99	1.32	1.37
23	D	405	CLA	C1B-NB	-3.99	1.32	1.37
23	d	405	CLA	C1B-NB	-3.99	1.32	1.37
23	D	402	CLA	C1B-NB	-3.99	1.32	1.37
23	d	402	CLA	C1B-NB	-3.99	1.32	1.37
23	C	509	CLA	O2D-CGD	3.98	1.42	1.33
23	c	509	CLA	O2D-CGD	3.98	1.42	1.33
23	C	512	CLA	CHB-C1B	3.97	1.48	1.39
23	c	512	CLA	CHB-C1B	3.97	1.48	1.39
23	C	511	CLA	CHC-C1C	3.97	1.46	1.38
23	c	511	CLA	CHC-C1C	3.97	1.46	1.38
23	C	509	CLA	CHC-C1C	3.97	1.46	1.38
23	c	509	CLA	CHC-C1C	3.97	1.46	1.38
23	C	507	CLA	CHC-C1C	3.96	1.46	1.38
23	c	507	CLA	CHC-C1C	3.96	1.46	1.38
23	C	508	CLA	O2D-CGD	3.96	1.42	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	O2D-CGD	3.96	1.42	1.33
26	A	410	LMG	O7-C10	3.96	1.45	1.34
26	a	410	LMG	O7-C10	3.96	1.45	1.34
23	B	601	CLA	O2D-CGD	3.95	1.42	1.33
23	b	601	CLA	O2D-CGD	3.95	1.42	1.33
23	B	613	CLA	O2D-CGD	3.95	1.42	1.33
23	b	613	CLA	O2D-CGD	3.95	1.42	1.33
23	C	502	CLA	CHC-C1C	3.93	1.46	1.38
23	c	502	CLA	CHC-C1C	3.93	1.46	1.38
34	F	101	HEM	FE-NC	3.91	2.08	1.95
34	f	101	HEM	FE-NC	3.91	2.08	1.95
28	T	103	SQD	O47-C7	3.91	1.45	1.33
28	t	101	SQD	O47-C7	3.91	1.45	1.33
23	C	512	CLA	CHD-C1D	3.89	1.45	1.38
23	c	512	CLA	CHD-C1D	3.89	1.45	1.38
23	C	511	CLA	O2D-CGD	3.89	1.42	1.33
23	c	511	CLA	O2D-CGD	3.89	1.42	1.33
23	C	506	CLA	CHB-C1B	3.89	1.48	1.39
23	c	506	CLA	CHB-C1B	3.89	1.48	1.39
34	F	101	HEM	FE-NB	3.89	2.06	1.94
34	f	101	HEM	FE-NB	3.89	2.06	1.94
26	C	520	LMG	O7-C10	3.88	1.45	1.34
26	c	520	LMG	O7-C10	3.88	1.45	1.34
23	A	406	CLA	C3C-C2C	3.88	1.45	1.36
23	a	406	CLA	C3C-C2C	3.88	1.45	1.36
23	B	612	CLA	CHB-C1B	3.88	1.48	1.39
23	b	612	CLA	CHB-C1B	3.88	1.48	1.39
23	c	510	CLA	CHC-C1C	3.88	1.46	1.38
23	B	613	CLA	C3C-C2C	3.88	1.45	1.36
23	b	613	CLA	C3C-C2C	3.88	1.45	1.36
23	A	408	CLA	O2D-CGD	3.87	1.42	1.33
23	a	408	CLA	O2D-CGD	3.87	1.42	1.33
23	B	610	CLA	CHB-C1B	3.87	1.48	1.39
23	b	610	CLA	CHB-C1B	3.87	1.48	1.39
23	B	612	CLA	O2D-CGD	3.87	1.42	1.33
23	b	612	CLA	O2D-CGD	3.87	1.42	1.33
37	V	201	HEC	CHD-C4C	3.86	1.45	1.38
37	v	201	HEC	CHD-C4C	3.86	1.45	1.38
23	C	511	CLA	C4B-NB	-3.86	1.33	1.37
23	c	511	CLA	C4B-NB	-3.86	1.33	1.37
23	C	510	CLA	CHC-C1C	3.86	1.46	1.38
23	C	514	CLA	C3D-C2D	3.85	1.49	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	514	CLA	C3D-C2D	3.85	1.49	1.39
23	D	405	CLA	CHC-C1C	3.85	1.46	1.38
23	d	405	CLA	CHC-C1C	3.85	1.46	1.38
23	D	405	CLA	CHB-C1B	3.84	1.48	1.39
23	d	405	CLA	CHB-C1B	3.84	1.48	1.39
25	T	101	BCR	C23-C22	-3.84	1.39	1.50
25	t	103	BCR	C23-C22	-3.84	1.39	1.50
23	C	504	CLA	C3D-C2D	3.83	1.49	1.39
23	c	504	CLA	C3D-C2D	3.83	1.49	1.39
23	C	512	CLA	C4B-NB	-3.82	1.33	1.37
23	c	512	CLA	C4B-NB	-3.82	1.33	1.37
23	B	604	CLA	C1B-NB	-3.82	1.33	1.37
23	C	506	CLA	O2D-CGD	3.81	1.42	1.33
23	C	512	CLA	O2D-CGD	3.81	1.42	1.33
23	c	512	CLA	O2D-CGD	3.81	1.42	1.33
23	A	408	CLA	O2A-CGA	3.81	1.44	1.33
23	a	408	CLA	O2A-CGA	3.81	1.44	1.33
23	c	506	CLA	O2D-CGD	3.80	1.42	1.33
24	A	407	PHO	OBD-CAD	3.80	1.27	1.22
24	a	407	PHO	OBD-CAD	3.80	1.27	1.22
26	B	620	LMG	O8-C28	3.80	1.44	1.33
26	b	620	LMG	O8-C28	3.80	1.44	1.33
23	C	513	CLA	C3D-C2D	3.79	1.49	1.39
23	c	513	CLA	C3D-C2D	3.79	1.49	1.39
23	C	505	CLA	O2D-CGD	3.78	1.42	1.33
23	c	505	CLA	O2D-CGD	3.78	1.42	1.33
23	B	606	CLA	CHC-C1C	3.78	1.46	1.38
23	b	606	CLA	CHC-C1C	3.78	1.46	1.38
23	B	615	CLA	C3D-C2D	3.77	1.49	1.39
23	b	615	CLA	C3D-C2D	3.77	1.49	1.39
23	B	601	CLA	CHB-C1B	3.77	1.47	1.39
23	b	601	CLA	CHB-C1B	3.77	1.47	1.39
35	H	101	RRX	C19-C18	-3.77	1.37	1.45
35	h	101	RRX	C19-C18	-3.77	1.37	1.45
23	b	604	CLA	C1B-NB	-3.76	1.33	1.37
23	B	601	CLA	C1B-NB	-3.75	1.33	1.37
23	b	601	CLA	C1B-NB	-3.75	1.33	1.37
23	C	504	CLA	C1B-NB	-3.75	1.33	1.37
23	c	504	CLA	C1B-NB	-3.75	1.33	1.37
23	B	611	CLA	C3B-C2B	3.75	1.53	1.41
23	b	611	CLA	C3B-C2B	3.75	1.53	1.41
23	D	406	CLA	O2D-CGD	3.75	1.42	1.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	406	CLA	O2D-CGD	3.75	1.42	1.33
23	C	502	CLA	CHC-C4B	3.75	1.47	1.39
23	c	502	CLA	CHC-C4B	3.75	1.47	1.39
23	B	603	CLA	CHB-C1B	3.74	1.47	1.39
23	b	603	CLA	CHB-C1B	3.74	1.47	1.39
23	B	613	CLA	CHB-C1B	3.72	1.47	1.39
23	b	613	CLA	CHB-C1B	3.72	1.47	1.39
23	B	603	CLA	CHC-C1C	3.72	1.46	1.38
23	b	603	CLA	CHC-C1C	3.72	1.46	1.38
23	C	508	CLA	CHC-C1C	3.72	1.46	1.38
23	c	508	CLA	CHC-C1C	3.72	1.46	1.38
24	D	401	PHO	C3A-C2A	-3.72	1.51	1.54
24	d	401	PHO	C3A-C2A	-3.72	1.51	1.54
23	A	408	CLA	C4B-NB	-3.71	1.33	1.37
23	a	408	CLA	C4B-NB	-3.71	1.33	1.37
23	C	512	CLA	CHC-C1C	3.71	1.46	1.38
23	c	512	CLA	CHC-C1C	3.71	1.46	1.38
23	C	510	CLA	CHD-C4C	3.70	1.47	1.39
23	c	510	CLA	CHD-C4C	3.70	1.47	1.39
23	B	605	CLA	CHC-C1C	3.70	1.46	1.38
23	b	605	CLA	CHC-C1C	3.70	1.46	1.38
23	C	509	CLA	C3D-C2D	3.69	1.49	1.39
23	c	509	CLA	C3D-C2D	3.69	1.49	1.39
23	C	511	CLA	CHB-C1B	3.68	1.47	1.39
23	c	511	CLA	CHB-C1B	3.68	1.47	1.39
23	B	616	CLA	C4B-NB	-3.68	1.33	1.37
23	b	616	CLA	C4B-NB	-3.68	1.33	1.37
31	C	519	DGD	O1G-C1A	3.68	1.44	1.33
31	c	519	DGD	O1G-C1A	3.68	1.44	1.33
23	C	509	CLA	CHB-C1B	3.68	1.47	1.39
23	c	509	CLA	CHB-C1B	3.68	1.47	1.39
23	B	609	CLA	CHB-C1B	3.65	1.47	1.39
23	b	609	CLA	CHB-C1B	3.65	1.47	1.39
24	A	407	PHO	C3D-C2D	3.65	1.46	1.39
24	a	407	PHO	C3D-C2D	3.65	1.46	1.39
23	B	607	CLA	OBD-CAD	3.64	1.28	1.22
23	b	607	CLA	OBD-CAD	3.64	1.28	1.22
23	B	609	CLA	C1D-ND	3.64	1.42	1.37
23	b	609	CLA	C1D-ND	3.64	1.42	1.37
23	C	507	CLA	CHB-C1B	3.64	1.47	1.39
23	c	507	CLA	CHB-C1B	3.64	1.47	1.39
33	E	101	LHG	O7-C7	3.64	1.44	1.34

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	e	101	LHG	O7-C7	3.64	1.44	1.34
28	C	501	SQD	O47-C7	3.64	1.44	1.34
28	c	501	SQD	O47-C7	3.64	1.44	1.34
23	C	511	CLA	CHC-C4B	3.64	1.47	1.39
23	c	511	CLA	CHC-C4B	3.64	1.47	1.39
23	B	616	CLA	C3D-C2D	3.63	1.49	1.39
23	b	616	CLA	C3D-C2D	3.63	1.49	1.39
23	A	405	CLA	CHD-C1D	3.63	1.45	1.38
23	a	405	CLA	CHD-C1D	3.63	1.45	1.38
23	B	609	CLA	CHD-C1D	3.62	1.45	1.38
23	B	601	CLA	CHC-C4B	3.62	1.47	1.39
23	b	601	CLA	CHC-C4B	3.62	1.47	1.39
31	C	518	DGD	O1G-C1A	3.61	1.43	1.33
31	c	518	DGD	O1G-C1A	3.61	1.43	1.33
23	C	503	CLA	CHC-C1C	3.61	1.45	1.38
23	c	503	CLA	CHC-C1C	3.61	1.45	1.38
23	b	609	CLA	CHD-C1D	3.61	1.45	1.38
23	B	609	CLA	C4B-NB	-3.60	1.33	1.37
23	b	609	CLA	C4B-NB	-3.60	1.33	1.37
23	C	505	CLA	C1B-NB	-3.60	1.33	1.37
23	c	505	CLA	C1B-NB	-3.60	1.33	1.37
23	C	514	CLA	CHD-C4C	3.60	1.47	1.39
23	c	514	CLA	CHD-C4C	3.60	1.47	1.39
23	B	614	CLA	CHC-C4B	3.59	1.47	1.39
23	b	614	CLA	CHC-C4B	3.59	1.47	1.39
23	C	513	CLA	O2D-CGD	3.59	1.42	1.33
23	c	513	CLA	O2D-CGD	3.59	1.42	1.33
23	C	508	CLA	CHD-C4C	3.59	1.47	1.39
23	c	508	CLA	CHD-C4C	3.59	1.47	1.39
23	B	616	CLA	C1B-NB	-3.58	1.33	1.37
23	b	616	CLA	C1B-NB	-3.58	1.33	1.37
23	B	613	CLA	CHC-C1C	3.58	1.45	1.38
23	C	508	CLA	O2A-CGA	3.58	1.43	1.33
23	c	508	CLA	O2A-CGA	3.58	1.43	1.33
23	B	614	CLA	CHC-C1C	3.57	1.45	1.38
23	b	614	CLA	CHC-C1C	3.57	1.45	1.38
24	D	401	PHO	CBD-CGD	-3.57	1.47	1.52
24	d	401	PHO	CBD-CGD	-3.57	1.47	1.52
23	B	613	CLA	CHD-C1D	3.57	1.45	1.38
23	b	613	CLA	CHD-C1D	3.57	1.45	1.38
23	B	611	CLA	C1D-ND	3.56	1.42	1.37
23	b	611	CLA	C1D-ND	3.56	1.42	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	CHD-C1D	3.56	1.45	1.38
23	c	507	CLA	CHD-C1D	3.56	1.45	1.38
23	B	612	CLA	C1C-NC	-3.56	1.32	1.37
23	b	612	CLA	C1C-NC	-3.56	1.32	1.37
23	B	604	CLA	CHD-C1D	3.56	1.45	1.38
23	b	604	CLA	CHD-C1D	3.56	1.45	1.38
23	C	507	CLA	C1B-NB	-3.55	1.33	1.37
23	c	507	CLA	C1B-NB	-3.55	1.33	1.37
23	b	613	CLA	CHC-C1C	3.55	1.45	1.38
23	B	611	CLA	CHB-C1B	3.55	1.47	1.39
23	b	611	CLA	CHB-C1B	3.55	1.47	1.39
23	B	606	CLA	C3D-C2D	3.54	1.48	1.39
23	b	606	CLA	C3D-C2D	3.54	1.48	1.39
23	B	601	CLA	C3D-C2D	3.54	1.48	1.39
23	b	601	CLA	C3D-C2D	3.54	1.48	1.39
23	C	505	CLA	O2A-CGA	3.54	1.43	1.33
23	c	505	CLA	O2A-CGA	3.54	1.43	1.33
23	B	605	CLA	C1C-NC	-3.54	1.32	1.37
23	b	605	CLA	C1C-NC	-3.54	1.32	1.37
23	C	510	CLA	CHB-C1B	3.54	1.47	1.39
23	c	510	CLA	CHB-C1B	3.54	1.47	1.39
23	B	611	CLA	CHC-C4B	3.53	1.47	1.39
23	b	611	CLA	CHC-C4B	3.53	1.47	1.39
23	B	608	CLA	O2A-CGA	3.53	1.43	1.33
23	b	608	CLA	O2A-CGA	3.53	1.43	1.33
23	C	506	CLA	CHD-C4C	3.53	1.47	1.39
23	c	506	CLA	CHD-C4C	3.53	1.47	1.39
23	C	505	CLA	C4B-NB	-3.53	1.33	1.37
23	c	505	CLA	C4B-NB	-3.53	1.33	1.37
23	B	602	CLA	O2A-CGA	3.53	1.43	1.33
23	b	602	CLA	O2A-CGA	3.53	1.43	1.33
23	B	611	CLA	C3C-C2C	3.52	1.44	1.36
23	b	611	CLA	C3C-C2C	3.52	1.44	1.36
34	F	101	HEM	C1B-NB	-3.52	1.34	1.40
34	f	101	HEM	C1B-NB	-3.52	1.34	1.40
23	C	507	CLA	O2A-CGA	3.52	1.44	1.33
23	c	507	CLA	O2A-CGA	3.52	1.44	1.33
23	B	602	CLA	CHC-C4B	3.51	1.47	1.39
23	b	602	CLA	CHC-C4B	3.51	1.47	1.39
23	A	408	CLA	C1B-NB	-3.51	1.33	1.37
23	a	408	CLA	C1B-NB	-3.51	1.33	1.37
23	B	606	CLA	OBD-CAD	3.50	1.28	1.22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	OBD-CAD	3.50	1.28	1.22
23	D	402	CLA	C3D-C2D	3.50	1.48	1.39
23	d	402	CLA	C3D-C2D	3.50	1.48	1.39
25	K	102	BCR	C23-C22	-3.50	1.38	1.45
25	k	102	BCR	C23-C22	-3.50	1.38	1.45
23	D	406	CLA	C3D-C2D	3.49	1.48	1.39
23	d	406	CLA	C3D-C2D	3.49	1.48	1.39
23	B	616	CLA	OBD-CAD	3.49	1.28	1.22
23	b	616	CLA	OBD-CAD	3.49	1.28	1.22
23	B	616	CLA	CHB-C1B	3.48	1.47	1.39
23	B	610	CLA	CHC-C4B	3.48	1.47	1.39
23	b	610	CLA	CHC-C4B	3.48	1.47	1.39
23	b	616	CLA	CHB-C1B	3.48	1.47	1.39
23	C	509	CLA	C1B-NB	-3.48	1.33	1.37
23	c	509	CLA	C1B-NB	-3.48	1.33	1.37
23	C	514	CLA	CHB-C1B	3.48	1.47	1.39
23	c	514	CLA	CHB-C1B	3.48	1.47	1.39
23	C	509	CLA	C1D-ND	3.47	1.42	1.37
23	c	509	CLA	C1D-ND	3.47	1.42	1.37
23	C	509	CLA	O2A-CGA	3.47	1.43	1.33
23	c	509	CLA	O2A-CGA	3.47	1.43	1.33
23	C	510	CLA	OBD-CAD	3.47	1.28	1.22
23	c	510	CLA	OBD-CAD	3.47	1.28	1.22
23	B	612	CLA	CHC-C4B	3.46	1.47	1.39
23	b	612	CLA	CHC-C4B	3.46	1.47	1.39
23	B	615	CLA	OBD-CAD	3.46	1.28	1.22
23	b	615	CLA	OBD-CAD	3.46	1.28	1.22
23	B	615	CLA	O2D-CGD	3.46	1.41	1.33
23	b	615	CLA	O2D-CGD	3.46	1.41	1.33
23	B	607	CLA	C1D-ND	3.46	1.42	1.37
23	b	607	CLA	C1D-ND	3.46	1.42	1.37
23	C	508	CLA	C3D-C2D	3.46	1.48	1.39
23	c	508	CLA	C3D-C2D	3.46	1.48	1.39
24	D	401	PHO	O2D-CGD	3.46	1.41	1.33
24	d	401	PHO	O2D-CGD	3.46	1.41	1.33
23	B	608	CLA	CHD-C1D	3.45	1.45	1.38
23	b	608	CLA	CHD-C1D	3.45	1.45	1.38
23	B	610	CLA	CHC-C1C	3.45	1.45	1.38
23	b	610	CLA	CHC-C1C	3.45	1.45	1.38
23	A	408	CLA	CHC-C1C	3.44	1.45	1.38
23	a	408	CLA	CHC-C1C	3.44	1.45	1.38
24	A	407	PHO	O2A-CGA	3.44	1.43	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	407	PHO	O2A-CGA	3.44	1.43	1.33
23	B	612	CLA	C3C-C2C	3.44	1.44	1.36
23	b	612	CLA	C3C-C2C	3.44	1.44	1.36
23	C	502	CLA	O2D-CGD	3.43	1.41	1.33
23	c	502	CLA	O2D-CGD	3.43	1.41	1.33
23	A	406	CLA	O2A-CGA	3.43	1.43	1.33
23	a	406	CLA	O2A-CGA	3.43	1.43	1.33
23	C	503	CLA	C3C-C2C	3.42	1.44	1.36
23	c	503	CLA	C3C-C2C	3.42	1.44	1.36
23	C	502	CLA	O2A-CGA	3.42	1.43	1.33
23	c	502	CLA	O2A-CGA	3.42	1.43	1.33
23	C	508	CLA	OBD-CAD	3.42	1.28	1.22
23	D	402	CLA	C4B-NB	-3.42	1.33	1.37
23	d	402	CLA	C4B-NB	-3.42	1.33	1.37
23	c	508	CLA	OBD-CAD	3.41	1.28	1.22
24	D	401	PHO	C3D-C2D	3.41	1.45	1.39
24	d	401	PHO	C3D-C2D	3.41	1.45	1.39
23	C	508	CLA	C4B-NB	-3.41	1.33	1.37
23	c	508	CLA	C4B-NB	-3.41	1.33	1.37
23	B	615	CLA	CHC-C1C	3.41	1.45	1.38
23	b	615	CLA	CHC-C1C	3.41	1.45	1.38
23	C	503	CLA	O2D-CGD	3.41	1.41	1.33
23	c	503	CLA	O2D-CGD	3.41	1.41	1.33
23	B	616	CLA	O2D-CGD	3.41	1.41	1.33
23	b	616	CLA	O2D-CGD	3.41	1.41	1.33
23	A	408	CLA	CHB-C1B	3.41	1.47	1.39
23	a	408	CLA	CHB-C1B	3.41	1.47	1.39
23	C	507	CLA	C3D-C2D	3.41	1.48	1.39
23	c	507	CLA	C3D-C2D	3.41	1.48	1.39
23	C	502	CLA	CHB-C1B	3.40	1.47	1.39
23	c	502	CLA	CHB-C1B	3.40	1.47	1.39
23	B	614	CLA	C3D-C2D	3.40	1.48	1.39
23	b	614	CLA	C3D-C2D	3.40	1.48	1.39
23	c	507	CLA	C4B-NB	-3.40	1.33	1.37
23	C	506	CLA	C3D-C2D	3.40	1.48	1.39
23	c	506	CLA	C3D-C2D	3.40	1.48	1.39
23	A	406	CLA	O2D-CGD	3.40	1.41	1.33
23	B	611	CLA	O2D-CGD	3.40	1.41	1.33
23	a	406	CLA	O2D-CGD	3.40	1.41	1.33
23	b	611	CLA	O2D-CGD	3.40	1.41	1.33
31	C	517	DGD	O1G-C1A	3.40	1.43	1.33
31	c	517	DGD	O1G-C1A	3.40	1.43	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407	PHO	O2D-CGD	3.40	1.41	1.33
24	a	407	PHO	O2D-CGD	3.40	1.41	1.33
23	B	616	CLA	CHC-C4B	3.39	1.47	1.39
23	b	616	CLA	CHC-C4B	3.39	1.47	1.39
23	C	512	CLA	O2A-CGA	3.39	1.43	1.33
23	c	512	CLA	O2A-CGA	3.39	1.43	1.33
23	B	608	CLA	CHC-C1C	3.39	1.45	1.38
23	b	608	CLA	CHC-C1C	3.39	1.45	1.38
23	B	610	CLA	C3D-C2D	3.38	1.48	1.39
23	b	610	CLA	C3D-C2D	3.38	1.48	1.39
23	A	406	CLA	CHB-C1B	3.38	1.47	1.39
23	a	406	CLA	CHB-C1B	3.38	1.47	1.39
23	C	510	CLA	CHD-C1D	3.37	1.44	1.38
23	c	510	CLA	CHD-C1D	3.37	1.44	1.38
23	C	509	CLA	C4B-NB	-3.35	1.33	1.37
23	c	509	CLA	C4B-NB	-3.35	1.33	1.37
23	b	604	CLA	C3C-C2C	3.35	1.43	1.36
28	A	412	SQD	O48-C23	3.35	1.46	1.33
28	a	412	SQD	O48-C23	3.35	1.46	1.33
23	C	512	CLA	CHD-C4C	3.35	1.46	1.39
23	c	512	CLA	CHD-C4C	3.35	1.46	1.39
23	B	610	CLA	O2D-CGD	3.35	1.41	1.33
23	b	610	CLA	O2D-CGD	3.35	1.41	1.33
25	B	619	BCR	C23-C22	-3.35	1.38	1.45
25	b	619	BCR	C23-C22	-3.35	1.38	1.45
23	C	512	CLA	C3D-C2D	3.34	1.48	1.39
23	c	512	CLA	C3D-C2D	3.34	1.48	1.39
23	B	607	CLA	O2A-CGA	3.34	1.43	1.33
23	b	607	CLA	O2A-CGA	3.34	1.43	1.33
23	B	613	CLA	C1C-NC	-3.34	1.32	1.37
23	b	613	CLA	C1C-NC	-3.34	1.32	1.37
37	V	201	HEC	CHC-C4B	3.34	1.44	1.38
37	v	201	HEC	CHC-C4B	3.34	1.44	1.38
23	C	507	CLA	C4B-NB	-3.33	1.33	1.37
23	B	604	CLA	C3C-C2C	3.33	1.43	1.36
23	B	613	CLA	O2A-CGA	3.33	1.43	1.33
23	b	613	CLA	O2A-CGA	3.33	1.43	1.33
23	B	606	CLA	CHC-C4B	3.33	1.46	1.39
23	b	606	CLA	CHC-C4B	3.33	1.46	1.39
23	C	504	CLA	CHB-C1B	3.33	1.46	1.39
23	c	504	CLA	CHB-C1B	3.33	1.46	1.39
23	A	405	CLA	C1B-NB	-3.33	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	405	CLA	C1B-NB	-3.33	1.33	1.37
23	C	502	CLA	C1B-NB	-3.32	1.33	1.37
23	c	502	CLA	C1B-NB	-3.32	1.33	1.37
23	B	601	CLA	CHD-C4C	3.32	1.46	1.39
23	b	601	CLA	CHD-C4C	3.32	1.46	1.39
23	B	613	CLA	C1B-NB	-3.32	1.33	1.37
23	b	613	CLA	C1B-NB	-3.32	1.33	1.37
23	C	514	CLA	CHD-C1D	3.32	1.44	1.38
23	c	514	CLA	CHD-C1D	3.32	1.44	1.38
23	A	408	CLA	CHD-C4C	3.32	1.46	1.39
23	a	408	CLA	CHD-C4C	3.32	1.46	1.39
23	B	612	CLA	C4B-NB	-3.32	1.33	1.37
23	b	612	CLA	C4B-NB	-3.32	1.33	1.37
37	V	201	HEC	CHD-C1D	3.32	1.46	1.39
37	v	201	HEC	CHD-C1D	3.32	1.46	1.39
23	C	504	CLA	O2A-CGA	3.31	1.43	1.33
23	C	506	CLA	CHD-C1D	3.31	1.44	1.38
23	c	506	CLA	CHD-C1D	3.31	1.44	1.38
23	B	605	CLA	CHB-C1B	3.31	1.46	1.39
23	b	605	CLA	CHB-C1B	3.31	1.46	1.39
23	B	607	CLA	C1C-NC	-3.30	1.32	1.37
23	b	607	CLA	C1C-NC	-3.30	1.32	1.37
23	A	408	CLA	C1D-ND	3.30	1.41	1.37
23	a	408	CLA	C1D-ND	3.30	1.41	1.37
23	B	608	CLA	CHB-C1B	3.30	1.46	1.39
23	B	615	CLA	CHB-C1B	3.30	1.46	1.39
23	b	608	CLA	CHB-C1B	3.30	1.46	1.39
23	b	615	CLA	CHB-C1B	3.30	1.46	1.39
23	c	504	CLA	O2A-CGA	3.29	1.43	1.33
23	C	508	CLA	CHD-C1D	3.29	1.44	1.38
23	c	508	CLA	CHD-C1D	3.29	1.44	1.38
35	H	101	RRX	C12-C13	-3.29	1.38	1.45
35	h	101	RRX	C12-C13	-3.29	1.38	1.45
23	B	608	CLA	CHD-C4C	3.29	1.46	1.39
23	b	608	CLA	CHD-C4C	3.29	1.46	1.39
37	v	201	HEC	CHC-C1C	3.28	1.46	1.39
23	c	510	CLA	C4B-NB	-3.28	1.33	1.37
33	L	101	LHG	O8-C23	3.28	1.42	1.33
33	l	101	LHG	O8-C23	3.28	1.42	1.33
23	D	405	CLA	O2D-CGD	3.27	1.41	1.33
23	d	405	CLA	O2D-CGD	3.27	1.41	1.33
23	C	513	CLA	CHD-C4C	3.27	1.46	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	513	CLA	CHD-C4C	3.27	1.46	1.39
35	H	101	RRX	C8-C9	-3.27	1.38	1.45
35	h	101	RRX	C8-C9	-3.27	1.38	1.45
23	D	406	CLA	OBD-CAD	3.26	1.28	1.22
23	d	406	CLA	OBD-CAD	3.26	1.28	1.22
23	C	513	CLA	C1D-ND	3.26	1.41	1.37
23	c	513	CLA	C1D-ND	3.26	1.41	1.37
23	C	507	CLA	C1D-ND	3.25	1.41	1.37
23	c	507	CLA	C1D-ND	3.25	1.41	1.37
37	V	201	HEC	C4D-ND	-3.25	1.33	1.39
37	v	201	HEC	C4D-ND	-3.25	1.33	1.39
37	V	201	HEC	CHC-C1C	3.25	1.46	1.39
28	C	501	SQD	O48-C23	3.25	1.42	1.33
28	c	501	SQD	O48-C23	3.25	1.42	1.33
24	A	407	PHO	C3B-C4B	3.24	1.45	1.41
24	a	407	PHO	C3B-C4B	3.24	1.45	1.41
23	B	611	CLA	CHD-C1D	3.24	1.44	1.38
23	b	611	CLA	CHD-C1D	3.24	1.44	1.38
23	B	601	CLA	CHD-C1D	3.24	1.44	1.38
23	b	601	CLA	CHD-C1D	3.24	1.44	1.38
23	C	506	CLA	CHC-C1C	3.23	1.45	1.38
23	c	506	CLA	CHC-C1C	3.23	1.45	1.38
23	B	609	CLA	C3D-C2D	3.23	1.47	1.39
23	b	609	CLA	C3D-C2D	3.23	1.47	1.39
23	C	510	CLA	C4B-NB	-3.23	1.33	1.37
23	B	613	CLA	C3D-C2D	3.23	1.47	1.39
23	b	613	CLA	C3D-C2D	3.23	1.47	1.39
23	B	610	CLA	O2A-CGA	3.23	1.42	1.33
23	b	610	CLA	O2A-CGA	3.23	1.42	1.33
28	C	501	SQD	C6-S	-3.22	1.65	1.77
28	c	501	SQD	C6-S	-3.22	1.65	1.77
23	B	614	CLA	O2D-CGD	3.22	1.41	1.33
23	b	614	CLA	O2D-CGD	3.22	1.41	1.33
23	C	506	CLA	OBD-CAD	3.22	1.28	1.22
23	c	506	CLA	OBD-CAD	3.22	1.28	1.22
23	D	402	CLA	O2A-CGA	3.22	1.42	1.33
23	d	402	CLA	O2A-CGA	3.22	1.42	1.33
23	B	614	CLA	CHB-C1B	3.21	1.46	1.39
23	b	614	CLA	CHB-C1B	3.21	1.46	1.39
23	B	604	CLA	O2A-CGA	3.21	1.42	1.33
23	b	604	CLA	O2A-CGA	3.21	1.42	1.33
23	C	513	CLA	CHD-C1D	3.21	1.44	1.38

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	513	CLA	CHD-C1D	3.21	1.44	1.38
23	B	606	CLA	CHD-C4C	3.21	1.46	1.39
23	b	606	CLA	CHD-C4C	3.21	1.46	1.39
23	B	602	CLA	C3D-C2D	3.20	1.47	1.39
23	b	602	CLA	C3D-C2D	3.20	1.47	1.39
23	C	514	CLA	C1B-NB	-3.19	1.33	1.37
23	c	514	CLA	C1B-NB	-3.19	1.33	1.37
26	D	412	LMG	O8-C28	3.19	1.42	1.33
26	d	412	LMG	O8-C28	3.19	1.42	1.33
23	D	402	CLA	CHC-C1C	3.19	1.45	1.38
23	d	402	CLA	CHC-C1C	3.19	1.45	1.38
31	H	102	DGD	O1G-C1A	3.18	1.42	1.33
31	h	102	DGD	O1G-C1A	3.18	1.42	1.33
23	C	505	CLA	CHD-C4C	3.18	1.46	1.39
31	H	102	DGD	O2G-C1B	3.17	1.43	1.34
31	h	102	DGD	O2G-C1B	3.17	1.43	1.34
23	C	514	CLA	CHC-C4B	3.17	1.46	1.39
23	c	514	CLA	CHC-C4B	3.17	1.46	1.39
23	C	503	CLA	C1C-NC	-3.17	1.33	1.37
23	c	503	CLA	C1C-NC	-3.17	1.33	1.37
23	D	405	CLA	CHC-C4B	3.17	1.46	1.39
23	d	405	CLA	CHC-C4B	3.17	1.46	1.39
23	C	503	CLA	CHD-C4C	3.17	1.46	1.39
23	c	503	CLA	CHD-C4C	3.17	1.46	1.39
23	B	609	CLA	O2A-CGA	3.16	1.42	1.33
23	b	609	CLA	O2A-CGA	3.16	1.42	1.33
23	B	610	CLA	C1D-ND	3.16	1.41	1.37
23	b	610	CLA	C1D-ND	3.16	1.41	1.37
23	B	605	CLA	O2A-CGA	3.16	1.42	1.33
23	b	605	CLA	O2A-CGA	3.16	1.42	1.33
23	D	406	CLA	CHC-C4B	3.16	1.46	1.39
23	d	406	CLA	CHC-C4B	3.16	1.46	1.39
23	B	606	CLA	O2D-CGD	3.15	1.40	1.33
23	b	606	CLA	O2D-CGD	3.15	1.40	1.33
23	B	611	CLA	OBD-CAD	3.15	1.27	1.22
23	b	611	CLA	OBD-CAD	3.15	1.27	1.22
23	B	608	CLA	C1C-NC	-3.15	1.33	1.37
23	c	505	CLA	CHD-C4C	3.15	1.46	1.39
23	B	612	CLA	OBD-CAD	3.15	1.27	1.22
23	b	612	CLA	OBD-CAD	3.15	1.27	1.22
23	B	615	CLA	C4B-NB	-3.14	1.33	1.37
23	b	615	CLA	C4B-NB	-3.14	1.33	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405	CLA	C1C-NC	-3.14	1.33	1.37
23	a	405	CLA	C1C-NC	-3.14	1.33	1.37
26	D	412	LMG	O7-C10	3.14	1.43	1.34
26	d	412	LMG	O7-C10	3.14	1.43	1.34
23	B	602	CLA	C1B-NB	-3.13	1.33	1.37
23	b	602	CLA	C1B-NB	-3.13	1.33	1.37
23	B	611	CLA	C3D-C2D	3.13	1.47	1.39
23	b	611	CLA	C3D-C2D	3.13	1.47	1.39
23	b	604	CLA	C4B-NB	-3.13	1.33	1.37
23	b	608	CLA	C1C-NC	-3.13	1.33	1.37
25	B	618	BCR	C24-C25	3.12	1.51	1.45
25	b	618	BCR	C24-C25	3.12	1.51	1.45
23	B	610	CLA	C4C-C3C	3.12	1.50	1.45
23	b	610	CLA	C4C-C3C	3.12	1.50	1.45
23	B	607	CLA	CHB-C1B	3.12	1.46	1.39
23	b	607	CLA	CHB-C1B	3.12	1.46	1.39
33	L	101	LHG	O7-C5	-3.12	1.38	1.46
33	l	101	LHG	O7-C5	-3.12	1.38	1.46
23	B	608	CLA	C3D-C2D	3.12	1.47	1.39
23	b	608	CLA	C3D-C2D	3.12	1.47	1.39
23	B	604	CLA	C4B-NB	-3.11	1.34	1.37
24	A	407	PHO	C1B-NB	-3.11	1.32	1.38
23	C	514	CLA	OBD-CAD	3.10	1.27	1.22
23	B	603	CLA	CHC-C4B	3.10	1.46	1.39
23	b	603	CLA	CHC-C4B	3.10	1.46	1.39
24	D	401	PHO	O2A-CGA	3.09	1.42	1.33
24	d	401	PHO	O2A-CGA	3.09	1.42	1.33
23	B	606	CLA	CHB-C1B	3.09	1.46	1.39
23	b	606	CLA	CHB-C1B	3.09	1.46	1.39
24	a	407	PHO	C1B-NB	-3.09	1.32	1.38
23	A	408	CLA	C1C-NC	-3.08	1.33	1.37
23	a	408	CLA	C1C-NC	-3.08	1.33	1.37
23	c	514	CLA	OBD-CAD	3.08	1.27	1.22
23	C	507	CLA	CHD-C4C	3.08	1.46	1.39
23	c	507	CLA	CHD-C4C	3.08	1.46	1.39
27	A	411	PL9	C2-C3	3.07	1.42	1.34
27	a	411	PL9	C2-C3	3.07	1.42	1.34
23	D	406	CLA	CHD-C1D	3.07	1.44	1.38
23	d	406	CLA	CHD-C1D	3.07	1.44	1.38
23	B	610	CLA	C1C-NC	-3.07	1.33	1.37
23	b	610	CLA	C1C-NC	-3.07	1.33	1.37
23	B	602	CLA	C4B-NB	-3.06	1.34	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	602	CLA	C4B-NB	-3.06	1.34	1.37
23	C	508	CLA	CHC-C4B	3.06	1.46	1.39
23	c	508	CLA	CHC-C4B	3.06	1.46	1.39
23	C	512	CLA	C1B-NB	-3.06	1.34	1.37
23	c	512	CLA	C1B-NB	-3.06	1.34	1.37
23	B	615	CLA	CHD-C1D	3.06	1.44	1.38
23	b	615	CLA	CHD-C1D	3.06	1.44	1.38
23	B	614	CLA	CHD-C1D	3.06	1.44	1.38
23	b	614	CLA	CHD-C1D	3.06	1.44	1.38
31	C	519	DGD	O2G-C1B	3.06	1.42	1.34
31	c	519	DGD	O2G-C1B	3.06	1.42	1.34
31	C	517	DGD	O2G-C1B	3.05	1.42	1.34
23	D	405	CLA	O2A-CGA	3.05	1.42	1.33
23	d	405	CLA	O2A-CGA	3.05	1.42	1.33
23	C	505	CLA	C3D-C2D	3.04	1.47	1.39
23	c	505	CLA	C3D-C2D	3.04	1.47	1.39
23	D	406	CLA	C1D-ND	3.04	1.41	1.37
23	d	406	CLA	C1D-ND	3.04	1.41	1.37
23	B	613	CLA	C4B-NB	-3.04	1.34	1.37
23	b	613	CLA	C4B-NB	-3.04	1.34	1.37
31	c	517	DGD	O2G-C1B	3.03	1.42	1.34
23	A	408	CLA	C3D-C2D	3.03	1.47	1.39
23	a	408	CLA	C3D-C2D	3.03	1.47	1.39
33	D	410	LHG	O8-C23	3.03	1.42	1.33
33	d	410	LHG	O8-C23	3.03	1.42	1.33
24	D	401	PHO	OBD-CAD	3.02	1.26	1.22
24	d	401	PHO	OBD-CAD	3.02	1.26	1.22
23	C	503	CLA	C3D-C2D	3.02	1.47	1.39
23	c	503	CLA	C3D-C2D	3.02	1.47	1.39
23	B	609	CLA	CHC-C4B	3.02	1.46	1.39
23	b	609	CLA	CHC-C4B	3.02	1.46	1.39
23	B	606	CLA	C3B-C4B	3.02	1.49	1.42
23	b	606	CLA	C3B-C4B	3.02	1.49	1.42
23	A	405	CLA	C3D-C2D	3.01	1.47	1.39
23	a	405	CLA	C3D-C2D	3.01	1.47	1.39
23	B	613	CLA	MG-ND	-3.01	1.99	2.05
23	b	613	CLA	MG-ND	-3.01	1.99	2.05
23	B	615	CLA	C3B-C4B	3.01	1.49	1.42
23	b	615	CLA	C3B-C4B	3.01	1.49	1.42
37	V	201	HEC	CHB-C1B	3.01	1.46	1.39
37	v	201	HEC	CHB-C1B	3.01	1.46	1.39
23	C	505	CLA	CHC-C4B	3.01	1.46	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	505	CLA	CHC-C4B	3.01	1.46	1.39
37	V	201	HEC	C1A-NA	-3.01	1.33	1.39
37	v	201	HEC	C1A-NA	-3.01	1.33	1.39
23	B	603	CLA	O2D-CGD	3.00	1.40	1.33
23	b	603	CLA	O2D-CGD	3.00	1.40	1.33
23	D	406	CLA	C1C-NC	-3.00	1.33	1.37
23	d	406	CLA	C1C-NC	-3.00	1.33	1.37
23	B	608	CLA	O2D-CGD	2.99	1.40	1.33
23	b	608	CLA	O2D-CGD	2.99	1.40	1.33
23	b	613	CLA	C3D-C4D	-2.99	1.37	1.44
23	B	608	CLA	OBD-CAD	2.98	1.27	1.22
23	b	608	CLA	OBD-CAD	2.98	1.27	1.22
23	C	506	CLA	C1D-ND	2.98	1.41	1.37
23	c	506	CLA	C1D-ND	2.98	1.41	1.37
23	C	509	CLA	CHC-C4B	2.97	1.46	1.39
23	c	509	CLA	CHC-C4B	2.97	1.46	1.39
23	C	503	CLA	O2A-CGA	2.97	1.42	1.33
23	c	503	CLA	O2A-CGA	2.97	1.42	1.33
37	V	201	HEC	C4A-NA	-2.97	1.34	1.39
37	v	201	HEC	C4A-NA	-2.97	1.34	1.39
24	D	401	PHO	C1B-NB	-2.97	1.33	1.38
24	d	401	PHO	C1B-NB	-2.97	1.33	1.38
23	B	602	CLA	CHC-C1C	2.97	1.44	1.38
23	b	602	CLA	CHC-C1C	2.97	1.44	1.38
23	C	514	CLA	C3B-C4B	2.97	1.49	1.42
23	c	514	CLA	C3B-C4B	2.97	1.49	1.42
23	b	604	CLA	CHB-C1B	2.97	1.46	1.39
31	c	518	DGD	O2G-C1B	2.96	1.42	1.34
23	B	604	CLA	CHB-C1B	2.96	1.46	1.39
31	C	518	DGD	O2G-C1B	2.95	1.42	1.34
23	B	613	CLA	C3D-C4D	-2.95	1.37	1.44
23	c	502	CLA	C3D-C2D	2.95	1.47	1.39
23	B	601	CLA	C4B-NB	-2.95	1.34	1.37
23	b	601	CLA	C4B-NB	-2.95	1.34	1.37
23	c	507	CLA	CHC-C4B	2.95	1.46	1.39
23	B	606	CLA	CHD-C1D	2.95	1.44	1.38
23	b	606	CLA	CHD-C1D	2.95	1.44	1.38
23	C	514	CLA	C4B-NB	-2.95	1.34	1.37
23	c	514	CLA	C4B-NB	-2.95	1.34	1.37
23	C	502	CLA	C3D-C2D	2.94	1.47	1.39
23	D	402	CLA	O2D-CGD	2.94	1.40	1.33
23	C	510	CLA	C3D-C2D	2.94	1.47	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	510	CLA	C3D-C2D	2.94	1.47	1.39
37	v	201	HEC	C1C-NC	-2.94	1.34	1.39
23	A	408	CLA	OBD-CAD	2.93	1.27	1.22
23	a	408	CLA	OBD-CAD	2.93	1.27	1.22
23	B	603	CLA	C4B-NB	-2.93	1.34	1.37
23	b	603	CLA	C4B-NB	-2.93	1.34	1.37
23	B	603	CLA	CHD-C1D	2.93	1.44	1.38
23	b	603	CLA	CHD-C1D	2.93	1.44	1.38
23	B	602	CLA	CHB-C1B	2.93	1.46	1.39
23	b	602	CLA	CHB-C1B	2.93	1.46	1.39
23	B	610	CLA	OBD-CAD	2.93	1.27	1.22
23	b	610	CLA	OBD-CAD	2.93	1.27	1.22
23	B	615	CLA	CHC-C4B	2.93	1.46	1.39
23	b	615	CLA	CHC-C4B	2.93	1.46	1.39
23	d	402	CLA	O2D-CGD	2.92	1.40	1.33
23	C	502	CLA	C1D-ND	2.92	1.41	1.37
23	c	502	CLA	C1D-ND	2.92	1.41	1.37
35	H	101	RRX	C23-C22	-2.92	1.39	1.45
35	h	101	RRX	C23-C22	-2.92	1.39	1.45
23	C	507	CLA	CHC-C4B	2.92	1.46	1.39
23	C	504	CLA	CHD-C4C	2.92	1.45	1.39
23	B	613	CLA	CHC-C4B	2.91	1.45	1.39
23	C	510	CLA	CHC-C4B	2.91	1.45	1.39
23	b	613	CLA	CHC-C4B	2.91	1.45	1.39
23	C	513	CLA	CHC-C4B	2.91	1.45	1.39
23	c	513	CLA	CHC-C4B	2.91	1.45	1.39
23	B	612	CLA	O2A-CGA	2.91	1.41	1.33
23	b	612	CLA	O2A-CGA	2.91	1.41	1.33
23	C	505	CLA	C1C-NC	-2.91	1.33	1.37
23	c	505	CLA	C1C-NC	-2.91	1.33	1.37
23	B	604	CLA	CHC-C1C	2.91	1.44	1.38
23	b	604	CLA	CHC-C1C	2.91	1.44	1.38
23	C	504	CLA	CHD-C1D	2.91	1.44	1.38
23	c	504	CLA	CHD-C1D	2.91	1.44	1.38
23	c	510	CLA	CHC-C4B	2.91	1.45	1.39
23	D	405	CLA	C3D-C2D	2.90	1.47	1.39
23	d	405	CLA	C3D-C2D	2.90	1.47	1.39
33	D	409	LHG	O7-C7	2.90	1.42	1.34
33	d	409	LHG	O7-C7	2.90	1.42	1.34
24	A	407	PHO	C1D-ND	-2.90	1.33	1.38
24	a	407	PHO	C1D-ND	-2.90	1.33	1.38
25	B	617	BCR	C23-C22	-2.90	1.39	1.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	617	BCR	C23-C22	-2.90	1.39	1.45
37	V	201	HEC	C1C-NC	-2.90	1.34	1.39
23	B	605	CLA	O2D-CGD	2.90	1.40	1.33
23	b	605	CLA	O2D-CGD	2.90	1.40	1.33
23	A	406	CLA	C3D-C2D	2.90	1.47	1.39
23	a	406	CLA	C3D-C2D	2.90	1.47	1.39
23	B	614	CLA	C1D-ND	2.90	1.41	1.37
23	b	614	CLA	C1D-ND	2.90	1.41	1.37
23	B	612	CLA	C3D-C2D	2.89	1.47	1.39
23	b	612	CLA	C3D-C2D	2.89	1.47	1.39
23	B	611	CLA	C4B-NB	-2.89	1.34	1.37
23	b	611	CLA	C4B-NB	-2.89	1.34	1.37
23	C	505	CLA	CHB-C1B	2.89	1.45	1.39
23	c	505	CLA	CHB-C1B	2.89	1.45	1.39
23	c	504	CLA	CHD-C4C	2.89	1.45	1.39
23	C	502	CLA	CHD-C1D	2.89	1.44	1.38
23	c	502	CLA	CHD-C1D	2.89	1.44	1.38
23	D	402	CLA	C1C-NC	-2.89	1.33	1.37
23	d	402	CLA	C1C-NC	-2.89	1.33	1.37
23	B	604	CLA	OBD-CAD	2.89	1.27	1.22
23	b	604	CLA	OBD-CAD	2.89	1.27	1.22
23	B	602	CLA	C1B-C2B	2.88	1.50	1.43
23	b	602	CLA	C1B-C2B	2.88	1.50	1.43
23	B	604	CLA	CHD-C4C	2.88	1.45	1.39
23	b	604	CLA	CHD-C4C	2.88	1.45	1.39
23	B	607	CLA	CHD-C1D	2.88	1.44	1.38
23	b	607	CLA	CHD-C1D	2.88	1.44	1.38
23	B	603	CLA	C3D-C2D	2.87	1.47	1.39
23	b	603	CLA	C3D-C2D	2.87	1.47	1.39
23	A	406	CLA	C1C-NC	-2.87	1.33	1.37
23	a	406	CLA	C1C-NC	-2.87	1.33	1.37
23	C	508	CLA	CHB-C1B	2.87	1.45	1.39
23	c	508	CLA	CHB-C1B	2.87	1.45	1.39
23	A	405	CLA	C3B-C4B	2.86	1.49	1.42
23	a	405	CLA	C3B-C4B	2.86	1.49	1.42
23	B	605	CLA	C3D-C2D	2.86	1.46	1.39
23	b	605	CLA	C3D-C2D	2.86	1.46	1.39
23	A	405	CLA	CHD-C4C	2.86	1.45	1.39
23	B	610	CLA	C3D-C4D	-2.86	1.37	1.44
23	b	610	CLA	C3D-C4D	-2.86	1.37	1.44
23	B	616	CLA	C1D-ND	2.86	1.41	1.37
23	b	616	CLA	C1D-ND	2.86	1.41	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	OBD-CAD	2.86	1.27	1.22
23	c	509	CLA	OBD-CAD	2.86	1.27	1.22
23	C	503	CLA	CHB-C1B	2.86	1.45	1.39
23	c	503	CLA	CHB-C1B	2.86	1.45	1.39
23	B	605	CLA	C4B-NB	-2.86	1.34	1.37
23	b	605	CLA	C4B-NB	-2.86	1.34	1.37
23	B	604	CLA	C3D-C2D	2.85	1.46	1.39
23	b	604	CLA	C3D-C2D	2.85	1.46	1.39
23	a	405	CLA	CHD-C4C	2.85	1.45	1.39
23	B	604	CLA	O2D-CED	-2.85	1.38	1.45
23	b	604	CLA	O2D-CED	-2.85	1.38	1.45
23	B	613	CLA	CHD-C4C	2.85	1.45	1.39
23	B	612	CLA	CHD-C1D	2.85	1.43	1.38
23	b	612	CLA	CHD-C1D	2.85	1.43	1.38
23	C	514	CLA	C1C-C2C	2.83	1.50	1.44
23	c	514	CLA	C1C-C2C	2.83	1.50	1.44
28	A	412	SQD	C6-S	-2.83	1.66	1.77
28	a	412	SQD	C6-S	-2.83	1.66	1.77
23	A	405	CLA	O2A-CGA	2.83	1.41	1.33
23	a	405	CLA	O2A-CGA	2.83	1.41	1.33
23	C	507	CLA	C3D-C4D	-2.83	1.37	1.44
23	c	507	CLA	C3D-C4D	-2.83	1.37	1.44
23	b	613	CLA	CHD-C4C	2.83	1.45	1.39
23	B	616	CLA	CHC-C1C	2.81	1.44	1.38
23	b	616	CLA	CHC-C1C	2.81	1.44	1.38
23	b	609	CLA	CHD-C4C	2.81	1.45	1.39
23	B	604	CLA	O2D-CGD	2.81	1.40	1.33
23	b	604	CLA	O2D-CGD	2.81	1.40	1.33
23	C	514	CLA	C1C-NC	-2.80	1.33	1.37
23	c	514	CLA	C1C-NC	-2.80	1.33	1.37
23	c	506	CLA	O2A-CGA	2.80	1.41	1.33
23	C	506	CLA	O2A-CGA	2.80	1.41	1.33
23	B	603	CLA	O2A-CGA	2.80	1.41	1.33
23	b	603	CLA	O2A-CGA	2.80	1.41	1.33
23	C	506	CLA	CHC-C4B	2.79	1.45	1.39
23	c	506	CLA	CHC-C4B	2.79	1.45	1.39
23	C	504	CLA	OBD-CAD	2.79	1.27	1.22
23	c	504	CLA	OBD-CAD	2.79	1.27	1.22
23	C	512	CLA	OBD-CAD	2.79	1.27	1.22
23	c	512	CLA	OBD-CAD	2.79	1.27	1.22
23	C	513	CLA	CHB-C1B	2.79	1.45	1.39
23	c	513	CLA	CHB-C1B	2.79	1.45	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	609	CLA	CHD-C4C	2.79	1.45	1.39
23	C	502	CLA	C3B-C4B	2.79	1.49	1.42
23	c	502	CLA	C3B-C4B	2.79	1.49	1.42
23	D	406	CLA	C3D-C4D	-2.78	1.37	1.44
23	d	406	CLA	C3D-C4D	-2.78	1.37	1.44
23	C	513	CLA	OBD-CAD	2.78	1.27	1.22
23	c	513	CLA	OBD-CAD	2.78	1.27	1.22
26	B	620	LMG	O7-C10	2.78	1.42	1.34
26	b	620	LMG	O7-C10	2.78	1.42	1.34
23	C	502	CLA	CHD-C4C	2.77	1.45	1.39
23	c	502	CLA	CHD-C4C	2.77	1.45	1.39
23	C	507	CLA	C3B-C4B	2.77	1.49	1.42
23	c	507	CLA	C3B-C4B	2.77	1.49	1.42
23	A	408	CLA	C3D-C4D	-2.77	1.37	1.44
23	a	408	CLA	C3D-C4D	-2.77	1.37	1.44
23	A	408	CLA	CHD-C1D	2.77	1.43	1.38
23	a	408	CLA	CHD-C1D	2.77	1.43	1.38
23	C	505	CLA	C3D-C4D	-2.77	1.37	1.44
23	c	505	CLA	C3D-C4D	-2.77	1.37	1.44
23	B	609	CLA	OBD-CAD	2.77	1.27	1.22
23	b	609	CLA	OBD-CAD	2.77	1.27	1.22
23	C	512	CLA	C3B-C4B	2.76	1.49	1.42
23	c	512	CLA	C3B-C4B	2.76	1.49	1.42
23	C	511	CLA	OBD-CAD	2.76	1.27	1.22
23	A	408	CLA	CHC-C4B	2.76	1.45	1.39
23	a	408	CLA	CHC-C4B	2.76	1.45	1.39
23	C	511	CLA	CHD-C1D	2.76	1.43	1.38
23	c	511	CLA	CHD-C1D	2.76	1.43	1.38
25	T	101	BCR	C30-C25	2.75	1.55	1.51
25	t	103	BCR	C30-C25	2.75	1.55	1.51
23	C	509	CLA	C3B-C4B	2.75	1.49	1.42
23	c	509	CLA	C3B-C4B	2.75	1.49	1.42
35	H	101	RRX	C16-C17	-2.75	1.34	1.43
35	h	101	RRX	C16-C17	-2.75	1.34	1.43
37	V	201	HEC	CHA-C4D	2.74	1.45	1.39
37	v	201	HEC	CHA-C4D	2.74	1.45	1.39
23	B	607	CLA	CHD-C4C	2.74	1.45	1.39
23	b	607	CLA	CHD-C4C	2.74	1.45	1.39
23	B	604	CLA	C1D-ND	2.74	1.41	1.37
23	b	604	CLA	C1D-ND	2.74	1.41	1.37
37	v	201	HEC	C3D-C2D	2.74	1.46	1.38
23	C	504	CLA	CHC-C4B	2.74	1.45	1.39

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	CHC-C4B	2.74	1.45	1.39
37	V	201	HEC	C3D-C2D	2.73	1.46	1.38
23	B	608	CLA	C1D-ND	2.73	1.41	1.37
23	b	608	CLA	C1D-ND	2.73	1.41	1.37
23	B	603	CLA	C1D-ND	2.73	1.41	1.37
23	C	511	CLA	C1C-NC	-2.73	1.33	1.37
23	c	511	CLA	C1C-NC	-2.73	1.33	1.37
23	c	505	CLA	CHD-C1D	2.73	1.43	1.38
23	B	610	CLA	CHD-C1D	2.73	1.43	1.38
23	b	610	CLA	CHD-C1D	2.73	1.43	1.38
23	B	610	CLA	C4B-NB	-2.73	1.34	1.37
23	b	610	CLA	C4B-NB	-2.73	1.34	1.37
23	A	406	CLA	CHD-C1D	2.73	1.43	1.38
23	a	406	CLA	CHD-C1D	2.73	1.43	1.38
23	b	603	CLA	C1D-ND	2.72	1.41	1.37
23	B	604	CLA	CHC-C4B	2.72	1.45	1.39
23	b	604	CLA	CHC-C4B	2.72	1.45	1.39
23	B	606	CLA	O2A-CGA	2.72	1.41	1.33
23	b	606	CLA	O2A-CGA	2.72	1.41	1.33
23	B	605	CLA	CHD-C4C	2.72	1.45	1.39
23	b	605	CLA	CHD-C4C	2.72	1.45	1.39
23	C	505	CLA	CHD-C1D	2.72	1.43	1.38
33	D	409	LHG	O7-C5	-2.72	1.39	1.46
33	d	409	LHG	O7-C5	-2.72	1.39	1.46
23	B	613	CLA	OBD-CAD	2.72	1.27	1.22
23	b	613	CLA	OBD-CAD	2.72	1.27	1.22
25	B	617	BCR	C1-C6	-2.71	1.50	1.53
25	b	617	BCR	C1-C6	-2.71	1.50	1.53
23	B	602	CLA	CHD-C4C	2.71	1.45	1.39
23	c	511	CLA	OBD-CAD	2.71	1.27	1.22
33	D	411	LHG	O8-C23	2.71	1.41	1.33
33	d	411	LHG	O8-C23	2.71	1.41	1.33
23	B	615	CLA	CHD-C4C	2.71	1.45	1.39
23	b	615	CLA	CHD-C4C	2.71	1.45	1.39
25	D	407	BCR	C30-C25	-2.71	1.50	1.53
25	d	407	BCR	C30-C25	-2.71	1.50	1.53
23	C	512	CLA	C1D-ND	2.70	1.41	1.37
23	c	512	CLA	C1D-ND	2.70	1.41	1.37
23	b	602	CLA	CHD-C4C	2.70	1.45	1.39
23	C	503	CLA	CHC-C4B	2.69	1.45	1.39
23	c	503	CLA	CHC-C4B	2.69	1.45	1.39
23	D	402	CLA	CHB-C1B	2.69	1.45	1.39

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402	CLA	CHB-C1B	2.69	1.45	1.39
23	C	509	CLA	C4C-C3C	2.69	1.49	1.45
23	c	509	CLA	C4C-C3C	2.69	1.49	1.45
23	B	611	CLA	C1C-NC	-2.69	1.33	1.37
23	b	611	CLA	C1C-NC	-2.69	1.33	1.37
23	C	512	CLA	CHC-C4B	2.68	1.45	1.39
23	c	512	CLA	CHC-C4B	2.68	1.45	1.39
23	D	406	CLA	CHD-C4C	2.68	1.45	1.39
23	d	406	CLA	CHD-C4C	2.68	1.45	1.39
33	D	410	LHG	O7-C7	2.68	1.41	1.34
33	d	410	LHG	O7-C7	2.68	1.41	1.34
23	B	607	CLA	C3D-C2D	2.68	1.46	1.39
23	b	607	CLA	C3D-C2D	2.68	1.46	1.39
23	B	616	CLA	CHD-C4C	2.68	1.45	1.39
23	b	616	CLA	CHD-C4C	2.68	1.45	1.39
23	A	405	CLA	C3B-C2B	2.67	1.50	1.41
23	a	405	CLA	C3B-C2B	2.67	1.50	1.41
23	D	405	CLA	CHD-C1D	2.67	1.43	1.38
23	d	405	CLA	CHD-C1D	2.67	1.43	1.38
23	A	406	CLA	C4B-NB	-2.67	1.34	1.37
23	a	406	CLA	C4B-NB	-2.67	1.34	1.37
23	D	405	CLA	MG-ND	-2.65	2.00	2.05
23	d	405	CLA	MG-ND	-2.65	2.00	2.05
23	D	405	CLA	CHD-C4C	2.65	1.45	1.39
23	d	405	CLA	CHD-C4C	2.65	1.45	1.39
37	V	201	HEC	C4C-NC	-2.65	1.34	1.39
23	D	406	CLA	CHB-C1B	2.65	1.45	1.39
23	d	406	CLA	CHB-C1B	2.65	1.45	1.39
23	C	503	CLA	OBD-CAD	2.64	1.27	1.22
23	c	503	CLA	OBD-CAD	2.64	1.27	1.22
25	B	619	BCR	C30-C25	-2.64	1.50	1.53
25	b	619	BCR	C30-C25	-2.64	1.50	1.53
23	D	406	CLA	CHC-C1C	2.63	1.43	1.38
23	d	406	CLA	CHC-C1C	2.63	1.43	1.38
33	D	411	LHG	O7-C7	2.62	1.41	1.34
33	d	411	LHG	O7-C7	2.62	1.41	1.34
23	D	402	CLA	CHD-C1D	2.62	1.43	1.38
23	d	402	CLA	CHD-C1D	2.62	1.43	1.38
33	E	101	LHG	O8-C23	2.62	1.46	1.33
33	e	101	LHG	O8-C23	2.62	1.46	1.33
24	D	401	PHO	C1D-ND	-2.62	1.33	1.38
24	d	401	PHO	C1D-ND	-2.62	1.33	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	O2D-CGD	2.62	1.39	1.33
23	b	602	CLA	O2D-CGD	2.62	1.39	1.33
37	v	201	HEC	C4C-NC	-2.61	1.34	1.39
23	C	511	CLA	C4D-CHA	2.61	1.47	1.38
23	c	511	CLA	C4D-CHA	2.61	1.47	1.38
23	B	611	CLA	C3B-C4B	2.61	1.48	1.42
23	b	611	CLA	C3B-C4B	2.61	1.48	1.42
27	d	408	PL9	C3-C4	-2.61	1.45	1.49
23	B	610	CLA	C4D-CHA	2.60	1.47	1.38
23	b	610	CLA	C4D-CHA	2.60	1.47	1.38
23	C	509	CLA	CHD-C4C	2.59	1.45	1.39
23	c	509	CLA	CHD-C4C	2.59	1.45	1.39
23	C	505	CLA	C1D-ND	2.59	1.41	1.37
23	c	505	CLA	C1D-ND	2.59	1.41	1.37
23	B	602	CLA	C1C-NC	-2.59	1.33	1.37
23	b	602	CLA	C1C-NC	-2.59	1.33	1.37
23	C	511	CLA	CHD-C4C	2.59	1.45	1.39
23	c	511	CLA	CHD-C4C	2.59	1.45	1.39
23	B	615	CLA	C3D-C4D	-2.59	1.38	1.44
23	b	615	CLA	C3D-C4D	-2.59	1.38	1.44
24	D	401	PHO	CHA-CBD	-2.59	1.48	1.51
24	d	401	PHO	CHA-CBD	-2.59	1.48	1.51
35	H	101	RRX	C11-C10	-2.58	1.35	1.43
35	h	101	RRX	C11-C10	-2.58	1.35	1.43
23	D	402	CLA	C3B-C4B	2.58	1.48	1.42
23	B	611	CLA	CHD-C4C	2.58	1.45	1.39
23	b	611	CLA	CHD-C4C	2.58	1.45	1.39
23	C	510	CLA	C4C-C3C	2.57	1.49	1.45
23	c	510	CLA	C4C-C3C	2.57	1.49	1.45
23	D	406	CLA	C3B-C4B	2.57	1.48	1.42
23	d	406	CLA	C3B-C4B	2.57	1.48	1.42
28	C	501	SQD	O47-C45	-2.57	1.40	1.46
28	c	501	SQD	O47-C45	-2.57	1.40	1.46
23	d	402	CLA	C3B-C4B	2.57	1.48	1.42
23	C	509	CLA	C3D-C4D	-2.57	1.38	1.44
23	c	509	CLA	C3D-C4D	-2.57	1.38	1.44
23	C	512	CLA	C1B-C2B	2.56	1.49	1.43
23	c	512	CLA	C1B-C2B	2.56	1.49	1.43
26	D	412	LMG	O7-C8	-2.56	1.40	1.46
26	d	412	LMG	O7-C8	-2.56	1.40	1.46
33	L	101	LHG	O7-C7	2.56	1.41	1.34
33	l	101	LHG	O7-C7	2.56	1.41	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	415	SQD	C6-S	-2.56	1.68	1.77
28	d	415	SQD	C6-S	-2.56	1.68	1.77
27	D	408	PL9	C3-C4	-2.56	1.45	1.49
25	C	516	BCR	C1-C6	-2.55	1.50	1.53
25	c	516	BCR	C1-C6	-2.55	1.50	1.53
35	H	101	RRX	C17-C18	2.55	1.39	1.35
35	h	101	RRX	C17-C18	2.55	1.39	1.35
23	C	513	CLA	C3B-C4B	2.55	1.48	1.42
23	c	513	CLA	C3B-C4B	2.55	1.48	1.42
23	A	405	CLA	CHB-C1B	2.54	1.45	1.39
23	a	405	CLA	CHB-C1B	2.54	1.45	1.39
23	C	505	CLA	C3B-C2B	2.53	1.49	1.41
23	c	505	CLA	C3B-C2B	2.53	1.49	1.41
23	B	609	CLA	C3D-C4D	-2.53	1.38	1.44
23	b	609	CLA	C3D-C4D	-2.53	1.38	1.44
23	B	614	CLA	CHD-C4C	2.51	1.45	1.39
23	b	614	CLA	CHD-C4C	2.51	1.45	1.39
23	D	402	CLA	CHD-C4C	2.51	1.45	1.39
23	d	402	CLA	CHD-C4C	2.51	1.45	1.39
23	C	502	CLA	C1C-C2C	2.51	1.49	1.44
23	c	502	CLA	C1C-C2C	2.51	1.49	1.44
23	C	511	CLA	O2A-CGA	2.51	1.40	1.33
23	c	511	CLA	O2A-CGA	2.51	1.40	1.33
37	V	201	HEC	C4B-NB	-2.50	1.34	1.39
37	v	201	HEC	C4B-NB	-2.50	1.34	1.39
23	A	405	CLA	CHC-C4B	2.49	1.45	1.39
23	a	405	CLA	CHC-C4B	2.49	1.45	1.39
23	B	611	CLA	C4D-CHA	2.49	1.47	1.38
23	b	611	CLA	C4D-CHA	2.49	1.47	1.38
23	A	406	CLA	OBD-CAD	2.49	1.26	1.22
23	a	406	CLA	OBD-CAD	2.49	1.26	1.22
33	D	411	LHG	O7-C5	-2.49	1.40	1.46
33	d	411	LHG	O7-C5	-2.49	1.40	1.46
23	b	613	CLA	C4D-CHA	2.48	1.47	1.38
23	C	507	CLA	OBD-CAD	2.47	1.26	1.22
23	c	507	CLA	OBD-CAD	2.47	1.26	1.22
31	C	519	DGD	O2G-C2G	-2.47	1.40	1.46
31	c	519	DGD	O2G-C2G	-2.47	1.40	1.46
23	b	616	CLA	C4D-CHA	2.46	1.47	1.38
23	B	608	CLA	CHC-C4B	2.46	1.44	1.39
23	b	608	CLA	CHC-C4B	2.46	1.44	1.39
23	B	605	CLA	CHD-C1D	2.46	1.43	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	605	CLA	CHD-C1D	2.46	1.43	1.38
31	C	517	DGD	O1G-C1G	-2.46	1.39	1.45
31	c	517	DGD	O1G-C1G	-2.46	1.39	1.45
23	C	506	CLA	C1C-NC	-2.46	1.34	1.37
23	c	506	CLA	C1C-NC	-2.46	1.34	1.37
23	B	616	CLA	C4D-CHA	2.45	1.47	1.38
23	B	613	CLA	C4D-CHA	2.45	1.47	1.38
23	D	405	CLA	C3B-C4B	2.45	1.48	1.42
23	d	405	CLA	C3B-C4B	2.45	1.48	1.42
23	C	511	CLA	C3D-C2D	2.45	1.45	1.39
23	c	511	CLA	C3D-C2D	2.45	1.45	1.39
28	D	415	SQD	O48-C23	2.45	1.45	1.33
28	d	415	SQD	O48-C23	2.45	1.45	1.33
23	C	506	CLA	C4D-CHA	2.44	1.47	1.38
23	c	506	CLA	C4D-CHA	2.44	1.47	1.38
23	B	603	CLA	C3B-C2B	2.44	1.49	1.41
23	b	603	CLA	C3B-C2B	2.44	1.49	1.41
23	B	610	CLA	C3B-C4B	2.44	1.48	1.42
23	b	610	CLA	C3B-C4B	2.44	1.48	1.42
23	B	605	CLA	CHC-C4B	2.43	1.44	1.39
23	b	605	CLA	CHC-C4B	2.43	1.44	1.39
23	C	504	CLA	C1C-C2C	2.43	1.49	1.44
23	c	504	CLA	C1C-C2C	2.43	1.49	1.44
27	A	411	PL9	C6-C5	2.43	1.48	1.35
27	a	411	PL9	C6-C5	2.43	1.48	1.35
23	B	603	CLA	C1B-C2B	2.43	1.49	1.43
23	b	603	CLA	C1B-C2B	2.43	1.49	1.43
23	B	606	CLA	C1D-ND	2.42	1.40	1.37
23	D	406	CLA	C4B-NB	-2.42	1.34	1.37
23	b	606	CLA	C1D-ND	2.42	1.40	1.37
23	d	406	CLA	C4B-NB	-2.42	1.34	1.37
23	B	601	CLA	OBD-CAD	2.42	1.26	1.22
23	b	601	CLA	OBD-CAD	2.42	1.26	1.22
23	D	406	CLA	C1C-C2C	2.42	1.49	1.44
23	d	406	CLA	C1C-C2C	2.42	1.49	1.44
23	B	606	CLA	C1B-C2B	2.42	1.49	1.43
23	b	606	CLA	C1B-C2B	2.42	1.49	1.43
23	B	608	CLA	C4D-CHA	2.42	1.47	1.38
23	b	608	CLA	C4D-CHA	2.42	1.47	1.38
23	C	513	CLA	C4C-C3C	2.41	1.49	1.45
23	c	513	CLA	C4C-C3C	2.41	1.49	1.45
33	D	409	LHG	O8-C23	2.40	1.40	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	d	409	LHG	O8-C23	2.40	1.40	1.33
23	C	504	CLA	C3B-C4B	2.40	1.48	1.42
23	c	504	CLA	C3B-C4B	2.40	1.48	1.42
23	C	507	CLA	C4D-CHA	2.40	1.46	1.38
23	c	507	CLA	C4D-CHA	2.40	1.46	1.38
23	C	505	CLA	C1C-C2C	2.40	1.49	1.44
23	c	505	CLA	C1C-C2C	2.40	1.49	1.44
25	A	409	BCR	C23-C22	-2.40	1.40	1.45
25	a	409	BCR	C23-C22	-2.40	1.40	1.45
23	B	605	CLA	C3D-C4D	-2.39	1.38	1.44
23	b	605	CLA	C3D-C4D	-2.39	1.38	1.44
23	B	605	CLA	C3B-C4B	2.39	1.48	1.42
23	b	605	CLA	C3B-C4B	2.39	1.48	1.42
23	D	402	CLA	OBD-CAD	2.39	1.26	1.22
23	d	402	CLA	OBD-CAD	2.39	1.26	1.22
23	C	503	CLA	CHD-C1D	2.39	1.43	1.38
23	A	405	CLA	OBD-CAD	2.38	1.26	1.22
23	a	405	CLA	OBD-CAD	2.38	1.26	1.22
23	B	611	CLA	O2A-CGA	2.38	1.40	1.33
23	b	611	CLA	O2A-CGA	2.38	1.40	1.33
25	D	407	BCR	C1-C6	-2.36	1.50	1.53
25	d	407	BCR	C1-C6	-2.36	1.50	1.53
23	c	503	CLA	CHD-C1D	2.36	1.43	1.38
23	B	615	CLA	C1B-C2B	2.36	1.48	1.43
23	b	615	CLA	C1B-C2B	2.36	1.48	1.43
37	V	201	HEC	C4D-C3D	2.35	1.49	1.44
37	v	201	HEC	C4D-C3D	2.35	1.49	1.44
23	C	510	CLA	C1C-NC	-2.35	1.34	1.37
23	c	510	CLA	C1C-NC	-2.35	1.34	1.37
23	C	503	CLA	MG-ND	-2.35	2.01	2.05
23	c	503	CLA	MG-ND	-2.35	2.01	2.05
33	D	410	LHG	O7-C5	-2.34	1.40	1.46
33	d	410	LHG	O7-C5	-2.34	1.40	1.46
23	C	509	CLA	C1C-NC	-2.34	1.34	1.37
23	c	509	CLA	C1C-NC	-2.34	1.34	1.37
23	C	509	CLA	C1C-C2C	2.34	1.49	1.44
23	c	509	CLA	C1C-C2C	2.34	1.49	1.44
23	C	510	CLA	C4D-CHA	2.33	1.46	1.38
23	c	510	CLA	C4D-CHA	2.33	1.46	1.38
23	D	405	CLA	C1C-NC	-2.33	1.34	1.37
23	d	405	CLA	C1C-NC	-2.33	1.34	1.37
23	B	607	CLA	CHC-C4B	2.32	1.44	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	607	CLA	CHC-C4B	2.32	1.44	1.39
23	B	606	CLA	C4D-CHA	2.32	1.46	1.38
23	b	606	CLA	C4D-CHA	2.32	1.46	1.38
23	B	602	CLA	OBD-CAD	2.31	1.26	1.22
23	b	602	CLA	OBD-CAD	2.31	1.26	1.22
23	B	604	CLA	C4C-C3C	2.31	1.49	1.45
23	b	604	CLA	C4C-C3C	2.31	1.49	1.45
23	B	604	CLA	C4D-CHA	2.31	1.46	1.38
23	b	604	CLA	C4D-CHA	2.31	1.46	1.38
31	C	518	DGD	O2G-C2G	-2.31	1.40	1.46
31	c	518	DGD	O2G-C2G	-2.31	1.40	1.46
23	C	512	CLA	C4D-CHA	2.31	1.46	1.38
23	c	512	CLA	C4D-CHA	2.31	1.46	1.38
23	C	513	CLA	C3D-C4D	-2.31	1.39	1.44
23	c	513	CLA	C3D-C4D	-2.31	1.39	1.44
23	B	604	CLA	C1C-C2C	2.31	1.49	1.44
23	b	604	CLA	C1C-C2C	2.31	1.49	1.44
25	B	618	BCR	C26-C25	2.31	1.36	1.33
25	b	618	BCR	C26-C25	2.31	1.36	1.33
23	B	601	CLA	MG-ND	-2.30	2.01	2.05
23	b	601	CLA	MG-ND	-2.30	2.01	2.05
23	D	406	CLA	MG-ND	-2.30	2.01	2.05
23	d	406	CLA	MG-ND	-2.30	2.01	2.05
23	C	513	CLA	C4D-CHA	2.30	1.46	1.38
23	c	513	CLA	C4D-CHA	2.30	1.46	1.38
23	B	608	CLA	C1B-C2B	2.30	1.48	1.43
23	b	608	CLA	C1B-C2B	2.30	1.48	1.43
34	F	101	HEM	C1D-ND	-2.30	1.34	1.38
34	f	101	HEM	C1D-ND	-2.30	1.34	1.38
37	V	201	HEC	C1D-ND	-2.29	1.35	1.39
24	D	401	PHO	C4B-NB	-2.29	1.34	1.38
24	d	401	PHO	C4B-NB	-2.29	1.34	1.38
23	C	504	CLA	C3D-C4D	-2.29	1.39	1.44
23	c	504	CLA	C3D-C4D	-2.29	1.39	1.44
23	B	601	CLA	C4D-CHA	2.28	1.46	1.38
23	b	601	CLA	C4D-CHA	2.28	1.46	1.38
23	B	605	CLA	C4D-CHA	2.28	1.46	1.38
23	b	605	CLA	C4D-CHA	2.28	1.46	1.38
37	V	201	HEC	C1C-C2C	2.28	1.48	1.43
37	v	201	HEC	C1C-C2C	2.28	1.48	1.43
37	V	201	HEC	C1B-NB	-2.28	1.35	1.39
37	v	201	HEC	C1B-NB	-2.28	1.35	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	C1B-C2B	2.28	1.48	1.43
23	C	511	CLA	C1C-C2C	2.28	1.49	1.44
23	C	503	CLA	C3B-C4B	2.27	1.48	1.42
23	c	503	CLA	C3B-C4B	2.27	1.48	1.42
23	B	606	CLA	C1C-C2C	2.27	1.49	1.44
23	b	606	CLA	C1C-C2C	2.27	1.49	1.44
37	v	201	HEC	C1D-ND	-2.27	1.35	1.39
24	A	407	PHO	CBD-CGD	-2.27	1.49	1.52
24	a	407	PHO	CBD-CGD	-2.27	1.49	1.52
23	c	511	CLA	C1C-C2C	2.26	1.48	1.44
23	b	607	CLA	C1B-C2B	2.26	1.48	1.43
24	A	407	PHO	CHA-CBD	-2.26	1.48	1.51
24	a	407	PHO	CHA-CBD	-2.26	1.48	1.51
23	D	405	CLA	C1B-C2B	2.26	1.48	1.43
23	d	405	CLA	C1B-C2B	2.26	1.48	1.43
23	A	406	CLA	C3B-C4B	2.25	1.48	1.42
23	a	406	CLA	C3B-C4B	2.25	1.48	1.42
23	B	612	CLA	CHD-C4C	2.25	1.44	1.39
23	b	612	CLA	CHD-C4C	2.25	1.44	1.39
23	B	610	CLA	C1B-C2B	2.25	1.48	1.43
23	b	610	CLA	C1B-C2B	2.25	1.48	1.43
23	B	608	CLA	C3B-C4B	2.24	1.48	1.42
23	b	608	CLA	C3B-C4B	2.24	1.48	1.42
23	B	611	CLA	C1C-C2C	2.24	1.48	1.44
23	b	611	CLA	C1C-C2C	2.24	1.48	1.44
23	C	503	CLA	C1C-C2C	2.24	1.48	1.44
23	c	503	CLA	C1C-C2C	2.24	1.48	1.44
23	B	609	CLA	C3B-C4B	2.23	1.48	1.42
23	b	609	CLA	C3B-C4B	2.23	1.48	1.42
23	A	408	CLA	C4D-CHA	2.23	1.46	1.38
23	a	408	CLA	C4D-CHA	2.23	1.46	1.38
23	C	505	CLA	C4D-CHA	2.23	1.46	1.38
23	c	505	CLA	C4D-CHA	2.23	1.46	1.38
23	C	506	CLA	C3D-C4D	-2.23	1.39	1.44
23	c	506	CLA	C3D-C4D	-2.23	1.39	1.44
23	C	508	CLA	C3B-C4B	2.22	1.48	1.42
23	c	508	CLA	C3B-C4B	2.22	1.48	1.42
23	B	605	CLA	C1D-ND	2.22	1.40	1.37
23	b	605	CLA	C1D-ND	2.22	1.40	1.37
23	C	512	CLA	C1C-NC	-2.22	1.34	1.37
23	c	512	CLA	C1C-NC	-2.22	1.34	1.37
23	C	502	CLA	MG-ND	-2.22	2.01	2.05

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	502	CLA	MG-ND	-2.22	2.01	2.05
24	A	407	PHO	O2D-CED	-2.22	1.40	1.45
24	a	407	PHO	O2D-CED	-2.22	1.40	1.45
23	A	405	CLA	MG-ND	-2.21	2.01	2.05
23	a	405	CLA	MG-ND	-2.21	2.01	2.05
23	B	601	CLA	C3B-C4B	2.21	1.47	1.42
23	b	601	CLA	C3B-C4B	2.21	1.47	1.42
23	A	405	CLA	C4D-CHA	2.20	1.46	1.38
23	a	405	CLA	C4D-CHA	2.20	1.46	1.38
23	A	406	CLA	CHD-C4C	2.20	1.44	1.39
23	a	406	CLA	CHD-C4C	2.20	1.44	1.39
25	B	617	BCR	C15-C14	2.20	1.50	1.43
25	b	617	BCR	C15-C14	2.20	1.50	1.43
23	C	507	CLA	C1B-C2B	2.19	1.48	1.43
37	V	201	HEC	C1B-C2B	2.19	1.48	1.43
37	v	201	HEC	C1B-C2B	2.19	1.48	1.43
33	D	409	LHG	O8-C6	-2.19	1.40	1.45
33	d	409	LHG	O8-C6	-2.19	1.40	1.45
23	B	612	CLA	C3B-C4B	2.19	1.47	1.42
23	b	612	CLA	C3B-C4B	2.19	1.47	1.42
23	C	510	CLA	MG-ND	-2.19	2.01	2.05
23	c	510	CLA	MG-ND	-2.19	2.01	2.05
23	B	616	CLA	C1B-C2B	2.19	1.48	1.43
23	b	616	CLA	C1B-C2B	2.19	1.48	1.43
34	F	101	HEM	C4C-NC	-2.19	1.35	1.39
34	f	101	HEM	C4C-NC	-2.19	1.35	1.39
23	B	603	CLA	C3B-C4B	2.19	1.47	1.42
23	b	603	CLA	C3B-C4B	2.19	1.47	1.42
23	B	614	CLA	C4D-CHA	2.19	1.46	1.38
23	b	614	CLA	C4D-CHA	2.19	1.46	1.38
35	H	101	RRX	C15-C14	-2.18	1.36	1.43
35	h	101	RRX	C15-C14	-2.18	1.36	1.43
23	A	405	CLA	C4B-NB	-2.18	1.35	1.37
23	a	405	CLA	C4B-NB	-2.18	1.35	1.37
23	D	405	CLA	C1D-ND	2.18	1.40	1.37
23	d	405	CLA	C1D-ND	2.18	1.40	1.37
23	B	604	CLA	C1B-C2B	2.18	1.48	1.43
23	b	604	CLA	C1B-C2B	2.18	1.48	1.43
23	B	614	CLA	MG-ND	-2.18	2.01	2.05
23	C	506	CLA	C1C-C2C	2.18	1.48	1.44
24	A	407	PHO	C4B-NB	-2.18	1.34	1.38
24	a	407	PHO	C4B-NB	-2.18	1.34	1.38

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	C1B-C2B	2.18	1.48	1.43
23	B	616	CLA	C3B-C4B	2.17	1.47	1.42
23	b	616	CLA	C3B-C4B	2.17	1.47	1.42
23	C	504	CLA	C4D-CHA	2.17	1.46	1.38
23	c	504	CLA	C4D-CHA	2.17	1.46	1.38
23	B	603	CLA	C1C-NC	-2.17	1.34	1.37
23	b	603	CLA	C1C-NC	-2.17	1.34	1.37
23	C	514	CLA	C3D-C4D	-2.17	1.39	1.44
23	c	514	CLA	C3D-C4D	-2.17	1.39	1.44
23	C	507	CLA	C1C-NC	-2.16	1.34	1.37
23	c	507	CLA	C1C-NC	-2.16	1.34	1.37
23	A	406	CLA	CHC-C4B	2.16	1.44	1.39
23	a	406	CLA	CHC-C4B	2.16	1.44	1.39
23	C	502	CLA	C4D-CHA	2.16	1.46	1.38
23	c	502	CLA	C4D-CHA	2.16	1.46	1.38
23	B	611	CLA	MG-NA	2.15	2.11	2.06
23	b	611	CLA	MG-NA	2.15	2.11	2.06
23	B	607	CLA	C3D-C4D	-2.15	1.39	1.44
23	b	607	CLA	C3D-C4D	-2.15	1.39	1.44
23	B	606	CLA	C3D-C4D	-2.15	1.39	1.44
23	b	606	CLA	C3D-C4D	-2.15	1.39	1.44
23	A	408	CLA	C1B-C2B	2.15	1.48	1.43
23	a	408	CLA	C1B-C2B	2.15	1.48	1.43
23	c	506	CLA	C1C-C2C	2.14	1.48	1.44
23	b	603	CLA	C4D-CHA	2.14	1.46	1.38
23	C	509	CLA	CAA-C2A	2.14	1.58	1.54
23	c	509	CLA	CAA-C2A	2.14	1.58	1.54
23	C	503	CLA	C3D-C4D	-2.14	1.39	1.44
23	B	603	CLA	C4D-CHA	2.14	1.46	1.38
23	b	614	CLA	MG-ND	-2.14	2.01	2.05
23	C	508	CLA	C4D-CHA	2.13	1.46	1.38
23	c	508	CLA	C4D-CHA	2.13	1.46	1.38
23	C	507	CLA	C1C-C2C	2.13	1.48	1.44
23	c	507	CLA	C1C-C2C	2.13	1.48	1.44
23	C	506	CLA	C1B-C2B	2.13	1.48	1.43
23	c	506	CLA	C1B-C2B	2.13	1.48	1.43
23	b	609	CLA	C1C-C2C	2.13	1.48	1.44
23	B	609	CLA	C1C-C2C	2.13	1.48	1.44
23	C	504	CLA	C1B-C2B	2.12	1.48	1.43
23	c	504	CLA	C1B-C2B	2.12	1.48	1.43
23	c	503	CLA	C3D-C4D	-2.12	1.39	1.44
23	b	616	CLA	MG-NA	2.12	2.11	2.06

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	MG-NA	2.12	2.11	2.06
23	c	512	CLA	MG-NA	2.12	2.11	2.06
23	B	605	CLA	C1B-C2B	2.11	1.48	1.43
23	b	605	CLA	C1B-C2B	2.11	1.48	1.43
23	B	616	CLA	MG-NA	2.11	2.11	2.06
23	B	606	CLA	C1C-NC	-2.10	1.34	1.37
23	b	606	CLA	C1C-NC	-2.10	1.34	1.37
23	B	616	CLA	C1C-NC	-2.09	1.34	1.37
23	b	616	CLA	C1C-NC	-2.09	1.34	1.37
23	C	502	CLA	C3D-C4D	-2.09	1.39	1.44
23	c	502	CLA	C3D-C4D	-2.09	1.39	1.44
27	d	408	PL9	C6-C5	2.08	1.46	1.35
23	B	605	CLA	C1C-C2C	2.08	1.48	1.44
23	b	605	CLA	C1C-C2C	2.08	1.48	1.44
27	D	408	PL9	C6-C5	2.08	1.46	1.35
25	a	409	BCR	C8-C9	2.08	1.50	1.45
23	B	614	CLA	OBD-CAD	2.08	1.26	1.22
23	b	614	CLA	OBD-CAD	2.08	1.26	1.22
23	C	508	CLA	C3D-C4D	-2.08	1.39	1.44
23	c	508	CLA	C3D-C4D	-2.08	1.39	1.44
23	B	612	CLA	C4D-CHA	2.08	1.45	1.38
23	b	612	CLA	C4D-CHA	2.08	1.45	1.38
23	B	607	CLA	MG-ND	-2.07	2.01	2.05
23	b	607	CLA	MG-ND	-2.07	2.01	2.05
31	C	517	DGD	O2G-C2G	-2.07	1.41	1.46
23	B	608	CLA	MG-ND	-2.06	2.01	2.05
23	D	402	CLA	C3D-C4D	-2.06	1.39	1.44
23	d	402	CLA	C3D-C4D	-2.06	1.39	1.44
23	B	604	CLA	MG-ND	-2.06	2.01	2.05
23	b	604	CLA	MG-ND	-2.06	2.01	2.05
23	B	610	CLA	CHD-C4C	2.06	1.43	1.39
23	b	610	CLA	CHD-C4C	2.06	1.43	1.39
23	A	406	CLA	C1D-ND	2.06	1.40	1.37
23	a	406	CLA	C1D-ND	2.06	1.40	1.37
25	A	409	BCR	C8-C9	2.06	1.50	1.45
23	A	405	CLA	MG-NA	2.05	2.11	2.06
23	a	405	CLA	MG-NA	2.05	2.11	2.06
23	C	503	CLA	O2A-C1	-2.05	1.40	1.46
23	A	408	CLA	C3B-C2B	2.05	1.48	1.41
23	a	408	CLA	C3B-C2B	2.05	1.48	1.41
23	B	604	CLA	C3B-C2B	2.05	1.48	1.41
23	b	604	CLA	C3B-C2B	2.05	1.48	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406	CLA	C1B-C2B	2.05	1.48	1.43
23	a	406	CLA	C1B-C2B	2.05	1.48	1.43
23	C	514	CLA	C4D-CHA	2.04	1.45	1.38
23	c	514	CLA	C4D-CHA	2.04	1.45	1.38
23	C	508	CLA	CHB-C4A	-2.04	1.32	1.37
23	c	508	CLA	CHB-C4A	-2.04	1.32	1.37
31	c	517	DGD	O2G-C2G	-2.04	1.41	1.46
23	C	510	CLA	C1B-C2B	2.04	1.48	1.43
23	c	510	CLA	C1B-C2B	2.04	1.48	1.43
23	D	402	CLA	CHC-C4B	2.04	1.44	1.39
23	d	402	CLA	CHC-C4B	2.04	1.44	1.39
23	D	405	CLA	O2D-CED	-2.04	1.40	1.45
23	d	405	CLA	O2D-CED	-2.04	1.40	1.45
23	C	506	CLA	C4B-NB	-2.04	1.35	1.37
23	c	506	CLA	C4B-NB	-2.04	1.35	1.37
23	B	604	CLA	C3D-C4D	-2.04	1.39	1.44
23	b	604	CLA	C3D-C4D	-2.04	1.39	1.44
30	M	101	LMT	C3'-C2'	2.03	1.57	1.52
30	m	101	LMT	C3'-C2'	2.03	1.57	1.52
23	C	502	CLA	C1C-NC	-2.03	1.34	1.37
23	c	502	CLA	C1C-NC	-2.03	1.34	1.37
23	B	604	CLA	O2A-C1	-2.03	1.40	1.46
23	b	604	CLA	O2A-C1	-2.03	1.40	1.46
23	c	503	CLA	C1D-ND	2.03	1.40	1.37
23	C	511	CLA	MG-ND	-2.03	2.01	2.05
23	c	511	CLA	MG-ND	-2.03	2.01	2.05
23	C	503	CLA	C1B-C2B	2.03	1.48	1.43
23	c	503	CLA	C1B-C2B	2.03	1.48	1.43
23	A	405	CLA	C1C-C2C	2.03	1.48	1.44
23	a	405	CLA	C1C-C2C	2.03	1.48	1.44
23	b	608	CLA	MG-ND	-2.02	2.01	2.05
23	C	503	CLA	MG-NB	-2.02	2.01	2.05
23	c	503	CLA	MG-NB	-2.02	2.01	2.05
23	B	602	CLA	C3D-C4D	-2.02	1.39	1.44
23	b	602	CLA	C3D-C4D	-2.02	1.39	1.44
23	B	609	CLA	C4D-CHA	2.02	1.45	1.38
23	b	609	CLA	C4D-CHA	2.02	1.45	1.38
35	H	101	RRX	C20-C21	-2.02	1.37	1.43
35	h	101	RRX	C20-C21	-2.02	1.37	1.43
23	c	503	CLA	O2A-C1	-2.01	1.40	1.46
23	B	601	CLA	C1C-NC	-2.01	1.34	1.37
23	b	601	CLA	C1C-NC	-2.01	1.34	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	MG-ND	-2.01	2.01	2.05
23	c	512	CLA	MG-ND	-2.01	2.01	2.05
23	B	603	CLA	CHD-C4C	2.01	1.43	1.39
23	b	603	CLA	CHD-C4C	2.01	1.43	1.39
23	C	511	CLA	C3B-C4B	2.00	1.47	1.42
23	c	511	CLA	C3B-C4B	2.00	1.47	1.42
23	B	601	CLA	C3D-C4D	-2.00	1.39	1.44
23	b	601	CLA	C3D-C4D	-2.00	1.39	1.44
25	T	101	BCR	C20-C21	2.00	1.49	1.43
25	t	103	BCR	C20-C21	2.00	1.49	1.43
25	K	102	BCR	C20-C21	2.00	1.49	1.43
25	k	102	BCR	C20-C21	2.00	1.49	1.43

All (2580) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	407	PHO	C2D-C1D-ND	15.53	120.25	109.53
24	a	407	PHO	C2D-C1D-ND	15.53	120.25	109.53
23	B	611	CLA	C2B-C1B-NB	15.44	120.58	110.23
23	b	611	CLA	C2B-C1B-NB	15.44	120.58	110.23
24	D	401	PHO	C2D-C1D-ND	14.40	119.47	109.53
24	d	401	PHO	C2D-C1D-ND	14.40	119.47	109.53
23	B	611	CLA	C3B-C2B-C1B	-12.02	92.65	107.16
23	b	611	CLA	C3B-C2B-C1B	-12.02	92.65	107.16
23	B	603	CLA	C1D-ND-C4D	-11.57	98.11	106.33
23	b	603	CLA	C1D-ND-C4D	-11.53	98.14	106.33
23	B	603	CLA	C2D-C1D-ND	11.20	118.36	110.10
23	b	603	CLA	C2D-C1D-ND	11.17	118.34	110.10
23	C	502	CLA	C1D-ND-C4D	-10.87	98.62	106.33
23	c	502	CLA	C1D-ND-C4D	-10.87	98.62	106.33
23	B	605	CLA	C1D-ND-C4D	-10.64	98.78	106.33
23	b	605	CLA	C1D-ND-C4D	-10.64	98.78	106.33
23	C	505	CLA	C1D-ND-C4D	-10.33	99.00	106.33
23	c	505	CLA	C1D-ND-C4D	-10.33	99.00	106.33
37	V	201	HEC	CBB-CAB-C3B	-10.09	109.31	127.86
37	v	201	HEC	CBB-CAB-C3B	-10.09	109.31	127.86
23	B	605	CLA	C2D-C1D-ND	10.03	117.50	110.10
23	b	605	CLA	C2D-C1D-ND	10.03	117.50	110.10
23	c	502	CLA	C2D-C1D-ND	10.03	117.49	110.10
23	C	502	CLA	C2D-C1D-ND	10.02	117.49	110.10
23	D	406	CLA	C1D-ND-C4D	-9.92	99.29	106.33
23	d	406	CLA	C1D-ND-C4D	-9.92	99.29	106.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	514	CLA	C1D-ND-C4D	-9.82	99.36	106.33
23	c	514	CLA	C1D-ND-C4D	-9.82	99.36	106.33
23	C	505	CLA	C2D-C1D-ND	9.80	117.33	110.10
23	c	505	CLA	C2D-C1D-ND	9.79	117.32	110.10
23	C	514	CLA	C2D-C1D-ND	9.76	117.30	110.10
23	c	514	CLA	C2D-C1D-ND	9.76	117.30	110.10
23	B	611	CLA	C1D-ND-C4D	-9.71	99.43	106.33
23	b	611	CLA	C1D-ND-C4D	-9.71	99.43	106.33
23	b	612	CLA	C2D-C1D-ND	9.70	117.25	110.10
23	B	612	CLA	C2D-C1D-ND	9.68	117.24	110.10
23	B	614	CLA	C2D-C1D-ND	9.67	117.23	110.10
23	b	614	CLA	C2D-C1D-ND	9.67	117.23	110.10
23	C	510	CLA	C1D-ND-C4D	-9.62	99.50	106.33
23	c	510	CLA	C1D-ND-C4D	-9.62	99.50	106.33
23	C	511	CLA	C2D-C1D-ND	9.60	117.17	110.10
23	D	402	CLA	C2D-C1D-ND	9.57	117.16	110.10
23	d	402	CLA	C2D-C1D-ND	9.57	117.16	110.10
23	c	511	CLA	C2D-C1D-ND	9.56	117.15	110.10
23	C	513	CLA	C1D-ND-C4D	-9.56	99.54	106.33
23	c	513	CLA	C1D-ND-C4D	-9.56	99.54	106.33
23	b	612	CLA	C1D-ND-C4D	-9.55	99.55	106.33
23	B	612	CLA	C1D-ND-C4D	-9.52	99.57	106.33
23	B	616	CLA	C2D-C1D-ND	9.48	117.09	110.10
23	b	616	CLA	C2D-C1D-ND	9.48	117.09	110.10
24	D	401	PHO	C4D-ND-C1D	-9.47	99.19	108.83
24	d	401	PHO	C4D-ND-C1D	-9.47	99.19	108.83
23	A	408	CLA	C1D-ND-C4D	-9.45	99.62	106.33
23	a	408	CLA	C1D-ND-C4D	-9.45	99.62	106.33
23	C	511	CLA	C1D-ND-C4D	-9.41	99.65	106.33
24	A	407	PHO	C4D-ND-C1D	-9.40	99.26	108.83
24	a	407	PHO	C4D-ND-C1D	-9.40	99.26	108.83
23	B	611	CLA	C2D-C1D-ND	9.40	117.03	110.10
23	b	611	CLA	C2D-C1D-ND	9.40	117.03	110.10
37	V	201	HEC	CBC-CAC-C3C	-9.40	110.58	127.86
37	v	201	HEC	CBC-CAC-C3C	-9.40	110.58	127.86
23	c	511	CLA	C1D-ND-C4D	-9.37	99.68	106.33
23	A	406	CLA	C1D-ND-C4D	-9.31	99.72	106.33
23	a	406	CLA	C1D-ND-C4D	-9.31	99.72	106.33
23	B	609	CLA	C1D-ND-C4D	-9.29	99.74	106.33
23	b	609	CLA	C1D-ND-C4D	-9.29	99.74	106.33
23	C	510	CLA	C2D-C1D-ND	9.29	116.95	110.10
23	c	510	CLA	C2D-C1D-ND	9.29	116.95	110.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	616	CLA	C1D-ND-C4D	-9.28	99.74	106.33
23	b	616	CLA	C1D-ND-C4D	-9.28	99.74	106.33
23	B	604	CLA	C2D-C1D-ND	9.27	116.94	110.10
23	b	604	CLA	C2D-C1D-ND	9.27	116.94	110.10
23	C	513	CLA	C2D-C1D-ND	9.25	116.92	110.10
23	c	513	CLA	C2D-C1D-ND	9.25	116.92	110.10
23	D	406	CLA	C2D-C1D-ND	9.25	116.92	110.10
23	d	406	CLA	C2D-C1D-ND	9.25	116.92	110.10
23	B	609	CLA	C2D-C1D-ND	9.23	116.90	110.10
23	b	609	CLA	C2D-C1D-ND	9.23	116.90	110.10
23	C	508	CLA	C1D-ND-C4D	-9.22	99.78	106.33
23	c	508	CLA	C1D-ND-C4D	-9.22	99.78	106.33
23	B	615	CLA	C2D-C1D-ND	9.17	116.86	110.10
23	b	615	CLA	C2D-C1D-ND	9.17	116.86	110.10
23	D	405	CLA	C2D-C1D-ND	9.13	116.83	110.10
23	d	405	CLA	C2D-C1D-ND	9.13	116.83	110.10
23	B	601	CLA	C2D-C1D-ND	9.08	116.80	110.10
23	b	601	CLA	C2D-C1D-ND	9.08	116.80	110.10
23	C	503	CLA	C1D-ND-C4D	-9.05	99.91	106.33
23	c	503	CLA	C1D-ND-C4D	-9.05	99.91	106.33
23	C	512	CLA	C2D-C1D-ND	9.01	116.75	110.10
23	c	512	CLA	C2D-C1D-ND	9.01	116.75	110.10
23	C	508	CLA	C2D-C1D-ND	8.98	116.72	110.10
23	c	508	CLA	C2D-C1D-ND	8.98	116.72	110.10
23	A	406	CLA	C2D-C1D-ND	8.94	116.69	110.10
23	a	406	CLA	C2D-C1D-ND	8.94	116.69	110.10
23	B	614	CLA	C1D-ND-C4D	-8.93	99.99	106.33
23	B	601	CLA	C1D-ND-C4D	-8.92	100.00	106.33
23	b	601	CLA	C1D-ND-C4D	-8.92	100.00	106.33
23	C	509	CLA	C2D-C1D-ND	8.89	116.65	110.10
23	c	509	CLA	C2D-C1D-ND	8.89	116.65	110.10
23	b	614	CLA	C1D-ND-C4D	-8.88	100.03	106.33
23	B	606	CLA	C1D-ND-C4D	-8.82	100.07	106.33
23	b	606	CLA	C1D-ND-C4D	-8.82	100.07	106.33
23	C	503	CLA	C2D-C1D-ND	8.82	116.60	110.10
23	c	503	CLA	C2D-C1D-ND	8.81	116.60	110.10
23	D	405	CLA	C1D-ND-C4D	-8.81	100.08	106.33
23	d	405	CLA	C1D-ND-C4D	-8.81	100.08	106.33
23	B	602	CLA	C1D-ND-C4D	-8.81	100.08	106.33
23	b	602	CLA	C1D-ND-C4D	-8.81	100.08	106.33
23	B	604	CLA	C1D-ND-C4D	-8.76	100.11	106.33
23	b	604	CLA	C1D-ND-C4D	-8.76	100.11	106.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	C2D-C1D-ND	8.75	116.55	110.10
23	b	606	CLA	C2D-C1D-ND	8.75	116.55	110.10
23	B	608	CLA	C1D-ND-C4D	-8.73	100.13	106.33
23	b	608	CLA	C1D-ND-C4D	-8.73	100.13	106.33
23	A	408	CLA	C2D-C1D-ND	8.73	116.53	110.10
23	a	408	CLA	C2D-C1D-ND	8.73	116.53	110.10
23	C	509	CLA	C1D-ND-C4D	-8.70	100.16	106.33
23	c	509	CLA	C1D-ND-C4D	-8.70	100.16	106.33
23	B	610	CLA	C1D-ND-C4D	-8.66	100.18	106.33
23	b	610	CLA	C1D-ND-C4D	-8.66	100.18	106.33
23	C	512	CLA	C1D-ND-C4D	-8.46	100.33	106.33
23	c	512	CLA	C1D-ND-C4D	-8.46	100.33	106.33
23	B	613	CLA	C1D-ND-C4D	-8.45	100.33	106.33
23	C	506	CLA	C2D-C1D-ND	8.43	116.32	110.10
23	c	506	CLA	C2D-C1D-ND	8.43	116.32	110.10
23	b	613	CLA	C1D-ND-C4D	-8.39	100.38	106.33
23	D	402	CLA	C1D-ND-C4D	-8.38	100.38	106.33
23	d	402	CLA	C1D-ND-C4D	-8.38	100.38	106.33
23	C	506	CLA	C1D-ND-C4D	-8.37	100.39	106.33
23	c	506	CLA	C1D-ND-C4D	-8.37	100.39	106.33
23	C	507	CLA	C1D-ND-C4D	-8.24	100.48	106.33
23	c	507	CLA	C1D-ND-C4D	-8.24	100.48	106.33
23	B	615	CLA	C1D-ND-C4D	-8.23	100.49	106.33
23	b	615	CLA	C1D-ND-C4D	-8.23	100.49	106.33
23	A	405	CLA	C2D-C1D-ND	8.22	116.16	110.10
23	a	405	CLA	C2D-C1D-ND	8.22	116.16	110.10
24	D	401	PHO	C2B-C1B-NB	8.19	115.18	109.53
24	d	401	PHO	C2B-C1B-NB	8.19	115.18	109.53
23	C	504	CLA	C2D-C1D-ND	8.13	116.09	110.10
23	B	613	CLA	C2D-C1D-ND	8.11	116.08	110.10
23	c	504	CLA	C2D-C1D-ND	8.10	116.07	110.10
23	B	610	CLA	C2D-C1D-ND	8.08	116.06	110.10
23	b	610	CLA	C2D-C1D-ND	8.08	116.06	110.10
23	B	608	CLA	C2D-C1D-ND	8.07	116.05	110.10
23	b	608	CLA	C2D-C1D-ND	8.07	116.05	110.10
23	b	613	CLA	C2D-C1D-ND	8.03	116.02	110.10
23	A	405	CLA	C1D-ND-C4D	-8.02	100.64	106.33
23	a	405	CLA	C1D-ND-C4D	-8.02	100.64	106.33
23	C	514	CLA	C2B-C1B-NB	7.97	115.58	110.23
23	c	514	CLA	C2B-C1B-NB	7.97	115.58	110.23
23	B	607	CLA	C1D-ND-C4D	-7.94	100.69	106.33
23	b	607	CLA	C1D-ND-C4D	-7.94	100.69	106.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	501	SQD	O6-C1-C2	7.91	120.65	108.30
28	c	501	SQD	O6-C1-C2	7.91	120.65	108.30
23	C	504	CLA	C1D-ND-C4D	-7.88	100.74	106.33
23	c	504	CLA	C1D-ND-C4D	-7.82	100.78	106.33
23	B	602	CLA	C2D-C1D-ND	7.59	115.69	110.10
23	b	602	CLA	C2D-C1D-ND	7.59	115.69	110.10
28	D	415	SQD	O6-C1-C2	7.56	120.11	108.30
28	d	415	SQD	O6-C1-C2	7.56	120.11	108.30
23	B	607	CLA	C2D-C1D-ND	7.52	115.65	110.10
23	b	607	CLA	C2D-C1D-ND	7.52	115.65	110.10
23	B	602	CLA	CMD-C2D-C1D	7.43	137.81	124.71
23	b	602	CLA	CMD-C2D-C1D	7.43	137.81	124.71
24	A	407	PHO	O2D-CGD-CBD	7.28	120.23	111.00
24	a	407	PHO	O2D-CGD-CBD	7.28	120.23	111.00
25	C	515	BCR	C8-C7-C6	-7.20	117.72	126.86
25	c	515	BCR	C8-C7-C6	-7.20	117.72	126.86
23	B	602	CLA	CHD-C1D-ND	-7.07	117.96	124.45
23	b	602	CLA	CHD-C1D-ND	-7.07	117.96	124.45
23	C	505	CLA	O2D-CGD-CBD	6.96	123.63	111.27
23	c	505	CLA	O2D-CGD-CBD	6.96	123.63	111.27
23	A	406	CLA	O2D-CGD-CBD	6.95	123.62	111.27
23	a	406	CLA	O2D-CGD-CBD	6.95	123.62	111.27
23	B	611	CLA	CMB-C2B-C1B	6.85	135.80	125.37
23	b	611	CLA	CMB-C2B-C1B	6.85	135.80	125.37
23	B	616	CLA	C2B-C1B-NB	6.83	114.81	110.23
23	b	616	CLA	C2B-C1B-NB	6.83	114.81	110.23
23	C	507	CLA	C2D-C1D-ND	6.78	115.10	110.10
23	c	507	CLA	C2D-C1D-ND	6.78	115.10	110.10
23	B	614	CLA	C2C-C1C-NC	6.77	116.32	109.97
23	B	616	CLA	C2C-C1C-NC	6.76	116.31	109.97
23	b	616	CLA	C2C-C1C-NC	6.76	116.31	109.97
23	b	614	CLA	C2C-C1C-NC	6.74	116.29	109.97
23	B	603	CLA	O2D-CGD-CBD	6.71	123.18	111.27
23	b	603	CLA	O2D-CGD-CBD	6.71	123.18	111.27
23	B	615	CLA	C2B-C1B-NB	6.70	114.72	110.23
23	b	615	CLA	C2B-C1B-NB	6.70	114.72	110.23
23	C	514	CLA	CHD-C4C-C3C	-6.62	115.10	124.84
23	c	514	CLA	CHD-C4C-C3C	-6.62	115.10	124.84
24	D	401	PHO	O2D-CGD-CBD	6.53	119.27	111.00
24	d	401	PHO	O2D-CGD-CBD	6.53	119.27	111.00
23	B	606	CLA	CHD-C4C-C3C	-6.51	115.27	124.84
23	b	606	CLA	CHD-C4C-C3C	-6.51	115.27	124.84

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	C2B-C1B-NB	6.48	114.57	110.23
23	c	513	CLA	C2B-C1B-NB	6.48	114.57	110.23
23	C	509	CLA	C2B-C1B-NB	6.40	114.52	110.23
23	c	509	CLA	C2B-C1B-NB	6.40	114.52	110.23
23	C	510	CLA	C2C-C1C-NC	6.39	115.96	109.97
23	c	510	CLA	C2C-C1C-NC	6.39	115.96	109.97
24	A	407	PHO	C3D-C4D-ND	6.39	116.43	107.72
24	a	407	PHO	C3D-C4D-ND	6.39	116.43	107.72
23	B	610	CLA	C2C-C1C-NC	6.38	115.94	109.97
23	b	610	CLA	C2C-C1C-NC	6.38	115.94	109.97
23	C	508	CLA	C2B-C1B-NB	6.37	114.50	110.23
23	c	508	CLA	C2B-C1B-NB	6.37	114.50	110.23
24	A	407	PHO	C1C-C2C-C3C	-6.36	103.32	108.61
24	a	407	PHO	C1C-C2C-C3C	-6.36	103.32	108.61
23	B	604	CLA	C2C-C1C-NC	6.33	115.91	109.97
24	a	407	PHO	C2B-C1B-NB	6.31	113.88	109.53
23	b	604	CLA	C2C-C1C-NC	6.30	115.88	109.97
23	A	408	CLA	O2D-CGD-CBD	6.30	122.46	111.27
23	a	408	CLA	O2D-CGD-CBD	6.30	122.46	111.27
23	D	406	CLA	C2B-C1B-NB	6.28	114.44	110.23
23	d	406	CLA	C2B-C1B-NB	6.28	114.44	110.23
23	C	513	CLA	O2D-CGD-CBD	6.28	122.42	111.27
23	c	513	CLA	O2D-CGD-CBD	6.28	122.42	111.27
23	B	602	CLA	C2B-C1B-NB	6.27	114.43	110.23
23	b	602	CLA	C2B-C1B-NB	6.27	114.43	110.23
24	A	407	PHO	C2B-C1B-NB	6.27	113.85	109.53
23	A	408	CLA	C2C-C1C-NC	6.25	115.83	109.97
23	a	408	CLA	C2C-C1C-NC	6.25	115.83	109.97
23	B	603	CLA	CHD-C1D-ND	-6.24	118.72	124.45
23	C	502	CLA	CHD-C4C-C3C	-6.23	115.68	124.84
23	c	502	CLA	CHD-C4C-C3C	-6.23	115.68	124.84
23	b	603	CLA	CHD-C1D-ND	-6.22	118.73	124.45
23	B	609	CLA	C4A-NA-C1A	-6.21	103.91	106.71
23	b	609	CLA	C4A-NA-C1A	-6.21	103.91	106.71
23	C	512	CLA	C2C-C1C-NC	6.20	115.78	109.97
23	B	605	CLA	CHD-C1D-ND	-6.20	118.75	124.45
23	b	605	CLA	CHD-C1D-ND	-6.20	118.75	124.45
23	B	601	CLA	C2B-C1B-NB	6.20	114.39	110.23
23	b	601	CLA	C2B-C1B-NB	6.20	114.39	110.23
23	c	512	CLA	C2C-C1C-NC	6.19	115.77	109.97
23	B	604	CLA	C2B-C1B-NB	6.18	114.37	110.23
23	b	604	CLA	C2B-C1B-NB	6.18	114.37	110.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	602	CLA	O2D-CGD-CBD	6.17	122.24	111.27
23	b	602	CLA	O2D-CGD-CBD	6.17	122.24	111.27
23	B	607	CLA	C2C-C1C-NC	6.16	115.74	109.97
23	b	607	CLA	C2C-C1C-NC	6.16	115.74	109.97
23	B	608	CLA	C2C-C1C-NC	6.10	115.68	109.97
23	C	507	CLA	CMD-C2D-C1D	6.10	135.46	124.71
23	c	507	CLA	CMD-C2D-C1D	6.10	135.46	124.71
23	C	512	CLA	O2D-CGD-CBD	6.10	122.10	111.27
23	c	512	CLA	O2D-CGD-CBD	6.10	122.10	111.27
23	C	503	CLA	C2C-C1C-NC	6.09	115.68	109.97
23	c	503	CLA	C2C-C1C-NC	6.09	115.68	109.97
23	C	505	CLA	CMD-C2D-C1D	6.08	135.44	124.71
23	c	505	CLA	CMD-C2D-C1D	6.08	135.43	124.71
23	D	406	CLA	CMD-C2D-C1D	6.07	135.41	124.71
23	d	406	CLA	CMD-C2D-C1D	6.07	135.41	124.71
28	C	501	SQD	C1-O5-C5	-6.07	101.78	113.69
28	c	501	SQD	C1-O5-C5	-6.07	101.78	113.69
23	B	604	CLA	CMD-C2D-C1D	6.06	135.40	124.71
23	b	604	CLA	CMD-C2D-C1D	6.06	135.40	124.71
23	B	607	CLA	CHD-C4C-C3C	-6.06	115.94	124.84
23	b	607	CLA	CHD-C4C-C3C	-6.06	115.94	124.84
23	b	608	CLA	C2C-C1C-NC	6.04	115.63	109.97
23	B	602	CLA	C2C-C1C-NC	6.04	115.63	109.97
23	b	602	CLA	C2C-C1C-NC	6.04	115.63	109.97
23	C	511	CLA	CHD-C4C-C3C	-6.04	115.97	124.84
23	c	511	CLA	CHD-C4C-C3C	-6.04	115.97	124.84
23	D	402	CLA	C2C-C1C-NC	6.01	115.60	109.97
23	d	402	CLA	C2C-C1C-NC	6.01	115.60	109.97
23	b	614	CLA	O2D-CGD-CBD	6.00	121.93	111.27
23	C	511	CLA	C2B-C1B-NB	5.99	114.25	110.23
23	c	511	CLA	C2B-C1B-NB	5.99	114.25	110.23
23	B	614	CLA	O2D-CGD-CBD	5.98	121.90	111.27
24	D	401	PHO	C3D-C4D-ND	5.98	115.87	107.72
24	d	401	PHO	C3D-C4D-ND	5.98	115.87	107.72
23	C	505	CLA	C2B-C1B-NB	5.97	114.23	110.23
23	c	505	CLA	C2B-C1B-NB	5.97	114.23	110.23
23	B	612	CLA	CHD-C1D-ND	-5.93	119.00	124.45
23	b	612	CLA	CHD-C1D-ND	-5.93	119.00	124.45
23	b	609	CLA	CHD-C4C-C3C	-5.91	116.15	124.84
23	C	510	CLA	C2B-C1B-NB	5.91	114.19	110.23
23	B	609	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
23	B	606	CLA	C2C-C1C-NC	5.86	115.46	109.97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	C2C-C1C-NC	5.86	115.46	109.97
23	C	509	CLA	C3C-C4C-NC	5.86	117.14	110.57
23	c	509	CLA	C3C-C4C-NC	5.86	117.14	110.57
23	C	507	CLA	C2C-C1C-NC	5.86	115.46	109.97
23	c	507	CLA	C2C-C1C-NC	5.86	115.46	109.97
23	c	510	CLA	C2B-C1B-NB	5.86	114.16	110.23
23	D	406	CLA	CHD-C1D-ND	-5.83	119.10	124.45
23	d	406	CLA	CHD-C1D-ND	-5.83	119.10	124.45
23	B	602	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
23	b	602	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
23	B	608	CLA	C2B-C1B-NB	5.81	114.13	110.23
23	b	608	CLA	C2B-C1B-NB	5.81	114.13	110.23
23	C	505	CLA	C2C-C1C-NC	5.81	115.41	109.97
23	c	505	CLA	C2C-C1C-NC	5.81	115.41	109.97
23	C	504	CLA	CHD-C4C-C3C	-5.79	116.33	124.84
23	c	504	CLA	CHD-C4C-C3C	-5.78	116.35	124.84
23	C	502	CLA	O2D-CGD-CBD	5.77	121.53	111.27
23	c	502	CLA	O2D-CGD-CBD	5.77	121.53	111.27
23	B	614	CLA	C1C-C2C-C3C	-5.75	100.92	106.96
23	B	611	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
23	b	611	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
23	C	509	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
23	c	509	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
23	b	614	CLA	C1C-C2C-C3C	-5.72	100.94	106.96
23	A	406	CLA	CHD-C1D-ND	-5.69	119.22	124.45
23	a	406	CLA	CHD-C1D-ND	-5.69	119.22	124.45
23	B	610	CLA	CMD-C2D-C1D	5.69	134.75	124.71
23	b	610	CLA	CMD-C2D-C1D	5.69	134.75	124.71
23	C	513	CLA	CHD-C4C-C3C	-5.69	116.48	124.84
23	c	513	CLA	CHD-C4C-C3C	-5.69	116.48	124.84
23	C	504	CLA	CMD-C2D-C1D	5.68	134.73	124.71
23	c	504	CLA	CMD-C2D-C1D	5.68	134.73	124.71
23	C	511	CLA	O2D-CGD-CBD	5.66	121.33	111.27
23	c	511	CLA	O2D-CGD-CBD	5.66	121.33	111.27
23	C	504	CLA	C2B-C1B-NB	5.66	114.03	110.23
23	c	504	CLA	C2B-C1B-NB	5.66	114.03	110.23
23	B	605	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
23	b	605	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
23	D	406	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
23	d	406	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
23	B	606	CLA	O2D-CGD-CBD	5.62	121.26	111.27
23	b	606	CLA	O2D-CGD-CBD	5.62	121.26	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	F	101	HEM	CHC-C4B-NB	5.61	130.51	124.42
34	f	101	HEM	CHC-C4B-NB	5.61	130.51	124.42
23	B	614	CLA	CHD-C4C-C3C	-5.61	116.60	124.84
23	b	614	CLA	CHD-C4C-C3C	-5.61	116.60	124.84
23	C	502	CLA	C2B-C1B-NB	5.58	113.98	110.23
23	c	502	CLA	C2B-C1B-NB	5.58	113.98	110.23
23	D	405	CLA	C2C-C1C-NC	5.58	115.20	109.97
23	d	405	CLA	C2C-C1C-NC	5.58	115.20	109.97
23	C	514	CLA	C3D-C2D-C1D	-5.58	98.22	105.83
23	c	514	CLA	C3D-C2D-C1D	-5.58	98.22	105.83
23	B	601	CLA	O2D-CGD-CBD	5.56	121.15	111.27
23	b	601	CLA	O2D-CGD-CBD	5.56	121.15	111.27
25	K	102	BCR	C7-C8-C9	-5.53	117.87	126.23
25	k	102	BCR	C7-C8-C9	-5.53	117.87	126.23
23	A	405	CLA	CMD-C2D-C1D	5.52	134.45	124.71
23	a	405	CLA	CMD-C2D-C1D	5.52	134.45	124.71
23	C	510	CLA	CHD-C4C-C3C	-5.52	116.72	124.84
23	c	510	CLA	CHD-C4C-C3C	-5.52	116.72	124.84
23	B	603	CLA	C4-C3-C5	5.51	124.54	115.27
23	b	603	CLA	C4-C3-C5	5.51	124.54	115.27
23	d	402	CLA	C4A-NA-C1A	-5.50	104.23	106.71
23	B	603	CLA	CMD-C2D-C1D	5.49	134.38	124.71
23	b	603	CLA	CMD-C2D-C1D	5.49	134.38	124.71
23	B	611	CLA	CHB-C1B-NB	-5.49	118.45	124.26
23	b	611	CLA	CHB-C1B-NB	-5.49	118.45	124.26
23	B	601	CLA	CHD-C4C-C3C	-5.49	116.78	124.84
23	b	601	CLA	CHD-C4C-C3C	-5.49	116.78	124.84
23	B	604	CLA	CHD-C1D-ND	-5.48	119.42	124.45
23	b	604	CLA	CHD-C1D-ND	-5.48	119.42	124.45
23	D	402	CLA	C4A-NA-C1A	-5.45	104.25	106.71
23	C	504	CLA	C4A-NA-C1A	-5.45	104.26	106.71
23	c	504	CLA	C4A-NA-C1A	-5.45	104.26	106.71
25	B	617	BCR	C7-C8-C9	-5.44	118.01	126.23
25	b	617	BCR	C7-C8-C9	-5.44	118.01	126.23
23	C	514	CLA	O2D-CGD-CBD	5.44	120.93	111.27
23	c	514	CLA	O2D-CGD-CBD	5.44	120.93	111.27
25	C	515	BCR	C7-C8-C9	-5.42	118.04	126.23
25	c	515	BCR	C7-C8-C9	-5.42	118.04	126.23
23	A	405	CLA	C3B-C4B-NB	5.42	115.54	110.52
23	a	405	CLA	C3B-C4B-NB	5.42	115.54	110.52
23	C	508	CLA	O2D-CGD-CBD	5.42	120.89	111.27
23	c	508	CLA	O2D-CGD-CBD	5.42	120.89	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	C2C-C1C-NC	5.39	115.03	109.97
23	B	614	CLA	CMD-C2D-C1D	5.38	134.20	124.71
23	b	614	CLA	CMD-C2D-C1D	5.38	134.20	124.71
23	C	508	CLA	CHD-C1D-ND	-5.37	119.52	124.45
23	c	508	CLA	CHD-C1D-ND	-5.37	119.52	124.45
23	B	601	CLA	C2C-C1C-NC	5.36	115.00	109.97
23	b	601	CLA	C2C-C1C-NC	5.36	115.00	109.97
23	C	511	CLA	C2C-C1C-NC	5.36	115.00	109.97
23	C	508	CLA	CMD-C2D-C1D	5.35	134.14	124.71
23	c	508	CLA	CMD-C2D-C1D	5.35	134.14	124.71
23	C	507	CLA	CHD-C1D-ND	-5.34	119.54	124.45
23	c	507	CLA	CHD-C1D-ND	-5.34	119.54	124.45
28	D	415	SQD	O7-S-C6	5.34	113.29	106.94
28	d	415	SQD	O7-S-C6	5.34	113.29	106.94
23	C	514	CLA	CHD-C1D-ND	-5.33	119.55	124.45
23	c	514	CLA	CHD-C1D-ND	-5.33	119.55	124.45
23	A	406	CLA	CHD-C4C-C3C	-5.33	117.00	124.84
23	a	406	CLA	CHD-C4C-C3C	-5.33	117.00	124.84
24	D	401	PHO	C1C-C2C-C3C	-5.33	104.18	108.61
24	d	401	PHO	C1C-C2C-C3C	-5.33	104.18	108.61
23	C	513	CLA	C2C-C1C-NC	5.33	114.96	109.97
23	c	513	CLA	C2C-C1C-NC	5.33	114.96	109.97
25	A	409	BCR	C37-C22-C21	-5.31	115.49	122.92
25	a	409	BCR	C37-C22-C21	-5.31	115.49	122.92
23	C	503	CLA	CHD-C4C-C3C	-5.29	117.06	124.84
23	c	503	CLA	CHD-C4C-C3C	-5.29	117.06	124.84
23	b	613	CLA	CHD-C4C-C3C	-5.29	117.07	124.84
23	B	604	CLA	C3C-C4C-NC	5.28	116.49	110.57
23	b	604	CLA	C3C-C4C-NC	5.28	116.49	110.57
23	B	613	CLA	C3C-C4C-NC	5.27	116.49	110.57
23	b	613	CLA	C3C-C4C-NC	5.27	116.49	110.57
23	B	613	CLA	CHD-C4C-C3C	-5.27	117.10	124.84
23	B	609	CLA	C2C-C1C-NC	5.26	114.90	109.97
23	B	613	CLA	C2C-C1C-NC	5.26	114.90	109.97
23	b	613	CLA	C2C-C1C-NC	5.26	114.90	109.97
23	C	507	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
23	c	507	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
23	B	606	CLA	C3C-C4C-NC	5.25	116.46	110.57
23	b	606	CLA	C3C-C4C-NC	5.25	116.46	110.57
23	b	609	CLA	C2C-C1C-NC	5.25	114.89	109.97
23	C	509	CLA	C2C-C1C-NC	5.24	114.88	109.97
23	c	509	CLA	C2C-C1C-NC	5.24	114.88	109.97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	616	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
23	b	616	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
23	c	512	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
23	C	512	CLA	C2B-C1B-NB	5.23	113.73	110.23
23	c	512	CLA	C2B-C1B-NB	5.23	113.73	110.23
23	A	408	CLA	CHD-C4C-C3C	-5.22	117.16	124.84
23	a	408	CLA	CHD-C4C-C3C	-5.22	117.16	124.84
23	C	512	CLA	CHD-C4C-C3C	-5.22	117.17	124.84
23	c	506	CLA	CHD-C4C-C3C	-5.22	117.17	124.84
23	c	514	CLA	CMD-C2D-C1D	5.21	133.90	124.71
23	D	405	CLA	C3C-C4C-NC	5.21	116.42	110.57
23	d	405	CLA	C3C-C4C-NC	5.21	116.42	110.57
23	C	506	CLA	CHD-C4C-C3C	-5.21	117.18	124.84
23	C	514	CLA	CMD-C2D-C1D	5.21	133.89	124.71
25	C	516	BCR	C8-C7-C6	-5.21	112.58	127.20
25	c	516	BCR	C8-C7-C6	-5.21	112.58	127.20
23	A	405	CLA	CAC-C3C-C4C	5.20	131.56	124.81
23	a	405	CLA	CAC-C3C-C4C	5.20	131.56	124.81
23	C	511	CLA	CMD-C2D-C1D	5.19	133.87	124.71
23	c	511	CLA	CMD-C2D-C1D	5.19	133.87	124.71
23	c	511	CLA	C3C-C4C-NC	5.19	116.39	110.57
23	B	611	CLA	C3C-C4C-NC	5.18	116.38	110.57
23	b	611	CLA	C3C-C4C-NC	5.18	116.38	110.57
23	B	610	CLA	CAC-C3C-C4C	5.18	131.53	124.81
23	b	610	CLA	CAC-C3C-C4C	5.18	131.53	124.81
23	C	511	CLA	C3C-C4C-NC	5.17	116.37	110.57
23	B	604	CLA	O2D-CGD-CBD	5.17	120.45	111.27
23	b	604	CLA	O2D-CGD-CBD	5.17	120.45	111.27
23	B	605	CLA	O2D-CGD-CBD	5.16	120.43	111.27
23	b	605	CLA	O2D-CGD-CBD	5.16	120.43	111.27
28	C	501	SQD	C1-C2-C3	-5.16	99.26	110.00
28	c	501	SQD	C1-C2-C3	-5.16	99.26	110.00
23	c	506	CLA	C3C-C4C-NC	5.15	116.35	110.57
23	B	608	CLA	CMD-C2D-C1D	5.15	133.79	124.71
23	b	608	CLA	CMD-C2D-C1D	5.15	133.79	124.71
23	C	506	CLA	C2C-C1C-NC	5.15	114.79	109.97
23	C	505	CLA	CHD-C4C-C3C	-5.14	117.28	124.84
23	C	506	CLA	C3C-C4C-NC	5.14	116.34	110.57
23	B	603	CLA	CHD-C4C-C3C	-5.14	117.29	124.84
23	b	603	CLA	CHD-C4C-C3C	-5.14	117.29	124.84
23	B	612	CLA	CAC-C3C-C4C	5.14	131.48	124.81
23	b	612	CLA	CAC-C3C-C4C	5.14	131.48	124.81

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	505	CLA	CHD-C4C-C3C	-5.14	117.29	124.84
23	c	512	CLA	C3C-C4C-NC	5.14	116.33	110.57
23	b	609	CLA	CMD-C2D-C1D	5.14	133.76	124.71
23	C	508	CLA	C2C-C1C-NC	5.13	114.78	109.97
23	c	508	CLA	C2C-C1C-NC	5.13	114.78	109.97
23	B	609	CLA	CMD-C2D-C1D	5.13	133.75	124.71
23	B	606	CLA	C4A-NA-C1A	-5.12	104.40	106.71
23	b	606	CLA	C4A-NA-C1A	-5.12	104.40	106.71
23	c	506	CLA	C2C-C1C-NC	5.12	114.77	109.97
23	C	512	CLA	C3C-C4C-NC	5.12	116.31	110.57
23	C	510	CLA	CMD-C2D-C1D	5.10	133.70	124.71
23	c	510	CLA	CMD-C2D-C1D	5.10	133.70	124.71
23	B	603	CLA	C3D-C4D-ND	5.06	118.42	110.24
23	B	603	CLA	CAC-C3C-C4C	5.06	131.37	124.81
23	b	603	CLA	CAC-C3C-C4C	5.06	131.37	124.81
23	b	603	CLA	C3D-C4D-ND	5.05	118.41	110.24
23	C	507	CLA	O2D-CGD-CBD	5.05	120.25	111.27
23	c	507	CLA	O2D-CGD-CBD	5.05	120.25	111.27
23	D	402	CLA	CHD-C4C-C3C	-5.05	117.41	124.84
23	d	402	CLA	CHD-C4C-C3C	-5.05	117.41	124.84
23	b	615	CLA	CMD-C2D-C1D	5.04	133.59	124.71
23	C	509	CLA	O2D-CGD-CBD	5.04	120.22	111.27
23	c	509	CLA	O2D-CGD-CBD	5.04	120.22	111.27
23	B	605	CLA	C2C-C1C-NC	5.03	114.69	109.97
23	b	605	CLA	C2C-C1C-NC	5.03	114.69	109.97
23	B	615	CLA	CMD-C2D-C1D	5.02	133.57	124.71
23	B	601	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
23	b	601	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
23	B	603	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
23	b	603	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
23	B	610	CLA	O2D-CGD-CBD	5.01	120.18	111.27
23	b	610	CLA	O2D-CGD-CBD	5.01	120.18	111.27
23	c	505	CLA	CHD-C1D-ND	-5.01	119.85	124.45
23	D	406	CLA	O2D-CGD-CBD	5.01	120.16	111.27
23	d	406	CLA	O2D-CGD-CBD	5.01	120.16	111.27
23	B	603	CLA	C2C-C1C-NC	4.98	114.64	109.97
23	b	603	CLA	C2C-C1C-NC	4.98	114.64	109.97
23	C	505	CLA	CHD-C1D-ND	-4.98	119.88	124.45
23	B	606	CLA	C2B-C1B-NB	4.97	113.57	110.23
23	b	606	CLA	C2B-C1B-NB	4.97	113.57	110.23
25	K	102	BCR	C37-C22-C21	-4.97	115.96	122.92
25	k	102	BCR	C37-C22-C21	-4.97	115.96	122.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	O2D-CGD-O1D	-4.97	114.12	123.84
23	B	605	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
23	b	605	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
23	D	406	CLA	C3C-C4C-NC	4.96	116.13	110.57
23	d	406	CLA	C3C-C4C-NC	4.96	116.13	110.57
23	D	405	CLA	CHD-C4C-C3C	-4.96	117.56	124.84
23	d	405	CLA	CHD-C4C-C3C	-4.96	117.56	124.84
23	b	603	CLA	O2D-CGD-O1D	-4.95	114.16	123.84
23	B	612	CLA	C3C-C4C-NC	4.94	116.12	110.57
23	b	612	CLA	C3C-C4C-NC	4.94	116.12	110.57
37	V	201	HEC	C2A-C1A-NA	4.93	115.12	110.32
37	v	201	HEC	C2A-C1A-NA	4.93	115.12	110.32
23	A	408	CLA	C2B-C1B-NB	4.93	113.53	110.23
23	a	408	CLA	C2B-C1B-NB	4.93	113.53	110.23
25	a	409	BCR	C7-C8-C9	-4.92	118.80	126.23
23	D	402	CLA	CHD-C1D-ND	-4.92	119.94	124.45
23	d	402	CLA	CHD-C1D-ND	-4.92	119.94	124.45
23	C	513	CLA	CHD-C1D-ND	-4.91	119.94	124.45
23	c	513	CLA	CHD-C1D-ND	-4.91	119.94	124.45
23	A	406	CLA	C2B-C1B-NB	4.91	113.52	110.23
23	a	406	CLA	C2B-C1B-NB	4.91	113.52	110.23
25	A	409	BCR	C7-C8-C9	-4.91	118.82	126.23
23	b	612	CLA	CMD-C2D-C1D	4.91	133.36	124.71
23	c	502	CLA	CMD-C2D-C1D	4.91	133.36	124.71
23	B	615	CLA	C2C-C1C-NC	4.90	114.57	109.97
23	b	615	CLA	C2C-C1C-NC	4.90	114.57	109.97
25	T	101	BCR	C7-C8-C9	-4.90	118.83	126.23
25	t	103	BCR	C7-C8-C9	-4.90	118.83	126.23
23	A	408	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
23	a	408	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
23	C	502	CLA	CMD-C2D-C1D	4.90	133.35	124.71
23	B	612	CLA	CMD-C2D-C1D	4.90	133.35	124.71
23	B	612	CLA	CHD-C4C-C3C	-4.90	117.64	124.84
23	b	612	CLA	CHD-C4C-C3C	-4.90	117.64	124.84
27	A	411	PL9	C15-C14-C16	4.89	121.58	115.98
27	a	411	PL9	C15-C14-C16	4.89	121.58	115.98
23	B	605	CLA	CMD-C2D-C1D	4.89	133.32	124.71
23	b	605	CLA	CMD-C2D-C1D	4.89	133.32	124.71
23	c	507	CLA	C2B-C1B-NB	4.88	113.50	110.23
23	a	408	CLA	CMD-C2D-C1D	4.88	133.31	124.71
23	A	408	CLA	CMD-C2D-C1D	4.88	133.31	124.71
23	B	616	CLA	O2D-CGD-CBD	4.87	119.91	111.27

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	O2D-CGD-CBD	4.87	119.91	111.27
23	B	610	CLA	C2B-C1B-NB	4.86	113.49	110.23
23	b	610	CLA	C2B-C1B-NB	4.86	113.49	110.23
23	B	608	CLA	CHD-C1D-ND	-4.86	119.99	124.45
23	b	608	CLA	CHD-C1D-ND	-4.86	119.99	124.45
23	B	601	CLA	CHD-C1D-ND	-4.86	119.99	124.45
23	b	601	CLA	CHD-C1D-ND	-4.86	119.99	124.45
23	D	406	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
23	d	406	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
23	B	611	CLA	CMD-C2D-C1D	4.86	133.27	124.71
23	b	611	CLA	CMD-C2D-C1D	4.86	133.27	124.71
23	B	609	CLA	C3D-C2D-C1D	-4.86	99.21	105.83
23	b	609	CLA	C3D-C2D-C1D	-4.86	99.21	105.83
23	B	612	CLA	C2B-C1B-NB	4.85	113.48	110.23
23	b	612	CLA	C2B-C1B-NB	4.85	113.48	110.23
23	B	615	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
23	b	615	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
23	B	610	CLA	C3C-C4C-NC	4.84	116.00	110.57
23	b	610	CLA	C3C-C4C-NC	4.84	116.00	110.57
23	C	507	CLA	C2B-C1B-NB	4.84	113.47	110.23
23	C	504	CLA	CHD-C1D-ND	-4.84	120.01	124.45
23	B	605	CLA	C3C-C4C-NC	4.82	115.98	110.57
23	b	605	CLA	C3C-C4C-NC	4.82	115.98	110.57
23	B	604	CLA	CHD-C4C-C3C	-4.82	117.75	124.84
23	b	604	CLA	CHD-C4C-C3C	-4.82	117.75	124.84
23	C	504	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
23	c	504	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
23	B	605	CLA	C3D-C4D-ND	4.82	118.03	110.24
23	b	605	CLA	C3D-C4D-ND	4.82	118.03	110.24
23	c	504	CLA	CHD-C1D-ND	-4.81	120.03	124.45
23	B	602	CLA	C3C-C4C-NC	4.80	115.95	110.57
23	b	602	CLA	C3C-C4C-NC	4.80	115.95	110.57
23	B	608	CLA	CHD-C4C-C3C	-4.79	117.79	124.84
23	b	608	CLA	CHD-C4C-C3C	-4.79	117.79	124.84
23	B	615	CLA	CAC-C3C-C4C	4.79	131.03	124.81
23	b	615	CLA	CAC-C3C-C4C	4.79	131.03	124.81
23	B	614	CLA	C2B-C1B-NB	4.79	113.44	110.23
23	b	614	CLA	C2B-C1B-NB	4.79	113.44	110.23
23	C	511	CLA	CAC-C3C-C4C	4.79	131.02	124.81
23	c	511	CLA	CAC-C3C-C4C	4.79	131.02	124.81
23	C	508	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
23	c	508	CLA	C3D-C2D-C1D	-4.78	99.31	105.83

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406	CLA	C2C-C1C-NC	4.77	114.44	109.97
23	a	406	CLA	C2C-C1C-NC	4.77	114.44	109.97
23	C	502	CLA	C3C-C4C-NC	4.77	115.92	110.57
23	c	502	CLA	C3C-C4C-NC	4.77	115.92	110.57
23	C	509	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
23	c	509	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
23	B	610	CLA	CHD-C1D-ND	-4.76	120.08	124.45
23	b	610	CLA	CHD-C1D-ND	-4.76	120.08	124.45
23	C	514	CLA	C3B-C2B-C1B	-4.75	101.43	107.16
23	c	514	CLA	C3B-C2B-C1B	-4.75	101.43	107.16
23	B	610	CLA	CHD-C4C-C3C	-4.75	117.86	124.84
23	b	610	CLA	CHD-C4C-C3C	-4.75	117.86	124.84
23	B	613	CLA	C2B-C1B-NB	4.74	113.41	110.23
23	b	613	CLA	C2B-C1B-NB	4.74	113.41	110.23
23	A	406	CLA	C3C-C4C-NC	4.74	115.89	110.57
23	a	406	CLA	C3C-C4C-NC	4.74	115.89	110.57
23	B	616	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
23	b	616	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
23	B	601	CLA	CMD-C2D-C1D	4.74	133.07	124.71
23	b	601	CLA	CMD-C2D-C1D	4.74	133.07	124.71
23	D	405	CLA	C2B-C1B-NB	4.74	113.41	110.23
23	d	405	CLA	C2B-C1B-NB	4.74	113.41	110.23
23	B	605	CLA	C4A-NA-C1A	-4.73	104.58	106.71
23	b	605	CLA	C4A-NA-C1A	-4.73	104.58	106.71
23	C	505	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
23	B	611	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
23	b	611	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
23	C	503	CLA	CAC-C3C-C4C	4.72	130.94	124.81
23	c	503	CLA	CAC-C3C-C4C	4.72	130.94	124.81
23	B	611	CLA	CHD-C1D-ND	-4.72	120.11	124.45
23	b	611	CLA	CHD-C1D-ND	-4.72	120.11	124.45
23	b	603	CLA	C3C-C4C-NC	4.71	115.86	110.57
23	B	616	CLA	CAC-C3C-C4C	4.71	130.93	124.81
23	b	616	CLA	CAC-C3C-C4C	4.71	130.93	124.81
23	A	405	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
23	a	405	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
23	B	613	CLA	C4A-NA-C1A	-4.71	104.59	106.71
23	b	613	CLA	C4A-NA-C1A	-4.71	104.59	106.71
23	B	605	CLA	C4-C3-C5	4.71	123.19	115.27
23	b	605	CLA	C4-C3-C5	4.71	123.19	115.27
23	C	514	CLA	C3C-C4C-NC	4.71	115.85	110.57
23	c	514	CLA	C3C-C4C-NC	4.71	115.85	110.57

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	C3C-C4C-NC	4.71	115.85	110.57
23	c	505	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
23	C	505	CLA	C4A-NA-C1A	-4.70	104.59	106.71
23	c	505	CLA	C4A-NA-C1A	-4.70	104.59	106.71
23	C	508	CLA	CHD-C4C-C3C	-4.69	117.95	124.84
23	c	508	CLA	CHD-C4C-C3C	-4.69	117.95	124.84
23	C	502	CLA	CHD-C1D-ND	-4.68	120.15	124.45
23	c	502	CLA	CHD-C1D-ND	-4.68	120.15	124.45
23	B	604	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
23	b	604	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
23	C	514	CLA	C4A-NA-C1A	-4.67	104.61	106.71
23	c	514	CLA	C4A-NA-C1A	-4.67	104.61	106.71
23	C	505	CLA	C4-C3-C5	4.67	123.13	115.27
23	c	505	CLA	C4-C3-C5	4.67	123.13	115.27
34	F	101	HEM	C1B-NB-C4B	4.67	109.90	105.07
34	f	101	HEM	C1B-NB-C4B	4.67	109.90	105.07
23	C	511	CLA	C3D-C2D-C1D	-4.66	99.48	105.83
23	c	511	CLA	C3D-C2D-C1D	-4.66	99.48	105.83
23	B	616	CLA	C3C-C4C-NC	4.63	115.76	110.57
23	b	616	CLA	C3C-C4C-NC	4.63	115.76	110.57
23	B	614	CLA	CHD-C1D-ND	-4.63	120.20	124.45
23	b	614	CLA	CHD-C1D-ND	-4.63	120.20	124.45
23	B	607	CLA	O2D-CGD-CBD	4.63	119.49	111.27
23	b	607	CLA	O2D-CGD-CBD	4.63	119.49	111.27
23	B	602	CLA	C3B-C2B-C1B	-4.62	101.58	107.16
23	b	602	CLA	C3B-C2B-C1B	-4.62	101.58	107.16
23	B	615	CLA	CHD-C4C-C3C	-4.62	118.05	124.84
23	b	615	CLA	CHD-C4C-C3C	-4.62	118.05	124.84
23	C	507	CLA	O2D-CGD-O1D	-4.62	114.81	123.84
23	c	507	CLA	O2D-CGD-O1D	-4.62	114.81	123.84
23	C	506	CLA	CMD-C2D-C1D	4.62	132.85	124.71
23	c	506	CLA	CMD-C2D-C1D	4.62	132.85	124.71
23	D	402	CLA	CMD-C2D-C1D	4.62	132.85	124.71
23	d	402	CLA	CMD-C2D-C1D	4.62	132.85	124.71
23	C	504	CLA	C3C-C4C-NC	4.60	115.73	110.57
23	c	504	CLA	C3C-C4C-NC	4.60	115.73	110.57
23	C	512	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
23	c	512	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
23	B	605	CLA	CAC-C3C-C4C	4.60	130.77	124.81
23	b	605	CLA	CAC-C3C-C4C	4.60	130.77	124.81
25	B	617	BCR	C8-C7-C6	-4.59	114.30	127.20
25	b	617	BCR	C8-C7-C6	-4.59	114.30	127.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	505	CLA	O2D-CGD-O1D	-4.58	114.88	123.84
23	c	505	CLA	O2D-CGD-O1D	-4.58	114.88	123.84
23	b	609	CLA	C3C-C4C-NC	4.58	115.70	110.57
35	H	101	RRX	C34-C9-C10	-4.57	116.52	122.92
23	B	616	CLA	CMD-C2D-C1D	4.57	132.77	124.71
23	b	616	CLA	CMD-C2D-C1D	4.57	132.77	124.71
23	C	502	CLA	C3D-C4D-ND	4.57	117.63	110.24
23	c	502	CLA	C3D-C4D-ND	4.57	117.63	110.24
23	D	406	CLA	C3D-C4D-ND	4.57	117.63	110.24
23	d	406	CLA	C3D-C4D-ND	4.57	117.63	110.24
23	C	510	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
23	c	510	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
23	B	609	CLA	C3C-C4C-NC	4.56	115.69	110.57
23	A	408	CLA	C1-C2-C3	-4.56	118.17	126.04
23	a	408	CLA	C1-C2-C3	-4.56	118.17	126.04
35	h	101	RRX	C34-C9-C10	-4.55	116.54	122.92
23	B	608	CLA	C3B-C4B-NB	4.55	114.74	110.52
23	b	608	CLA	C3B-C4B-NB	4.55	114.74	110.52
23	C	513	CLA	C3D-C2D-C1D	-4.55	99.63	105.83
23	c	513	CLA	C3D-C2D-C1D	-4.55	99.63	105.83
23	B	604	CLA	CAC-C3C-C4C	4.54	130.70	124.81
23	b	604	CLA	CAC-C3C-C4C	4.54	130.70	124.81
23	B	603	CLA	C2B-C1B-NB	4.53	113.27	110.23
23	b	603	CLA	C2B-C1B-NB	4.53	113.27	110.23
23	C	510	CLA	C1-C2-C3	-4.53	118.21	126.04
23	c	510	CLA	C1-C2-C3	-4.53	118.21	126.04
26	B	620	LMG	O7-C10-C11	4.53	121.26	111.50
26	b	620	LMG	O7-C10-C11	4.53	121.26	111.50
23	C	504	CLA	C2C-C1C-NC	4.52	114.21	109.97
23	c	504	CLA	C2C-C1C-NC	4.52	114.21	109.97
24	A	407	PHO	C1A-C2A-C3A	-4.51	98.54	102.84
24	a	407	PHO	C1A-C2A-C3A	-4.51	98.54	102.84
23	B	608	CLA	C3C-C4C-NC	4.50	115.62	110.57
23	b	608	CLA	C3C-C4C-NC	4.50	115.62	110.57
23	B	614	CLA	O2D-CGD-O1D	-4.50	115.04	123.84
23	b	614	CLA	O2D-CGD-O1D	-4.50	115.04	123.84
28	D	415	SQD	C44-O6-C1	-4.49	104.96	113.74
28	d	415	SQD	C44-O6-C1	-4.49	104.96	113.74
37	V	201	HEC	C3D-C4D-ND	4.48	115.16	110.15
37	v	201	HEC	C3D-C4D-ND	4.48	115.16	110.15
23	A	406	CLA	CMD-C2D-C1D	4.48	132.61	124.71
23	a	406	CLA	CMD-C2D-C1D	4.48	132.61	124.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	616	CLA	C3B-C2B-C1B	-4.48	101.75	107.16
23	b	616	CLA	C3B-C2B-C1B	-4.48	101.75	107.16
23	B	611	CLA	O2D-CGD-CBD	4.46	119.20	111.27
23	b	611	CLA	O2D-CGD-CBD	4.46	119.20	111.27
23	B	609	CLA	C2B-C1B-NB	4.46	113.22	110.23
23	b	609	CLA	C2B-C1B-NB	4.46	113.22	110.23
23	B	611	CLA	C3D-C4D-ND	4.46	117.46	110.24
23	b	611	CLA	C3D-C4D-ND	4.46	117.46	110.24
23	C	502	CLA	O2D-CGD-O1D	-4.46	115.11	123.84
23	c	502	CLA	O2D-CGD-O1D	-4.46	115.11	123.84
23	A	405	CLA	C2B-C1B-NB	4.46	113.22	110.23
23	a	405	CLA	C2B-C1B-NB	4.46	113.22	110.23
23	B	614	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
23	b	614	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
23	C	503	CLA	C4A-NA-C1A	-4.45	104.70	106.71
23	c	503	CLA	C4A-NA-C1A	-4.45	104.70	106.71
23	B	613	CLA	CMD-C2D-C1D	4.44	132.54	124.71
23	b	613	CLA	CMD-C2D-C1D	4.44	132.54	124.71
23	C	511	CLA	C4A-NA-C1A	-4.43	104.71	106.71
23	c	511	CLA	C4A-NA-C1A	-4.43	104.71	106.71
23	C	502	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
23	B	607	CLA	CMD-C2D-C1D	4.43	132.51	124.71
23	b	607	CLA	CMD-C2D-C1D	4.43	132.51	124.71
23	C	513	CLA	O2D-CGD-O1D	-4.42	115.19	123.84
23	c	513	CLA	O2D-CGD-O1D	-4.42	115.19	123.84
23	b	612	CLA	C3D-C4D-ND	4.42	117.39	110.24
23	c	502	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
23	B	606	CLA	CHD-C1D-ND	-4.42	120.39	124.45
23	b	606	CLA	CHD-C1D-ND	-4.42	120.39	124.45
23	C	503	CLA	C3C-C4C-NC	4.42	115.52	110.57
23	c	503	CLA	C3C-C4C-NC	4.42	115.52	110.57
23	C	503	CLA	O2D-CGD-CBD	4.42	119.11	111.27
23	a	405	CLA	CHD-C4C-C3C	-4.41	118.36	124.84
23	B	612	CLA	C3D-C4D-ND	4.41	117.37	110.24
23	A	405	CLA	CHD-C4C-C3C	-4.41	118.36	124.84
23	B	606	CLA	C3D-C2D-C1D	-4.41	99.82	105.83
23	b	606	CLA	C3D-C2D-C1D	-4.41	99.82	105.83
23	C	509	CLA	CMD-C2D-C1D	4.40	132.47	124.71
23	c	509	CLA	CMD-C2D-C1D	4.40	132.47	124.71
23	C	510	CLA	CHD-C1D-ND	-4.40	120.41	124.45
23	c	510	CLA	CHD-C1D-ND	-4.40	120.41	124.45
23	C	513	CLA	C3C-C4C-NC	4.40	115.50	110.57

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	513	CLA	C3C-C4C-NC	4.40	115.50	110.57
23	C	513	CLA	C3D-C4D-ND	4.40	117.35	110.24
23	c	513	CLA	C3D-C4D-ND	4.40	117.35	110.24
23	c	503	CLA	O2D-CGD-CBD	4.40	119.08	111.27
23	B	602	CLA	C3D-C4D-ND	4.38	117.33	110.24
23	b	602	CLA	C3D-C4D-ND	4.38	117.33	110.24
23	B	608	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
23	b	608	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
24	D	401	PHO	C4A-C3A-C2A	-4.36	98.69	102.84
24	d	401	PHO	C4A-C3A-C2A	-4.36	98.69	102.84
23	B	602	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
23	b	602	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
23	B	607	CLA	C3C-C4C-NC	4.35	115.45	110.57
23	b	607	CLA	C3C-C4C-NC	4.35	115.45	110.57
23	C	506	CLA	CHD-C1D-ND	-4.35	120.45	124.45
23	c	506	CLA	CHD-C1D-ND	-4.35	120.45	124.45
23	c	512	CLA	CAC-C3C-C4C	4.35	130.46	124.81
23	B	607	CLA	C1D-CHD-C4C	-4.35	116.68	126.06
23	b	607	CLA	C1D-CHD-C4C	-4.35	116.68	126.06
23	C	507	CLA	C3C-C4C-NC	4.35	115.44	110.57
23	C	505	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
23	c	505	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
23	C	512	CLA	CAC-C3C-C4C	4.34	130.44	124.81
23	B	608	CLA	C3D-C4D-ND	4.33	117.24	110.24
23	b	608	CLA	C3D-C4D-ND	4.33	117.24	110.24
23	c	507	CLA	C3C-C4C-NC	4.32	115.42	110.57
23	b	613	CLA	CAC-C3C-C4C	4.32	130.42	124.81
23	A	408	CLA	C1C-C2C-C3C	-4.32	102.41	106.96
23	a	408	CLA	C1C-C2C-C3C	-4.32	102.41	106.96
23	B	601	CLA	C3B-C2B-C1B	-4.31	101.96	107.16
23	b	601	CLA	C3B-C2B-C1B	-4.31	101.96	107.16
23	D	402	CLA	C3C-C4C-NC	4.31	115.40	110.57
23	d	402	CLA	C3C-C4C-NC	4.31	115.40	110.57
34	F	101	HEM	C4C-NC-C1C	4.31	109.56	105.35
34	f	101	HEM	C4C-NC-C1C	4.31	109.56	105.35
23	B	613	CLA	CAC-C3C-C4C	4.30	130.39	124.81
23	C	505	CLA	C3C-C4C-NC	4.30	115.40	110.57
23	C	510	CLA	C3C-C4C-NC	4.30	115.40	110.57
23	c	505	CLA	C3C-C4C-NC	4.30	115.40	110.57
23	c	510	CLA	C3C-C4C-NC	4.30	115.40	110.57
35	H	101	RRX	C34-C9-C8	4.30	124.85	118.08
35	h	101	RRX	C34-C9-C8	4.30	124.85	118.08

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	C3C-C4C-NC	4.30	115.39	110.57
23	A	406	CLA	C3D-C4D-ND	4.30	117.19	110.24
23	a	406	CLA	C3D-C4D-ND	4.30	117.19	110.24
23	b	614	CLA	C3C-C4C-NC	4.30	115.39	110.57
23	C	503	CLA	CMC-C2C-C1C	4.30	131.58	125.04
23	c	503	CLA	CMC-C2C-C1C	4.30	131.58	125.04
23	B	606	CLA	C3D-C4D-ND	4.29	117.18	110.24
23	b	606	CLA	C3D-C4D-ND	4.29	117.18	110.24
23	c	503	CLA	CHD-C1D-ND	-4.29	120.51	124.45
23	C	503	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
23	c	503	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
23	B	601	CLA	C3C-C4C-NC	4.29	115.38	110.57
23	b	601	CLA	C3C-C4C-NC	4.29	115.38	110.57
23	C	507	CLA	C3D-C4D-ND	4.29	117.17	110.24
23	c	507	CLA	C3D-C4D-ND	4.29	117.17	110.24
23	A	408	CLA	C3D-C4D-ND	4.28	117.17	110.24
23	a	408	CLA	C3D-C4D-ND	4.28	117.17	110.24
23	B	616	CLA	CHD-C1D-ND	-4.28	120.52	124.45
23	b	616	CLA	CHD-C1D-ND	-4.28	120.52	124.45
23	C	505	CLA	C3D-C4D-ND	4.28	117.16	110.24
23	c	505	CLA	C3D-C4D-ND	4.28	117.16	110.24
23	c	506	CLA	CAC-C3C-C4C	4.28	130.36	124.81
23	C	503	CLA	CHD-C1D-ND	-4.27	120.53	124.45
23	C	506	CLA	CAC-C3C-C4C	4.27	130.35	124.81
23	B	609	CLA	CHD-C1D-ND	-4.26	120.54	124.45
23	C	509	CLA	C4C-C3C-C2C	-4.26	100.69	106.90
23	c	509	CLA	C4C-C3C-C2C	-4.26	100.69	106.90
23	A	408	CLA	C3C-C4C-NC	4.25	115.34	110.57
23	a	408	CLA	C3C-C4C-NC	4.25	115.34	110.57
23	b	609	CLA	CHD-C1D-ND	-4.24	120.55	124.45
23	B	612	CLA	C2C-C1C-NC	4.24	113.94	109.97
23	b	612	CLA	C2C-C1C-NC	4.24	113.94	109.97
23	C	511	CLA	C3B-C2B-C1B	-4.23	102.06	107.16
23	c	511	CLA	C3B-C2B-C1B	-4.23	102.06	107.16
23	B	610	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
23	b	610	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
23	A	408	CLA	C3B-C2B-C1B	-4.23	102.06	107.16
23	a	408	CLA	C3B-C2B-C1B	-4.23	102.06	107.16
23	C	511	CLA	CHD-C1D-ND	-4.22	120.58	124.45
23	C	503	CLA	C1-C2-C3	-4.21	118.76	126.04
23	c	503	CLA	C1-C2-C3	-4.21	118.76	126.04
23	D	405	CLA	CMD-C2D-C1D	4.20	132.12	124.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	405	CLA	CMD-C2D-C1D	4.20	132.12	124.71
34	F	101	HEM	CBD-CAD-C3D	-4.20	100.96	112.63
23	A	408	CLA	CAC-C3C-C4C	4.20	130.25	124.81
23	a	408	CLA	CAC-C3C-C4C	4.19	130.25	124.81
34	f	101	HEM	CBD-CAD-C3D	-4.19	100.98	112.63
23	c	511	CLA	CHD-C1D-ND	-4.19	120.60	124.45
23	C	506	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
23	c	506	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
25	C	516	BCR	C7-C8-C9	-4.19	119.91	126.23
25	c	516	BCR	C7-C8-C9	-4.19	119.91	126.23
23	B	606	CLA	CMD-C2D-C1D	4.18	132.09	124.71
23	B	615	CLA	C3B-C2B-C1B	-4.18	102.12	107.16
23	b	615	CLA	C3B-C2B-C1B	-4.18	102.12	107.16
23	D	405	CLA	C3B-C2B-C1B	-4.18	102.12	107.16
23	d	405	CLA	C3B-C2B-C1B	-4.18	102.12	107.16
23	b	606	CLA	CMD-C2D-C1D	4.17	132.07	124.71
34	F	101	HEM	CHD-C4C-NC	4.17	128.95	124.44
34	f	101	HEM	CHD-C4C-NC	4.17	128.95	124.44
23	C	503	CLA	C3D-C4D-ND	4.16	116.97	110.24
23	c	503	CLA	C3D-C4D-ND	4.15	116.96	110.24
23	C	510	CLA	O2D-CGD-CBD	4.15	118.63	111.27
23	c	510	CLA	O2D-CGD-CBD	4.15	118.63	111.27
23	D	405	CLA	CHD-C1D-ND	-4.14	120.64	124.45
23	d	405	CLA	CHD-C1D-ND	-4.14	120.64	124.45
23	D	405	CLA	O2D-CGD-CBD	4.14	118.62	111.27
23	d	405	CLA	O2D-CGD-CBD	4.14	118.62	111.27
23	A	405	CLA	C3C-C4C-NC	4.13	115.20	110.57
23	a	405	CLA	C3C-C4C-NC	4.13	115.20	110.57
23	B	615	CLA	C3D-C4D-ND	4.13	116.92	110.24
23	b	615	CLA	C3D-C4D-ND	4.13	116.92	110.24
23	A	405	CLA	C2C-C1C-NC	4.13	113.84	109.97
23	a	405	CLA	C2C-C1C-NC	4.13	113.84	109.97
23	c	506	CLA	C2B-C1B-NB	4.12	113.00	110.23
23	C	505	CLA	C1C-C2C-C3C	-4.12	102.62	106.96
23	c	505	CLA	C1C-C2C-C3C	-4.12	102.62	106.96
23	C	513	CLA	CMD-C2D-C1D	4.12	131.98	124.71
23	c	513	CLA	CMD-C2D-C1D	4.12	131.98	124.71
23	C	514	CLA	C3D-C4D-ND	4.11	116.89	110.24
23	c	514	CLA	C3D-C4D-ND	4.11	116.89	110.24
23	B	616	CLA	C3D-C4D-ND	4.11	116.88	110.24
23	b	616	CLA	C3D-C4D-ND	4.11	116.88	110.24
23	C	506	CLA	C2B-C1B-NB	4.11	112.98	110.23

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	408	CLA	O2D-CGD-O1D	-4.11	115.81	123.84
23	a	408	CLA	O2D-CGD-O1D	-4.11	115.81	123.84
23	D	402	CLA	C2B-C1B-NB	4.11	112.98	110.23
23	d	402	CLA	C2B-C1B-NB	4.11	112.98	110.23
23	B	608	CLA	O2D-CGD-CBD	4.09	118.54	111.27
23	b	608	CLA	O2D-CGD-CBD	4.09	118.54	111.27
23	D	406	CLA	C2C-C1C-NC	4.08	113.80	109.97
23	d	406	CLA	C2C-C1C-NC	4.08	113.80	109.97
23	B	609	CLA	C3D-C4D-ND	4.08	116.84	110.24
23	b	609	CLA	C3D-C4D-ND	4.08	116.84	110.24
23	C	512	CLA	CMD-C2D-C1D	4.07	131.89	124.71
23	c	512	CLA	CMD-C2D-C1D	4.07	131.89	124.71
23	A	406	CLA	CAC-C3C-C4C	4.07	130.09	124.81
23	a	406	CLA	CAC-C3C-C4C	4.07	130.09	124.81
23	B	607	CLA	C3D-C2D-C1D	-4.07	100.28	105.83
23	b	607	CLA	C3D-C2D-C1D	-4.07	100.28	105.83
23	B	616	CLA	C1C-C2C-C3C	-4.07	102.68	106.96
23	b	616	CLA	C1C-C2C-C3C	-4.07	102.68	106.96
35	H	101	RRX	C35-C13-C14	-4.06	117.23	122.92
35	h	101	RRX	C35-C13-C14	-4.06	117.23	122.92
23	C	508	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
23	c	508	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
23	C	506	CLA	C4A-NA-C1A	-4.06	104.88	106.71
23	c	506	CLA	C4A-NA-C1A	-4.06	104.88	106.71
23	C	508	CLA	C3D-C4D-ND	4.06	116.80	110.24
23	c	508	CLA	C3D-C4D-ND	4.06	116.80	110.24
23	c	507	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
23	D	402	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
23	d	402	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
23	B	604	CLA	C3B-C2B-C1B	-4.05	102.27	107.16
23	b	604	CLA	C3B-C2B-C1B	-4.05	102.27	107.16
23	B	615	CLA	CHD-C1D-ND	-4.05	120.73	124.45
23	b	615	CLA	CHD-C1D-ND	-4.05	120.73	124.45
23	B	601	CLA	C3D-C4D-ND	4.04	116.78	110.24
23	b	601	CLA	C3D-C4D-ND	4.04	116.78	110.24
23	b	612	CLA	C3D-C2D-C1D	-4.04	100.32	105.83
23	C	512	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
23	A	406	CLA	C3D-C2D-C1D	-4.04	100.32	105.83
23	a	406	CLA	C3D-C2D-C1D	-4.04	100.32	105.83
23	C	510	CLA	C3B-C2B-C1B	-4.04	102.29	107.16
23	c	510	CLA	C3B-C2B-C1B	-4.04	102.29	107.16
23	C	507	CLA	C1C-C2C-C3C	-4.04	102.71	106.96

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	C3D-C2D-C1D	-4.03	100.33	105.83
23	B	605	CLA	CMC-C2C-C1C	4.03	131.18	125.04
23	b	605	CLA	CMC-C2C-C1C	4.03	131.18	125.04
23	c	512	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
23	B	608	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
23	B	610	CLA	C4C-C3C-C2C	-4.01	101.05	106.90
23	b	610	CLA	C4C-C3C-C2C	-4.01	101.05	106.90
23	B	605	CLA	O2D-CGD-O1D	-4.00	116.02	123.84
23	b	605	CLA	O2D-CGD-O1D	-4.00	116.02	123.84
23	b	608	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
23	C	511	CLA	C3D-C4D-ND	3.98	116.68	110.24
23	c	511	CLA	C3D-C4D-ND	3.98	116.68	110.24
26	C	520	LMG	O8-C28-C29	3.98	124.38	111.91
26	c	520	LMG	O8-C28-C29	3.98	124.38	111.91
23	B	610	CLA	C3D-C4D-ND	3.97	116.67	110.24
23	b	610	CLA	C3D-C4D-ND	3.97	116.67	110.24
23	d	402	CLA	O2D-CGD-CBD	3.97	118.33	111.27
23	D	402	CLA	C3D-C2D-C1D	-3.97	100.41	105.83
23	d	402	CLA	C3D-C2D-C1D	-3.97	100.41	105.83
23	B	602	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
23	b	602	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
23	B	601	CLA	C4A-NA-C1A	-3.97	104.92	106.71
23	b	601	CLA	C4A-NA-C1A	-3.97	104.92	106.71
23	C	509	CLA	C3D-C4D-ND	3.97	116.66	110.24
23	c	509	CLA	C3D-C4D-ND	3.97	116.66	110.24
23	D	405	CLA	C3D-C2D-C1D	-3.97	100.42	105.83
23	d	405	CLA	C3D-C2D-C1D	-3.97	100.42	105.83
23	B	607	CLA	CAC-C3C-C4C	3.96	129.95	124.81
23	b	607	CLA	CAC-C3C-C4C	3.96	129.95	124.81
23	B	609	CLA	CBC-CAC-C3C	-3.96	101.50	112.43
23	b	609	CLA	CBC-CAC-C3C	-3.96	101.50	112.43
23	B	603	CLA	C5-C3-C2	-3.95	113.12	121.12
23	b	603	CLA	C5-C3-C2	-3.95	113.12	121.12
23	D	402	CLA	O2D-CGD-CBD	3.95	118.29	111.27
23	C	514	CLA	O2D-CGD-O1D	-3.94	116.13	123.84
23	c	514	CLA	O2D-CGD-O1D	-3.94	116.13	123.84
23	b	613	CLA	C3D-C4D-ND	3.94	116.61	110.24
23	B	613	CLA	C3D-C4D-ND	3.93	116.60	110.24
23	B	613	CLA	C3D-C2D-C1D	-3.93	100.46	105.83
23	b	613	CLA	C3D-C2D-C1D	-3.93	100.46	105.83
25	D	407	BCR	C29-C30-C25	3.93	116.53	110.48
25	d	407	BCR	C29-C30-C25	3.93	116.53	110.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	503	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
23	c	503	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
25	C	515	BCR	C37-C22-C21	-3.93	117.42	122.92
25	c	515	BCR	C37-C22-C21	-3.93	117.42	122.92
23	D	406	CLA	CAC-C3C-C4C	3.93	129.90	124.81
23	d	406	CLA	CAC-C3C-C4C	3.93	129.90	124.81
23	B	612	CLA	O2D-CGD-CBD	3.92	118.24	111.27
23	b	612	CLA	O2D-CGD-CBD	3.92	118.24	111.27
23	C	508	CLA	CMC-C2C-C1C	3.92	131.00	125.04
23	C	503	CLA	CMD-C2D-C1D	3.91	131.61	124.71
23	c	503	CLA	CMD-C2D-C1D	3.91	131.61	124.71
23	C	508	CLA	C4-C3-C5	3.91	121.84	115.27
23	c	508	CLA	C4-C3-C5	3.91	121.84	115.27
23	B	614	CLA	C3B-C2B-C1B	-3.90	102.45	107.16
23	b	614	CLA	C3B-C2B-C1B	-3.90	102.45	107.16
34	F	101	HEM	CAD-CBD-CGD	3.90	122.00	113.60
34	f	101	HEM	CAD-CBD-CGD	3.90	121.99	113.60
23	B	602	CLA	C3B-C4B-NB	3.90	114.13	110.52
23	b	602	CLA	C3B-C4B-NB	3.90	114.13	110.52
23	c	508	CLA	CMC-C2C-C1C	3.90	130.97	125.04
23	B	613	CLA	C3B-C2B-C1B	-3.89	102.47	107.16
23	b	613	CLA	C3B-C2B-C1B	-3.89	102.47	107.16
25	D	407	BCR	C24-C23-C22	-3.89	120.36	126.23
25	d	407	BCR	C24-C23-C22	-3.89	120.36	126.23
23	c	507	CLA	C3B-C4B-NB	3.88	114.12	110.52
23	B	605	CLA	C2B-C1B-NB	3.88	112.84	110.23
23	b	605	CLA	C2B-C1B-NB	3.88	112.84	110.23
28	C	501	SQD	O9-S-C6	3.88	111.55	106.94
28	c	501	SQD	O9-S-C6	3.88	111.55	106.94
23	B	608	CLA	CMC-C2C-C1C	3.88	130.95	125.04
23	B	609	CLA	CMC-C2C-C1C	3.88	130.95	125.04
23	b	609	CLA	CMC-C2C-C1C	3.87	130.93	125.04
23	C	507	CLA	C3B-C4B-NB	3.87	114.11	110.52
23	b	604	CLA	C3B-C4B-NB	3.87	114.10	110.52
23	b	604	CLA	C4C-C3C-C2C	-3.87	101.26	106.90
23	b	608	CLA	CMC-C2C-C1C	3.87	130.93	125.04
23	C	508	CLA	C3B-C2B-C1B	-3.86	102.50	107.16
23	c	508	CLA	C3B-C2B-C1B	-3.86	102.50	107.16
25	B	617	BCR	C37-C22-C21	-3.85	117.52	122.92
25	b	617	BCR	C37-C22-C21	-3.85	117.52	122.92
23	C	513	CLA	C1-O2A-CGA	3.85	126.56	116.44
23	c	513	CLA	C1-O2A-CGA	3.85	126.56	116.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	604	CLA	C4C-C3C-C2C	-3.85	101.28	106.90
23	C	510	CLA	C3D-C4D-ND	3.85	116.47	110.24
23	c	510	CLA	C3D-C4D-ND	3.85	116.47	110.24
23	D	402	CLA	C3D-C4D-ND	3.85	116.46	110.24
23	d	402	CLA	C3D-C4D-ND	3.85	116.46	110.24
23	c	511	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
28	A	412	SQD	C1-O5-C5	-3.84	106.14	113.69
28	a	412	SQD	C1-O5-C5	-3.84	106.14	113.69
23	C	506	CLA	C3D-C4D-ND	3.84	116.45	110.24
23	c	506	CLA	C3D-C4D-ND	3.84	116.45	110.24
23	c	506	CLA	O2D-CGD-CBD	3.84	118.09	111.27
23	A	408	CLA	CHD-C1D-ND	-3.84	120.93	124.45
23	a	408	CLA	CHD-C1D-ND	-3.84	120.93	124.45
23	B	604	CLA	C3B-C4B-NB	3.83	114.07	110.52
23	b	609	CLA	CAC-C3C-C4C	3.83	129.78	124.81
23	c	506	CLA	C4C-C3C-C2C	-3.83	101.32	106.90
23	C	510	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
23	c	510	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
23	B	615	CLA	CMC-C2C-C1C	3.82	130.86	125.04
23	b	615	CLA	CMC-C2C-C1C	3.82	130.86	125.04
25	C	515	BCR	C7-C6-C5	-3.82	116.44	122.75
25	c	515	BCR	C7-C6-C5	-3.82	116.44	122.75
23	C	506	CLA	C4C-C3C-C2C	-3.82	101.33	106.90
23	C	506	CLA	O2D-CGD-CBD	3.82	118.05	111.27
23	B	609	CLA	CAC-C3C-C4C	3.82	129.76	124.81
23	B	614	CLA	C3D-C4D-ND	3.82	116.41	110.24
23	C	511	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
23	B	605	CLA	C1C-C2C-C3C	-3.81	102.96	106.96
23	b	605	CLA	C1C-C2C-C3C	-3.81	102.96	106.96
23	C	514	CLA	CMC-C2C-C1C	3.80	130.83	125.04
23	c	514	CLA	CMC-C2C-C1C	3.80	130.83	125.04
23	C	514	CLA	C2C-C1C-NC	3.80	113.53	109.97
23	c	514	CLA	C2C-C1C-NC	3.80	113.53	109.97
23	C	507	CLA	C3D-C2D-C1D	-3.79	100.66	105.83
23	c	507	CLA	C3D-C2D-C1D	-3.79	100.66	105.83
23	b	614	CLA	C3D-C4D-ND	3.79	116.36	110.24
23	D	406	CLA	C3B-C2B-C1B	-3.78	102.59	107.16
23	d	406	CLA	C3B-C2B-C1B	-3.78	102.59	107.16
23	B	602	CLA	O2D-CGD-O1D	-3.78	116.44	123.84
23	b	602	CLA	O2D-CGD-O1D	-3.78	116.44	123.84
23	C	513	CLA	C3B-C2B-C1B	-3.78	102.60	107.16
23	c	513	CLA	C3B-C2B-C1B	-3.78	102.60	107.16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	CMC-C2C-C1C	3.78	130.80	125.04
25	C	516	BCR	C24-C23-C22	-3.78	120.52	126.23
25	c	516	BCR	C24-C23-C22	-3.78	120.52	126.23
23	C	514	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
23	c	514	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
23	C	512	CLA	C3D-C4D-ND	3.77	116.34	110.24
23	c	512	CLA	C3D-C4D-ND	3.77	116.34	110.24
23	B	606	CLA	CMB-C2B-C1B	3.77	131.11	125.37
23	b	606	CLA	CMB-C2B-C1B	3.77	131.11	125.37
23	B	609	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
28	D	415	SQD	C1-C2-C3	-3.76	102.16	110.00
28	d	415	SQD	C1-C2-C3	-3.76	102.16	110.00
23	B	603	CLA	C3B-C2B-C1B	-3.76	102.62	107.16
23	b	603	CLA	C3B-C2B-C1B	-3.76	102.62	107.16
23	c	511	CLA	CMC-C2C-C1C	3.76	130.76	125.04
23	b	609	CLA	C1C-C2C-C3C	-3.76	103.01	106.96
23	B	615	CLA	C3C-C4C-NC	3.75	114.78	110.57
23	b	615	CLA	C3C-C4C-NC	3.75	114.78	110.57
23	C	512	CLA	O2D-CGD-O1D	-3.75	116.50	123.84
23	c	512	CLA	O2D-CGD-O1D	-3.75	116.50	123.84
23	C	509	CLA	C3B-C2B-C1B	-3.75	102.64	107.16
23	c	509	CLA	C3B-C2B-C1B	-3.75	102.64	107.16
23	A	405	CLA	C4A-NA-C1A	-3.74	105.02	106.71
23	a	405	CLA	C4A-NA-C1A	-3.74	105.02	106.71
23	b	614	CLA	CMC-C2C-C1C	3.74	130.73	125.04
23	C	511	CLA	CMC-C2C-C1C	3.74	130.73	125.04
23	B	608	CLA	C3B-C2B-C1B	-3.72	102.67	107.16
23	b	608	CLA	C3B-C2B-C1B	-3.72	102.67	107.16
23	C	510	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
23	c	510	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
23	B	609	CLA	O2D-CGD-CBD	3.71	117.85	111.27
23	b	609	CLA	O2D-CGD-CBD	3.71	117.85	111.27
31	H	102	DGD	O2G-C1B-C2B	3.70	119.47	111.50
31	h	102	DGD	O2G-C1B-C2B	3.70	119.47	111.50
23	D	405	CLA	CAC-C3C-C4C	3.69	129.60	124.81
23	d	405	CLA	CAC-C3C-C4C	3.69	129.60	124.81
34	f	101	HEM	CBA-CAA-C2A	-3.69	102.39	112.63
34	F	101	HEM	CBA-CAA-C2A	-3.68	102.39	112.63
23	C	512	CLA	C3B-C2B-C1B	-3.68	102.72	107.16
23	c	512	CLA	C3B-C2B-C1B	-3.68	102.72	107.16
23	C	509	CLA	CHD-C1D-ND	-3.68	121.08	124.45
23	c	509	CLA	CHD-C1D-ND	-3.68	121.08	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	618	BCR	C7-C8-C9	-3.68	120.68	126.23
23	D	406	CLA	CMC-C2C-C1C	3.67	130.63	125.04
23	d	406	CLA	CMC-C2C-C1C	3.67	130.63	125.04
25	b	618	BCR	C7-C8-C9	-3.66	120.71	126.23
23	D	405	CLA	C3D-C4D-ND	3.66	116.15	110.24
23	d	405	CLA	C3D-C4D-ND	3.66	116.15	110.24
25	B	618	BCR	C24-C23-C22	-3.66	120.71	126.23
25	b	618	BCR	C24-C23-C22	-3.66	120.71	126.23
23	C	507	CLA	CAC-C3C-C4C	3.65	129.55	124.81
23	c	507	CLA	CAC-C3C-C4C	3.65	129.55	124.81
25	A	409	BCR	C8-C7-C6	-3.65	116.96	127.20
25	a	409	BCR	C8-C7-C6	-3.65	116.96	127.20
23	B	611	CLA	CAC-C3C-C4C	3.65	129.54	124.81
23	b	611	CLA	CAC-C3C-C4C	3.65	129.54	124.81
27	a	411	PL9	C12-C13-C14	-3.62	118.93	127.66
28	D	415	SQD	C1-O5-C5	-3.62	106.58	113.69
28	d	415	SQD	C1-O5-C5	-3.62	106.58	113.69
23	b	603	CLA	C4C-C3C-C2C	-3.62	101.62	106.90
23	B	603	CLA	C4C-C3C-C2C	-3.62	101.62	106.90
23	b	609	CLA	C1D-CHD-C4C	-3.61	118.27	126.06
27	A	411	PL9	C12-C13-C14	-3.61	118.97	127.66
23	B	606	CLA	C1D-CHD-C4C	-3.61	118.28	126.06
23	b	606	CLA	C1D-CHD-C4C	-3.61	118.28	126.06
23	B	609	CLA	C1D-CHD-C4C	-3.61	118.28	126.06
23	C	504	CLA	C1C-C2C-C3C	-3.61	103.17	106.96
23	c	504	CLA	C1C-C2C-C3C	-3.61	103.17	106.96
25	D	407	BCR	C7-C8-C9	-3.60	120.79	126.23
25	d	407	BCR	C7-C8-C9	-3.60	120.79	126.23
23	C	504	CLA	CMB-C2B-C1B	3.60	130.85	125.37
23	c	504	CLA	CMB-C2B-C1B	3.60	130.85	125.37
23	C	510	CLA	CAC-C3C-C4C	3.60	129.48	124.81
23	c	510	CLA	CAC-C3C-C4C	3.60	129.48	124.81
23	C	510	CLA	CHC-C1C-C2C	-3.60	116.74	126.73
23	D	405	CLA	C1-C2-C3	-3.59	119.83	126.04
23	d	405	CLA	C1-C2-C3	-3.59	119.83	126.04
23	c	510	CLA	CHC-C1C-C2C	-3.59	116.75	126.73
23	C	508	CLA	C4A-NA-C1A	-3.59	105.09	106.71
23	c	508	CLA	C4A-NA-C1A	-3.59	105.09	106.71
27	A	411	PL9	C37-C38-C39	-3.59	119.02	127.66
27	a	411	PL9	C37-C38-C39	-3.59	119.02	127.66
23	c	505	CLA	CAC-C3C-C4C	3.59	129.46	124.81
23	C	513	CLA	C1C-C2C-C3C	-3.58	103.19	106.96

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	513	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
23	B	611	CLA	C2C-C1C-NC	3.58	113.32	109.97
23	b	611	CLA	C2C-C1C-NC	3.58	113.32	109.97
23	C	505	CLA	CAC-C3C-C4C	3.57	129.44	124.81
23	B	605	CLA	C4C-C3C-C2C	-3.56	101.72	106.90
23	b	605	CLA	C4C-C3C-C2C	-3.56	101.72	106.90
23	b	604	CLA	C4A-NA-C1A	-3.55	105.11	106.71
27	D	408	PL9	C42-C43-C44	-3.55	119.10	127.66
27	d	408	PL9	C42-C43-C44	-3.55	119.10	127.66
24	A	407	PHO	C4D-CHA-CBD	3.55	110.12	108.52
23	D	406	CLA	C4C-C3C-C2C	-3.54	101.74	106.90
23	d	406	CLA	C4C-C3C-C2C	-3.54	101.74	106.90
23	B	612	CLA	C4C-C3C-C2C	-3.54	101.74	106.90
23	b	612	CLA	C4C-C3C-C2C	-3.54	101.74	106.90
23	C	509	CLA	O2D-CGD-O1D	-3.54	116.92	123.84
23	c	509	CLA	O2D-CGD-O1D	-3.54	116.92	123.84
23	C	512	CLA	CHD-C1D-ND	-3.54	121.20	124.45
23	c	512	CLA	CHD-C1D-ND	-3.54	121.20	124.45
23	C	511	CLA	C4-C3-C5	3.53	121.21	115.27
23	c	511	CLA	C4-C3-C5	3.53	121.21	115.27
23	B	608	CLA	CAC-C3C-C4C	3.53	129.39	124.81
23	b	608	CLA	CAC-C3C-C4C	3.53	129.39	124.81
28	D	415	SQD	O5-C1-C2	-3.52	102.89	110.35
28	d	415	SQD	O5-C1-C2	-3.52	102.89	110.35
23	B	601	CLA	CAC-C3C-C4C	3.52	129.38	124.81
23	b	601	CLA	CAC-C3C-C4C	3.52	129.38	124.81
23	b	602	CLA	C4A-NA-C1A	-3.51	105.13	106.71
23	B	616	CLA	C3B-C4B-NB	3.51	113.77	110.52
23	b	616	CLA	C3B-C4B-NB	3.51	113.77	110.52
23	B	607	CLA	C2B-C1B-NB	3.51	112.59	110.23
23	B	608	CLA	C1-C2-C3	-3.51	119.97	126.04
23	b	608	CLA	C1-C2-C3	-3.51	119.97	126.04
25	Y	101	BCR	C37-C22-C23	3.51	123.60	118.08
25	y	101	BCR	C37-C22-C23	3.51	123.60	118.08
23	C	509	CLA	C4A-NA-C1A	-3.51	105.13	106.71
23	c	509	CLA	C4A-NA-C1A	-3.51	105.13	106.71
23	B	613	CLA	CHD-C1D-ND	-3.51	121.23	124.45
23	A	408	CLA	C1D-CHD-C4C	-3.51	118.50	126.06
23	a	408	CLA	C1D-CHD-C4C	-3.51	118.50	126.06
26	B	620	LMG	O7-C10-O9	-3.51	115.23	123.70
26	b	620	LMG	O7-C10-O9	-3.51	115.23	123.70
23	c	502	CLA	CBC-CAC-C3C	-3.50	102.77	112.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	509	CLA	O2A-CGA-O1A	-3.50	114.76	123.59
23	c	509	CLA	O2A-CGA-O1A	-3.50	114.76	123.59
23	b	607	CLA	C2B-C1B-NB	3.50	112.58	110.23
23	B	607	CLA	C1C-C2C-C3C	-3.49	103.28	106.96
23	b	607	CLA	C1C-C2C-C3C	-3.49	103.28	106.96
23	B	602	CLA	C4A-NA-C1A	-3.49	105.14	106.71
23	C	502	CLA	CBC-CAC-C3C	-3.49	102.81	112.43
23	B	608	CLA	C4A-NA-C1A	-3.49	105.14	106.71
23	b	608	CLA	C4A-NA-C1A	-3.49	105.14	106.71
23	b	607	CLA	CHC-C1C-C2C	-3.49	117.05	126.73
37	v	201	HEC	C2D-C1D-ND	3.48	115.38	110.08
25	A	409	BCR	C37-C22-C23	3.48	123.56	118.08
25	a	409	BCR	C37-C22-C23	3.48	123.56	118.08
37	v	201	HEC	C1D-C2D-C3D	-3.48	102.76	106.83
23	B	604	CLA	C4A-NA-C1A	-3.48	105.14	106.71
23	D	402	CLA	CAC-C3C-C4C	3.48	129.32	124.81
23	d	402	CLA	CAC-C3C-C4C	3.48	129.32	124.81
24	a	407	PHO	C4D-CHA-CBD	3.48	110.09	108.52
25	D	407	BCR	C28-C27-C26	-3.47	107.88	114.08
25	d	407	BCR	C28-C27-C26	-3.47	107.88	114.08
23	B	607	CLA	CHC-C1C-C2C	-3.47	117.09	126.73
23	C	502	CLA	C4C-C3C-C2C	-3.47	101.84	106.90
23	c	502	CLA	C4C-C3C-C2C	-3.47	101.84	106.90
23	C	507	CLA	CMC-C2C-C1C	3.46	130.31	125.04
23	c	507	CLA	CMC-C2C-C1C	3.46	130.31	125.04
37	V	201	HEC	C2D-C1D-ND	3.46	115.35	110.08
23	C	504	CLA	C3B-C2B-C1B	-3.46	102.98	107.16
23	c	504	CLA	C3B-C2B-C1B	-3.46	102.98	107.16
23	B	607	CLA	C3B-C2B-C1B	-3.46	102.99	107.16
23	B	604	CLA	O2D-CGD-O1D	-3.46	117.08	123.84
23	b	604	CLA	O2D-CGD-O1D	-3.46	117.08	123.84
23	B	611	CLA	CMC-C2C-C1C	3.46	130.30	125.04
23	b	611	CLA	CMC-C2C-C1C	3.46	130.30	125.04
23	B	611	CLA	C4C-C3C-C2C	-3.45	101.86	106.90
23	b	611	CLA	C4C-C3C-C2C	-3.45	101.86	106.90
23	B	604	CLA	C3D-C4D-ND	3.45	115.82	110.24
23	b	604	CLA	C3D-C4D-ND	3.45	115.82	110.24
23	B	606	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
23	B	613	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
23	b	606	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
23	b	613	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
37	V	201	HEC	C1D-C2D-C3D	-3.45	102.79	106.83

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	515	BCR	C11-C10-C9	-3.45	122.38	127.31
25	c	515	BCR	C11-C10-C9	-3.45	122.38	127.31
23	b	607	CLA	C3B-C2B-C1B	-3.45	103.00	107.16
23	B	603	CLA	O2A-CGA-O1A	-3.45	114.89	123.59
23	b	603	CLA	O2A-CGA-O1A	-3.45	114.89	123.59
23	C	513	CLA	C1D-CHD-C4C	-3.44	118.63	126.06
23	c	513	CLA	C1D-CHD-C4C	-3.44	118.63	126.06
23	b	613	CLA	CHD-C1D-ND	-3.44	121.29	124.45
23	B	610	CLA	O2A-CGA-CBA	3.44	122.71	111.91
23	b	610	CLA	O2A-CGA-CBA	3.44	122.71	111.91
23	B	616	CLA	C1D-CHD-C4C	-3.42	118.68	126.06
23	b	616	CLA	C1D-CHD-C4C	-3.42	118.68	126.06
25	Y	101	BCR	C23-C24-C25	-3.42	117.60	127.20
23	A	405	CLA	C7-C6-C5	-3.41	104.09	113.36
23	a	405	CLA	C7-C6-C5	-3.41	104.09	113.36
23	A	405	CLA	C4C-C3C-C2C	-3.41	101.93	106.90
23	a	405	CLA	C4C-C3C-C2C	-3.41	101.93	106.90
25	B	617	BCR	C37-C22-C23	3.41	123.45	118.08
25	b	617	BCR	C37-C22-C23	3.41	123.45	118.08
25	D	407	BCR	C23-C24-C25	-3.41	117.63	127.20
25	d	407	BCR	C23-C24-C25	-3.41	117.63	127.20
25	y	101	BCR	C23-C24-C25	-3.41	117.64	127.20
23	C	504	CLA	C1D-CHD-C4C	-3.40	118.71	126.06
27	A	411	PL9	C53-C6-C1	3.40	121.94	114.99
27	a	411	PL9	C53-C6-C1	3.40	121.94	114.99
23	c	504	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
23	A	405	CLA	C1D-CHD-C4C	-3.40	118.73	126.06
23	a	405	CLA	C1D-CHD-C4C	-3.40	118.73	126.06
23	C	502	CLA	C3B-C2B-C1B	-3.39	103.06	107.16
23	c	502	CLA	C3B-C2B-C1B	-3.39	103.06	107.16
23	D	405	CLA	C4C-C3C-C2C	-3.39	101.96	106.90
23	d	405	CLA	C4C-C3C-C2C	-3.39	101.96	106.90
23	B	606	CLA	C4C-C3C-C2C	-3.38	101.97	106.90
23	b	606	CLA	C4C-C3C-C2C	-3.38	101.97	106.90
23	C	504	CLA	C3D-C4D-ND	3.37	115.69	110.24
23	B	613	CLA	C4C-C3C-C2C	-3.37	101.98	106.90
23	b	613	CLA	C4C-C3C-C2C	-3.37	101.98	106.90
23	B	607	CLA	C3D-C4D-ND	3.37	115.69	110.24
23	b	607	CLA	C3D-C4D-ND	3.37	115.69	110.24
23	B	604	CLA	CHC-C1C-C2C	-3.37	117.38	126.73
23	b	604	CLA	CHC-C1C-C2C	-3.37	117.38	126.73
23	D	406	CLA	C4A-NA-C1A	-3.36	105.19	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	406	CLA	C4A-NA-C1A	-3.36	105.19	106.71
23	c	512	CLA	C4C-C3C-C2C	-3.36	102.00	106.90
37	V	201	HEC	C1A-C2A-C3A	-3.36	102.75	107.13
37	v	201	HEC	C1A-C2A-C3A	-3.36	102.75	107.13
23	B	615	CLA	C1C-C2C-C3C	-3.36	103.43	106.96
23	b	615	CLA	C1C-C2C-C3C	-3.36	103.43	106.96
23	c	504	CLA	C3D-C4D-ND	3.36	115.67	110.24
23	A	405	CLA	C3D-C4D-ND	3.35	115.66	110.24
23	a	405	CLA	C3D-C4D-ND	3.35	115.66	110.24
23	C	512	CLA	C4C-C3C-C2C	-3.35	102.02	106.90
23	B	614	CLA	C1-C2-C3	-3.34	120.26	126.04
23	b	614	CLA	C1-C2-C3	-3.34	120.26	126.04
23	c	507	CLA	C4A-NA-C1A	-3.34	105.20	106.71
25	C	516	BCR	C3-C4-C5	-3.34	108.11	114.08
25	c	516	BCR	C3-C4-C5	-3.34	108.11	114.08
23	C	514	CLA	CMB-C2B-C1B	3.34	130.46	125.37
23	c	514	CLA	CMB-C2B-C1B	3.34	130.46	125.37
23	C	508	CLA	CMB-C2B-C1B	3.34	130.46	125.37
23	c	508	CLA	CMB-C2B-C1B	3.34	130.46	125.37
23	B	611	CLA	C1-C2-C3	-3.34	120.27	126.04
23	b	611	CLA	C1-C2-C3	-3.34	120.27	126.04
23	B	601	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
23	b	601	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
23	B	613	CLA	C1-C2-C3	-3.33	120.28	126.04
23	b	613	CLA	C1-C2-C3	-3.33	120.28	126.04
23	C	514	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
23	c	514	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
23	C	505	CLA	C1D-CHD-C4C	-3.33	118.88	126.06
23	C	507	CLA	C4A-NA-C1A	-3.32	105.21	106.71
23	c	505	CLA	C1D-CHD-C4C	-3.32	118.91	126.06
23	B	609	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
23	b	609	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
23	B	601	CLA	C1D-CHD-C4C	-3.30	118.93	126.06
23	b	601	CLA	C1D-CHD-C4C	-3.30	118.93	126.06
23	D	405	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
23	d	405	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
23	A	406	CLA	C3B-C2B-C1B	-3.29	103.19	107.16
23	a	406	CLA	C3B-C2B-C1B	-3.29	103.19	107.16
23	A	408	CLA	CHB-C4A-NA	3.29	129.06	124.51
23	a	408	CLA	CHB-C4A-NA	3.29	129.06	124.51
23	B	616	CLA	C4C-C3C-C2C	-3.29	102.11	106.90
23	b	616	CLA	C4C-C3C-C2C	-3.29	102.11	106.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	CLA	CAA-C2A-C3A	-3.29	103.78	112.78
23	B	614	CLA	O2A-CGA-CBA	3.28	122.21	111.91
23	b	614	CLA	O2A-CGA-CBA	3.28	122.21	111.91
23	d	402	CLA	C2A-C1A-CHA	-3.28	118.12	123.86
23	A	406	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
23	a	406	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
23	C	505	CLA	C3B-C4B-NB	3.28	113.56	110.52
23	c	505	CLA	C3B-C4B-NB	3.28	113.56	110.52
23	C	504	CLA	CMC-C2C-C1C	3.27	130.03	125.04
23	c	504	CLA	CMC-C2C-C1C	3.27	130.03	125.04
24	A	407	PHO	O2D-CGD-O1D	-3.27	117.44	123.84
24	a	407	PHO	O2D-CGD-O1D	-3.27	117.44	123.84
23	D	402	CLA	CAA-C2A-C3A	-3.27	103.81	112.78
23	C	504	CLA	O2D-CGD-CBD	3.27	117.08	111.27
23	c	504	CLA	O2D-CGD-CBD	3.27	117.08	111.27
28	A	412	SQD	O47-C7-C8	3.27	118.55	111.50
23	A	406	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
23	a	406	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
28	a	412	SQD	O47-C7-C8	3.26	118.53	111.50
25	C	515	BCR	C37-C22-C23	3.26	123.21	118.08
25	c	515	BCR	C37-C22-C23	3.26	123.21	118.08
23	C	512	CLA	C1-C2-C3	-3.26	120.41	126.04
23	c	512	CLA	C1-C2-C3	-3.26	120.41	126.04
31	H	102	DGD	O1G-C1A-O1A	-3.26	115.37	123.59
31	h	102	DGD	O1G-C1A-O1A	-3.26	115.37	123.59
23	C	505	CLA	C5-C3-C2	-3.26	114.53	121.12
23	c	505	CLA	C5-C3-C2	-3.26	114.53	121.12
23	B	606	CLA	CHC-C1C-C2C	-3.26	117.68	126.73
23	b	606	CLA	CHC-C1C-C2C	-3.26	117.68	126.73
23	B	602	CLA	CMC-C2C-C1C	3.26	130.00	125.04
23	b	602	CLA	CMC-C2C-C1C	3.26	130.00	125.04
23	D	402	CLA	C2A-C1A-CHA	-3.26	118.16	123.86
23	C	508	CLA	C3C-C4C-NC	3.25	114.22	110.57
23	c	508	CLA	C3C-C4C-NC	3.25	114.22	110.57
23	C	504	CLA	CAC-C3C-C4C	3.25	129.03	124.81
23	c	504	CLA	CAC-C3C-C4C	3.25	129.03	124.81
23	B	608	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
23	b	608	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
23	B	614	CLA	CHC-C1C-C2C	-3.25	117.71	126.73
25	B	619	BCR	C37-C22-C21	-3.25	118.37	122.92
25	b	619	BCR	C37-C22-C21	-3.25	118.37	122.92
23	C	507	CLA	CHC-C1C-C2C	-3.24	117.72	126.73

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	507	CLA	CHC-C1C-C2C	-3.24	117.72	126.73
23	B	611	CLA	C4A-NA-C1A	-3.24	105.25	106.71
23	b	611	CLA	C4A-NA-C1A	-3.24	105.25	106.71
25	T	101	BCR	C27-C26-C25	3.24	125.53	122.00
25	t	103	BCR	C27-C26-C25	3.24	125.53	122.00
23	B	612	CLA	C3B-C4B-NB	3.24	113.52	110.52
23	b	612	CLA	C3B-C4B-NB	3.24	113.52	110.52
23	b	614	CLA	CHC-C1C-C2C	-3.24	117.73	126.73
23	C	513	CLA	C4A-NA-C1A	-3.24	105.25	106.71
23	c	513	CLA	C4A-NA-C1A	-3.24	105.25	106.71
23	B	610	CLA	CHC-C1C-C2C	-3.24	117.74	126.73
23	b	610	CLA	CHC-C1C-C2C	-3.24	117.74	126.73
23	B	607	CLA	C4A-NA-C1A	-3.23	105.25	106.71
23	B	602	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
23	b	602	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
23	C	502	CLA	C2A-C1A-CHA	-3.23	118.22	123.86
23	c	502	CLA	C2A-C1A-CHA	-3.23	118.22	123.86
23	B	605	CLA	CMB-C2B-C1B	3.22	130.28	125.37
23	b	605	CLA	CMB-C2B-C1B	3.22	130.28	125.37
23	B	607	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
23	b	607	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
25	A	409	BCR	C24-C23-C22	-3.22	121.36	126.23
25	a	409	BCR	C24-C23-C22	-3.22	121.36	126.23
23	C	511	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
23	c	511	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
23	C	513	CLA	C1-C2-C3	-3.22	120.47	126.04
23	c	513	CLA	C1-C2-C3	-3.22	120.47	126.04
23	C	510	CLA	C3B-C4B-NB	3.22	113.50	110.52
23	B	614	CLA	C4-C3-C5	3.22	120.68	115.27
23	b	614	CLA	C4-C3-C5	3.22	120.68	115.27
23	B	604	CLA	C1C-C2C-C3C	-3.22	103.57	106.96
23	c	505	CLA	CBC-CAC-C3C	-3.21	103.57	112.43
37	V	201	HEC	C2B-C1B-NB	3.21	114.97	110.08
37	v	201	HEC	C2B-C1B-NB	3.21	114.97	110.08
23	B	615	CLA	C4A-NA-C1A	-3.21	105.26	106.71
23	b	615	CLA	C4A-NA-C1A	-3.21	105.26	106.71
23	C	505	CLA	CBC-CAC-C3C	-3.21	103.58	112.43
23	C	505	CLA	CMC-C2C-C1C	3.20	129.91	125.04
23	c	505	CLA	CMC-C2C-C1C	3.20	129.91	125.04
23	b	604	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
37	v	201	HEC	C2C-C1C-NC	3.19	114.94	110.08
23	C	506	CLA	C3B-C2B-C1B	-3.19	103.31	107.16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	506	CLA	C3B-C2B-C1B	-3.19	103.31	107.16
23	c	510	CLA	C3B-C4B-NB	3.19	113.47	110.52
23	a	408	CLA	CBC-CAC-C3C	-3.19	103.64	112.43
23	B	610	CLA	C3B-C4B-NB	3.19	113.47	110.52
23	b	610	CLA	C3B-C4B-NB	3.19	113.47	110.52
23	A	406	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
23	a	406	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
25	D	407	BCR	C37-C22-C21	-3.18	118.47	122.92
25	d	407	BCR	C37-C22-C21	-3.18	118.47	122.92
31	H	102	DGD	O1G-C1A-C2A	3.18	121.89	111.91
31	h	102	DGD	O1G-C1A-C2A	3.18	121.89	111.91
23	C	513	CLA	CAC-C3C-C4C	3.18	128.94	124.81
23	c	513	CLA	CAC-C3C-C4C	3.18	128.94	124.81
23	C	513	CLA	CHC-C1C-C2C	-3.18	117.91	126.73
23	c	513	CLA	CHC-C1C-C2C	-3.18	117.91	126.73
37	V	201	HEC	C2C-C1C-NC	3.18	114.92	110.08
23	A	408	CLA	CBC-CAC-C3C	-3.18	103.68	112.43
23	C	502	CLA	C2C-C1C-NC	3.17	112.94	109.97
23	c	502	CLA	C2C-C1C-NC	3.17	112.94	109.97
26	B	620	LMG	C1-O6-C5	-3.17	107.47	113.69
26	b	620	LMG	C1-O6-C5	-3.17	107.47	113.69
25	B	617	BCR	C24-C23-C22	-3.16	121.45	126.23
25	b	617	BCR	C24-C23-C22	-3.16	121.45	126.23
23	A	408	CLA	CAA-C2A-C3A	-3.16	104.12	112.78
23	a	408	CLA	CAA-C2A-C3A	-3.16	104.12	112.78
23	C	503	CLA	C2B-C1B-NB	3.16	112.35	110.23
23	c	503	CLA	C2B-C1B-NB	3.16	112.35	110.23
23	B	613	CLA	CMC-C2C-C1C	3.16	129.85	125.04
23	b	613	CLA	CMC-C2C-C1C	3.16	129.85	125.04
23	B	601	CLA	CMB-C2B-C1B	3.15	130.17	125.37
23	b	601	CLA	CMB-C2B-C1B	3.15	130.17	125.37
23	C	512	CLA	CMC-C2C-C1C	3.15	129.84	125.04
25	c	516	BCR	C23-C24-C25	-3.15	118.36	127.20
23	c	512	CLA	CMC-C2C-C1C	3.14	129.83	125.04
23	b	607	CLA	C4A-NA-C1A	-3.14	105.29	106.71
23	B	608	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
23	b	608	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
25	B	619	BCR	C7-C8-C9	-3.14	121.49	126.23
25	b	619	BCR	C7-C8-C9	-3.14	121.49	126.23
25	C	516	BCR	C23-C24-C25	-3.14	118.38	127.20
23	D	402	CLA	C1D-CHD-C4C	-3.14	119.28	126.06
23	d	402	CLA	C1D-CHD-C4C	-3.14	119.28	126.06

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	601	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
23	b	601	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
23	C	508	CLA	C1D-CHD-C4C	-3.13	119.30	126.06
23	c	508	CLA	C1D-CHD-C4C	-3.13	119.30	126.06
23	C	510	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
23	c	510	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
23	C	503	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
23	c	503	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
23	C	509	CLA	C2A-C1A-CHA	-3.13	118.39	123.86
23	c	509	CLA	C2A-C1A-CHA	-3.13	118.39	123.86
23	B	615	CLA	C1D-CHD-C4C	-3.13	119.31	126.06
23	b	615	CLA	C1D-CHD-C4C	-3.13	119.31	126.06
23	C	507	CLA	CBC-CAC-C3C	-3.13	103.81	112.43
23	c	507	CLA	CBC-CAC-C3C	-3.13	103.81	112.43
33	L	101	LHG	C6-C5-C4	-3.13	104.39	111.79
33	l	101	LHG	C6-C5-C4	-3.13	104.39	111.79
23	C	513	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
23	c	513	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
35	h	101	RRX	C37-C22-C21	-3.13	118.54	122.92
23	D	402	CLA	CHC-C1C-C2C	-3.13	118.05	126.73
23	d	402	CLA	CHC-C1C-C2C	-3.13	118.05	126.73
23	A	405	CLA	CHD-C1D-ND	-3.12	121.58	124.45
23	a	405	CLA	CHD-C1D-ND	-3.12	121.58	124.45
23	B	616	CLA	CHC-C1C-C2C	-3.12	118.06	126.73
23	b	616	CLA	CHC-C1C-C2C	-3.12	118.06	126.73
25	A	409	BCR	C23-C24-C25	-3.11	118.46	127.20
25	a	409	BCR	C23-C24-C25	-3.11	118.46	127.20
23	B	601	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
23	b	601	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
35	H	101	RRX	C37-C22-C21	-3.11	118.56	122.92
23	B	602	CLA	CHC-C1C-C2C	-3.11	118.08	126.73
23	b	602	CLA	CHC-C1C-C2C	-3.11	118.08	126.73
23	B	612	CLA	C1-C2-C3	-3.11	120.66	126.04
23	b	612	CLA	C1-C2-C3	-3.11	120.66	126.04
23	C	514	CLA	CAC-C3C-C4C	3.11	128.84	124.81
23	c	514	CLA	CAC-C3C-C4C	3.11	128.84	124.81
23	B	602	CLA	CAA-C2A-C3A	-3.10	104.28	112.78
23	b	602	CLA	CAA-C2A-C3A	-3.10	104.28	112.78
23	C	505	CLA	CHC-C1C-C2C	-3.10	118.12	126.73
23	c	505	CLA	CHC-C1C-C2C	-3.10	118.12	126.73
23	B	602	CLA	C1-C2-C3	-3.10	120.69	126.04
23	b	602	CLA	C1-C2-C3	-3.10	120.69	126.04

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	616	CLA	CMC-C2C-C1C	3.09	129.75	125.04
23	b	616	CLA	CMC-C2C-C1C	3.09	129.75	125.04
23	C	511	CLA	C1D-CHD-C4C	-3.09	119.39	126.06
23	c	511	CLA	C1D-CHD-C4C	-3.09	119.39	126.06
27	D	408	PL9	C36-C37-C38	-3.09	101.72	111.88
27	d	408	PL9	C36-C37-C38	-3.09	101.72	111.88
25	Y	101	BCR	C37-C22-C21	-3.09	118.60	122.92
25	y	101	BCR	C37-C22-C21	-3.09	118.60	122.92
23	B	612	CLA	CHC-C1C-C2C	-3.09	118.15	126.73
23	b	612	CLA	CHC-C1C-C2C	-3.09	118.15	126.73
23	C	512	CLA	C3B-C4B-NB	3.09	113.38	110.52
23	c	512	CLA	C3B-C4B-NB	3.09	113.38	110.52
23	b	607	CLA	C3B-C4B-NB	3.08	113.38	110.52
23	B	614	CLA	CMB-C2B-C1B	3.08	130.06	125.37
23	b	614	CLA	CMB-C2B-C1B	3.08	130.06	125.37
23	B	607	CLA	C3B-C4B-NB	3.08	113.37	110.52
23	B	601	CLA	CMC-C2C-C1C	3.08	129.73	125.04
23	b	601	CLA	CMC-C2C-C1C	3.08	129.73	125.04
23	A	408	CLA	C4-C3-C5	3.08	120.44	115.27
23	a	408	CLA	C4-C3-C5	3.08	120.44	115.27
27	d	408	PL9	C25-C24-C26	3.07	120.44	115.27
23	B	615	CLA	C4-C3-C5	3.07	120.43	115.27
23	b	615	CLA	C4-C3-C5	3.07	120.43	115.27
23	A	405	CLA	CHC-C1C-C2C	-3.07	118.21	126.73
23	a	405	CLA	CHC-C1C-C2C	-3.07	118.21	126.73
27	D	408	PL9	C25-C24-C26	3.06	120.41	115.27
23	C	514	CLA	CHD-C4C-NC	3.06	129.02	124.20
23	c	514	CLA	CHD-C4C-NC	3.06	129.02	124.20
23	A	408	CLA	CHC-C1C-C2C	-3.05	118.25	126.73
23	a	408	CLA	CHC-C1C-C2C	-3.05	118.25	126.73
23	C	502	CLA	C1D-CHD-C4C	-3.05	119.48	126.06
23	c	502	CLA	C1D-CHD-C4C	-3.05	119.48	126.06
23	C	508	CLA	CBC-CAC-C3C	-3.05	104.02	112.43
23	c	508	CLA	CBC-CAC-C3C	-3.05	104.02	112.43
23	B	609	CLA	C2A-C1A-CHA	-3.05	118.53	123.86
23	b	609	CLA	C2A-C1A-CHA	-3.05	118.53	123.86
24	A	407	PHO	CBC-CAC-C3C	-3.05	108.42	112.88
24	a	407	PHO	CBC-CAC-C3C	-3.05	108.42	112.88
23	B	610	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
23	b	610	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
24	A	407	PHO	CMB-C2B-C3B	3.03	130.35	124.68
23	B	603	CLA	CAA-C2A-C3A	-3.03	104.48	112.78

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	603	CLA	CAA-C2A-C3A	-3.03	104.48	112.78
28	D	415	SQD	O9-S-C6	3.02	110.53	106.94
28	d	415	SQD	O9-S-C6	3.02	110.53	106.94
24	a	407	PHO	CMB-C2B-C3B	3.02	130.33	124.68
23	C	513	CLA	CMB-C2B-C1B	3.02	129.97	125.37
23	c	513	CLA	CMB-C2B-C1B	3.02	129.97	125.37
23	D	402	CLA	CMC-C2C-C1C	3.02	129.63	125.04
23	d	402	CLA	CMC-C2C-C1C	3.02	129.63	125.04
23	C	512	CLA	CHC-C1C-C2C	-3.02	118.35	126.73
23	c	512	CLA	CHC-C1C-C2C	-3.01	118.36	126.73
23	C	512	CLA	C1D-CHD-C4C	-3.01	119.56	126.06
23	c	512	CLA	C1D-CHD-C4C	-3.01	119.56	126.06
33	E	101	LHG	O7-C7-C8	3.01	117.99	111.50
33	e	101	LHG	O7-C7-C8	3.01	117.99	111.50
23	B	603	CLA	CHC-C1C-C2C	-3.01	118.37	126.73
23	b	603	CLA	CHC-C1C-C2C	-3.01	118.37	126.73
23	B	609	CLA	CHC-C1C-C2C	-3.00	118.41	126.73
24	D	401	PHO	CMC-C2C-C1C	3.00	130.39	124.73
24	d	401	PHO	CMC-C2C-C1C	3.00	130.39	124.73
26	A	410	LMG	O7-C10-C11	2.99	117.95	111.50
26	a	410	LMG	O7-C10-C11	2.99	117.95	111.50
23	D	402	CLA	CMB-C2B-C1B	2.99	129.93	125.37
23	d	402	CLA	CMB-C2B-C1B	2.99	129.93	125.37
27	A	411	PL9	C40-C39-C41	2.99	120.31	115.27
27	a	411	PL9	C40-C39-C41	2.99	120.31	115.27
23	b	609	CLA	CHC-C1C-C2C	-2.99	118.42	126.73
23	D	405	CLA	C1D-CHD-C4C	-2.99	119.61	126.06
23	d	405	CLA	C1D-CHD-C4C	-2.99	119.61	126.06
25	B	619	BCR	C40-C30-C25	-2.99	105.45	110.30
25	b	619	BCR	C40-C30-C25	-2.99	105.45	110.30
23	C	503	CLA	CMB-C2B-C1B	2.99	129.92	125.37
23	c	503	CLA	CMB-C2B-C1B	2.99	129.92	125.37
23	B	616	CLA	CBC-CAC-C3C	-2.99	104.19	112.43
23	b	616	CLA	CBC-CAC-C3C	-2.99	104.19	112.43
23	B	614	CLA	C4-C3-C2	-2.98	116.03	123.68
23	b	614	CLA	C4-C3-C2	-2.98	116.03	123.68
25	C	515	BCR	C36-C18-C19	2.98	122.78	118.08
25	c	515	BCR	C36-C18-C19	2.98	122.78	118.08
25	A	409	BCR	C15-C16-C17	-2.98	117.38	123.47
25	a	409	BCR	C15-C16-C17	-2.98	117.38	123.47
23	B	603	CLA	O2A-CGA-CBA	2.98	121.24	111.91
23	b	603	CLA	O2A-CGA-CBA	2.98	121.24	111.91

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	512	CLA	CBC-CAC-C3C	-2.97	104.24	112.43
23	c	512	CLA	CBC-CAC-C3C	-2.97	104.24	112.43
23	B	605	CLA	C3B-C2B-C1B	-2.97	103.58	107.16
23	b	605	CLA	C3B-C2B-C1B	-2.97	103.58	107.16
23	B	601	CLA	CHC-C1C-C2C	-2.96	118.50	126.73
23	b	601	CLA	CHC-C1C-C2C	-2.96	118.50	126.73
24	A	407	PHO	CBA-CAA-C2A	-2.96	105.15	113.81
24	a	407	PHO	CBA-CAA-C2A	-2.96	105.15	113.81
23	C	506	CLA	CHC-C1C-C2C	-2.96	118.50	126.73
23	B	602	CLA	CAC-C3C-C4C	2.96	128.65	124.81
23	b	602	CLA	CAC-C3C-C4C	2.96	128.65	124.81
23	D	402	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
23	d	402	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
25	Y	101	BCR	C7-C8-C9	-2.96	121.76	126.23
25	y	101	BCR	C7-C8-C9	-2.96	121.76	126.23
23	C	506	CLA	C2A-C1A-CHA	-2.95	118.69	123.86
23	c	506	CLA	C2A-C1A-CHA	-2.95	118.69	123.86
23	C	513	CLA	C2A-C1A-CHA	-2.95	118.69	123.86
23	c	513	CLA	C2A-C1A-CHA	-2.95	118.69	123.86
23	B	610	CLA	C3B-C2B-C1B	-2.95	103.60	107.16
23	b	610	CLA	C3B-C2B-C1B	-2.95	103.60	107.16
23	c	506	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
24	D	401	PHO	C1-C2-C3	-2.94	120.95	126.04
24	d	401	PHO	C1-C2-C3	-2.94	120.95	126.04
28	C	501	SQD	O5-C1-C2	-2.94	104.12	110.35
28	c	501	SQD	O5-C1-C2	-2.94	104.12	110.35
23	A	408	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
23	a	408	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
23	B	603	CLA	C6-C7-C8	-2.93	106.44	115.92
23	b	603	CLA	C6-C7-C8	-2.93	106.44	115.92
23	B	607	CLA	CBC-CAC-C3C	-2.93	104.35	112.43
23	b	607	CLA	CBC-CAC-C3C	-2.93	104.35	112.43
23	D	405	CLA	CHC-C1C-C2C	-2.93	118.59	126.73
23	d	405	CLA	CHC-C1C-C2C	-2.93	118.59	126.73
23	C	514	CLA	C1C-C2C-C3C	-2.92	103.88	106.96
23	c	514	CLA	C1C-C2C-C3C	-2.92	103.88	106.96
23	B	616	CLA	C4A-NA-C1A	-2.92	105.39	106.71
23	b	616	CLA	C4A-NA-C1A	-2.92	105.39	106.71
23	C	508	CLA	CHC-C1C-C2C	-2.92	118.62	126.73
23	c	508	CLA	CHC-C1C-C2C	-2.92	118.62	126.73
23	B	605	CLA	CED-O2D-CGD	2.92	122.54	115.94
23	b	605	CLA	CED-O2D-CGD	2.92	122.54	115.94

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	C1D-CHD-C4C	-2.92	119.77	126.06
23	c	507	CLA	C1D-CHD-C4C	-2.92	119.77	126.06
23	D	402	CLA	C1-O2A-CGA	2.91	124.08	116.44
23	d	402	CLA	C1-O2A-CGA	2.91	124.08	116.44
23	C	503	CLA	CHC-C1C-C2C	-2.91	118.65	126.73
23	c	503	CLA	CHC-C1C-C2C	-2.91	118.65	126.73
25	K	102	BCR	C24-C23-C22	-2.91	121.84	126.23
25	k	102	BCR	C24-C23-C22	-2.91	121.84	126.23
23	C	509	CLA	C3B-C4B-NB	2.91	113.21	110.52
23	c	509	CLA	C3B-C4B-NB	2.91	113.21	110.52
23	D	406	CLA	C2A-C1A-CHA	-2.90	118.78	123.86
23	d	406	CLA	C2A-C1A-CHA	-2.90	118.78	123.86
23	c	506	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
28	A	412	SQD	O6-C1-C2	2.89	112.81	108.30
28	a	412	SQD	O6-C1-C2	2.89	112.81	108.30
23	C	506	CLA	CMB-C2B-C1B	2.89	129.76	125.37
23	c	506	CLA	CMB-C2B-C1B	2.89	129.76	125.37
25	B	617	BCR	C36-C18-C19	2.89	122.62	118.08
25	b	617	BCR	C36-C18-C19	2.89	122.62	118.08
23	C	506	CLA	C1D-CHD-C4C	-2.88	119.84	126.06
23	c	506	CLA	C1D-CHD-C4C	-2.88	119.84	126.06
23	C	504	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
23	c	504	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
23	C	506	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
23	B	607	CLA	CMC-C2C-C1C	2.88	129.42	125.04
23	b	607	CLA	CMC-C2C-C1C	2.88	129.42	125.04
23	D	406	CLA	CMB-C2B-C1B	2.88	129.75	125.37
23	d	406	CLA	CMB-C2B-C1B	2.88	129.75	125.37
23	B	614	CLA	O2A-CGA-O1A	-2.88	116.33	123.59
23	b	614	CLA	O2A-CGA-O1A	-2.88	116.33	123.59
23	B	610	CLA	C1C-C2C-C3C	-2.87	103.93	106.96
23	b	610	CLA	C1C-C2C-C3C	-2.87	103.93	106.96
24	D	401	PHO	C4D-CHA-CBD	2.87	109.81	108.52
24	d	401	PHO	C4D-CHA-CBD	2.87	109.81	108.52
23	B	615	CLA	O2D-CGD-CBD	2.87	116.36	111.27
23	b	615	CLA	O2D-CGD-CBD	2.87	116.36	111.27
23	A	405	CLA	C4-C3-C5	2.87	120.09	115.27
23	a	405	CLA	C4-C3-C5	2.87	120.09	115.27
23	C	503	CLA	C1D-CHD-C4C	-2.86	119.88	126.06
23	B	614	CLA	C1D-CHD-C4C	-2.86	119.88	126.06
23	C	509	CLA	C1D-CHD-C4C	-2.86	119.88	126.06
23	b	614	CLA	C1D-CHD-C4C	-2.86	119.88	126.06

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	509	CLA	C1D-CHD-C4C	-2.86	119.88	126.06
23	C	503	CLA	C4C-C3C-C2C	-2.86	102.72	106.90
23	c	503	CLA	C4C-C3C-C2C	-2.86	102.72	106.90
28	A	412	SQD	C44-O6-C1	-2.86	108.15	113.74
28	a	412	SQD	C44-O6-C1	-2.86	108.15	113.74
23	A	406	CLA	CMC-C2C-C1C	2.86	129.39	125.04
23	a	406	CLA	CMC-C2C-C1C	2.86	129.39	125.04
23	B	612	CLA	C3B-C2B-C1B	-2.86	103.71	107.16
23	b	612	CLA	C3B-C2B-C1B	-2.86	103.71	107.16
23	D	405	CLA	O2A-CGA-CBA	2.86	120.87	111.91
23	d	405	CLA	O2A-CGA-CBA	2.86	120.87	111.91
23	c	503	CLA	C1D-CHD-C4C	-2.86	119.90	126.06
23	B	615	CLA	CMB-C2B-C1B	2.85	129.71	125.37
23	b	615	CLA	CMB-C2B-C1B	2.85	129.71	125.37
23	B	603	CLA	CBC-CAC-C3C	-2.85	104.57	112.43
23	b	603	CLA	CBC-CAC-C3C	-2.85	104.57	112.43
25	C	515	BCR	C20-C21-C22	-2.85	123.24	127.31
25	c	515	BCR	C20-C21-C22	-2.85	123.24	127.31
26	b	620	LMG	O8-C28-C29	2.85	120.85	111.91
35	H	101	RRX	C15-C16-C17	2.85	129.31	123.47
35	h	101	RRX	C15-C16-C17	2.85	129.31	123.47
23	B	612	CLA	O2A-CGA-CBA	2.84	120.82	111.91
26	B	620	LMG	O8-C28-C29	2.84	120.81	111.91
23	b	612	CLA	O2A-CGA-CBA	2.84	120.81	111.91
23	D	406	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
23	d	406	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
25	B	618	BCR	C37-C22-C21	-2.83	118.95	122.92
25	b	618	BCR	C37-C22-C21	-2.83	118.95	122.92
23	B	603	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
28	a	412	SQD	C9-C8-C7	-2.83	103.33	113.62
23	b	603	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
25	C	515	BCR	C24-C23-C22	-2.83	121.96	126.23
25	c	515	BCR	C24-C23-C22	-2.83	121.96	126.23
28	A	412	SQD	C9-C8-C7	-2.82	103.35	113.62
25	B	618	BCR	C8-C7-C6	-2.82	119.27	127.20
23	B	608	CLA	C1D-CHD-C4C	-2.82	119.97	126.06
23	b	608	CLA	C1D-CHD-C4C	-2.82	119.97	126.06
25	b	618	BCR	C8-C7-C6	-2.82	119.29	127.20
24	D	401	PHO	C1A-C2A-C3A	-2.82	100.16	102.84
24	d	401	PHO	C1A-C2A-C3A	-2.82	100.16	102.84
27	A	411	PL9	C42-C43-C44	-2.81	120.88	127.66
27	a	411	PL9	C42-C43-C44	-2.81	120.88	127.66

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	619	BCR	C37-C22-C23	2.81	122.51	118.08
25	b	619	BCR	C37-C22-C23	2.81	122.51	118.08
23	C	514	CLA	CAA-C2A-C3A	-2.81	107.23	114.26
23	c	514	CLA	CAA-C2A-C3A	-2.81	107.23	114.26
23	B	609	CLA	C3B-C2B-C1B	-2.81	103.77	107.16
23	b	609	CLA	C3B-C2B-C1B	-2.81	103.77	107.16
25	B	619	BCR	C23-C24-C25	-2.81	119.31	127.20
25	b	619	BCR	C23-C24-C25	-2.81	119.31	127.20
23	A	406	CLA	O1D-CGD-CBD	-2.81	118.74	124.48
23	a	406	CLA	O1D-CGD-CBD	-2.81	118.74	124.48
23	C	502	CLA	CMC-C2C-C1C	2.81	129.31	125.04
23	c	502	CLA	CMC-C2C-C1C	2.81	129.31	125.04
23	C	514	CLA	CBA-CAA-C2A	2.80	119.71	113.47
23	c	514	CLA	CBA-CAA-C2A	2.80	119.71	113.47
23	B	616	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	b	616	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	B	606	CLA	O2A-CGA-O1A	-2.80	116.52	123.59
23	b	606	CLA	O2A-CGA-O1A	-2.80	116.52	123.59
31	C	517	DGD	O2G-C1B-C2B	2.80	117.53	111.50
25	C	516	BCR	C15-C16-C17	-2.80	117.74	123.47
25	c	516	BCR	C15-C16-C17	-2.80	117.74	123.47
25	C	515	BCR	C16-C17-C18	-2.80	123.32	127.31
25	c	515	BCR	C16-C17-C18	-2.80	123.32	127.31
23	C	502	CLA	C4A-NA-C1A	-2.80	105.45	106.71
23	c	502	CLA	C4A-NA-C1A	-2.80	105.45	106.71
23	B	606	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
23	b	606	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
23	B	608	CLA	CHC-C1C-C2C	-2.79	118.97	126.73
31	c	517	DGD	O2G-C1B-C2B	2.79	117.52	111.50
24	D	401	PHO	O2D-CGD-O1D	-2.79	118.38	123.84
24	d	401	PHO	O2D-CGD-O1D	-2.79	118.38	123.84
24	D	401	PHO	CMB-C2B-C3B	2.78	129.89	124.68
24	d	401	PHO	CMB-C2B-C3B	2.78	129.89	124.68
34	F	101	HEM	CHD-C1D-ND	2.78	127.44	124.42
34	f	101	HEM	CHD-C1D-ND	2.78	127.44	124.42
23	D	405	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
23	d	405	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
23	b	608	CLA	CHC-C1C-C2C	-2.78	119.00	126.73
28	C	501	SQD	C44-O6-C1	-2.78	108.30	113.74
28	c	501	SQD	C44-O6-C1	-2.78	108.30	113.74
23	b	613	CLA	C1D-CHD-C4C	-2.78	120.06	126.06
23	C	510	CLA	O2D-CGD-O1D	-2.78	118.40	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
23	A	405	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
23	a	405	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
23	C	507	CLA	CAA-C2A-C3A	-2.78	105.17	112.78
23	c	507	CLA	CAA-C2A-C3A	-2.78	105.17	112.78
25	T	101	BCR	C3-C4-C5	-2.77	109.13	114.08
25	t	103	BCR	C3-C4-C5	-2.77	109.13	114.08
23	C	511	CLA	O1D-CGD-CBD	-2.77	118.82	124.48
23	c	511	CLA	O1D-CGD-CBD	-2.77	118.82	124.48
25	C	516	BCR	C37-C22-C21	-2.77	119.04	122.92
25	c	516	BCR	C37-C22-C21	-2.77	119.04	122.92
23	C	502	CLA	C4-C3-C5	2.77	119.93	115.27
23	c	502	CLA	C4-C3-C5	2.77	119.93	115.27
23	B	613	CLA	C1D-CHD-C4C	-2.77	120.09	126.06
23	B	601	CLA	C2A-C1A-CHA	-2.76	119.03	123.86
23	b	601	CLA	C2A-C1A-CHA	-2.76	119.03	123.86
23	A	406	CLA	CHC-C1C-C2C	-2.76	119.05	126.73
23	a	406	CLA	CHC-C1C-C2C	-2.76	119.05	126.73
23	D	402	CLA	CMA-C3A-C2A	-2.76	102.69	113.83
23	d	402	CLA	CMA-C3A-C2A	-2.76	102.69	113.83
28	A	412	SQD	O9-S-C6	2.76	110.22	106.94
28	a	412	SQD	O9-S-C6	2.76	110.22	106.94
25	K	102	BCR	C8-C7-C6	-2.76	119.45	127.20
25	k	102	BCR	C8-C7-C6	-2.76	119.45	127.20
23	b	607	CLA	C4-C3-C5	2.75	119.90	115.27
23	B	607	CLA	C4-C3-C5	2.75	119.90	115.27
23	C	505	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
23	c	505	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
31	C	519	DGD	O3G-C3G-C2G	-2.75	104.27	110.90
31	c	519	DGD	O3G-C3G-C2G	-2.75	104.27	110.90
23	C	513	CLA	CHB-C4A-NA	2.75	128.31	124.51
23	c	513	CLA	CHB-C4A-NA	2.75	128.31	124.51
23	B	613	CLA	CHC-C1C-C2C	-2.75	119.11	126.73
23	C	504	CLA	C7-C6-C5	-2.74	105.90	113.36
23	c	504	CLA	C7-C6-C5	-2.74	105.90	113.36
23	B	605	CLA	C2A-C1A-CHA	-2.74	119.06	123.86
23	b	605	CLA	C2A-C1A-CHA	-2.74	119.06	123.86
23	c	507	CLA	C3B-C2B-C1B	-2.74	103.85	107.16
23	b	613	CLA	CHC-C1C-C2C	-2.74	119.12	126.73
37	V	201	HEC	CBD-CAD-C3D	-2.74	105.02	112.63
23	b	609	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
25	D	407	BCR	C40-C30-C25	-2.74	105.86	110.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	407	BCR	C40-C30-C25	-2.74	105.86	110.30
23	C	509	CLA	O2A-CGA-CBA	2.74	120.50	111.91
23	c	509	CLA	O2A-CGA-CBA	2.74	120.50	111.91
23	B	605	CLA	CHC-C1C-C2C	-2.73	119.14	126.73
23	b	605	CLA	CHC-C1C-C2C	-2.73	119.14	126.73
37	v	201	HEC	CBD-CAD-C3D	-2.73	105.04	112.63
25	Y	101	BCR	C39-C30-C25	-2.73	105.87	110.30
25	y	101	BCR	C39-C30-C25	-2.73	105.87	110.30
23	A	405	CLA	C1-C2-C3	-2.73	121.32	126.04
23	a	405	CLA	C1-C2-C3	-2.73	121.32	126.04
37	V	201	HEC	C3A-C4A-NA	2.73	114.72	109.69
37	v	201	HEC	C3A-C4A-NA	2.73	114.72	109.69
25	D	407	BCR	C39-C30-C25	-2.73	105.88	110.30
25	d	407	BCR	C39-C30-C25	-2.73	105.88	110.30
23	B	609	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
23	D	406	CLA	C1-O2A-CGA	2.73	123.60	116.44
23	d	406	CLA	C1-O2A-CGA	2.73	123.60	116.44
25	K	102	BCR	C37-C22-C23	2.72	122.37	118.08
25	k	102	BCR	C37-C22-C23	2.72	122.37	118.08
33	D	411	LHG	O7-C7-C8	2.72	117.36	111.50
33	d	411	LHG	O7-C7-C8	2.72	117.36	111.50
26	D	412	LMG	O1-C7-C8	-2.72	104.34	110.90
26	d	412	LMG	O1-C7-C8	-2.72	104.34	110.90
23	C	507	CLA	C3B-C2B-C1B	-2.72	103.88	107.16
23	B	607	CLA	CHD-C4C-NC	2.72	128.49	124.20
23	b	607	CLA	CHD-C4C-NC	2.72	128.49	124.20
25	B	619	BCR	C36-C18-C17	-2.71	119.12	122.92
25	b	619	BCR	C36-C18-C17	-2.71	119.12	122.92
23	C	507	CLA	C4C-C3C-C2C	-2.71	102.94	106.90
23	b	602	CLA	C1D-CHD-C4C	-2.71	120.21	126.06
23	C	510	CLA	C11-C12-C13	-2.71	107.16	115.92
23	c	510	CLA	C11-C12-C13	-2.71	107.16	115.92
23	B	602	CLA	C1D-CHD-C4C	-2.71	120.21	126.06
23	C	512	CLA	OBD-CAD-C3D	-2.71	122.00	128.52
23	c	512	CLA	OBD-CAD-C3D	-2.71	122.00	128.52
23	d	402	CLA	C1-C2-C3	-2.71	121.36	126.04
28	D	415	SQD	C3-C4-C5	2.70	115.06	110.24
28	d	415	SQD	C3-C4-C5	2.70	115.06	110.24
23	C	511	CLA	O2A-CGA-CBA	2.70	120.39	111.91
23	c	511	CLA	O2A-CGA-CBA	2.70	120.39	111.91
23	D	402	CLA	C1-C2-C3	-2.70	121.37	126.04
37	V	201	HEC	C4A-C3A-C2A	-2.70	103.00	106.94

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	v	201	HEC	C4A-C3A-C2A	-2.70	103.00	106.94
23	B	603	CLA	C3B-C4B-NB	2.70	113.02	110.52
23	b	603	CLA	C3B-C4B-NB	2.70	113.02	110.52
34	F	101	HEM	CHA-C4D-ND	2.70	127.70	124.37
34	f	101	HEM	CHA-C4D-ND	2.70	127.70	124.37
33	L	101	LHG	O4-P-O5	2.70	125.58	112.24
33	l	101	LHG	O4-P-O5	2.70	125.58	112.24
23	c	507	CLA	C4C-C3C-C2C	-2.70	102.97	106.90
23	D	406	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
23	d	406	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
25	C	516	BCR	C11-C10-C9	-2.69	123.47	127.31
25	c	516	BCR	C11-C10-C9	-2.69	123.47	127.31
27	D	408	PL9	C12-C13-C14	-2.68	121.20	127.66
27	d	408	PL9	C12-C13-C14	-2.68	121.20	127.66
34	F	101	HEM	CHB-C1B-NB	2.68	127.68	124.37
34	f	101	HEM	CHB-C1B-NB	2.68	127.68	124.37
31	C	519	DGD	O1G-C1A-C2A	2.68	120.33	111.91
31	c	519	DGD	O1G-C1A-C2A	2.68	120.33	111.91
23	B	614	CLA	CAC-C3C-C4C	2.68	128.29	124.81
23	b	614	CLA	CAC-C3C-C4C	2.68	128.29	124.81
23	A	406	CLA	C1D-CHD-C4C	-2.68	120.27	126.06
23	a	406	CLA	C1D-CHD-C4C	-2.68	120.27	126.06
23	B	606	CLA	C3B-C4B-NB	2.68	113.00	110.52
23	b	606	CLA	C3B-C4B-NB	2.68	113.00	110.52
23	B	615	CLA	CHC-C1C-C2C	-2.68	119.30	126.73
23	b	615	CLA	CHC-C1C-C2C	-2.68	119.30	126.73
23	c	511	CLA	CHC-C1C-C2C	-2.68	119.30	126.73
27	D	408	PL9	C40-C39-C41	2.67	119.77	115.27
27	d	408	PL9	C40-C39-C41	2.67	119.77	115.27
23	C	502	CLA	CHD-C4C-NC	2.67	128.40	124.20
23	c	502	CLA	CHD-C4C-NC	2.67	128.40	124.20
37	V	201	HEC	C4D-C3D-C2D	-2.66	102.70	106.89
23	C	511	CLA	CHC-C1C-C2C	-2.66	119.33	126.73
34	F	101	HEM	C4A-NA-C1A	2.66	107.96	105.35
34	f	101	HEM	C4A-NA-C1A	2.66	107.96	105.35
23	C	509	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
23	c	509	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
25	B	618	BCR	C36-C18-C17	-2.66	119.20	122.92
25	b	618	BCR	C36-C18-C17	-2.66	119.20	122.92
23	B	610	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
23	b	610	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
27	D	408	PL9	C10-C9-C11	2.66	119.74	115.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d	408	PL9	C10-C9-C11	2.66	119.74	115.27
25	T	101	BCR	C36-C18-C19	2.66	122.26	118.08
25	t	103	BCR	C36-C18-C19	2.66	122.26	118.08
23	B	606	CLA	C11-C12-C13	-2.65	107.35	115.92
23	b	606	CLA	C11-C12-C13	-2.65	107.35	115.92
23	C	504	CLA	C4C-C3C-C2C	-2.65	103.03	106.90
23	c	504	CLA	C4C-C3C-C2C	-2.65	103.03	106.90
23	D	402	CLA	C3B-C2B-C1B	-2.65	103.97	107.16
23	d	402	CLA	C3B-C2B-C1B	-2.65	103.97	107.16
37	v	201	HEC	C4D-C3D-C2D	-2.64	102.73	106.89
37	V	201	HEC	CBA-CAA-C2A	-2.64	105.28	112.63
37	v	201	HEC	CBA-CAA-C2A	-2.64	105.28	112.63
23	C	502	CLA	CMB-C2B-C1B	2.64	129.39	125.37
23	c	502	CLA	CMB-C2B-C1B	2.64	129.39	125.37
23	B	602	CLA	O2A-CGA-CBA	2.64	120.19	111.91
23	b	602	CLA	O2A-CGA-CBA	2.64	120.19	111.91
23	B	616	CLA	O2A-CGA-CBA	2.64	120.18	111.91
23	b	616	CLA	O2A-CGA-CBA	2.64	120.18	111.91
23	D	405	CLA	CAA-C2A-C3A	-2.64	105.56	112.78
23	d	405	CLA	CAA-C2A-C3A	-2.64	105.56	112.78
34	F	101	HEM	C4D-ND-C1D	2.63	107.79	105.07
34	f	101	HEM	C4D-ND-C1D	2.63	107.79	105.07
23	B	614	CLA	CHC-C4B-NB	2.63	127.04	124.26
23	b	614	CLA	CHC-C4B-NB	2.63	127.04	124.26
23	B	604	CLA	CMA-C3A-C4A	2.63	118.84	111.77
23	b	604	CLA	CMA-C3A-C4A	2.63	118.84	111.77
35	H	101	RRX	C23-C22-C21	2.63	122.97	118.94
35	h	101	RRX	C23-C22-C21	2.63	122.97	118.94
23	B	607	CLA	CHD-C1D-ND	-2.63	122.04	124.45
23	b	607	CLA	CHD-C1D-ND	-2.63	122.04	124.45
23	B	606	CLA	C3B-C2B-C1B	-2.63	103.99	107.16
23	b	606	CLA	C3B-C2B-C1B	-2.63	103.99	107.16
23	b	606	CLA	CBC-CAC-C3C	-2.62	105.20	112.43
23	C	513	CLA	CBC-CAC-C3C	-2.62	105.20	112.43
23	c	513	CLA	CBC-CAC-C3C	-2.62	105.20	112.43
23	B	604	CLA	CMC-C2C-C1C	2.62	129.03	125.04
23	b	604	CLA	CMC-C2C-C1C	2.62	129.03	125.04
23	B	606	CLA	CBC-CAC-C3C	-2.61	105.22	112.43
23	C	502	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
23	c	502	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
23	b	614	CLA	CBC-CAC-C3C	-2.61	105.24	112.43
23	A	408	CLA	C3B-C4B-NB	2.61	112.93	110.52

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	408	CLA	C3B-C4B-NB	2.61	112.93	110.52
23	D	406	CLA	C1D-CHD-C4C	-2.60	120.44	126.06
23	d	406	CLA	C1D-CHD-C4C	-2.60	120.44	126.06
25	C	516	BCR	C36-C18-C19	2.60	122.18	118.08
25	c	516	BCR	C36-C18-C19	2.60	122.18	118.08
23	B	611	CLA	CBC-CAC-C3C	-2.60	105.25	112.43
23	b	611	CLA	CBC-CAC-C3C	-2.60	105.25	112.43
23	D	402	CLA	CBC-CAC-C3C	-2.60	105.26	112.43
23	d	402	CLA	CBC-CAC-C3C	-2.60	105.26	112.43
23	D	405	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
23	d	405	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
23	C	508	CLA	CAC-C3C-C4C	2.60	128.18	124.81
23	c	508	CLA	CAC-C3C-C4C	2.60	128.18	124.81
25	B	619	BCR	C2-C3-C4	-2.60	105.57	111.38
25	b	619	BCR	C2-C3-C4	-2.60	105.57	111.38
23	B	614	CLA	CBC-CAC-C3C	-2.60	105.27	112.43
23	B	611	CLA	C1D-CHD-C4C	-2.59	120.47	126.06
23	b	611	CLA	C1D-CHD-C4C	-2.59	120.47	126.06
23	C	504	CLA	C2A-C1A-CHA	-2.59	119.33	123.86
23	C	506	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
23	B	608	CLA	CMA-C3A-C2A	-2.59	103.38	113.83
23	b	608	CLA	CMA-C3A-C2A	-2.59	103.38	113.83
25	T	101	BCR	C19-C18-C17	-2.59	114.97	118.94
25	t	103	BCR	C19-C18-C17	-2.59	114.97	118.94
23	c	504	CLA	C2A-C1A-CHA	-2.59	119.34	123.86
25	C	516	BCR	C2-C1-C6	2.59	114.46	110.48
25	c	516	BCR	C2-C1-C6	2.59	114.46	110.48
24	A	407	PHO	CMC-C2C-C1C	2.59	129.61	124.73
24	a	407	PHO	CMC-C2C-C1C	2.59	129.61	124.73
23	A	406	CLA	C4A-NA-C1A	-2.58	105.55	106.71
23	a	406	CLA	C4A-NA-C1A	-2.58	105.55	106.71
23	C	508	CLA	CHB-C1B-C2B	-2.57	119.97	127.24
23	c	508	CLA	CHB-C1B-C2B	-2.57	119.97	127.24
23	B	612	CLA	C2A-C1A-CHA	-2.57	119.36	123.86
23	b	612	CLA	C2A-C1A-CHA	-2.57	119.36	123.86
23	B	606	CLA	CHD-C4C-NC	2.57	128.25	124.20
23	b	606	CLA	CHD-C4C-NC	2.57	128.25	124.20
25	D	407	BCR	C31-C1-C6	-2.57	106.13	110.30
25	d	407	BCR	C31-C1-C6	-2.57	106.13	110.30
27	D	408	PL9	C36-C34-C33	-2.57	115.92	121.12
27	d	408	PL9	C36-C34-C33	-2.57	115.92	121.12
23	c	506	CLA	C1C-C2C-C3C	-2.57	104.26	106.96

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	514	CLA	CHB-C1B-C2B	-2.56	120.00	127.24
23	c	514	CLA	CHB-C1B-C2B	-2.56	120.00	127.24
25	C	515	BCR	C15-C16-C17	-2.56	118.22	123.47
25	c	515	BCR	C15-C16-C17	-2.56	118.22	123.47
25	C	515	BCR	C39-C30-C25	-2.56	106.14	110.30
25	c	515	BCR	C39-C30-C25	-2.56	106.14	110.30
27	D	408	PL9	C32-C33-C34	-2.56	121.50	127.66
27	d	408	PL9	C32-C33-C34	-2.56	121.50	127.66
25	B	619	BCR	C2-C1-C6	2.56	114.42	110.48
25	b	619	BCR	C2-C1-C6	2.56	114.42	110.48
27	A	411	PL9	C37-C36-C34	-2.56	104.56	112.98
27	a	411	PL9	C37-C36-C34	-2.56	104.56	112.98
23	B	606	CLA	CMC-C2C-C1C	2.56	128.93	125.04
23	b	606	CLA	CMC-C2C-C1C	2.56	128.93	125.04
23	B	613	CLA	C2A-C1A-CHA	-2.55	119.39	123.86
23	b	613	CLA	C2A-C1A-CHA	-2.55	119.39	123.86
23	C	504	CLA	CBC-CAC-C3C	-2.55	105.39	112.43
23	c	504	CLA	CBC-CAC-C3C	-2.55	105.39	112.43
23	A	405	CLA	OBD-CAD-C3D	-2.55	122.38	128.52
23	a	405	CLA	OBD-CAD-C3D	-2.55	122.38	128.52
23	c	506	CLA	O2A-C1-C2	-2.55	101.93	108.64
26	B	620	LMG	C9-C8-C7	-2.55	105.76	111.79
26	b	620	LMG	C9-C8-C7	-2.55	105.76	111.79
27	D	408	PL9	C22-C23-C24	-2.55	121.53	127.66
27	d	408	PL9	C22-C23-C24	-2.55	121.53	127.66
25	K	102	BCR	C40-C30-C25	-2.54	106.18	110.30
25	k	102	BCR	C40-C30-C25	-2.54	106.18	110.30
23	D	405	CLA	C2A-C1A-CHA	-2.53	119.43	123.86
23	d	405	CLA	C2A-C1A-CHA	-2.53	119.43	123.86
23	B	603	CLA	C1D-CHD-C4C	-2.53	120.59	126.06
23	b	603	CLA	C1D-CHD-C4C	-2.53	120.59	126.06
23	C	506	CLA	O2A-C1-C2	-2.53	101.98	108.64
23	C	513	CLA	CMC-C2C-C1C	2.53	128.89	125.04
23	c	513	CLA	CMC-C2C-C1C	2.53	128.89	125.04
23	A	405	CLA	O2A-CGA-O1A	-2.53	117.21	123.59
23	a	405	CLA	O2A-CGA-O1A	-2.53	117.21	123.59
23	C	514	CLA	CHC-C1C-C2C	-2.53	119.71	126.73
23	c	514	CLA	CHC-C1C-C2C	-2.53	119.71	126.73
31	C	518	DGD	O2G-C1B-C2B	2.53	116.94	111.50
31	c	518	DGD	O2G-C1B-C2B	2.52	116.94	111.50
23	D	406	CLA	CBC-CAC-C3C	-2.52	105.49	112.43
23	d	406	CLA	CBC-CAC-C3C	-2.52	105.49	112.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	408	CLA	CMC-C2C-C1C	2.51	128.87	125.04
23	a	408	CLA	CMC-C2C-C1C	2.51	128.87	125.04
23	B	612	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
23	b	612	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
23	D	406	CLA	CHC-C1C-C2C	-2.51	119.76	126.73
23	d	406	CLA	CHC-C1C-C2C	-2.51	119.76	126.73
23	C	505	CLA	C7-C6-C5	-2.50	106.56	113.36
23	c	505	CLA	C7-C6-C5	-2.50	106.56	113.36
31	C	517	DGD	C6D-O5D-C1E	2.50	118.63	113.74
31	c	517	DGD	C6D-O5D-C1E	2.50	118.63	113.74
23	B	613	CLA	CMB-C2B-C1B	2.50	129.18	125.37
23	b	613	CLA	CMB-C2B-C1B	2.50	129.18	125.37
23	A	406	CLA	CMB-C2B-C1B	2.50	129.18	125.37
23	a	406	CLA	CMB-C2B-C1B	2.50	129.18	125.37
25	B	618	BCR	C29-C30-C25	-2.49	104.63	113.63
23	A	408	CLA	CMA-C3A-C2A	-2.49	103.77	113.83
23	a	408	CLA	CMA-C3A-C2A	-2.49	103.77	113.83
23	B	612	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
23	b	612	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
25	b	618	BCR	C29-C30-C25	-2.49	104.65	113.63
25	A	409	BCR	C16-C17-C18	-2.49	123.76	127.31
25	a	409	BCR	C16-C17-C18	-2.49	123.76	127.31
27	D	408	PL9	C7-C8-C9	-2.48	122.66	126.79
27	d	408	PL9	C7-C8-C9	-2.48	122.66	126.79
27	A	411	PL9	C35-C34-C36	2.48	119.44	115.27
27	a	411	PL9	C35-C34-C36	2.48	119.44	115.27
23	B	602	CLA	C2A-C1A-CHA	-2.48	119.53	123.86
23	b	602	CLA	C2A-C1A-CHA	-2.48	119.53	123.86
23	C	511	CLA	CMB-C2B-C1B	2.47	129.13	125.37
23	c	511	CLA	CMB-C2B-C1B	2.47	129.13	125.37
25	B	618	BCR	C36-C18-C19	2.47	121.96	118.08
25	b	618	BCR	C36-C18-C19	2.47	121.96	118.08
23	B	615	CLA	C5-C3-C2	-2.47	116.13	121.12
23	b	615	CLA	C5-C3-C2	-2.47	116.13	121.12
23	B	610	CLA	O2A-CGA-O1A	-2.47	117.37	123.59
23	b	610	CLA	O2A-CGA-O1A	-2.47	117.37	123.59
25	y	101	BCR	C16-C17-C18	-2.46	123.80	127.31
23	B	613	CLA	C3B-C4B-NB	2.46	112.80	110.52
23	b	613	CLA	C3B-C4B-NB	2.46	112.80	110.52
23	A	406	CLA	CBC-CAC-C3C	-2.46	105.65	112.43
23	a	406	CLA	CBC-CAC-C3C	-2.46	105.65	112.43
23	C	514	CLA	CBC-CAC-C3C	-2.46	105.66	112.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	514	CLA	CBC-CAC-C3C	-2.46	105.66	112.43
25	D	407	BCR	C27-C26-C25	-2.46	119.17	122.73
25	d	407	BCR	C27-C26-C25	-2.46	119.17	122.73
23	B	604	CLA	C6-C5-C3	-2.45	107.02	113.45
23	b	604	CLA	C6-C5-C3	-2.45	107.02	113.45
23	C	514	CLA	C2A-C1A-CHA	-2.45	119.58	123.86
23	c	514	CLA	C2A-C1A-CHA	-2.45	119.58	123.86
25	C	515	BCR	C23-C24-C25	-2.44	120.34	127.20
25	c	515	BCR	C23-C24-C25	-2.44	120.34	127.20
25	Y	101	BCR	C16-C17-C18	-2.44	123.83	127.31
23	A	408	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
23	a	408	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
28	C	501	SQD	O7-S-C6	2.44	109.84	106.94
28	c	501	SQD	O7-S-C6	2.44	109.84	106.94
23	c	510	CLA	O2A-CGA-CBA	2.44	119.55	111.91
23	A	405	CLA	C5-C3-C2	-2.44	116.19	121.12
23	a	405	CLA	C5-C3-C2	-2.44	116.19	121.12
23	B	612	CLA	CHC-C1C-NC	2.44	127.90	124.20
23	b	612	CLA	CHC-C1C-NC	2.44	127.90	124.20
23	C	510	CLA	O2A-CGA-CBA	2.44	119.55	111.91
23	C	505	CLA	CMB-C2B-C1B	2.43	129.08	125.37
23	c	505	CLA	CMB-C2B-C1B	2.43	129.08	125.37
23	C	508	CLA	O1D-CGD-CBD	-2.43	119.50	124.48
23	c	508	CLA	O1D-CGD-CBD	-2.43	119.50	124.48
23	D	405	CLA	C4-C3-C5	2.43	119.36	115.27
23	d	405	CLA	C4-C3-C5	2.43	119.36	115.27
23	B	613	CLA	C7-C6-C5	-2.43	106.76	113.36
23	b	613	CLA	C7-C6-C5	-2.43	106.76	113.36
23	A	406	CLA	C3B-C4B-NB	2.43	112.77	110.52
23	a	406	CLA	C3B-C4B-NB	2.43	112.77	110.52
23	C	505	CLA	OBD-CAD-C3D	-2.43	122.67	128.52
23	c	505	CLA	OBD-CAD-C3D	-2.43	122.67	128.52
23	C	514	CLA	OBD-CAD-C3D	-2.43	122.68	128.52
26	A	410	LMG	C1-O6-C5	-2.43	108.92	113.69
26	a	410	LMG	C1-O6-C5	-2.43	108.92	113.69
23	B	608	CLA	OBD-CAD-C3D	-2.43	122.68	128.52
23	b	608	CLA	OBD-CAD-C3D	-2.43	122.68	128.52
23	A	405	CLA	CHC-C1C-NC	2.42	127.88	124.20
23	a	405	CLA	CHC-C1C-NC	2.42	127.88	124.20
23	B	603	CLA	C2A-C1A-CHA	-2.42	119.62	123.86
23	b	603	CLA	C2A-C1A-CHA	-2.42	119.62	123.86
23	B	611	CLA	CHB-C4A-NA	2.42	127.86	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	611	CLA	CHB-C4A-NA	2.42	127.86	124.51
23	B	604	CLA	CMB-C2B-C1B	2.42	129.06	125.37
23	C	513	CLA	CHD-C4C-NC	2.42	128.02	124.20
23	c	513	CLA	CHD-C4C-NC	2.42	128.02	124.20
23	c	514	CLA	OBD-CAD-C3D	-2.42	122.70	128.52
24	D	401	PHO	CBA-CAA-C2A	-2.42	106.75	113.81
24	d	401	PHO	CBA-CAA-C2A	-2.42	106.75	113.81
23	b	612	CLA	C11-C12-C13	-2.41	108.12	115.92
25	B	618	BCR	C30-C25-C24	-2.41	118.11	119.86
23	b	609	CLA	CHD-C4C-NC	2.41	127.99	124.20
23	B	609	CLA	CHD-C4C-NC	2.40	127.99	124.20
23	B	610	CLA	C1-C2-C3	-2.40	121.88	126.04
23	b	610	CLA	C1-C2-C3	-2.40	121.88	126.04
23	B	615	CLA	C1-O2A-CGA	2.40	122.75	116.44
23	b	615	CLA	C1-O2A-CGA	2.40	122.75	116.44
23	B	612	CLA	C11-C12-C13	-2.40	108.15	115.92
23	b	604	CLA	CMB-C2B-C1B	2.40	129.03	125.37
23	b	614	CLA	CHD-C4C-NC	2.40	127.99	124.20
23	B	615	CLA	C4C-C3C-C2C	-2.40	103.40	106.90
23	b	615	CLA	C4C-C3C-C2C	-2.40	103.40	106.90
23	B	614	CLA	CHD-C4C-NC	2.40	127.98	124.20
23	C	509	CLA	CHC-C1C-C2C	-2.40	120.07	126.73
23	c	509	CLA	CHC-C1C-C2C	-2.40	120.07	126.73
23	B	610	CLA	CHB-C4A-NA	2.39	127.82	124.51
23	b	610	CLA	CHB-C4A-NA	2.39	127.82	124.51
25	b	618	BCR	C30-C25-C24	-2.39	118.12	119.86
25	K	102	BCR	C11-C10-C9	-2.39	123.90	127.31
25	k	102	BCR	C11-C10-C9	-2.39	123.90	127.31
23	B	608	CLA	CAA-C2A-C3A	-2.39	106.24	112.78
23	b	608	CLA	CAA-C2A-C3A	-2.39	106.24	112.78
24	D	401	PHO	CAC-C3C-C4C	2.38	130.31	124.27
24	d	401	PHO	CAC-C3C-C4C	2.38	130.31	124.27
25	C	516	BCR	C37-C22-C23	2.38	121.83	118.08
25	c	516	BCR	C37-C22-C23	2.38	121.83	118.08
23	B	616	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
23	b	616	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
28	C	501	SQD	O48-C23-C24	2.38	119.38	111.91
28	c	501	SQD	O48-C23-C24	2.38	119.38	111.91
23	C	509	CLA	CAC-C3C-C4C	2.38	127.89	124.81
23	c	509	CLA	CAC-C3C-C4C	2.38	127.89	124.81
23	B	609	CLA	C3B-C4B-NB	2.38	112.72	110.52
23	b	609	CLA	C3B-C4B-NB	2.38	112.72	110.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	501	SQD	O5-C1-O6	2.38	115.60	109.97
28	c	501	SQD	O5-C1-O6	2.38	115.60	109.97
28	D	415	SQD	O48-C23-C24	2.37	122.73	112.38
28	d	415	SQD	O48-C23-C24	2.37	122.73	112.38
37	V	201	HEC	CHD-C4C-C3C	-2.37	121.20	125.26
37	v	201	HEC	CHD-C4C-C3C	-2.37	121.20	125.26
26	D	412	LMG	O2-C2-C1	-2.37	104.28	110.05
26	d	412	LMG	O2-C2-C1	-2.37	104.28	110.05
24	A	407	PHO	CMD-C2D-C3D	2.37	129.11	124.68
24	a	407	PHO	CMD-C2D-C3D	2.37	129.11	124.68
25	D	407	BCR	C20-C21-C22	-2.37	123.93	127.31
25	d	407	BCR	C20-C21-C22	-2.37	123.93	127.31
31	C	517	DGD	O3G-C3G-C2G	-2.37	105.19	110.90
31	c	517	DGD	O3G-C3G-C2G	-2.37	105.19	110.90
33	D	409	LHG	O8-C23-O10	-2.36	117.62	123.59
33	d	409	LHG	O8-C23-O10	-2.36	117.62	123.59
27	D	408	PL9	C53-C6-C1	2.36	119.82	114.99
27	d	408	PL9	C53-C6-C1	2.36	119.82	114.99
25	B	619	BCR	C36-C18-C19	2.36	121.79	118.08
25	b	619	BCR	C36-C18-C19	2.36	121.79	118.08
25	K	102	BCR	C32-C1-C6	-2.36	106.47	110.30
25	k	102	BCR	C32-C1-C6	-2.36	106.47	110.30
23	C	502	CLA	CHC-C1C-C2C	-2.35	120.19	126.73
23	c	502	CLA	CHC-C1C-C2C	-2.35	120.19	126.73
23	B	602	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
23	b	602	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
25	K	102	BCR	C20-C21-C22	-2.35	123.95	127.31
25	k	102	BCR	C20-C21-C22	-2.35	123.95	127.31
23	C	507	CLA	CGD-CBD-CAD	-2.35	103.13	110.73
23	c	507	CLA	CGD-CBD-CAD	-2.35	103.13	110.73
23	B	609	CLA	CMB-C2B-C1B	2.34	128.94	125.37
23	b	609	CLA	CMB-C2B-C1B	2.34	128.94	125.37
23	B	605	CLA	C1D-CHD-C4C	-2.34	121.00	126.06
23	b	605	CLA	C1D-CHD-C4C	-2.34	121.00	126.06
23	B	610	CLA	CMC-C2C-C1C	2.34	128.61	125.04
23	b	610	CLA	CMC-C2C-C1C	2.34	128.61	125.04
23	B	611	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
23	b	611	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
28	C	501	SQD	O48-C23-O10	-2.34	117.69	123.59
28	c	501	SQD	O48-C23-O10	-2.34	117.69	123.59
23	C	510	CLA	CHD-C4C-NC	2.33	127.88	124.20
23	c	510	CLA	CHD-C4C-NC	2.33	127.88	124.20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	618	BCR	C30-C25-C26	-2.33	119.04	121.15
31	C	518	DGD	O1G-C1A-O1A	-2.33	117.72	123.59
31	c	518	DGD	O1G-C1A-O1A	-2.33	117.72	123.59
23	B	608	CLA	CHB-C4A-NA	2.32	127.72	124.51
23	b	608	CLA	CHB-C4A-NA	2.32	127.72	124.51
23	B	608	CLA	C11-C10-C8	-2.32	108.41	115.92
23	b	608	CLA	C11-C10-C8	-2.32	108.41	115.92
35	H	101	RRX	C24-C23-C22	-2.32	122.73	126.23
35	h	101	RRX	C24-C23-C22	-2.32	122.73	126.23
25	Y	101	BCR	C10-C11-C12	-2.32	115.98	123.22
25	y	101	BCR	C10-C11-C12	-2.32	115.98	123.22
23	A	405	CLA	CAA-C2A-C3A	-2.32	106.43	112.78
23	a	405	CLA	CAA-C2A-C3A	-2.32	106.43	112.78
37	V	201	HEC	CAA-C2A-C1A	2.32	129.26	124.89
37	v	201	HEC	CAA-C2A-C1A	2.32	129.26	124.89
25	B	618	BCR	C30-C25-C26	-2.32	119.06	121.15
34	F	101	HEM	O2A-CGA-CBA	2.31	121.46	114.03
34	f	101	HEM	O2A-CGA-CBA	2.31	121.46	114.03
23	B	602	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
23	b	602	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
23	B	601	CLA	CHD-C4C-NC	2.31	127.84	124.20
23	b	601	CLA	CHD-C4C-NC	2.31	127.84	124.20
23	C	512	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
23	c	512	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
25	B	619	BCR	C16-C17-C18	-2.31	124.02	127.31
25	b	619	BCR	C16-C17-C18	-2.31	124.02	127.31
23	C	506	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
23	c	502	CLA	CAC-C3C-C4C	2.30	127.80	124.81
23	C	507	CLA	CED-O2D-CGD	2.30	121.15	115.94
23	c	507	CLA	CED-O2D-CGD	2.30	121.15	115.94
23	B	608	CLA	C11-C12-C13	-2.30	108.47	115.92
23	b	608	CLA	C11-C12-C13	-2.30	108.47	115.92
23	C	505	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
23	c	505	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
25	D	407	BCR	C37-C22-C23	2.30	121.70	118.08
25	d	407	BCR	C37-C22-C23	2.30	121.70	118.08
27	D	408	PL9	C37-C38-C39	-2.30	122.12	127.66
27	d	408	PL9	C37-C38-C39	-2.30	122.12	127.66
23	B	611	CLA	C1C-C2C-C3C	-2.30	104.54	106.96
23	b	611	CLA	C1C-C2C-C3C	-2.30	104.54	106.96
23	B	615	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
23	b	615	CLA	O2D-CGD-O1D	-2.30	119.35	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406	CLA	CMA-C3A-C2A	-2.30	104.57	113.83
23	a	406	CLA	CMA-C3A-C2A	-2.30	104.57	113.83
23	B	610	CLA	C4A-NA-C1A	-2.29	105.67	106.71
23	b	610	CLA	C4A-NA-C1A	-2.29	105.67	106.71
23	B	614	CLA	C4C-C3C-C2C	-2.29	103.56	106.90
23	b	614	CLA	C4C-C3C-C2C	-2.29	103.56	106.90
23	c	506	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
23	C	502	CLA	CAC-C3C-C4C	2.29	127.78	124.81
23	B	609	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
23	b	609	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
25	C	515	BCR	C4-C5-C6	-2.29	121.45	124.37
25	c	515	BCR	C4-C5-C6	-2.29	121.45	124.37
26	A	410	LMG	O8-C28-C29	2.29	119.09	111.91
26	a	410	LMG	O8-C28-C29	2.29	119.09	111.91
23	C	506	CLA	CMC-C2C-C1C	2.29	128.52	125.04
23	C	504	CLA	CHD-C4C-NC	2.29	127.81	124.20
23	B	611	CLA	C2A-C1A-CHA	-2.28	119.86	123.86
23	b	611	CLA	C2A-C1A-CHA	-2.28	119.86	123.86
23	B	613	CLA	O2A-CGA-CBA	2.28	119.07	111.91
23	b	613	CLA	O2A-CGA-CBA	2.28	119.07	111.91
23	B	603	CLA	CMA-C3A-C2A	-2.28	104.63	113.83
23	b	603	CLA	CMA-C3A-C2A	-2.28	104.63	113.83
23	D	406	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
23	d	406	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
23	c	504	CLA	CHD-C4C-NC	2.28	127.80	124.20
25	B	618	BCR	C15-C16-C17	-2.28	118.81	123.47
25	b	618	BCR	C15-C16-C17	-2.28	118.81	123.47
23	C	508	CLA	CHD-C4C-NC	2.28	127.79	124.20
23	c	508	CLA	CHD-C4C-NC	2.28	127.79	124.20
23	c	506	CLA	CED-O2D-CGD	2.28	121.09	115.94
23	C	511	CLA	CHA-C1A-NA	-2.28	121.18	126.40
23	c	511	CLA	CHA-C1A-NA	-2.28	121.18	126.40
23	B	606	CLA	CAA-C2A-C3A	-2.27	106.55	112.78
23	b	606	CLA	CAA-C2A-C3A	-2.27	106.55	112.78
25	D	407	BCR	C8-C7-C6	-2.27	120.82	127.20
25	d	407	BCR	C8-C7-C6	-2.27	120.82	127.20
25	B	619	BCR	C3-C4-C5	-2.27	110.02	114.08
25	b	619	BCR	C3-C4-C5	-2.27	110.02	114.08
23	C	502	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
23	c	502	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
23	c	506	CLA	CMC-C2C-C1C	2.27	128.50	125.04
23	A	405	CLA	C2A-C1A-CHA	-2.27	119.89	123.86

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	405	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
23	C	512	CLA	C1-O2A-CGA	2.27	122.40	116.44
23	c	512	CLA	C1-O2A-CGA	2.27	122.40	116.44
27	A	411	PL9	C10-C9-C11	2.27	119.08	115.27
27	a	411	PL9	C10-C9-C11	2.27	119.08	115.27
25	T	101	BCR	C20-C21-C22	-2.26	124.05	127.30
25	t	103	BCR	C20-C21-C22	-2.26	124.05	127.30
23	b	616	CLA	OBD-CAD-C3D	-2.26	123.08	128.52
25	d	407	BCR	C15-C16-C17	-2.26	118.84	123.47
23	B	613	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
23	b	613	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
23	C	506	CLA	CED-O2D-CGD	2.26	121.05	115.94
23	B	602	CLA	CMB-C2B-C3B	2.26	132.06	126.59
23	b	602	CLA	CMB-C2B-C3B	2.26	132.06	126.59
23	B	609	CLA	CHB-C1B-C2B	-2.26	120.86	127.24
23	b	609	CLA	CHB-C1B-C2B	-2.26	120.86	127.24
37	V	201	HEC	CHA-C1A-C2A	-2.26	121.28	124.94
37	v	201	HEC	CHA-C1A-C2A	-2.26	121.28	124.94
23	C	506	CLA	C11-C10-C8	-2.26	108.63	115.92
23	c	506	CLA	C11-C10-C8	-2.26	108.63	115.92
25	D	407	BCR	C15-C16-C17	-2.25	118.86	123.47
25	B	617	BCR	C11-C10-C9	-2.25	124.10	127.31
25	b	617	BCR	C11-C10-C9	-2.25	124.10	127.31
23	B	616	CLA	OBD-CAD-C3D	-2.25	123.11	128.52
26	C	520	LMG	O8-C9-C8	2.24	114.97	108.43
26	c	520	LMG	O8-C9-C8	2.24	114.97	108.43
37	V	201	HEC	CHB-C1B-C2B	-2.24	120.90	127.24
37	v	201	HEC	CHB-C1B-C2B	-2.24	120.90	127.24
23	C	509	CLA	CAC-C3C-C2C	2.24	131.36	127.53
23	c	509	CLA	CAC-C3C-C2C	2.24	131.36	127.53
23	b	605	CLA	C5-C3-C2	-2.24	116.58	121.12
23	C	511	CLA	C3B-C4B-NB	2.24	112.59	110.52
23	c	511	CLA	C3B-C4B-NB	2.24	112.59	110.52
25	Y	101	BCR	C15-C16-C17	-2.24	118.89	123.47
25	y	101	BCR	C15-C16-C17	-2.24	118.89	123.47
23	C	509	CLA	CMB-C2B-C1B	2.24	128.78	125.37
23	c	509	CLA	CMB-C2B-C1B	2.24	128.78	125.37
23	C	509	CLA	CHB-C4A-NA	2.24	127.61	124.51
23	c	509	CLA	CHB-C4A-NA	2.24	127.61	124.51
23	B	602	CLA	CMA-C3A-C2A	-2.24	104.81	113.83
23	b	602	CLA	CMA-C3A-C2A	-2.24	104.81	113.83
23	B	614	CLA	C3B-C4B-NB	2.24	112.59	110.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	614	CLA	C3B-C4B-NB	2.24	112.59	110.52
23	B	607	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
23	b	607	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
23	B	605	CLA	C5-C3-C2	-2.24	116.59	121.12
23	A	405	CLA	CAA-C2A-C1A	-2.23	104.65	111.97
23	a	405	CLA	CAA-C2A-C1A	-2.23	104.65	111.97
31	H	102	DGD	O6D-C5D-C4D	-2.23	105.64	109.69
31	h	102	DGD	O6D-C5D-C4D	-2.23	105.64	109.69
25	Y	101	BCR	C1-C6-C5	-2.23	119.47	122.61
25	y	101	BCR	C1-C6-C5	-2.23	119.47	122.61
23	B	607	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
23	b	607	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
23	B	613	CLA	CHB-C4A-NA	2.23	127.60	124.51
23	b	613	CLA	CHB-C4A-NA	2.23	127.60	124.51
33	D	409	LHG	O7-C7-C8	2.23	116.31	111.50
33	d	409	LHG	O7-C7-C8	2.23	116.31	111.50
24	A	407	PHO	CAC-C3C-C4C	2.23	129.92	124.27
24	a	407	PHO	CAC-C3C-C4C	2.23	129.92	124.27
27	D	408	PL9	O1-C4-C3	-2.23	118.27	120.72
23	B	615	CLA	CHB-C1B-C2B	-2.23	120.95	127.24
23	b	615	CLA	CHB-C1B-C2B	-2.23	120.95	127.24
23	C	505	CLA	CHB-C1B-NB	-2.23	121.90	124.26
23	c	505	CLA	CHB-C1B-NB	-2.23	121.90	124.26
25	B	617	BCR	C19-C18-C17	-2.22	115.53	118.94
25	b	617	BCR	C19-C18-C17	-2.22	115.53	118.94
23	C	506	CLA	C16-C15-C13	-2.22	108.74	115.92
23	c	506	CLA	C16-C15-C13	-2.22	108.74	115.92
23	B	611	CLA	CHB-C1B-C2B	-2.22	120.97	127.24
23	b	611	CLA	CHB-C1B-C2B	-2.22	120.97	127.24
23	B	610	CLA	CED-O2D-CGD	2.22	120.95	115.94
23	b	610	CLA	CED-O2D-CGD	2.22	120.95	115.94
37	v	201	HEC	CHC-C1C-C2C	-2.22	120.98	127.24
28	C	501	SQD	C9-C8-C7	-2.22	105.24	114.34
28	c	501	SQD	C9-C8-C7	-2.22	105.24	114.34
23	C	504	CLA	C3B-C4B-NB	2.22	112.57	110.52
23	c	504	CLA	C3B-C4B-NB	2.22	112.57	110.52
23	C	505	CLA	C11-C10-C8	-2.21	108.76	115.92
23	c	505	CLA	C11-C10-C8	-2.21	108.76	115.92
23	b	602	CLA	CHD-C4C-NC	2.21	127.69	124.20
37	V	201	HEC	CHC-C1C-C2C	-2.21	120.99	127.24
23	B	602	CLA	CHD-C4C-NC	2.21	127.69	124.20
23	C	511	CLA	C4-C3-C2	-2.21	118.01	123.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	C4-C3-C2	-2.21	118.01	123.68
27	d	408	PL9	O1-C4-C3	-2.21	118.29	120.72
37	V	201	HEC	C3B-C4B-NB	2.21	113.66	110.58
37	v	201	HEC	C3B-C4B-NB	2.21	113.66	110.58
23	A	406	CLA	CAA-C2A-C3A	-2.20	106.75	112.78
23	a	406	CLA	CAA-C2A-C3A	-2.20	106.75	112.78
25	B	619	BCR	C1-C6-C5	-2.20	119.51	122.61
25	b	619	BCR	C1-C6-C5	-2.20	119.51	122.61
25	K	102	BCR	C23-C24-C25	-2.20	121.03	127.20
25	k	102	BCR	C23-C24-C25	-2.20	121.03	127.20
23	B	610	CLA	C1D-CHD-C4C	-2.20	121.32	126.06
23	b	610	CLA	C1D-CHD-C4C	-2.20	121.32	126.06
37	V	201	HEC	CMA-C3A-C4A	2.19	128.58	124.71
37	v	201	HEC	CMA-C3A-C4A	2.19	128.58	124.71
23	B	602	CLA	C4-C3-C5	2.19	118.96	115.27
23	b	602	CLA	C4-C3-C5	2.19	118.96	115.27
23	B	606	CLA	C4-C3-C5	2.19	118.95	115.27
23	b	606	CLA	C4-C3-C5	2.19	118.95	115.27
23	C	509	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
23	c	509	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
23	B	614	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
23	b	614	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
23	B	605	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
23	b	605	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
26	c	520	LMG	O8-C28-O10	-2.19	118.07	123.59
23	C	511	CLA	CHD-C4C-NC	2.19	127.65	124.20
23	D	406	CLA	CHB-C4A-NA	2.19	127.54	124.51
23	d	406	CLA	CHB-C4A-NA	2.19	127.54	124.51
25	B	617	BCR	C16-C15-C14	-2.19	118.99	123.47
25	b	617	BCR	C16-C15-C14	-2.19	118.99	123.47
26	C	520	LMG	O8-C28-O10	-2.19	118.07	123.59
24	a	407	PHO	C4B-NB-C1B	-2.19	105.44	108.83
23	B	613	CLA	O2D-CGD-CBD	2.18	115.15	111.27
23	b	613	CLA	O2D-CGD-CBD	2.18	115.15	111.27
23	C	510	CLA	C16-C15-C13	-2.18	108.86	115.92
23	c	510	CLA	C16-C15-C13	-2.18	108.86	115.92
25	B	619	BCR	C24-C23-C22	-2.18	122.94	126.23
25	b	619	BCR	C24-C23-C22	-2.18	122.94	126.23
23	A	408	CLA	CMB-C2B-C3B	2.18	131.87	126.59
23	a	408	CLA	CMB-C2B-C3B	2.18	131.87	126.59
23	C	507	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
23	B	610	CLA	OBD-CAD-C3D	-2.18	123.28	128.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	OBD-CAD-C3D	-2.18	123.28	128.52
23	c	511	CLA	CHD-C4C-NC	2.17	127.63	124.20
23	C	508	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
23	c	508	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
26	D	412	LMG	O8-C28-O10	-2.17	118.12	123.59
26	d	412	LMG	O8-C28-O10	-2.17	118.12	123.59
23	c	507	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
23	A	408	CLA	CMA-C3A-C4A	-2.17	105.95	111.77
23	a	408	CLA	CMA-C3A-C4A	-2.17	105.95	111.77
23	C	504	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
23	c	504	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
23	c	504	CLA	O2A-CGA-CBA	2.17	118.70	111.91
24	A	407	PHO	C4B-NB-C1B	-2.16	105.48	108.83
37	V	201	HEC	CHB-C4A-C3A	-2.16	120.94	125.48
37	v	201	HEC	CHB-C4A-C3A	-2.16	120.94	125.48
23	C	504	CLA	O2A-CGA-CBA	2.16	118.69	111.91
28	T	103	SQD	C9-C8-C7	-2.16	105.76	113.62
28	t	101	SQD	C9-C8-C7	-2.16	105.76	113.62
23	B	608	CLA	CMA-C3A-C4A	-2.16	105.98	111.77
23	b	608	CLA	CMA-C3A-C4A	-2.16	105.98	111.77
27	D	408	PL9	C20-C19-C21	2.16	118.90	115.27
23	C	503	CLA	CHA-C1A-NA	-2.15	121.46	126.40
23	c	503	CLA	CHA-C1A-NA	-2.15	121.46	126.40
25	C	515	BCR	C2-C1-C6	2.15	112.92	109.20
25	c	515	BCR	C2-C1-C6	2.15	112.92	109.20
25	B	618	BCR	C2-C1-C6	2.15	113.79	110.48
25	b	618	BCR	C2-C1-C6	2.15	113.79	110.48
23	B	609	CLA	C1-C2-C3	-2.15	122.33	126.04
23	b	609	CLA	C1-C2-C3	-2.15	122.33	126.04
23	B	607	CLA	C2A-C1A-CHA	-2.14	120.11	123.86
23	b	607	CLA	C2A-C1A-CHA	-2.14	120.11	123.86
24	A	407	PHO	C4A-C3A-C2A	-2.14	100.80	102.84
24	a	407	PHO	C4A-C3A-C2A	-2.14	100.80	102.84
23	C	510	CLA	CMC-C2C-C1C	2.14	128.30	125.04
23	c	510	CLA	CMC-C2C-C1C	2.14	128.30	125.04
23	B	609	CLA	C1-O2A-CGA	2.14	122.06	116.44
23	b	609	CLA	C1-O2A-CGA	2.14	122.06	116.44
23	B	607	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
23	b	607	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
33	L	101	LHG	O8-C23-C24	2.14	118.61	111.91
33	l	101	LHG	O8-C23-C24	2.14	118.61	111.91
30	B	621	LMT	O1B-C4'-C5'	-2.14	103.59	109.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	621	LMT	O1B-C4'-C5'	-2.14	103.59	109.45
23	B	605	CLA	C14-C13-C12	-2.13	103.58	111.29
23	b	605	CLA	C14-C13-C12	-2.13	103.58	111.29
27	d	408	PL9	C20-C19-C21	2.13	118.85	115.27
23	D	405	CLA	C3B-C4B-NB	2.13	112.49	110.52
23	d	405	CLA	C3B-C4B-NB	2.13	112.49	110.52
23	B	615	CLA	CHB-C4A-NA	2.12	127.45	124.51
23	b	615	CLA	CHB-C4A-NA	2.12	127.45	124.51
33	D	411	LHG	O8-C23-O10	-2.12	118.24	123.59
33	d	411	LHG	O8-C23-O10	-2.12	118.24	123.59
31	H	102	DGD	O2G-C1B-O1B	-2.12	118.58	123.70
31	h	102	DGD	O2G-C1B-O1B	-2.12	118.58	123.70
23	B	604	CLA	OBD-CAD-C3D	-2.12	123.42	128.52
23	b	604	CLA	OBD-CAD-C3D	-2.12	123.42	128.52
23	B	606	CLA	O2A-CGA-CBA	2.11	118.54	111.91
23	b	606	CLA	O2A-CGA-CBA	2.11	118.54	111.91
23	B	615	CLA	CBC-CAC-C3C	-2.11	106.61	112.43
23	b	615	CLA	CBC-CAC-C3C	-2.11	106.61	112.43
23	B	613	CLA	CBC-CAC-C3C	-2.11	106.61	112.43
23	d	402	CLA	C3A-C2A-C1A	-2.11	98.18	101.34
23	C	507	CLA	CHB-C4A-NA	2.11	127.43	124.51
23	c	507	CLA	CHB-C4A-NA	2.11	127.43	124.51
23	D	406	CLA	CED-O2D-CGD	2.11	120.70	115.94
23	d	406	CLA	CED-O2D-CGD	2.11	120.70	115.94
23	B	616	CLA	CHB-C4A-NA	2.11	127.42	124.51
23	b	616	CLA	CHB-C4A-NA	2.11	127.42	124.51
23	b	613	CLA	CBC-CAC-C3C	-2.11	106.62	112.43
23	B	605	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
23	b	605	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
23	B	603	CLA	CMC-C2C-C1C	2.10	128.23	125.04
23	b	603	CLA	CMC-C2C-C1C	2.10	128.23	125.04
23	C	506	CLA	CAA-C2A-C1A	2.10	118.85	111.97
23	c	506	CLA	CAA-C2A-C1A	2.10	118.85	111.97
25	B	619	BCR	C15-C16-C17	-2.10	119.18	123.47
25	b	619	BCR	C15-C16-C17	-2.10	119.18	123.47
37	V	201	HEC	CHA-C4D-C3D	-2.09	120.78	125.36
37	v	201	HEC	CHA-C4D-C3D	-2.09	120.78	125.36
23	C	508	CLA	C1-C2-C3	-2.09	122.42	126.04
23	c	508	CLA	C1-C2-C3	-2.09	122.42	126.04
23	C	504	CLA	OBD-CAD-C3D	-2.09	123.49	128.52
23	c	504	CLA	OBD-CAD-C3D	-2.09	123.49	128.52
25	B	617	BCR	C21-C20-C19	-2.09	116.69	123.22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	617	BCR	C21-C20-C19	-2.09	116.69	123.22
25	C	516	BCR	C34-C9-C10	-2.09	120.00	122.92
25	c	516	BCR	C34-C9-C10	-2.09	120.00	122.92
23	B	611	CLA	C4-C3-C5	2.09	118.78	115.27
23	b	611	CLA	C4-C3-C5	2.09	118.78	115.27
23	A	408	CLA	CHD-C4C-NC	2.09	127.49	124.20
23	a	408	CLA	CHD-C4C-NC	2.09	127.49	124.20
23	C	505	CLA	C1-C2-C3	-2.09	122.44	126.04
23	c	505	CLA	C1-C2-C3	-2.09	122.44	126.04
30	M	101	LMT	C1'-O5'-C5'	-2.09	109.59	113.69
30	m	101	LMT	C1'-O5'-C5'	-2.09	109.59	113.69
23	B	603	CLA	CHC-C4B-NB	2.09	126.47	124.26
23	b	603	CLA	CHC-C4B-NB	2.09	126.47	124.26
23	B	615	CLA	C11-C10-C8	-2.09	109.18	115.92
23	b	615	CLA	C11-C10-C8	-2.09	109.18	115.92
23	B	611	CLA	CHC-C1C-C2C	-2.08	120.94	126.73
23	b	611	CLA	CHC-C1C-C2C	-2.08	120.94	126.73
25	K	102	BCR	C3-C4-C5	-2.08	110.36	114.08
25	k	102	BCR	C3-C4-C5	-2.08	110.36	114.08
31	C	519	DGD	O5E-C6E-C5E	-2.08	104.15	111.29
31	c	519	DGD	O5E-C6E-C5E	-2.08	104.15	111.29
37	V	201	HEC	CMB-C2B-C3B	2.08	131.62	126.59
37	v	201	HEC	CMB-C2B-C3B	2.08	131.62	126.59
23	D	402	CLA	C3A-C2A-C1A	-2.08	98.23	101.34
23	B	605	CLA	CHD-C4C-NC	2.08	127.48	124.20
23	b	605	CLA	CHD-C4C-NC	2.08	127.48	124.20
23	A	405	CLA	O2A-CGA-CBA	2.08	118.43	111.91
23	a	405	CLA	O2A-CGA-CBA	2.08	118.43	111.91
23	C	504	CLA	CHB-C1B-C2B	-2.08	121.37	127.24
23	c	504	CLA	CHB-C1B-C2B	-2.08	121.37	127.24
35	H	101	RRX	C36-C18-C17	-2.08	120.01	122.92
35	h	101	RRX	C36-C18-C17	-2.08	120.01	122.92
23	D	406	CLA	CMA-C3A-C4A	-2.08	106.19	111.77
23	d	406	CLA	CMA-C3A-C4A	-2.08	106.19	111.77
23	C	503	CLA	C3B-C4B-NB	2.08	112.44	110.52
23	c	503	CLA	C3B-C4B-NB	2.08	112.44	110.52
23	A	408	CLA	OBD-CAD-C3D	-2.07	123.53	128.52
23	a	408	CLA	OBD-CAD-C3D	-2.07	123.53	128.52
27	A	411	PL9	C11-C9-C8	-2.07	116.93	121.12
27	a	411	PL9	C11-C9-C8	-2.07	116.93	121.12
23	A	405	CLA	CMA-C3A-C4A	-2.07	106.21	111.77
23	a	405	CLA	CMA-C3A-C4A	-2.07	106.21	111.77

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	CHB-C1B-C2B	-2.07	121.39	127.24
23	c	513	CLA	CHB-C1B-C2B	-2.07	121.39	127.24
23	c	507	CLA	CHD-C4C-NC	2.07	127.46	124.20
28	A	412	SQD	C3-C4-C5	2.06	113.92	110.24
28	a	412	SQD	C3-C4-C5	2.06	113.92	110.24
30	M	101	LMT	O1'-C1'-C2'	2.06	111.52	108.30
28	C	501	SQD	C45-O47-C7	-2.06	112.72	117.79
28	c	501	SQD	C45-O47-C7	-2.06	112.72	117.79
23	B	606	CLA	C1-C2-C3	-2.06	122.48	126.04
23	b	606	CLA	C1-C2-C3	-2.06	122.48	126.04
23	B	601	CLA	C3B-C4B-NB	2.06	112.43	110.52
23	b	601	CLA	C3B-C4B-NB	2.06	112.43	110.52
23	A	406	CLA	C4-C3-C5	2.06	118.74	115.27
23	a	406	CLA	C4-C3-C5	2.06	118.74	115.27
25	K	102	BCR	C36-C18-C19	2.06	121.32	118.08
25	k	102	BCR	C36-C18-C19	2.06	121.32	118.08
33	D	410	LHG	O7-C7-C8	2.06	115.94	111.50
23	C	512	CLA	C4-C3-C5	2.06	118.73	115.27
23	c	512	CLA	C4-C3-C5	2.06	118.73	115.27
35	H	101	RRX	C12-C13-C14	2.06	122.10	118.94
35	h	101	RRX	C12-C13-C14	2.06	122.10	118.94
25	B	618	BCR	C32-C1-C6	-2.06	106.97	110.30
25	b	618	BCR	C32-C1-C6	-2.06	106.97	110.30
23	C	511	CLA	O2A-C1-C2	-2.05	103.24	108.64
23	c	511	CLA	O2A-C1-C2	-2.05	103.24	108.64
23	C	507	CLA	CHD-C4C-NC	2.05	127.44	124.20
27	D	408	PL9	C51-C49-C50	2.05	119.13	114.60
27	d	408	PL9	C51-C49-C50	2.05	119.13	114.60
23	C	511	CLA	C2A-C1A-CHA	-2.05	120.27	123.86
23	c	511	CLA	C2A-C1A-CHA	-2.05	120.27	123.86
25	Y	101	BCR	C21-C20-C19	-2.05	116.82	123.22
25	y	101	BCR	C21-C20-C19	-2.05	116.82	123.22
23	B	610	CLA	CAA-CBA-CGA	-2.05	107.26	113.25
23	b	610	CLA	CAA-CBA-CGA	-2.05	107.26	113.25
23	C	512	CLA	CMB-C2B-C1B	2.05	128.49	125.37
23	c	512	CLA	CMB-C2B-C1B	2.05	128.49	125.37
23	c	504	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
23	B	615	CLA	CHA-C1A-NA	-2.05	121.71	126.40
23	b	615	CLA	CHA-C1A-NA	-2.05	121.71	126.40
30	m	101	LMT	O1'-C1'-C2'	2.05	111.50	108.30
23	b	611	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
23	C	504	CLA	O2A-CGA-O1A	-2.04	118.44	123.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	620	LMG	C30-C29-C28	-2.04	106.19	113.62
33	d	410	LHG	O7-C7-C8	2.04	115.90	111.50
23	A	405	CLA	CHB-C4A-NA	2.04	127.33	124.51
25	D	407	BCR	C11-C10-C9	-2.04	124.40	127.31
25	d	407	BCR	C11-C10-C9	-2.04	124.40	127.31
23	a	405	CLA	CHB-C4A-NA	2.04	127.33	124.51
26	B	620	LMG	C30-C29-C28	-2.04	106.20	113.62
23	B	611	CLA	CMB-C2B-C3B	2.04	131.53	126.59
23	b	611	CLA	CMB-C2B-C3B	2.04	131.53	126.59
23	C	511	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
23	c	511	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
23	C	511	CLA	O2D-CGD-O1D	-2.04	119.86	123.84
23	c	511	CLA	O2D-CGD-O1D	-2.04	119.86	123.84
23	B	611	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
28	T	103	SQD	O47-C7-C8	2.03	120.27	112.23
28	t	101	SQD	O47-C7-C8	2.03	120.27	112.23
23	B	611	CLA	CHA-C1A-NA	-2.03	121.74	126.40
23	b	611	CLA	CHA-C1A-NA	-2.03	121.74	126.40
23	C	510	CLA	CHC-C1C-NC	2.03	127.29	124.20
23	B	608	CLA	C2A-C1A-CHA	-2.03	120.30	123.86
26	D	412	LMG	O8-C28-C29	2.03	118.29	111.91
26	d	412	LMG	O8-C28-C29	2.03	118.29	111.91
23	C	509	CLA	OBD-CAD-C3D	-2.03	123.63	128.52
23	c	509	CLA	OBD-CAD-C3D	-2.03	123.63	128.52
23	b	608	CLA	C2A-C1A-CHA	-2.03	120.31	123.86
25	C	515	BCR	C1-C6-C7	-2.03	118.43	122.84
25	c	515	BCR	C1-C6-C7	-2.03	118.43	122.84
24	A	407	PHO	CMA-C3A-C4A	-2.03	109.93	114.38
24	a	407	PHO	CMA-C3A-C4A	-2.03	109.93	114.38
37	V	201	HEC	CHD-C1D-C2D	-2.03	121.51	127.24
37	v	201	HEC	CHD-C1D-C2D	-2.03	121.51	127.24
23	B	603	CLA	CMB-C2B-C1B	2.03	128.46	125.37
23	b	603	CLA	CMB-C2B-C1B	2.03	128.46	125.37
33	E	101	LHG	O8-C23-C24	2.03	121.22	112.38
33	e	101	LHG	O8-C23-C24	2.03	121.22	112.38
23	C	503	CLA	C3B-C2B-C1B	-2.03	104.71	107.16
23	c	503	CLA	C3B-C2B-C1B	-2.03	104.71	107.16
23	B	611	CLA	C7-C6-C5	-2.03	107.85	113.36
23	b	611	CLA	C7-C6-C5	-2.03	107.85	113.36
23	c	510	CLA	CHC-C1C-NC	2.03	127.28	124.20
23	C	508	CLA	C4C-C3C-C2C	-2.03	103.94	106.90
23	c	508	CLA	C4C-C3C-C2C	-2.03	103.94	106.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	H	102	DGD	O5E-C6E-C5E	-2.03	104.34	111.29
31	h	102	DGD	O5E-C6E-C5E	-2.03	104.34	111.29
23	B	606	CLA	CHB-C1B-C2B	-2.03	121.52	127.24
23	b	606	CLA	CHB-C1B-C2B	-2.03	121.52	127.24
25	B	617	BCR	C33-C5-C6	-2.02	122.25	124.53
25	b	617	BCR	C33-C5-C6	-2.02	122.25	124.53
23	B	612	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
23	b	612	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
23	B	606	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
23	b	606	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
25	C	515	BCR	C36-C18-C17	-2.02	120.10	122.92
25	c	515	BCR	C36-C18-C17	-2.02	120.10	122.92
23	A	405	CLA	C4D-CHA-C1A	-2.02	118.80	121.25
23	a	405	CLA	C4D-CHA-C1A	-2.02	118.80	121.25
24	D	401	PHO	C4B-NB-C1B	-2.02	105.71	108.83
24	d	401	PHO	C4B-NB-C1B	-2.02	105.71	108.83
23	C	512	CLA	CMA-C3A-C4A	2.01	117.19	111.77
23	c	512	CLA	CMA-C3A-C4A	2.01	117.19	111.77
23	B	602	CLA	CHB-C4A-NA	2.01	127.30	124.51
25	A	409	BCR	C40-C30-C25	-2.01	107.04	110.30
25	a	409	BCR	C40-C30-C25	-2.01	107.04	110.30
23	b	602	CLA	CHB-C4A-NA	2.01	127.29	124.51
24	A	407	PHO	C7-C6-C5	-2.01	107.91	113.36
24	a	407	PHO	C7-C6-C5	-2.01	107.91	113.36
28	A	412	SQD	C46-C45-C44	-2.00	107.05	111.79
28	a	412	SQD	C46-C45-C44	-2.00	107.05	111.79
23	C	509	CLA	CMC-C2C-C1C	2.00	128.09	125.04
23	c	509	CLA	CMC-C2C-C1C	2.00	128.09	125.04
23	D	406	CLA	CGD-CBD-CAD	-2.00	104.25	110.73
23	d	406	CLA	CGD-CBD-CAD	-2.00	104.25	110.73
35	H	101	RRX	C24-C25-C26	-2.00	116.62	121.46
35	h	101	RRX	C24-C25-C26	-2.00	116.62	121.46
23	B	604	CLA	O2A-CGA-CBA	2.00	118.18	111.91
23	b	604	CLA	O2A-CGA-CBA	2.00	118.18	111.91

There are no chirality outliers.

All (782) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	605	CLA	C2-C3-C5-C6
23	B	605	CLA	C4-C3-C5-C6
23	B	606	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	B	614	CLA	C2-C3-C5-C6
23	B	614	CLA	C4-C3-C5-C6
23	B	616	CLA	C11-C10-C8-C9
23	C	503	CLA	CHA-CBD-CGD-O1D
23	C	505	CLA	C2-C3-C5-C6
23	C	505	CLA	C4-C3-C5-C6
23	C	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	C	513	CLA	C3-C5-C6-C7
23	b	605	CLA	C2-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
23	b	606	CLA	CHA-CBD-CGD-O1D
23	b	606	CLA	CHA-CBD-CGD-O2D
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	b	614	CLA	C2-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
23	b	616	CLA	C11-C10-C8-C9
23	c	503	CLA	CHA-CBD-CGD-O1D
23	c	505	CLA	C2-C3-C5-C6
23	c	505	CLA	C4-C3-C5-C6
23	c	509	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O2D
23	c	513	CLA	C3-C5-C6-C7
25	B	618	BCR	C23-C24-C25-C26
25	B	618	BCR	C23-C24-C25-C30
25	b	618	BCR	C23-C24-C25-C26
25	b	618	BCR	C23-C24-C25-C30
27	A	411	PL9	C13-C14-C16-C17
27	A	411	PL9	C15-C14-C16-C17
27	a	411	PL9	C13-C14-C16-C17
27	a	411	PL9	C15-C14-C16-C17
28	D	415	SQD	O6-C44-C45-O47
28	d	415	SQD	O6-C44-C45-O47
33	D	410	LHG	C3-O3-P-O5
33	D	410	LHG	C4-O6-P-O4
33	L	101	LHG	C4-O6-P-O5
33	d	410	LHG	C3-O3-P-O5
33	d	410	LHG	C4-O6-P-O4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
33	l	101	LHG	C4-O6-P-O5
33	E	101	LHG	C1-C2-C3-O3
33	E	101	LHG	C3-O3-P-O4
33	E	101	LHG	C3-O3-P-O5
33	e	101	LHG	C1-C2-C3-O3
33	e	101	LHG	C3-O3-P-O4
33	e	101	LHG	C3-O3-P-O5
35	H	101	RRX	C23-C24-C25-C30
35	H	101	RRX	C23-C24-C25-C26
35	H	101	RRX	C37-C22-C23-C24
35	H	101	RRX	C21-C22-C23-C24
35	h	101	RRX	C23-C24-C25-C30
35	h	101	RRX	C23-C24-C25-C26
35	h	101	RRX	C37-C22-C23-C24
35	h	101	RRX	C21-C22-C23-C24
37	V	201	HEC	C2B-C3B-CAB-CBB
37	V	201	HEC	C4B-C3B-CAB-CBB
37	V	201	HEC	C2C-C3C-CAC-CBC
37	V	201	HEC	C4C-C3C-CAC-CBC
37	v	201	HEC	C2B-C3B-CAB-CBB
37	v	201	HEC	C4B-C3B-CAB-CBB
37	v	201	HEC	C2C-C3C-CAC-CBC
37	v	201	HEC	C4C-C3C-CAC-CBC
23	B	616	CLA	C3-C5-C6-C7
23	b	616	CLA	C3-C5-C6-C7
30	B	621	LMT	O5B-C5B-C6B-O6B
30	b	621	LMT	O5B-C5B-C6B-O6B
23	B	604	CLA	C3-C5-C6-C7
23	b	604	CLA	C3-C5-C6-C7
30	J	102	LMT	O5'-C5'-C6'-O6'
30	j	102	LMT	O5'-C5'-C6'-O6'
33	E	101	LHG	O2-C2-C3-O3
33	e	101	LHG	O2-C2-C3-O3
31	C	519	DGD	C8A-C9A-CAA-CBA
31	c	519	DGD	C8A-C9A-CAA-CBA
30	J	102	LMT	C4'-C5'-C6'-O6'
30	j	102	LMT	C4'-C5'-C6'-O6'
23	B	603	CLA	C4-C3-C5-C6
23	C	508	CLA	C4-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	c	508	CLA	C4-C3-C5-C6
23	B	603	CLA	C2-C3-C5-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
23	C	508	CLA	C2-C3-C5-C6
23	b	603	CLA	C2-C3-C5-C6
23	c	508	CLA	C2-C3-C5-C6
23	B	606	CLA	C2A-CAA-CBA-CGA
23	b	606	CLA	C2A-CAA-CBA-CGA
30	B	621	LMT	C4B-C5B-C6B-O6B
30	b	621	LMT	C4B-C5B-C6B-O6B
27	D	408	PL9	C39-C41-C42-C43
27	d	408	PL9	C39-C41-C42-C43
23	C	513	CLA	CBA-CGA-O2A-C1
23	c	513	CLA	CBA-CGA-O2A-C1
31	C	518	DGD	C3B-C4B-C5B-C6B
31	c	518	DGD	C3B-C4B-C5B-C6B
23	B	604	CLA	C6-C7-C8-C9
23	C	510	CLA	C6-C7-C8-C9
23	b	604	CLA	C6-C7-C8-C9
23	c	510	CLA	C6-C7-C8-C9
26	C	520	LMG	C39-C40-C41-C42
26	c	520	LMG	C39-C40-C41-C42
31	C	517	DGD	C1B-C2B-C3B-C4B
31	c	517	DGD	C1B-C2B-C3B-C4B
30	B	621	LMT	C4'-C5'-C6'-O6'
30	b	621	LMT	C4'-C5'-C6'-O6'
26	B	620	LMG	C28-C29-C30-C31
26	b	620	LMG	C28-C29-C30-C31
23	C	509	CLA	C11-C10-C8-C7
23	c	509	CLA	C11-C10-C8-C7
23	C	513	CLA	O1A-CGA-O2A-C1
23	c	513	CLA	O1A-CGA-O2A-C1
33	L	101	LHG	C4-O6-P-O3
33	l	101	LHG	C4-O6-P-O3
33	E	101	LHG	C3-O3-P-O6
33	e	101	LHG	C3-O3-P-O6
23	B	608	CLA	C13-C15-C16-C17
23	b	608	CLA	C13-C15-C16-C17
26	A	410	LMG	C39-C40-C41-C42
26	a	410	LMG	C39-C40-C41-C42
28	D	415	SQD	O6-C44-C45-C46
28	d	415	SQD	O6-C44-C45-C46
28	A	412	SQD	C17-C18-C19-C20
28	a	412	SQD	C17-C18-C19-C20
30	B	623	LMT	C5-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
30	T	104	LMT	C5-C6-C7-C8
33	D	411	LHG	C29-C30-C31-C32
33	d	411	LHG	C29-C30-C31-C32
33	D	409	LHG	C26-C27-C28-C29
33	L	101	LHG	C27-C28-C29-C30
33	d	409	LHG	C26-C27-C28-C29
33	l	101	LHG	C27-C28-C29-C30
26	A	410	LMG	C38-C39-C40-C41
26	a	410	LMG	C38-C39-C40-C41
33	D	409	LHG	C23-C24-C25-C26
33	d	409	LHG	C23-C24-C25-C26
26	A	410	LMG	C2-C1-O1-C7
26	a	410	LMG	C2-C1-O1-C7
30	B	621	LMT	C4-C5-C6-C7
30	b	621	LMT	C4-C5-C6-C7
30	B	621	LMT	C6-C7-C8-C9
30	b	621	LMT	C6-C7-C8-C9
23	B	603	CLA	C6-C7-C8-C9
23	C	511	CLA	C6-C7-C8-C9
23	b	603	CLA	C6-C7-C8-C9
23	c	511	CLA	C6-C7-C8-C9
26	C	520	LMG	C20-C21-C22-C23
26	c	520	LMG	C20-C21-C22-C23
33	E	101	LHG	C18-C19-C20-C21
33	e	101	LHG	C18-C19-C20-C21
30	B	623	LMT	C7-C8-C9-C10
30	T	104	LMT	C7-C8-C9-C10
28	T	103	SQD	C12-C13-C14-C15
28	t	101	SQD	C12-C13-C14-C15
31	H	102	DGD	C6A-C7A-C8A-C9A
31	h	102	DGD	C6A-C7A-C8A-C9A
33	E	101	LHG	C13-C14-C15-C16
33	e	101	LHG	C13-C14-C15-C16
26	A	410	LMG	O6-C1-O1-C7
26	a	410	LMG	O6-C1-O1-C7
30	B	623	LMT	C11-C10-C9-C8
30	T	104	LMT	C11-C10-C9-C8
33	D	411	LHG	C12-C13-C14-C15
33	d	411	LHG	C12-C13-C14-C15
26	A	410	LMG	C30-C31-C32-C33
26	a	410	LMG	C30-C31-C32-C33
30	M	101	LMT	C2-C1-O1'-C1'

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
30	m	101	LMT	C2-C1-O1'-C1'
26	B	620	LMG	C36-C37-C38-C39
26	b	620	LMG	C36-C37-C38-C39
28	A	412	SQD	C10-C11-C12-C13
28	a	412	SQD	C10-C11-C12-C13
27	D	408	PL9	C43-C44-C46-C47
27	d	408	PL9	C43-C44-C46-C47
26	A	410	LMG	C11-C10-O7-C8
26	a	410	LMG	C11-C10-O7-C8
26	D	412	LMG	C12-C13-C14-C15
26	d	412	LMG	C12-C13-C14-C15
23	B	601	CLA	C11-C10-C8-C7
23	b	601	CLA	C11-C10-C8-C7
26	A	410	LMG	O9-C10-O7-C8
26	a	410	LMG	O9-C10-O7-C8
26	A	410	LMG	C16-C17-C18-C19
26	B	620	LMG	C17-C18-C19-C20
26	B	620	LMG	C34-C35-C36-C37
26	a	410	LMG	C16-C17-C18-C19
26	b	620	LMG	C17-C18-C19-C20
26	b	620	LMG	C34-C35-C36-C37
30	B	621	LMT	O5'-C5'-C6'-O6'
30	b	621	LMT	O5'-C5'-C6'-O6'
23	B	606	CLA	C8-C10-C11-C12
23	b	606	CLA	C8-C10-C11-C12
25	B	617	BCR	C1-C6-C7-C8
25	b	617	BCR	C1-C6-C7-C8
26	B	620	LMG	C31-C32-C33-C34
26	b	620	LMG	C31-C32-C33-C34
31	C	517	DGD	O6E-C5E-C6E-O5E
31	c	517	DGD	O6E-C5E-C6E-O5E
28	D	415	SQD	C24-C23-O48-C46
28	d	415	SQD	C24-C23-O48-C46
23	C	513	CLA	C4-C3-C5-C6
23	c	513	CLA	C4-C3-C5-C6
27	D	408	PL9	C45-C44-C46-C47
27	d	408	PL9	C45-C44-C46-C47
23	B	603	CLA	C6-C7-C8-C10
23	B	606	CLA	C12-C13-C15-C16
23	B	611	CLA	C12-C13-C15-C16
23	C	511	CLA	C6-C7-C8-C10
23	b	603	CLA	C6-C7-C8-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
23	b	606	CLA	C12-C13-C15-C16
23	b	611	CLA	C12-C13-C15-C16
23	c	511	CLA	C6-C7-C8-C10
28	A	412	SQD	C13-C14-C15-C16
28	a	412	SQD	C13-C14-C15-C16
30	B	623	LMT	C6-C7-C8-C9
30	T	104	LMT	C6-C7-C8-C9
31	H	102	DGD	CAB-CBB-CCB-CDB
31	h	102	DGD	CAB-CBB-CCB-CDB
33	L	101	LHG	C31-C32-C33-C34
33	l	101	LHG	C31-C32-C33-C34
31	C	519	DGD	CAA-CBA-CCA-CDA
31	c	519	DGD	CAA-CBA-CCA-CDA
30	T	105	LMT	C7-C8-C9-C10
30	t	102	LMT	C7-C8-C9-C10
26	A	410	LMG	C13-C14-C15-C16
26	a	410	LMG	C13-C14-C15-C16
25	C	515	BCR	C5-C6-C7-C8
25	c	515	BCR	C5-C6-C7-C8
28	C	501	SQD	O6-C44-C45-O47
28	c	501	SQD	O6-C44-C45-O47
26	C	520	LMG	C19-C20-C21-C22
26	c	520	LMG	C19-C20-C21-C22
33	d	410	LHG	C32-C33-C34-C35
33	D	410	LHG	C32-C33-C34-C35
28	T	103	SQD	C11-C12-C13-C14
28	t	101	SQD	C11-C12-C13-C14
23	B	611	CLA	C14-C13-C15-C16
23	C	509	CLA	C11-C10-C8-C9
23	b	611	CLA	C14-C13-C15-C16
23	c	509	CLA	C11-C10-C8-C9
28	T	103	SQD	C16-C17-C18-C19
28	t	101	SQD	C16-C17-C18-C19
23	C	513	CLA	C1A-C2A-CAA-CBA
23	c	513	CLA	C1A-C2A-CAA-CBA
33	D	410	LHG	C4-O6-P-O3
33	d	410	LHG	C4-O6-P-O3
31	H	102	DGD	CCB-CDB-CEB-CFB
31	h	102	DGD	CCB-CDB-CEB-CFB
31	C	518	DGD	C1B-C2B-C3B-C4B
31	c	518	DGD	C1B-C2B-C3B-C4B
26	D	412	LMG	O6-C5-C6-O5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
26	d	412	LMG	O6-C5-C6-O5
33	L	101	LHG	C33-C34-C35-C36
33	l	101	LHG	C33-C34-C35-C36
28	A	412	SQD	O6-C44-C45-C46
28	a	412	SQD	O6-C44-C45-C46
31	C	518	DGD	CBB-CCB-CDB-CEB
31	c	518	DGD	CBB-CCB-CDB-CEB
33	L	101	LHG	C14-C15-C16-C17
33	l	101	LHG	C14-C15-C16-C17
31	C	518	DGD	C2G-C3G-O3G-C1D
31	C	518	DGD	C5D-C6D-O5D-C1E
31	c	518	DGD	C2G-C3G-O3G-C1D
31	c	518	DGD	C5D-C6D-O5D-C1E
23	B	616	CLA	C13-C15-C16-C17
23	b	616	CLA	C13-C15-C16-C17
33	D	409	LHG	C24-C23-O8-C6
33	d	409	LHG	C24-C23-O8-C6
23	B	615	CLA	C10-C11-C12-C13
23	b	615	CLA	C10-C11-C12-C13
30	T	105	LMT	O1'-C1-C2-C3
30	t	102	LMT	O1'-C1-C2-C3
23	B	601	CLA	C8-C10-C11-C12
23	b	601	CLA	C8-C10-C11-C12
30	B	621	LMT	C5'-C4'-O1B-C1B
30	b	621	LMT	C5'-C4'-O1B-C1B
23	D	406	CLA	CBA-CGA-O2A-C1
23	d	406	CLA	CBA-CGA-O2A-C1
26	B	620	LMG	C10-C11-C12-C13
26	b	620	LMG	C10-C11-C12-C13
28	T	103	SQD	C15-C16-C17-C18
28	t	101	SQD	C15-C16-C17-C18
33	L	101	LHG	C30-C31-C32-C33
33	l	101	LHG	C30-C31-C32-C33
28	A	412	SQD	C2-C1-O6-C44
28	a	412	SQD	C2-C1-O6-C44
33	D	411	LHG	C31-C32-C33-C34
33	d	411	LHG	C31-C32-C33-C34
26	C	520	LMG	C22-C23-C24-C25
26	c	520	LMG	C22-C23-C24-C25
28	a	412	SQD	C15-C16-C17-C18
33	D	409	LHG	O10-C23-O8-C6
33	d	409	LHG	O10-C23-O8-C6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
28	A	412	SQD	C15-C16-C17-C18
33	E	101	LHG	C17-C18-C19-C20
33	e	101	LHG	C17-C18-C19-C20
26	c	520	LMG	C21-C22-C23-C24
23	B	604	CLA	C6-C7-C8-C10
23	B	616	CLA	C12-C13-C15-C16
23	C	510	CLA	C6-C7-C8-C10
23	D	405	CLA	C12-C13-C15-C16
23	b	604	CLA	C6-C7-C8-C10
23	b	616	CLA	C12-C13-C15-C16
23	c	510	CLA	C6-C7-C8-C10
23	d	405	CLA	C12-C13-C15-C16
26	C	520	LMG	C21-C22-C23-C24
23	C	506	CLA	C11-C12-C13-C14
23	c	506	CLA	C11-C12-C13-C14
30	B	621	LMT	C3'-C4'-O1B-C1B
30	b	621	LMT	C3'-C4'-O1B-C1B
31	c	517	DGD	C3B-C4B-C5B-C6B
31	C	517	DGD	C3B-C4B-C5B-C6B
30	B	621	LMT	C3-C4-C5-C6
30	b	621	LMT	C3-C4-C5-C6
28	A	412	SQD	C11-C10-C9-C8
28	a	412	SQD	C11-C10-C9-C8
33	L	101	LHG	O6-C4-C5-C6
33	l	101	LHG	O6-C4-C5-C6
23	B	601	CLA	CAA-CBA-CGA-O2A
23	b	601	CLA	CAA-CBA-CGA-O2A
23	B	616	CLA	C8-C10-C11-C12
23	b	616	CLA	C8-C10-C11-C12
23	B	601	CLA	C3-C5-C6-C7
23	b	601	CLA	C3-C5-C6-C7
33	E	101	LHG	C24-C23-O8-C6
33	e	101	LHG	C24-C23-O8-C6
26	C	521	LMG	C10-C11-C12-C13
26	c	521	LMG	C10-C11-C12-C13
30	B	621	LMT	C11-C10-C9-C8
30	b	621	LMT	C11-C10-C9-C8
31	H	102	DGD	CDA-CEA-CFA-CGA
31	h	102	DGD	CDA-CEA-CFA-CGA
33	L	101	LHG	C16-C17-C18-C19
33	l	101	LHG	C16-C17-C18-C19
28	C	501	SQD	O6-C44-C45-C46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
28	c	501	SQD	O6-C44-C45-C46
26	D	412	LMG	C30-C31-C32-C33
26	d	412	LMG	C30-C31-C32-C33
31	C	518	DGD	C4B-C5B-C6B-C7B
31	c	518	DGD	C4B-C5B-C6B-C7B
26	C	520	LMG	C10-C11-C12-C13
26	c	520	LMG	C10-C11-C12-C13
23	B	601	CLA	C10-C11-C12-C13
23	b	601	CLA	C10-C11-C12-C13
30	B	623	LMT	C9-C10-C11-C12
30	T	104	LMT	C9-C10-C11-C12
26	A	410	LMG	C29-C30-C31-C32
26	a	410	LMG	C29-C30-C31-C32
23	D	406	CLA	O1A-CGA-O2A-C1
23	d	406	CLA	O1A-CGA-O2A-C1
28	A	412	SQD	O6-C44-C45-O47
28	a	412	SQD	O6-C44-C45-O47
23	C	509	CLA	C11-C12-C13-C14
23	c	509	CLA	C11-C12-C13-C14
28	A	412	SQD	O5-C1-O6-C44
28	a	412	SQD	O5-C1-O6-C44
33	E	101	LHG	C12-C13-C14-C15
33	e	101	LHG	C12-C13-C14-C15
23	B	614	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
23	B	616	CLA	C6-C7-C8-C9
23	b	616	CLA	C6-C7-C8-C9
23	C	505	CLA	C15-C16-C17-C18
23	c	505	CLA	C15-C16-C17-C18
25	B	617	BCR	C5-C6-C7-C8
25	b	617	BCR	C5-C6-C7-C8
23	B	616	CLA	C11-C10-C8-C7
23	b	616	CLA	C11-C10-C8-C7
23	D	402	CLA	C2C-C3C-CAC-CBC
23	d	402	CLA	C2C-C3C-CAC-CBC
28	T	103	SQD	C14-C15-C16-C17
28	t	101	SQD	C14-C15-C16-C17
23	B	604	CLA	CAD-CBD-CGD-O2D
23	C	513	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	c	513	CLA	CAD-CBD-CGD-O2D
28	A	412	SQD	C19-C20-C21-C22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
28	a	412	SQD	C19-C20-C21-C22
23	B	601	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	CHA-CBD-CGD-O2D
23	C	503	CLA	CHA-CBD-CGD-O2D
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	CHA-CBD-CGD-O1D
23	b	601	CLA	CHA-CBD-CGD-O2D
23	c	503	CLA	CHA-CBD-CGD-O2D
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O2D
31	H	102	DGD	C7A-C8A-C9A-CAA
31	h	102	DGD	C7A-C8A-C9A-CAA
33	D	411	LHG	C19-C20-C21-C22
33	d	411	LHG	C19-C20-C21-C22
28	T	103	SQD	C28-C29-C30-C31
28	t	101	SQD	C28-C29-C30-C31
26	A	410	LMG	O1-C7-C8-O7
26	a	410	LMG	O1-C7-C8-O7
23	C	512	CLA	CBA-CGA-O2A-C1
23	c	512	CLA	CBA-CGA-O2A-C1
26	C	520	LMG	C37-C38-C39-C40
26	c	520	LMG	C37-C38-C39-C40
23	C	507	CLA	O1D-CGD-O2D-CED
23	c	507	CLA	O1D-CGD-O2D-CED
31	C	517	DGD	O6D-C5D-C6D-O5D
31	c	517	DGD	O6D-C5D-C6D-O5D
33	L	101	LHG	C28-C29-C30-C31
33	l	101	LHG	C28-C29-C30-C31
28	D	415	SQD	O10-C23-O48-C46
28	d	415	SQD	O10-C23-O48-C46
27	A	411	PL9	C4-C3-C7-C8
27	a	411	PL9	C4-C3-C7-C8
26	A	410	LMG	C34-C35-C36-C37
26	a	410	LMG	C34-C35-C36-C37
23	C	512	CLA	O1A-CGA-O2A-C1
23	c	512	CLA	O1A-CGA-O2A-C1
23	B	601	CLA	C11-C12-C13-C15
23	b	601	CLA	C11-C12-C13-C15
23	C	509	CLA	C1A-C2A-CAA-CBA
23	c	509	CLA	C1A-C2A-CAA-CBA
23	C	508	CLA	C2-C1-O2A-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
23	c	508	CLA	C2-C1-O2A-CGA
33	D	411	LHG	C2-C3-O3-P
33	d	411	LHG	C2-C3-O3-P
25	C	515	BCR	C1-C6-C7-C8
25	c	515	BCR	C1-C6-C7-C8
33	D	410	LHG	C4-O6-P-O5
33	d	410	LHG	C4-O6-P-O5
33	E	101	LHG	C9-C10-C11-C12
33	e	101	LHG	C9-C10-C11-C12
27	A	411	PL9	C9-C11-C12-C13
27	a	411	PL9	C9-C11-C12-C13
26	A	410	LMG	C19-C20-C21-C22
26	a	410	LMG	C19-C20-C21-C22
31	H	102	DGD	C9B-CAB-CBB-CCB
31	h	102	DGD	C9B-CAB-CBB-CCB
28	a	412	SQD	C7-C8-C9-C10
23	C	513	CLA	C2A-CAA-CBA-CGA
23	c	513	CLA	C2A-CAA-CBA-CGA
33	D	411	LHG	C11-C12-C13-C14
33	d	411	LHG	C11-C12-C13-C14
31	C	517	DGD	C5B-C6B-C7B-C8B
31	c	517	DGD	C5B-C6B-C7B-C8B
23	B	601	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	505	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CAD-CBD-CGD-O1D
23	b	601	CLA	CAD-CBD-CGD-O1D
23	c	503	CLA	CAD-CBD-CGD-O1D
23	c	505	CLA	CAD-CBD-CGD-O1D
23	c	507	CLA	CAD-CBD-CGD-O1D
28	A	412	SQD	C7-C8-C9-C10
31	C	517	DGD	C4D-C5D-C6D-O5D
31	c	517	DGD	C4D-C5D-C6D-O5D
31	H	102	DGD	C5B-C6B-C7B-C8B
31	h	102	DGD	C5B-C6B-C7B-C8B
31	H	102	DGD	C6B-C7B-C8B-C9B
31	h	102	DGD	C6B-C7B-C8B-C9B
26	C	520	LMG	C34-C35-C36-C37
26	c	520	LMG	C34-C35-C36-C37
31	H	102	DGD	O2G-C1B-C2B-C3B
31	h	102	DGD	O2G-C1B-C2B-C3B
23	B	603	CLA	C11-C10-C8-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
23	B	606	CLA	C11-C12-C13-C15
23	C	508	CLA	C6-C7-C8-C10
23	C	508	CLA	C12-C13-C15-C16
23	b	603	CLA	C11-C10-C8-C7
23	b	606	CLA	C11-C12-C13-C15
23	c	508	CLA	C6-C7-C8-C10
23	c	508	CLA	C12-C13-C15-C16
33	L	101	LHG	O6-C4-C5-O7
33	l	101	LHG	O6-C4-C5-O7
28	A	412	SQD	C18-C19-C20-C21
28	a	412	SQD	C18-C19-C20-C21
23	C	508	CLA	C5-C6-C7-C8
23	c	508	CLA	C5-C6-C7-C8
23	A	408	CLA	O1A-CGA-O2A-C1
23	a	408	CLA	O1A-CGA-O2A-C1
26	A	410	LMG	C11-C12-C13-C14
26	a	410	LMG	C11-C12-C13-C14
23	B	604	CLA	CBD-CGD-O2D-CED
23	b	604	CLA	CBD-CGD-O2D-CED
23	B	606	CLA	C3-C5-C6-C7
23	b	606	CLA	C3-C5-C6-C7
26	A	410	LMG	O1-C7-C8-C9
26	a	410	LMG	O1-C7-C8-C9
31	H	102	DGD	O1G-C1G-C2G-O2G
31	h	102	DGD	O1G-C1G-C2G-O2G
23	B	601	CLA	C12-C13-C15-C16
23	b	601	CLA	C12-C13-C15-C16
23	A	408	CLA	CBA-CGA-O2A-C1
23	a	408	CLA	CBA-CGA-O2A-C1
26	A	410	LMG	C35-C36-C37-C38
26	a	410	LMG	C35-C36-C37-C38
23	B	606	CLA	C14-C13-C15-C16
23	C	508	CLA	C14-C13-C15-C16
23	b	606	CLA	C14-C13-C15-C16
23	c	508	CLA	C14-C13-C15-C16
23	B	611	CLA	C13-C15-C16-C17
37	V	201	HEC	C3D-CAD-CBD-CGD
37	v	201	HEC	C3D-CAD-CBD-CGD
23	b	611	CLA	C13-C15-C16-C17
23	B	616	CLA	C5-C6-C7-C8
23	b	616	CLA	C5-C6-C7-C8
23	B	612	CLA	O1A-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
23	b	612	CLA	O1A-CGA-O2A-C1
23	C	511	CLA	C8-C10-C11-C12
23	c	511	CLA	C8-C10-C11-C12
23	A	405	CLA	C2-C1-O2A-CGA
23	a	405	CLA	C2-C1-O2A-CGA
31	C	519	DGD	O6D-C5D-C6D-O5D
31	c	519	DGD	O6D-C5D-C6D-O5D
24	D	401	PHO	C2C-C3C-CAC-CBC
24	d	401	PHO	C2C-C3C-CAC-CBC
26	C	520	LMG	C18-C19-C20-C21
26	c	520	LMG	C18-C19-C20-C21
33	l	101	LHG	C34-C35-C36-C37
33	L	101	LHG	C34-C35-C36-C37
23	B	611	CLA	C16-C17-C18-C20
23	b	611	CLA	C16-C17-C18-C20
30	B	623	LMT	O1'-C1'-C2'-C3'
30	T	104	LMT	O1'-C1'-C2'-C3'
31	H	102	DGD	CBB-CCB-CDB-CEB
31	h	102	DGD	CBB-CCB-CDB-CEB
33	L	101	LHG	C32-C33-C34-C35
33	l	101	LHG	C32-C33-C34-C35
30	J	102	LMT	O5'-C1'-O1'-C1
30	j	102	LMT	O5'-C1'-O1'-C1
30	J	102	LMT	C2'-C1'-O1'-C1
30	j	102	LMT	C2'-C1'-O1'-C1
33	D	410	LHG	C3-O3-P-O6
33	d	410	LHG	C3-O3-P-O6
23	B	601	CLA	C6-C7-C8-C10
23	b	601	CLA	C6-C7-C8-C10
33	D	410	LHG	C14-C15-C16-C17
33	d	410	LHG	C14-C15-C16-C17
23	B	603	CLA	C11-C10-C8-C9
23	B	606	CLA	C11-C12-C13-C14
23	B	616	CLA	C14-C13-C15-C16
23	b	603	CLA	C11-C10-C8-C9
23	b	606	CLA	C11-C12-C13-C14
23	b	616	CLA	C14-C13-C15-C16
23	D	405	CLA	C2C-C3C-CAC-CBC
23	d	405	CLA	C2C-C3C-CAC-CBC
23	B	604	CLA	C15-C16-C17-C18
23	b	604	CLA	C15-C16-C17-C18
23	A	405	CLA	C2C-C3C-CAC-CBC

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
23	a	405	CLA	C2C-C3C-CAC-CBC
23	A	406	CLA	C11-C10-C8-C7
23	a	406	CLA	C11-C10-C8-C7
23	C	513	CLA	C2-C3-C5-C6
23	c	513	CLA	C2-C3-C5-C6
33	L	101	LHG	C17-C18-C19-C20
33	l	101	LHG	C17-C18-C19-C20
23	B	612	CLA	CBA-CGA-O2A-C1
23	b	612	CLA	CBA-CGA-O2A-C1
23	C	510	CLA	C10-C11-C12-C13
23	c	510	CLA	C10-C11-C12-C13
23	B	610	CLA	C8-C10-C11-C12
23	b	610	CLA	C8-C10-C11-C12
23	B	612	CLA	C10-C11-C12-C13
23	b	612	CLA	C10-C11-C12-C13
26	C	520	LMG	C30-C31-C32-C33
26	c	520	LMG	C30-C31-C32-C33
31	C	518	DGD	C2E-C1E-O5D-C6D
31	c	518	DGD	C2E-C1E-O5D-C6D
23	B	610	CLA	C2A-CAA-CBA-CGA
23	b	610	CLA	C2A-CAA-CBA-CGA
23	C	513	CLA	C3A-C2A-CAA-CBA
23	c	513	CLA	C3A-C2A-CAA-CBA
23	C	509	CLA	C11-C12-C13-C15
23	c	509	CLA	C11-C12-C13-C15
30	B	623	LMT	C1-C2-C3-C4
30	T	104	LMT	C1-C2-C3-C4
23	B	602	CLA	C6-C7-C8-C9
23	C	508	CLA	C6-C7-C8-C9
23	b	602	CLA	C6-C7-C8-C9
23	c	508	CLA	C6-C7-C8-C9
31	H	102	DGD	O1G-C1G-C2G-C3G
31	h	102	DGD	O1G-C1G-C2G-C3G
23	B	602	CLA	O2A-C1-C2-C3
23	b	602	CLA	O2A-C1-C2-C3
31	C	518	DGD	O6E-C1E-O5D-C6D
31	c	518	DGD	O6E-C1E-O5D-C6D
30	J	102	LMT	C6-C7-C8-C9
30	j	102	LMT	C6-C7-C8-C9
23	B	616	CLA	C4-C3-C5-C6
23	b	616	CLA	C4-C3-C5-C6
33	E	101	LHG	O10-C23-O8-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
33	e	101	LHG	O10-C23-O8-C6
28	T	103	SQD	C24-C25-C26-C27
28	t	101	SQD	C24-C25-C26-C27
26	B	620	LMG	C39-C40-C41-C42
26	b	620	LMG	C39-C40-C41-C42
23	C	507	CLA	CBD-CGD-O2D-CED
23	c	507	CLA	CBD-CGD-O2D-CED
26	C	520	LMG	C12-C13-C14-C15
26	c	520	LMG	C12-C13-C14-C15
26	D	412	LMG	C39-C40-C41-C42
26	d	412	LMG	C39-C40-C41-C42
23	A	408	CLA	C4-C3-C5-C6
23	a	408	CLA	C4-C3-C5-C6
23	D	405	CLA	C2-C1-O2A-CGA
23	d	405	CLA	C2-C1-O2A-CGA
31	C	518	DGD	C2A-C3A-C4A-C5A
31	c	518	DGD	C2A-C3A-C4A-C5A
26	C	520	LMG	C35-C36-C37-C38
26	c	520	LMG	C35-C36-C37-C38
33	D	410	LHG	C26-C27-C28-C29
33	d	410	LHG	C26-C27-C28-C29
26	A	410	LMG	C15-C16-C17-C18
26	a	410	LMG	C15-C16-C17-C18
23	A	405	CLA	C4C-C3C-CAC-CBC
23	a	405	CLA	C4C-C3C-CAC-CBC
34	f	101	HEM	CAD-CBD-CGD-O1D
34	F	101	HEM	CAD-CBD-CGD-O1D
31	C	517	DGD	C5D-C6D-O5D-C1E
31	c	517	DGD	C5D-C6D-O5D-C1E
23	B	603	CLA	O1D-CGD-O2D-CED
28	T	103	SQD	C9-C10-C11-C12
28	t	101	SQD	C9-C10-C11-C12
23	b	603	CLA	O1D-CGD-O2D-CED
33	E	101	LHG	O6-C4-C5-O7
33	e	101	LHG	O6-C4-C5-O7
23	A	406	CLA	C11-C10-C8-C9
23	a	406	CLA	C11-C10-C8-C9
31	C	519	DGD	C3B-C4B-C5B-C6B
31	c	519	DGD	C3B-C4B-C5B-C6B
23	A	408	CLA	C2-C3-C5-C6
23	B	606	CLA	C11-C10-C8-C7
23	B	609	CLA	C2-C3-C5-C6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
23	C	504	CLA	C6-C7-C8-C10
23	a	408	CLA	C2-C3-C5-C6
23	b	606	CLA	C11-C10-C8-C7
23	b	609	CLA	C2-C3-C5-C6
23	c	504	CLA	C6-C7-C8-C10
31	C	519	DGD	C2A-C3A-C4A-C5A
31	c	519	DGD	C2A-C3A-C4A-C5A
23	B	616	CLA	CBA-CGA-O2A-C1
23	b	616	CLA	CBA-CGA-O2A-C1
23	C	504	CLA	C8-C10-C11-C12
23	c	504	CLA	C8-C10-C11-C12
23	B	616	CLA	C2-C3-C5-C6
23	b	616	CLA	C2-C3-C5-C6
33	L	101	LHG	C11-C10-C9-C8
33	l	101	LHG	C11-C10-C9-C8
31	c	517	DGD	O2G-C1B-C2B-C3B
23	B	610	CLA	CAD-CBD-CGD-O2D
23	C	504	CLA	CAD-CBD-CGD-O2D
23	C	506	CLA	CAD-CBD-CGD-O2D
23	C	510	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	CAD-CBD-CGD-O2D
23	c	504	CLA	CAD-CBD-CGD-O2D
23	c	506	CLA	CAD-CBD-CGD-O2D
23	c	510	CLA	CAD-CBD-CGD-O2D
24	A	407	PHO	CAD-CBD-CGD-O2D
24	a	407	PHO	CAD-CBD-CGD-O2D
31	C	517	DGD	O2G-C1B-C2B-C3B
26	A	410	LMG	O8-C28-C29-C30
26	a	410	LMG	O8-C28-C29-C30
25	K	102	BCR	C7-C8-C9-C10
25	k	102	BCR	C7-C8-C9-C10
26	A	410	LMG	C28-C29-C30-C31
26	a	410	LMG	C28-C29-C30-C31
23	B	603	CLA	CBD-CGD-O2D-CED
23	b	603	CLA	CBD-CGD-O2D-CED
23	B	613	CLA	O2A-C1-C2-C3
23	C	510	CLA	O2A-C1-C2-C3
23	b	613	CLA	O2A-C1-C2-C3
23	c	510	CLA	O2A-C1-C2-C3
24	A	407	PHO	O2A-C1-C2-C3
24	a	407	PHO	O2A-C1-C2-C3
23	B	616	CLA	O1A-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
23	b	616	CLA	O1A-CGA-O2A-C1
26	C	520	LMG	C14-C15-C16-C17
26	c	520	LMG	C14-C15-C16-C17
28	C	501	SQD	O47-C7-C8-C9
28	c	501	SQD	O47-C7-C8-C9
23	A	406	CLA	CHA-CBD-CGD-O1D
23	A	406	CLA	CHA-CBD-CGD-O2D
23	B	602	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	C	505	CLA	CHA-CBD-CGD-O1D
23	D	402	CLA	CHA-CBD-CGD-O1D
23	D	402	CLA	CHA-CBD-CGD-O2D
23	a	406	CLA	CHA-CBD-CGD-O1D
23	a	406	CLA	CHA-CBD-CGD-O2D
23	b	602	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O2D
23	c	505	CLA	CHA-CBD-CGD-O1D
23	d	402	CLA	CHA-CBD-CGD-O1D
23	d	402	CLA	CHA-CBD-CGD-O2D
28	T	103	SQD	C17-C18-C19-C20
28	t	101	SQD	C17-C18-C19-C20
23	C	506	CLA	C12-C13-C15-C16
23	c	506	CLA	C12-C13-C15-C16
28	T	103	SQD	O47-C7-C8-C9
28	t	101	SQD	O47-C7-C8-C9
30	B	621	LMT	C9-C10-C11-C12
30	b	621	LMT	C9-C10-C11-C12
31	H	102	DGD	C3B-C4B-C5B-C6B
31	h	102	DGD	C3B-C4B-C5B-C6B
30	T	105	LMT	C4-C5-C6-C7
30	t	102	LMT	C4-C5-C6-C7
28	A	412	SQD	C11-C12-C13-C14
31	C	517	DGD	O1B-C1B-C2B-C3B
31	c	517	DGD	O1B-C1B-C2B-C3B
26	B	620	LMG	C33-C34-C35-C36
26	b	620	LMG	C33-C34-C35-C36
28	a	412	SQD	C11-C12-C13-C14
25	A	409	BCR	C36-C18-C19-C20
25	a	409	BCR	C36-C18-C19-C20
33	l	101	LHG	C7-C8-C9-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
34	F	101	HEM	CAD-CBD-CGD-O2D
34	f	101	HEM	CAD-CBD-CGD-O2D
33	L	101	LHG	C29-C30-C31-C32
33	l	101	LHG	C29-C30-C31-C32
33	E	101	LHG	O1-C1-C2-C3
33	e	101	LHG	O1-C1-C2-C3
33	L	101	LHG	C7-C8-C9-C10
28	C	501	SQD	O49-C7-C8-C9
28	c	501	SQD	O49-C7-C8-C9
31	H	102	DGD	C9A-CAA-CBA-CCA
31	h	102	DGD	C9A-CAA-CBA-CCA
23	C	502	CLA	C2A-CAA-CBA-CGA
23	c	502	CLA	C2A-CAA-CBA-CGA
23	D	402	CLA	C4C-C3C-CAC-CBC
23	d	402	CLA	C4C-C3C-CAC-CBC
31	C	519	DGD	O1G-C1A-C2A-C3A
31	c	519	DGD	O1G-C1A-C2A-C3A
31	C	517	DGD	O6E-C1E-O5D-C6D
31	c	517	DGD	O6E-C1E-O5D-C6D
25	Y	101	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8
25	y	101	BCR	C1-C6-C7-C8
25	y	101	BCR	C5-C6-C7-C8
26	D	412	LMG	C36-C37-C38-C39
26	d	412	LMG	C36-C37-C38-C39
23	B	609	CLA	C4-C3-C5-C6
23	b	609	CLA	C4-C3-C5-C6
23	A	406	CLA	CAD-CBD-CGD-O1D
23	B	602	CLA	CAD-CBD-CGD-O1D
23	B	605	CLA	CAD-CBD-CGD-O1D
23	B	607	CLA	CAD-CBD-CGD-O1D
23	B	609	CLA	CAD-CBD-CGD-O1D
23	a	406	CLA	CAD-CBD-CGD-O1D
23	b	602	CLA	CAD-CBD-CGD-O1D
23	b	605	CLA	CAD-CBD-CGD-O1D
23	b	607	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
28	T	103	SQD	O49-C7-C8-C9
28	t	101	SQD	O49-C7-C8-C9
23	A	406	CLA	C6-C7-C8-C9
23	B	612	CLA	C11-C10-C8-C9
23	a	406	CLA	C6-C7-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
23	b	612	CLA	C11-C10-C8-C9
23	C	502	CLA	CAA-CBA-CGA-O2A
23	c	502	CLA	CAA-CBA-CGA-O2A
26	C	520	LMG	O7-C10-C11-C12
26	c	520	LMG	O7-C10-C11-C12
23	C	506	CLA	CAA-CBA-CGA-O2A
23	c	506	CLA	CAA-CBA-CGA-O2A
31	C	518	DGD	C8B-C9B-CAB-CBB
31	c	518	DGD	C8B-C9B-CAB-CBB
26	C	520	LMG	O9-C10-C11-C12
26	c	520	LMG	O9-C10-C11-C12
23	C	511	CLA	CAA-CBA-CGA-O2A
23	c	511	CLA	CAA-CBA-CGA-O2A
33	D	410	LHG	C16-C17-C18-C19
33	d	410	LHG	C16-C17-C18-C19
31	C	519	DGD	O1A-C1A-C2A-C3A
31	c	519	DGD	O1A-C1A-C2A-C3A
23	b	612	CLA	C8-C10-C11-C12
23	C	502	CLA	CAA-CBA-CGA-O1A
23	c	502	CLA	CAA-CBA-CGA-O1A
28	a	412	SQD	C12-C13-C14-C15
23	B	612	CLA	C8-C10-C11-C12
28	A	412	SQD	C12-C13-C14-C15

There are no ring outliers.

106 monomers are involved in 225 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	508	CLA	1	0
23	B	604	CLA	1	0
33	d	411	LHG	1	0
28	d	415	SQD	1	0
30	B	623	LMT	1	0
23	D	405	CLA	2	0
23	c	506	CLA	2	0
23	b	611	CLA	2	0
23	B	616	CLA	2	0
23	b	610	CLA	2	0
30	T	105	LMT	1	0
33	e	101	LHG	1	0
23	B	611	CLA	2	0
23	a	406	CLA	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	512	CLA	4	0
23	b	605	CLA	3	0
31	C	518	DGD	1	0
23	a	405	CLA	3	0
33	E	101	LHG	1	0
23	B	610	CLA	2	0
23	b	604	CLA	1	0
30	M	101	LMT	1	0
25	b	618	BCR	4	0
25	y	101	BCR	4	0
23	B	601	CLA	2	0
34	F	101	HEM	3	0
23	b	613	CLA	2	0
25	D	407	BCR	3	0
23	c	502	CLA	1	0
34	f	101	HEM	3	0
23	C	511	CLA	1	0
30	T	104	LMT	1	0
23	b	601	CLA	2	0
23	B	609	CLA	1	0
23	d	405	CLA	1	0
23	C	513	CLA	5	0
23	B	613	CLA	2	0
25	B	617	BCR	1	0
23	A	406	CLA	3	0
25	k	102	BCR	2	0
35	h	101	RRX	2	0
35	H	101	RRX	1	0
23	c	504	CLA	5	0
24	A	407	PHO	2	0
23	b	615	CLA	3	0
23	b	606	CLA	4	0
27	D	408	PL9	1	0
33	D	411	LHG	1	0
23	b	616	CLA	2	0
28	T	103	SQD	1	0
23	B	605	CLA	3	0
30	J	102	LMT	1	0
25	c	516	BCR	8	0
23	C	504	CLA	5	0
25	t	103	BCR	5	0
23	C	507	CLA	1	0

*Continued on next page...*

*Continued from previous page...*

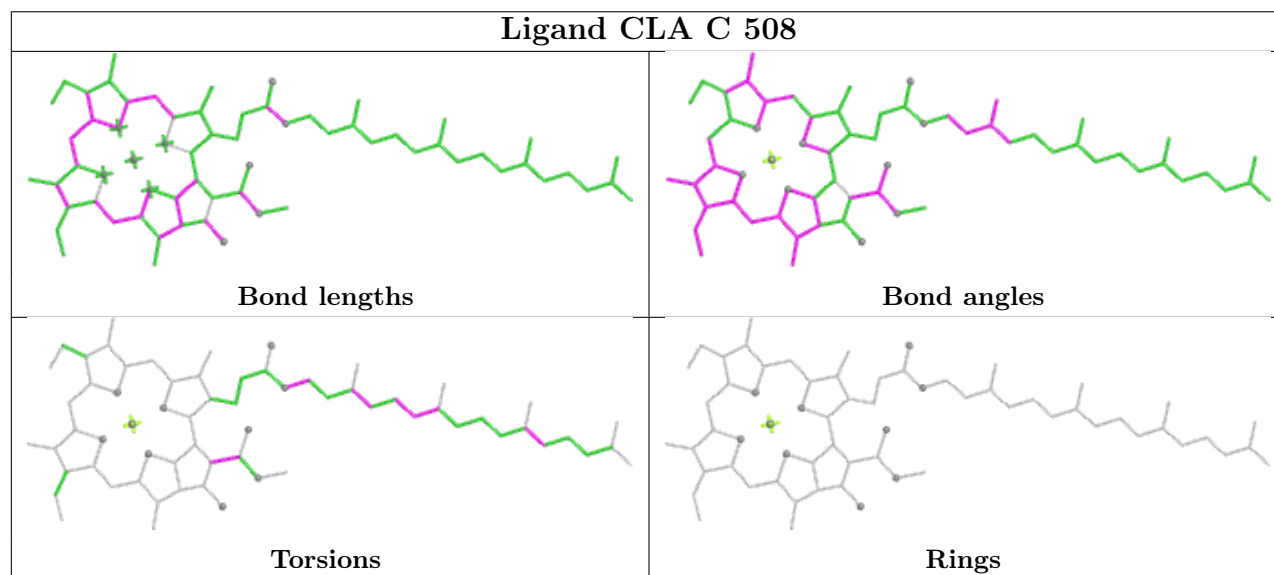
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	603	CLA	1	0
23	d	402	CLA	3	0
23	b	607	CLA	1	0
23	C	514	CLA	2	0
23	B	606	CLA	5	0
23	B	607	CLA	1	0
23	C	505	CLA	1	0
23	c	513	CLA	4	0
25	d	407	BCR	2	0
25	b	617	BCR	2	0
25	C	516	BCR	6	0
30	j	102	LMT	1	0
23	b	603	CLA	1	0
25	B	618	BCR	5	0
30	m	101	LMT	1	0
23	D	402	CLA	3	0
23	C	506	CLA	2	0
23	d	406	CLA	2	0
27	a	411	PL9	2	0
25	C	515	BCR	3	0
23	C	512	CLA	4	0
26	A	410	LMG	1	0
31	c	518	DGD	1	0
23	c	514	CLA	2	0
27	A	411	PL9	2	0
23	C	503	CLA	2	0
23	b	609	CLA	1	0
24	a	407	PHO	3	0
23	A	405	CLA	3	0
25	b	619	BCR	6	0
25	K	102	BCR	2	0
23	C	502	CLA	1	0
25	c	515	BCR	3	0
23	B	615	CLA	3	0
24	D	401	PHO	3	0
25	T	101	BCR	6	0
24	d	401	PHO	3	0
23	b	612	CLA	2	0
25	B	619	BCR	8	0
25	A	409	BCR	1	0
23	c	503	CLA	2	0
23	c	510	CLA	2	0

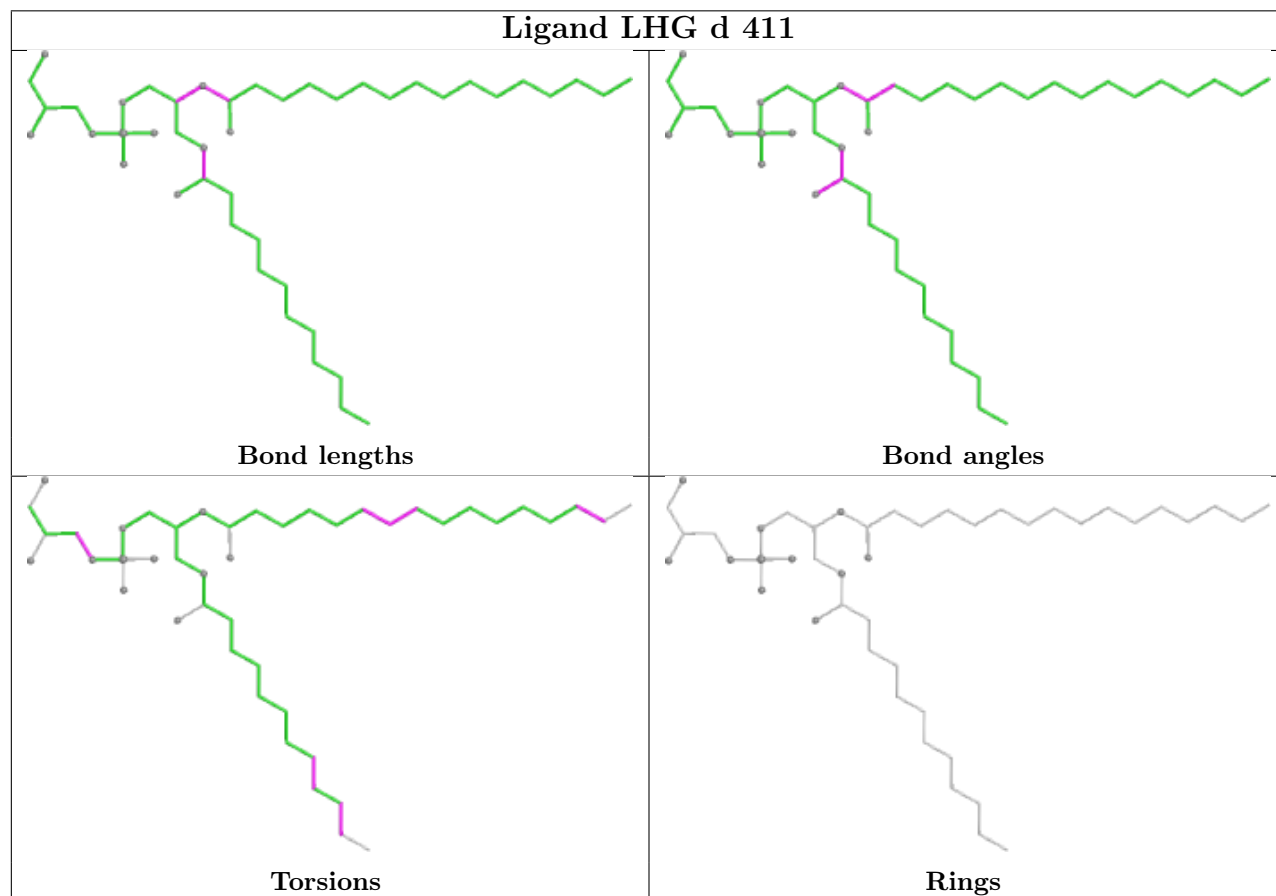
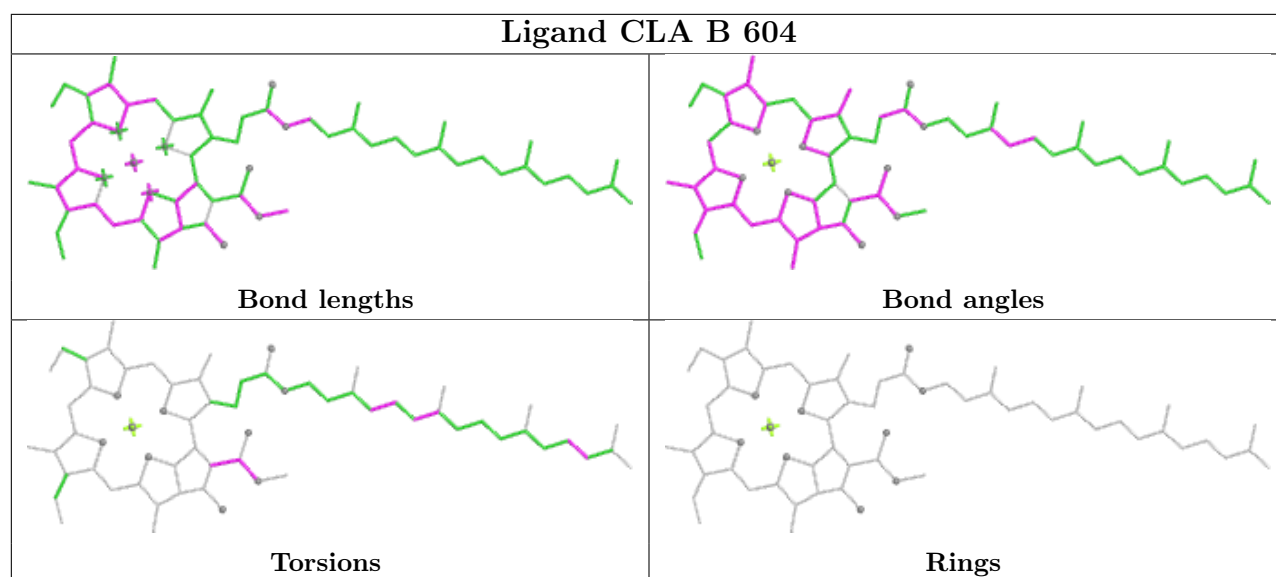
*Continued on next page...*

*Continued from previous page...*

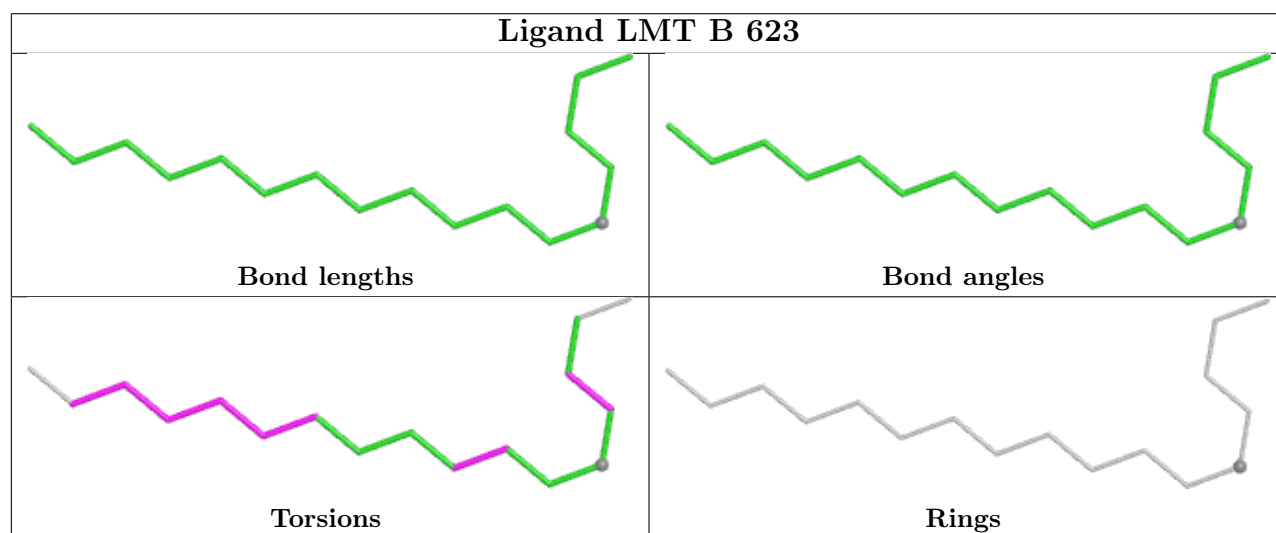
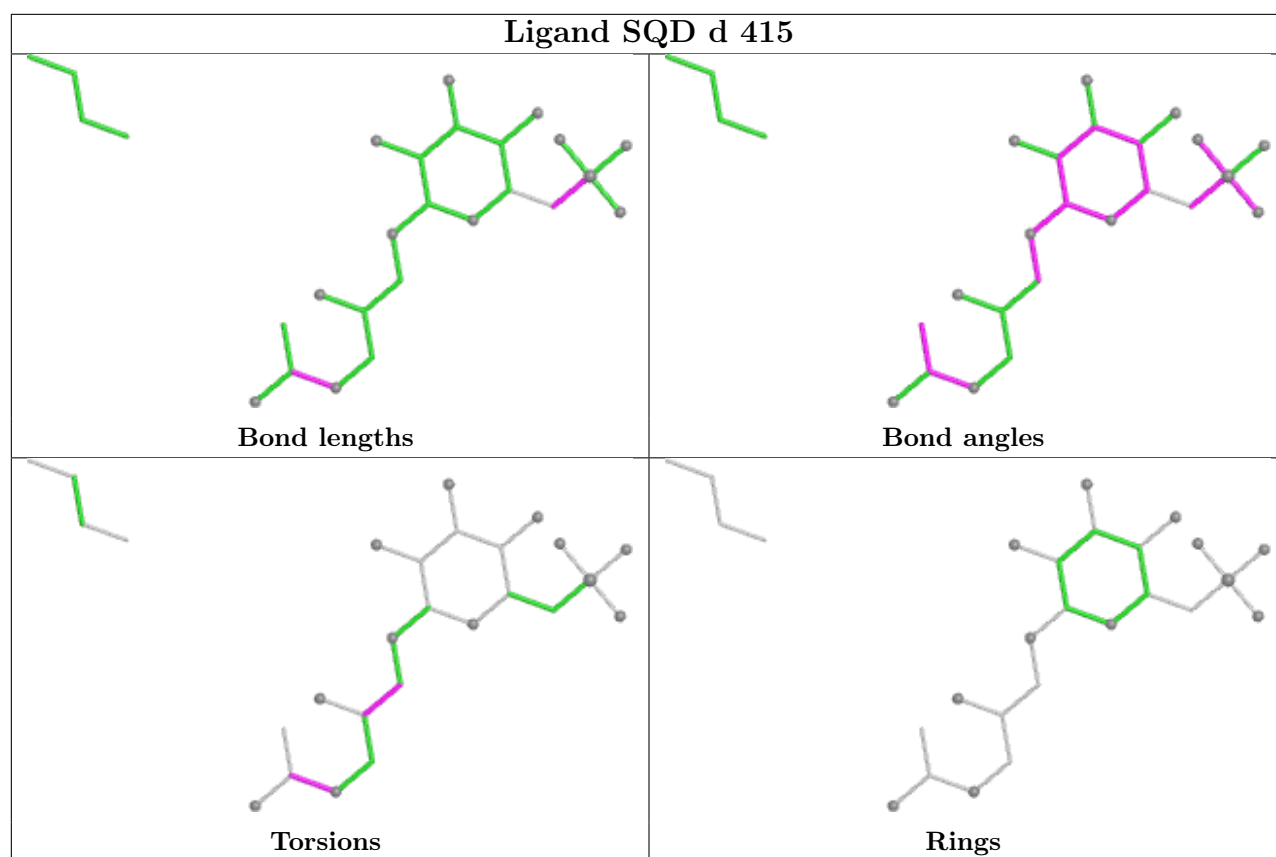
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	d	408	PL9	1	0
25	a	409	BCR	1	0
26	a	410	LMG	1	0
23	c	505	CLA	1	0
23	B	612	CLA	2	0
25	Y	101	BCR	3	0
23	C	510	CLA	2	0
23	D	406	CLA	2	0

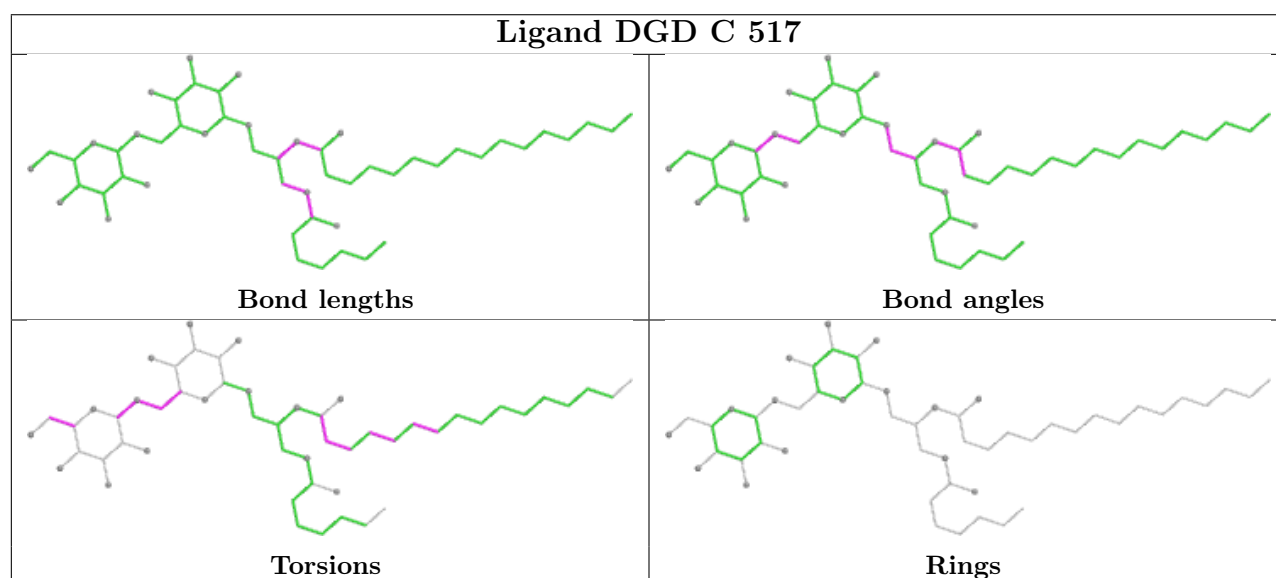
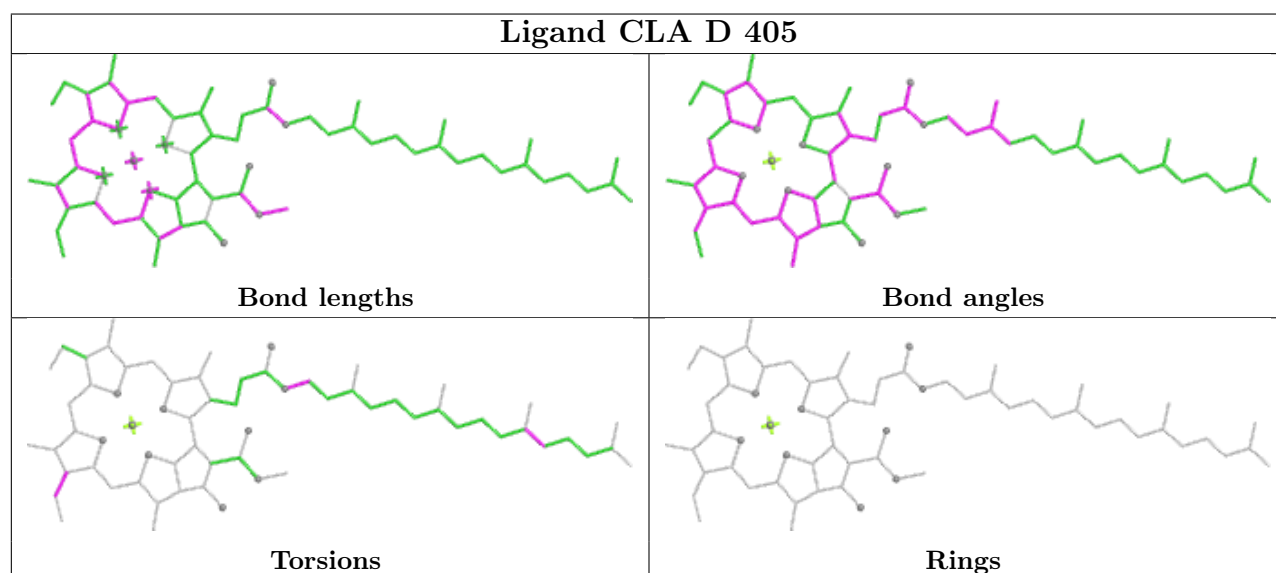
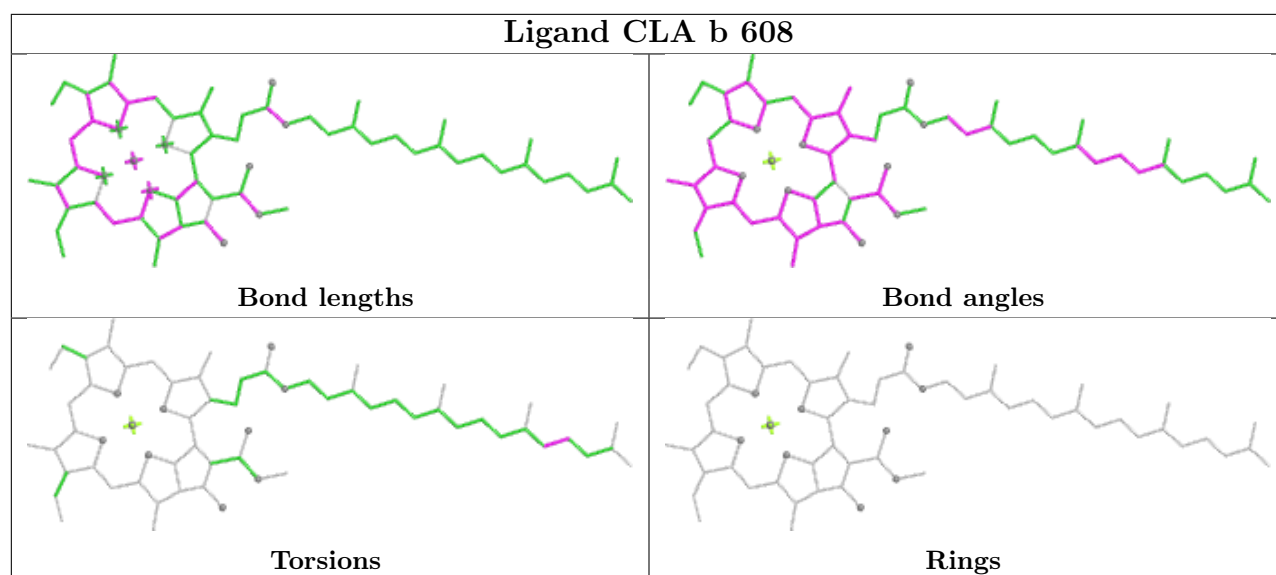
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

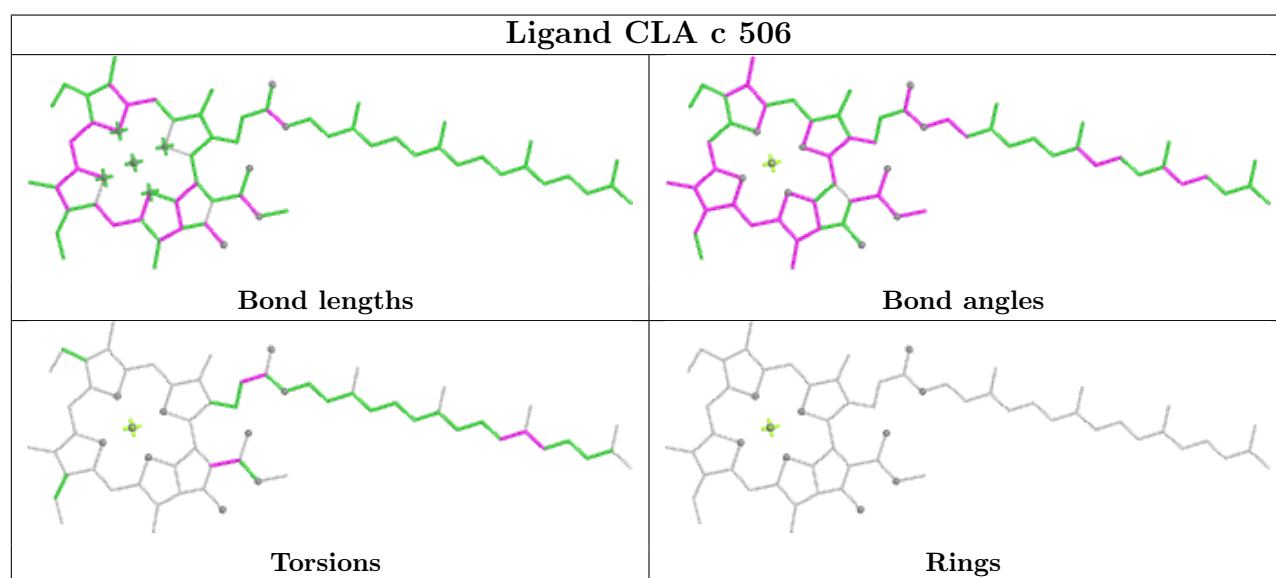
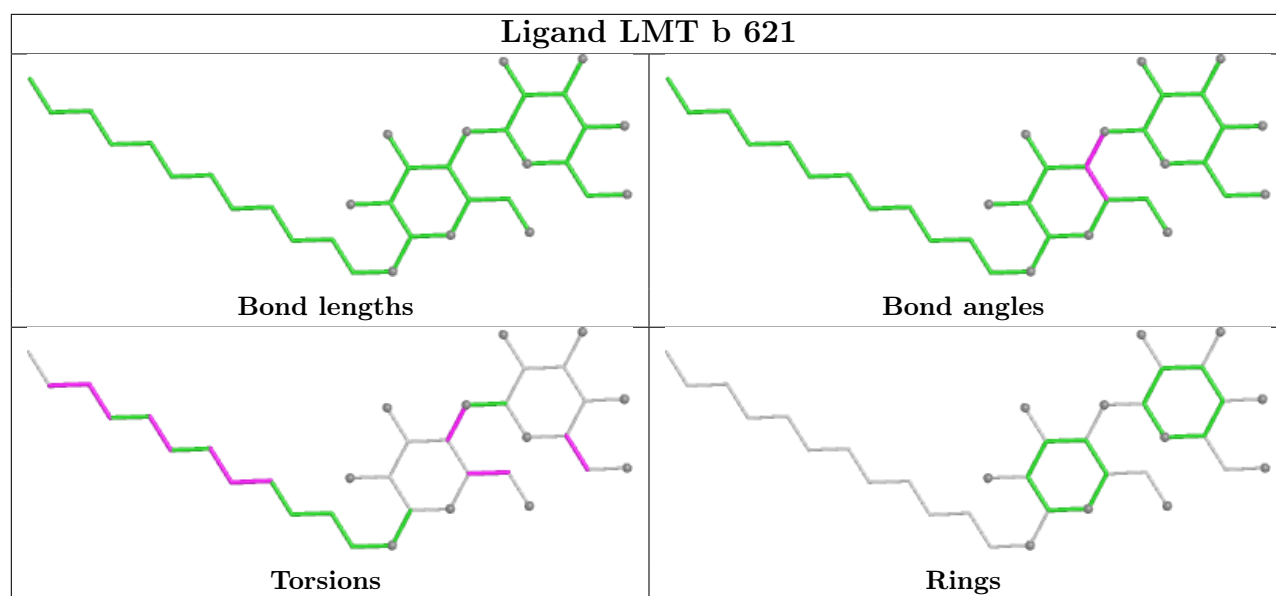


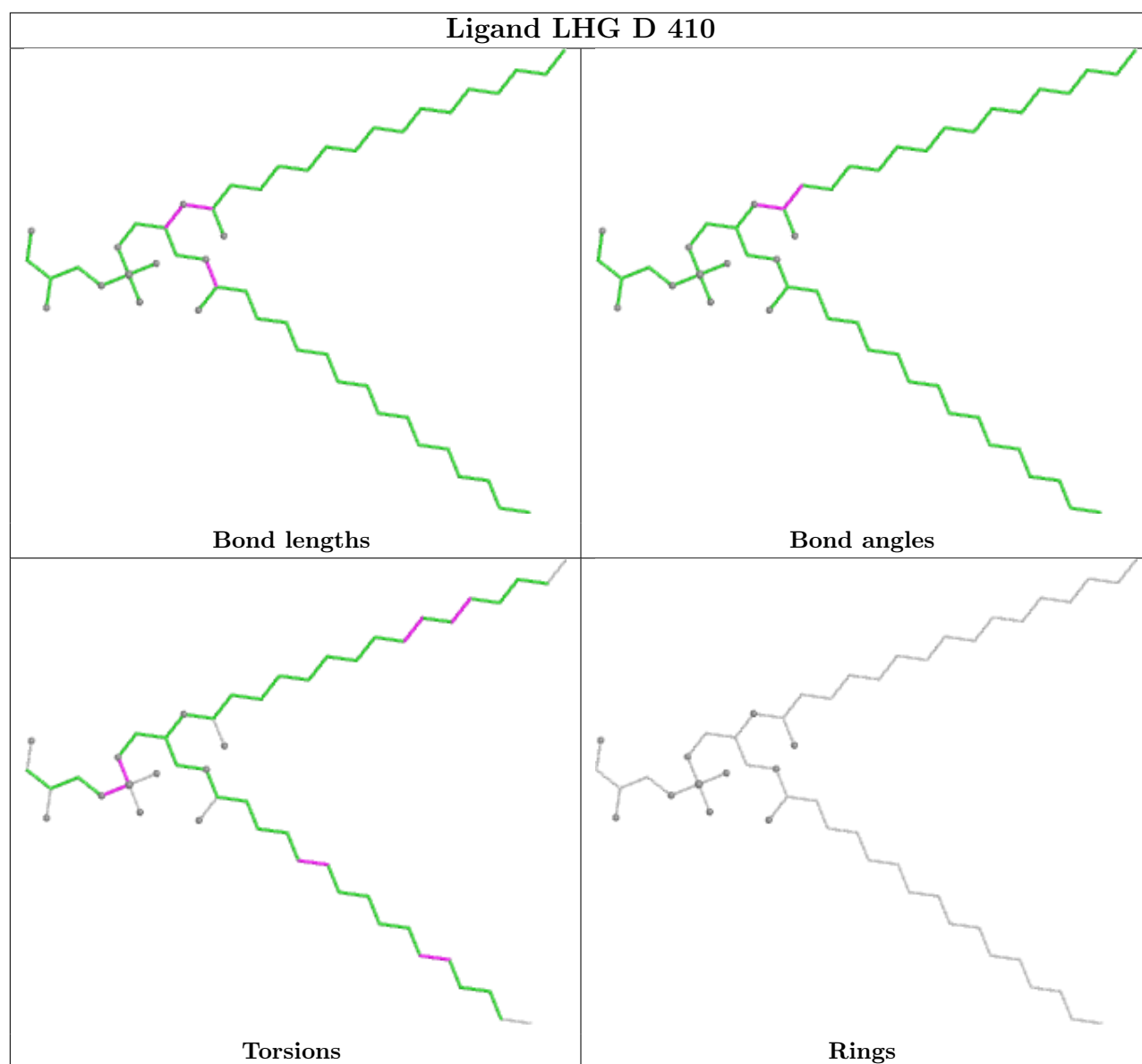


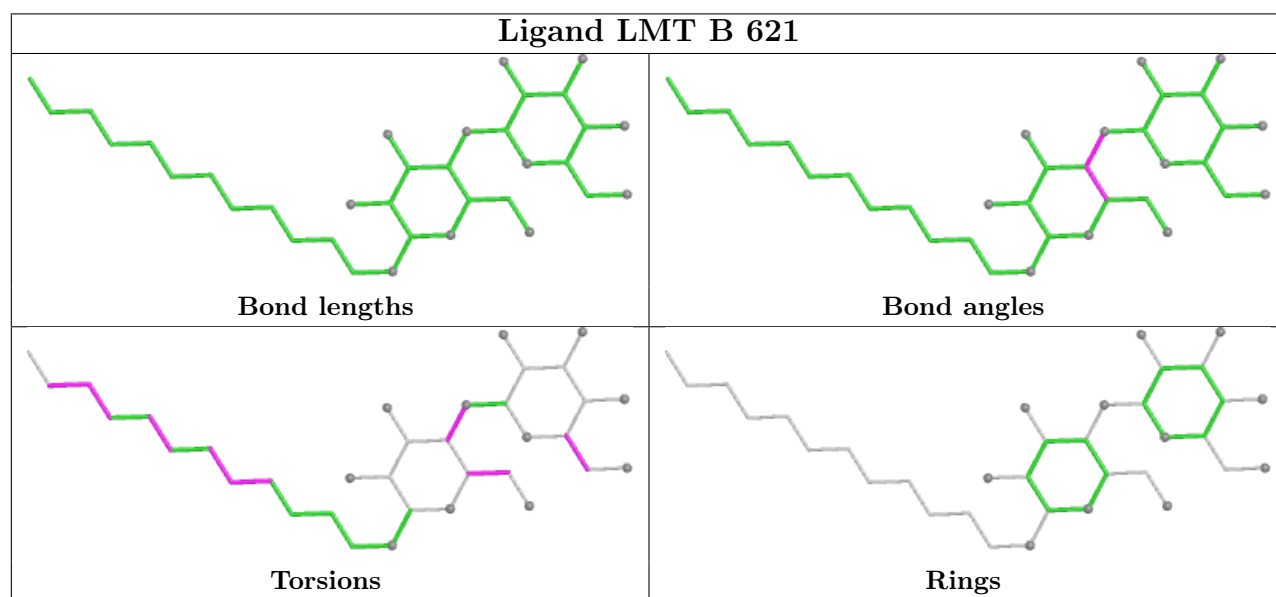
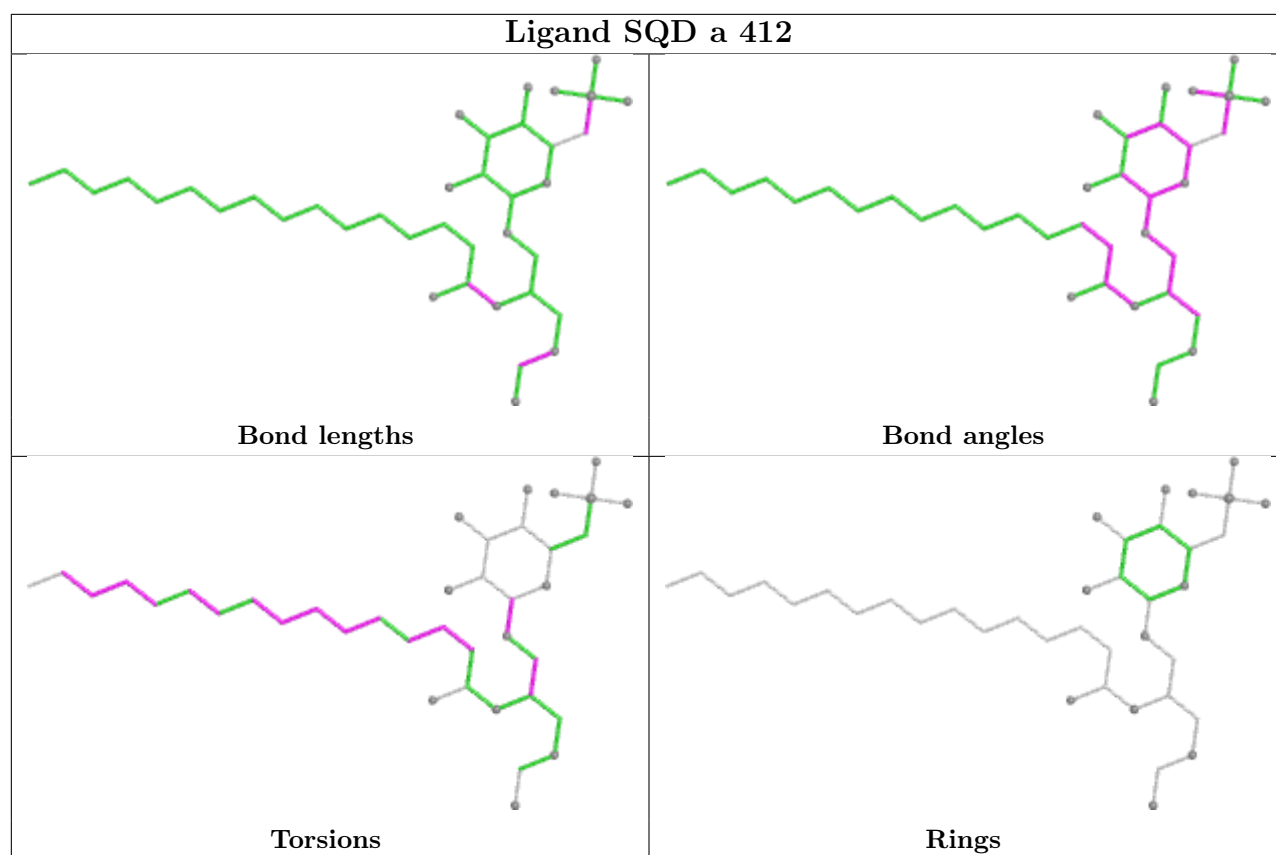


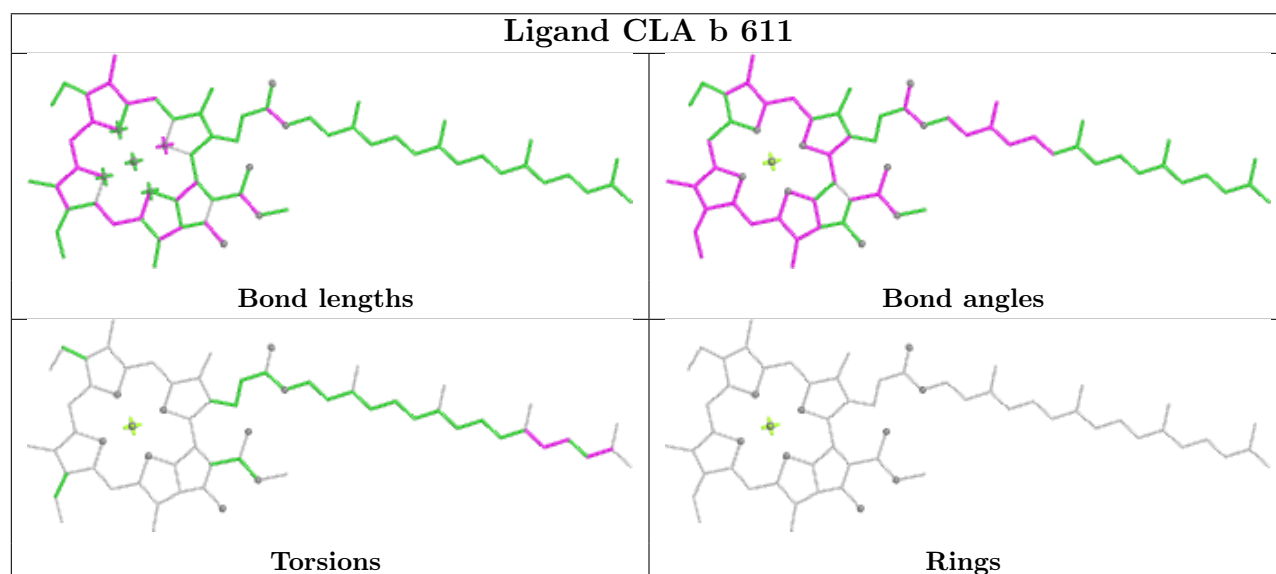
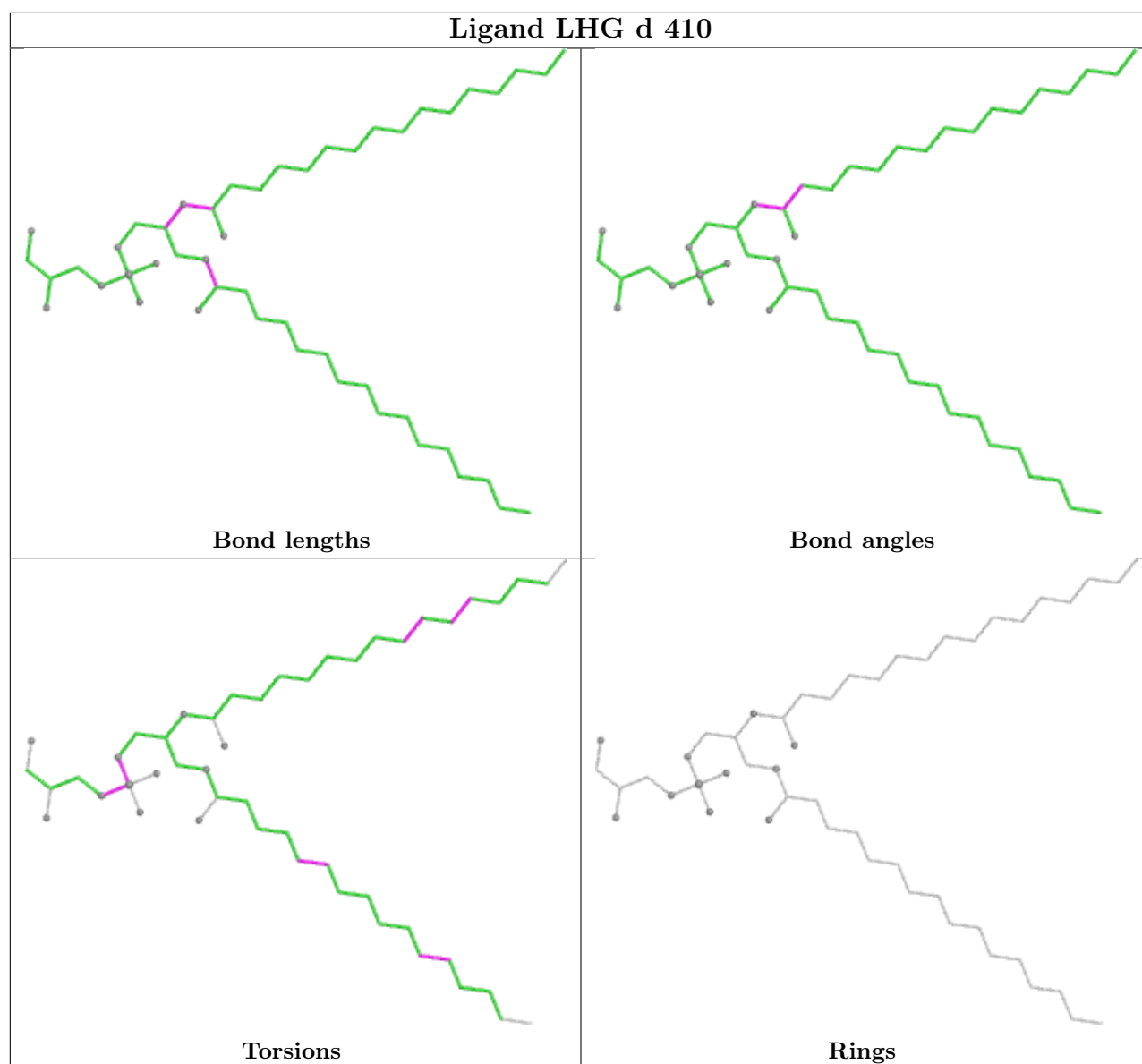


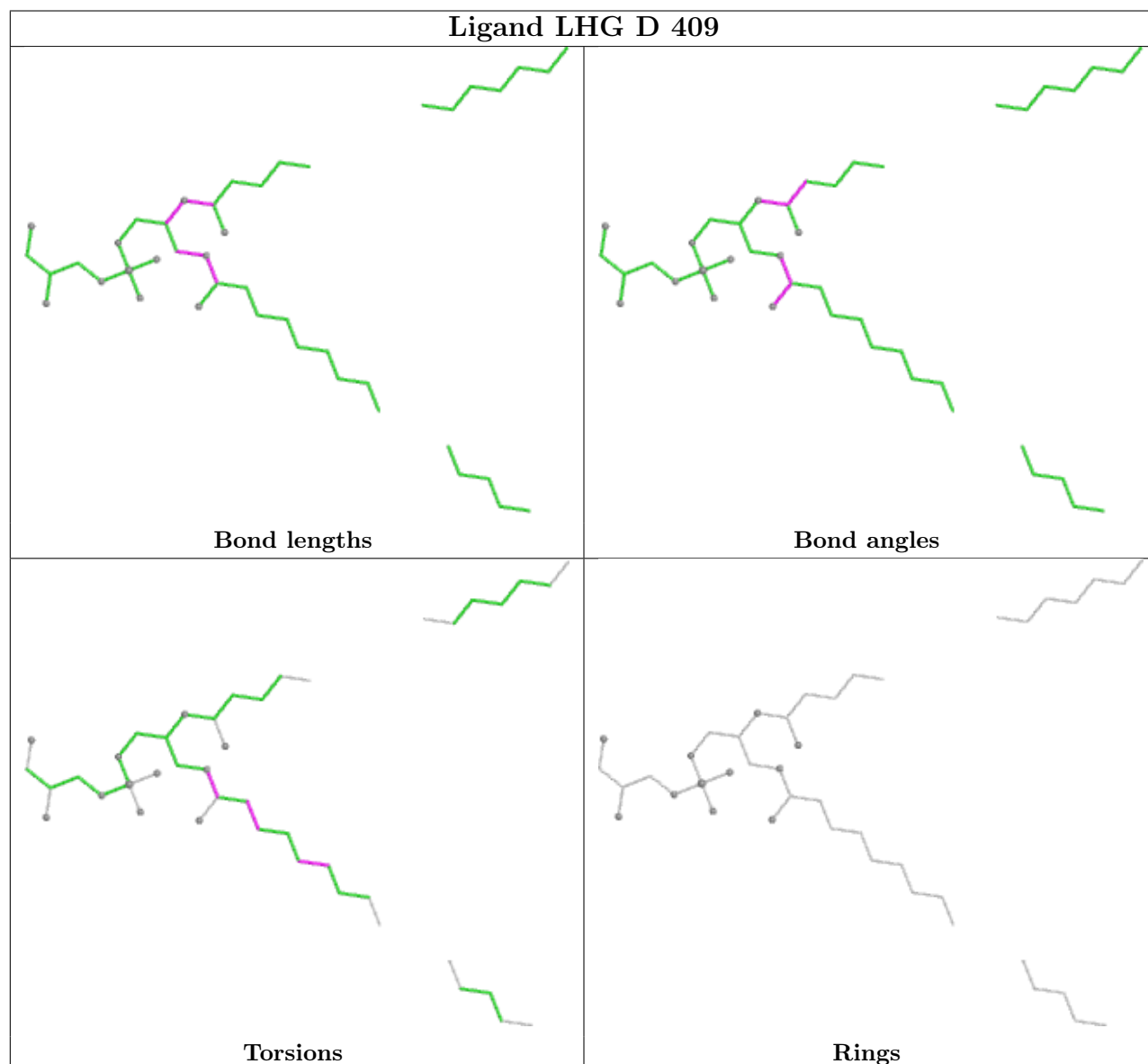
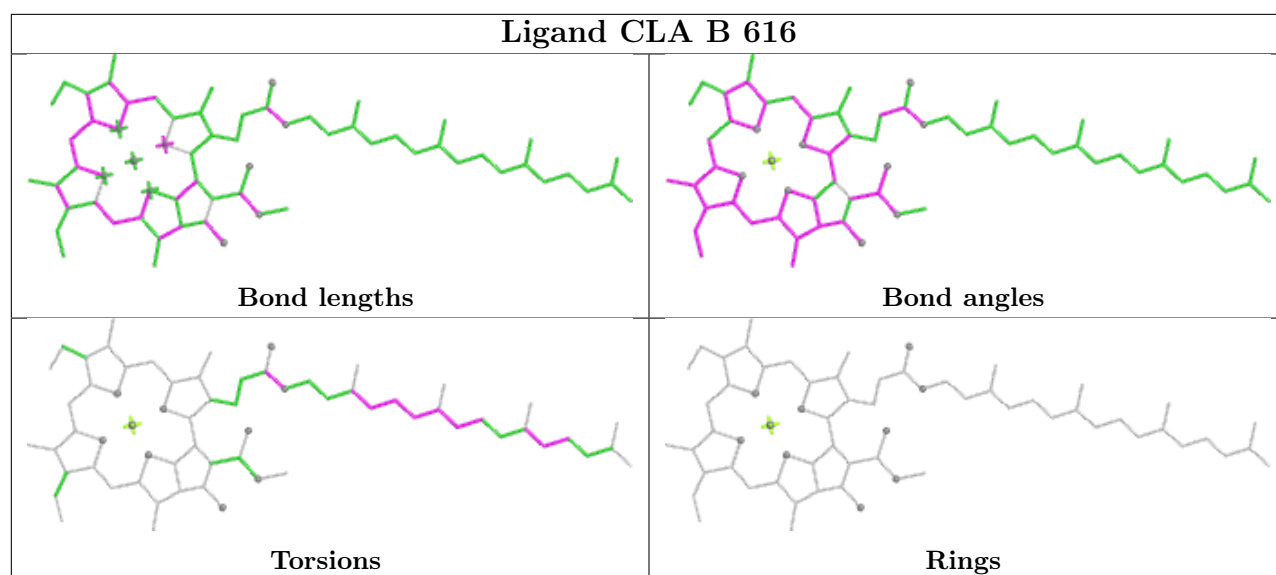


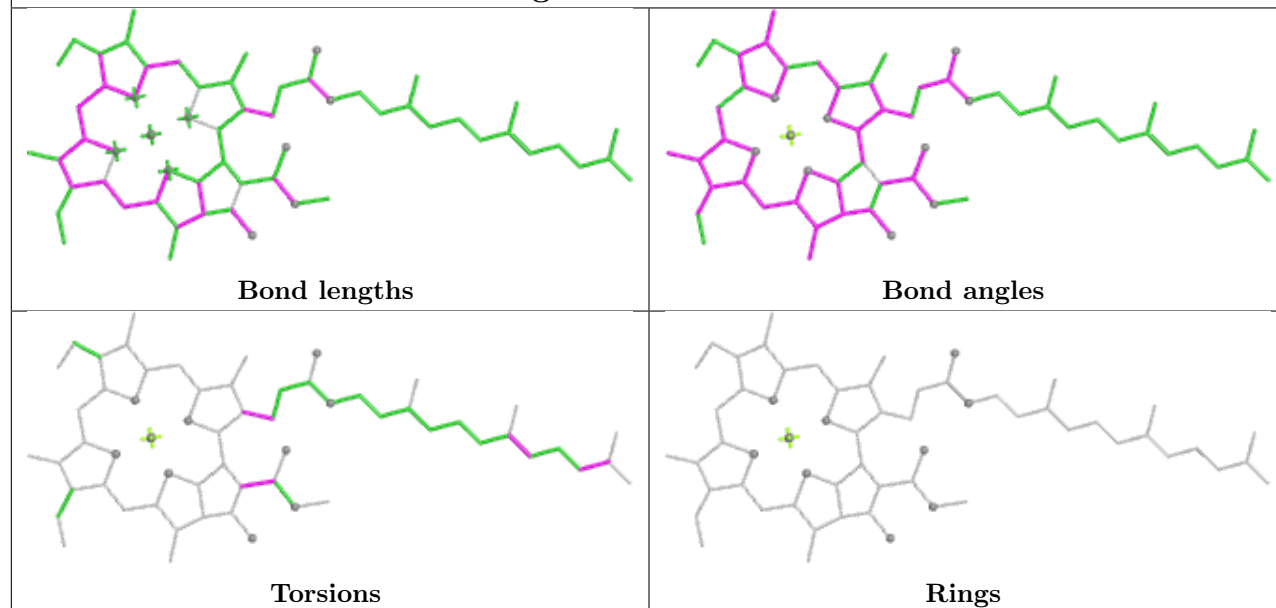
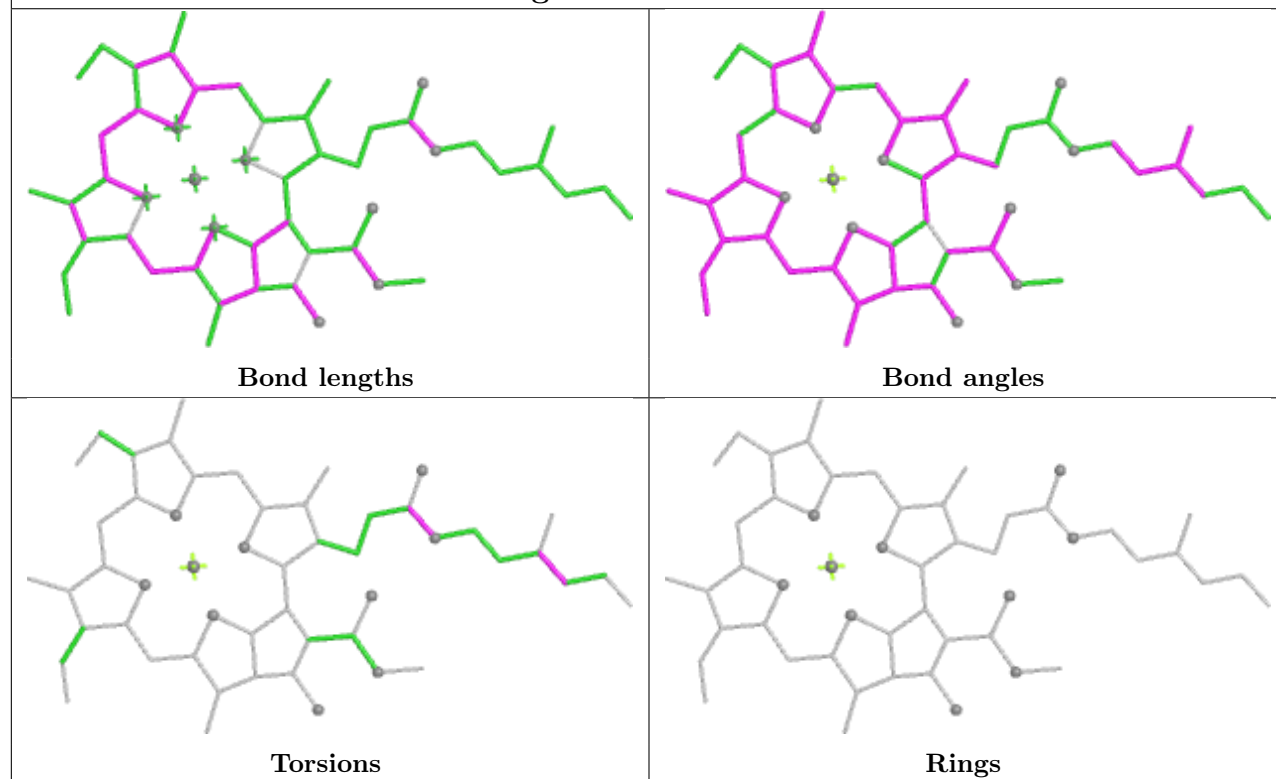




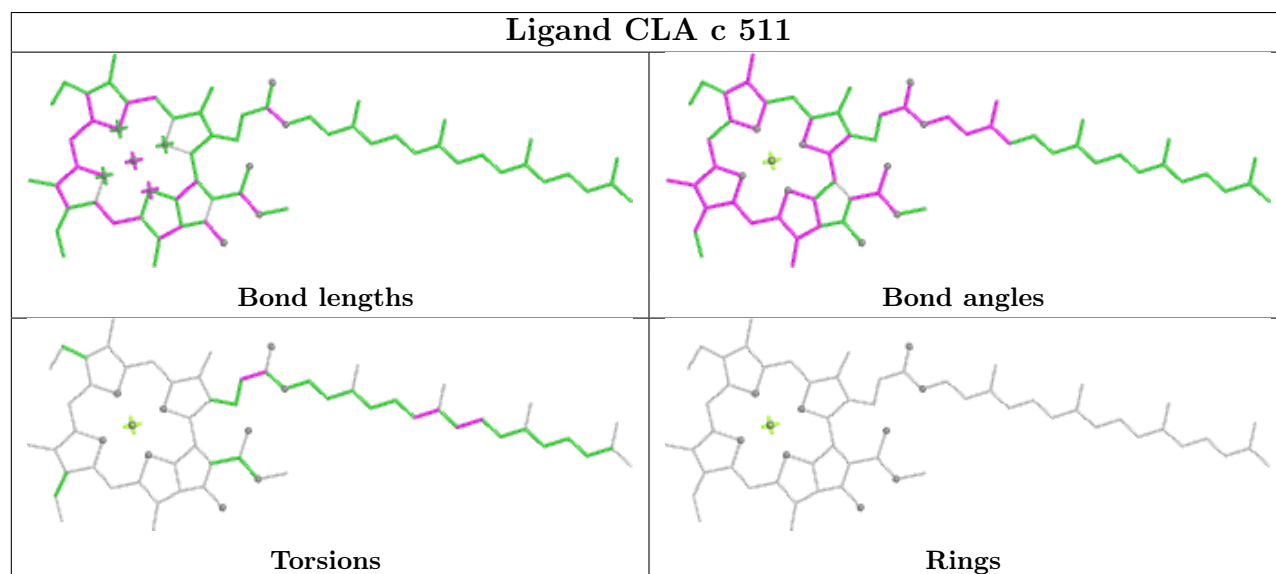
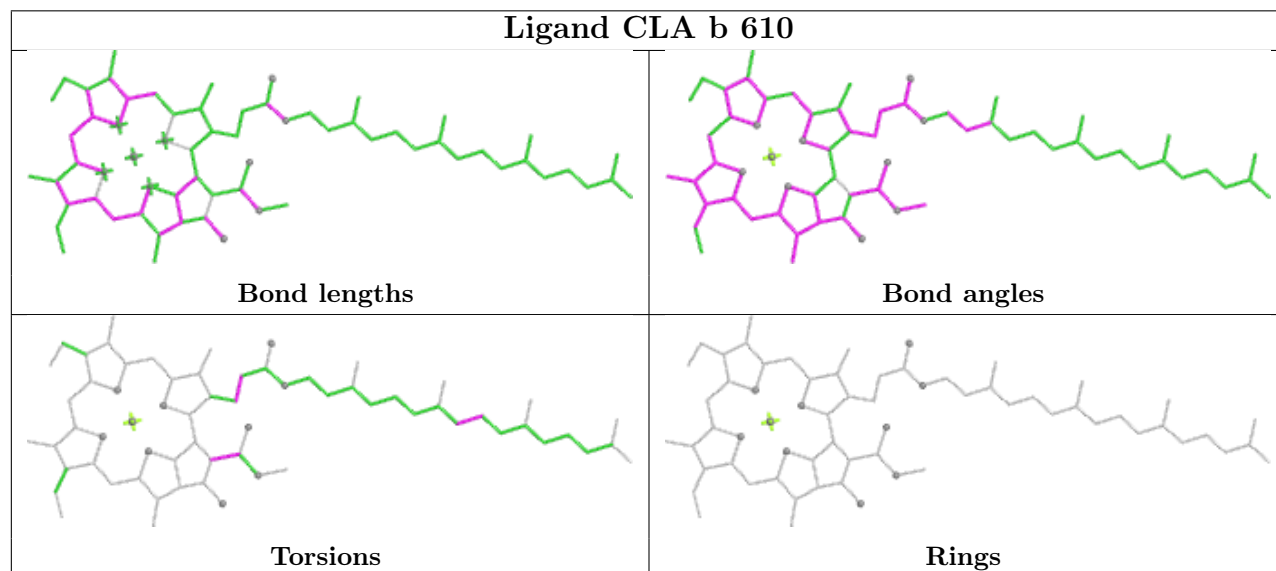
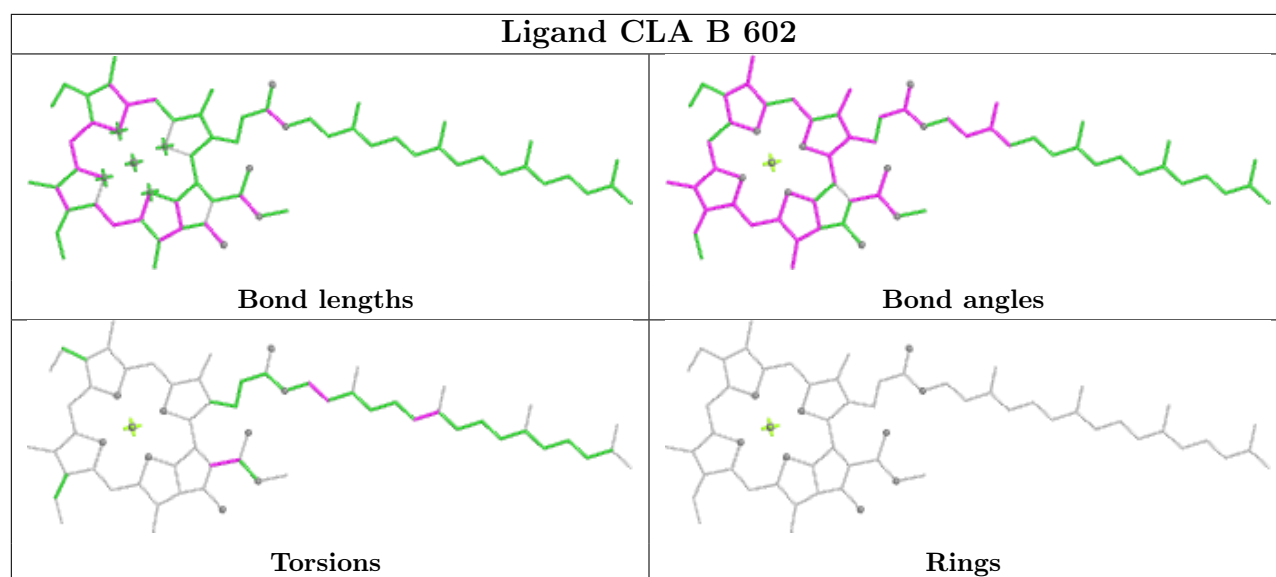


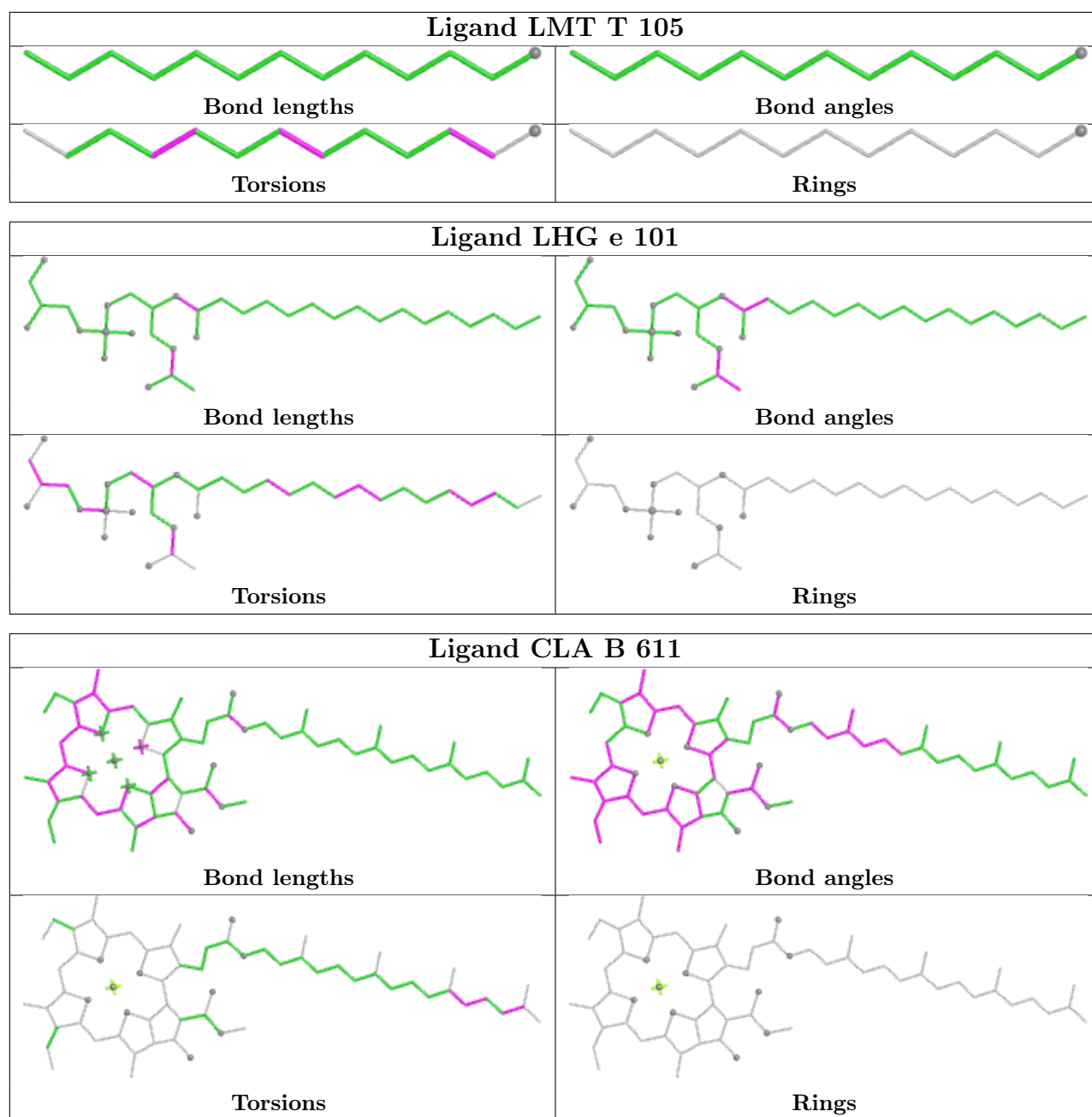


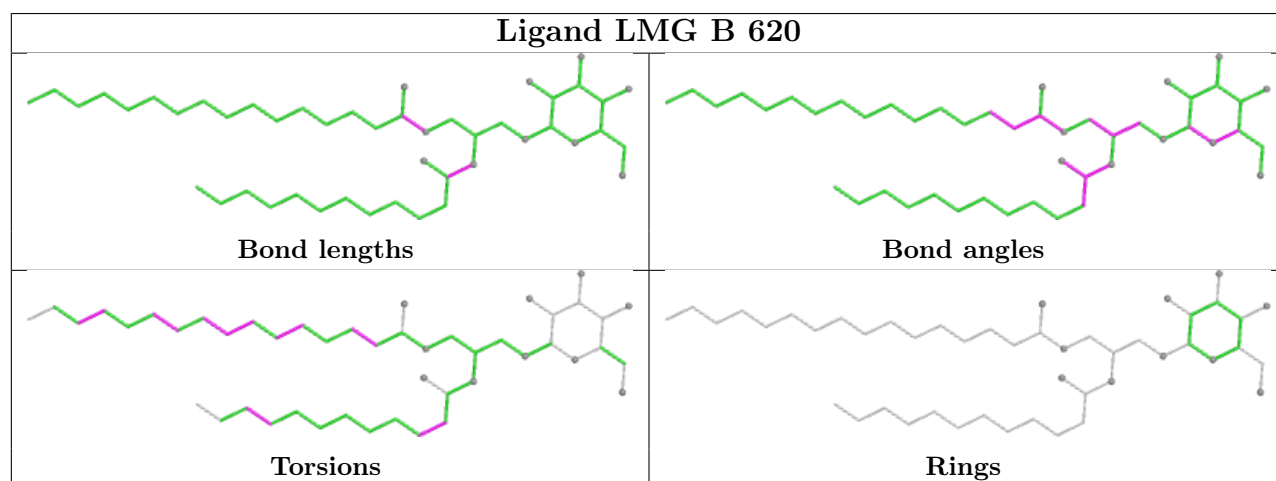
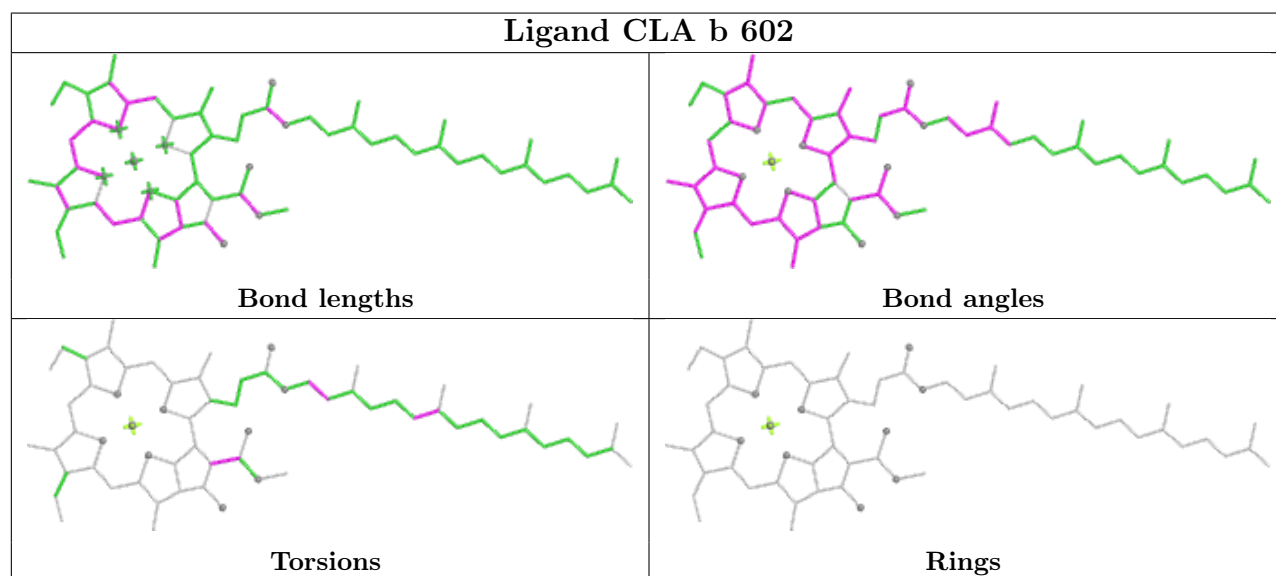
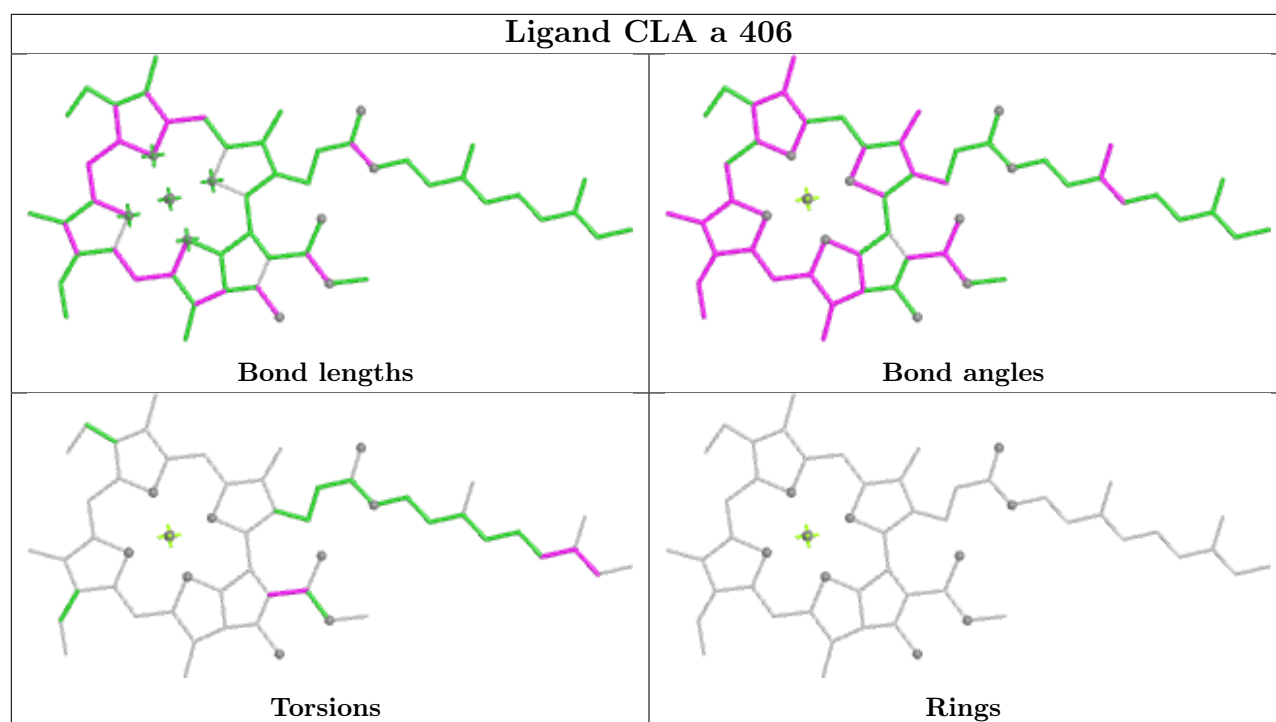


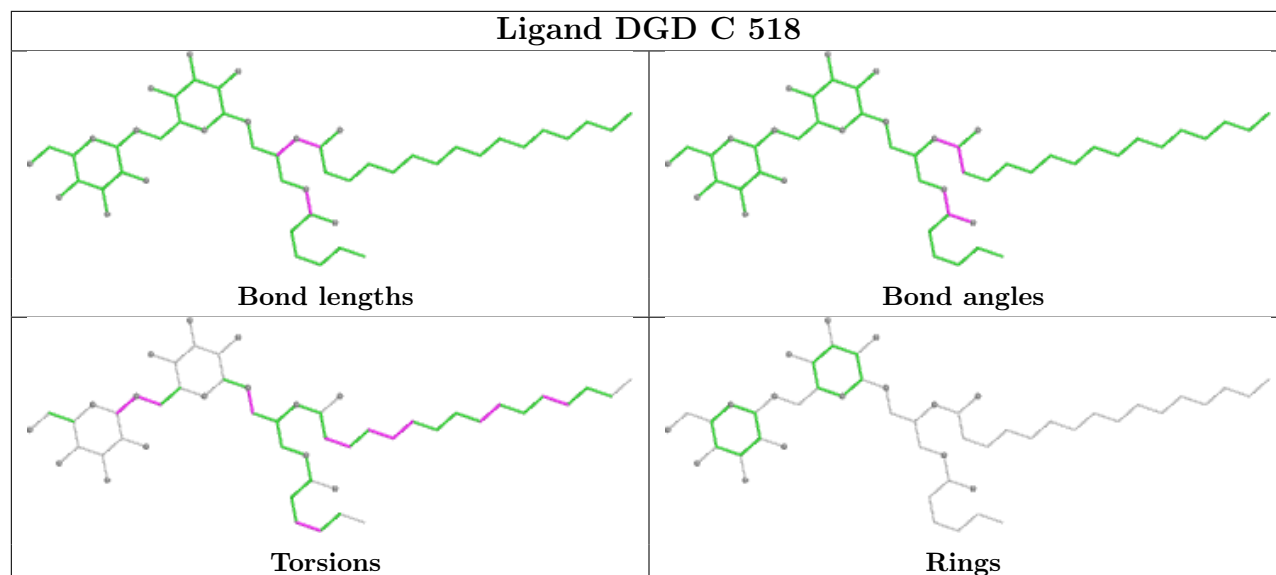
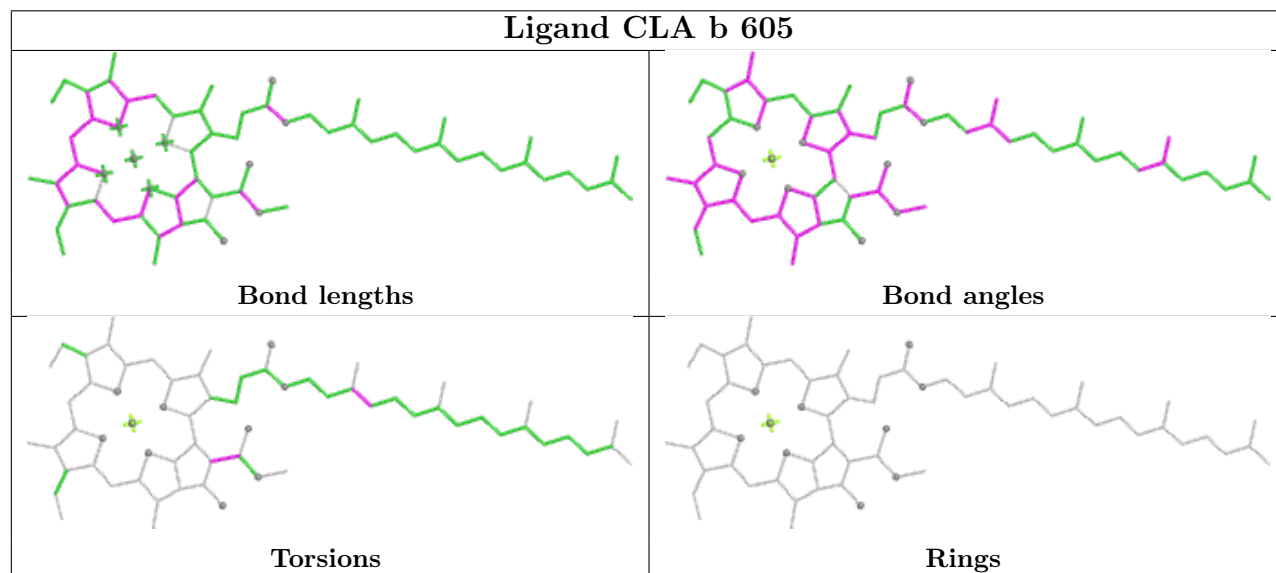
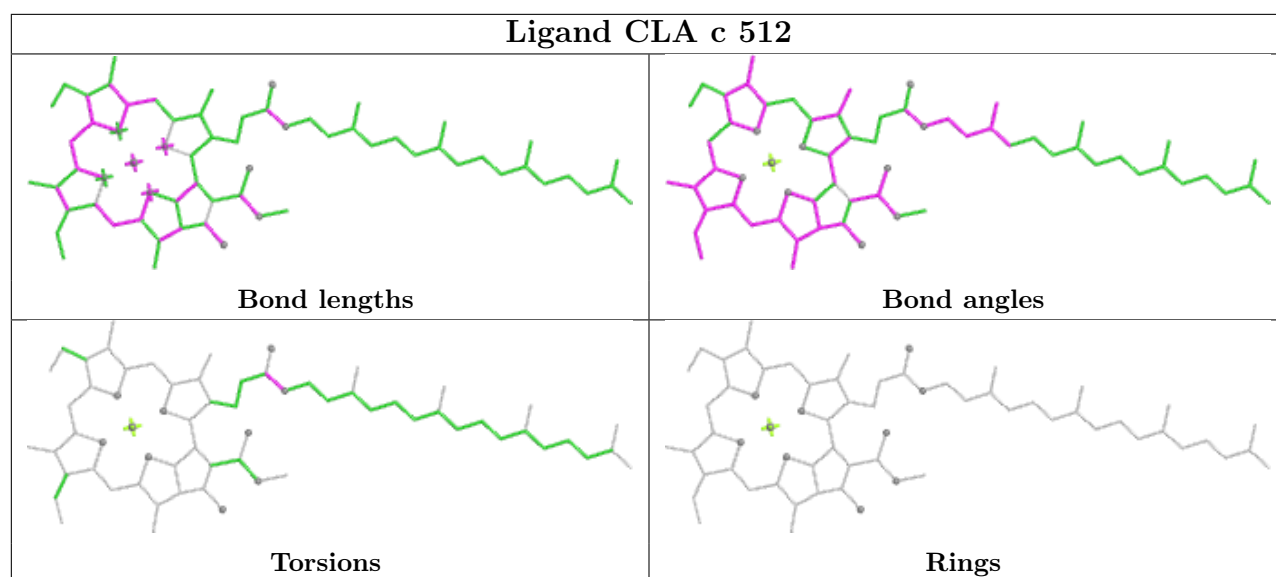
**Ligand CLA C 509****Ligand CLA A 408**



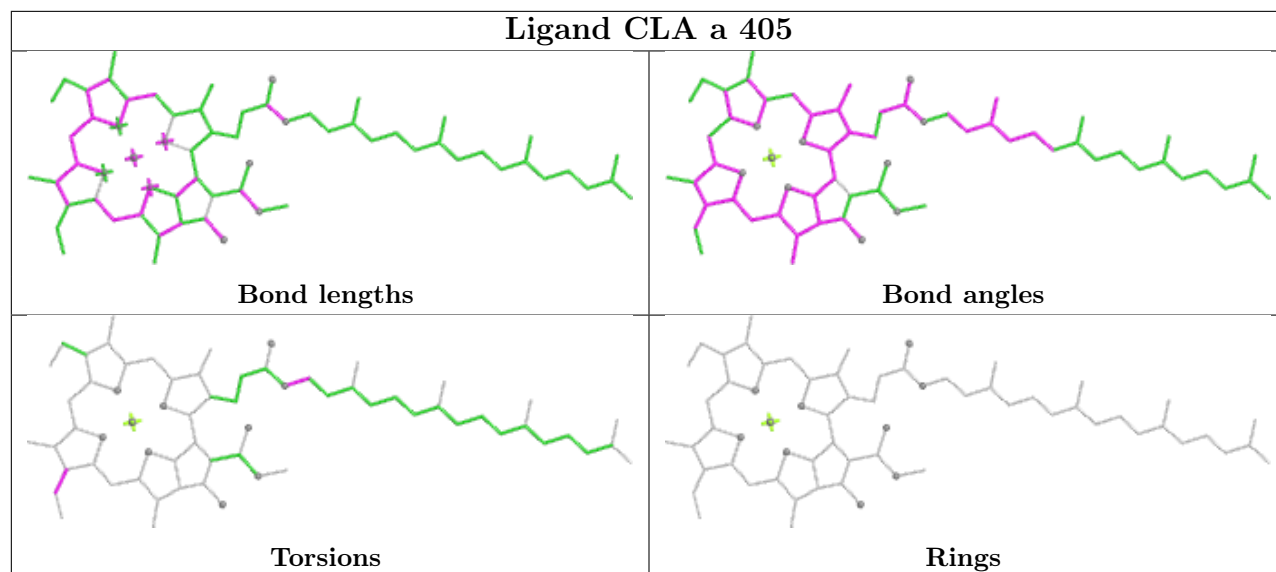




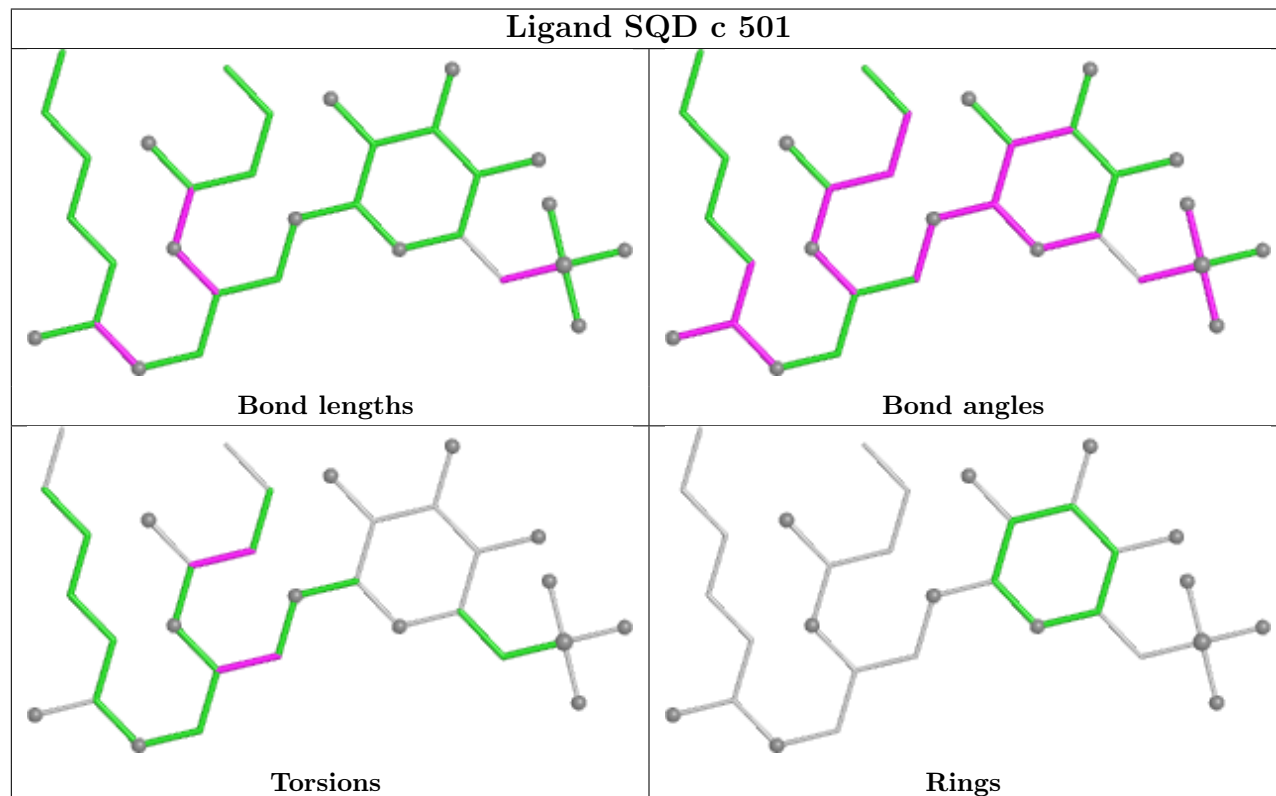


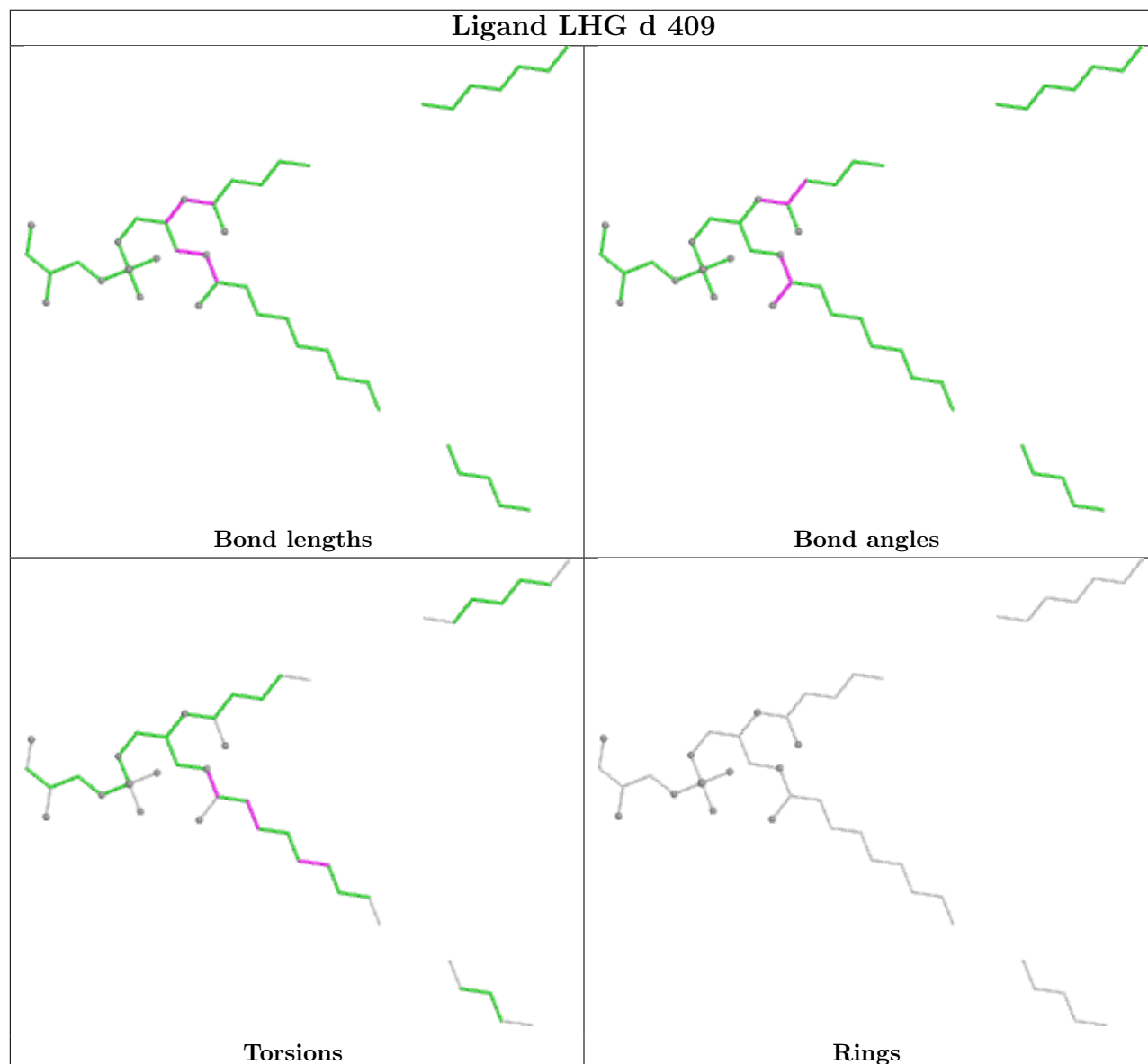
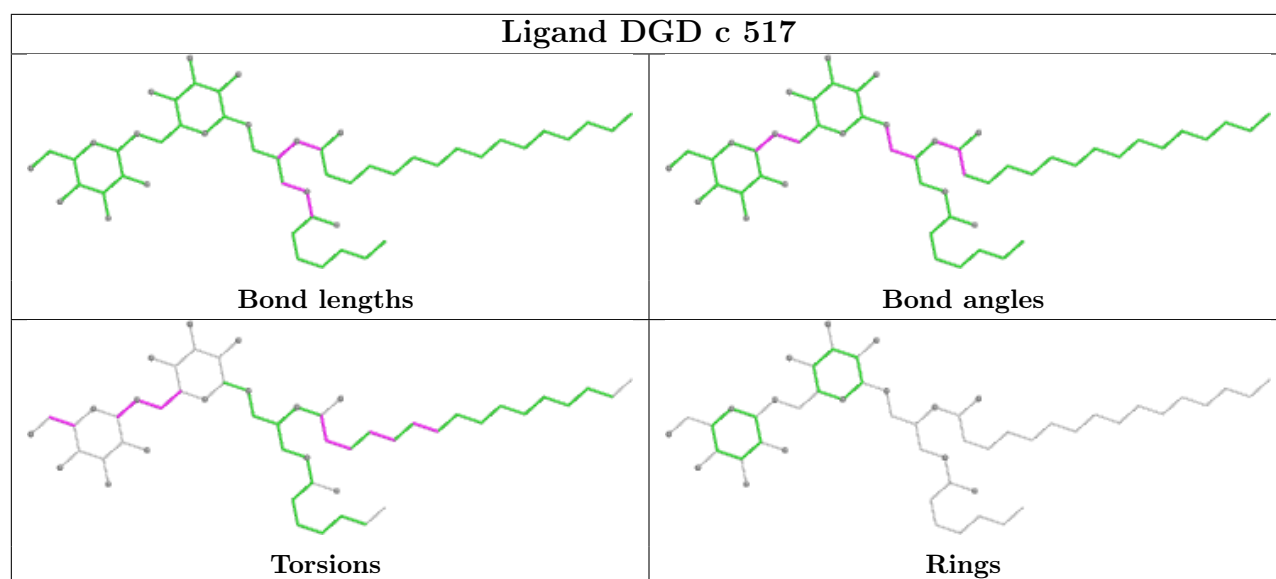


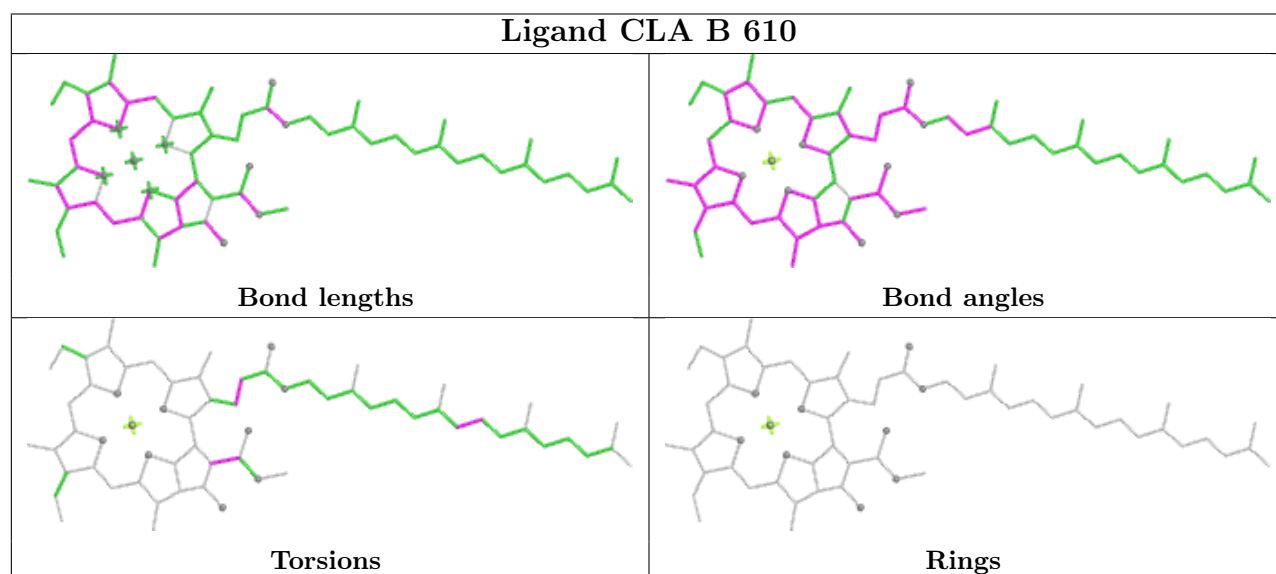
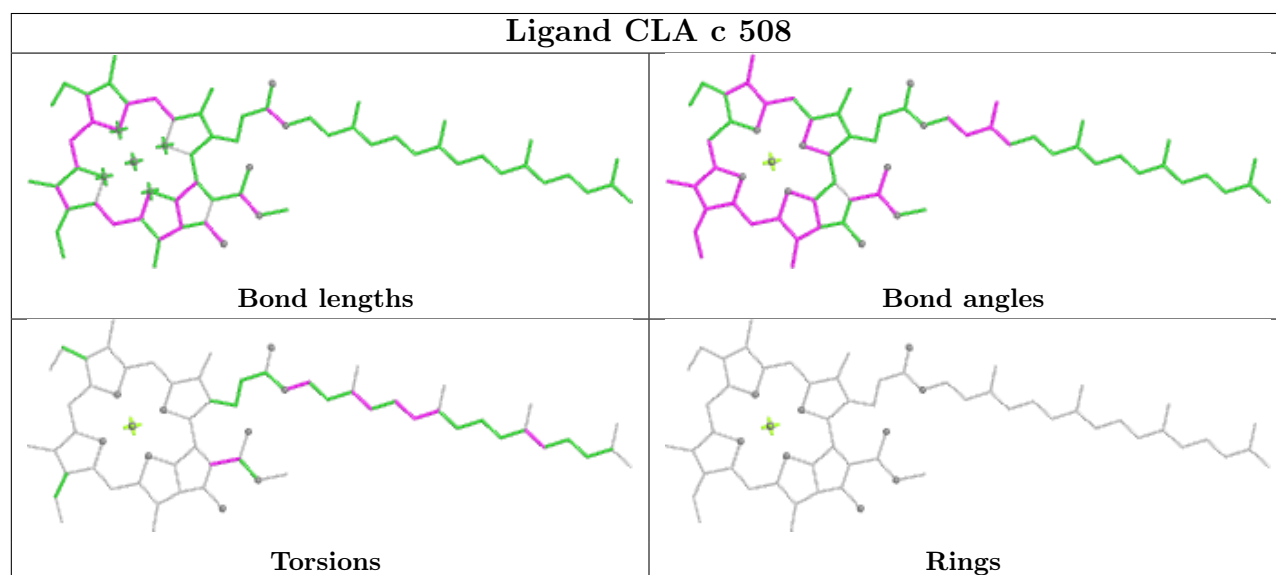
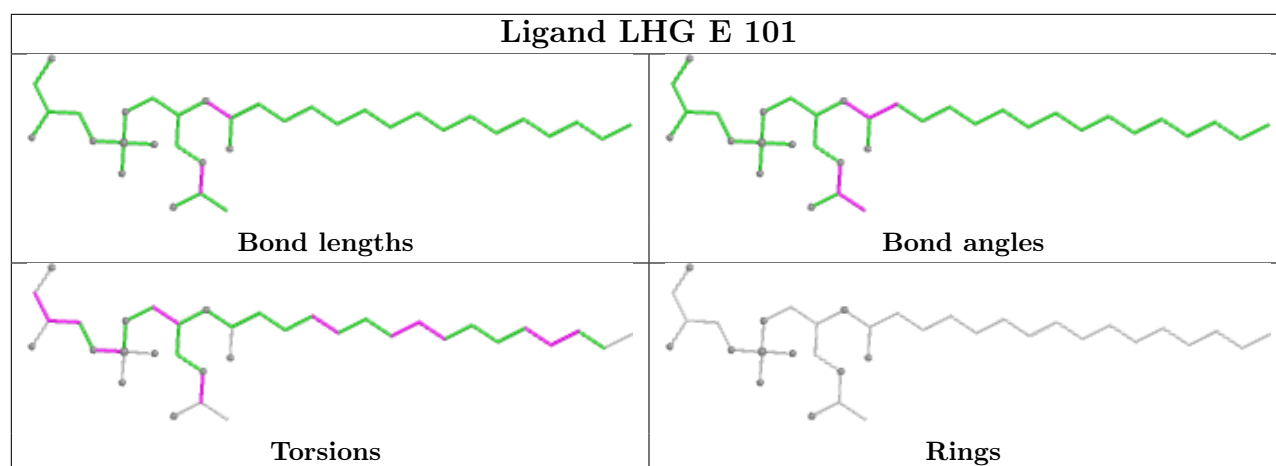
## Ligand CLA a 405

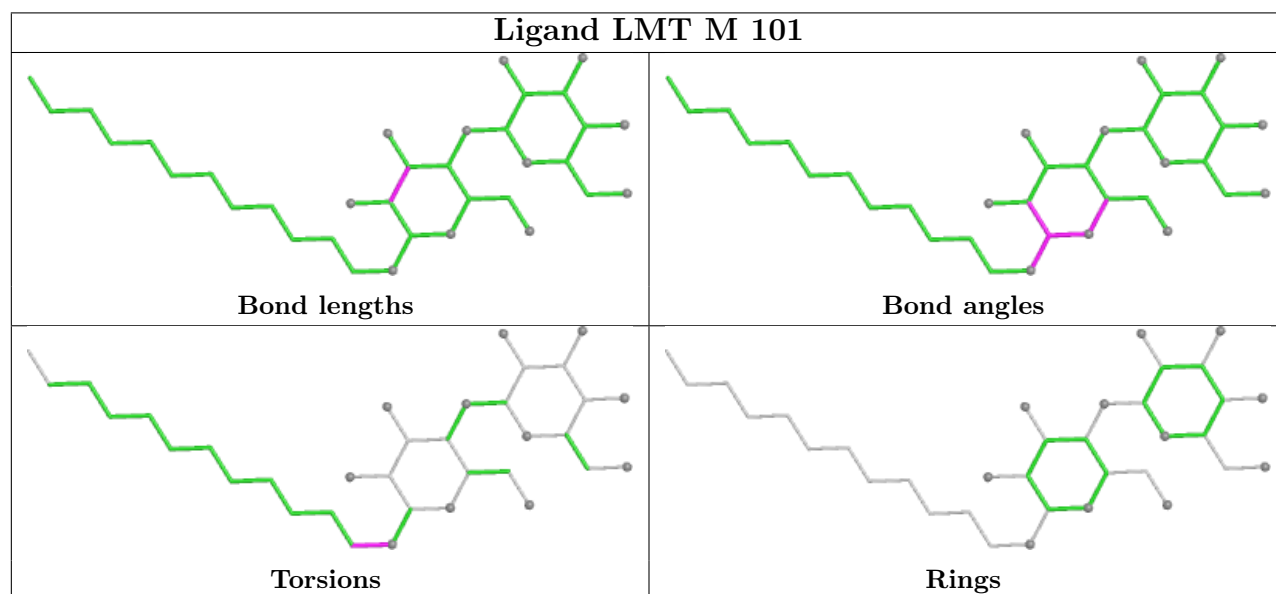
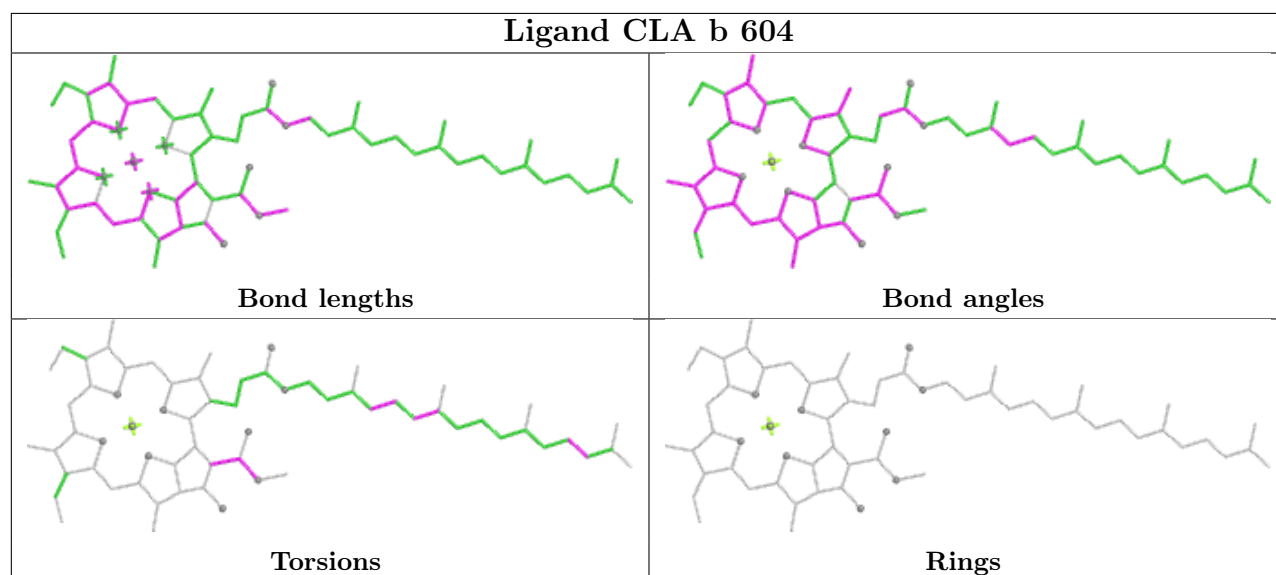
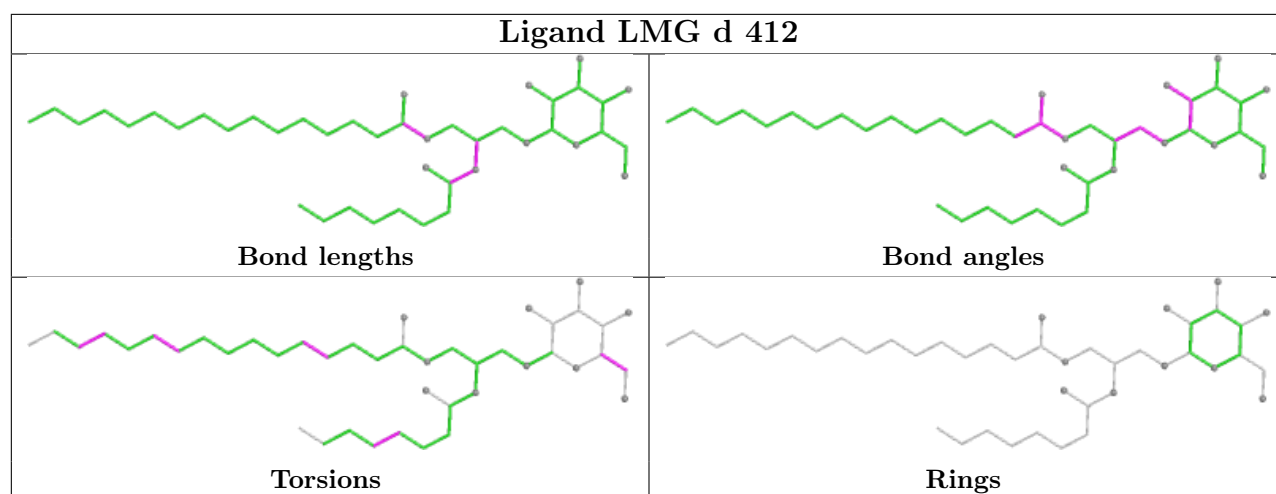


## Ligand SQD c 501

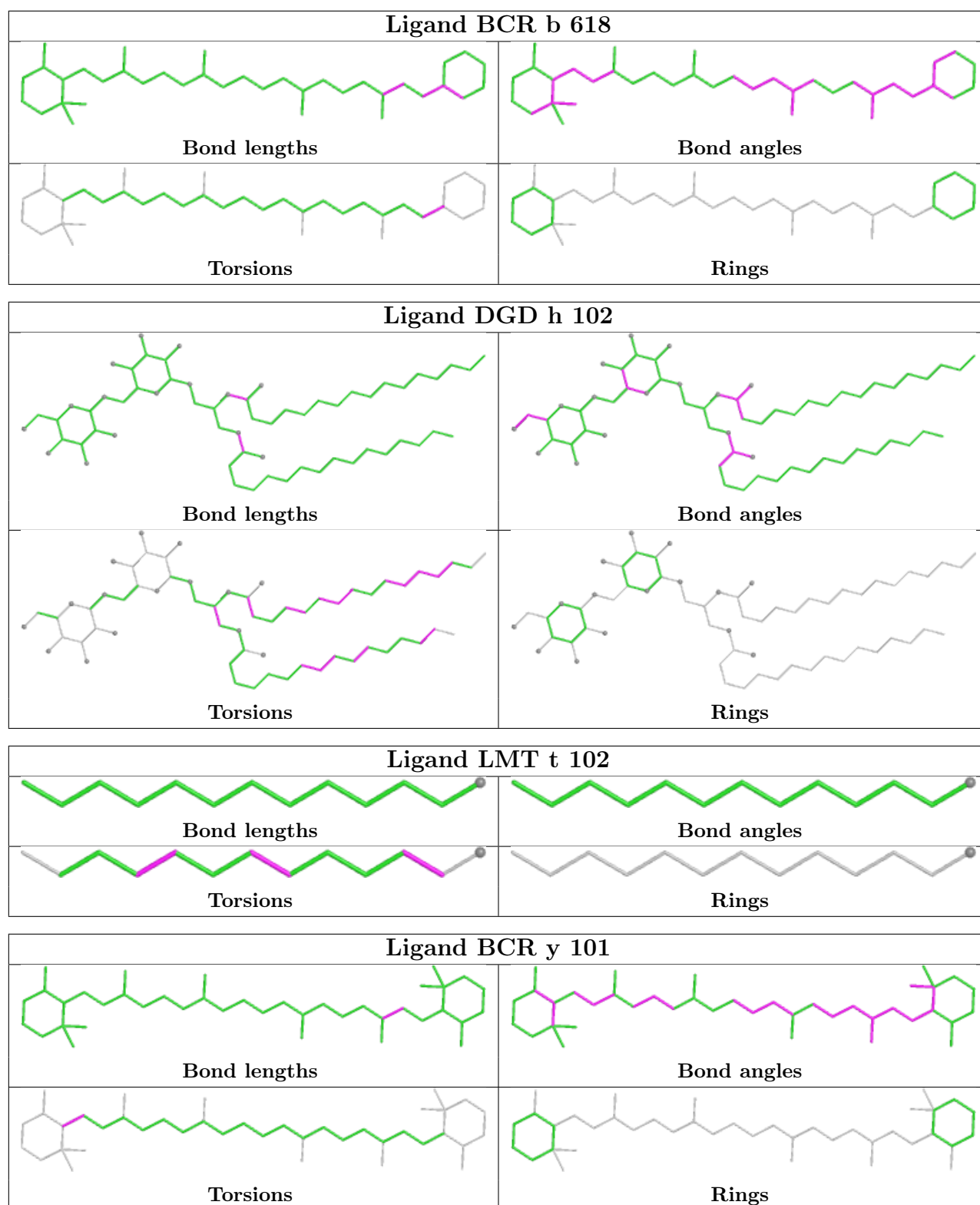


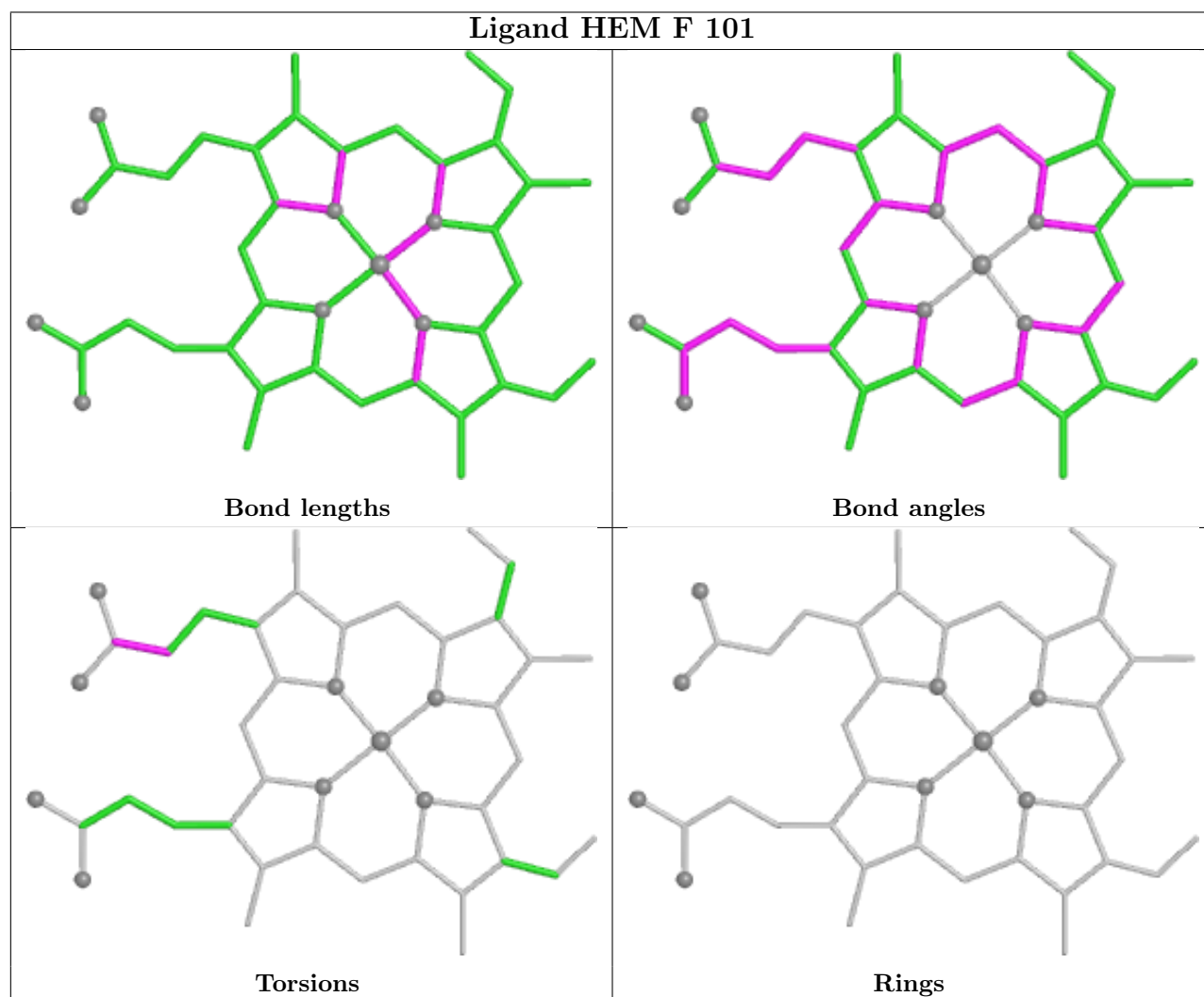
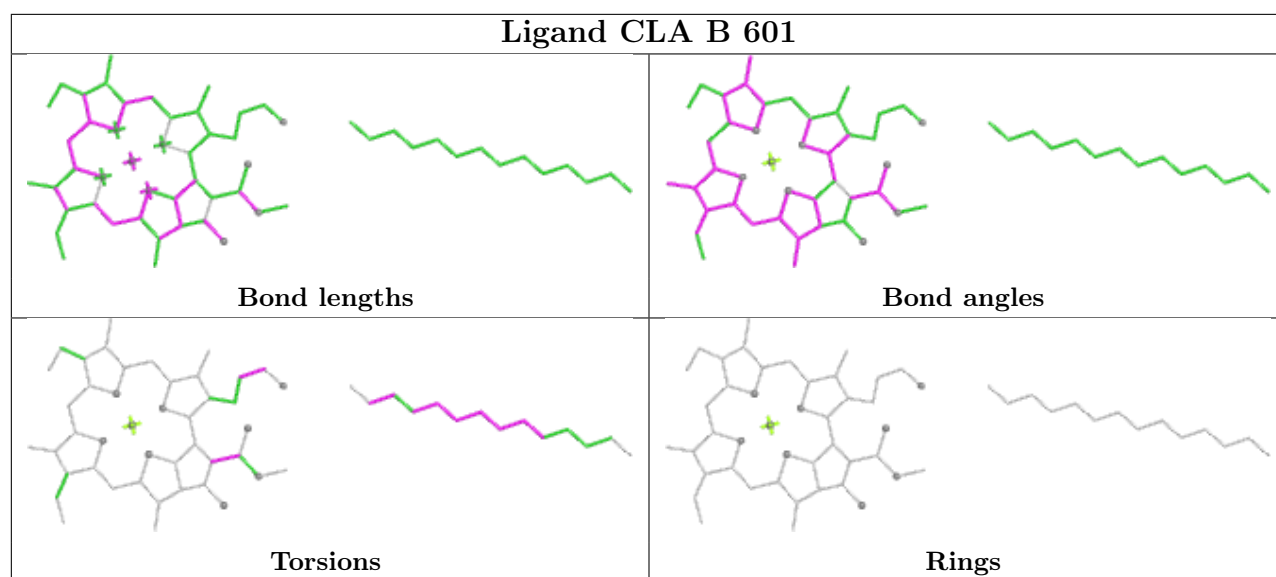


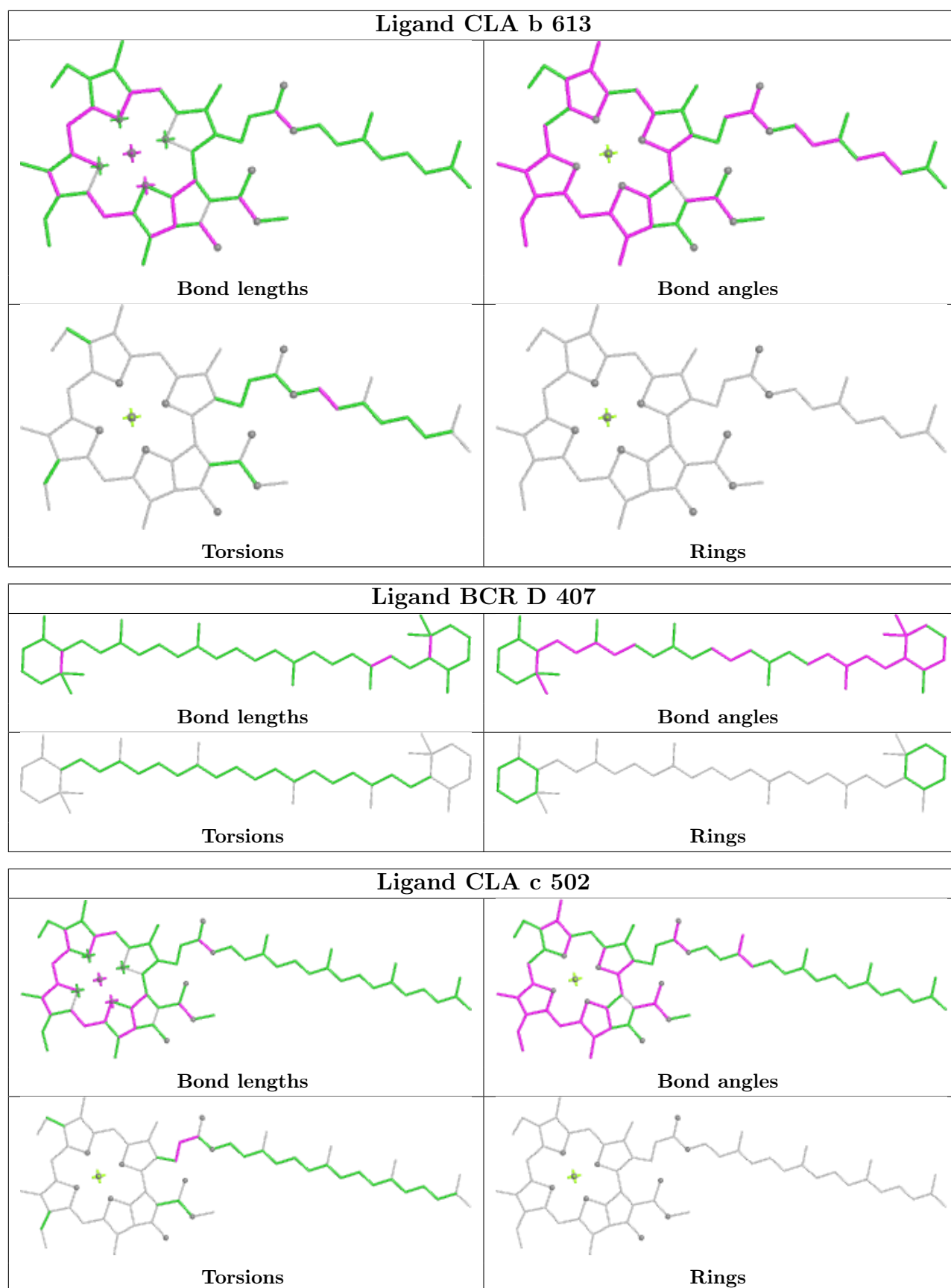




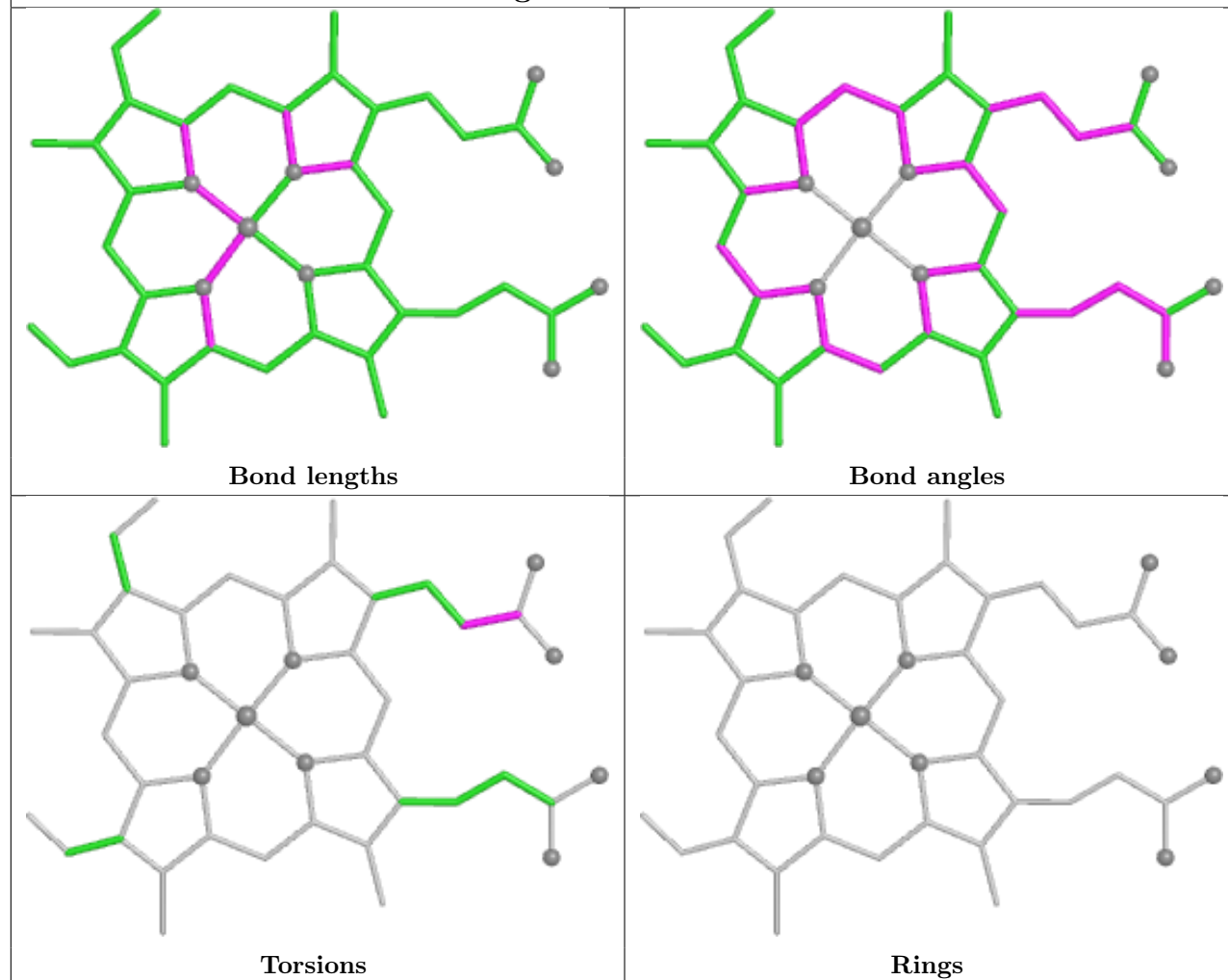




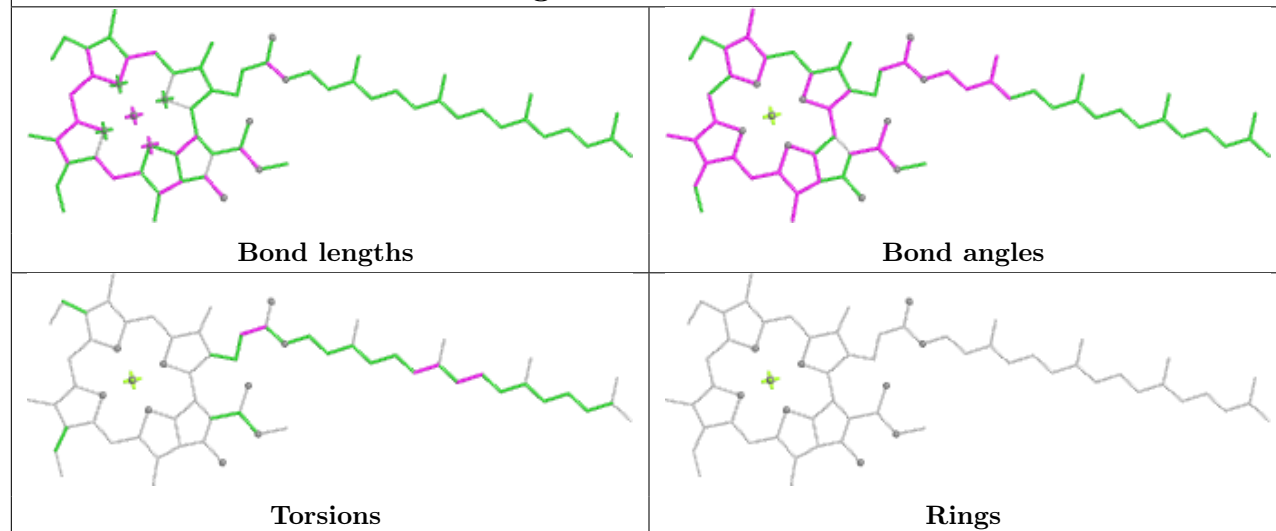


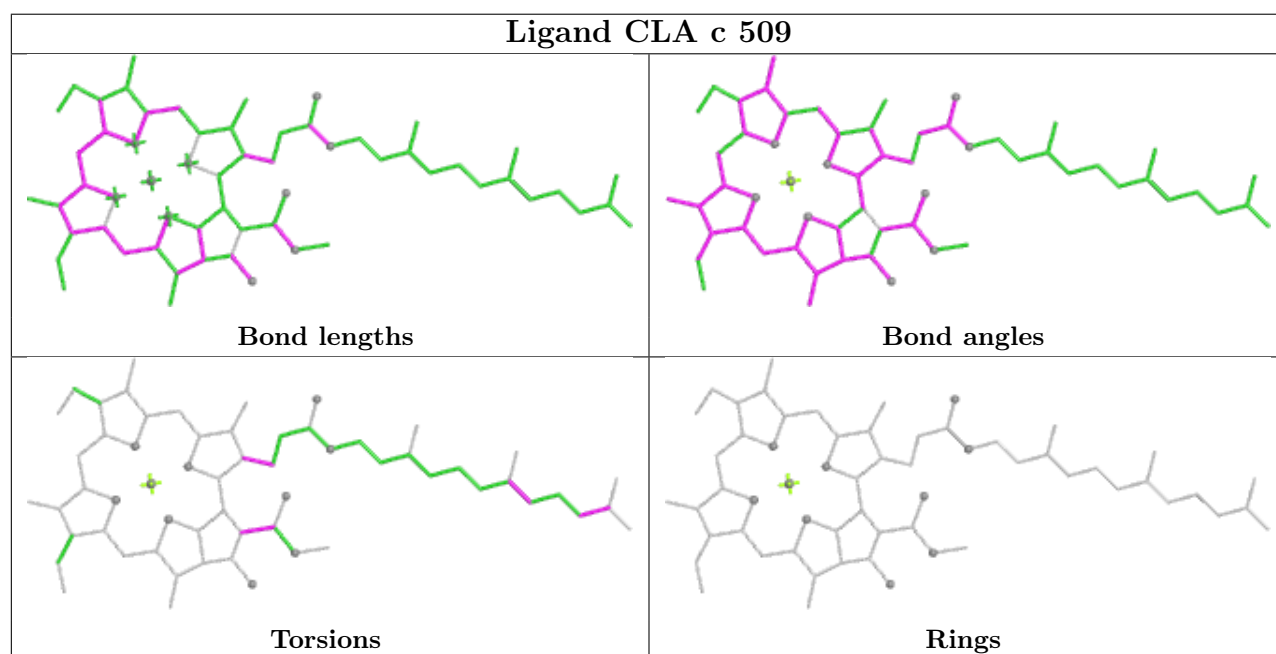
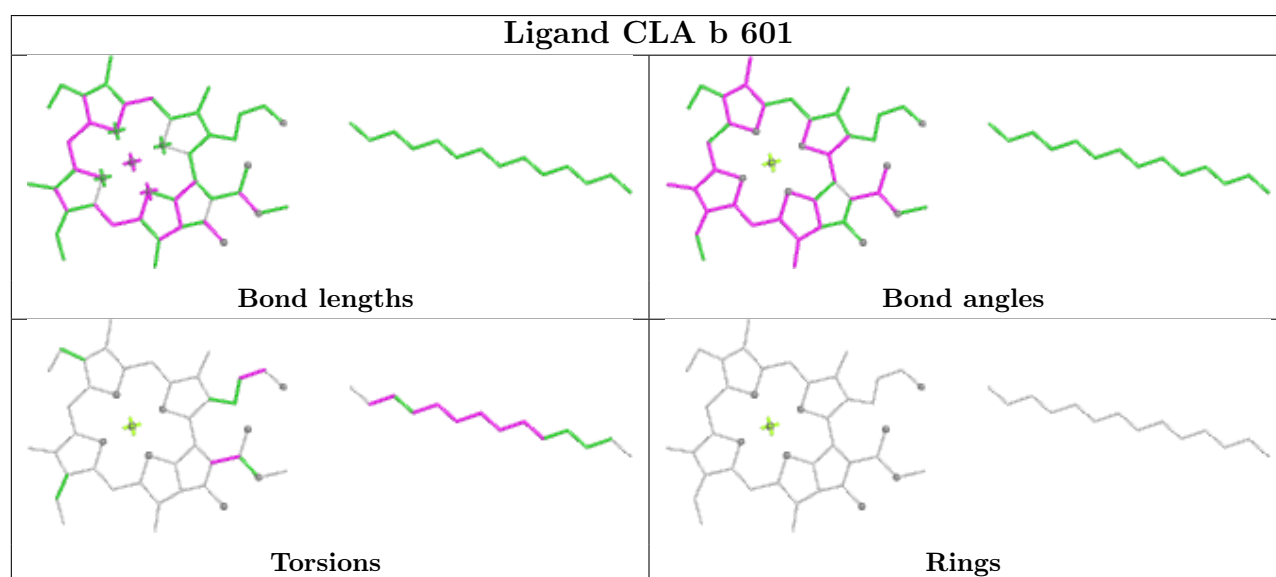
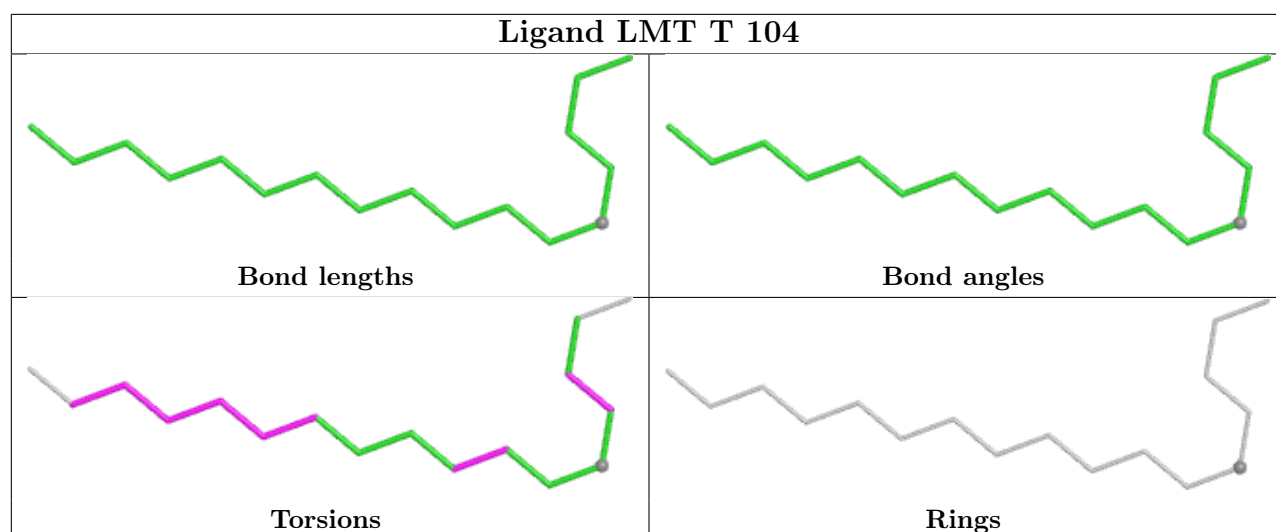


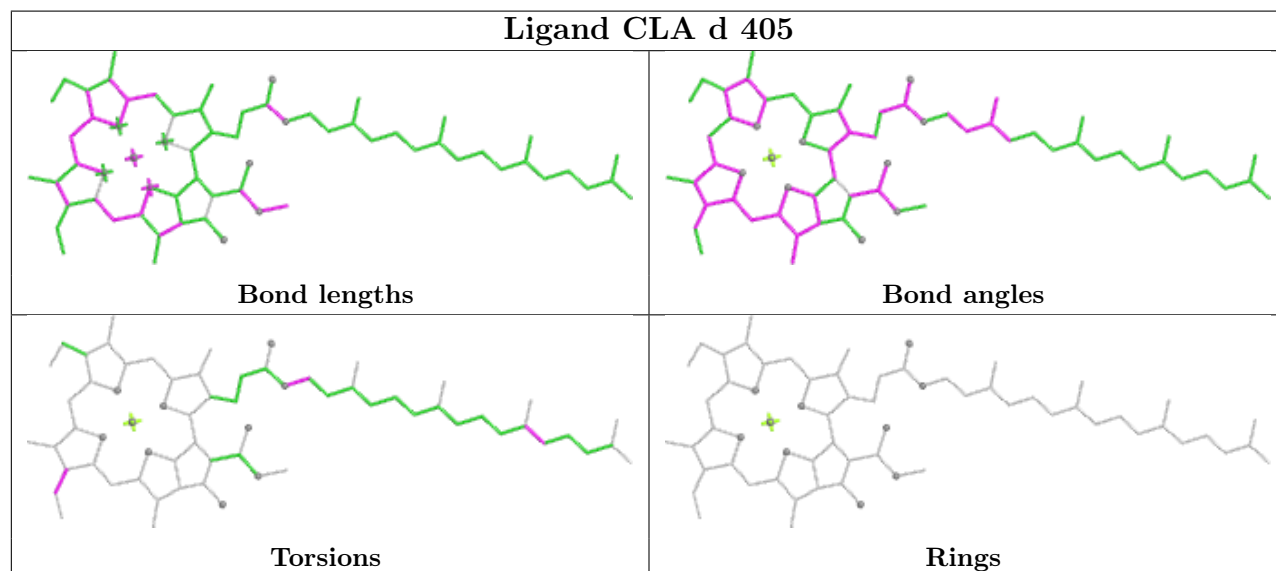
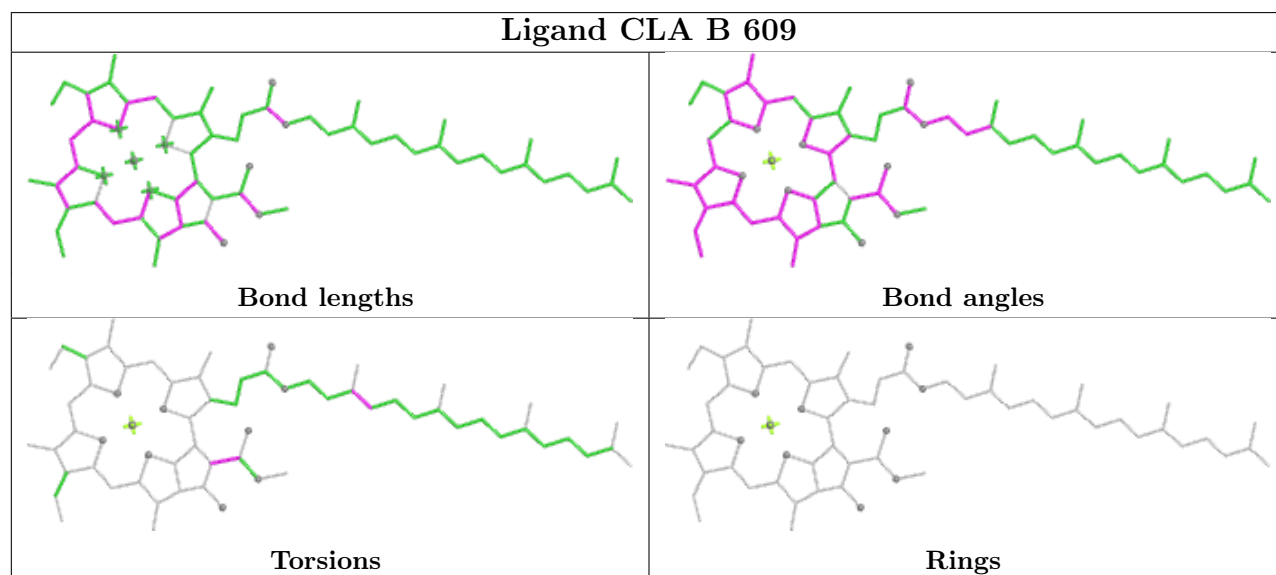
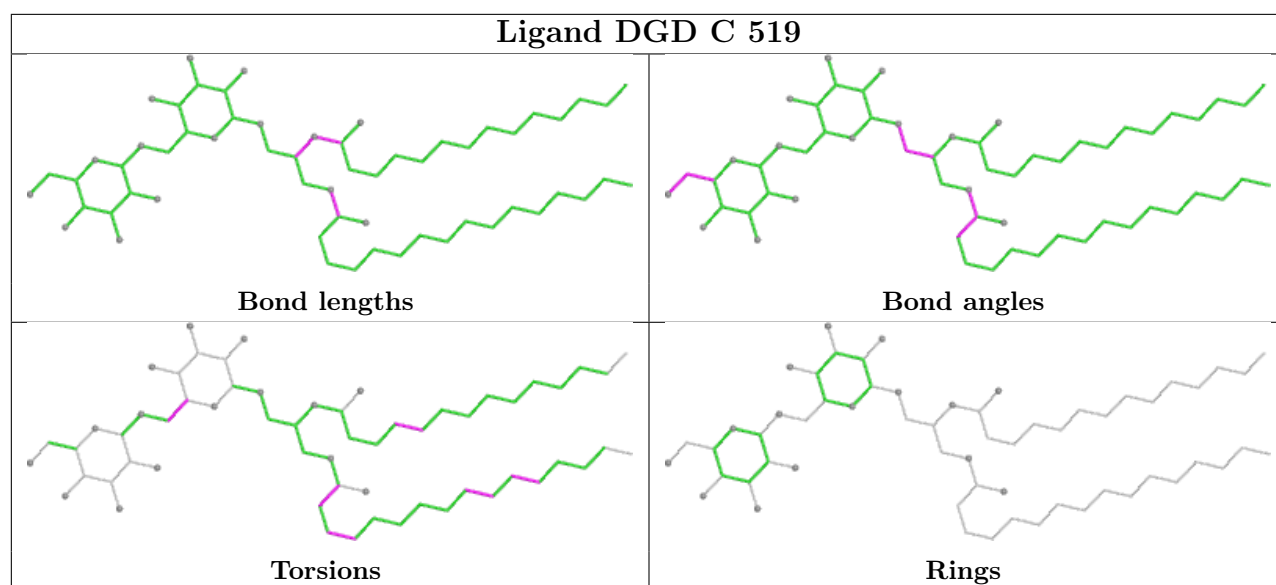
## Ligand HEM f 101



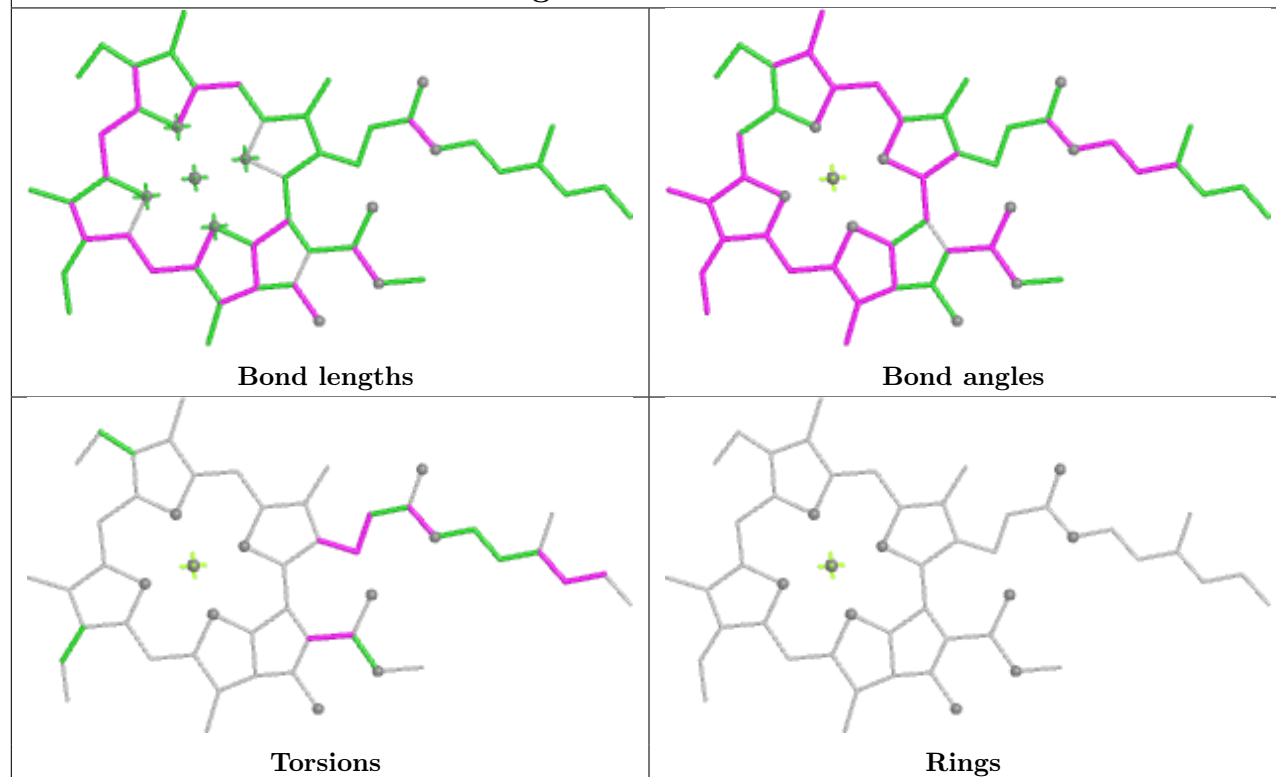
## Ligand CLA C 511



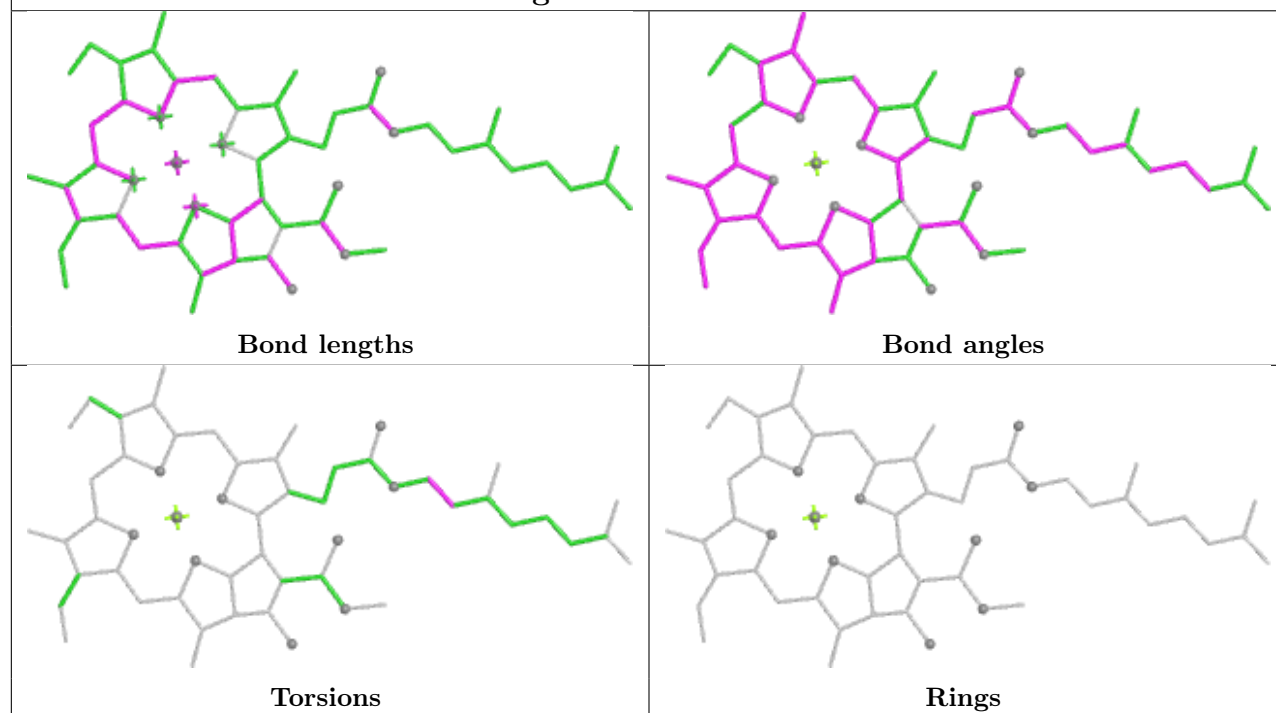


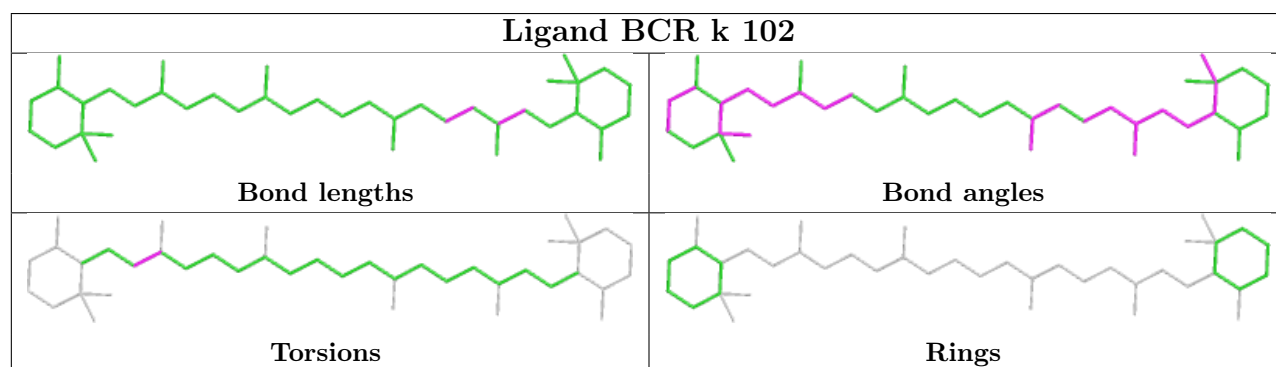
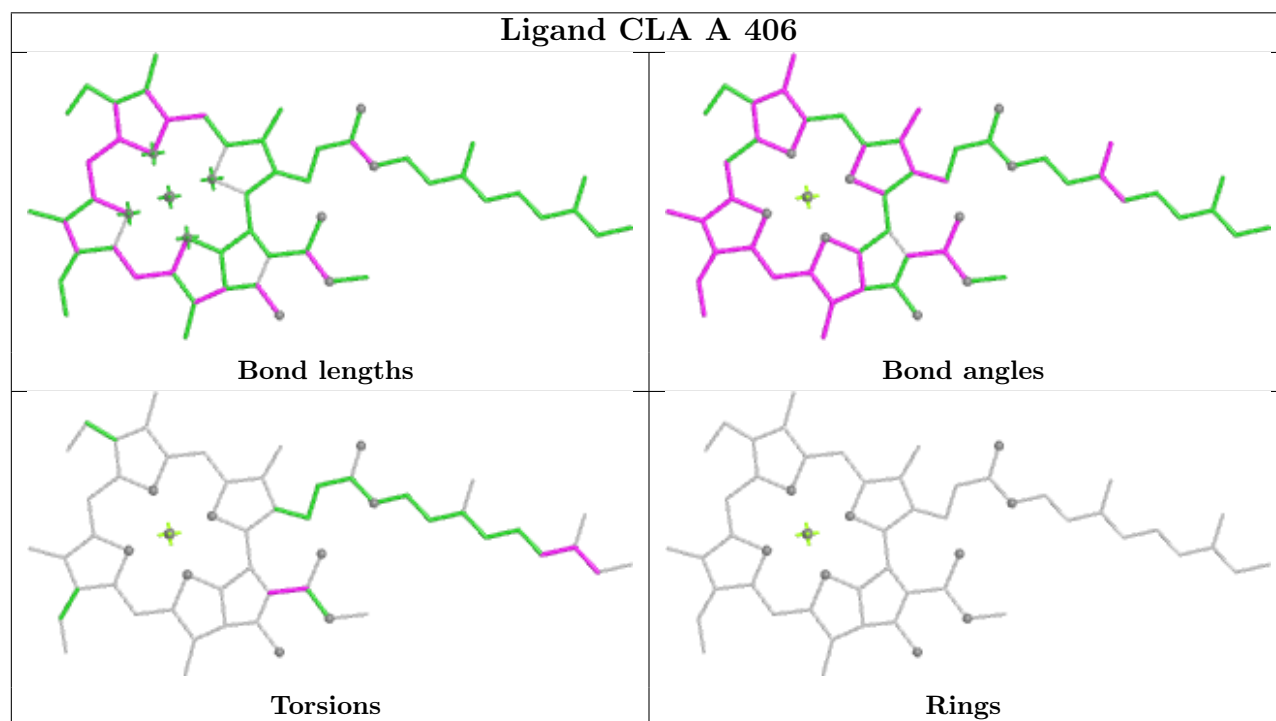
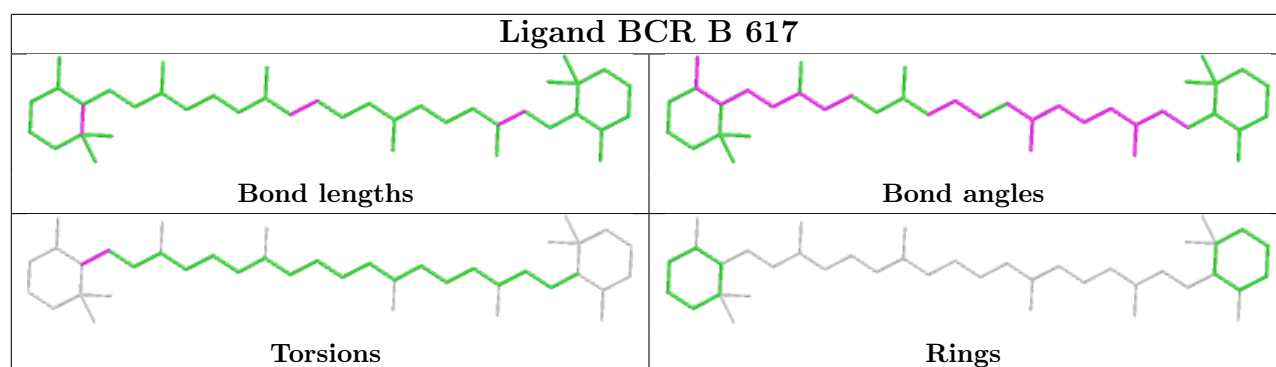


## Ligand CLA C 513

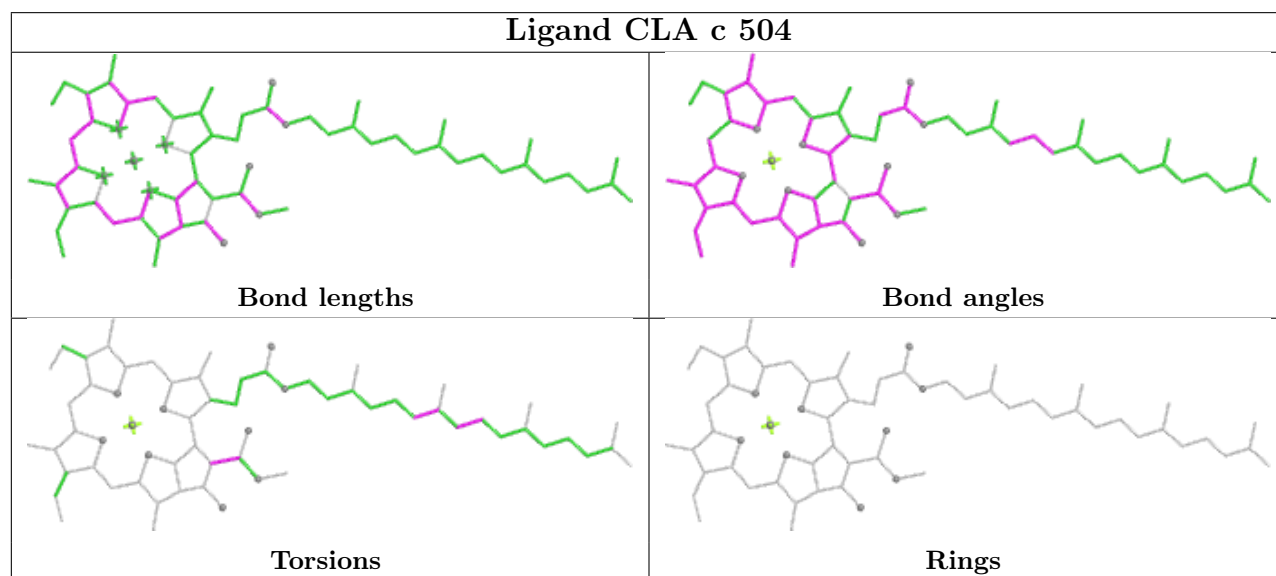
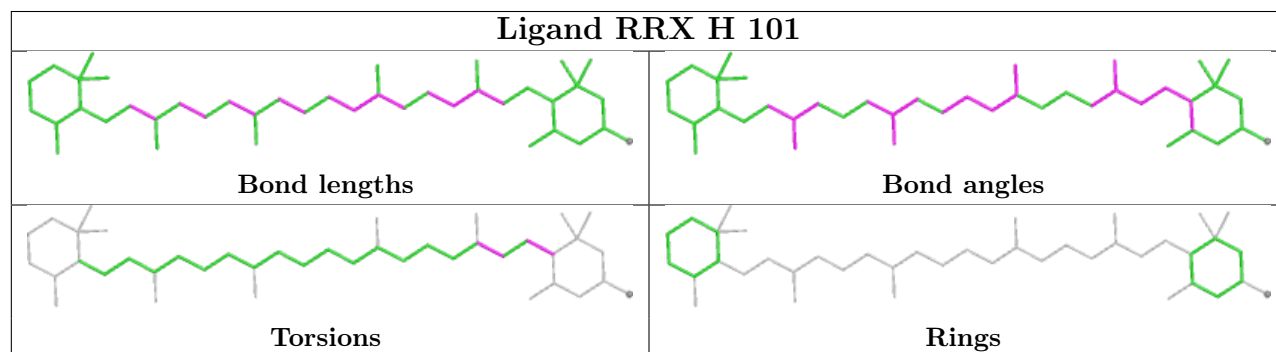
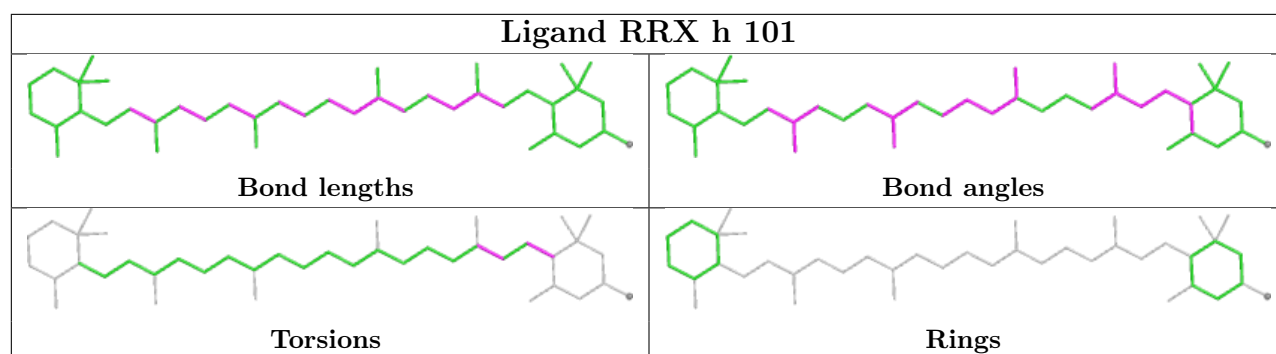


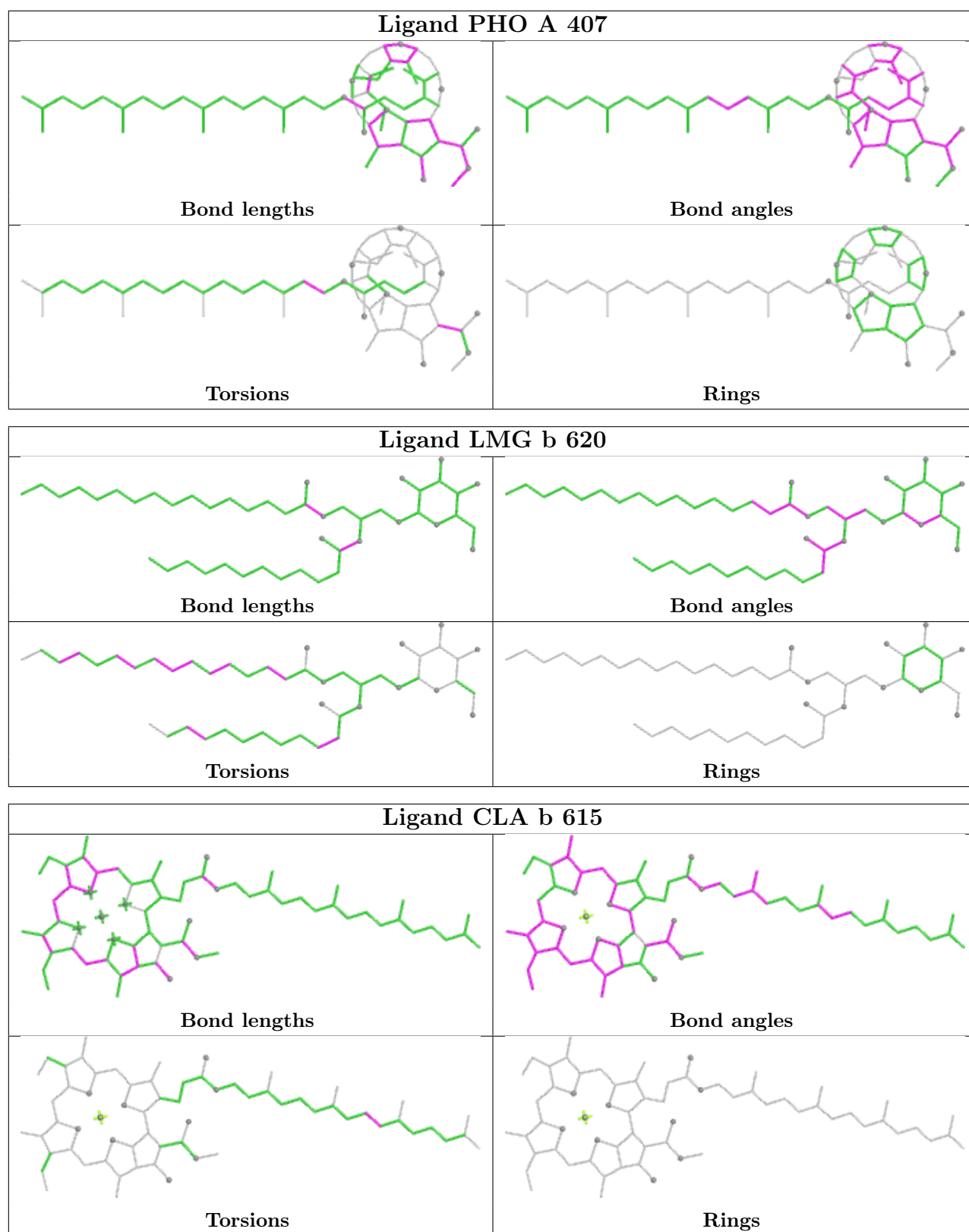
## Ligand CLA B 613

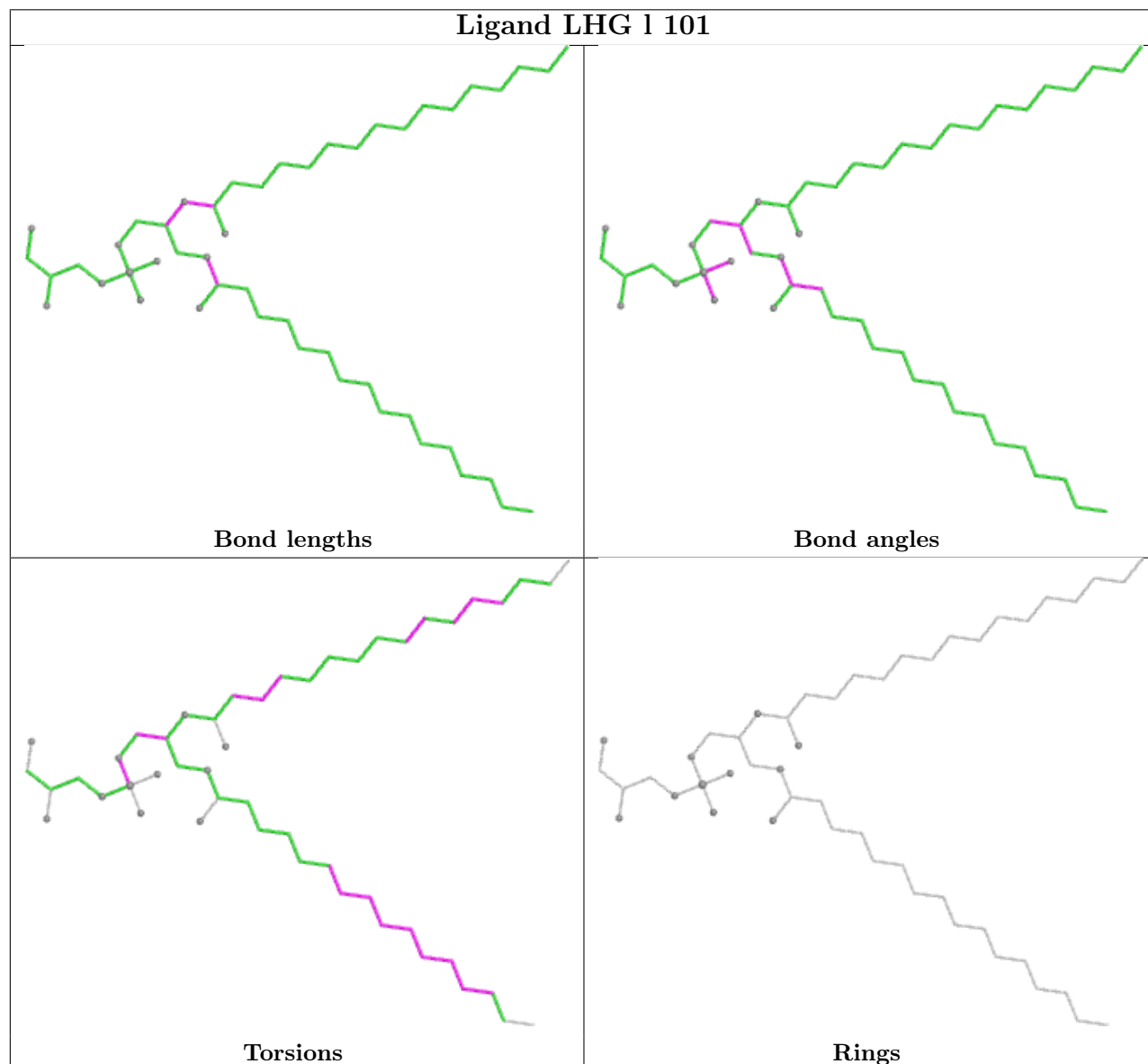
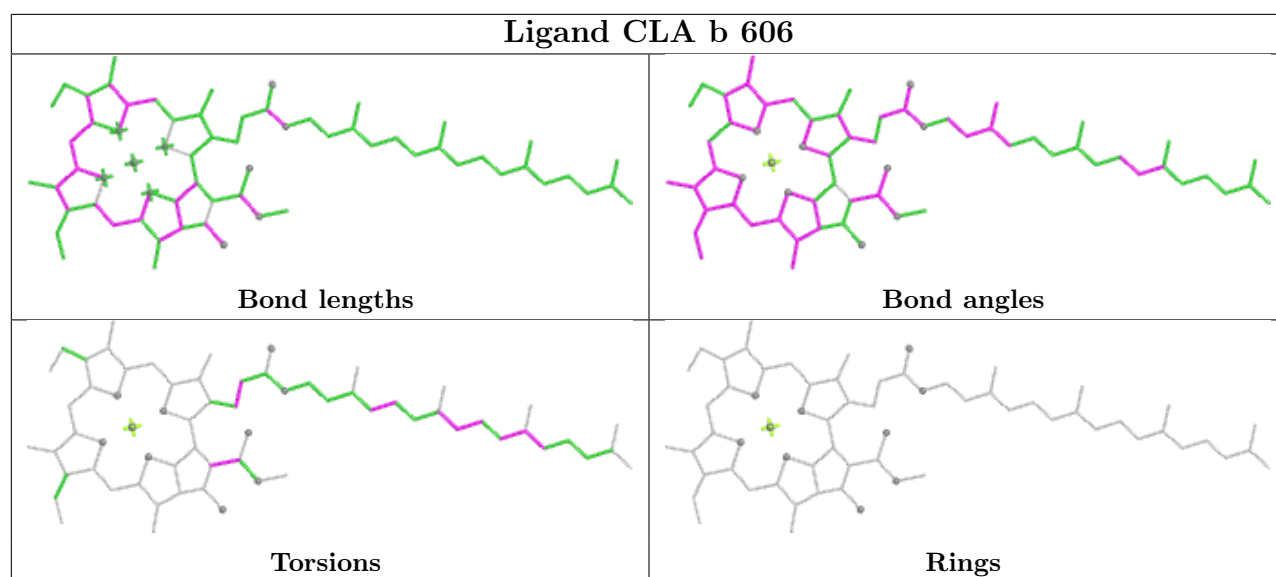


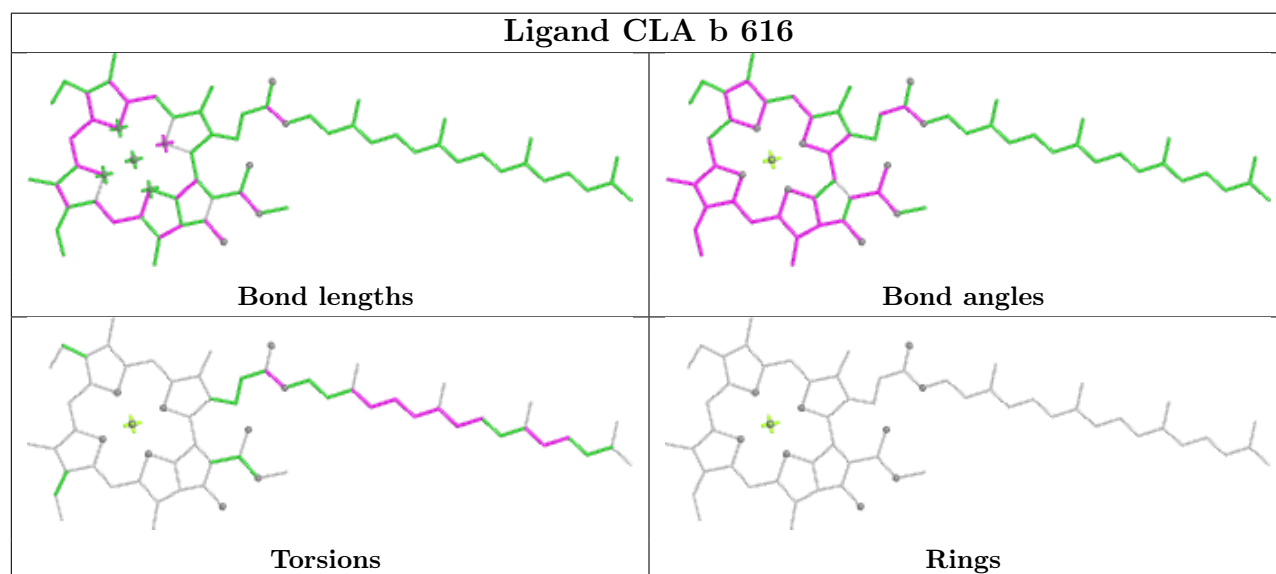
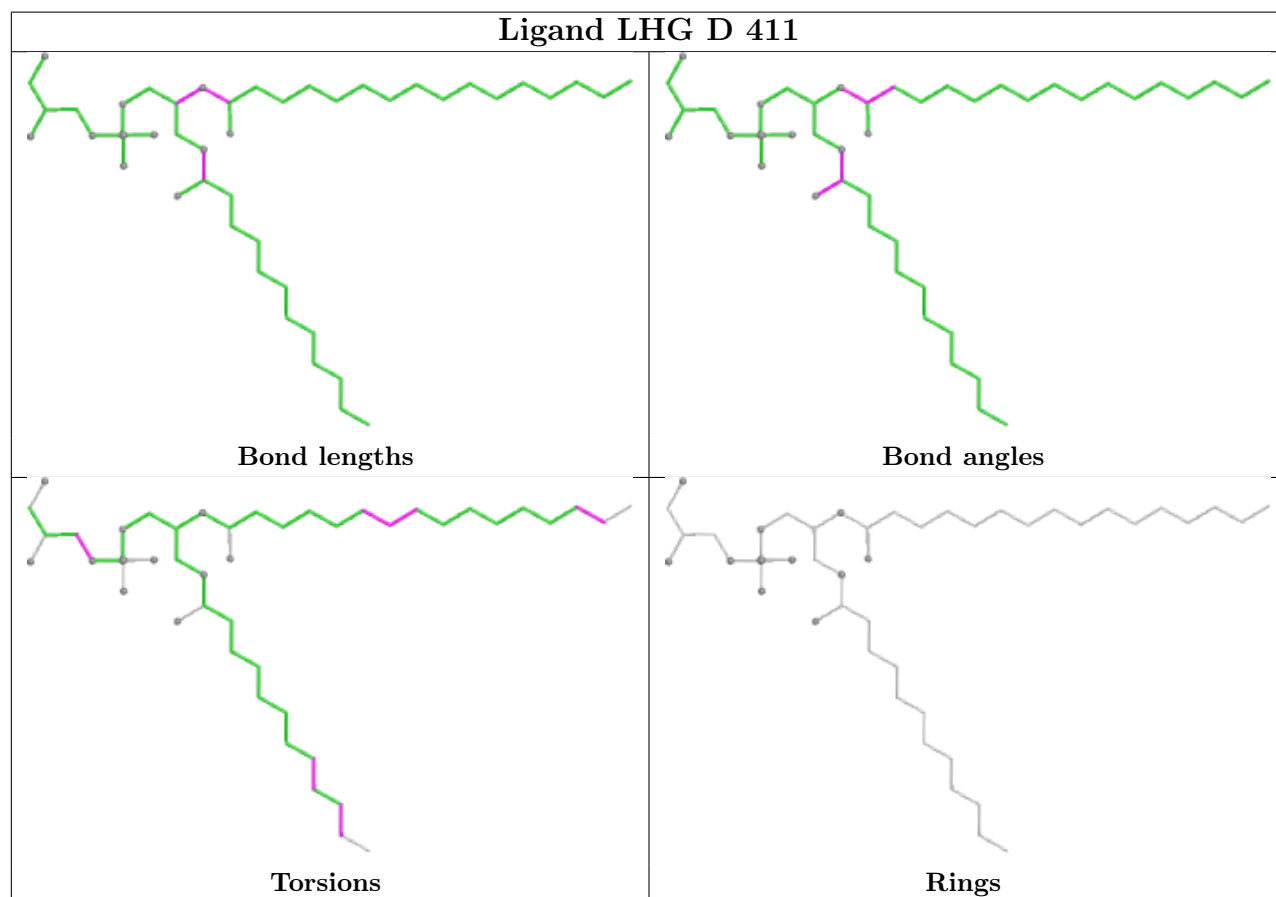
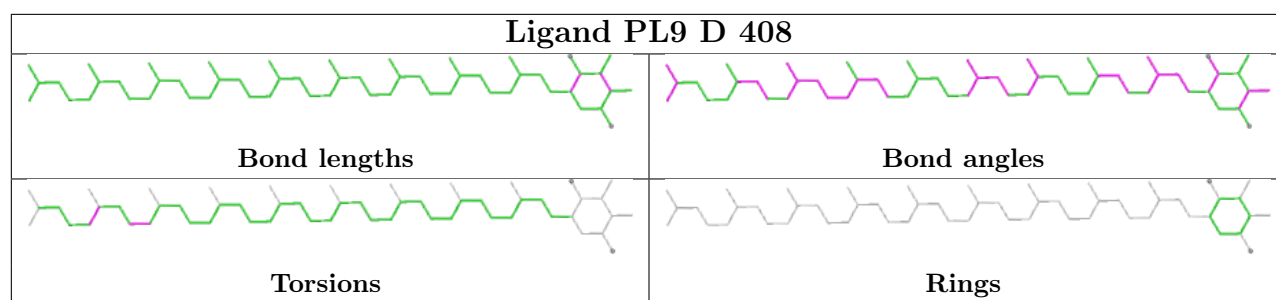


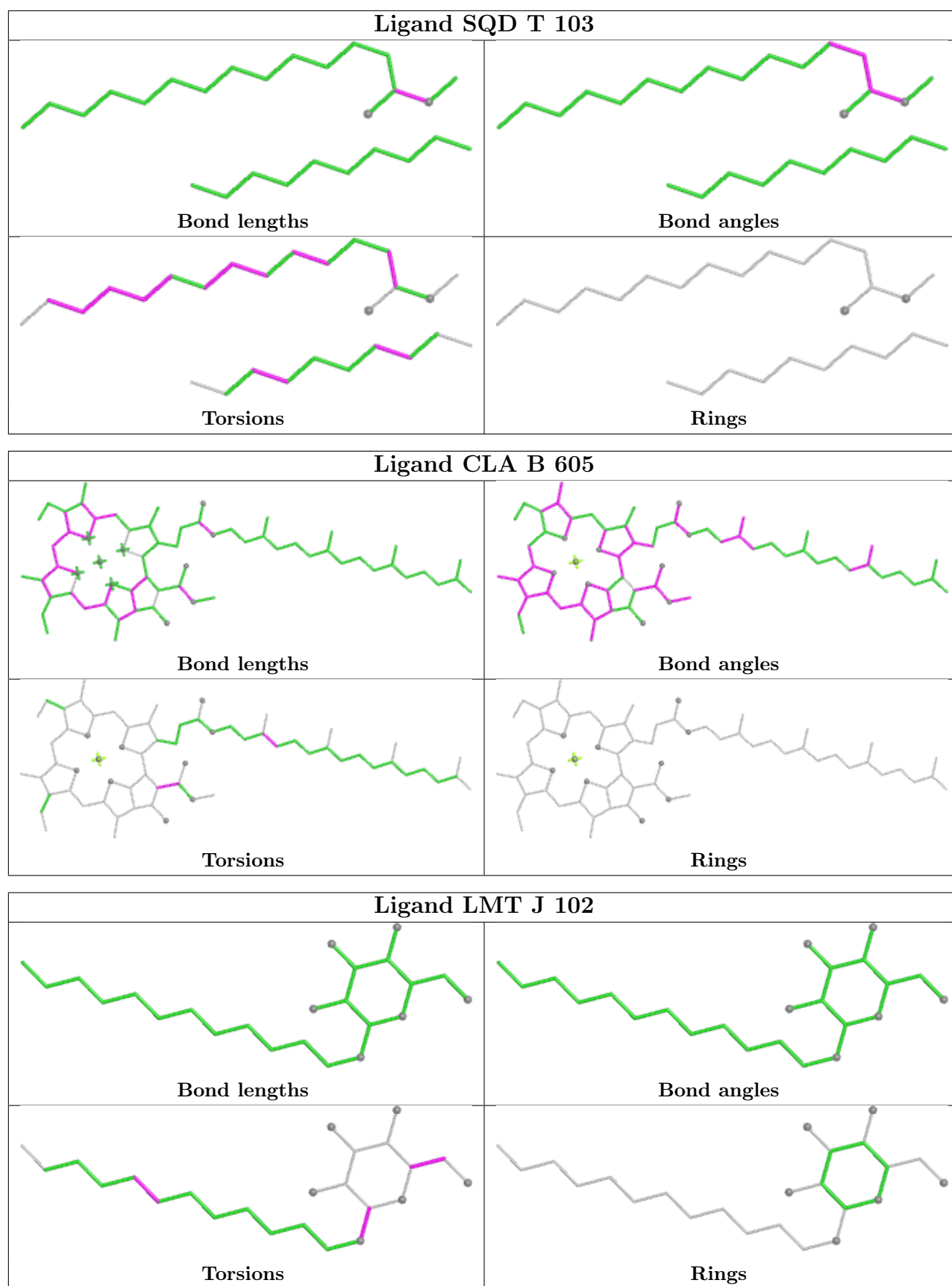


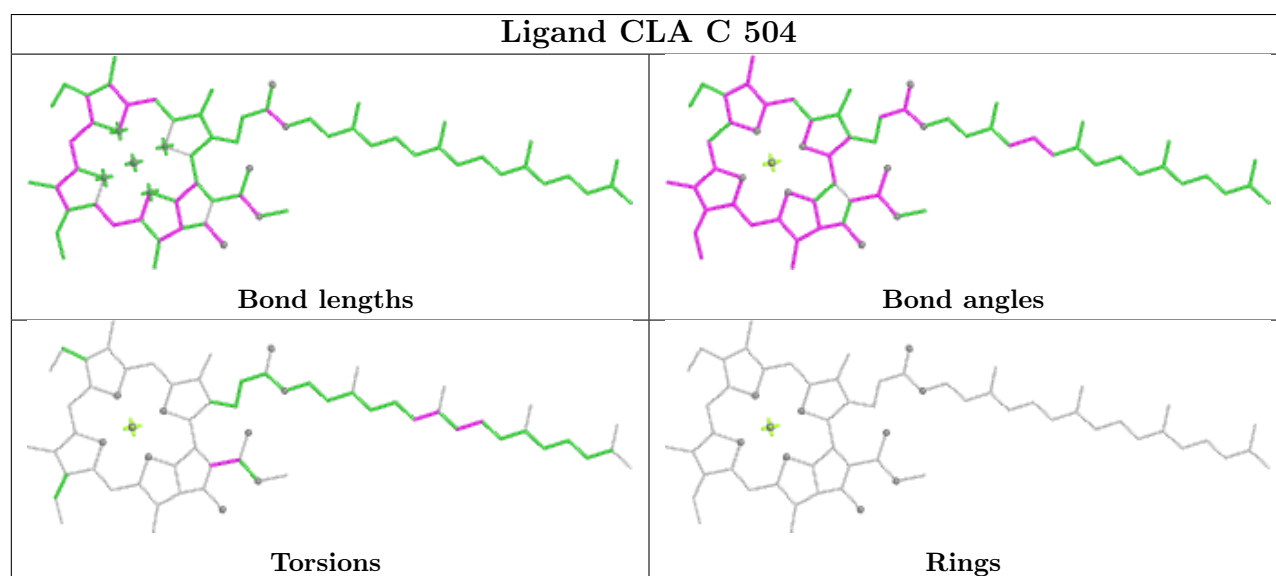
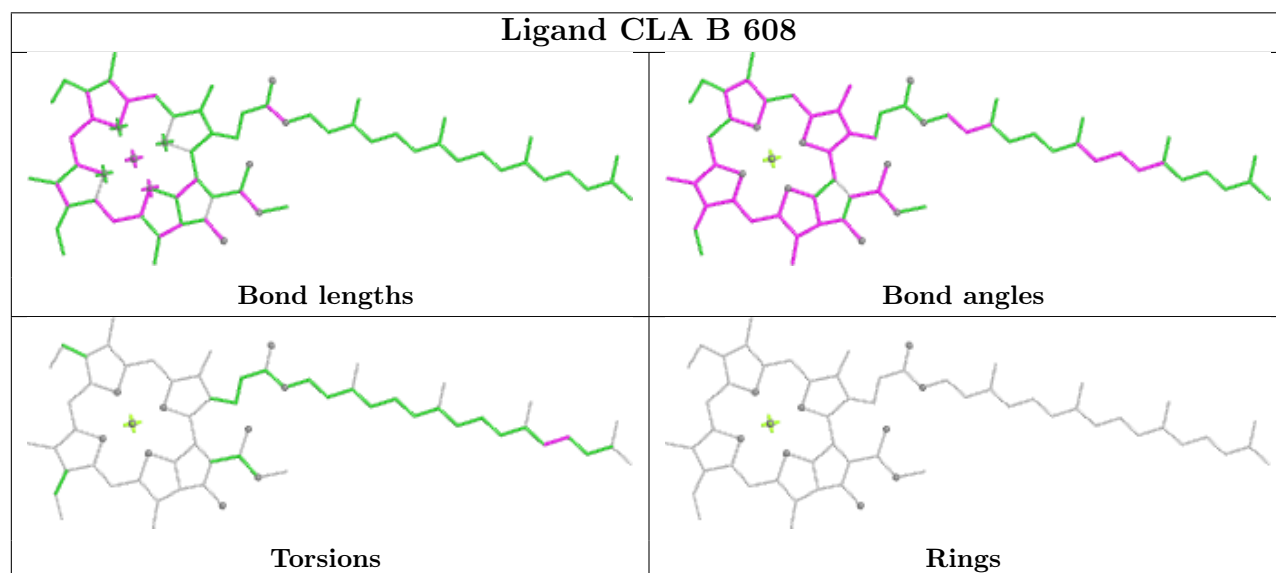
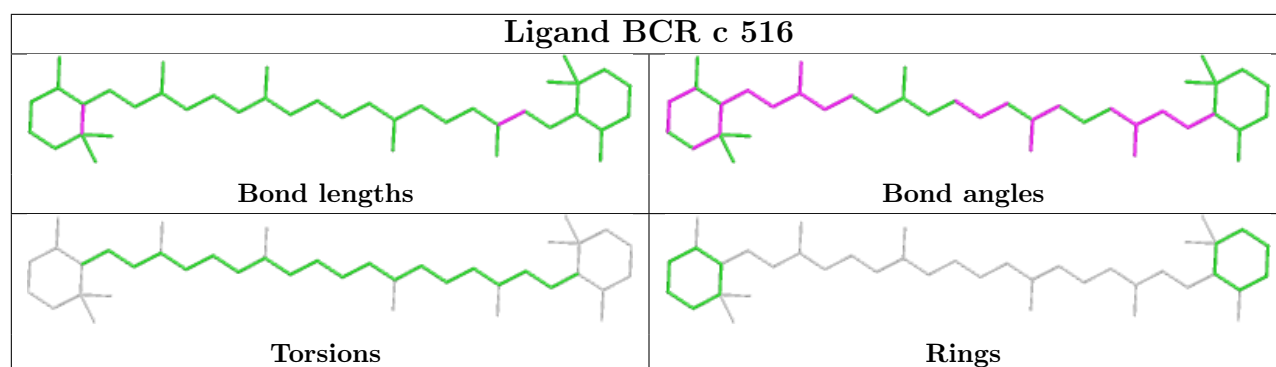


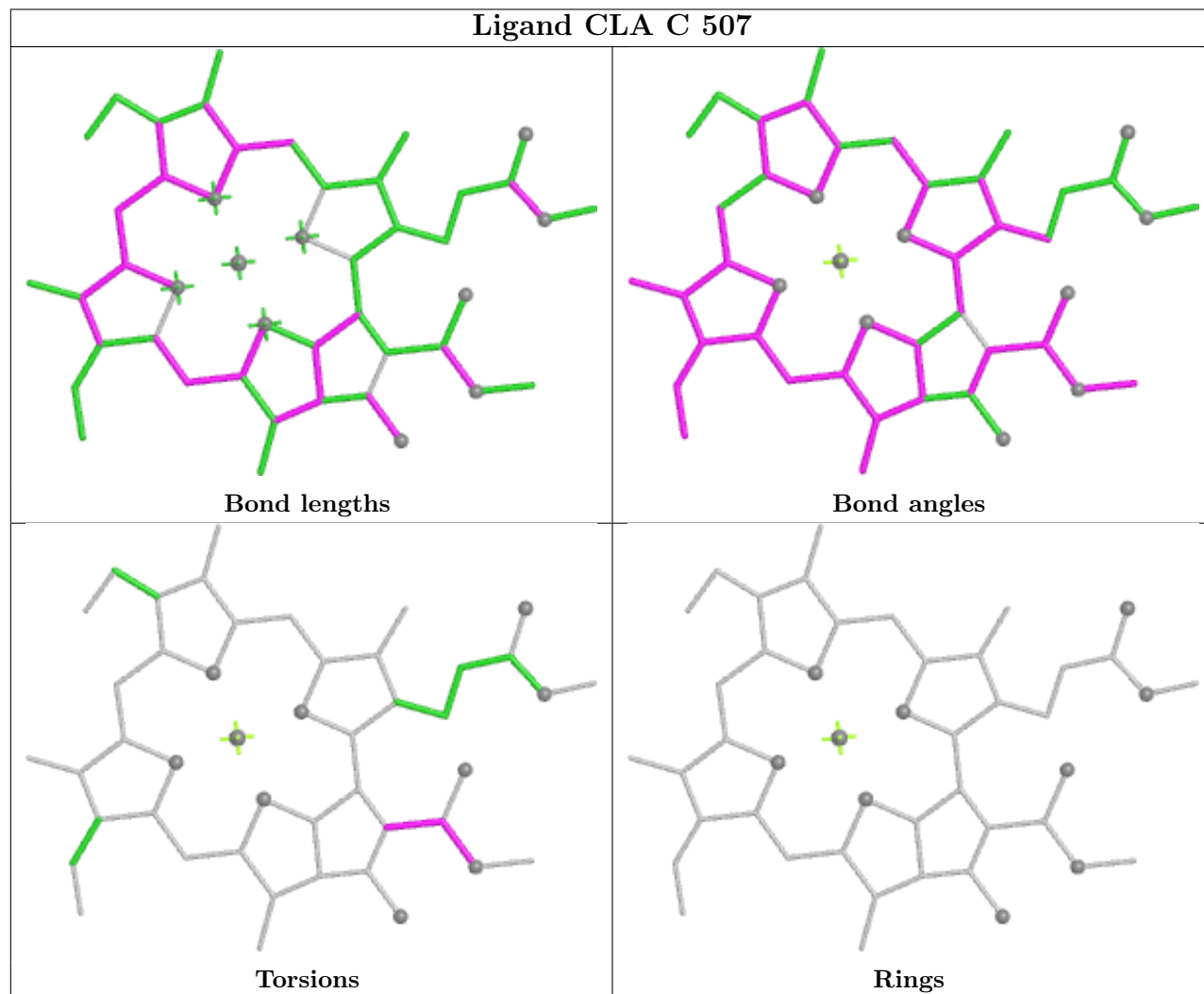
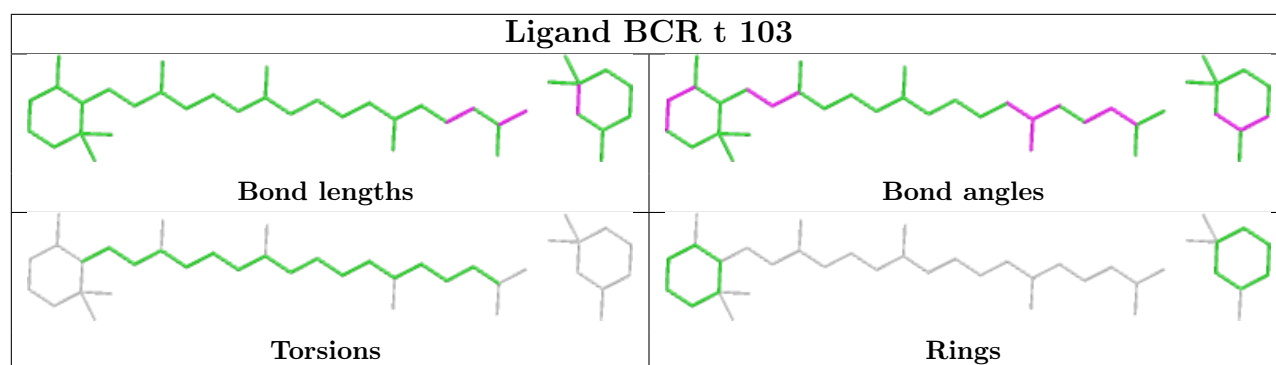


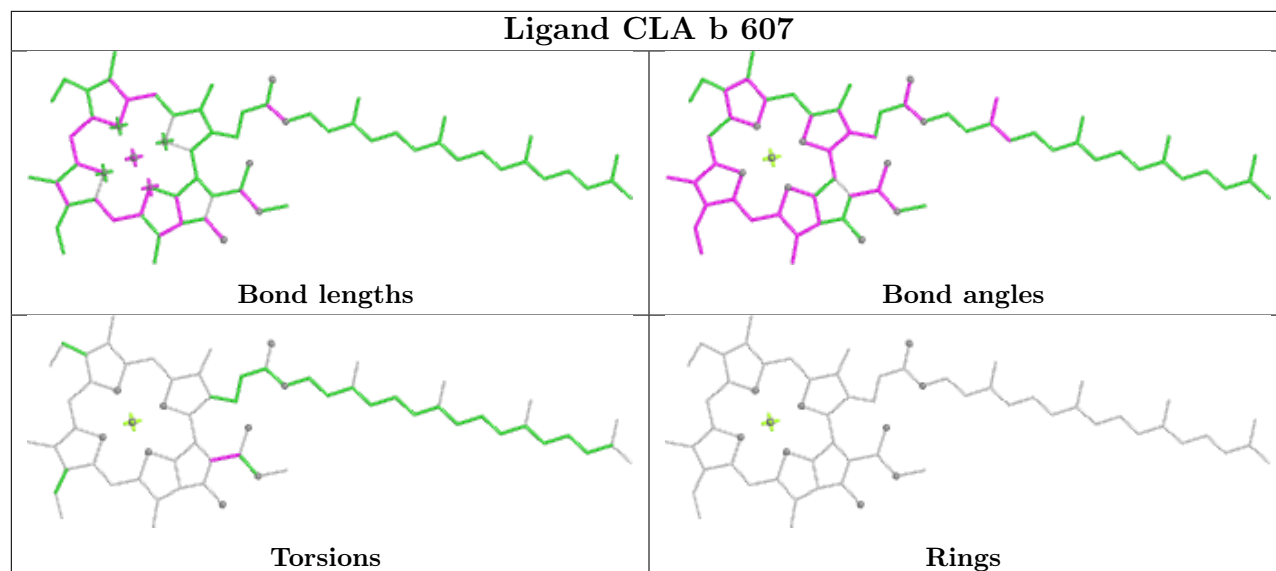
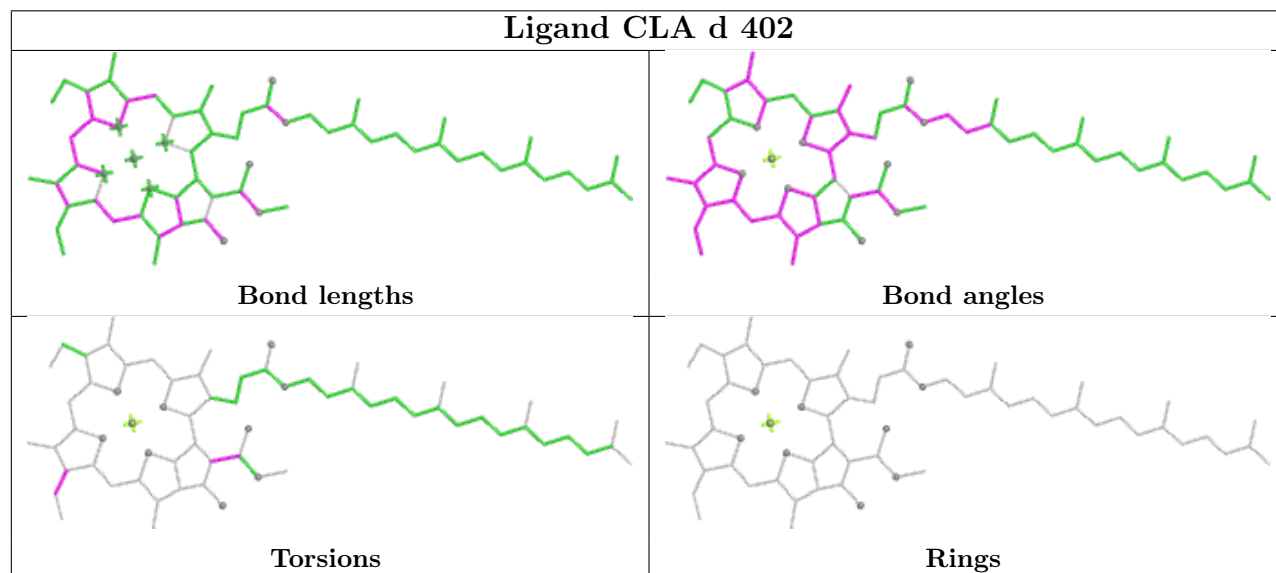
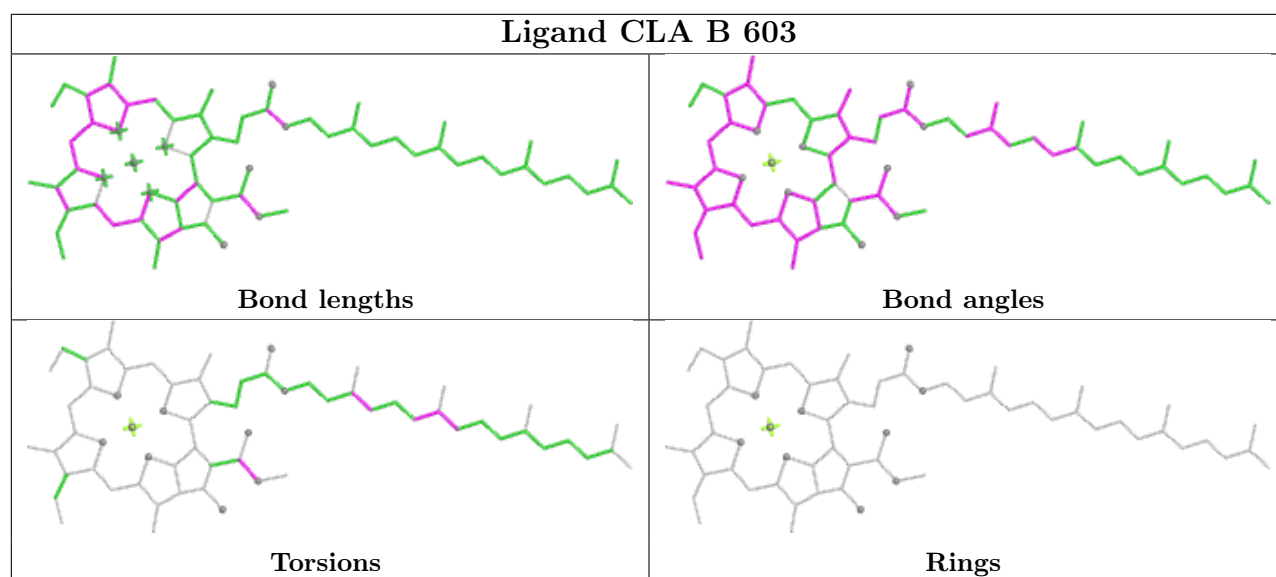




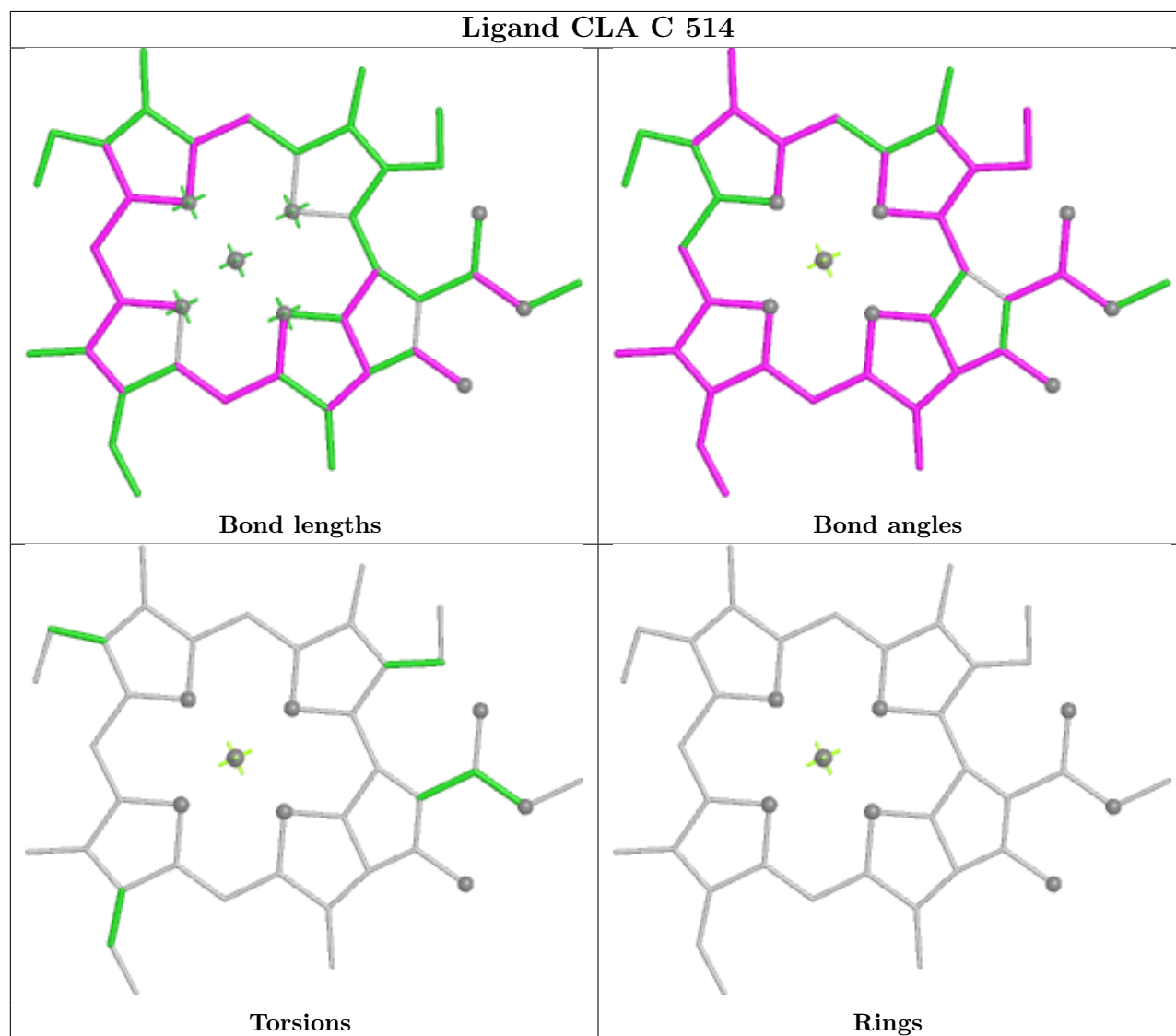
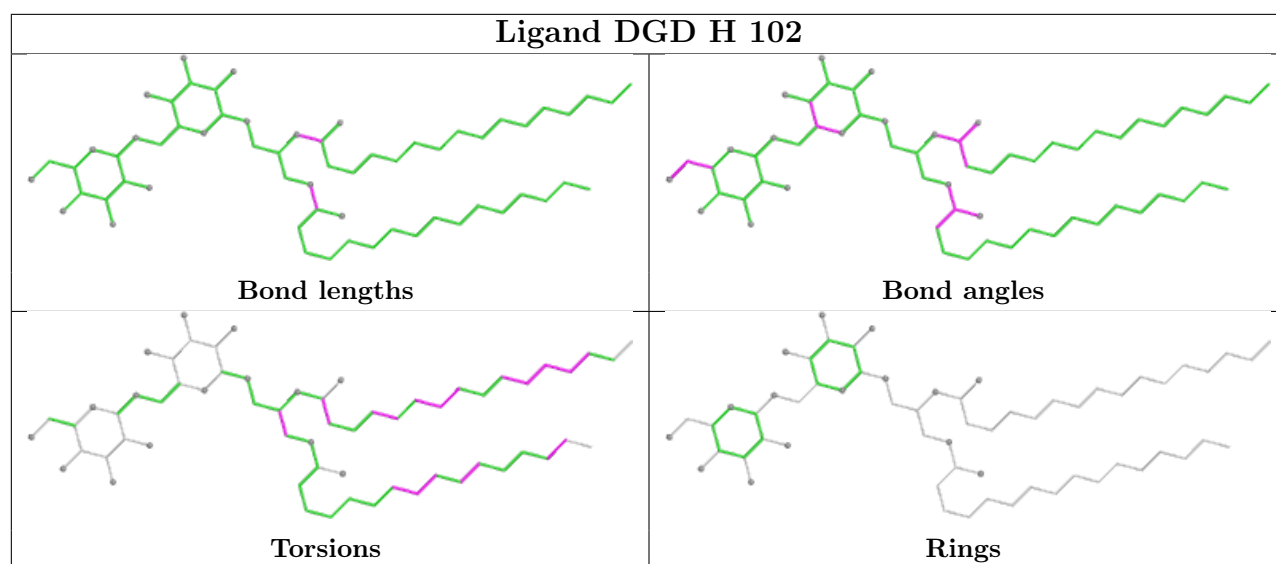


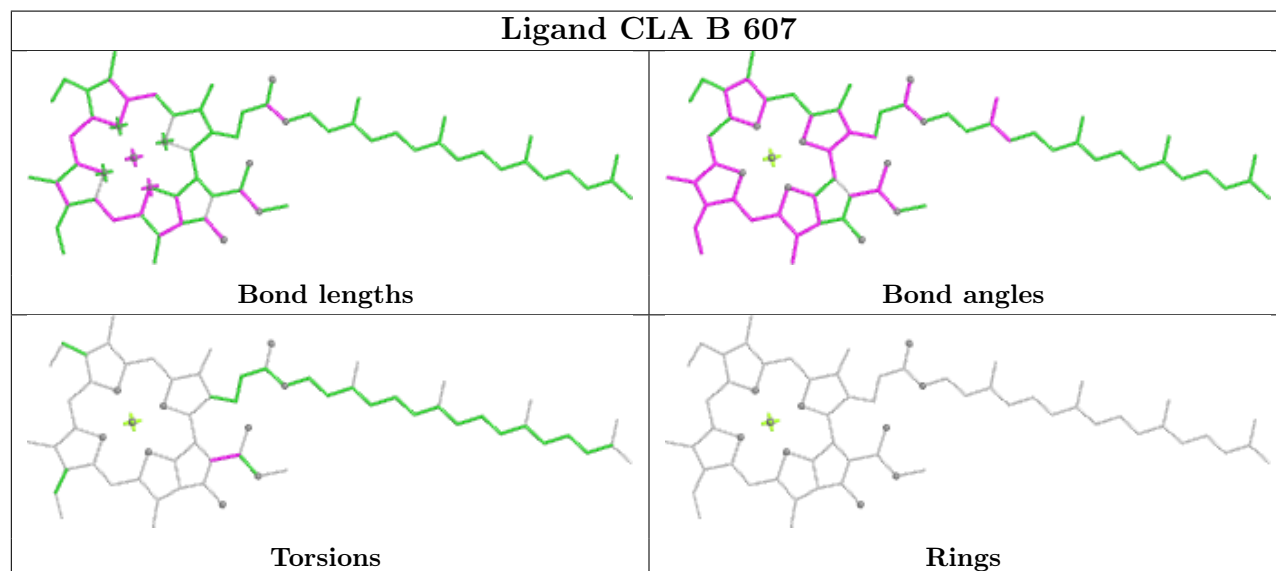
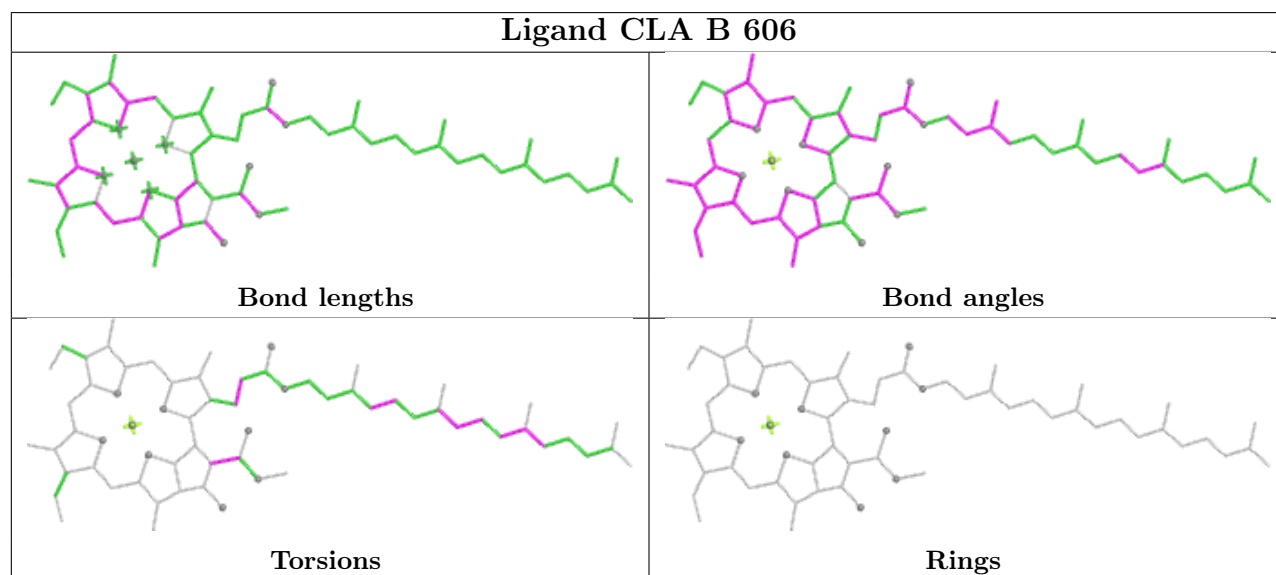
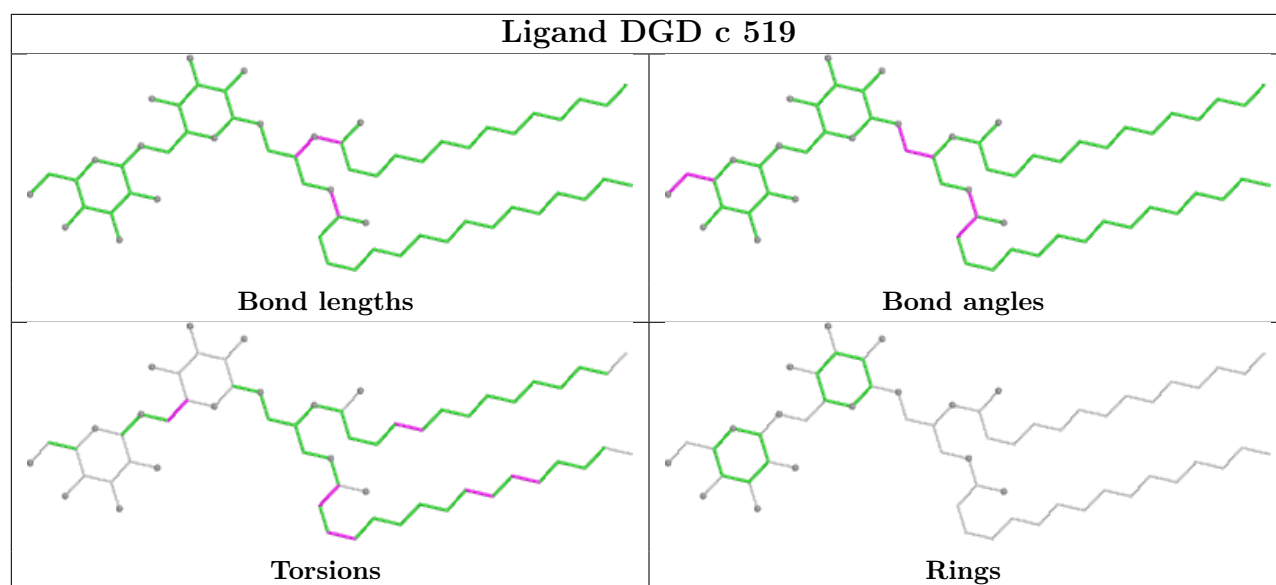


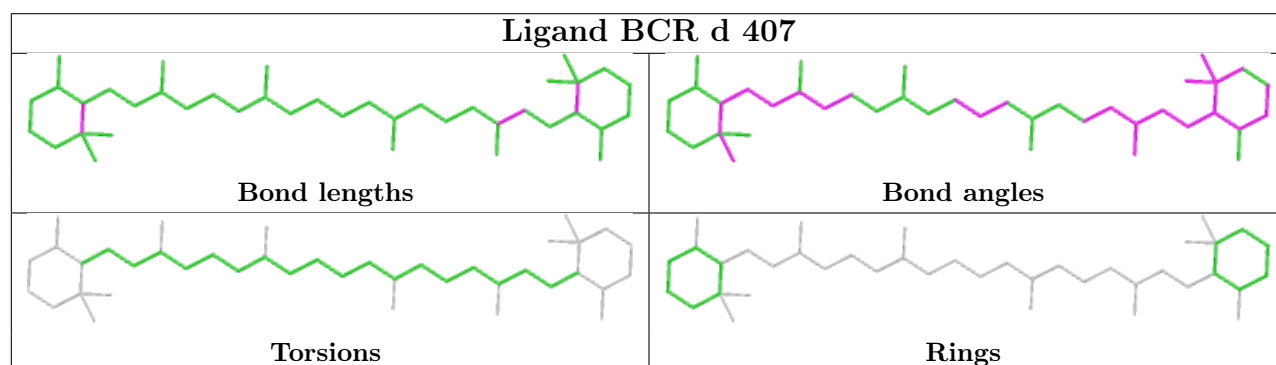
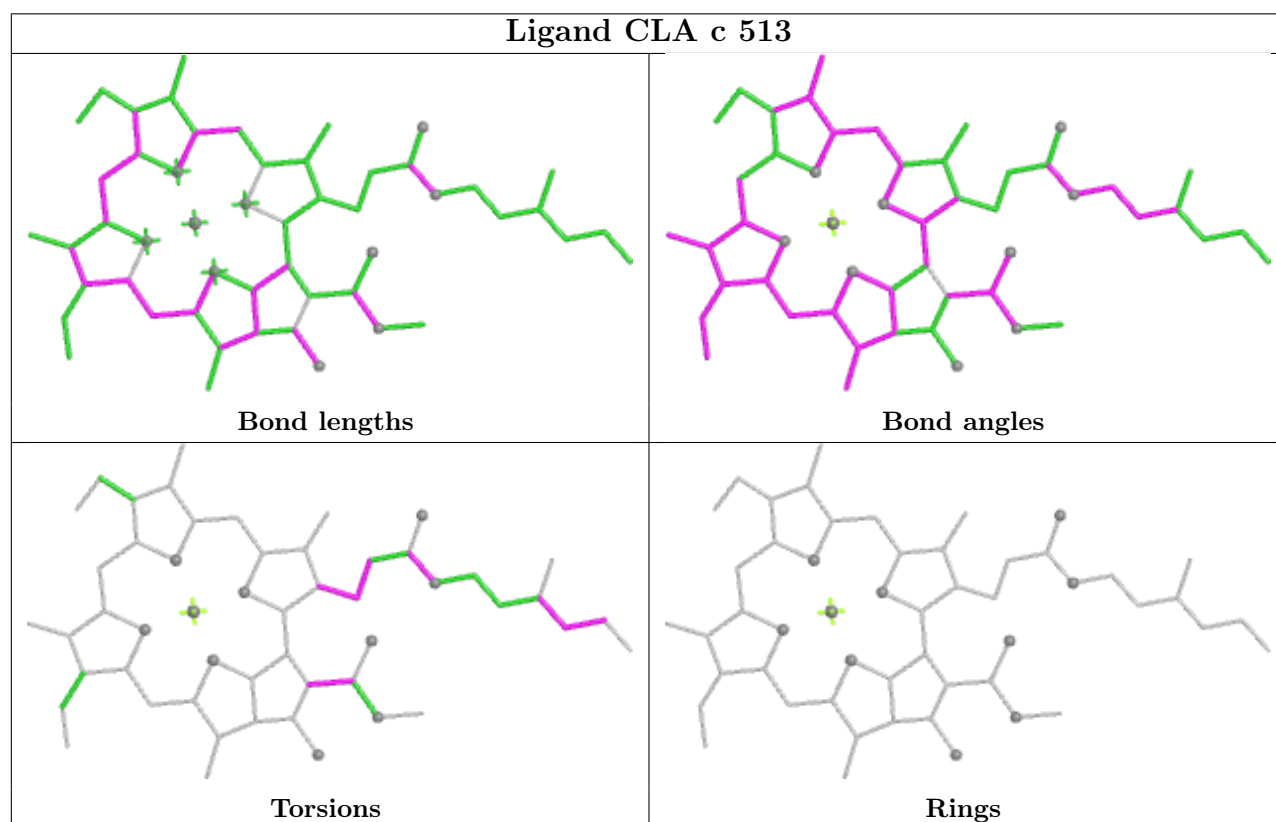
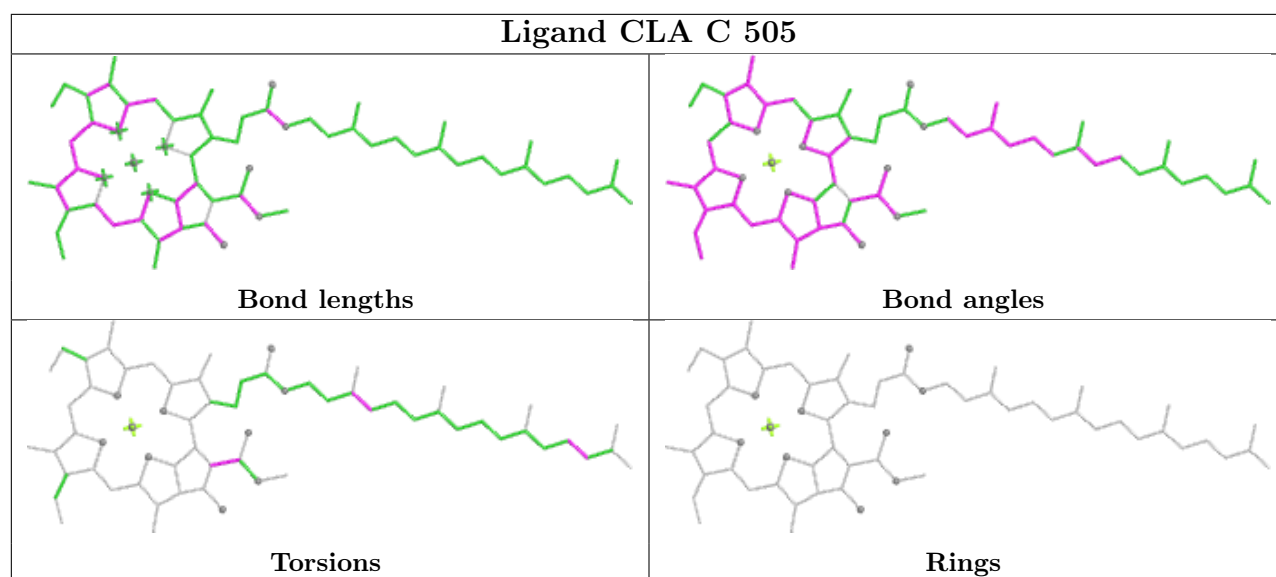


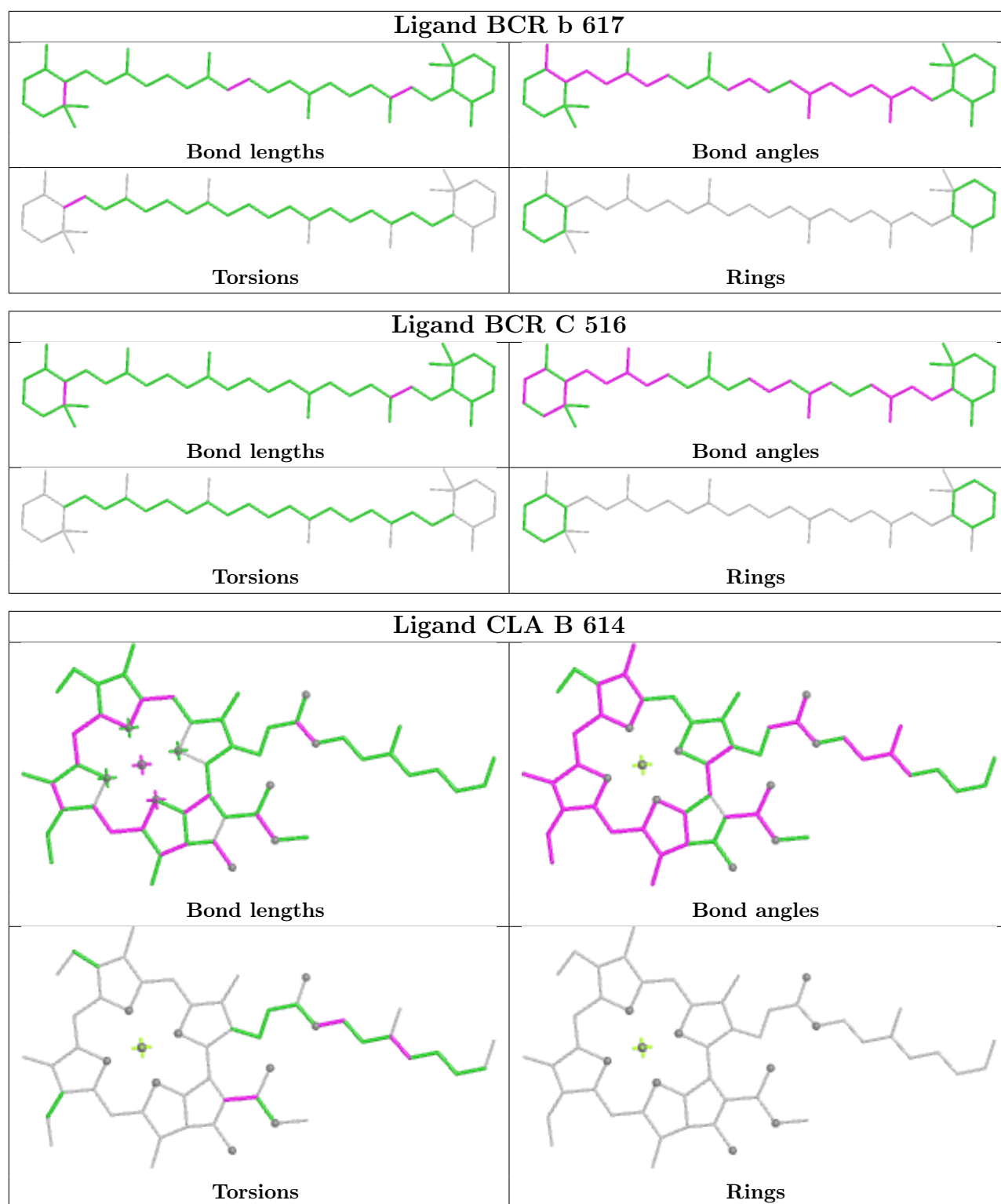


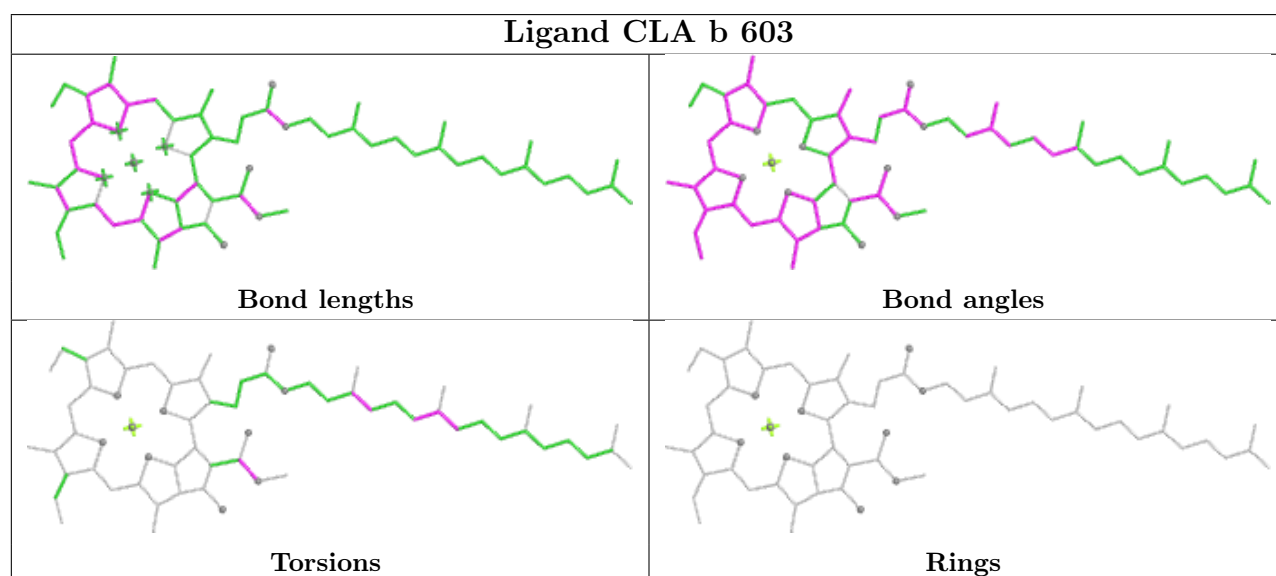
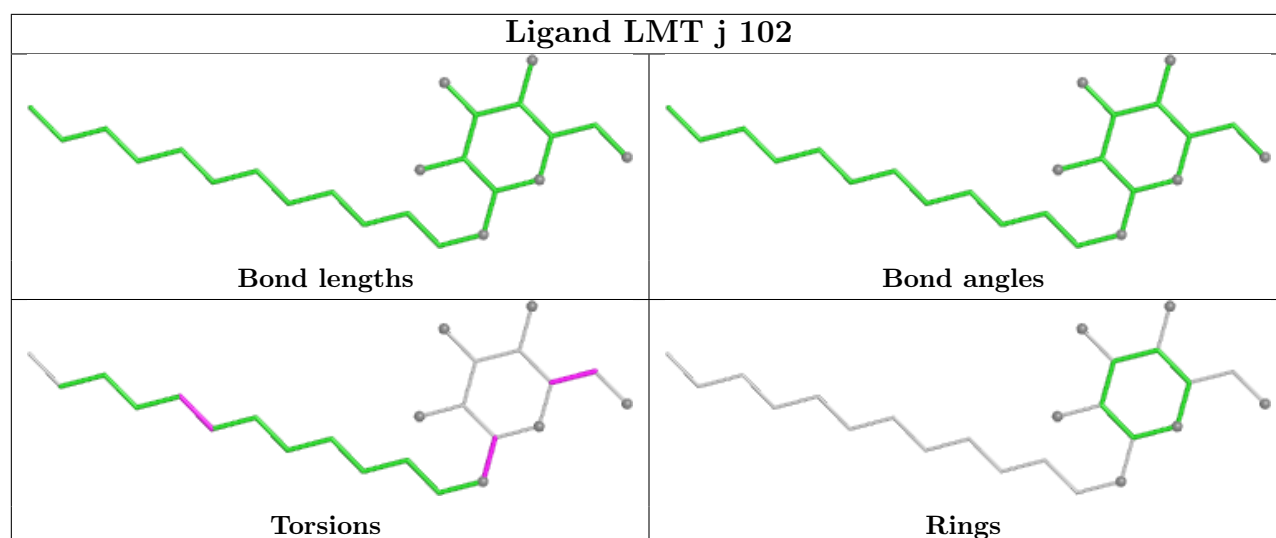


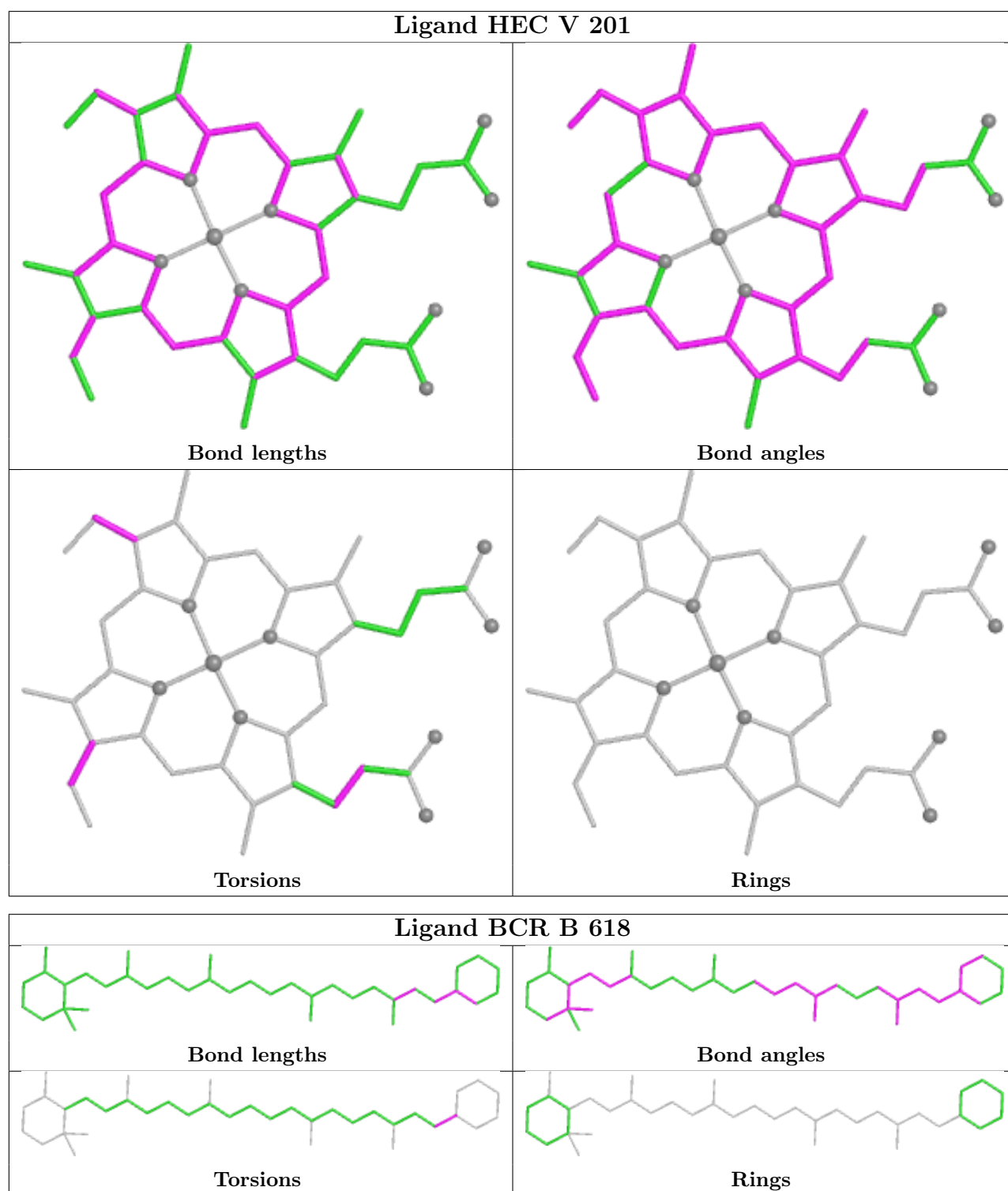


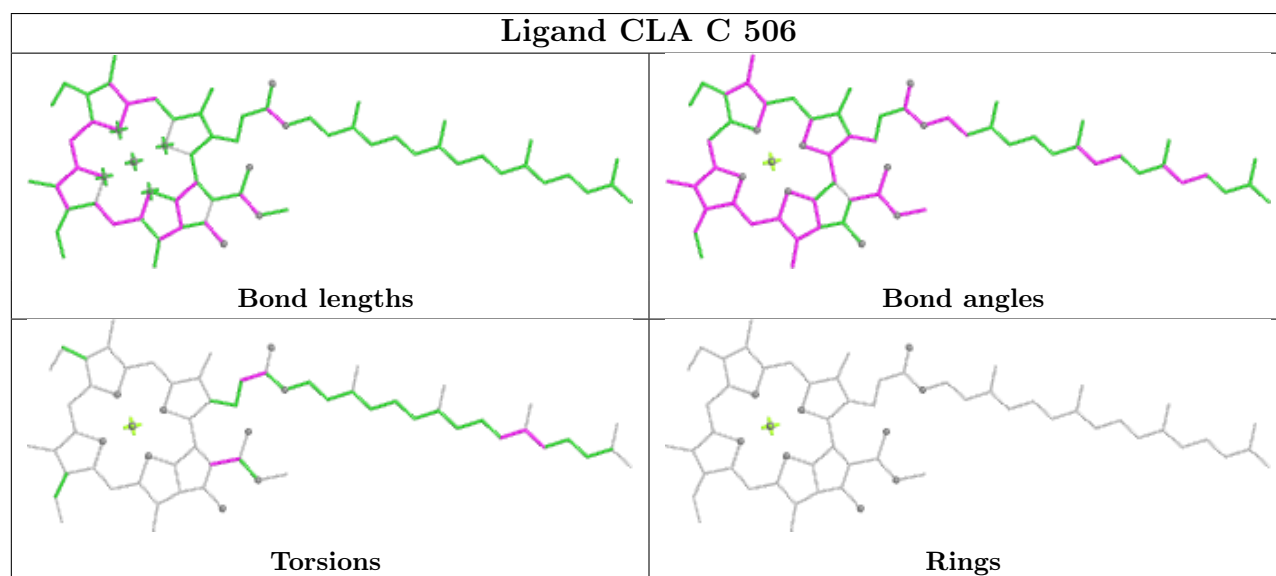
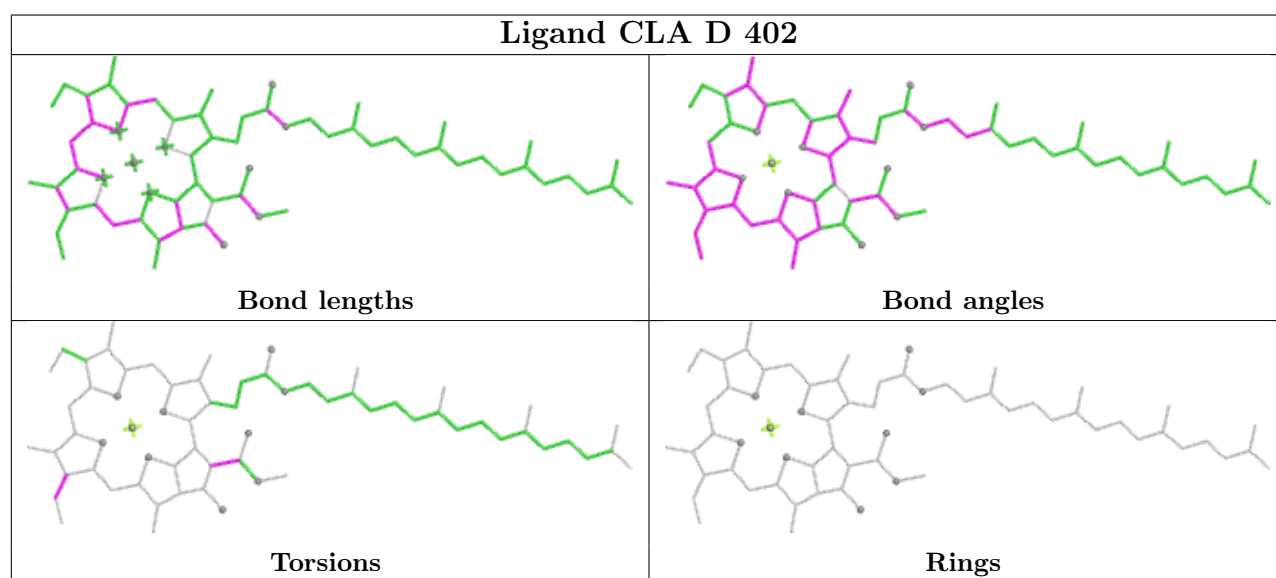
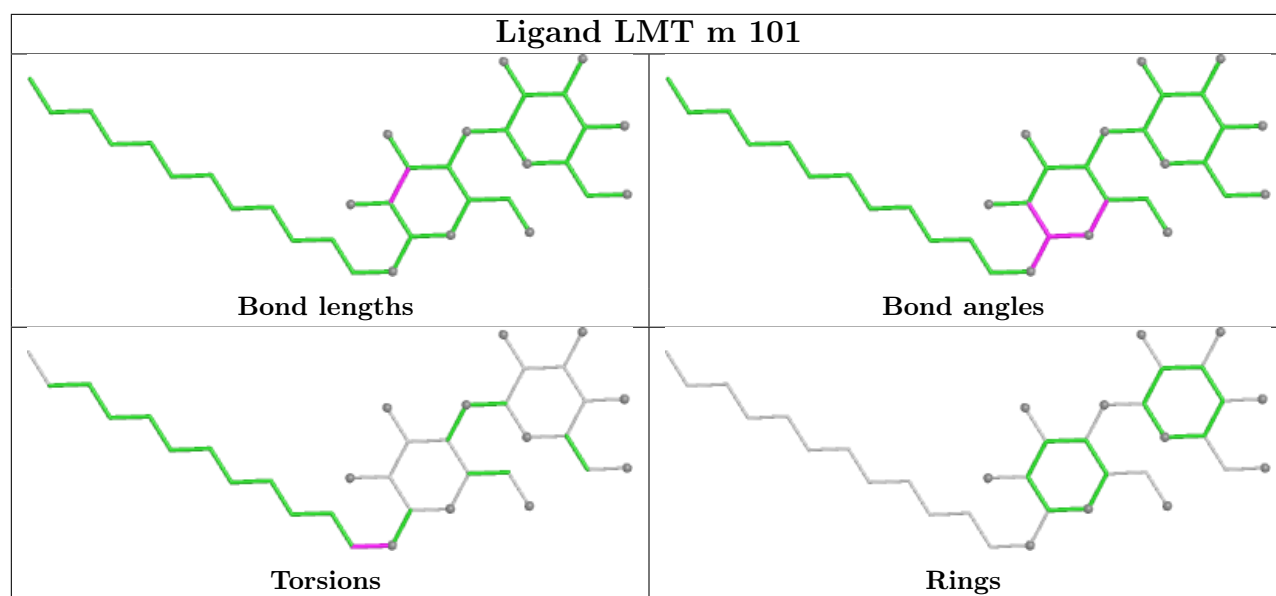


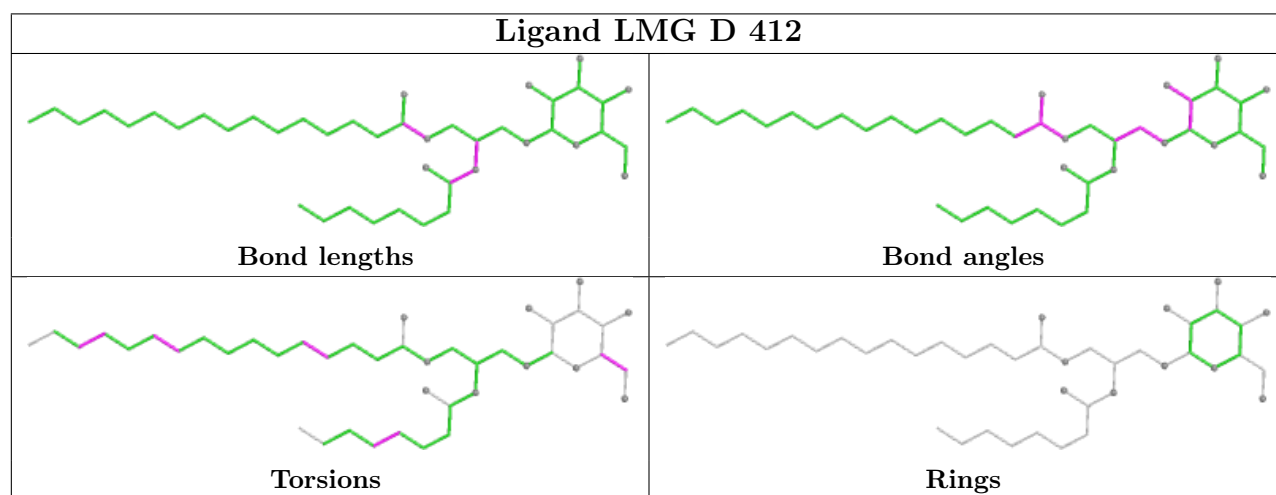
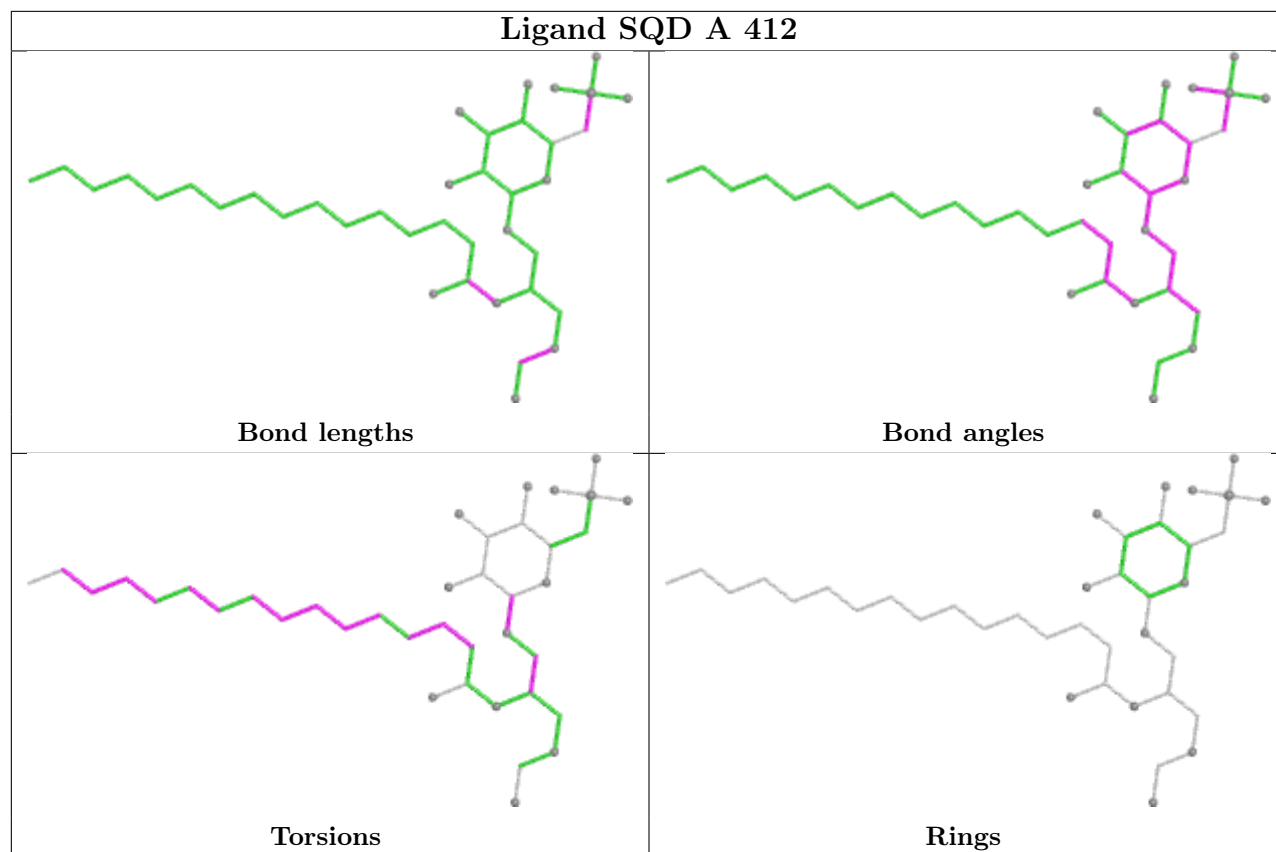




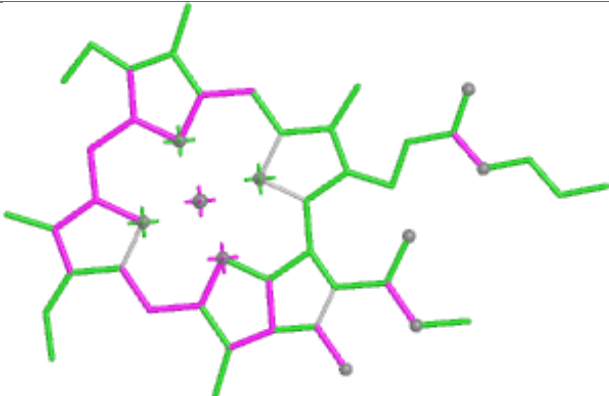
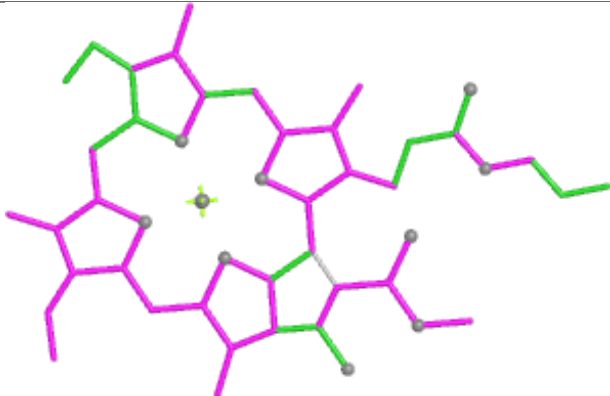
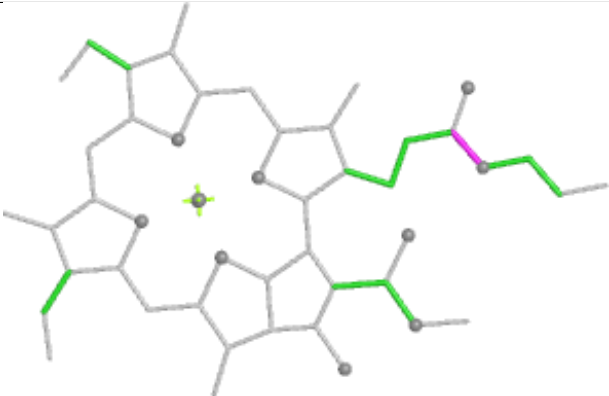
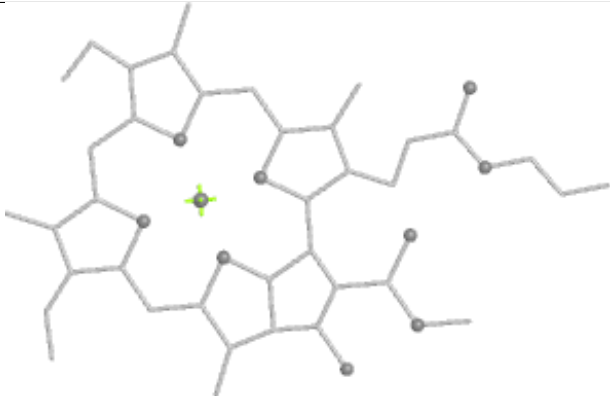










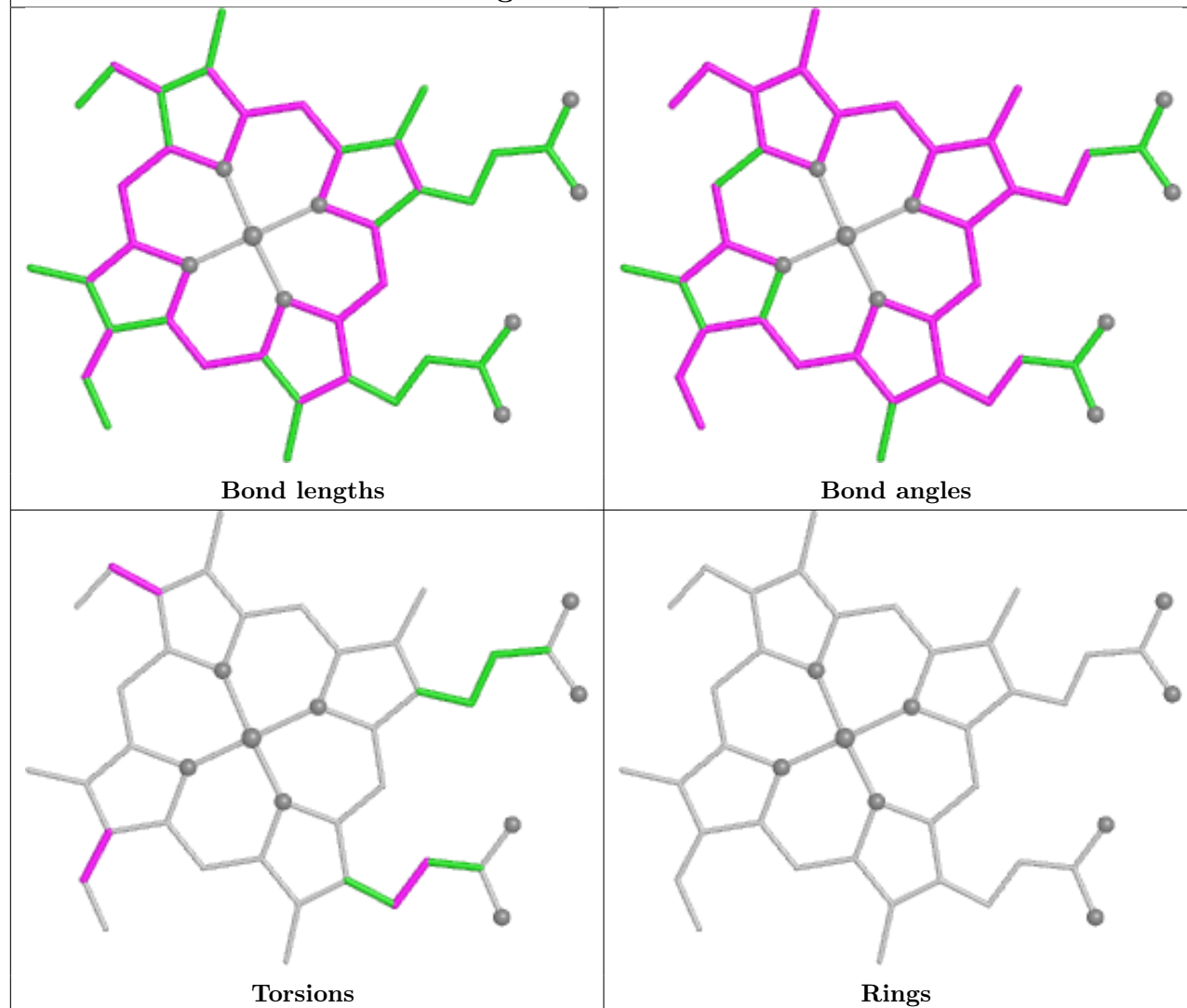




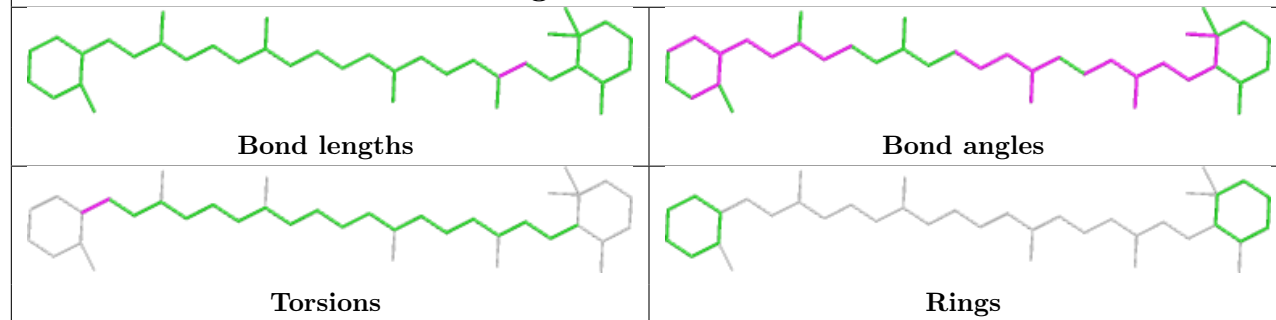
Ligand CLA d 406			
			
Bond lengths		Bond angles	
			
Torsions		Rings	

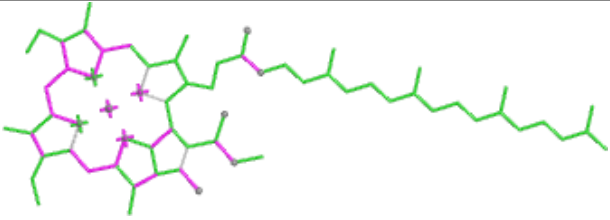
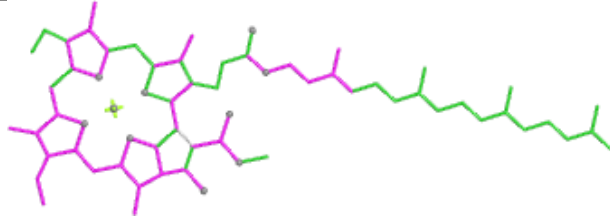
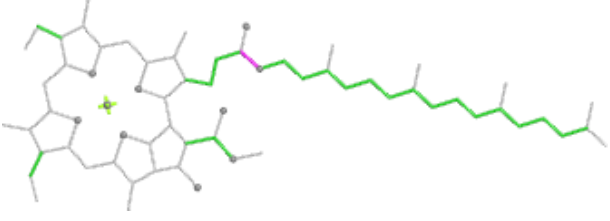
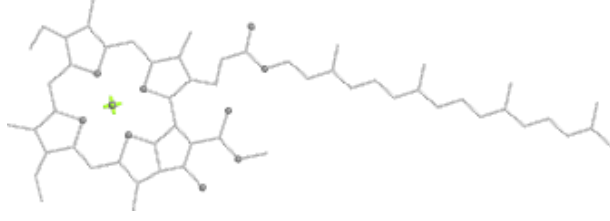
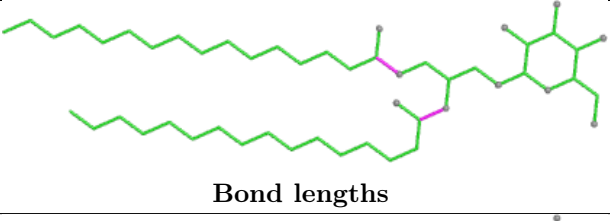
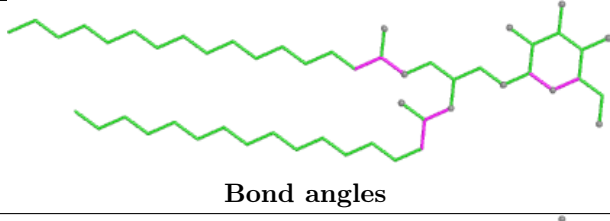
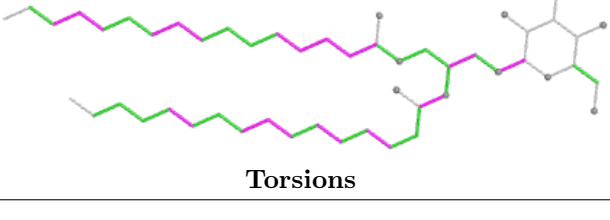
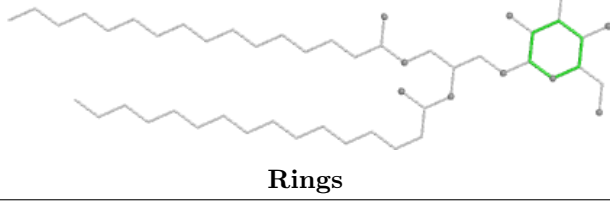
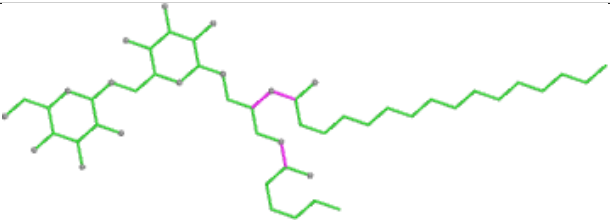
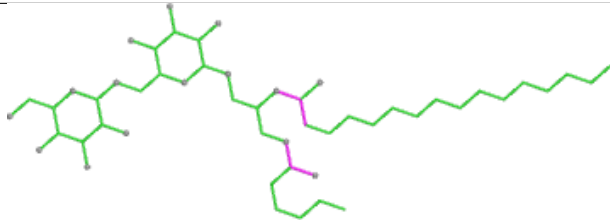
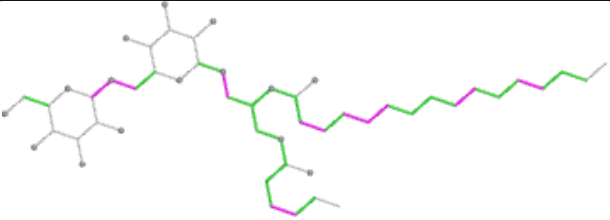
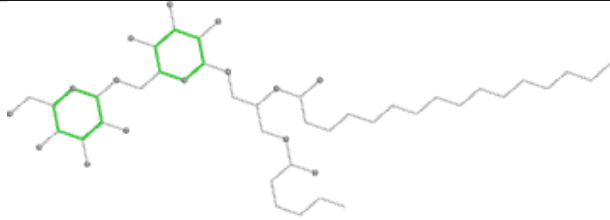
Ligand PL9 a 411			
			
Bond lengths		Bond angles	
			
Torsions		Rings	

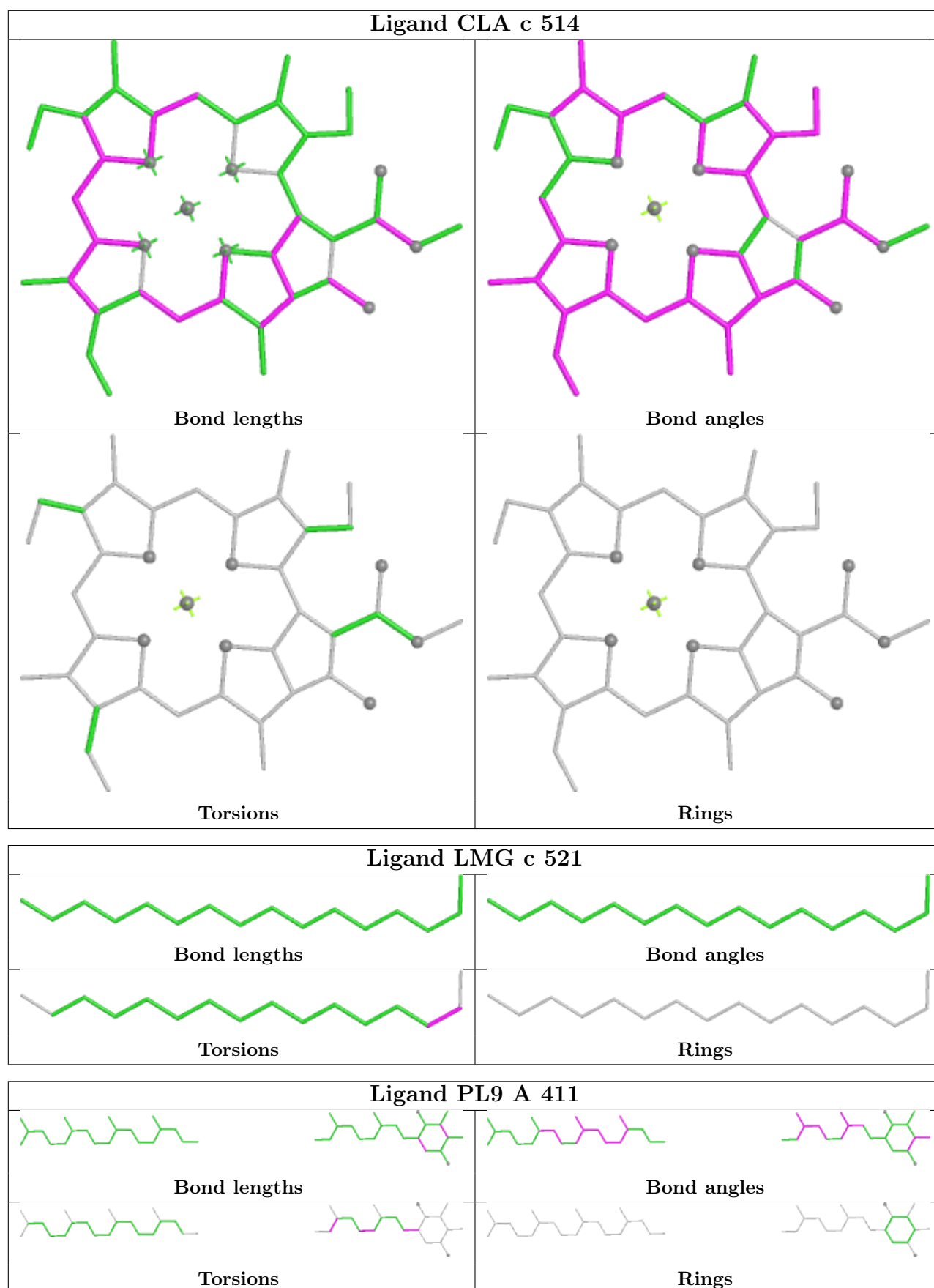
## Ligand HEC v 201

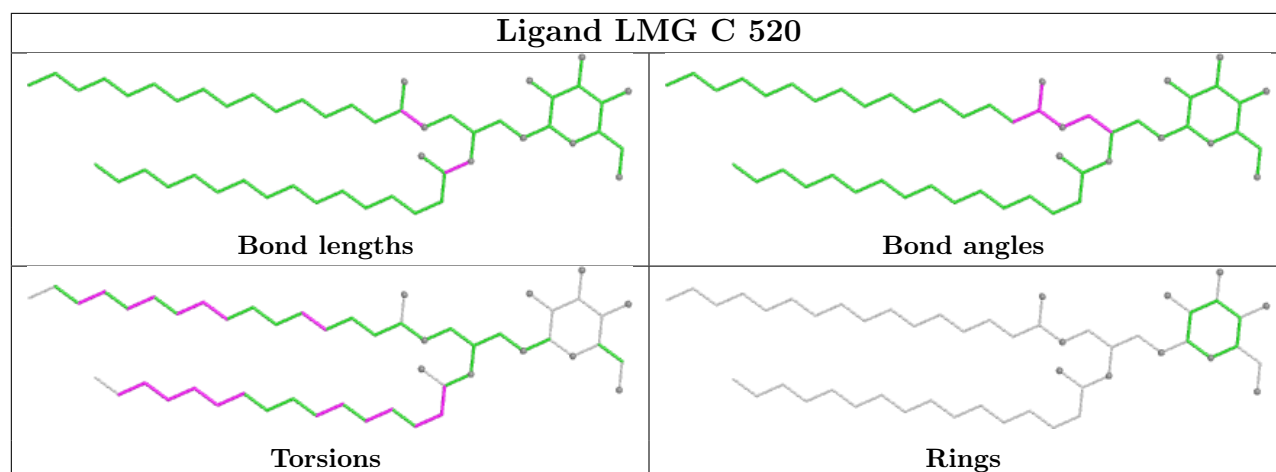
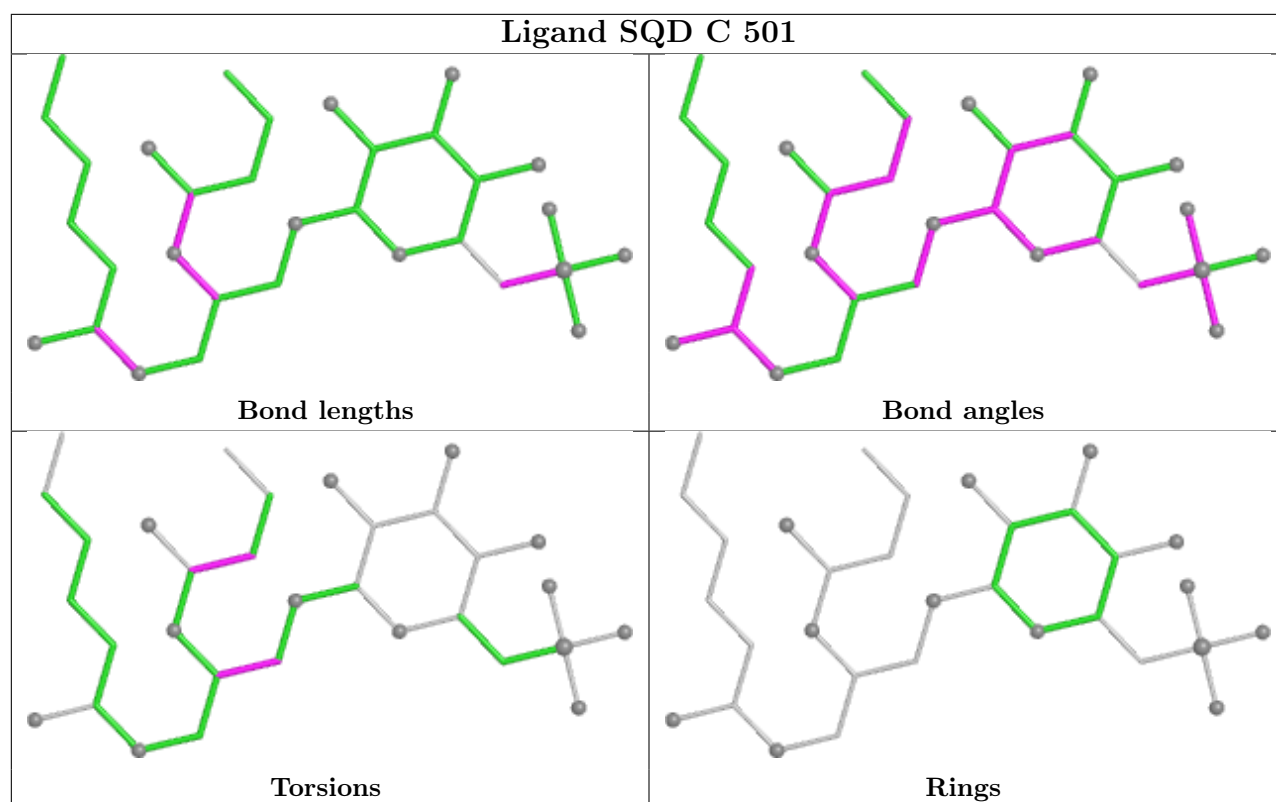


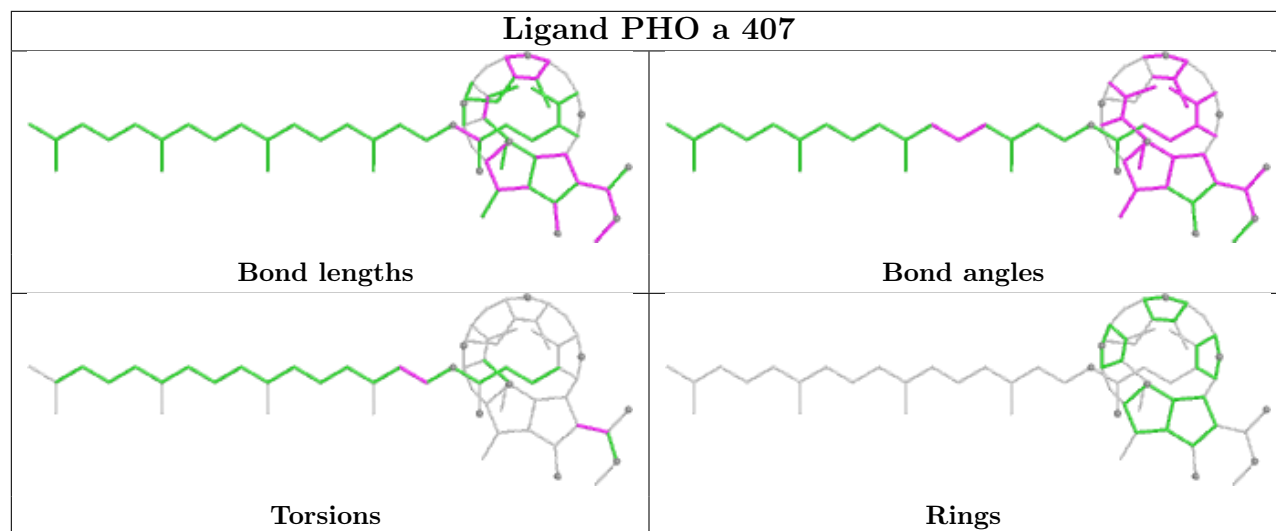
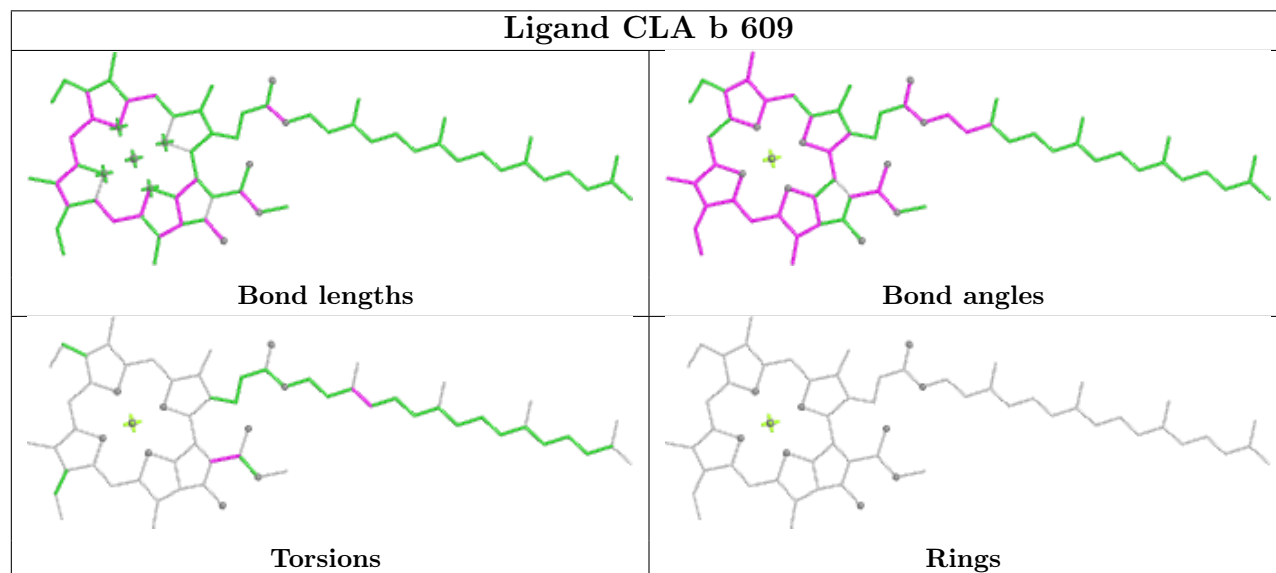
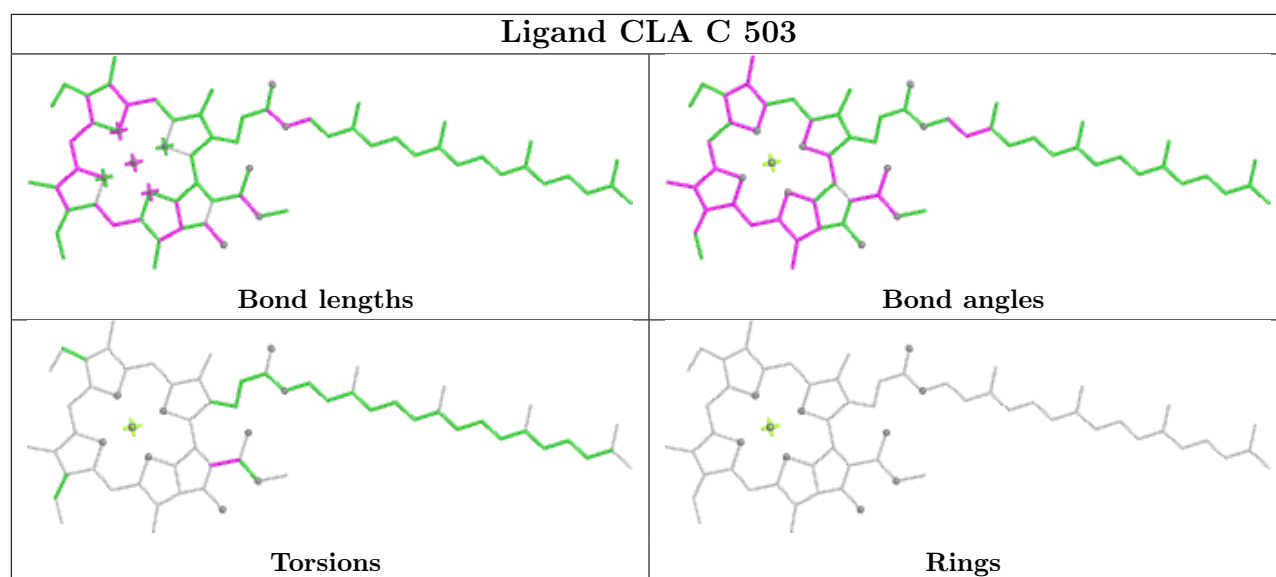
## Ligand BCR C 515

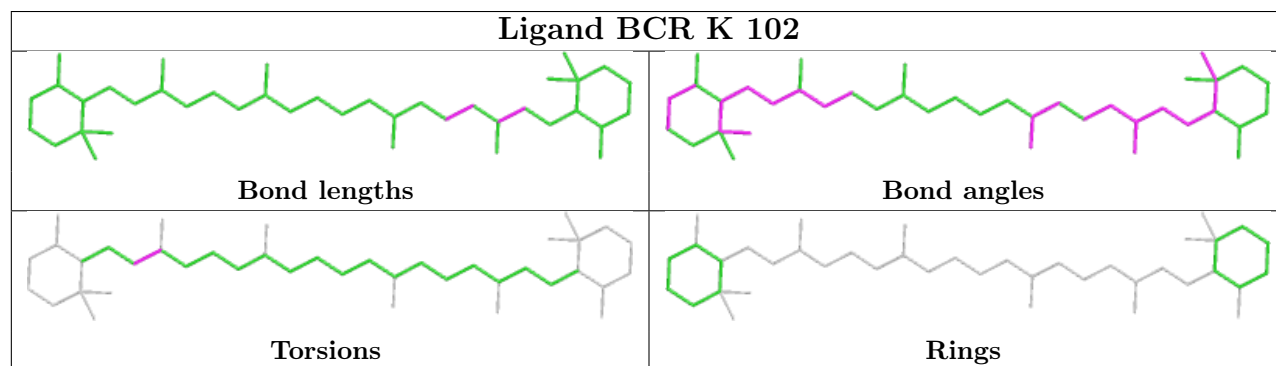
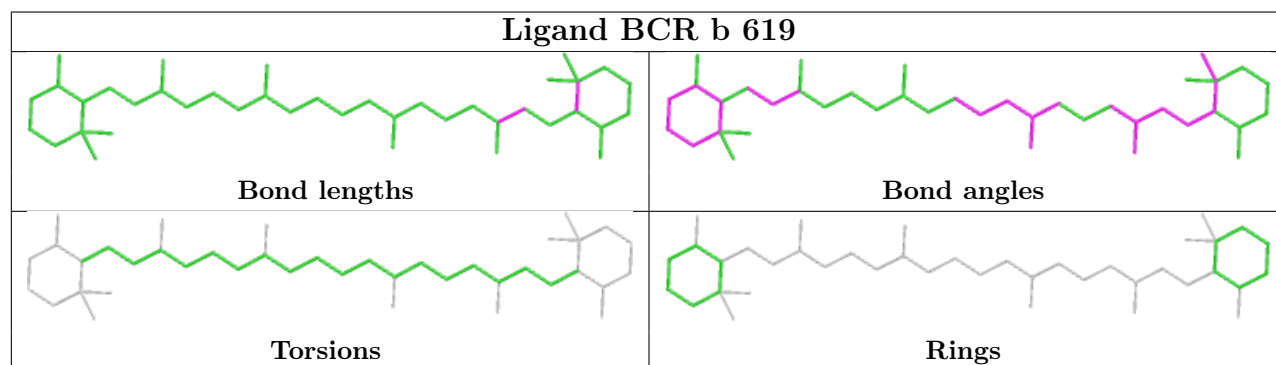
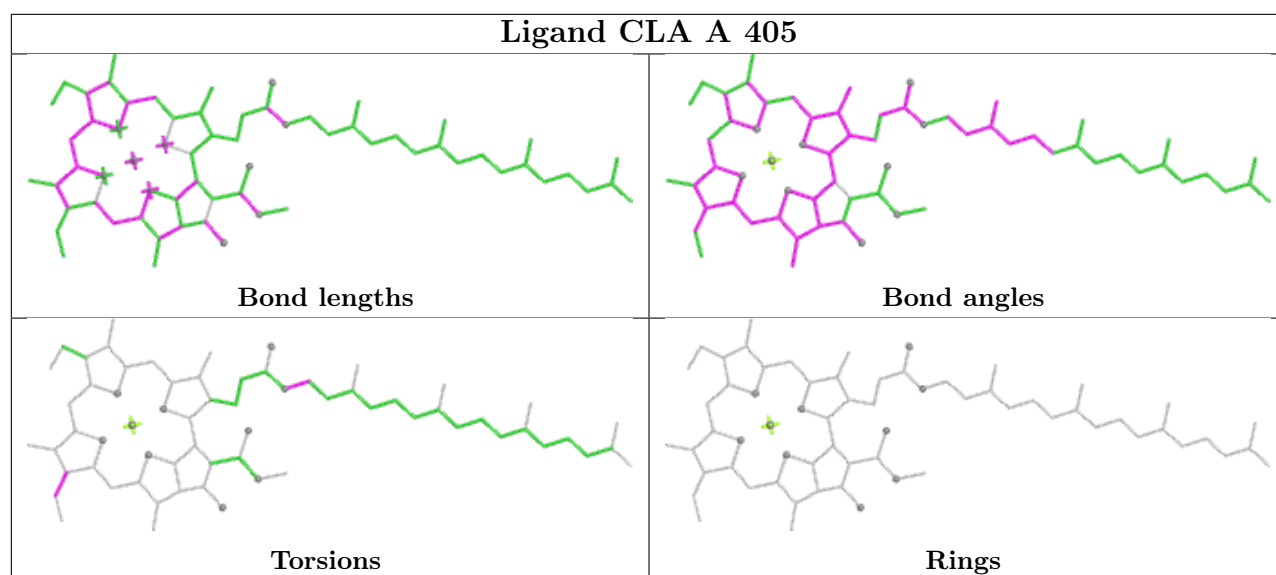


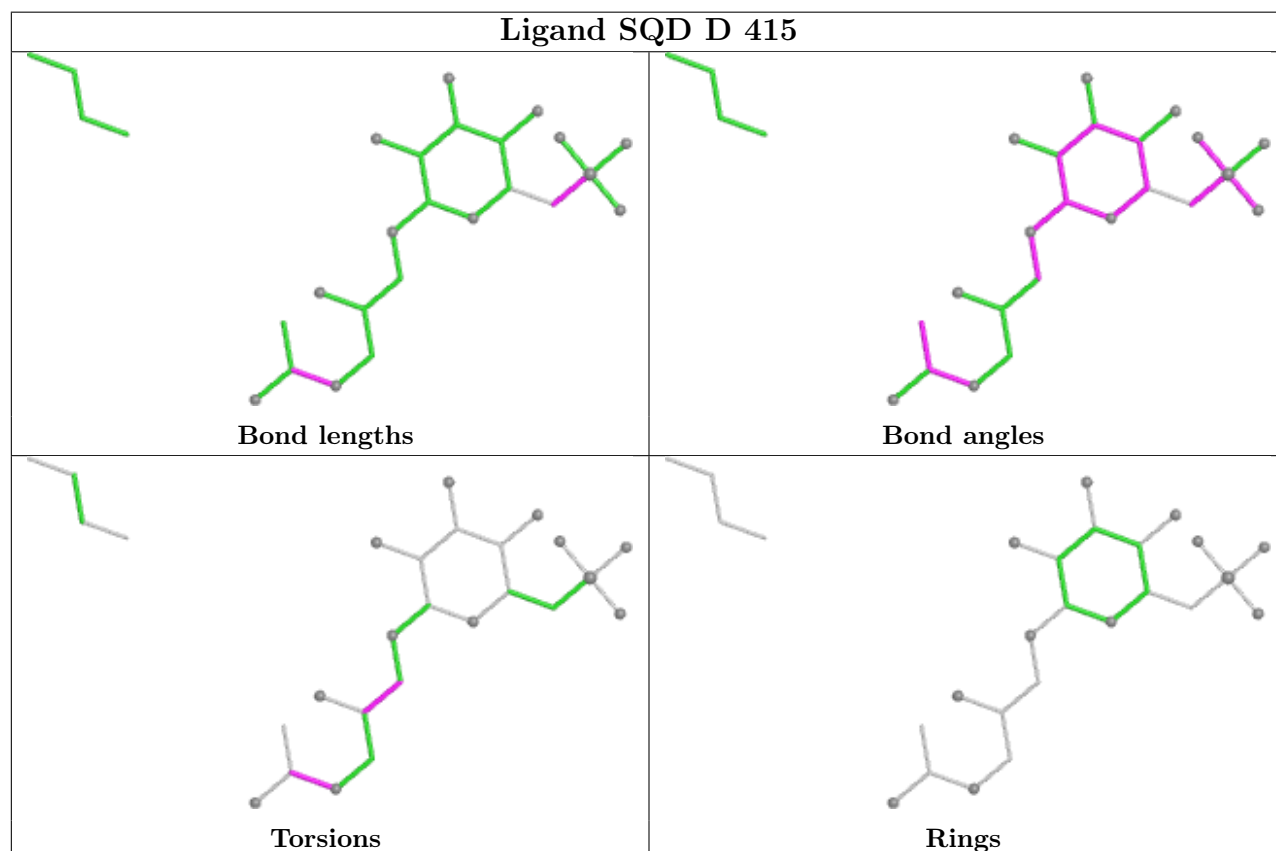
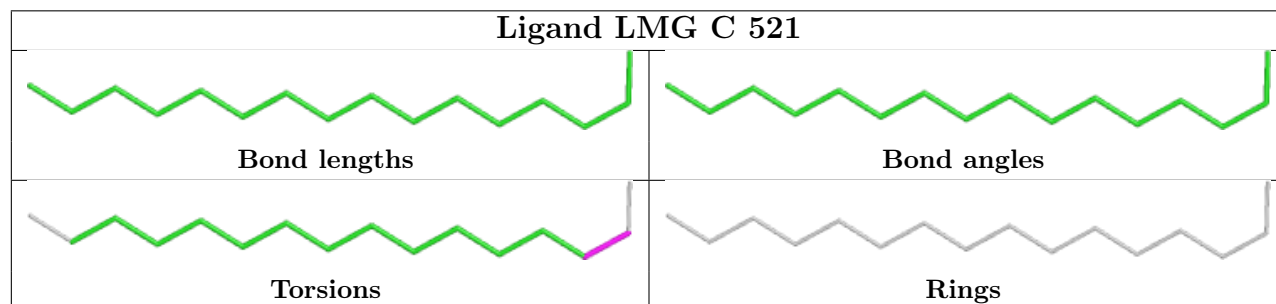
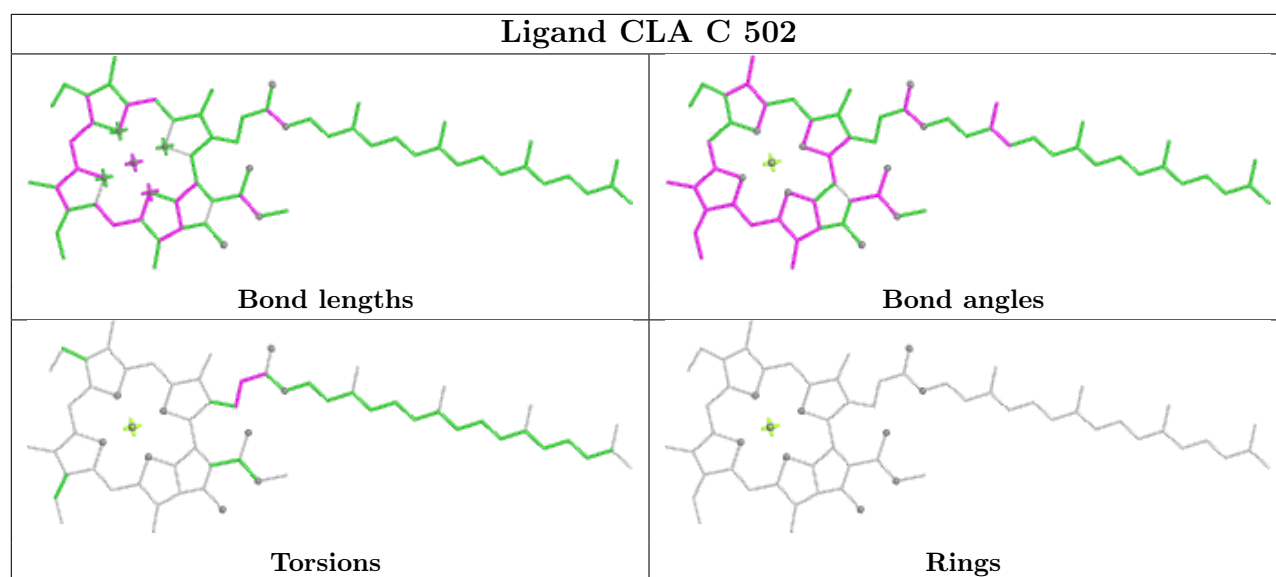
Ligand CLA C 512	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMG A 410	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand DGD c 518	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



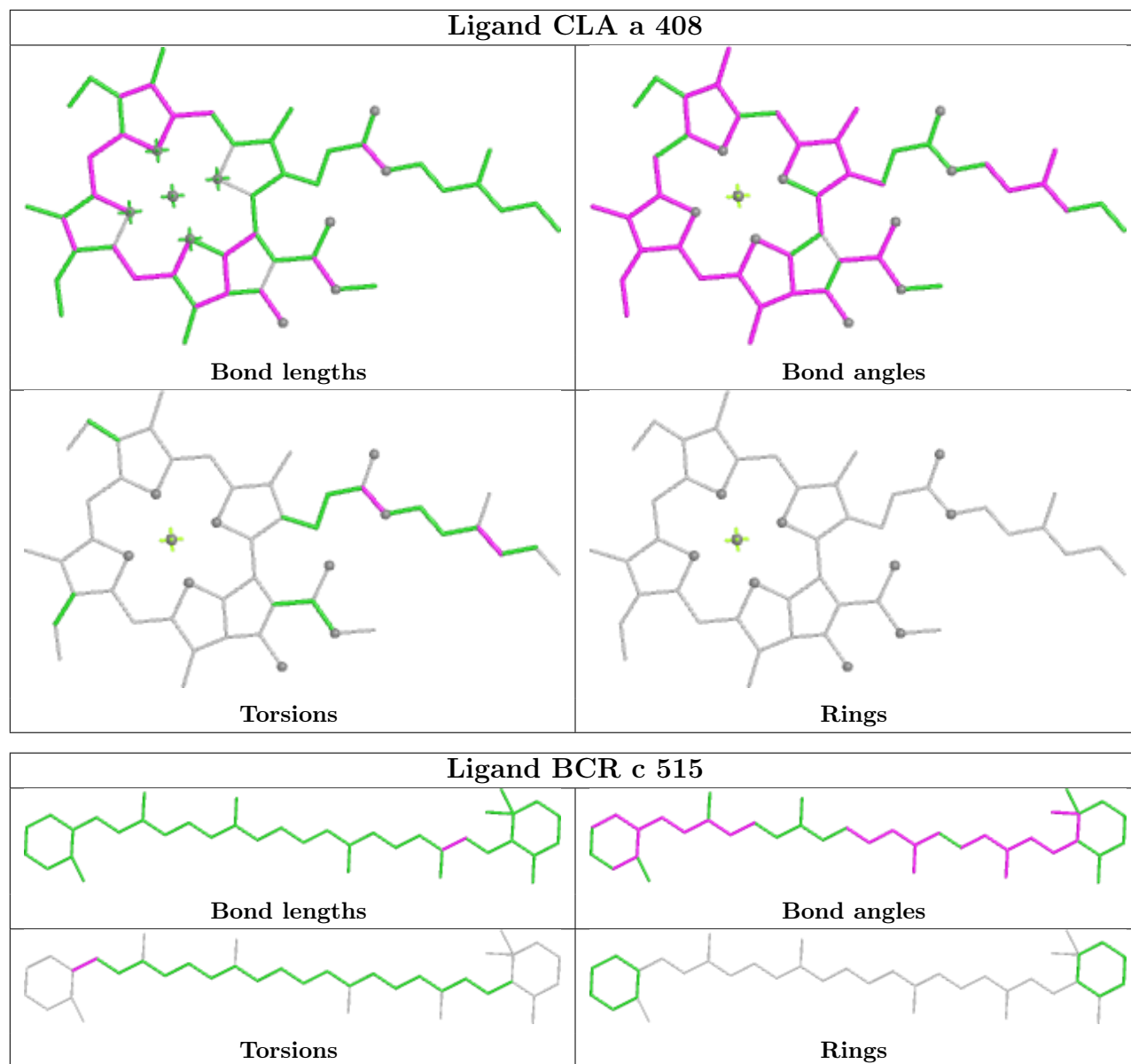


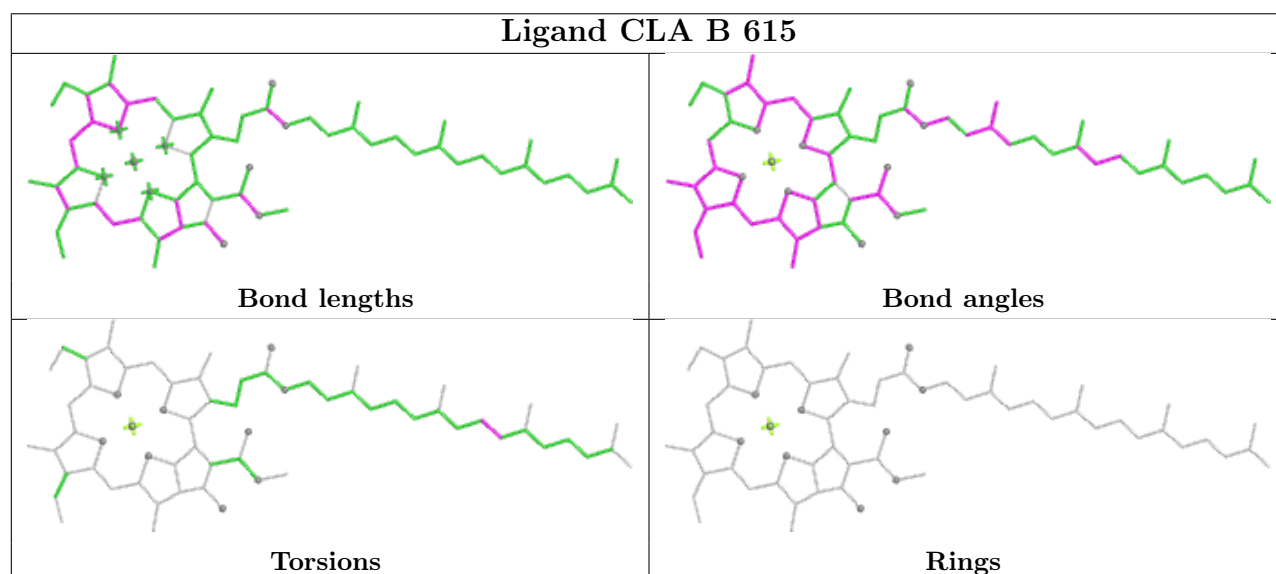
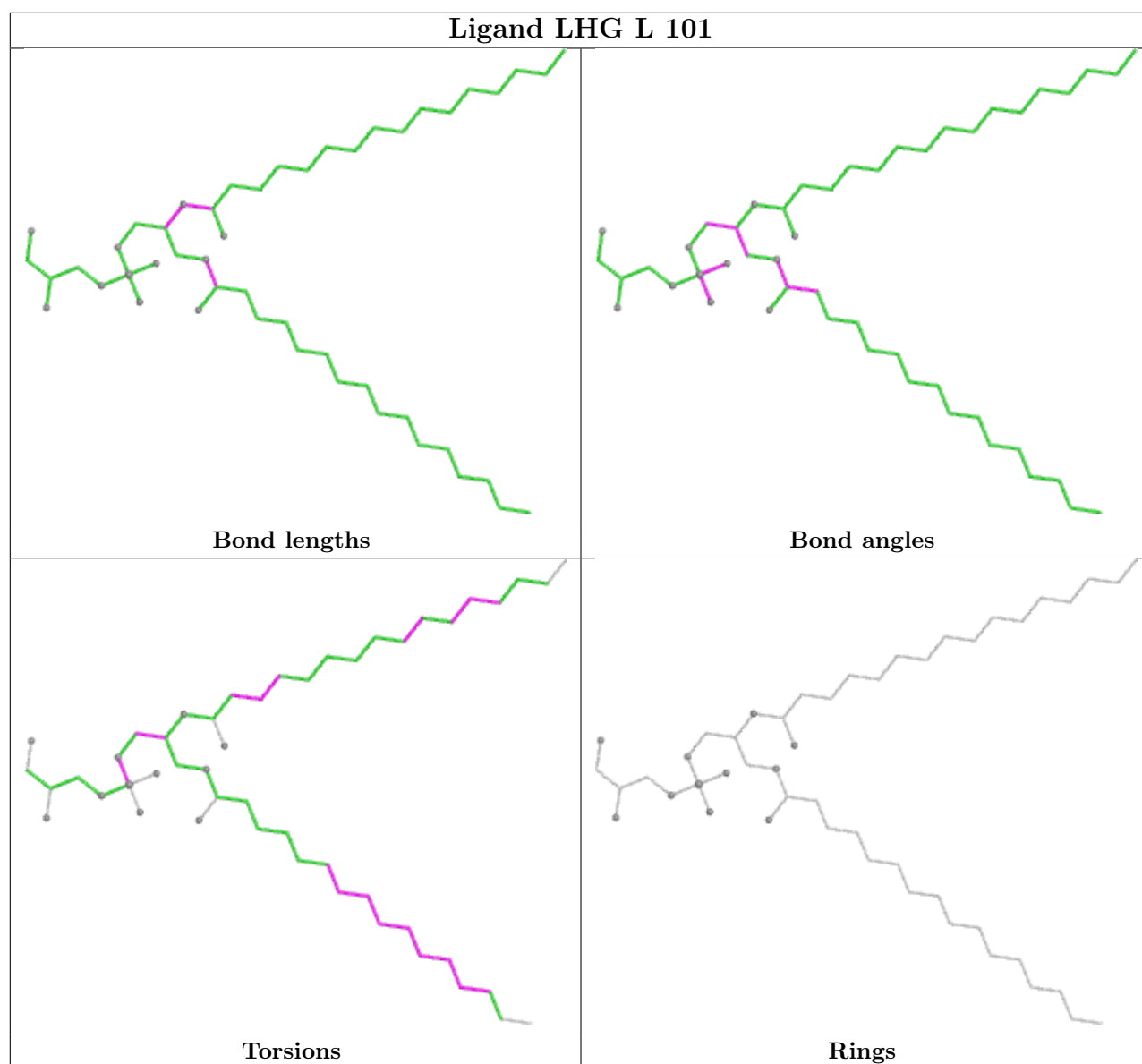


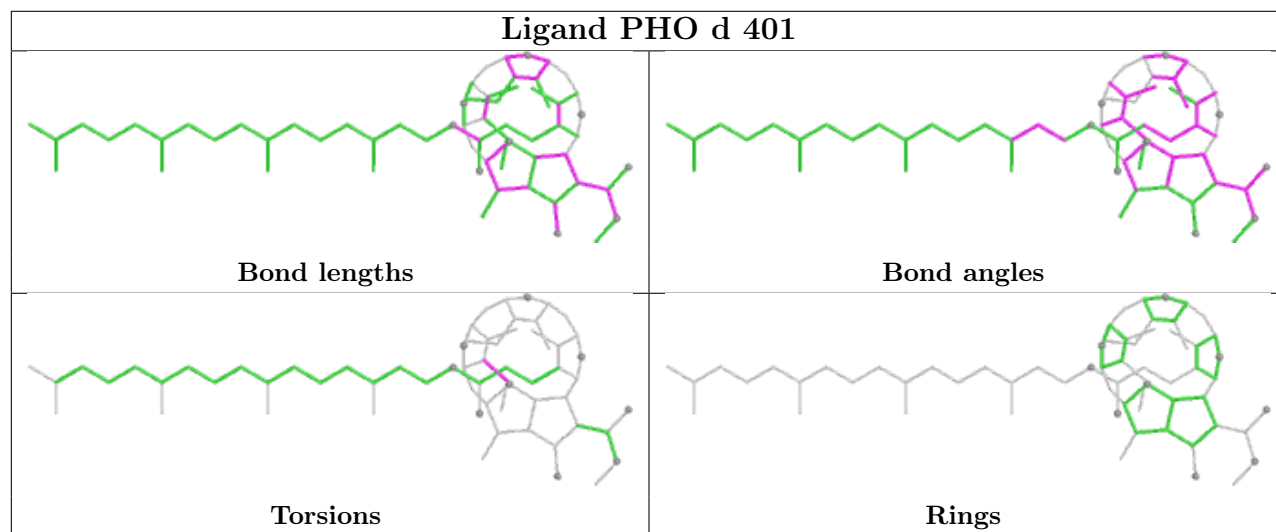
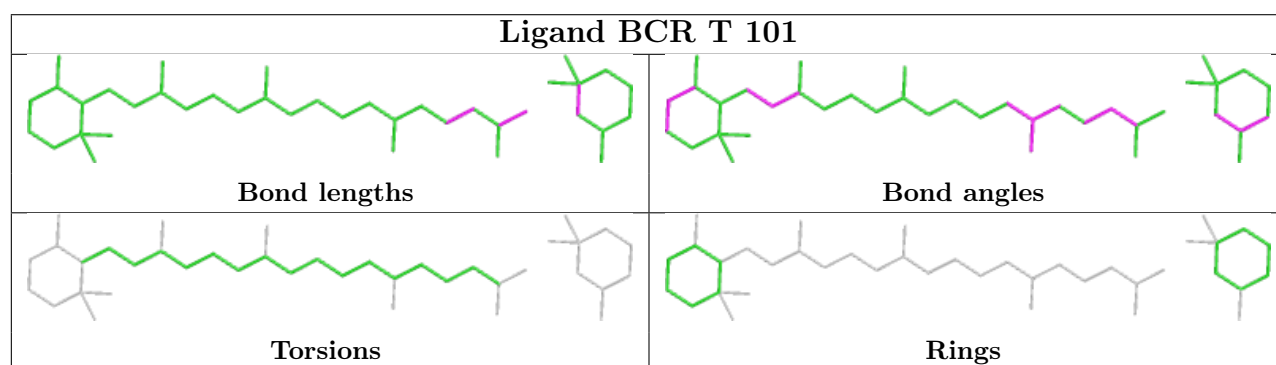
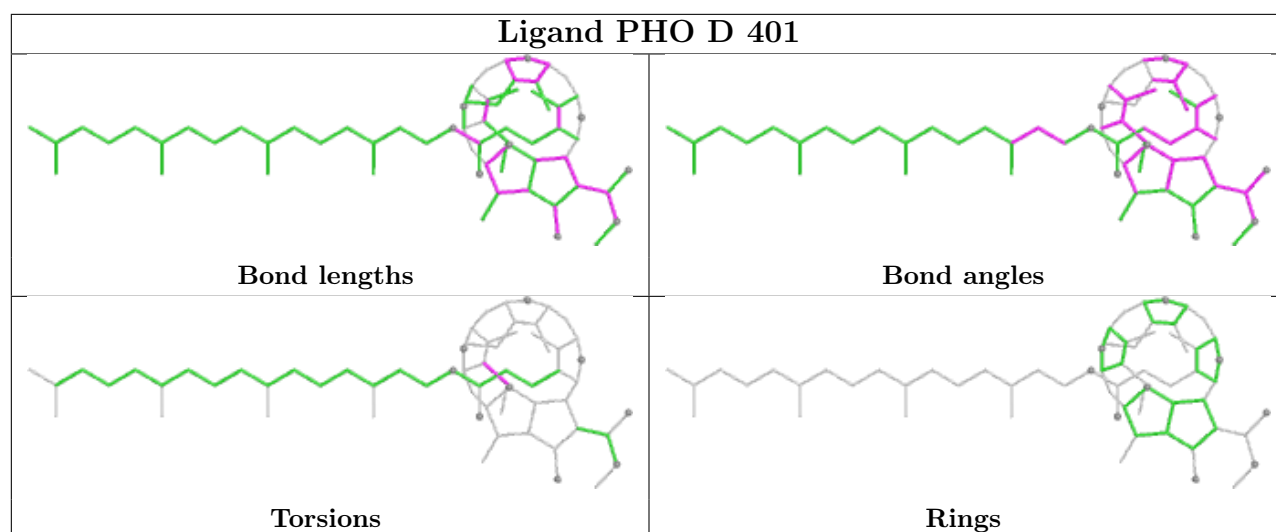


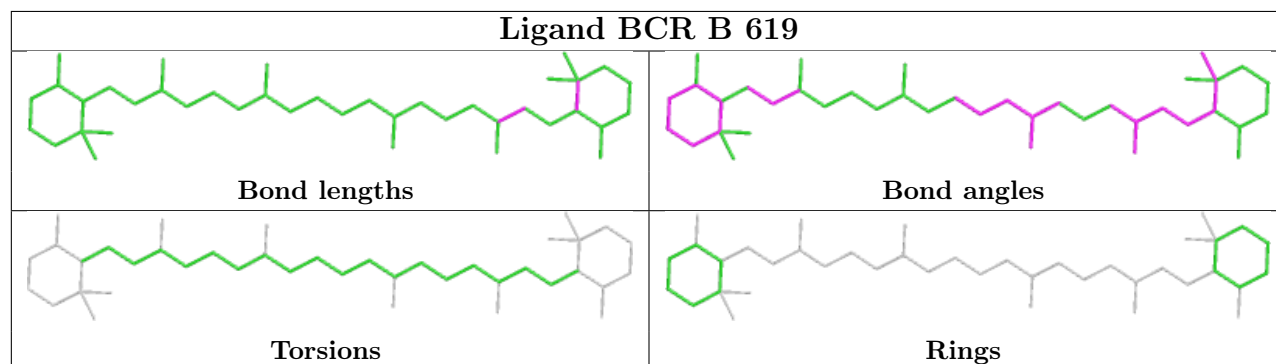
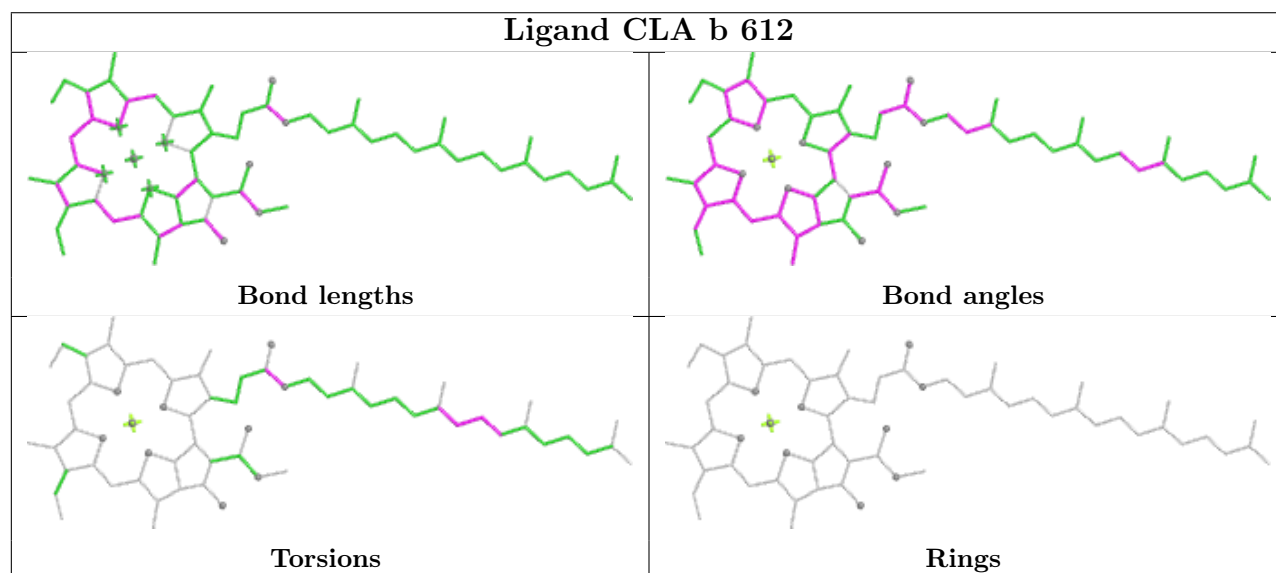
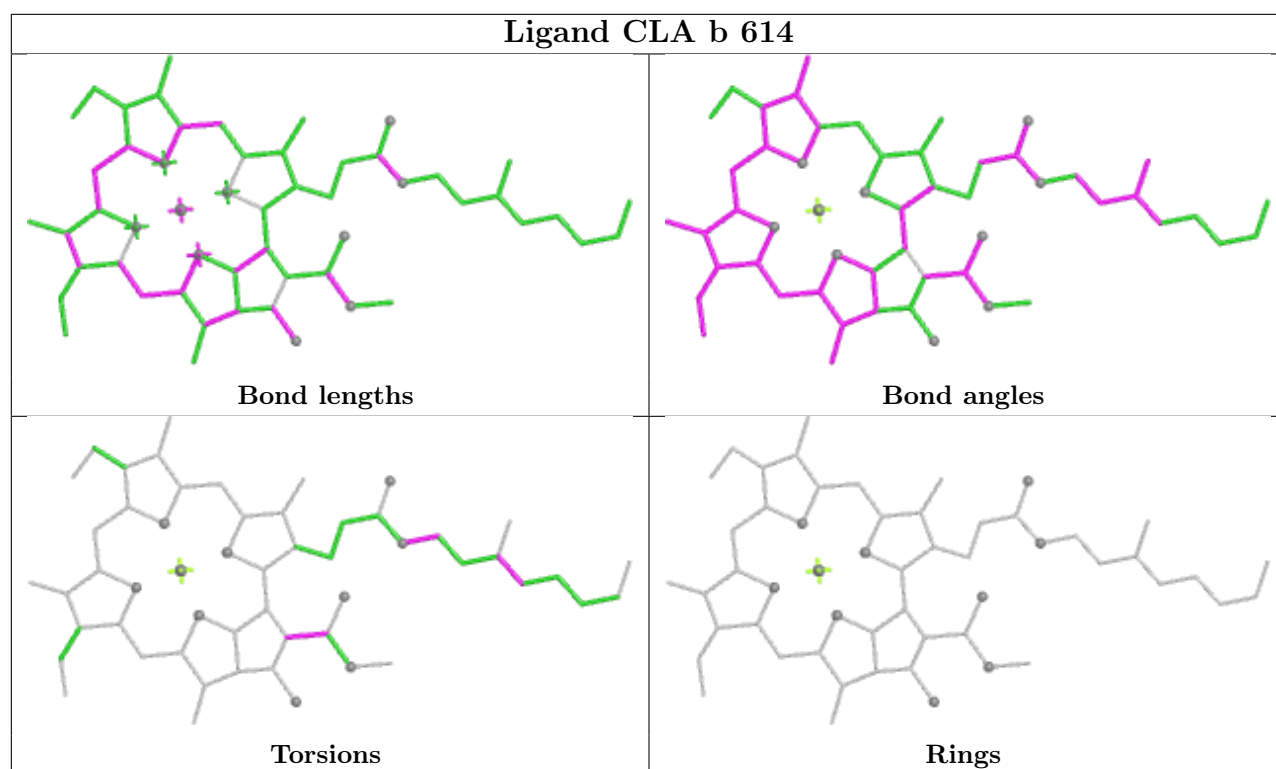


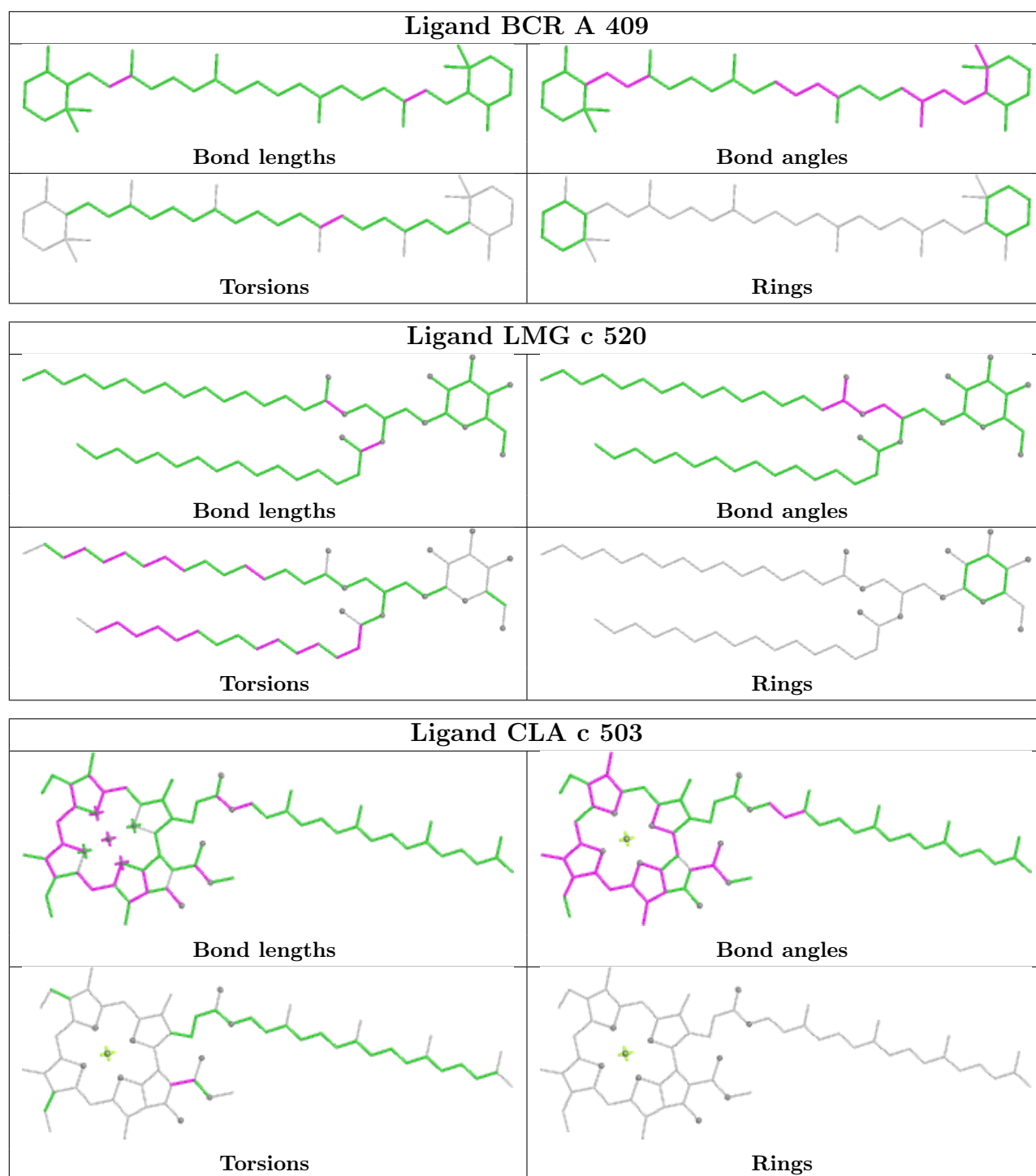




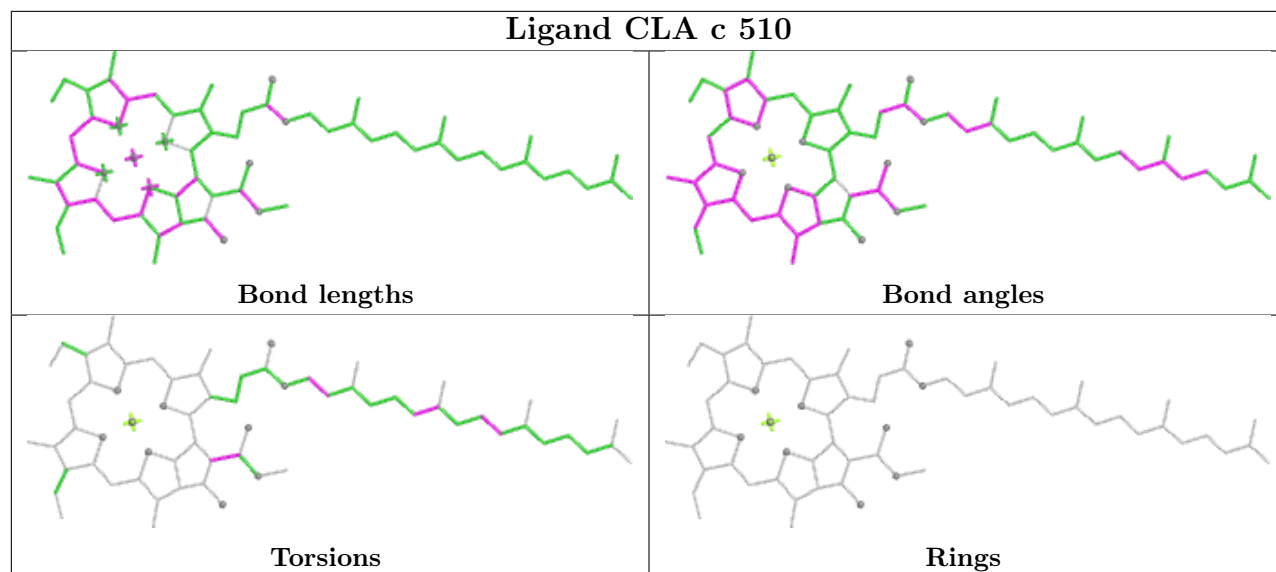




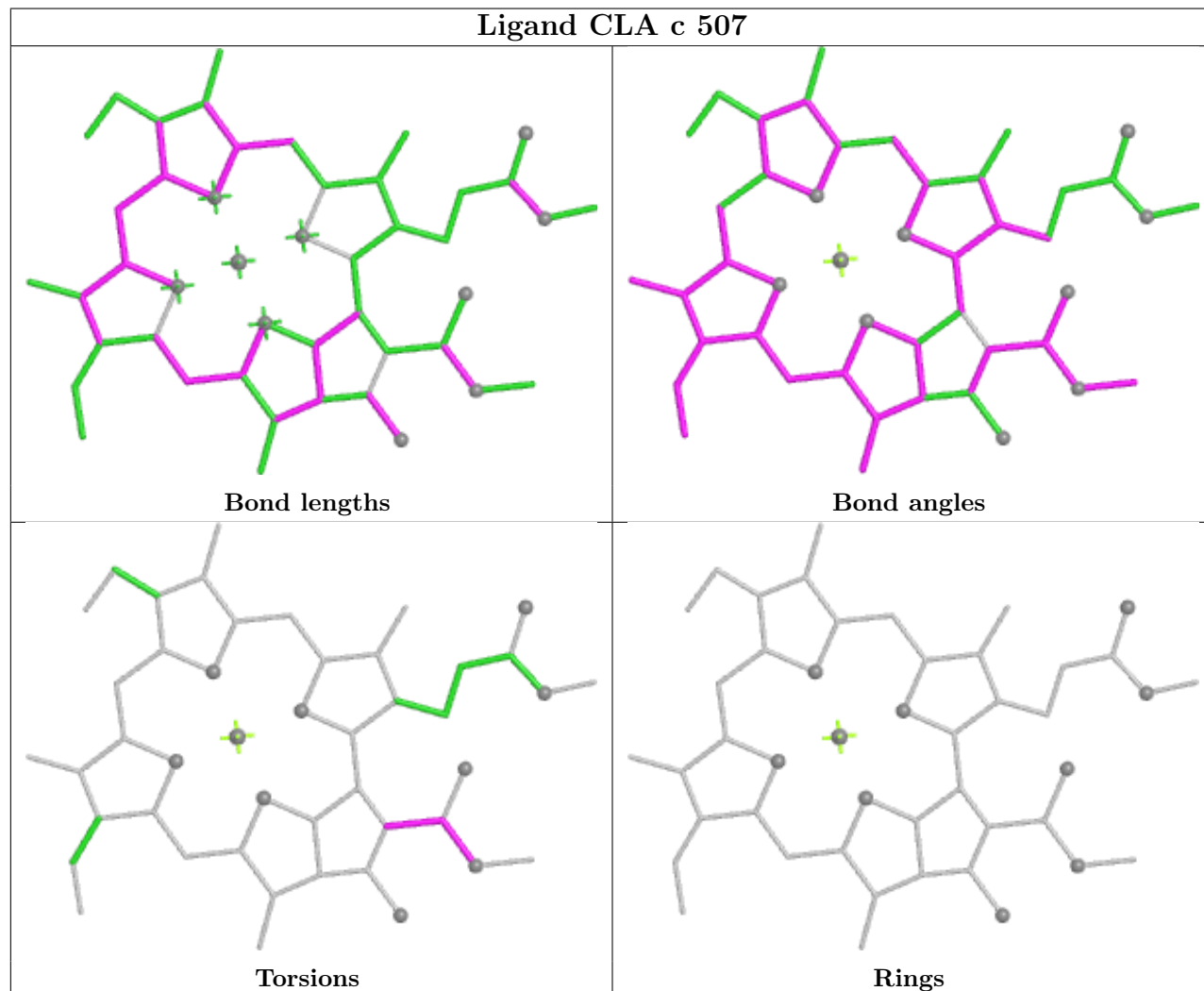


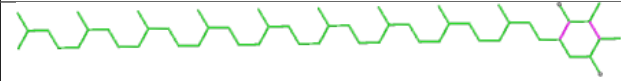
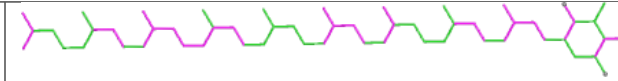

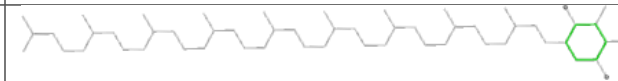
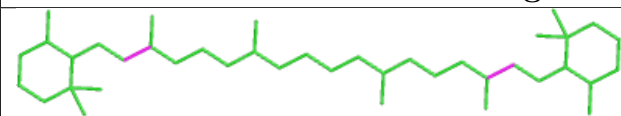
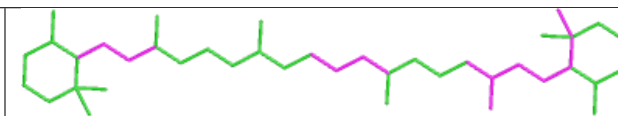
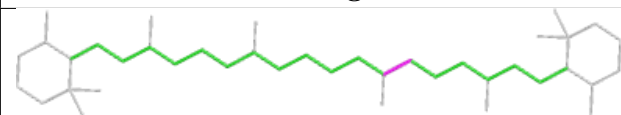
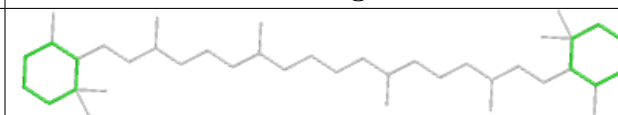
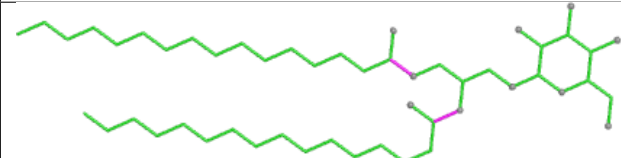
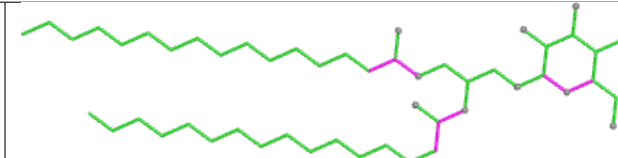
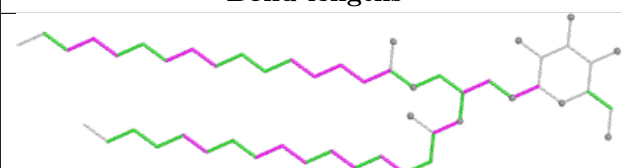
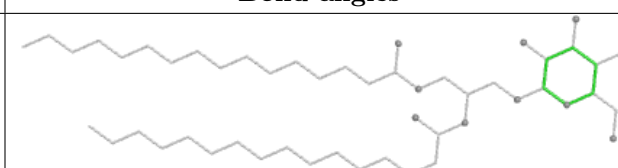
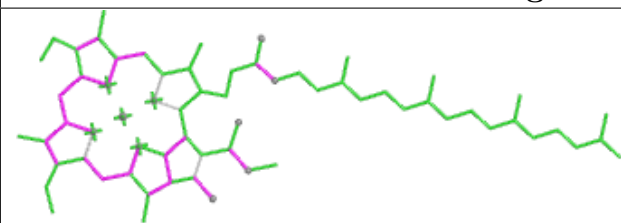
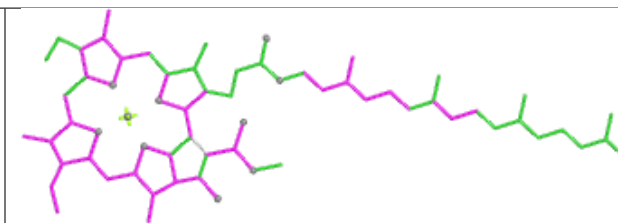
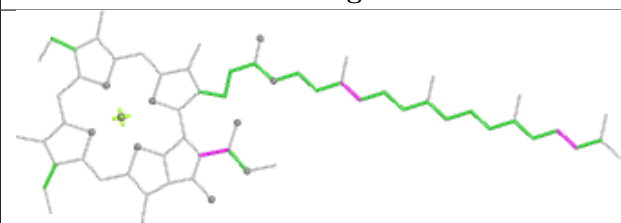
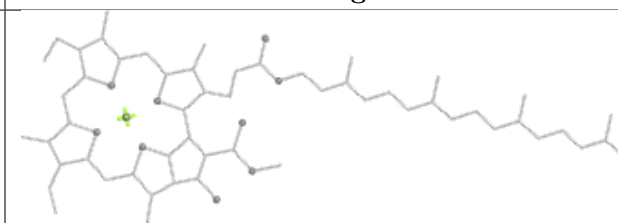


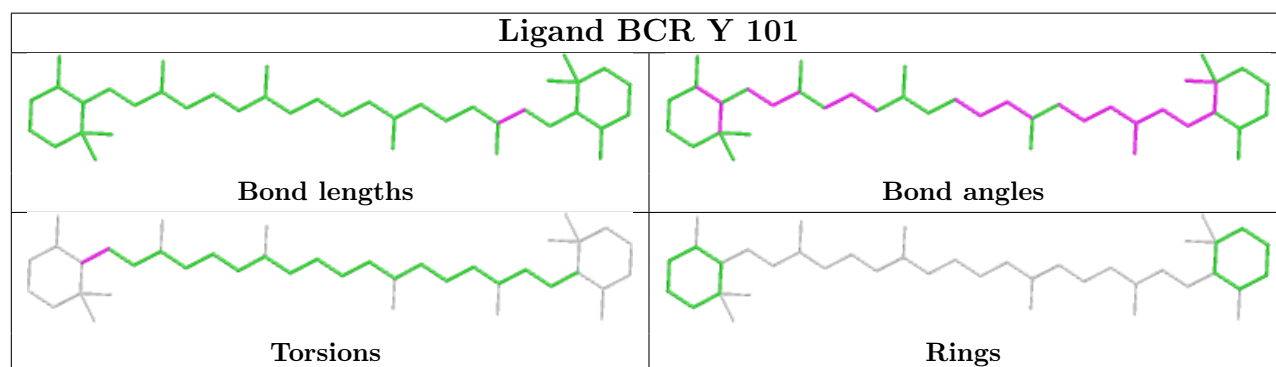
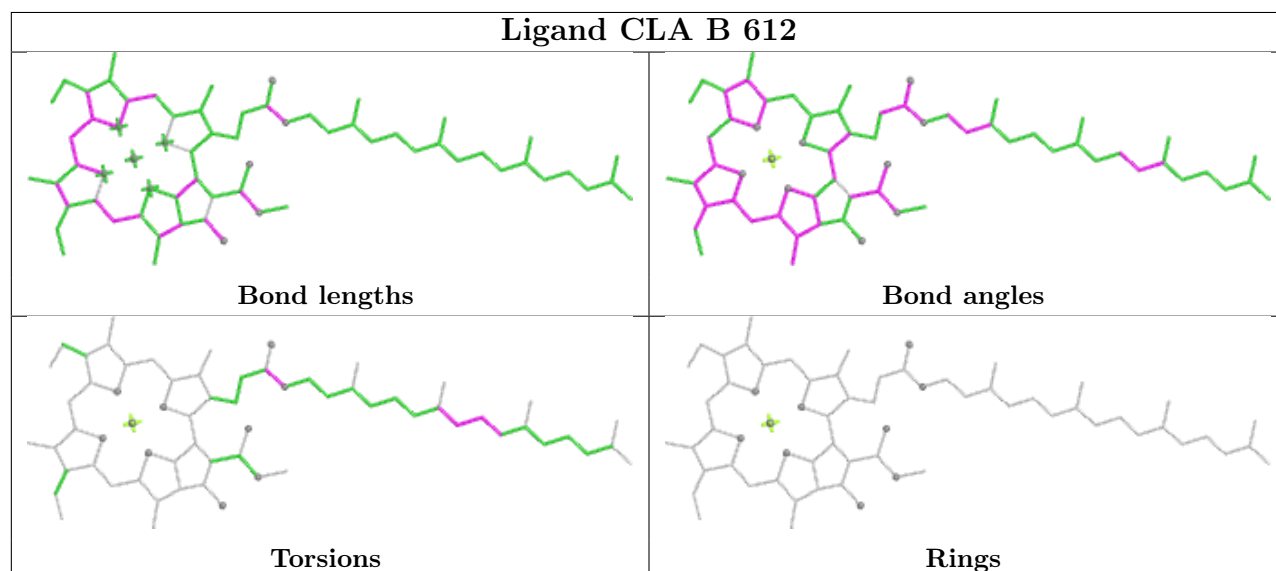
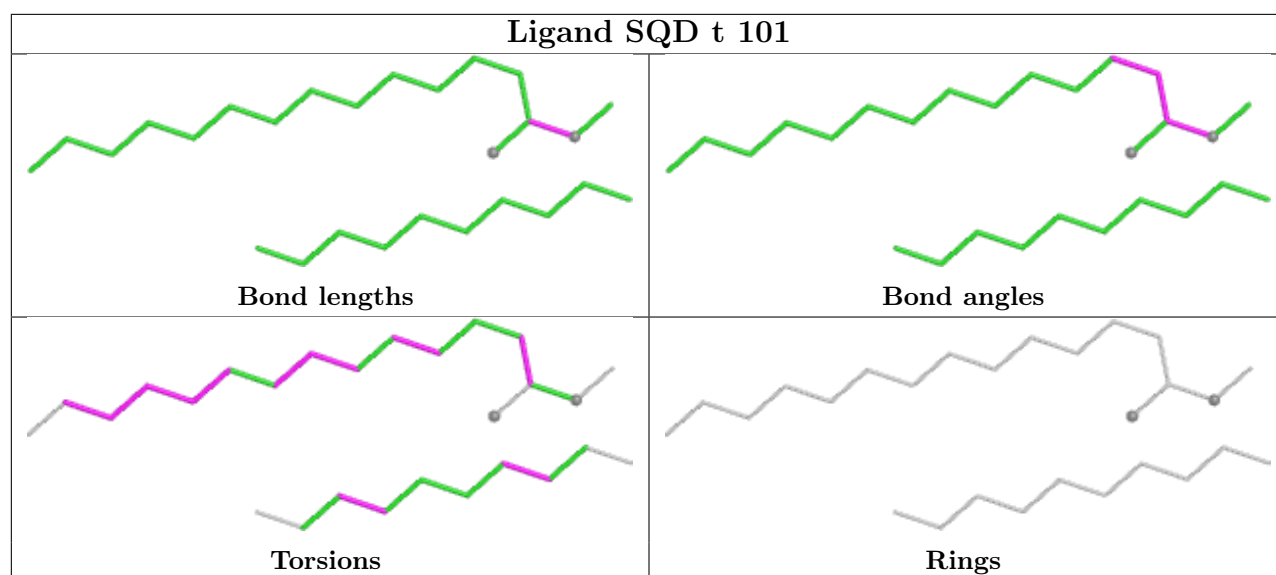
## Ligand CLA c 510



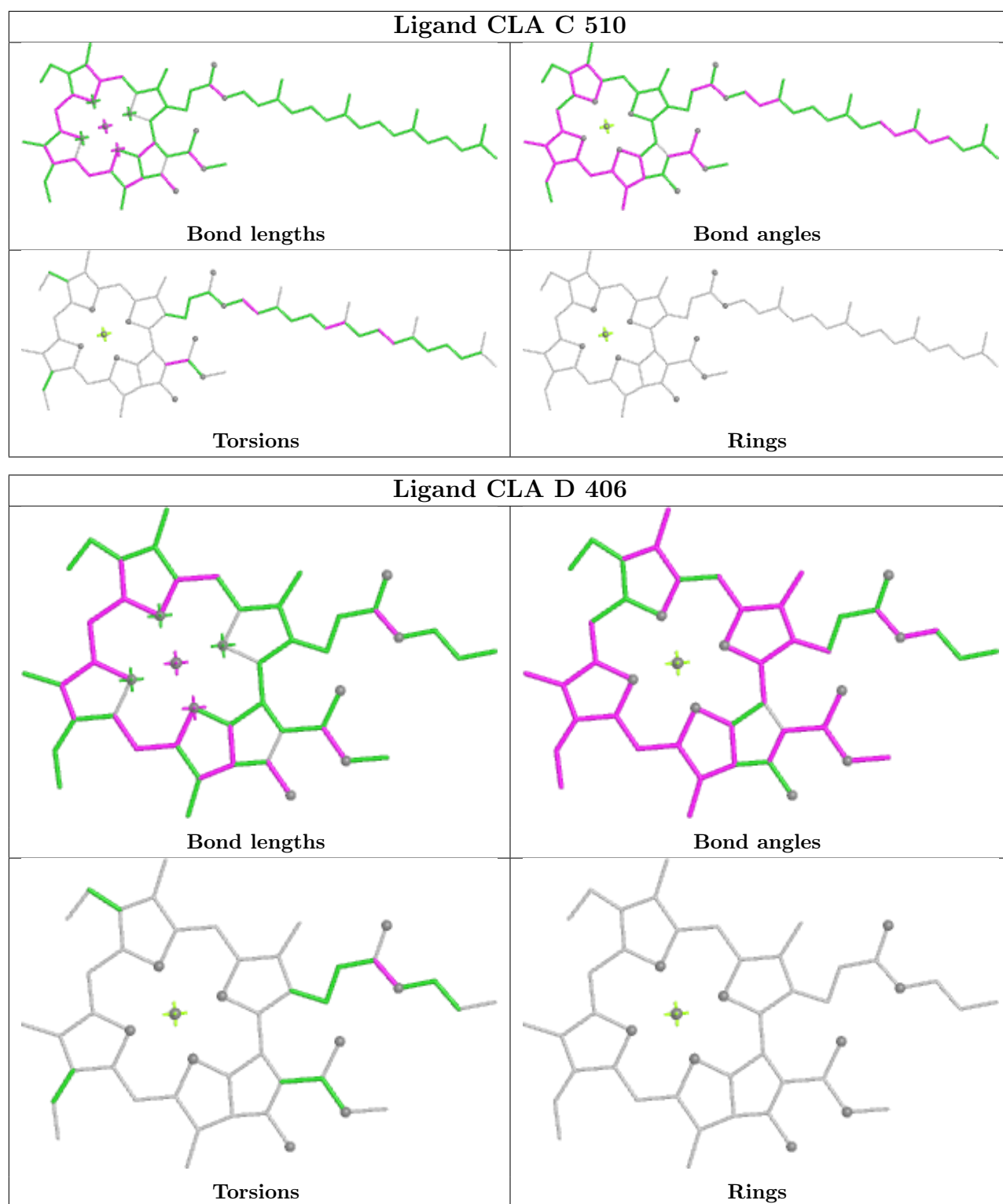
## Ligand CLA c 507



Ligand PL9 d 408	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR a 409	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG a 410	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA c 505	
 Bond lengths	 Bond angles
 Torsions	 Rings







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

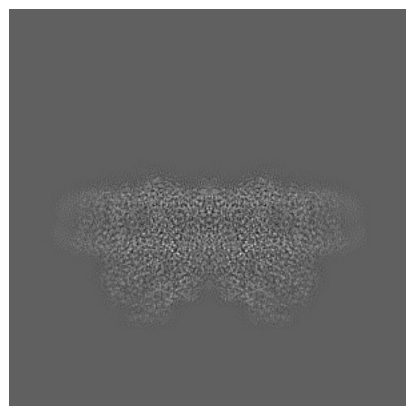
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63639. These allow visual inspection of the internal detail of the map and identification of artifacts.

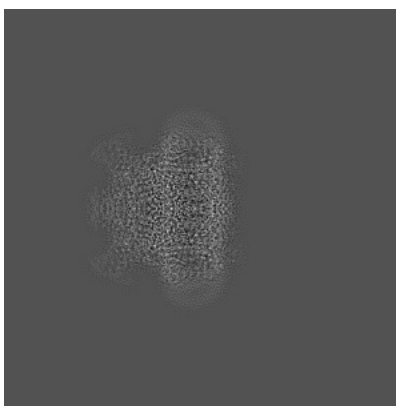
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

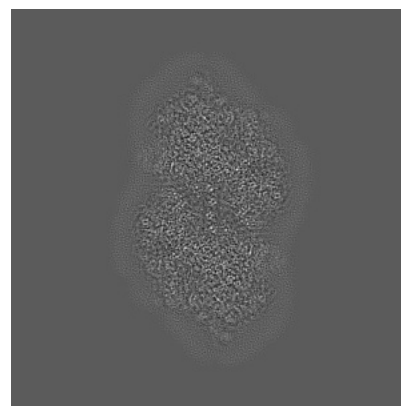
#### 6.1.1 Primary map



X

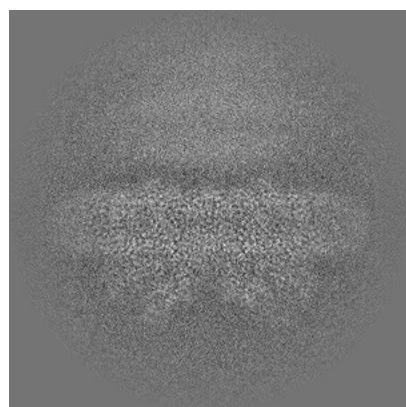


Y

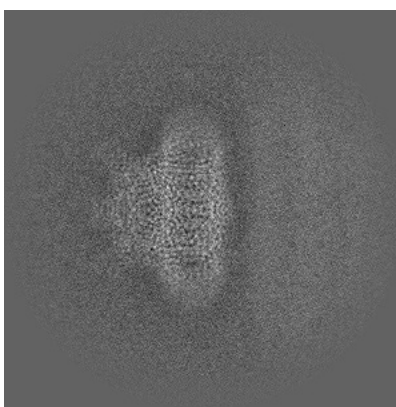


Z

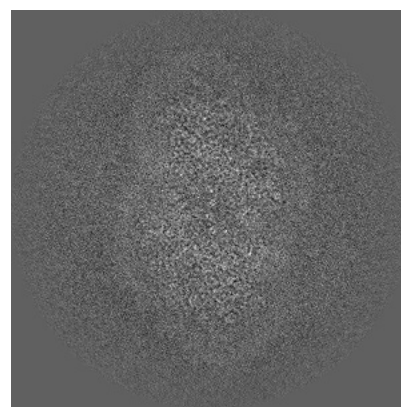
#### 6.1.2 Raw map



X



Y



Z

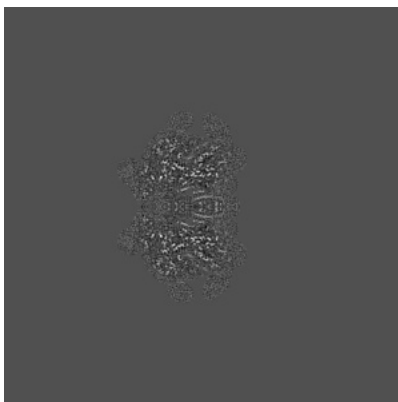
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

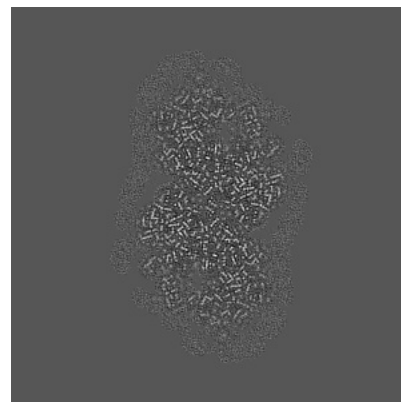
### 6.2.1 Primary map



X Index: 320

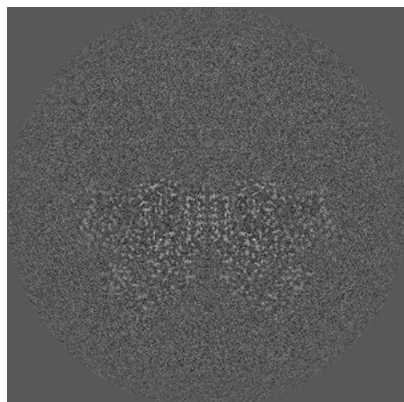


Y Index: 320

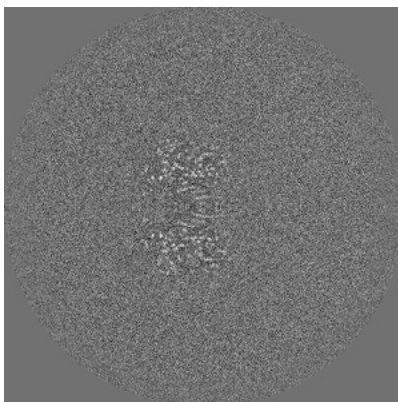


Z Index: 320

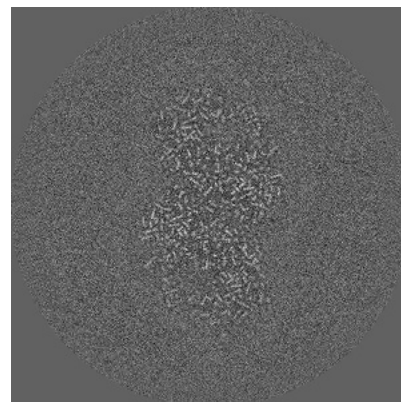
### 6.2.2 Raw map



X Index: 320



Y Index: 320



Z Index: 320

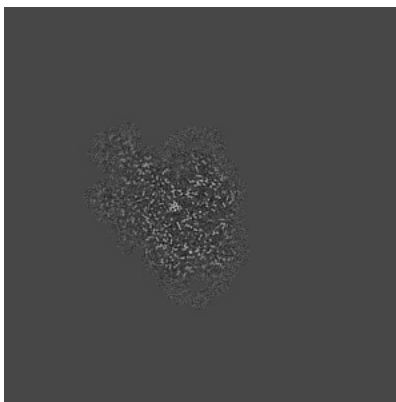
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

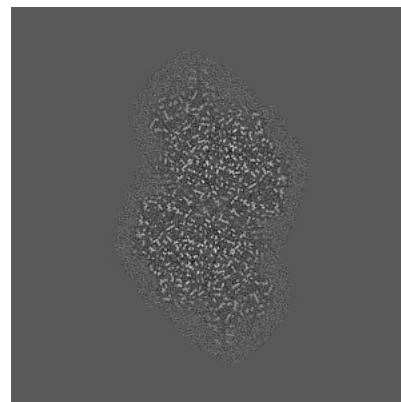
### 6.3.1 Primary map



X Index: 320

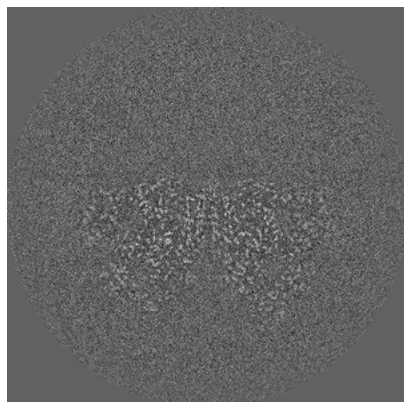


Y Index: 235

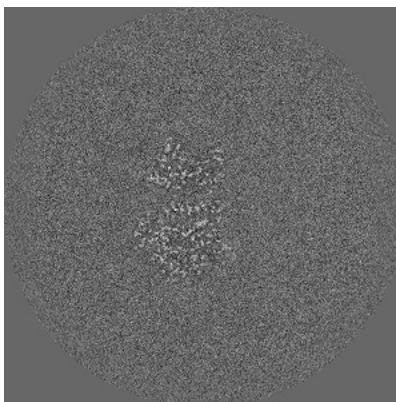


Z Index: 262

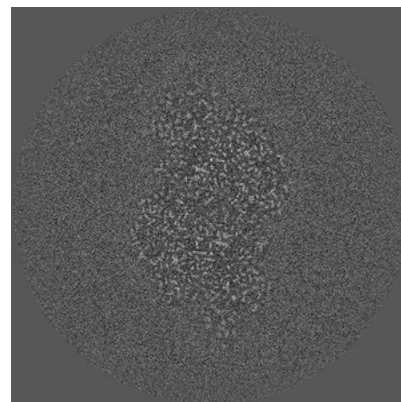
### 6.3.2 Raw map



X Index: 319



Y Index: 312



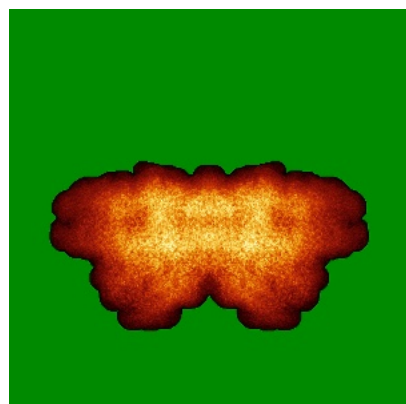
Z Index: 267

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

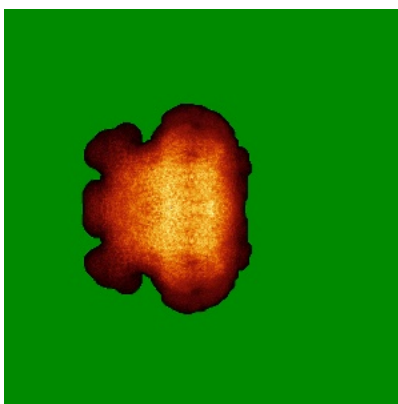


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

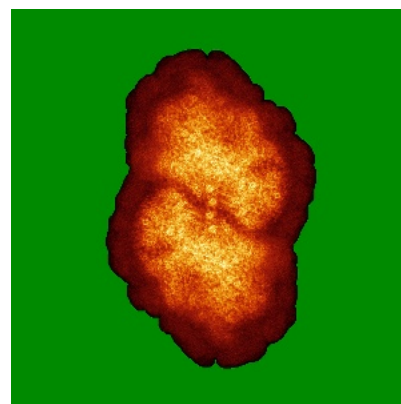
### 6.4.1 Primary map



X

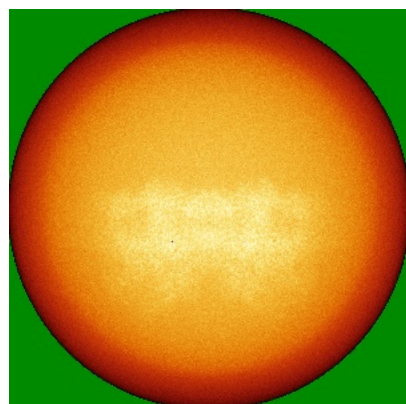


Y

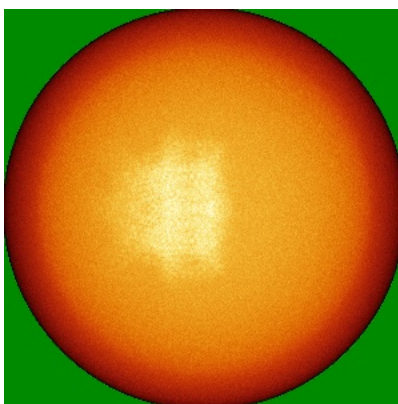


Z

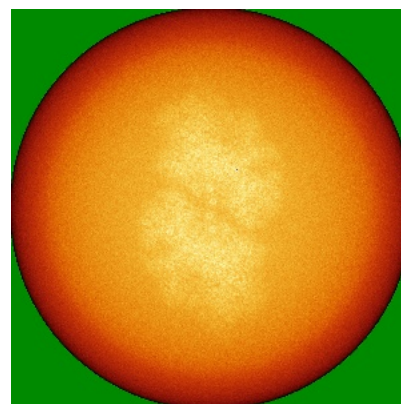
### 6.4.2 Raw map



X



Y

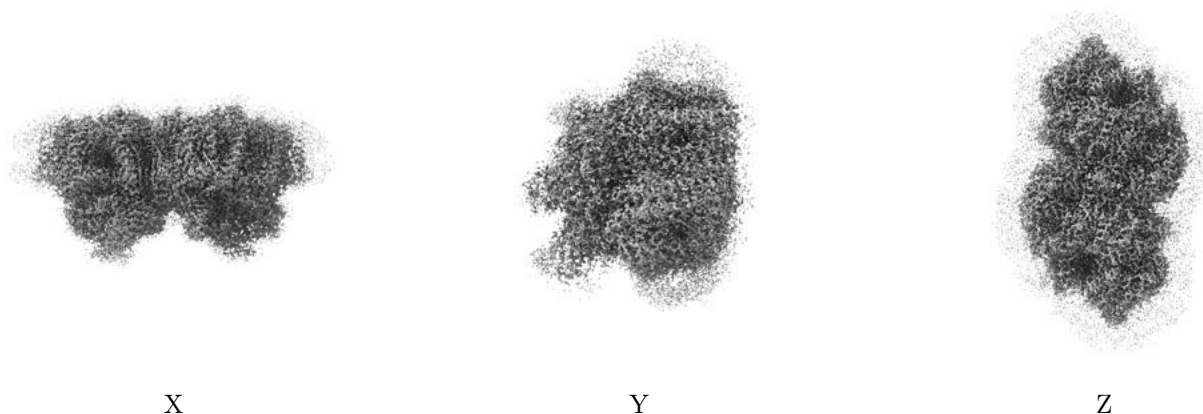


Z

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.

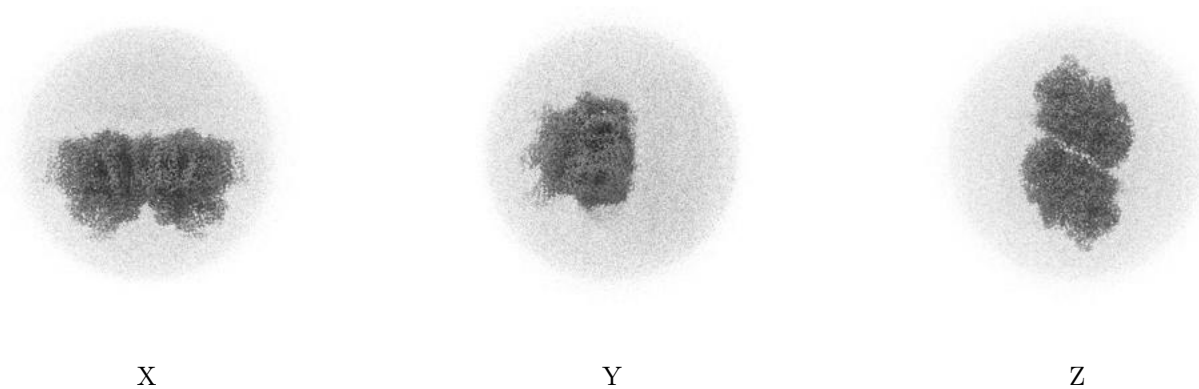
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. 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.

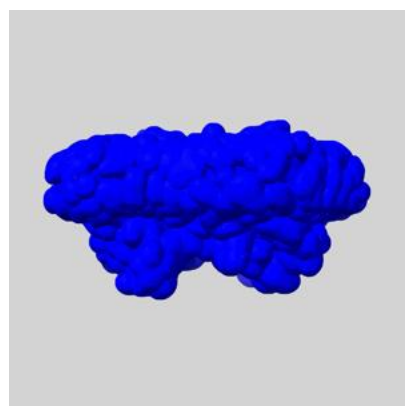
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

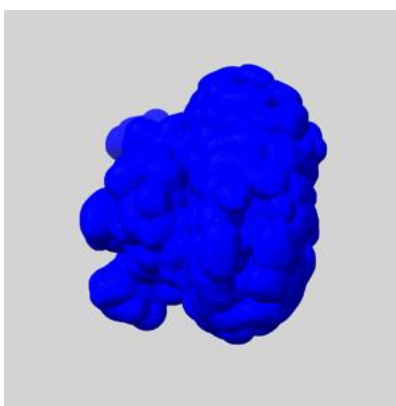
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

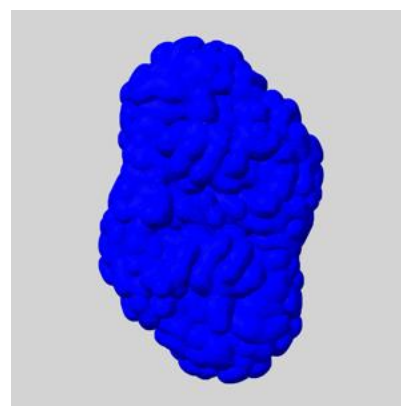
### 6.6.1 emd\_63639\_msk\_1.map [i](#)



X



Y



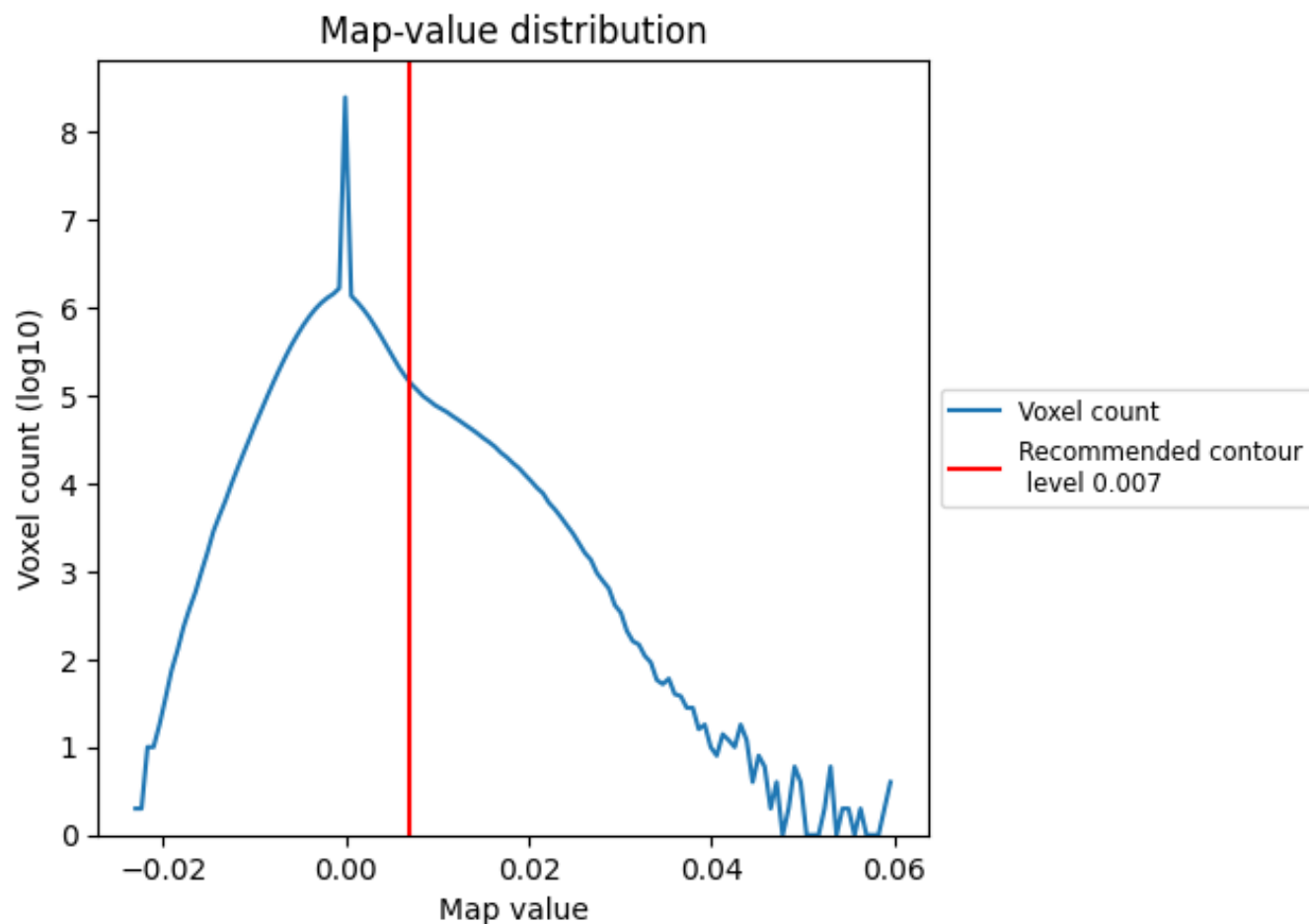
Z



## 7 Map analysis [i](#)

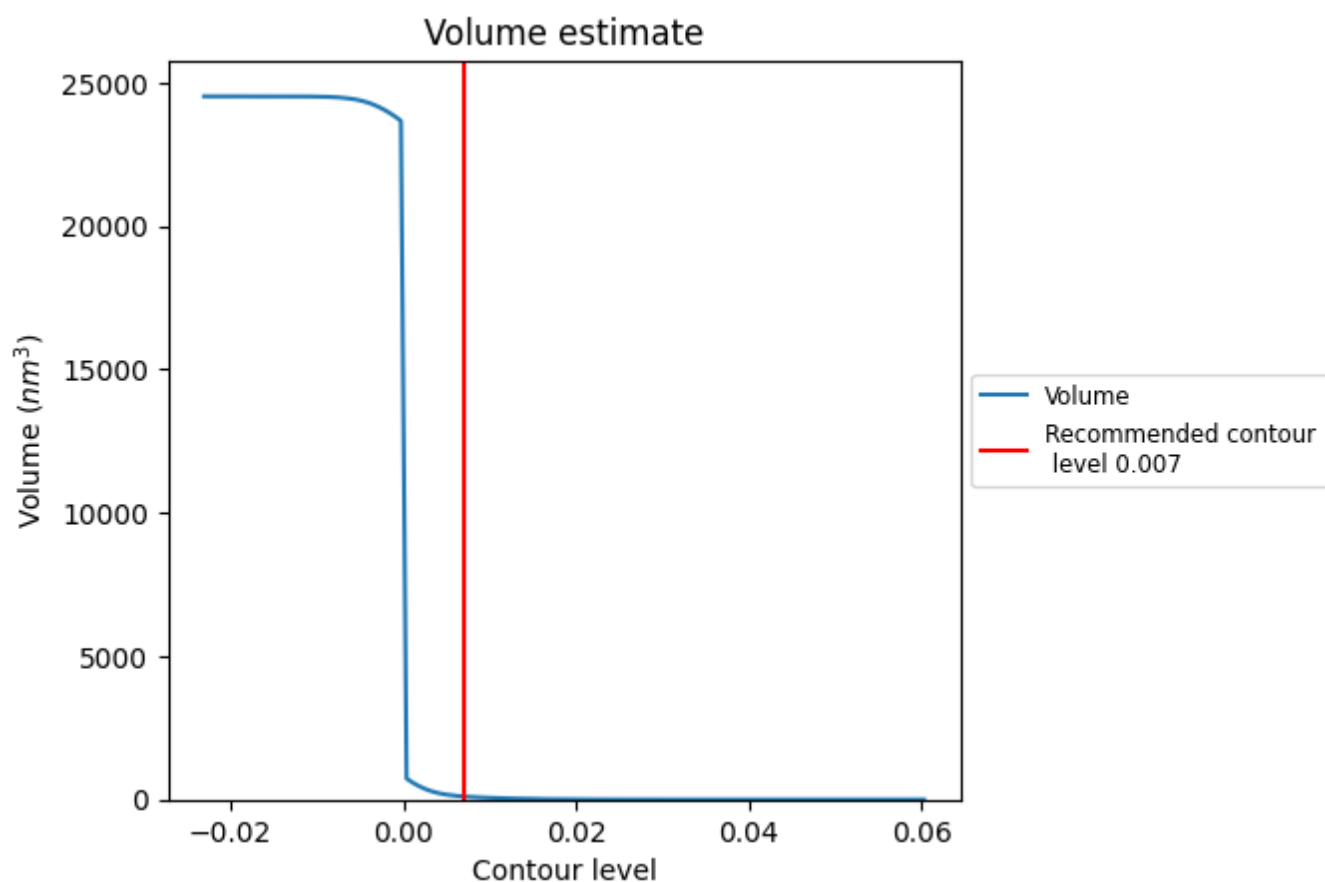
This section contains the results of statistical analysis of the map.

### 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.

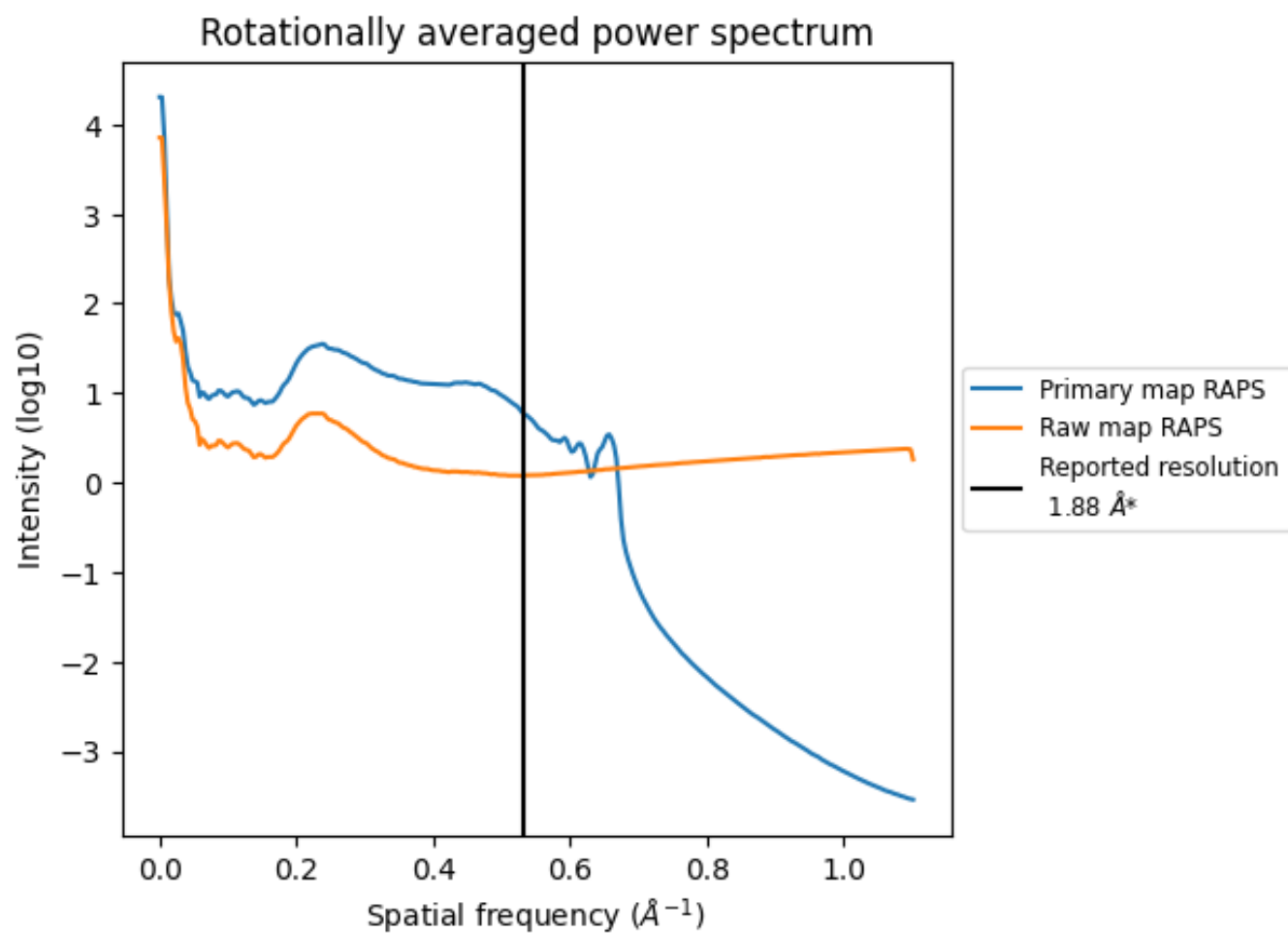
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 107  $\text{nm}^3$ ; this corresponds to an approximate mass of 97 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 ⓘ

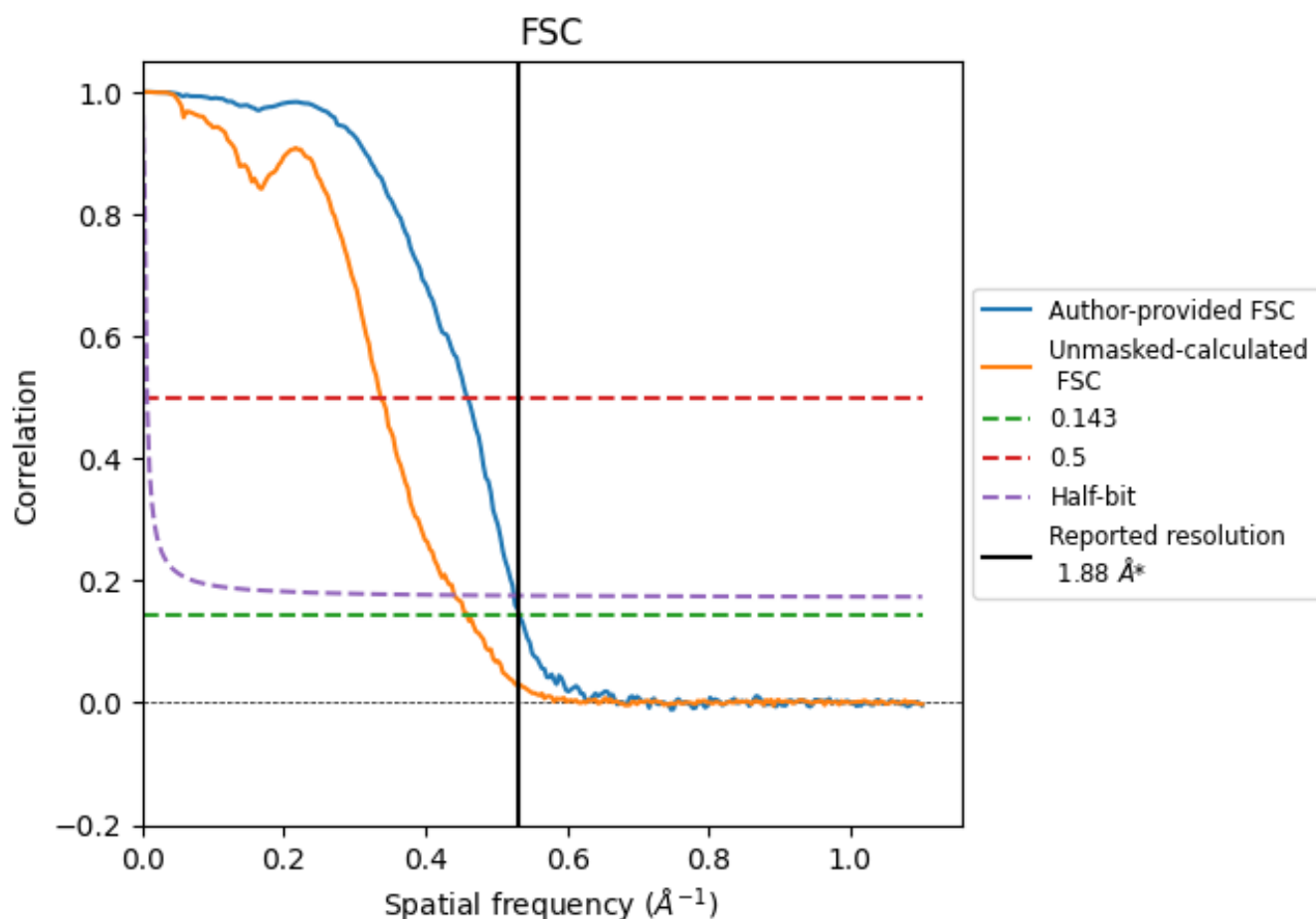


\*Reported resolution corresponds to spatial frequency of 0.532 Å<sup>-1</sup>

## 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 0.532  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

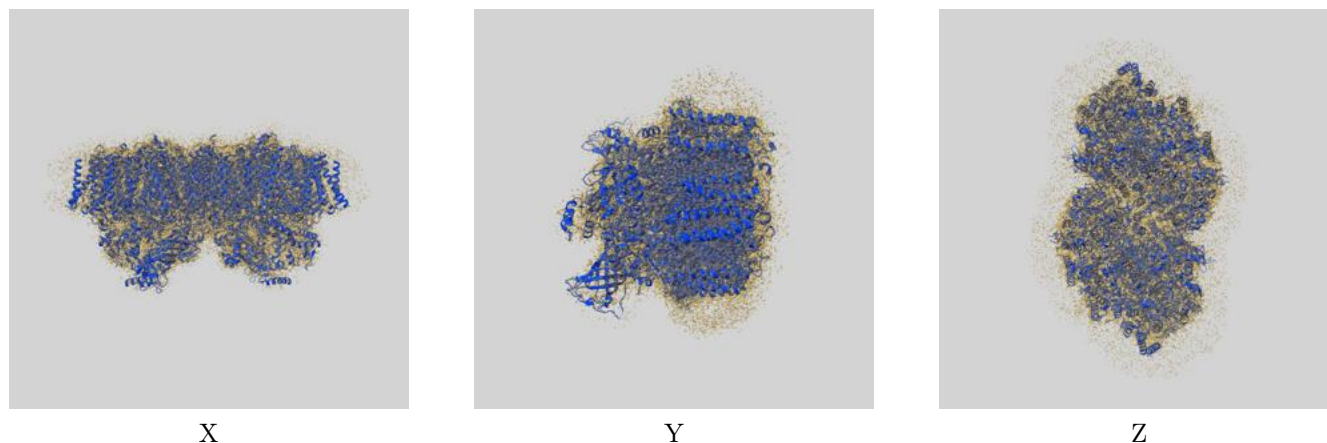
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.88	-	-
Author-provided FSC curve	1.88	2.18	1.91
Unmasked-calculated*	2.18	2.97	2.27

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.18 differs from the reported value 1.88 by more than 10 %

## 9 Map-model fit [i](#)

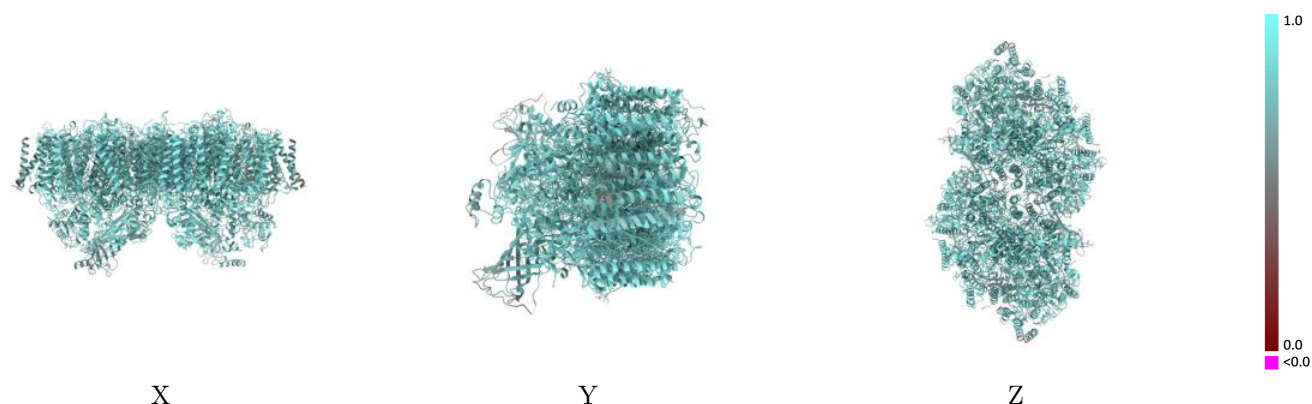
This section contains information regarding the fit between EMDB map EMD-63639 and PDB model 9M5A. Per-residue inclusion information can be found in section 3 on page 27.

### 9.1 Map-model overlay [i](#)



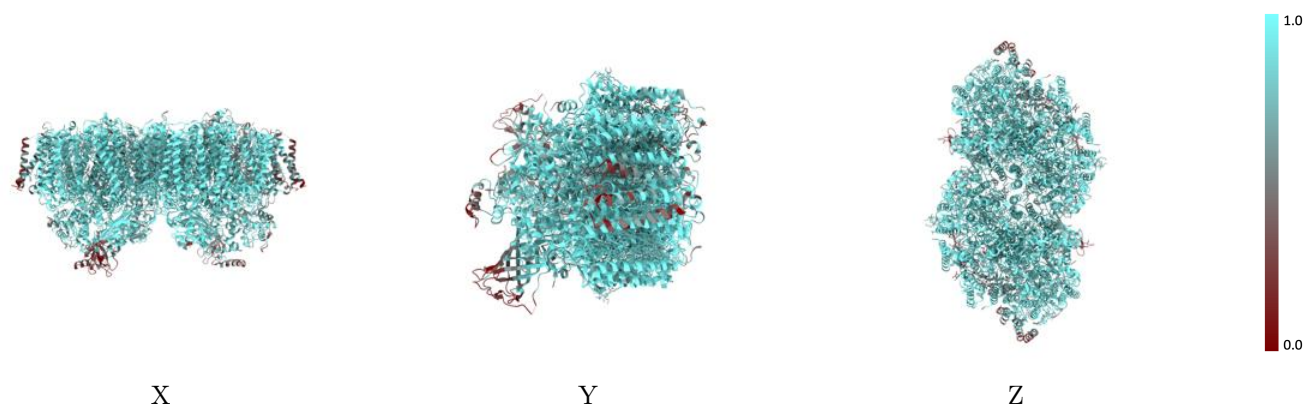
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



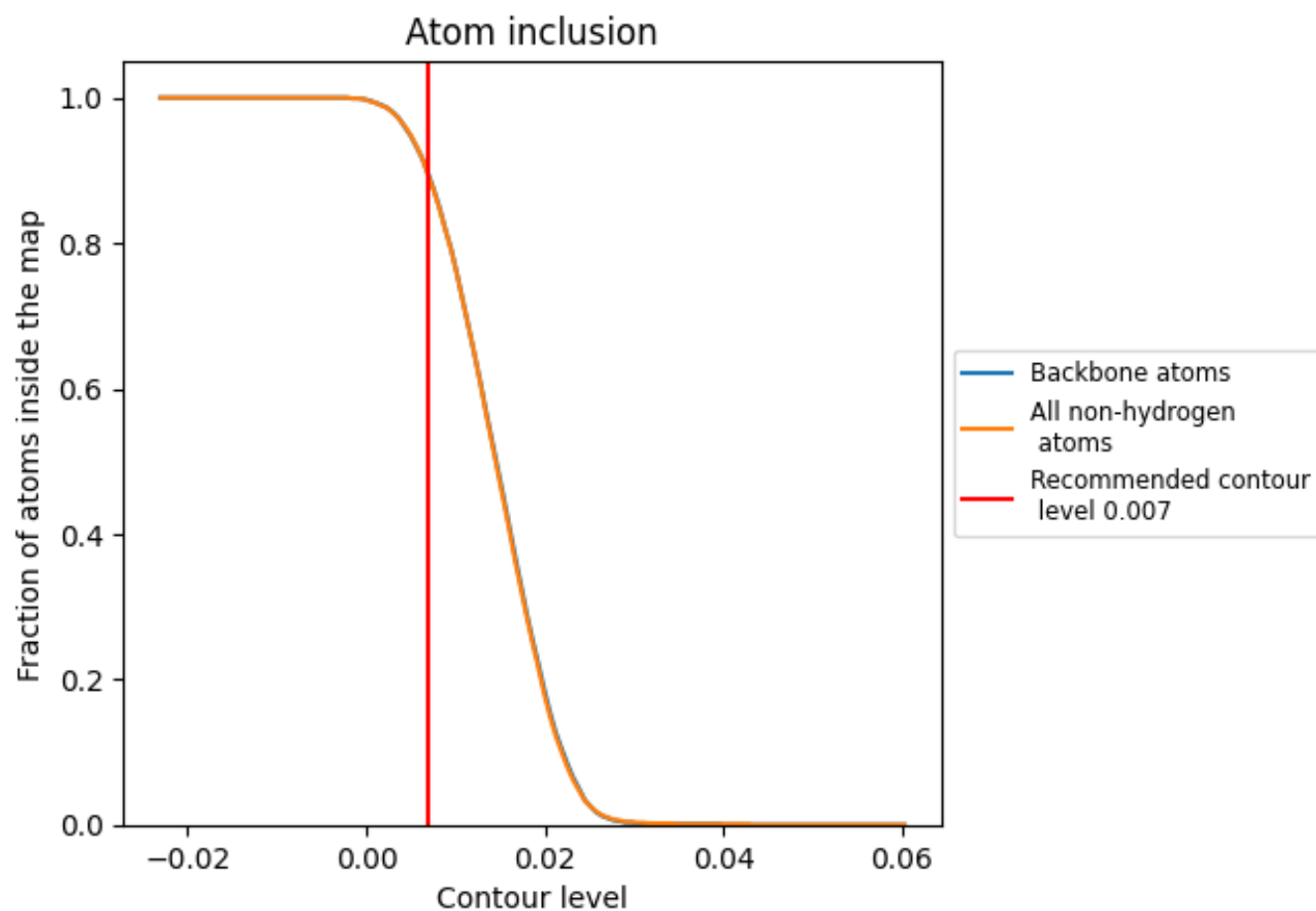
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

## 9.4 Atom inclusion ⓘ









































































At the recommended contour level, 89% of all backbone atoms, 89% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8910	 0.8100
A	 0.9550	 0.8470
B	 0.9320	 0.8240
C	 0.9160	 0.8110
D	 0.9640	 0.8490
E	 0.8090	 0.7600
F	 0.9440	 0.8170
H	 0.9510	 0.8210
I	 0.9420	 0.8210
J	 0.8530	 0.7750
K	 0.8390	 0.7730
L	 0.9310	 0.8420
M	 0.8970	 0.8240
O	 0.7210	 0.7410
T	 0.8910	 0.8050
U	 0.7300	 0.7560
V	 0.7950	 0.7690
X	 0.8330	 0.7830
Y	 0.6190	 0.7240
Z	 0.5010	 0.6690
a	 0.9540	 0.8480
b	 0.9330	 0.8240
c	 0.9150	 0.8100
d	 0.9640	 0.8480
e	 0.8100	 0.7600
f	 0.9440	 0.8180
h	 0.9490	 0.8190
i	 0.9450	 0.8240
j	 0.8530	 0.7750
k	 0.8360	 0.7760
l	 0.9310	 0.8400
m	 0.8970	 0.8250
o	 0.7210	 0.7400
t	 0.9070	 0.8160
u	 0.7300	 0.7550



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
v	 0.7950	 0.7690
x	 0.8330	 0.7860
y	 0.6190	 0.7280
z	 0.5040	 0.6670