



Full wwPDB EM Validation Report ⓘ

Aug 13, 2026 – 03:23 pm BST

PDB ID : 9I82 / pdb_00009i82
EMDB ID : EMD-52705
Title : Cryo-EM structure of PSII intermediate Psb27-PSII
Authors : Bohn, S.; Lo, Y.K.; Lambertz, J.; Furtges, T.; Rudack, T.; Nowaczyk, M.M.; Schuller, J.M.
Deposited on : 2025-02-04
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

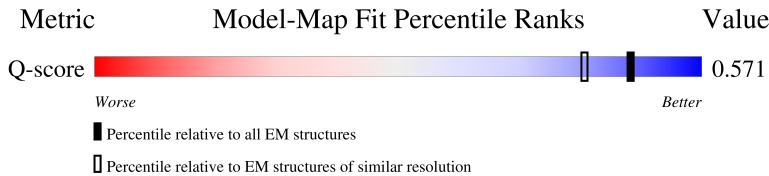
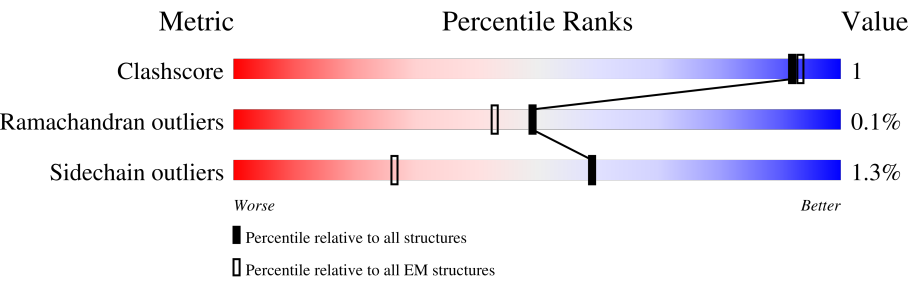
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 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.



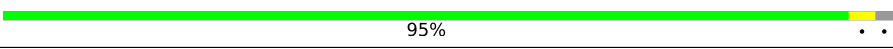
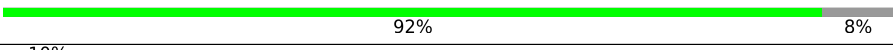
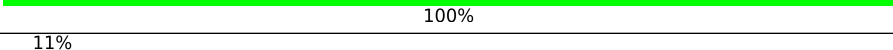
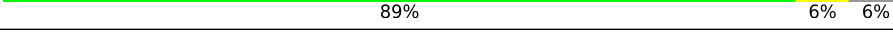
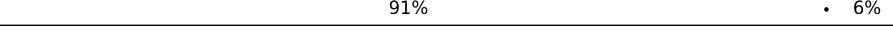
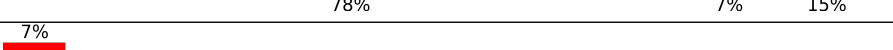
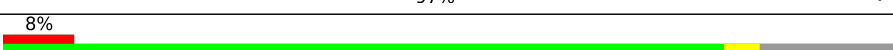
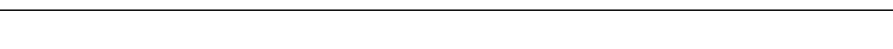
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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

Mol	Chain	Length	Quality of chain
1	A	360	86% 10%
2	B	510	90% 5% 5%
3	C	461	95%
4	D	352	91% 5%

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Mol	Chain	Length	Quality of chain
5	E	84	
6	F	45	
7	H	66	
8	I	38	
9	J	40	
10	K	46	
11	L	37	
12	M	36	
13	T	32	
14	X	41	
15	Y	46	
16	Z	62	
17	1	134	

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 20990 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	325	Total	C	N	O	S	1	0
			2559	1676	421	447	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	485	Total	C	N	O	S	0	0
			3812	2505	635	659	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	448	Total	C	N	O	S	0	0
			3466	2270	580	603	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	340	Total	C	N	O	S	0	0
			2706	1794	440	460	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	77	Total	C	N	O	0	0
			635	417	103	115		

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	38	Total	C	N	O	S	0	0
			307	207	50	49	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	65	Total	C	N	O	S	0	0
			511	341	82	86	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	35	Total	C	N	O	S	0	0
			286	195	45	45	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	34	Total	C	N	O	S	0	0
			249	170	38	40	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	37	Total	C	N	O	0	0
			293	204	43	46		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	37	Total	C	N	O	S	0	0
			304	202	48	53	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	34	Total	C	N	O	S	0	0
			267	178	40	48	1		

- Molecule 13 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	30	Total	C	N	O	S	0	0
			256	180	36	38	2		

- Molecule 14 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	X	35	Total	C	N	O	0	0
			254	172	38	44		

- Molecule 15 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Y	28	Total	C	N	O	S	0	0
			208	137	36	32	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Z	62	Total	C	N	O	S	0	0
			479	328	72	77	2		

- Molecule 17 is a protein called Photosystem II lipoprotein Psb27.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1	113	Total	C	N	O	S	0	0
			893	556	161	173	3		

- Molecule 18 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Fe	0
			1	1	

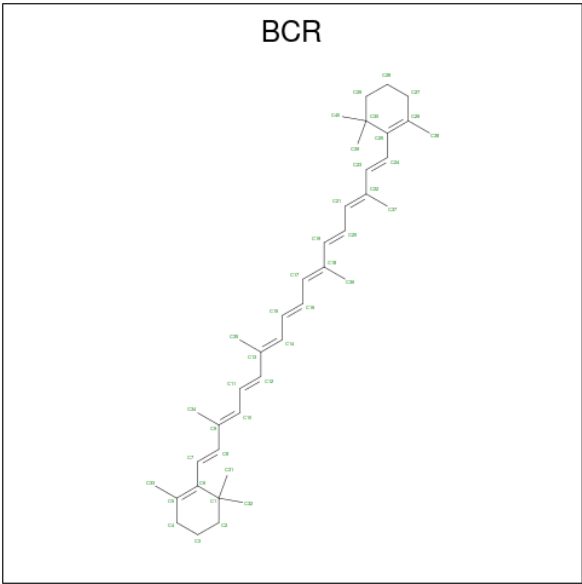
- Molecule 19 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	Mn	0
			1	1	

- Molecule 20 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

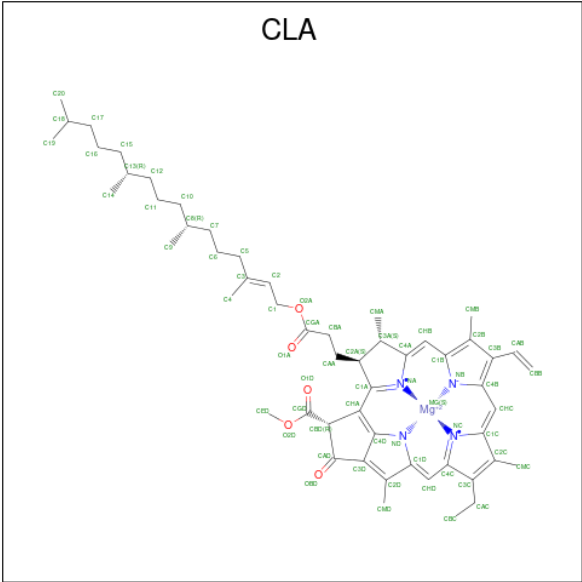
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	Cl	0
			1	1	

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	C	1	Total C 40 40	0
21	C	1	Total C 40 40	0
21	C	1	Total C 40 40	0
21	D	1	Total C 40 40	0
21	H	1	Total C 40 40	0
21	J	1	Total C 40 40	0
21	J	1	Total C 40 40	0
21	M	1	Total C 40 40	0

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



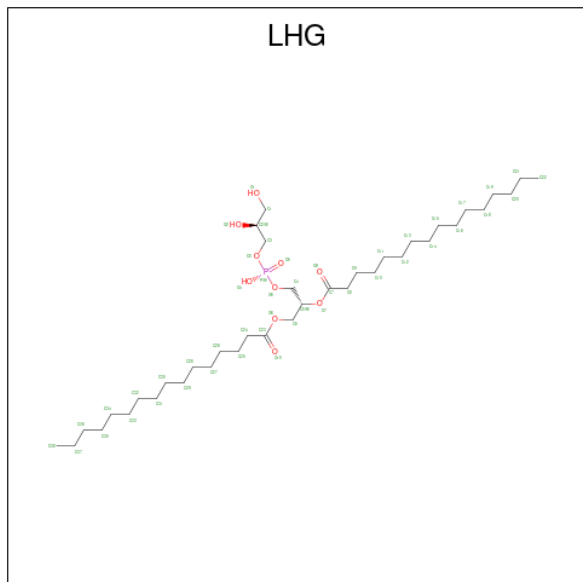
Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	C	N	O	0
			64	55	4	5	
22	A	1	Total	C	N	O	0
			64	55	4	5	
22	A	1	Total	C	N	O	0
			64	55	4	5	
22	A	1	Total	C	N	O	0
			64	55	4	5	
22	B	1	Total	C	N	O	0
			64	55	4	5	
22	B	1	Total	C	N	O	0
			64	55	4	5	
22	B	1	Total	C	N	O	0
			64	55	4	5	
22	B	1	Total	C	N	O	0
			64	55	4	5	
22	B	1	Total	C	N	O	0
			64	55	4	5	
22	B	1	Total	C	N	O	0
			64	55	4	5	
22	B	1	Total	C	N	O	0
			64	55	4	5	
22	B	1	Total	C	N	O	0
			64	55	4	5	
22	B	1	Total	C	N	O	0
			64	55	4	5	

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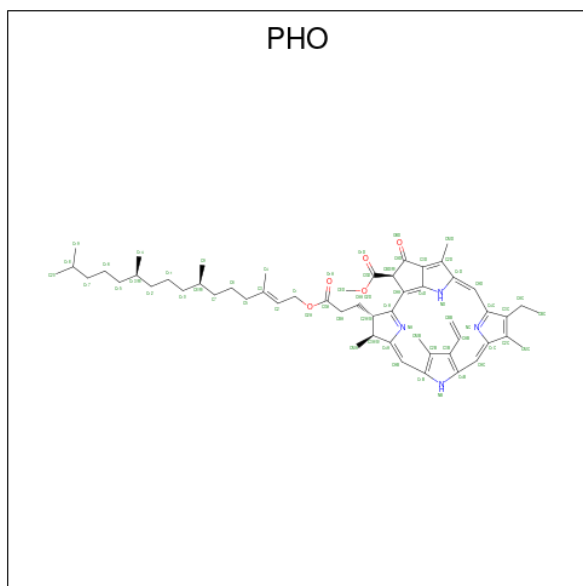
Mol	Chain	Residues	Atoms				AltConf
22	B	1	Total 64	C 55	N 4	O 5	0
22	B	1	Total 64	C 55	N 4	O 5	0
22	B	1	Total 64	C 55	N 4	O 5	0
22	B	1	Total 64	C 55	N 4	O 5	0
22	B	1	Total 64	C 55	N 4	O 5	0
22	B	1	Total 64	C 55	N 4	O 5	0
22	C	1	Total 64	C 55	N 4	O 5	0
22	C	1	Total 64	C 55	N 4	O 5	0
22	C	1	Total 64	C 55	N 4	O 5	0
22	C	1	Total 64	C 55	N 4	O 5	0
22	C	1	Total 64	C 55	N 4	O 5	0
22	C	1	Total 64	C 55	N 4	O 5	0
22	C	1	Total 64	C 55	N 4	O 5	0
22	C	1	Total 64	C 55	N 4	O 5	0
22	C	1	Total 64	C 55	N 4	O 5	0
22	C	1	Total 64	C 55	N 4	O 5	0
22	C	1	Total 64	C 55	N 4	O 5	0
22	C	1	Total 64	C 55	N 4	O 5	0
22	C	1	Total 64	C 55	N 4	O 5	0
22	D	1	Total 64	C 55	N 4	O 5	0
22	D	1	Total 64	C 55	N 4	O 5	0

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



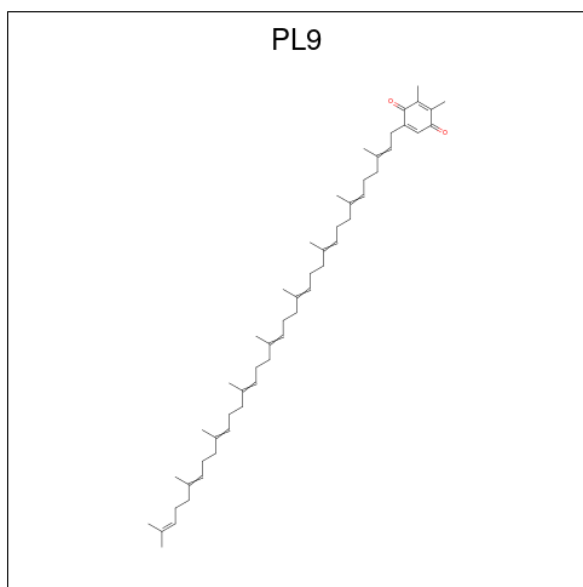
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	P	0
			49	38	10	1	
23	A	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



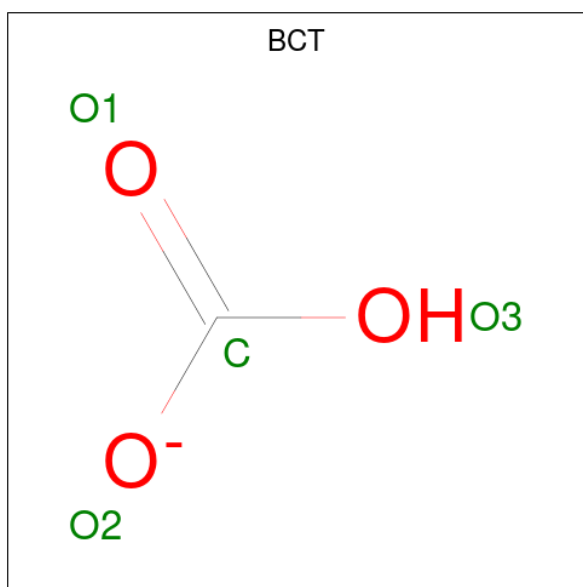
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	N	O	0
			64	55	4	5	
24	D	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 25 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: C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



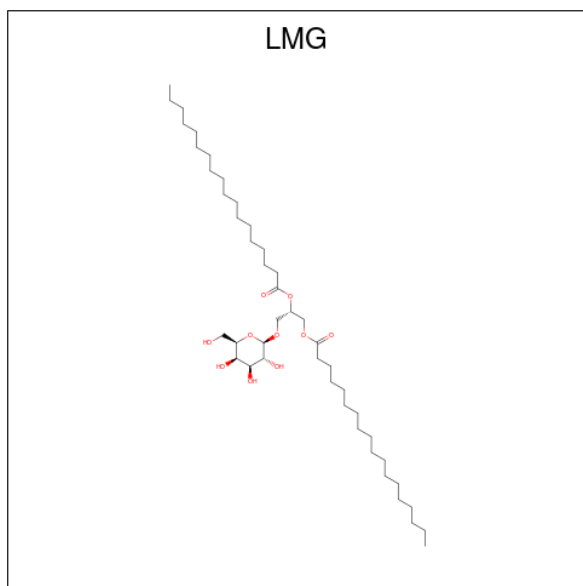
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			55	53	2	
25	D	1	Total	C	O	0
			55	53	2	

- Molecule 26 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			4	1	3	

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
27	C	1	Total	C	O	0
			55	45	10	
27	D	1	Total	C	O	0
			55	45	10	

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Mol	Chain	Residues	Atoms			AltConf
27	D	1	Total 55	C 45	O 10	0
27	D	1	Total 55	C 45	O 10	0
27	I	1	Total 55	C 45	O 10	0
27	K	1	Total 55	C 45	O 10	0
27	L	1	Total 55	C 45	O 10	0
27	M	1	Total 55	C 45	O 10	0

- # HEM

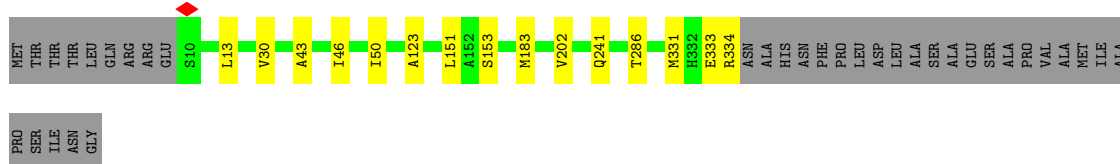
Mol	Chain	Residues	Atoms				AltConf
28	F	1	Total	C	N	O	0
			42	34	4	4	

3 Residue-property plots [i](#)

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.

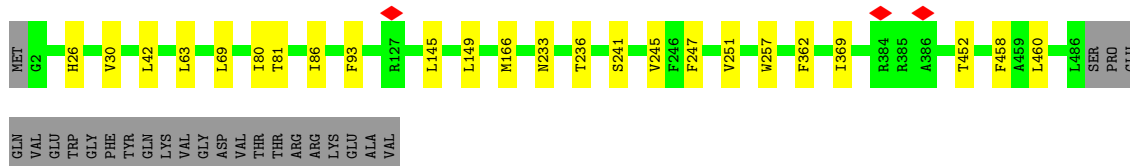
- Molecule 1: Photosystem II protein D1 1

Chain A:  86% 10%

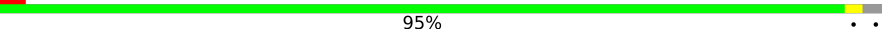


- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  90% 5% 5%



- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  95%



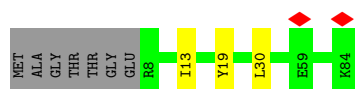
- Molecule 4: Photosystem II D2 protein

Chain D:  91% 5%



- Molecule 5: Cytochrome b559 subunit alpha

Chain E:  88% 8%

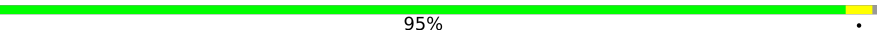


- Molecule 6: Cytochrome b559 subunit beta

Chain F:  11% 80% 16%



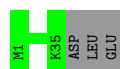
- Molecule 7: Photosystem II reaction center protein H

Chain H:  95%



- Molecule 8: Photosystem II reaction center protein I

Chain I:  92% 8%



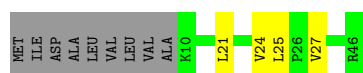
- Molecule 9: Photosystem II reaction center protein J

Chain J:  10% 78% 8% 15%



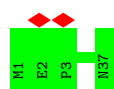
- Molecule 10: Photosystem II reaction center protein K

Chain K:  72% 9% 20%

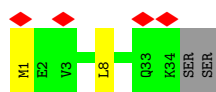
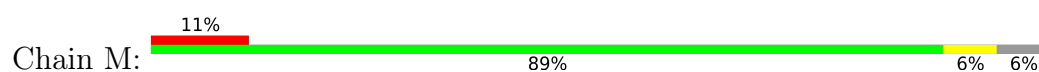


- Molecule 11: Photosystem II reaction center protein L

Chain L:  5% 100%



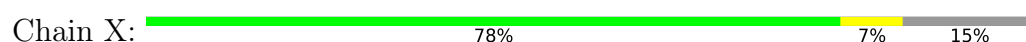
- Molecule 12: Photosystem II reaction center protein M



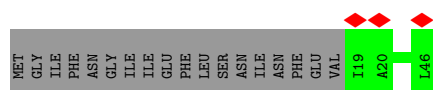
- Molecule 13: Photosystem II reaction center protein T



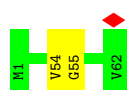
- Molecule 14: Photosystem II reaction center X protein



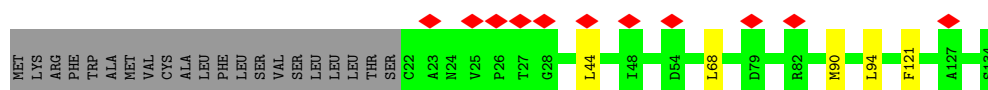
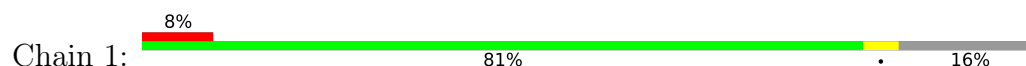
- Molecule 15: Photosystem II reaction center protein Ycf12



- Molecule 16: Photosystem II reaction center protein Z



- Molecule 17: Photosystem II lipoprotein Psb27



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	325601	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 ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.127	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0061	Depositor
Map size (Å)	268.8, 268.8, 268.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	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, MN, PHO, CL, FE, LHG, BCT, BCR, LMG, HEM, PL9

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	0.16	0/2642	0.36	0/3603
2	B	0.15	0/3947	0.35	0/5379
3	C	0.16	0/3579	0.34	0/4872
4	D	0.14	0/2801	0.31	0/3818
5	E	0.15	0/654	0.34	0/891
6	F	0.16	0/317	0.38	0/433
7	H	0.15	0/524	0.39	0/713
8	I	0.20	0/293	0.38	0/395
9	J	0.17	0/255	0.37	0/346
10	K	0.16	0/303	0.35	0/416
11	L	0.17	0/311	0.32	0/422
12	M	0.17	0/270	0.33	0/367
13	T	0.20	0/265	0.34	0/359
14	X	0.15	0/257	0.28	0/348
15	Y	0.16	0/209	0.40	0/279
16	Z	0.18	0/490	0.32	0/669
17	1	0.14	0/907	0.31	0/1220
All	All	0.16	0/18024	0.34	0/24530

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
7	H	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	H	35	MET	Peptide

5.2 Too-close contacts [i](#)

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	2559	0	2459	7	0
2	B	3812	0	3683	13	0
3	C	3466	0	3389	7	0
4	D	2706	0	2608	14	0
5	E	635	0	625	3	0
6	F	307	0	312	1	0
7	H	511	0	532	0	0
8	I	286	0	308	0	0
9	J	249	0	262	2	0
10	K	293	0	305	2	0
11	L	304	0	316	0	0
12	M	267	0	289	0	0
13	T	256	0	262	1	0
14	X	254	0	282	0	0
15	Y	208	0	237	0	0
16	Z	479	0	516	2	0
17	1	893	0	896	2	0
18	A	1	0	0	0	0
19	A	1	0	0	0	0
20	A	1	0	0	0	0
21	A	40	0	56	1	0
21	B	80	0	112	0	0
21	C	120	0	168	7	0
21	D	40	0	56	0	0
21	H	40	0	56	0	0
21	J	80	0	112	3	0
21	M	40	0	56	1	0
22	A	256	0	288	5	0
22	B	1024	0	1152	9	0
22	C	832	0	936	6	0
22	D	128	0	144	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	A	98	0	148	0	0
24	A	64	0	74	0	0
24	D	64	0	74	2	0
25	A	55	0	80	0	0
25	D	55	0	80	0	0
26	A	4	0	1	0	0
27	C	55	0	86	0	0
27	D	165	0	258	1	0
27	I	55	0	86	0	0
27	K	55	0	86	0	0
27	L	55	0	86	0	0
27	M	55	0	86	0	0
28	F	42	0	30	4	0
All	All	20990	0	21592	63	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 1.

All (63) 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)
3:C:104:VAL:HG11	21:C:517:BCR:H323	1.70	0.72
17:1:44:LEU:HD11	17:1:121:PHE:CZ	2.31	0.65
21:C:502:BCR:H403	22:C:503:CLA:HMB2	1.79	0.64
17:1:68:LEU:HD22	17:1:94:LEU:HD22	1.83	0.61
4:D:186:GLN:HB2	22:D:403:CLA:HBC1	1.84	0.58
2:B:149:LEU:HG	22:B:605:CLA:HBC1	1.87	0.57
3:C:147:THR:HG22	3:C:151:PHE:CE2	2.40	0.56
2:B:241:SER:O	2:B:245:VAL:HG23	2.06	0.55
2:B:460:LEU:HD22	4:D:287:VAL:HG21	1.89	0.54
4:D:192:THR:HG23	22:D:403:CLA:HBC2	1.88	0.54
2:B:458:PHE:HB3	22:B:606:CLA:HBC2	1.89	0.53
4:D:90:LEU:O	22:D:404:CLA:HED1	2.07	0.53
3:C:325:LEU:O	3:C:325:LEU:HD13	2.09	0.53
27:D:406:LMG:H241	13:T:13:ILE:HG21	1.91	0.53
5:E:13:ILE:HG21	28:F:101:HEM:HAD1	1.92	0.52
1:A:183:MET:HE1	22:A:406:CLA:HMD2	1.91	0.52
6:F:43:ILE:HD11	9:J:36:LEU:HD11	1.92	0.52
22:B:610:CLA:C4	4:D:127:LEU:HD21	2.40	0.52
21:C:517:BCR:H311	16:Z:55:GLY:HA2	1.92	0.52
1:A:153:SER:HB3	22:A:405:CLA:HED1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:221:THR:HG22	4:D:221:THR:O	2.11	0.51
28:F:101:HEM:HMC2	28:F:101:HEM:HBC2	1.93	0.51
2:B:80:ILE:HD12	2:B:81:THR:N	2.27	0.50
2:B:241:SER:HB3	22:B:614:CLA:HED3	1.94	0.50
10:K:24:VAL:O	10:K:27:VAL:HG12	2.12	0.49
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.94	0.49
2:B:69:LEU:HD21	22:B:605:CLA:OBD	2.13	0.48
1:A:202:VAL:HG23	22:A:405:CLA:HMB3	1.95	0.48
1:A:43:ALA:HB1	21:A:404:BCR:H362	1.95	0.48
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.48	0.47
4:D:197:HIS:O	4:D:201:VAL:HG23	2.15	0.47
5:E:30:LEU:HD11	28:F:101:HEM:HAB	1.97	0.47
2:B:257:TRP:CE3	2:B:452:THR:HG21	2.50	0.47
2:B:233:ASN:O	2:B:236:THR:HG22	2.15	0.46
9:J:14:ALA:O	21:J:101:BCR:H382	2.14	0.46
22:B:616:CLA:H141	21:M:101:BCR:H372	1.97	0.46
5:E:13:ILE:HG22	5:E:19:TYR:CD1	2.51	0.45
22:B:604:CLA:HED3	22:B:604:CLA:O2A	2.16	0.45
22:C:507:CLA:HBC3	22:C:507:CLA:HHD	1.99	0.45
3:C:112:VAL:HB	21:C:517:BCR:H362	1.99	0.45
2:B:26:HIS:O	2:B:30:VAL:HG23	2.16	0.45
22:B:605:CLA:H42	22:B:605:CLA:C4A	2.47	0.45
3:C:265:GLY:C	22:C:507:CLA:HBC2	2.41	0.45
1:A:46:ILE:HG22	1:A:50:ILE:HD12	2.00	0.44
3:C:228:ILE:CD1	21:C:502:BCR:H372	2.48	0.44
22:A:407:CLA:HMA2	24:D:407:PHO:H203	2.01	0.43
21:J:101:BCR:H313	10:K:25:LEU:CD1	2.48	0.43
22:C:503:CLA:HBB1	22:C:503:CLA:HHC	2.01	0.43
2:B:42:LEU:HD21	2:B:93:PHE:CB	2.49	0.42
3:C:216:ASN:HA	3:C:283:THR:HG21	2.02	0.42
2:B:247:PHE:O	2:B:251:VAL:HG23	2.20	0.42
21:C:502:BCR:H343	22:C:507:CLA:HMD2	2.02	0.42
2:B:145:LEU:HD11	22:B:617:CLA:HMB2	2.01	0.42
1:A:123:ALA:HB1	1:A:151:LEU:HD13	2.01	0.42
4:D:201:VAL:HG22	22:D:403:CLA:C1B	2.51	0.41
4:D:209:LEU:HD11	4:D:213:ILE:HD12	2.03	0.41
28:F:101:HEM:HBC2	28:F:101:HEM:CMC	2.51	0.41
1:A:202:VAL:HG23	22:A:405:CLA:CMB	2.51	0.40
22:C:506:CLA:H42	21:J:102:BCR:H381	2.02	0.40
4:D:80:THR:HG22	4:D:111:TRP:CE2	2.56	0.40
4:D:259:ILE:O	4:D:259:ILE:HD12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:C:517:BCR:H313	16:Z:54:VAL:HG12	2.03	0.40
4:D:48:TRP:CG	24:D:407:PHO:H143	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	324/360 (90%)	304 (94%)	20 (6%)	0	100	100
2	B	483/510 (95%)	470 (97%)	13 (3%)	0	100	100
3	C	446/461 (97%)	428 (96%)	18 (4%)	0	100	100
4	D	338/352 (96%)	330 (98%)	8 (2%)	0	100	100
5	E	75/84 (89%)	72 (96%)	3 (4%)	0	100	100
6	F	36/45 (80%)	32 (89%)	3 (8%)	1 (3%)	4	14
7	H	63/66 (96%)	58 (92%)	4 (6%)	1 (2%)	7	27
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
9	J	32/40 (80%)	31 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
13	T	28/32 (88%)	28 (100%)	0	0	100	100
14	X	33/41 (80%)	32 (97%)	1 (3%)	0	100	100
15	Y	26/46 (56%)	23 (88%)	3 (12%)	0	100	100
16	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
17	1	111/134 (83%)	110 (99%)	1 (1%)	0	100	100
All	All	2190/2390 (92%)	2109 (96%)	79 (4%)	2 (0%)	49	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	H	36	GLY
6	F	9	GLU

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	264/291 (91%)	257 (97%)	7 (3%)	39	74
2	B	385/407 (95%)	380 (99%)	5 (1%)	61	86
3	C	350/362 (97%)	348 (99%)	2 (1%)	78	92
4	D	275/283 (97%)	273 (99%)	2 (1%)	76	91
5	E	69/73 (94%)	69 (100%)	0	100	100
6	F	32/39 (82%)	32 (100%)	0	100	100
7	H	54/55 (98%)	54 (100%)	0	100	100
8	I	32/35 (91%)	32 (100%)	0	100	100
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	61
10	K	30/37 (81%)	29 (97%)	1 (3%)	33	69
11	L	35/35 (100%)	35 (100%)	0	100	100
12	M	31/33 (94%)	29 (94%)	2 (6%)	15	43
13	T	27/29 (93%)	27 (100%)	0	100	100
14	X	28/34 (82%)	25 (89%)	3 (11%)	6	21
15	Y	21/37 (57%)	21 (100%)	0	100	100
16	Z	52/52 (100%)	52 (100%)	0	100	100
17	1	96/115 (84%)	95 (99%)	1 (1%)	68	88
All	All	1805/1945 (93%)	1781 (99%)	24 (1%)	59	86

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	30	VAL
1	A	241	GLN
1	A	286	THR
1	A	331	MET
1	A	333	GLU
1	A	334	ARG
2	B	63	LEU
2	B	86	ILE
2	B	166	MET
2	B	362	PHE
2	B	369	ILE
3	C	277	PHE
3	C	382	GLU
4	D	90	LEU
4	D	243	THR
9	J	30	TYR
10	K	21	LEU
12	M	1	MET
12	M	8	LEU
14	X	3	ILE
14	X	21	LEU
14	X	23	LEU
17	1	90	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	58	GLN
2	B	100	HIS
2	B	274	GLN
2	B	338	GLN
2	B	395	GLN
3	C	370	ASN
3	C	373	GLN
4	D	186	GLN
4	D	224	GLN
4	D	322	ASN
11	L	6	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 65 ligands modelled in this entry, 3 are monoatomic - leaving 62 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	$\# Z > 2$
22	CLA	B	612	-	58,69,73	2.25	10 (17%)	56,99,113	1.41	8 (14%)
22	CLA	B	618	-	58,69,73	2.27	11 (18%)	56,99,113	1.31	8 (14%)
22	CLA	B	611	-	58,69,73	2.25	10 (17%)	56,99,113	1.34	9 (16%)
21	BCR	M	101	-	41,41,41	0.40	0	56,56,56	0.63	0
22	CLA	C	504	-	58,69,73	2.21	11 (18%)	56,99,113	1.56	10 (17%)
21	BCR	J	102	-	41,41,41	0.36	0	56,56,56	0.69	0
22	CLA	C	512	-	58,69,73	2.24	11 (18%)	56,99,113	1.41	8 (14%)
23	LHG	A	409	-	48,48,48	0.51	0	51,54,54	0.53	1 (1%)
22	CLA	B	610	-	58,69,73	2.22	12 (20%)	56,99,113	1.48	9 (16%)
22	CLA	B	614	-	58,69,73	2.24	10 (17%)	56,99,113	1.46	11 (19%)
27	LMG	D	405	-	55,55,55	0.46	0	63,63,63	0.66	1 (1%)
25	PL9	D	408	-	55,55,55	0.96	3 (5%)	68,69,69	1.50	10 (14%)
22	CLA	B	604	-	58,69,73	2.26	11 (18%)	56,99,113	1.49	8 (14%)
22	CLA	A	408	-	58,69,73	2.21	11 (18%)	56,99,113	1.43	9 (16%)
21	BCR	B	601	-	41,41,41	0.35	0	56,56,56	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	608	-	58,69,73	2.24	11 (18%)	56,99,113	1.37	9 (16%)
22	CLA	C	509	-	58,69,73	2.24	12 (20%)	56,99,113	1.50	8 (14%)
22	CLA	D	403	-	58,69,73	2.25	10 (17%)	56,99,113	1.45	9 (16%)
21	BCR	J	101	-	41,41,41	0.36	0	56,56,56	0.77	1 (1%)
22	CLA	C	508	-	58,69,73	2.24	12 (20%)	56,99,113	1.39	8 (14%)
27	LMG	I	101	-	55,55,55	0.48	0	63,63,63	0.56	0
21	BCR	H	101	-	41,41,41	0.38	0	56,56,56	1.09	4 (7%)
24	PHO	D	407	-	58,69,69	2.09	9 (15%)	56,99,99	1.67	7 (12%)
22	CLA	B	606	-	58,69,73	2.24	9 (15%)	56,99,113	1.32	9 (16%)
27	LMG	D	401	-	55,55,55	0.47	0	63,63,63	0.62	1 (1%)
27	LMG	L	101	-	55,55,55	0.49	0	63,63,63	0.58	0
22	CLA	B	617	-	58,69,73	2.25	10 (17%)	56,99,113	1.41	8 (14%)
21	BCR	C	501	-	41,41,41	0.36	0	56,56,56	0.67	0
25	PL9	A	411	-	55,55,55	0.90	3 (5%)	68,69,69	1.44	11 (16%)
21	BCR	C	502	-	41,41,41	0.36	0	56,56,56	0.76	2 (3%)
22	CLA	C	507	-	58,69,73	2.24	11 (18%)	56,99,113	1.50	8 (14%)
21	BCR	D	402	-	41,41,41	0.34	0	56,56,56	0.61	0
22	CLA	B	609	-	58,69,73	2.24	11 (18%)	56,99,113	1.63	11 (19%)
23	LHG	A	412	-	48,48,48	0.52	0	51,54,54	0.49	0
22	CLA	B	615	-	58,69,73	2.26	12 (20%)	56,99,113	1.33	6 (10%)
22	CLA	C	503	-	58,69,73	2.32	9 (15%)	56,99,113	1.31	8 (14%)
24	PHO	A	410	-	58,69,69	2.08	10 (17%)	56,99,99	1.63	7 (12%)
22	CLA	A	405	-	58,69,73	2.29	12 (20%)	56,99,113	1.30	7 (12%)
22	CLA	B	607	-	58,69,73	2.23	10 (17%)	56,99,113	1.42	10 (17%)
22	CLA	A	406	-	58,69,73	2.26	13 (22%)	56,99,113	1.70	9 (16%)
22	CLA	C	516	-	58,69,73	2.26	11 (18%)	56,99,113	1.39	9 (16%)
22	CLA	C	514	-	58,69,73	2.26	12 (20%)	56,99,113	1.49	8 (14%)
21	BCR	B	602	-	41,41,41	0.35	0	56,56,56	0.74	0
22	CLA	B	616	-	58,69,73	2.23	11 (18%)	56,99,113	1.39	8 (14%)
22	CLA	B	603	-	58,69,73	2.27	12 (20%)	56,99,113	1.51	8 (14%)
22	CLA	C	506	-	58,69,73	2.28	12 (20%)	56,99,113	1.49	8 (14%)
26	BCT	A	413	18	2,3,3	0.88	0	2,3,3	3.19	2 (100%)
22	CLA	D	404	-	58,69,73	2.26	10 (17%)	56,99,113	1.40	8 (14%)
28	HEM	F	101	-	35,46,50	2.23	11 (31%)	28,68,82	1.26	3 (10%)
22	CLA	C	505	-	58,69,73	2.26	12 (20%)	56,99,113	1.48	7 (12%)
22	CLA	B	613	-	58,69,73	2.28	12 (20%)	56,99,113	1.51	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	C	513	-	58,69,73	2.23	10 (17%)	56,99,113	1.39	7 (12%)
27	LMG	D	406	-	55,55,55	0.48	0	63,63,63	0.79	3 (4%)
27	LMG	K	101	-	55,55,55	0.48	0	63,63,63	0.62	0
22	CLA	A	407	-	58,69,73	2.23	11 (18%)	56,99,113	1.38	8 (14%)
27	LMG	M	102	-	55,55,55	0.46	0	63,63,63	0.67	0
22	CLA	B	605	-	58,69,73	2.24	10 (17%)	56,99,113	1.59	12 (21%)
22	CLA	C	510	-	58,69,73	2.25	11 (18%)	56,99,113	1.56	10 (17%)
22	CLA	C	511	-	58,69,73	2.26	12 (20%)	56,99,113	1.39	7 (12%)
21	BCR	A	404	-	41,41,41	0.32	0	56,56,56	0.54	0
27	LMG	C	515	-	55,55,55	0.46	0	63,63,63	0.63	1 (1%)
21	BCR	C	517	-	41,41,41	0.41	0	56,56,56	0.64	1 (1%)

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
22	CLA	B	612	-	-	19/37/87/115	0/5/5/9
22	CLA	B	618	-	-	15/37/87/115	0/5/5/9
22	CLA	B	611	-	-	12/37/87/115	0/5/5/9
21	BCR	M	101	-	-	7/29/63/63	0/2/2/2
22	CLA	C	504	-	-	19/37/87/115	0/5/5/9
21	BCR	J	102	-	-	9/29/63/63	0/2/2/2
22	CLA	C	512	-	-	12/37/87/115	0/5/5/9
23	LHG	A	409	-	-	17/53/53/53	-
22	CLA	B	610	-	-	12/37/87/115	0/5/5/9
22	CLA	B	614	-	-	11/37/87/115	0/5/5/9
27	LMG	D	405	-	-	11/50/70/70	0/1/1/1
25	PL9	D	408	-	-	11/53/73/73	0/1/1/1
22	CLA	B	604	-	-	13/37/87/115	0/5/5/9
22	CLA	A	408	-	-	11/37/87/115	0/5/5/9
21	BCR	B	601	-	-	7/29/63/63	0/2/2/2
22	CLA	B	608	-	-	9/37/87/115	0/5/5/9
22	CLA	C	509	-	-	6/37/87/115	0/5/5/9
22	CLA	D	403	-	-	13/37/87/115	0/5/5/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	J	101	-	-	6/29/63/63	0/2/2/2
22	CLA	C	508	-	-	11/37/87/115	0/5/5/9
27	LMG	I	101	-	-	8/50/70/70	0/1/1/1
21	BCR	H	101	-	-	15/29/63/63	0/2/2/2
24	PHO	D	407	-	-	7/37/103/103	0/5/6/6
22	CLA	B	606	-	-	6/37/87/115	0/5/5/9
27	LMG	D	401	-	-	10/50/70/70	0/1/1/1
27	LMG	L	101	-	-	14/50/70/70	0/1/1/1
22	CLA	B	617	-	-	9/37/87/115	0/5/5/9
21	BCR	C	501	-	-	8/29/63/63	0/2/2/2
25	PL9	A	411	-	-	17/53/73/73	0/1/1/1
21	BCR	C	502	-	-	7/29/63/63	0/2/2/2
22	CLA	C	507	-	-	16/37/87/115	0/5/5/9
21	BCR	D	402	-	-	11/29/63/63	0/2/2/2
22	CLA	B	609	-	-	11/37/87/115	0/5/5/9
23	LHG	A	412	-	-	14/53/53/53	-
22	CLA	B	615	-	-	6/37/87/115	0/5/5/9
22	CLA	C	503	-	-	11/37/87/115	0/5/5/9
24	PHO	A	410	-	-	10/37/103/103	0/5/6/6
22	CLA	A	405	-	-	11/37/87/115	0/5/5/9
22	CLA	B	607	-	-	15/37/87/115	0/5/5/9
22	CLA	A	406	-	-	11/37/87/115	0/5/5/9
22	CLA	C	516	-	-	9/37/87/115	0/5/5/9
22	CLA	C	514	-	-	9/37/87/115	0/5/5/9
21	BCR	B	602	-	-	14/29/63/63	0/2/2/2
22	CLA	B	616	-	-	11/37/87/115	0/5/5/9
22	CLA	B	603	-	-	8/37/87/115	0/5/5/9
22	CLA	C	506	-	-	7/37/87/115	0/5/5/9
22	CLA	D	404	-	-	9/37/87/115	0/5/5/9
28	HEM	F	101	-	-	4/12/30/54	0/4/4/8
22	CLA	C	505	-	-	12/37/87/115	0/5/5/9
22	CLA	B	613	-	-	13/37/87/115	0/5/5/9
22	CLA	C	513	-	-	4/37/87/115	0/5/5/9
27	LMG	D	406	-	-	11/50/70/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	K	101	-	-	12/50/70/70	0/1/1/1
22	CLA	A	407	-	-	9/37/87/115	0/5/5/9
27	LMG	M	102	-	-	14/50/70/70	0/1/1/1
22	CLA	B	605	-	-	11/37/87/115	0/5/5/9
22	CLA	C	510	-	-	11/37/87/115	0/5/5/9
22	CLA	C	511	-	-	11/37/87/115	0/5/5/9
21	BCR	A	404	-	-	8/29/63/63	0/2/2/2
27	LMG	C	515	-	-	13/50/70/70	0/1/1/1
21	BCR	C	517	-	-	6/29/63/63	0/2/2/2

All (421) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	407	PHO	C1B-C2B	9.60	1.50	1.39
24	A	410	PHO	C1B-C2B	9.50	1.50	1.39
22	B	605	CLA	C1B-C2B	9.36	1.50	1.39
22	C	506	CLA	C1B-C2B	9.35	1.49	1.39
22	C	516	CLA	C1B-C2B	9.28	1.49	1.39
22	B	618	CLA	C1B-C2B	9.28	1.49	1.39
22	B	614	CLA	C1B-C2B	9.27	1.49	1.39
22	C	503	CLA	C1B-C2B	9.26	1.49	1.39
22	C	511	CLA	C1B-C2B	9.18	1.49	1.39
22	B	616	CLA	C1B-C2B	9.18	1.49	1.39
22	D	404	CLA	C1B-C2B	9.12	1.49	1.39
22	B	611	CLA	C1B-C2B	9.12	1.49	1.39
22	A	405	CLA	C1B-C2B	9.11	1.49	1.39
22	B	617	CLA	C1B-C2B	9.09	1.49	1.39
22	A	406	CLA	C1B-C2B	9.08	1.49	1.39
22	C	504	CLA	C1B-C2B	9.05	1.49	1.39
22	B	604	CLA	C1B-C2B	9.03	1.49	1.39
22	B	607	CLA	C1B-C2B	9.03	1.49	1.39
22	B	608	CLA	C1B-C2B	9.03	1.49	1.39
22	B	609	CLA	C1B-C2B	9.02	1.49	1.39
22	B	615	CLA	C1B-C2B	9.02	1.49	1.39
22	B	603	CLA	C1B-C2B	9.01	1.49	1.39
22	C	513	CLA	C1B-C2B	8.95	1.49	1.39
22	C	505	CLA	C1B-C2B	8.94	1.49	1.39
22	A	408	CLA	C1B-C2B	8.91	1.49	1.39
22	A	407	CLA	C1B-C2B	8.89	1.49	1.39
22	B	606	CLA	C1B-C2B	8.84	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	403	CLA	C1B-C2B	8.81	1.49	1.39
22	C	508	CLA	C1B-C2B	8.76	1.49	1.39
22	C	512	CLA	C1B-C2B	8.75	1.49	1.39
22	B	610	CLA	C1B-C2B	8.74	1.49	1.39
22	C	507	CLA	C1B-C2B	8.74	1.49	1.39
22	B	612	CLA	C1B-C2B	8.73	1.49	1.39
22	B	613	CLA	C1B-C2B	8.69	1.49	1.39
22	C	514	CLA	C1B-C2B	8.49	1.49	1.39
22	C	510	CLA	C1B-C2B	8.45	1.48	1.39
22	C	503	CLA	C3B-C4B	8.45	1.51	1.41
22	C	509	CLA	C1B-C2B	8.23	1.48	1.39
22	D	404	CLA	C1D-C2D	8.21	1.48	1.39
22	C	512	CLA	C1D-C2D	8.18	1.48	1.39
22	A	405	CLA	C1D-C2D	8.14	1.48	1.39
22	A	407	CLA	C1D-C2D	8.13	1.48	1.39
22	B	608	CLA	C1D-C2D	8.12	1.48	1.39
22	A	408	CLA	C1D-C2D	8.03	1.48	1.39
22	A	406	CLA	C1D-C2D	8.01	1.48	1.39
22	C	503	CLA	C1D-C2D	8.00	1.48	1.39
22	C	514	CLA	C3B-C4B	8.00	1.50	1.41
22	B	606	CLA	C1D-C2D	7.99	1.48	1.39
22	B	613	CLA	C1D-C2D	7.98	1.48	1.39
22	B	609	CLA	C1D-C2D	7.97	1.48	1.39
22	B	607	CLA	C1D-C2D	7.97	1.48	1.39
22	B	618	CLA	C1D-C2D	7.96	1.48	1.39
22	C	508	CLA	C1D-C2D	7.90	1.48	1.39
24	A	410	PHO	C3B-C4B	7.89	1.50	1.41
22	C	516	CLA	C1D-C2D	7.87	1.48	1.39
22	B	612	CLA	C1D-C2D	7.86	1.48	1.39
22	B	617	CLA	C1D-C2D	7.86	1.48	1.39
22	C	507	CLA	C1D-C2D	7.86	1.48	1.39
22	B	616	CLA	C1D-C2D	7.84	1.48	1.39
22	B	611	CLA	C1D-C2D	7.84	1.48	1.39
22	B	604	CLA	C1D-C2D	7.84	1.48	1.39
22	C	510	CLA	C3B-C4B	7.83	1.50	1.41
22	C	511	CLA	C1D-C2D	7.81	1.48	1.39
22	C	509	CLA	C1D-C2D	7.81	1.48	1.39
22	C	513	CLA	C1D-C2D	7.80	1.48	1.39
24	D	407	PHO	C3B-C4B	7.80	1.50	1.41
22	C	509	CLA	C3B-C4B	7.78	1.50	1.41
22	C	514	CLA	C1D-C2D	7.78	1.48	1.39
22	C	506	CLA	C1D-C2D	7.76	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	403	CLA	C1D-C2D	7.73	1.48	1.39
22	D	403	CLA	C3B-C4B	7.71	1.50	1.41
22	B	613	CLA	C3B-C4B	7.70	1.50	1.41
22	B	614	CLA	C1D-C2D	7.69	1.48	1.39
22	B	615	CLA	C1D-C2D	7.68	1.48	1.39
22	C	505	CLA	C1D-C2D	7.63	1.48	1.39
22	B	610	CLA	C1D-C2D	7.62	1.48	1.39
22	C	510	CLA	C1D-C2D	7.60	1.48	1.39
22	B	615	CLA	C3B-C4B	7.59	1.50	1.41
22	A	405	CLA	C3B-C4B	7.58	1.50	1.41
22	B	612	CLA	C3B-C4B	7.58	1.50	1.41
22	B	603	CLA	C1D-C2D	7.53	1.47	1.39
22	B	605	CLA	C1D-C2D	7.52	1.47	1.39
22	C	507	CLA	C3B-C4B	7.37	1.49	1.41
22	B	604	CLA	C3B-C4B	7.28	1.49	1.41
22	B	603	CLA	C3B-C4B	7.28	1.49	1.41
22	C	504	CLA	C1D-C2D	7.28	1.47	1.39
22	C	508	CLA	C3B-C4B	7.21	1.49	1.41
22	B	606	CLA	C3B-C4B	7.17	1.49	1.41
22	A	407	CLA	C3B-C4B	7.14	1.49	1.41
22	C	512	CLA	C3B-C4B	7.14	1.49	1.41
22	B	617	CLA	C3B-C4B	7.12	1.49	1.41
22	B	611	CLA	C3B-C4B	7.12	1.49	1.41
22	C	505	CLA	C3B-C4B	7.12	1.49	1.41
22	B	610	CLA	C3B-C4B	7.06	1.49	1.41
22	B	618	CLA	C3B-C4B	7.01	1.49	1.41
22	C	511	CLA	C3B-C4B	7.00	1.49	1.41
22	B	607	CLA	C3B-C4B	6.97	1.49	1.41
22	C	513	CLA	C3B-C4B	6.96	1.49	1.41
22	C	506	CLA	C3B-C4B	6.94	1.49	1.41
22	C	516	CLA	C3B-C4B	6.90	1.49	1.41
22	D	404	CLA	C3B-C4B	6.88	1.49	1.41
22	B	616	CLA	C3B-C4B	6.87	1.49	1.41
22	B	614	CLA	C3B-C4B	6.84	1.49	1.41
22	B	608	CLA	C3B-C4B	6.84	1.49	1.41
22	B	609	CLA	C3B-C4B	6.80	1.49	1.41
22	B	605	CLA	C3B-C4B	6.77	1.49	1.41
22	A	408	CLA	C3B-C4B	6.70	1.49	1.41
22	A	406	CLA	C3B-C4B	6.68	1.49	1.41
22	C	504	CLA	C3B-C4B	6.62	1.49	1.41
28	F	101	HEM	C1A-C2A	5.64	1.45	1.39
28	F	101	HEM	C1C-C2C	5.23	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	F	101	HEM	C4A-C3A	4.98	1.45	1.39
22	B	603	CLA	C3D-C4D	4.89	1.48	1.41
22	C	506	CLA	C3D-C4D	4.81	1.48	1.41
22	C	516	CLA	C3D-C4D	4.74	1.48	1.41
22	C	514	CLA	C3D-C4D	4.73	1.48	1.41
22	C	513	CLA	C3D-C4D	4.72	1.48	1.41
22	C	505	CLA	C3D-C4D	4.72	1.48	1.41
22	B	604	CLA	C3D-C4D	4.70	1.48	1.41
22	A	406	CLA	C3D-C4D	4.69	1.48	1.41
22	B	606	CLA	C3D-C4D	4.69	1.48	1.41
22	B	609	CLA	C3D-C4D	4.68	1.48	1.41
22	B	618	CLA	C3D-C4D	4.67	1.48	1.41
22	C	510	CLA	C3D-C4D	4.66	1.48	1.41
22	B	617	CLA	C3D-C4D	4.66	1.48	1.41
22	B	612	CLA	C3D-C4D	4.65	1.48	1.41
22	D	403	CLA	C3D-C4D	4.64	1.48	1.41
22	C	504	CLA	C3D-C4D	4.64	1.48	1.41
22	C	511	CLA	C3D-C4D	4.64	1.48	1.41
22	C	508	CLA	C3D-C4D	4.64	1.48	1.41
22	B	605	CLA	C3D-C4D	4.62	1.48	1.41
22	B	611	CLA	C3D-C4D	4.62	1.48	1.41
22	B	608	CLA	C3D-C4D	4.61	1.48	1.41
22	B	614	CLA	C3D-C4D	4.60	1.48	1.41
22	C	509	CLA	C3D-C4D	4.60	1.48	1.41
22	A	405	CLA	C3D-C4D	4.59	1.48	1.41
22	B	613	CLA	C3D-C4D	4.59	1.48	1.41
22	A	408	CLA	C3D-C4D	4.58	1.47	1.41
22	B	607	CLA	C3D-C4D	4.56	1.47	1.41
22	B	610	CLA	C3D-C4D	4.54	1.47	1.41
22	C	512	CLA	C3D-C4D	4.52	1.47	1.41
22	D	404	CLA	C3D-C4D	4.52	1.47	1.41
22	A	407	CLA	C3D-C4D	4.51	1.47	1.41
22	C	503	CLA	C3D-C4D	4.51	1.47	1.41
22	B	616	CLA	C3D-C4D	4.49	1.47	1.41
22	B	615	CLA	C3D-C4D	4.48	1.47	1.41
24	D	407	PHO	C1D-C2D	4.46	1.44	1.39
22	C	507	CLA	C3D-C4D	4.45	1.47	1.41
24	A	410	PHO	C1D-C2D	4.31	1.44	1.39
28	F	101	HEM	C3C-C2C	-3.84	1.35	1.40
28	F	101	HEM	C3C-CAC	3.73	1.55	1.47
22	D	404	CLA	C4D-ND	-3.72	1.33	1.38
22	B	607	CLA	C4D-ND	-3.64	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	516	CLA	C4D-ND	-3.63	1.33	1.38
22	B	612	CLA	C4D-ND	-3.62	1.33	1.38
22	B	618	CLA	C4D-ND	-3.62	1.33	1.38
22	C	503	CLA	C4D-ND	-3.62	1.33	1.38
22	B	613	CLA	C4D-ND	-3.61	1.33	1.38
22	A	408	CLA	C4D-ND	-3.60	1.33	1.38
22	B	608	CLA	C4D-ND	-3.59	1.33	1.38
22	B	614	CLA	C4D-ND	-3.59	1.33	1.38
22	B	616	CLA	C4D-ND	-3.59	1.33	1.38
22	B	615	CLA	C4D-ND	-3.58	1.33	1.38
22	C	504	CLA	C4D-ND	-3.58	1.33	1.38
22	D	403	CLA	C4D-ND	-3.58	1.33	1.38
22	B	605	CLA	C4D-ND	-3.57	1.33	1.38
22	A	407	CLA	C4D-ND	-3.55	1.33	1.38
22	B	611	CLA	C4D-ND	-3.54	1.33	1.38
22	C	505	CLA	C4D-ND	-3.54	1.33	1.38
22	B	609	CLA	C4D-ND	-3.52	1.33	1.38
24	D	407	PHO	C4D-CHA	3.51	1.45	1.39
22	C	511	CLA	C4D-ND	-3.51	1.33	1.38
22	B	604	CLA	C4D-ND	-3.51	1.33	1.38
22	C	508	CLA	C4D-ND	-3.50	1.33	1.38
22	C	512	CLA	C4D-ND	-3.49	1.33	1.38
22	C	510	CLA	C4D-ND	-3.48	1.33	1.38
22	C	513	CLA	C4D-ND	-3.47	1.33	1.38
22	C	509	CLA	C4D-ND	-3.45	1.33	1.38
22	A	405	CLA	C4D-ND	-3.44	1.33	1.38
22	B	606	CLA	C4D-ND	-3.42	1.33	1.38
22	B	610	CLA	C4D-ND	-3.42	1.33	1.38
22	B	617	CLA	C4D-ND	-3.41	1.33	1.38
22	C	507	CLA	C4D-ND	-3.37	1.33	1.38
24	A	410	PHO	C4D-CHA	3.34	1.44	1.39
22	C	506	CLA	C4D-ND	-3.32	1.33	1.38
22	C	514	CLA	C4D-ND	-3.32	1.33	1.38
28	F	101	HEM	C3C-C4C	3.31	1.45	1.41
22	B	603	CLA	C4D-ND	-3.30	1.34	1.38
22	A	406	CLA	C4D-ND	-3.28	1.34	1.38
25	D	408	PL9	C7-C3	-3.27	1.48	1.51
22	B	603	CLA	C4D-CHA	2.99	1.44	1.39
22	A	406	CLA	C4D-CHA	2.97	1.44	1.39
28	F	101	HEM	CAB-C3B	2.97	1.55	1.47
25	D	408	PL9	C3-C4	-2.90	1.44	1.49
22	C	514	CLA	C4D-CHA	2.86	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	506	CLA	C4D-CHA	2.85	1.44	1.39
22	C	505	CLA	C4D-CHA	2.85	1.44	1.39
28	F	101	HEM	CMB-C2B	2.77	1.55	1.50
22	C	507	CLA	CMD-C2D	-2.76	1.45	1.51
22	C	510	CLA	C4D-CHA	2.76	1.44	1.39
22	B	604	CLA	C4D-CHA	2.73	1.44	1.39
22	C	509	CLA	C4D-CHA	2.73	1.43	1.39
22	B	615	CLA	C4D-CHA	2.72	1.43	1.39
28	F	101	HEM	CMD-C2D	2.71	1.55	1.50
22	C	513	CLA	C4D-CHA	2.71	1.43	1.39
22	C	504	CLA	CMD-C2D	-2.71	1.46	1.51
22	B	610	CLA	C4D-CHA	2.70	1.43	1.39
22	C	512	CLA	C4D-CHA	2.70	1.43	1.39
22	C	506	CLA	C1A-C2A	2.68	1.55	1.51
22	B	617	CLA	C4D-CHA	2.68	1.43	1.39
22	C	511	CLA	C4D-CHA	2.67	1.43	1.39
22	B	605	CLA	CMD-C2D	-2.67	1.46	1.51
22	B	609	CLA	C4D-CHA	2.61	1.43	1.39
22	B	603	CLA	C1A-C2A	2.61	1.54	1.51
22	C	505	CLA	C1A-C2A	2.61	1.54	1.51
22	C	503	CLA	CMD-C2D	-2.60	1.46	1.51
22	B	616	CLA	C4D-CHA	2.60	1.43	1.39
22	A	406	CLA	C1A-C2A	2.59	1.54	1.51
22	C	508	CLA	C4D-CHA	2.59	1.43	1.39
22	A	407	CLA	CMD-C2D	-2.58	1.46	1.51
22	B	614	CLA	CMD-C2D	-2.57	1.46	1.51
22	D	403	CLA	CMD-C2D	-2.57	1.46	1.51
22	C	507	CLA	C4D-CHA	2.56	1.43	1.39
22	C	508	CLA	CMB-C2B	-2.56	1.46	1.51
22	C	504	CLA	CMB-C2B	-2.55	1.46	1.51
25	A	411	PL9	C3-C4	-2.55	1.45	1.49
22	B	611	CLA	C4D-CHA	2.55	1.43	1.39
22	B	605	CLA	CAC-C3C	-2.55	1.47	1.51
22	C	516	CLA	C4D-CHA	2.55	1.43	1.39
22	B	614	CLA	C4D-CHA	2.55	1.43	1.39
22	B	606	CLA	C4D-CHA	2.55	1.43	1.39
22	B	612	CLA	C4D-CHA	2.54	1.43	1.39
22	B	618	CLA	CMC-C2C	-2.53	1.46	1.50
22	D	404	CLA	CMD-C2D	-2.53	1.46	1.51
22	A	406	CLA	CMD-C2D	-2.51	1.46	1.51
22	C	509	CLA	CMD-C2D	-2.48	1.46	1.51
22	B	618	CLA	CMD-C2D	-2.48	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	405	CLA	C4D-CHA	2.48	1.43	1.39
22	B	617	CLA	CMD-C2D	-2.47	1.46	1.51
22	A	408	CLA	CMD-C2D	-2.47	1.46	1.51
22	B	606	CLA	CMD-C2D	-2.47	1.46	1.51
22	A	405	CLA	CMD-C2D	-2.47	1.46	1.51
22	B	612	CLA	CMD-C2D	-2.47	1.46	1.51
22	B	610	CLA	CMB-C2B	-2.47	1.46	1.51
22	B	607	CLA	CMD-C2D	-2.47	1.46	1.51
22	B	618	CLA	C4D-CHA	2.47	1.43	1.39
24	A	410	PHO	CMD-C2D	-2.47	1.46	1.51
22	B	616	CLA	CMD-C2D	-2.46	1.46	1.51
24	D	407	PHO	C4D-ND	-2.46	1.35	1.38
22	A	406	CLA	CMB-C2B	-2.46	1.46	1.51
22	C	511	CLA	CMD-C2D	-2.46	1.46	1.51
22	B	613	CLA	CMB-C2B	-2.45	1.46	1.51
22	B	610	CLA	CMD-C2D	-2.45	1.46	1.51
22	B	615	CLA	CMD-C2D	-2.45	1.46	1.51
22	C	508	CLA	CMD-C2D	-2.45	1.46	1.51
22	A	407	CLA	C4D-CHA	2.45	1.43	1.39
22	C	516	CLA	CMD-C2D	-2.45	1.46	1.51
22	A	408	CLA	C4D-CHA	2.45	1.43	1.39
22	C	512	CLA	CMD-C2D	-2.44	1.46	1.51
24	A	410	PHO	C4D-ND	-2.44	1.35	1.38
22	B	609	CLA	CMD-C2D	-2.44	1.46	1.51
22	C	507	CLA	CMB-C2B	-2.44	1.46	1.51
22	D	403	CLA	C4D-CHA	2.43	1.43	1.39
22	C	505	CLA	CMD-C2D	-2.43	1.46	1.51
22	B	614	CLA	CMB-C2B	-2.43	1.46	1.51
22	B	604	CLA	CMD-C2D	-2.43	1.46	1.51
22	C	514	CLA	CMD-C2D	-2.43	1.46	1.51
22	C	504	CLA	C4D-CHA	2.42	1.43	1.39
22	C	506	CLA	CMD-C2D	-2.42	1.46	1.51
22	C	516	CLA	CMB-C2B	-2.42	1.46	1.51
22	B	606	CLA	CMB-C2B	-2.42	1.46	1.51
22	C	513	CLA	CMD-C2D	-2.42	1.46	1.51
22	C	503	CLA	CAC-C3C	-2.42	1.47	1.51
22	C	513	CLA	CMB-C2B	-2.41	1.46	1.51
22	C	510	CLA	CMB-C2B	-2.41	1.46	1.51
22	C	503	CLA	CMC-C2C	-2.41	1.46	1.50
22	C	504	CLA	CMC-C2C	-2.41	1.46	1.50
22	B	608	CLA	CMB-C2B	-2.41	1.46	1.51
22	B	613	CLA	CMD-C2D	-2.40	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	603	CLA	CMD-C2D	-2.40	1.46	1.51
22	C	505	CLA	CMB-C2B	-2.40	1.46	1.51
22	B	608	CLA	CMD-C2D	-2.40	1.46	1.51
22	C	511	CLA	CMB-C2B	-2.40	1.46	1.51
22	B	611	CLA	CMB-C2B	-2.40	1.46	1.51
22	B	605	CLA	CMB-C2B	-2.40	1.46	1.51
22	B	611	CLA	CMD-C2D	-2.40	1.46	1.51
22	C	510	CLA	CMD-C2D	-2.39	1.46	1.51
22	B	608	CLA	C4D-CHA	2.38	1.43	1.39
22	C	516	CLA	CAC-C3C	-2.38	1.47	1.51
22	C	512	CLA	CMB-C2B	-2.37	1.46	1.51
22	B	607	CLA	CMB-C2B	-2.37	1.46	1.51
22	C	510	CLA	CMC-C2C	-2.37	1.46	1.50
22	B	612	CLA	CMB-C2B	-2.37	1.46	1.51
24	A	410	PHO	CMB-C2B	-2.37	1.46	1.51
22	B	605	CLA	CMC-C2C	-2.37	1.46	1.50
22	B	613	CLA	CAC-C3C	-2.37	1.47	1.51
22	C	506	CLA	CMB-C2B	-2.36	1.46	1.51
22	C	505	CLA	CMC-C2C	-2.36	1.46	1.50
22	B	609	CLA	CMB-C2B	-2.35	1.46	1.51
24	D	407	PHO	CMD-C2D	-2.35	1.46	1.51
22	A	408	CLA	CMB-C2B	-2.35	1.46	1.51
22	C	506	CLA	CMC-C2C	-2.35	1.46	1.50
22	B	618	CLA	CMB-C2B	-2.35	1.46	1.51
22	B	606	CLA	CMC-C2C	-2.35	1.46	1.50
22	C	516	CLA	CMC-C2C	-2.34	1.46	1.50
22	B	616	CLA	CMB-C2B	-2.34	1.46	1.51
22	B	605	CLA	C4D-CHA	2.34	1.43	1.39
22	D	404	CLA	CMB-C2B	-2.34	1.46	1.51
22	D	404	CLA	CMC-C2C	-2.34	1.46	1.50
22	C	514	CLA	CMB-C2B	-2.34	1.46	1.51
22	D	403	CLA	CMB-C2B	-2.33	1.46	1.51
22	A	405	CLA	CMB-C2B	-2.33	1.46	1.51
22	B	607	CLA	CAC-C3C	-2.33	1.47	1.51
22	C	508	CLA	CMC-C2C	-2.33	1.46	1.50
22	C	509	CLA	CMB-C2B	-2.31	1.46	1.51
22	B	608	CLA	CMC-C2C	-2.31	1.46	1.50
22	B	607	CLA	CMC-C2C	-2.31	1.46	1.50
22	A	407	CLA	CMB-C2B	-2.31	1.46	1.51
22	B	611	CLA	CMC-C2C	-2.31	1.46	1.50
22	B	613	CLA	C4D-CHA	2.31	1.43	1.39
22	B	603	CLA	CMB-C2B	-2.29	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	405	CLA	CMC-C2C	-2.29	1.46	1.50
22	C	512	CLA	CMC-C2C	-2.29	1.46	1.50
22	B	611	CLA	CAC-C3C	-2.29	1.47	1.51
22	B	612	CLA	CMC-C2C	-2.29	1.46	1.50
22	B	604	CLA	CMB-C2B	-2.28	1.46	1.51
22	B	609	CLA	CAC-C3C	-2.28	1.47	1.51
22	D	404	CLA	CAC-C3C	-2.28	1.47	1.51
22	C	509	CLA	CMC-C2C	-2.28	1.46	1.50
22	B	604	CLA	CMC-C2C	-2.28	1.46	1.50
22	B	617	CLA	CMB-C2B	-2.28	1.46	1.51
22	C	511	CLA	CMC-C2C	-2.27	1.46	1.50
22	B	613	CLA	CMC-C2C	-2.27	1.46	1.50
22	B	609	CLA	CMC-C2C	-2.27	1.46	1.50
24	D	407	PHO	CMC-C2C	-2.26	1.46	1.50
24	D	407	PHO	CMB-C2B	-2.26	1.46	1.51
22	B	615	CLA	CMC-C2C	-2.26	1.46	1.50
24	A	410	PHO	CAC-C3C	-2.26	1.47	1.51
22	C	504	CLA	CAC-C3C	-2.26	1.47	1.51
22	C	514	CLA	CMC-C2C	-2.25	1.46	1.50
22	B	610	CLA	CAC-C3C	-2.25	1.47	1.51
22	B	617	CLA	CMC-C2C	-2.25	1.47	1.50
22	A	406	CLA	CAC-C3C	-2.25	1.47	1.51
22	B	610	CLA	CMC-C2C	-2.25	1.47	1.50
22	B	607	CLA	C4D-CHA	2.24	1.43	1.39
22	B	604	CLA	CAC-C3C	-2.24	1.47	1.51
22	A	408	CLA	CMC-C2C	-2.24	1.47	1.50
22	D	403	CLA	CMC-C2C	-2.24	1.47	1.50
22	C	505	CLA	CAC-C3C	-2.24	1.47	1.51
22	B	608	CLA	CAC-C3C	-2.23	1.47	1.51
22	B	615	CLA	CAC-C3C	-2.23	1.47	1.51
22	C	513	CLA	CMC-C2C	-2.22	1.47	1.50
22	B	603	CLA	CMC-C2C	-2.22	1.47	1.50
22	B	615	CLA	CMB-C2B	-2.21	1.47	1.51
22	A	408	CLA	CAC-C3C	-2.21	1.47	1.51
22	C	509	CLA	C1A-C2A	2.21	1.54	1.51
25	A	411	PL9	C7-C3	-2.21	1.49	1.51
22	D	404	CLA	C4D-CHA	2.20	1.43	1.39
22	B	616	CLA	CMC-C2C	-2.20	1.47	1.50
22	A	407	CLA	CMC-C2C	-2.20	1.47	1.50
22	C	510	CLA	CAC-C3C	-2.19	1.47	1.51
22	B	617	CLA	CAC-C3C	-2.19	1.47	1.51
22	C	503	CLA	C4B-NB	2.18	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	407	PHO	C3D-C4D	2.18	1.44	1.41
22	A	406	CLA	CMC-C2C	-2.18	1.47	1.50
22	A	406	CLA	C1D-ND	2.18	1.42	1.38
22	B	614	CLA	CAC-C3C	-2.18	1.47	1.51
22	B	618	CLA	CAC-C3C	-2.18	1.47	1.51
22	C	506	CLA	CAC-C3C	-2.17	1.47	1.51
22	B	603	CLA	CAC-C3C	-2.17	1.47	1.51
22	B	615	CLA	C3B-C2B	-2.17	1.37	1.40
22	B	614	CLA	CMC-C2C	-2.16	1.47	1.50
22	C	508	CLA	CAC-C3C	-2.16	1.47	1.51
22	C	509	CLA	CAC-C3C	-2.16	1.47	1.51
24	A	410	PHO	CMC-C2C	-2.15	1.47	1.50
22	C	507	CLA	CMC-C2C	-2.14	1.47	1.50
22	D	403	CLA	CAC-C3C	-2.14	1.47	1.51
22	C	513	CLA	CAC-C3C	-2.13	1.47	1.51
22	C	512	CLA	CAC-C3C	-2.13	1.47	1.51
22	C	514	CLA	C1D-ND	2.13	1.42	1.38
22	C	508	CLA	C3B-C2B	-2.12	1.37	1.40
22	C	504	CLA	C1A-C2A	2.12	1.54	1.51
22	A	407	CLA	CAC-C3C	-2.12	1.47	1.51
22	B	616	CLA	CAC-C3C	-2.11	1.47	1.51
22	C	514	CLA	CAC-C3C	-2.11	1.47	1.51
25	D	408	PL9	C6-C1	-2.11	1.44	1.48
22	C	512	CLA	C1D-ND	2.11	1.42	1.38
24	A	410	PHO	C3D-C4D	2.10	1.44	1.41
22	A	405	CLA	CAC-C3C	-2.10	1.47	1.51
22	B	604	CLA	C1D-ND	2.10	1.42	1.38
22	C	505	CLA	C1D-ND	2.09	1.42	1.38
22	B	603	CLA	C1D-ND	2.09	1.42	1.38
22	B	609	CLA	C1D-ND	2.09	1.42	1.38
22	A	407	CLA	C1D-ND	2.07	1.42	1.38
22	B	610	CLA	C1D-ND	2.07	1.42	1.38
22	B	608	CLA	C1D-ND	2.07	1.42	1.38
28	F	101	HEM	CAD-C3D	2.07	1.54	1.51
22	B	613	CLA	C1D-ND	2.07	1.42	1.38
22	A	405	CLA	C3B-C2B	-2.07	1.37	1.40
22	B	615	CLA	C1D-ND	2.07	1.42	1.38
22	A	408	CLA	C1D-ND	2.06	1.42	1.38
22	C	509	CLA	C1D-ND	2.06	1.42	1.38
22	B	616	CLA	C1D-ND	2.06	1.42	1.38
22	C	506	CLA	C1D-ND	2.05	1.42	1.38
22	C	507	CLA	CAC-C3C	-2.05	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	511	CLA	CAC-C3C	-2.05	1.48	1.51
22	C	508	CLA	C1D-ND	2.05	1.42	1.38
28	F	101	HEM	CAA-C2A	2.04	1.55	1.52
22	B	612	CLA	C1D-ND	2.04	1.42	1.38
22	B	618	CLA	C1D-ND	2.04	1.42	1.38
22	C	510	CLA	C1D-ND	2.04	1.42	1.38
22	C	514	CLA	C4B-NB	2.03	1.42	1.38
22	B	613	CLA	C1A-C2A	2.03	1.54	1.51
22	A	406	CLA	CMA-C3A	-2.03	1.49	1.53
22	B	610	CLA	C3B-C2B	-2.02	1.37	1.40
22	C	516	CLA	C1D-ND	2.01	1.42	1.38
25	A	411	PL9	C53-C6	-2.01	1.46	1.50
22	C	511	CLA	C1A-C2A	2.01	1.54	1.51
22	C	507	CLA	C1D-ND	2.00	1.42	1.38
22	A	405	CLA	C1D-ND	2.00	1.42	1.38
22	C	511	CLA	C1D-ND	2.00	1.42	1.38

All (358) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	407	PHO	C4D-CHA-CBD	-8.17	104.82	108.52
22	A	406	CLA	C4D-CHA-CBD	-7.68	105.04	108.52
22	B	603	CLA	C4D-CHA-CBD	-7.54	105.11	108.52
24	A	410	PHO	C4D-CHA-CBD	-7.08	105.31	108.52
22	C	505	CLA	C4D-CHA-CBD	-6.91	105.39	108.52
22	B	609	CLA	C4D-CHA-CBD	-6.82	105.43	108.52
22	C	506	CLA	C4D-CHA-CBD	-6.68	105.50	108.52
22	C	514	CLA	C4D-CHA-CBD	-6.19	105.72	108.52
22	C	509	CLA	C4D-CHA-CBD	-6.15	105.74	108.52
22	B	604	CLA	C4D-CHA-CBD	-6.12	105.75	108.52
22	C	510	CLA	C4D-CHA-CBD	-6.09	105.76	108.52
22	C	511	CLA	C4D-CHA-CBD	-6.08	105.77	108.52
22	C	504	CLA	C4D-CHA-CBD	-6.07	105.77	108.52
22	C	507	CLA	C4D-CHA-CBD	-6.05	105.78	108.52
25	D	408	PL9	C7-C3-C4	5.91	121.68	116.88
22	C	512	CLA	C4D-CHA-CBD	-5.90	105.85	108.52
22	B	605	CLA	C4D-CHA-CBD	-5.81	105.89	108.52
22	C	513	CLA	C4D-CHA-CBD	-5.80	105.89	108.52
22	C	516	CLA	C4D-CHA-CBD	-5.64	105.96	108.52
22	B	617	CLA	C4D-CHA-CBD	-5.61	105.98	108.52
22	D	403	CLA	C4D-CHA-CBD	-5.60	105.98	108.52
22	B	610	CLA	C4D-CHA-CBD	-5.48	106.04	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	614	CLA	C4D-CHA-CBD	-5.44	106.06	108.52
22	B	615	CLA	C4D-CHA-CBD	-5.27	106.13	108.52
22	B	612	CLA	C4D-CHA-CBD	-5.23	106.15	108.52
22	B	616	CLA	C4D-CHA-CBD	-5.22	106.16	108.52
22	B	611	CLA	C4D-CHA-CBD	-5.19	106.17	108.52
22	C	508	CLA	C4D-CHA-CBD	-5.19	106.17	108.52
22	B	606	CLA	C4D-CHA-CBD	-5.04	106.24	108.52
22	B	618	CLA	C4D-CHA-CBD	-4.98	106.26	108.52
22	A	405	CLA	C4D-CHA-CBD	-4.87	106.31	108.52
22	B	613	CLA	C4D-CHA-CBD	-4.81	106.34	108.52
22	A	408	CLA	C4D-CHA-CBD	-4.65	106.42	108.52
25	A	411	PL9	C7-C3-C4	4.64	120.65	116.88
22	B	608	CLA	C4D-CHA-CBD	-4.63	106.42	108.52
24	A	410	PHO	C2B-C1B-NB	-4.48	106.43	109.53
22	B	607	CLA	C4D-CHA-CBD	-4.42	106.52	108.52
24	D	407	PHO	C2B-C1B-NB	-4.26	106.58	109.53
22	B	610	CLA	O2D-CGD-CBD	4.18	116.29	111.00
22	C	514	CLA	O2D-CGD-CBD	4.15	116.25	111.00
22	A	407	CLA	C4D-CHA-CBD	-4.14	106.64	108.52
22	D	404	CLA	C4D-CHA-CBD	-4.14	106.65	108.52
22	B	609	CLA	CAA-C2A-C3A	-3.96	101.93	112.78
26	A	413	BCT	O2-C-O1	3.93	129.74	119.55
22	A	407	CLA	CMB-C2B-C3B	3.89	131.96	124.68
25	D	408	PL9	C7-C3-C2	-3.84	118.25	123.30
22	C	509	CLA	O2D-CGD-O1D	-3.65	116.70	123.84
22	C	504	CLA	O2D-CGD-CBD	3.54	115.48	111.00
22	C	503	CLA	C3D-C4D-ND	3.54	112.54	107.72
22	D	404	CLA	C3D-C4D-ND	3.46	112.44	107.72
22	C	503	CLA	C4D-CHA-CBD	-3.41	106.97	108.52
22	C	514	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
22	B	610	CLA	O2D-CGD-O1D	-3.37	117.26	123.84
22	B	607	CLA	C3D-C4D-ND	3.26	112.17	107.72
22	D	404	CLA	O2D-CGD-CBD	3.22	115.07	111.00
21	H	101	BCR	C1-C6-C5	-3.22	118.08	122.61
22	B	613	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
22	B	616	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
22	A	406	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
22	A	407	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
22	B	613	CLA	C3D-C4D-ND	3.17	112.04	107.72
22	B	608	CLA	C3D-C4D-ND	3.14	112.00	107.72
22	B	612	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
22	C	506	CLA	O2D-CGD-O1D	-3.13	117.71	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	407	PHO	O1D-CGD-CBD	3.13	129.95	124.74
22	A	408	CLA	CMB-C2B-C3B	3.13	130.53	124.68
22	C	507	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
22	A	407	CLA	C3D-C4D-ND	3.12	111.98	107.72
22	A	406	CLA	O2D-CGD-CBD	3.12	114.95	111.00
22	B	618	CLA	C3D-C4D-ND	3.12	111.97	107.72
22	A	407	CLA	O2D-CGD-CBD	3.12	114.95	111.00
22	D	403	CLA	O2D-CGD-CBD	3.12	114.94	111.00
22	B	604	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
22	B	607	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
22	B	608	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
22	A	406	CLA	C7-C6-C5	3.08	121.73	113.36
22	C	510	CLA	O2D-CGD-CBD	3.08	114.90	111.00
22	C	512	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
22	C	504	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
22	C	513	CLA	CMB-C2B-C3B	3.06	130.40	124.68
22	A	408	CLA	C3D-C4D-ND	3.06	111.89	107.72
22	B	613	CLA	O2D-CGD-CBD	3.04	114.85	111.00
22	B	607	CLA	CMB-C2B-C3B	3.04	130.37	124.68
22	C	506	CLA	O2D-CGD-CBD	3.04	114.84	111.00
22	B	609	CLA	C3D-C4D-ND	3.03	111.85	107.72
22	C	510	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
22	B	606	CLA	C3D-C4D-ND	3.00	111.81	107.72
22	C	512	CLA	CMB-C2B-C3B	3.00	130.29	124.68
24	D	407	PHO	C2D-C1D-ND	-3.00	107.46	109.53
22	D	403	CLA	C3D-C4D-ND	2.99	111.80	107.72
22	A	408	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
22	B	609	CLA	O2D-CGD-CBD	2.97	114.76	111.00
22	B	606	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
22	A	405	CLA	C3D-C4D-ND	2.96	111.75	107.72
22	D	403	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
22	B	605	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
22	B	617	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
22	C	504	CLA	CMD-C2D-C3D	2.94	130.19	124.68
22	C	516	CLA	C3D-C4D-ND	2.94	111.73	107.72
22	B	615	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
22	B	605	CLA	C5-C3-C2	-2.93	115.19	121.12
22	C	508	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
22	B	608	CLA	O2D-CGD-CBD	2.93	114.70	111.00
22	B	605	CLA	C3D-C4D-ND	2.93	111.71	107.72
22	C	511	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
22	B	611	CLA	C3D-C4D-ND	2.92	111.69	107.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	614	CLA	C3D-C4D-ND	2.92	111.69	107.72
22	B	612	CLA	C3D-C4D-ND	2.91	111.68	107.72
22	C	509	CLA	CMB-C2B-C3B	2.90	130.11	124.68
22	A	406	CLA	C1C-C2C-C3C	-2.90	106.20	108.61
27	D	405	LMG	C8-O7-C10	2.90	124.92	117.79
21	H	101	BCR	C15-C14-C13	2.88	131.43	127.31
22	B	605	CLA	C1C-C2C-C3C	-2.88	106.21	108.61
25	D	408	PL9	C36-C34-C33	-2.87	115.31	121.12
22	C	513	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
25	A	411	PL9	C7-C3-C2	-2.87	119.53	123.30
22	C	504	CLA	CMB-C2B-C3B	2.87	130.04	124.68
22	B	610	CLA	C1C-C2C-C3C	-2.86	106.23	108.61
24	A	410	PHO	C1C-C2C-C3C	-2.86	106.23	108.61
22	B	611	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
22	C	508	CLA	C3D-C4D-ND	2.85	111.60	107.72
24	A	410	PHO	O2D-CGD-O1D	-2.84	118.28	123.84
28	F	101	HEM	C2A-C1A-NA	-2.83	107.57	109.53
22	C	503	CLA	C4D-ND-C1D	-2.83	105.95	108.83
22	B	618	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
22	C	511	CLA	C3D-C4D-ND	2.83	111.57	107.72
22	C	516	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
22	B	616	CLA	CMB-C2B-C3B	2.82	129.96	124.68
22	B	616	CLA	C3D-C4D-ND	2.82	111.56	107.72
22	B	609	CLA	CMB-C2B-C3B	2.81	129.93	124.68
22	C	504	CLA	C3D-C4D-ND	2.81	111.55	107.72
22	C	510	CLA	C3D-C4D-ND	2.81	111.54	107.72
22	C	507	CLA	O2D-CGD-CBD	2.81	114.55	111.00
22	B	614	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
22	A	408	CLA	O2D-CGD-CBD	2.80	114.54	111.00
25	A	411	PL9	C40-C39-C41	2.80	119.97	115.27
22	C	505	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
22	C	507	CLA	C1C-C2C-C3C	-2.79	106.29	108.61
22	B	612	CLA	O2D-CGD-CBD	2.79	114.53	111.00
22	B	604	CLA	CMB-C2B-C3B	2.78	129.88	124.68
22	C	503	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
22	B	609	CLA	O2A-CGA-O1A	-2.77	116.60	123.59
22	D	404	CLA	CMB-C2B-C3B	2.77	129.86	124.68
22	C	512	CLA	C3D-C4D-ND	2.76	111.48	107.72
22	C	507	CLA	C3D-C4D-ND	2.76	111.48	107.72
22	B	617	CLA	C3D-C4D-ND	2.75	111.47	107.72
22	B	609	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
22	D	403	CLA	CMB-C2B-C3B	2.75	129.82	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	407	PHO	O2D-CGD-O1D	-2.75	118.46	123.84
22	C	513	CLA	C3D-C4D-ND	2.75	111.46	107.72
22	C	509	CLA	O2D-CGD-CBD	2.75	114.47	111.00
22	B	610	CLA	CMD-C2D-C3D	2.75	129.81	124.68
22	B	604	CLA	O2D-CGD-CBD	2.74	114.47	111.00
22	B	611	CLA	C1C-C2C-C3C	-2.73	106.34	108.61
22	C	510	CLA	CMB-C2B-C3B	2.73	129.79	124.68
22	B	606	CLA	O2D-CGD-CBD	2.72	114.44	111.00
22	A	406	CLA	CMA-C3A-C4A	-2.71	108.45	114.38
22	B	613	CLA	CMB-C2B-C3B	2.70	129.74	124.68
22	B	605	CLA	C4-C3-C5	2.70	119.81	115.27
24	A	410	PHO	O1D-CGD-CBD	2.70	129.24	124.74
22	B	603	CLA	CMD-C2D-C3D	2.70	129.73	124.68
22	C	507	CLA	CMB-C2B-C3B	2.70	129.73	124.68
24	A	410	PHO	C2D-C1D-ND	-2.70	107.67	109.53
22	C	509	CLA	C3D-C4D-ND	2.69	111.39	107.72
22	B	609	CLA	C1C-C2C-C3C	-2.69	106.38	108.61
22	B	604	CLA	C3D-C4D-ND	2.68	111.38	107.72
22	A	405	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
22	B	603	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
22	C	514	CLA	C3D-C4D-ND	2.68	111.37	107.72
25	D	408	PL9	C40-C39-C41	2.66	119.75	115.27
22	C	507	CLA	CBA-CAA-C2A	2.66	121.59	113.81
22	B	615	CLA	C1C-C2C-C3C	-2.66	106.40	108.61
22	D	404	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
22	B	610	CLA	C3D-C4D-ND	2.64	111.32	107.72
22	C	510	CLA	CMD-C2D-C3D	2.64	129.62	124.68
22	A	406	CLA	CMB-C2B-C3B	2.64	129.62	124.68
22	B	604	CLA	CMD-C2D-C3D	2.63	129.59	124.68
21	H	101	BCR	C16-C17-C18	2.62	131.05	127.31
25	A	411	PL9	C22-C23-C24	-2.62	121.36	127.66
22	B	615	CLA	C3D-C4D-ND	2.61	111.28	107.72
22	B	617	CLA	CMD-C2D-C3D	2.61	129.56	124.68
22	C	506	CLA	CMD-C2D-C3D	2.60	129.54	124.68
22	B	613	CLA	CAA-CBA-CGA	-2.60	105.66	113.25
22	B	614	CLA	CMD-C2D-C3D	2.59	129.53	124.68
22	B	605	CLA	CMB-C2B-C3B	2.59	129.53	124.68
22	B	603	CLA	C1C-C2C-C3C	-2.59	106.46	108.61
22	B	612	CLA	CMD-C2D-C3D	2.58	129.51	124.68
27	D	406	LMG	C8-O7-C10	2.58	124.15	117.79
22	B	613	CLA	C1C-C2C-C3C	-2.58	106.47	108.61
22	C	505	CLA	C1C-C2C-C3C	-2.58	106.47	108.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	505	CLA	C3D-C4D-ND	2.58	111.23	107.72
22	C	511	CLA	O2D-CGD-CBD	2.58	114.26	111.00
22	B	617	CLA	CMB-C2B-C3B	2.58	129.50	124.68
22	C	513	CLA	CMD-C2D-C3D	2.57	129.49	124.68
21	J	101	BCR	C2-C1-C6	2.57	114.44	110.48
22	A	405	CLA	O2D-CGD-CBD	2.57	114.25	111.00
22	B	607	CLA	C1C-C2C-C3C	-2.56	106.48	108.61
22	B	614	CLA	C1C-C2C-C3C	-2.56	106.48	108.61
22	D	403	CLA	C1C-C2C-C3C	-2.56	106.48	108.61
22	B	615	CLA	O2D-CGD-CBD	2.56	114.24	111.00
22	C	506	CLA	C1C-C2C-C3C	-2.55	106.49	108.61
22	C	512	CLA	O2D-CGD-CBD	2.55	114.23	111.00
22	B	607	CLA	O2D-CGD-CBD	2.55	114.23	111.00
22	D	403	CLA	CMD-C2D-C3D	2.54	129.44	124.68
22	B	605	CLA	CMD-C2D-C3D	2.54	129.43	124.68
22	C	516	CLA	C1C-C2C-C3C	-2.54	106.50	108.61
22	A	408	CLA	C1C-C2C-C3C	-2.53	106.50	108.61
22	B	616	CLA	C1C-C2C-C3C	-2.53	106.50	108.61
22	B	617	CLA	C1C-C2C-C3C	-2.53	106.51	108.61
22	B	614	CLA	O2A-CGA-O1A	-2.52	117.22	123.59
22	C	506	CLA	C3D-C4D-ND	2.52	111.16	107.72
22	B	612	CLA	CMB-C2B-C3B	2.52	129.39	124.68
22	C	508	CLA	CMD-C2D-C3D	2.52	129.39	124.68
22	B	613	CLA	CBA-CAA-C2A	2.52	121.17	113.81
22	C	505	CLA	CMD-C2D-C3D	2.51	129.38	124.68
22	B	615	CLA	CMD-C2D-C3D	2.51	129.38	124.68
21	C	517	BCR	C32-C1-C6	2.51	114.37	110.30
22	C	509	CLA	C1C-C2C-C3C	-2.51	106.53	108.61
22	C	513	CLA	C1C-C2C-C3C	-2.51	106.53	108.61
22	B	604	CLA	C1C-C2C-C3C	-2.49	106.54	108.61
22	C	516	CLA	CMD-C2D-C3D	2.49	129.34	124.68
22	C	503	CLA	O2D-CGD-CBD	2.48	114.14	111.00
22	B	609	CLA	C4D-ND-C1D	-2.48	106.31	108.83
22	B	618	CLA	CMD-C2D-C3D	2.48	129.31	124.68
22	C	509	CLA	CMD-C2D-C3D	2.47	129.29	124.68
22	C	512	CLA	C1C-C2C-C3C	-2.47	106.56	108.61
22	C	509	CLA	O1D-CGD-CBD	2.45	128.82	124.74
22	D	404	CLA	C1C-C2C-C3C	-2.45	106.57	108.61
22	B	608	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
25	D	408	PL9	C32-C33-C34	-2.45	121.77	127.66
22	B	614	CLA	C1-O2A-CGA	2.44	122.86	116.44
22	C	511	CLA	CMD-C2D-C3D	2.44	129.24	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	404	CLA	C4D-ND-C1D	-2.43	106.35	108.83
24	D	407	PHO	C1C-C2C-C3C	-2.43	106.59	108.61
22	B	608	CLA	CMD-C2D-C3D	2.43	129.23	124.68
22	B	611	CLA	CMD-C2D-C3D	2.43	129.22	124.68
22	C	503	CLA	C1C-C2C-C3C	-2.43	106.59	108.61
28	F	101	HEM	C3A-C4A-NA	-2.42	107.85	109.53
22	C	514	CLA	CMD-C2D-C3D	2.42	129.21	124.68
22	B	605	CLA	C4D-ND-C1D	-2.42	106.37	108.83
24	D	407	PHO	CMB-C2B-C3B	2.42	129.20	124.68
22	B	607	CLA	C4D-ND-C1D	-2.41	106.37	108.83
21	C	502	BCR	C27-C26-C25	-2.41	119.24	122.73
22	D	404	CLA	CMD-C2D-C3D	2.41	129.18	124.68
22	B	607	CLA	CMD-C2D-C3D	2.41	129.18	124.68
22	C	507	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
22	C	510	CLA	C4D-ND-C1D	-2.40	106.39	108.83
22	C	508	CLA	C1C-C2C-C3C	-2.40	106.61	108.61
22	C	505	CLA	CMB-C2B-C3B	2.40	129.17	124.68
22	B	613	CLA	CMD-C2D-C3D	2.40	129.16	124.68
22	B	608	CLA	CMB-C2B-C3B	2.40	129.16	124.68
22	C	510	CLA	C1C-C2C-C3C	-2.39	106.62	108.61
27	D	406	LMG	O1-C7-C8	-2.39	105.13	110.90
22	B	616	CLA	CMD-C2D-C3D	2.38	129.14	124.68
22	B	605	CLA	O2D-CGD-CBD	2.38	114.02	111.00
22	C	510	CLA	CBA-CAA-C2A	2.38	120.77	113.81
22	C	514	CLA	CMB-C2B-C3B	2.38	129.13	124.68
22	B	606	CLA	CMD-C2D-C3D	2.37	129.12	124.68
22	C	504	CLA	C1C-C2C-C3C	-2.36	106.65	108.61
22	C	504	CLA	CBA-CAA-C2A	2.36	120.70	113.81
22	B	605	CLA	C1-C2-C3	2.35	130.11	126.04
22	B	608	CLA	C1C-C2C-C3C	-2.35	106.66	108.61
22	B	613	CLA	C4D-ND-C1D	-2.35	106.44	108.83
22	C	514	CLA	C1C-C2C-C3C	-2.35	106.66	108.61
22	A	408	CLA	CMD-C2D-C3D	2.35	129.07	124.68
22	B	616	CLA	O2D-CGD-CBD	2.34	113.96	111.00
25	D	408	PL9	O2-C1-C6	2.34	124.64	120.59
22	B	603	CLA	C3D-C4D-ND	2.34	110.90	107.72
21	C	502	BCR	C30-C25-C26	-2.33	119.33	122.61
22	A	407	CLA	C1C-C2C-C3C	-2.33	106.67	108.61
25	D	408	PL9	O2-C1-C2	-2.33	116.45	121.78
22	B	613	CLA	CAA-C2A-C3A	2.32	119.14	112.78
22	A	406	CLA	C3D-C4D-ND	2.32	110.88	107.72
22	D	403	CLA	O2A-CGA-O1A	-2.31	117.75	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	403	CLA	C4D-ND-C1D	-2.31	106.48	108.83
22	B	607	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
22	B	613	CLA	C1-C2-C3	-2.30	122.06	126.04
22	C	508	CLA	O2D-CGD-CBD	2.30	113.91	111.00
22	B	617	CLA	O2D-CGD-CBD	2.30	113.91	111.00
25	A	411	PL9	O2-C1-C6	2.30	124.57	120.59
22	C	516	CLA	O2D-CGD-CBD	2.29	113.90	111.00
22	B	614	CLA	O2D-CGD-CBD	2.28	113.88	111.00
22	B	609	CLA	CMD-C2D-C3D	2.27	128.93	124.68
22	B	610	CLA	C4D-ND-C1D	-2.27	106.52	108.83
22	C	516	CLA	CMB-C2B-C3B	2.26	128.91	124.68
22	C	511	CLA	C1C-C2C-C3C	-2.26	106.73	108.61
22	A	405	CLA	C1C-C2C-C3C	-2.26	106.73	108.61
22	B	618	CLA	C4D-ND-C1D	-2.26	106.53	108.83
25	A	411	PL9	O2-C1-C2	-2.26	116.61	121.78
27	D	401	LMG	C8-O7-C10	2.25	123.32	117.79
22	B	611	CLA	CMB-C2B-C3B	2.24	128.88	124.68
22	C	508	CLA	CMB-C2B-C3B	2.24	128.87	124.68
26	A	413	BCT	O3-C-O1	-2.23	113.77	119.55
25	A	411	PL9	O1-C4-C3	-2.22	118.27	120.72
22	B	616	CLA	O1D-CGD-CBD	2.22	128.43	124.74
25	D	408	PL9	C20-C19-C21	2.22	119.00	115.27
22	C	503	CLA	CMD-C2D-C3D	2.21	128.81	124.68
22	C	513	CLA	O2D-CGD-CBD	2.20	113.78	111.00
22	C	508	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
27	D	406	LMG	C7-O1-C1	2.19	118.02	113.74
25	D	408	PL9	C50-C49-C48	-2.19	116.32	122.65
22	C	516	CLA	C4D-ND-C1D	-2.19	106.60	108.83
22	B	618	CLA	C1C-C2C-C3C	-2.19	106.79	108.61
22	B	608	CLA	C4D-ND-C1D	-2.18	106.61	108.83
22	B	606	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
25	A	411	PL9	C7-C8-C9	-2.18	123.16	126.79
22	C	504	CLA	CAA-CBA-CGA	-2.18	106.89	113.25
22	C	506	CLA	CMB-C2B-C3B	2.17	128.74	124.68
22	B	603	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
22	C	506	CLA	O2A-CGA-O1A	-2.17	118.13	123.59
22	B	606	CLA	C4D-ND-C1D	-2.15	106.64	108.83
27	C	515	LMG	C7-O1-C1	2.15	117.94	113.74
22	C	510	CLA	O2A-C1-C2	-2.15	103.00	108.64
22	C	505	CLA	O2D-CGD-CBD	2.14	113.71	111.00
22	B	604	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
24	A	410	PHO	CMB-C2B-C3B	2.14	128.68	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	614	CLA	C4D-ND-C1D	-2.14	106.66	108.83
22	B	606	CLA	CMB-C2B-C3B	2.14	128.67	124.68
22	B	614	CLA	CMB-C2B-C3B	2.13	128.67	124.68
22	B	610	CLA	OBD-CAD-CBD	-2.13	122.70	125.82
22	B	610	CLA	CMB-C2B-C3B	2.12	128.65	124.68
22	A	407	CLA	CMD-C2D-C3D	2.12	128.65	124.68
21	H	101	BCR	C36-C18-C17	2.12	125.89	122.92
22	B	612	CLA	C4D-ND-C1D	-2.12	106.67	108.83
22	B	617	CLA	C4D-ND-C1D	-2.12	106.67	108.83
22	B	605	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
22	B	603	CLA	CMB-C2B-C3B	2.11	128.63	124.68
22	B	614	CLA	C1-C2-C3	-2.11	122.39	126.04
28	F	101	HEM	CMC-C2C-C3C	2.11	128.62	124.68
22	A	405	CLA	CMD-C2D-C3D	2.11	128.62	124.68
25	A	411	PL9	C20-C19-C21	2.11	118.81	115.27
22	B	618	CLA	O2D-CGD-CBD	2.10	113.66	111.00
22	A	405	CLA	C4D-ND-C1D	-2.10	106.69	108.83
22	C	504	CLA	C4D-ND-C1D	-2.09	106.70	108.83
22	B	618	CLA	CMB-C2B-C3B	2.09	128.58	124.68
22	B	612	CLA	C1C-C2C-C3C	-2.08	106.88	108.61
22	B	606	CLA	C1C-C2C-C3C	-2.07	106.89	108.61
22	C	503	CLA	C1-C2-C3	-2.07	122.46	126.04
22	C	511	CLA	C4D-ND-C1D	-2.07	106.73	108.83
22	B	611	CLA	O1D-CGD-CBD	2.06	128.16	124.74
22	C	512	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
25	A	411	PL9	C42-C43-C44	-2.05	122.71	127.66
22	C	514	CLA	C4D-ND-C1D	-2.05	106.74	108.83
22	A	408	CLA	C4D-ND-C1D	-2.05	106.75	108.83
22	B	611	CLA	O2D-CGD-CBD	2.04	113.58	111.00
22	A	408	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
22	B	609	CLA	CBA-CAA-C2A	2.04	119.78	113.81
22	C	512	CLA	C4D-ND-C1D	-2.04	106.75	108.83
25	D	408	PL9	C37-C38-C39	-2.04	122.75	127.66
22	B	611	CLA	C4D-ND-C1D	-2.04	106.75	108.83
22	B	603	CLA	O2D-CGD-CBD	2.04	113.58	111.00
25	A	411	PL9	C31-C32-C33	-2.03	105.20	111.88
22	C	516	CLA	C1-O2A-CGA	2.03	121.78	116.44
22	A	407	CLA	C4D-ND-C1D	-2.02	106.77	108.83
23	A	409	LHG	C5-O7-C7	2.02	122.77	117.79
22	B	607	CLA	C9-C8-C10	2.01	118.58	111.29
22	B	613	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
22	A	406	CLA	CBA-CAA-C2A	2.01	119.68	113.81

There are no chirality outliers.

All (654) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	404	BCR	C1-C6-C7-C8
21	A	404	BCR	C5-C6-C7-C8
21	B	601	BCR	C11-C12-C13-C14
21	B	601	BCR	C11-C12-C13-C35
21	B	602	BCR	C1-C6-C7-C8
21	B	602	BCR	C11-C12-C13-C14
21	B	602	BCR	C11-C12-C13-C35
21	B	602	BCR	C13-C14-C15-C16
21	B	602	BCR	C15-C16-C17-C18
21	B	602	BCR	C17-C18-C19-C20
21	B	602	BCR	C36-C18-C19-C20
21	B	602	BCR	C21-C22-C23-C24
21	B	602	BCR	C37-C22-C23-C24
21	C	501	BCR	C7-C8-C9-C10
21	C	501	BCR	C7-C8-C9-C34
21	C	502	BCR	C19-C20-C21-C22
21	C	502	BCR	C21-C22-C23-C24
21	C	502	BCR	C37-C22-C23-C24
21	C	517	BCR	C7-C8-C9-C10
21	C	517	BCR	C7-C8-C9-C34
21	C	517	BCR	C19-C20-C21-C22
21	D	402	BCR	C1-C6-C7-C8
21	D	402	BCR	C7-C8-C9-C10
21	D	402	BCR	C7-C8-C9-C34
21	D	402	BCR	C17-C18-C19-C20
21	D	402	BCR	C36-C18-C19-C20
21	D	402	BCR	C23-C24-C25-C26
21	D	402	BCR	C23-C24-C25-C30
21	H	101	BCR	C7-C8-C9-C10
21	H	101	BCR	C7-C8-C9-C34
21	H	101	BCR	C9-C10-C11-C12
21	H	101	BCR	C11-C12-C13-C14
21	H	101	BCR	C11-C12-C13-C35
21	H	101	BCR	C21-C22-C23-C24
21	H	101	BCR	C37-C22-C23-C24
21	H	101	BCR	C23-C24-C25-C30
21	J	101	BCR	C9-C10-C11-C12
21	J	102	BCR	C7-C8-C9-C10
21	J	102	BCR	C7-C8-C9-C34
21	J	102	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	J	102	BCR	C11-C12-C13-C35
21	J	102	BCR	C21-C22-C23-C24
21	J	102	BCR	C37-C22-C23-C24
22	A	405	CLA	CBD-CGD-O2D-CED
22	A	406	CLA	C3A-C2A-CAA-CBA
22	A	406	CLA	C4C-C3C-CAC-CBC
22	A	407	CLA	C4C-C3C-CAC-CBC
22	A	408	CLA	C3A-C2A-CAA-CBA
22	B	605	CLA	CBD-CGD-O2D-CED
22	B	605	CLA	O2A-C1-C2-C3
22	B	605	CLA	C4-C3-C5-C6
22	B	606	CLA	C4C-C3C-CAC-CBC
22	B	607	CLA	C3A-C2A-CAA-CBA
22	B	607	CLA	C2-C3-C5-C6
22	B	607	CLA	C4-C3-C5-C6
22	B	608	CLA	C3A-C2A-CAA-CBA
22	B	609	CLA	O2A-C1-C2-C3
22	B	612	CLA	C4C-C3C-CAC-CBC
22	B	613	CLA	C1A-C2A-CAA-CBA
22	B	613	CLA	C3A-C2A-CAA-CBA
22	B	614	CLA	C2A-CAA-CBA-CGA
22	B	614	CLA	CBD-CGD-O2D-CED
22	B	615	CLA	CBD-CGD-O2D-CED
22	B	616	CLA	C1A-C2A-CAA-CBA
22	B	617	CLA	C1A-C2A-CAA-CBA
22	B	618	CLA	C1A-C2A-CAA-CBA
22	B	618	CLA	C2A-CAA-CBA-CGA
22	B	618	CLA	CBD-CGD-O2D-CED
22	C	503	CLA	C1A-C2A-CAA-CBA
22	C	503	CLA	C3A-C2A-CAA-CBA
22	C	504	CLA	C1A-C2A-CAA-CBA
22	C	504	CLA	C3A-C2A-CAA-CBA
22	C	506	CLA	CBD-CGD-O2D-CED
22	C	508	CLA	CAD-CBD-CGD-O1D
22	C	508	CLA	CAD-CBD-CGD-O2D
22	C	509	CLA	C1A-C2A-CAA-CBA
22	C	510	CLA	C1A-C2A-CAA-CBA
22	C	511	CLA	CBD-CGD-O2D-CED
22	C	512	CLA	CBD-CGD-O2D-CED
22	C	516	CLA	CBD-CGD-O2D-CED
22	D	403	CLA	O2A-C1-C2-C3
22	D	404	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	D	404	CLA	C3A-C2A-CAA-CBA
23	A	412	LHG	C2-C3-O3-P
24	A	410	PHO	C6-C7-C8-C9
25	A	411	PL9	C12-C13-C14-C16
25	A	411	PL9	C37-C38-C39-C41
25	D	408	PL9	C29-C31-C32-C33
25	D	408	PL9	C32-C33-C34-C36
25	D	408	PL9	C42-C43-C44-C46
27	C	515	LMG	C2-C1-O1-C7
27	C	515	LMG	O6-C1-O1-C7
27	C	515	LMG	O9-C10-O7-C8
27	C	515	LMG	C11-C10-O7-C8
27	D	405	LMG	O9-C10-O7-C8
27	D	405	LMG	O10-C28-O8-C9
27	I	101	LMG	C11-C10-O7-C8
27	M	102	LMG	C11-C10-O7-C8
22	B	604	CLA	O1D-CGD-O2D-CED
22	C	508	CLA	O1D-CGD-O2D-CED
22	B	615	CLA	O1D-CGD-O2D-CED
22	C	511	CLA	O1D-CGD-O2D-CED
22	C	512	CLA	O1D-CGD-O2D-CED
22	B	604	CLA	CBD-CGD-O2D-CED
22	B	607	CLA	CBD-CGD-O2D-CED
22	B	611	CLA	CBD-CGD-O2D-CED
22	C	505	CLA	CBD-CGD-O2D-CED
22	C	508	CLA	CBD-CGD-O2D-CED
22	C	514	CLA	CBD-CGD-O2D-CED
22	D	404	CLA	CBD-CGD-O2D-CED
27	C	515	LMG	O10-C28-O8-C9
22	B	614	CLA	O1D-CGD-O2D-CED
22	A	405	CLA	O1D-CGD-O2D-CED
22	B	607	CLA	O1D-CGD-O2D-CED
22	B	618	CLA	O1D-CGD-O2D-CED
22	C	506	CLA	O1D-CGD-O2D-CED
22	C	516	CLA	O1D-CGD-O2D-CED
22	A	406	CLA	CBD-CGD-O2D-CED
22	B	612	CLA	CBD-CGD-O2D-CED
22	B	603	CLA	O1A-CGA-O2A-C1
22	B	605	CLA	O1A-CGA-O2A-C1
22	B	614	CLA	O1A-CGA-O2A-C1
22	B	618	CLA	O1A-CGA-O2A-C1
22	D	403	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	M	102	LMG	O10-C28-O8-C9
22	B	605	CLA	O1D-CGD-O2D-CED
22	B	610	CLA	CBD-CGD-O2D-CED
22	C	514	CLA	O1D-CGD-O2D-CED
27	I	101	LMG	O9-C10-O7-C8
27	M	102	LMG	O9-C10-O7-C8
22	C	505	CLA	O1A-CGA-O2A-C1
22	B	617	CLA	C3-C5-C6-C7
22	B	609	CLA	CBA-CGA-O2A-C1
22	B	614	CLA	CBA-CGA-O2A-C1
22	D	403	CLA	CBA-CGA-O2A-C1
27	C	515	LMG	C29-C28-O8-C9
27	D	405	LMG	C29-C28-O8-C9
27	D	405	LMG	C11-C10-O7-C8
22	B	611	CLA	O1D-CGD-O2D-CED
22	C	507	CLA	CBD-CGD-O2D-CED
22	C	504	CLA	CBD-CGD-O2D-CED
22	C	512	CLA	C2A-CAA-CBA-CGA
22	B	603	CLA	CBA-CGA-O2A-C1
22	B	605	CLA	CBA-CGA-O2A-C1
22	B	610	CLA	CBA-CGA-O2A-C1
22	B	618	CLA	CBA-CGA-O2A-C1
22	C	505	CLA	CBA-CGA-O2A-C1
27	K	101	LMG	C29-C28-O8-C9
27	M	102	LMG	C29-C28-O8-C9
25	D	408	PL9	C47-C48-C49-C50
25	D	408	PL9	C47-C48-C49-C51
25	D	408	PL9	C32-C33-C34-C35
22	A	408	CLA	O1A-CGA-O2A-C1
22	B	610	CLA	O1A-CGA-O2A-C1
21	B	601	BCR	C13-C14-C15-C16
21	B	602	BCR	C9-C10-C11-C12
21	C	502	BCR	C15-C16-C17-C18
21	D	402	BCR	C19-C20-C21-C22
22	A	408	CLA	CBA-CGA-O2A-C1
22	C	510	CLA	CBA-CGA-O2A-C1
27	D	401	LMG	C29-C28-O8-C9
22	C	505	CLA	O1D-CGD-O2D-CED
22	D	404	CLA	O1D-CGD-O2D-CED
27	D	401	LMG	C11-C10-O7-C8
22	B	615	CLA	CBA-CGA-O2A-C1
22	B	609	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	C	510	CLA	O1A-CGA-O2A-C1
27	D	401	LMG	O10-C28-O8-C9
22	B	605	CLA	C2-C3-C5-C6
27	K	101	LMG	O10-C28-O8-C9
25	A	411	PL9	C44-C46-C47-C48
25	D	408	PL9	C34-C36-C37-C38
22	B	614	CLA	C3-C5-C6-C7
22	C	512	CLA	CBA-CGA-O2A-C1
22	A	406	CLA	O1D-CGD-O2D-CED
27	D	401	LMG	O9-C10-O7-C8
22	B	615	CLA	O1A-CGA-O2A-C1
22	C	512	CLA	O1A-CGA-O2A-C1
22	B	604	CLA	CBA-CGA-O2A-C1
22	B	606	CLA	CBA-CGA-O2A-C1
22	C	508	CLA	CBA-CGA-O2A-C1
22	C	514	CLA	CBA-CGA-O2A-C1
27	I	101	LMG	C29-C28-O8-C9
22	C	503	CLA	C8-C10-C11-C12
22	C	512	CLA	C8-C10-C11-C12
22	B	607	CLA	C11-C10-C8-C9
22	B	608	CLA	C11-C10-C8-C9
22	B	612	CLA	C14-C13-C15-C16
22	C	504	CLA	C6-C7-C8-C9
21	B	602	BCR	C7-C8-C9-C34
21	C	501	BCR	C37-C22-C23-C24
21	D	402	BCR	C37-C22-C23-C24
21	H	101	BCR	C36-C18-C19-C20
21	D	402	BCR	C21-C22-C23-C24
22	B	604	CLA	O1A-CGA-O2A-C1
22	B	606	CLA	O1A-CGA-O2A-C1
22	C	514	CLA	O1A-CGA-O2A-C1
22	A	405	CLA	C10-C11-C12-C13
22	B	617	CLA	C8-C10-C11-C12
28	F	101	HEM	C2A-CAA-CBA-CGA
22	B	618	CLA	C10-C11-C12-C13
22	B	613	CLA	CBA-CGA-O2A-C1
22	B	612	CLA	O1D-CGD-O2D-CED
22	B	614	CLA	C2-C1-O2A-CGA
22	B	612	CLA	C11-C10-C8-C7
22	B	613	CLA	C6-C7-C8-C10
22	B	616	CLA	C11-C10-C8-C7
22	D	403	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	B	613	CLA	O1A-CGA-O2A-C1
21	B	601	BCR	C15-C16-C17-C18
21	M	101	BCR	C9-C10-C11-C12
22	B	610	CLA	O1D-CGD-O2D-CED
22	D	403	CLA	C5-C6-C7-C8
22	C	508	CLA	O1A-CGA-O2A-C1
25	A	411	PL9	C14-C16-C17-C18
24	D	407	PHO	C5-C6-C7-C8
22	C	506	CLA	CBA-CGA-O2A-C1
27	I	101	LMG	O10-C28-O8-C9
22	B	609	CLA	C5-C6-C7-C8
22	C	513	CLA	C8-C10-C11-C12
23	A	409	LHG	C3-O3-P-O6
22	C	513	CLA	CBA-CGA-O2A-C1
27	D	401	LMG	C13-C14-C15-C16
24	D	407	PHO	CBA-CGA-O2A-C1
22	B	618	CLA	C3-C5-C6-C7
22	C	504	CLA	O1D-CGD-O2D-CED
22	C	507	CLA	O1D-CGD-O2D-CED
22	D	404	CLA	CBA-CGA-O2A-C1
27	L	101	LMG	C23-C24-C25-C26
27	M	102	LMG	C10-C11-C12-C13
27	D	406	LMG	C33-C34-C35-C36
28	F	101	HEM	C3D-CAD-CBD-CGD
22	B	611	CLA	C16-C17-C18-C19
25	D	408	PL9	C42-C43-C44-C45
27	L	101	LMG	C11-C12-C13-C14
27	L	101	LMG	C17-C18-C19-C20
22	A	405	CLA	C14-C13-C15-C16
22	A	406	CLA	C14-C13-C15-C16
22	B	612	CLA	C6-C7-C8-C9
22	B	616	CLA	C11-C10-C8-C9
27	D	401	LMG	C15-C16-C17-C18
24	A	410	PHO	C2A-CAA-CBA-CGA
22	C	506	CLA	O1A-CGA-O2A-C1
23	A	409	LHG	C27-C28-C29-C30
23	A	412	LHG	O1-C1-C2-C3
21	M	101	BCR	C7-C8-C9-C10
23	A	412	LHG	C23-C24-C25-C26
22	B	605	CLA	C8-C10-C11-C12
27	C	515	LMG	C16-C17-C18-C19
22	C	513	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	C	504	CLA	C3-C5-C6-C7
22	B	616	CLA	CBA-CGA-O2A-C1
22	B	616	CLA	C3A-C2A-CAA-CBA
22	B	617	CLA	C3A-C2A-CAA-CBA
22	B	618	CLA	C3A-C2A-CAA-CBA
22	C	509	CLA	C3A-C2A-CAA-CBA
22	C	510	CLA	C3A-C2A-CAA-CBA
22	B	611	CLA	C16-C17-C18-C20
27	K	101	LMG	C38-C39-C40-C41
22	A	405	CLA	O2A-C1-C2-C3
22	B	610	CLA	O2A-C1-C2-C3
24	D	407	PHO	O1A-CGA-O2A-C1
27	D	405	LMG	C12-C13-C14-C15
22	D	404	CLA	O1A-CGA-O2A-C1
27	D	406	LMG	C28-C29-C30-C31
22	B	608	CLA	C2-C1-O2A-CGA
21	A	404	BCR	C23-C24-C25-C26
21	A	404	BCR	C23-C24-C25-C30
21	B	601	BCR	C23-C24-C25-C26
21	B	602	BCR	C23-C24-C25-C26
21	D	402	BCR	C5-C6-C7-C8
21	H	101	BCR	C1-C6-C7-C8
21	H	101	BCR	C5-C6-C7-C8
21	H	101	BCR	C23-C24-C25-C26
21	J	102	BCR	C5-C6-C7-C8
21	M	101	BCR	C1-C6-C7-C8
22	B	616	CLA	O1A-CGA-O2A-C1
22	A	405	CLA	C12-C13-C15-C16
22	A	406	CLA	C12-C13-C15-C16
22	A	407	CLA	C6-C7-C8-C10
22	B	612	CLA	C12-C13-C15-C16
22	C	505	CLA	C6-C7-C8-C10
22	C	504	CLA	C15-C16-C17-C18
23	A	412	LHG	O9-C7-O7-C5
27	K	101	LMG	O9-C10-O7-C8
22	C	504	CLA	CBA-CGA-O2A-C1
22	A	406	CLA	C2A-CAA-CBA-CGA
22	A	408	CLA	C10-C11-C12-C13
27	D	406	LMG	C18-C19-C20-C21
25	A	411	PL9	C12-C13-C14-C15
25	A	411	PL9	C32-C33-C34-C35
25	A	411	PL9	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
22	B	616	CLA	C3-C5-C6-C7
22	B	607	CLA	CBA-CGA-O2A-C1
23	A	412	LHG	C8-C7-O7-C5
27	K	101	LMG	C11-C10-O7-C8
22	A	407	CLA	C6-C7-C8-C9
22	B	613	CLA	C6-C7-C8-C9
22	C	505	CLA	C6-C7-C8-C9
22	C	508	CLA	C14-C13-C15-C16
22	B	603	CLA	C2A-CAA-CBA-CGA
22	B	605	CLA	C2A-CAA-CBA-CGA
27	C	515	LMG	C31-C32-C33-C34
21	A	404	BCR	C7-C8-C9-C34
21	J	101	BCR	C11-C12-C13-C35
21	J	101	BCR	C37-C22-C23-C24
21	M	101	BCR	C7-C8-C9-C34
21	M	101	BCR	C36-C18-C19-C20
27	K	101	LMG	C22-C23-C24-C25
21	J	101	BCR	C11-C12-C13-C14
21	J	101	BCR	C21-C22-C23-C24
21	H	101	BCR	C13-C14-C15-C16
23	A	409	LHG	C4-O6-P-O3
22	C	509	CLA	C5-C6-C7-C8
22	B	604	CLA	C8-C10-C11-C12
22	B	606	CLA	C5-C6-C7-C8
22	B	606	CLA	C10-C11-C12-C13
22	C	504	CLA	O1A-CGA-O2A-C1
22	B	608	CLA	C3-C5-C6-C7
27	M	102	LMG	C8-C7-O1-C1
27	D	401	LMG	C33-C34-C35-C36
27	M	102	LMG	C36-C37-C38-C39
22	C	508	CLA	C4-C3-C5-C6
27	C	515	LMG	C12-C13-C14-C15
22	C	506	CLA	C2-C1-O2A-CGA
22	B	613	CLA	C8-C10-C11-C12
22	B	607	CLA	O1A-CGA-O2A-C1
23	A	412	LHG	C12-C13-C14-C15
27	L	101	LMG	C8-C9-O8-C28
22	A	405	CLA	CHA-CBD-CGD-O1D
22	A	405	CLA	CHA-CBD-CGD-O2D
22	B	610	CLA	CHA-CBD-CGD-O1D
22	B	610	CLA	CHA-CBD-CGD-O2D
22	C	506	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	C	506	CLA	CHA-CBD-CGD-O2D
22	C	507	CLA	CHA-CBD-CGD-O1D
22	B	618	CLA	C4-C3-C5-C6
22	B	609	CLA	C11-C12-C13-C15
22	B	610	CLA	C12-C13-C15-C16
22	C	503	CLA	C6-C7-C8-C10
22	C	508	CLA	C2-C3-C5-C6
22	C	508	CLA	C12-C13-C15-C16
24	A	410	PHO	C6-C7-C8-C10
22	B	610	CLA	C14-C13-C15-C16
22	B	612	CLA	C11-C10-C8-C9
22	C	503	CLA	C6-C7-C8-C9
27	C	515	LMG	C17-C18-C19-C20
27	K	101	LMG	C40-C41-C42-C43
27	D	406	LMG	C35-C36-C37-C38
22	B	610	CLA	C3-C5-C6-C7
27	D	401	LMG	C20-C21-C22-C23
27	M	102	LMG	C13-C14-C15-C16
22	C	507	CLA	C13-C15-C16-C17
22	B	617	CLA	C5-C6-C7-C8
25	A	411	PL9	C9-C11-C12-C13
22	B	618	CLA	C2-C3-C5-C6
27	D	405	LMG	C13-C14-C15-C16
27	K	101	LMG	C17-C18-C19-C20
22	B	611	CLA	CBA-CGA-O2A-C1
24	A	410	PHO	CBA-CGA-O2A-C1
22	C	507	CLA	C3A-C2A-CAA-CBA
23	A	409	LHG	C4-C5-C6-O8
27	L	101	LMG	C7-C8-C9-O8
22	B	603	CLA	O2A-C1-C2-C3
22	B	608	CLA	O2A-C1-C2-C3
22	C	508	CLA	O2A-C1-C2-C3
22	C	511	CLA	O2A-C1-C2-C3
22	C	514	CLA	O2A-C1-C2-C3
22	B	607	CLA	CAA-CBA-CGA-O2A
22	B	603	CLA	C3-C5-C6-C7
22	D	403	CLA	C2A-CAA-CBA-CGA
23	A	409	LHG	O6-C4-C5-O7
27	M	102	LMG	C15-C16-C17-C18
23	A	409	LHG	O7-C5-C6-O8
27	D	405	LMG	O7-C8-C9-O8
27	L	101	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
21	H	101	BCR	C15-C16-C17-C18
22	B	613	CLA	C2-C1-O2A-CGA
22	B	609	CLA	C11-C12-C13-C14
22	B	617	CLA	C14-C13-C15-C16
22	C	509	CLA	C14-C13-C15-C16
22	C	510	CLA	C14-C13-C15-C16
22	C	511	CLA	C11-C12-C13-C14
22	A	408	CLA	C1A-C2A-CAA-CBA
22	B	607	CLA	C1A-C2A-CAA-CBA
22	B	608	CLA	C1A-C2A-CAA-CBA
21	M	101	BCR	C5-C6-C7-C8
21	C	501	BCR	C21-C22-C23-C24
21	H	101	BCR	C17-C18-C19-C20
22	C	512	CLA	C13-C15-C16-C17
22	D	403	CLA	C10-C11-C12-C13
22	B	612	CLA	C4-C3-C5-C6
22	B	607	CLA	C11-C10-C8-C7
22	B	611	CLA	C11-C12-C13-C15
22	B	612	CLA	C6-C7-C8-C10
22	B	617	CLA	C12-C13-C15-C16
22	C	503	CLA	C11-C12-C13-C15
22	C	510	CLA	C12-C13-C15-C16
21	A	404	BCR	C19-C20-C21-C22
21	C	502	BCR	C13-C14-C15-C16
22	B	608	CLA	CBA-CGA-O2A-C1
22	A	408	CLA	CAD-CBD-CGD-O2D
22	B	607	CLA	CAD-CBD-CGD-O2D
22	B	614	CLA	CAD-CBD-CGD-O2D
22	B	618	CLA	CAD-CBD-CGD-O2D
22	D	404	CLA	CAD-CBD-CGD-O2D
25	A	411	PL9	C20-C19-C21-C22
23	A	409	LHG	C2-C3-O3-P
23	A	412	LHG	C32-C33-C34-C35
27	D	405	LMG	C15-C16-C17-C18
22	B	611	CLA	O1A-CGA-O2A-C1
24	A	410	PHO	O1A-CGA-O2A-C1
22	C	507	CLA	CAA-CBA-CGA-O2A
27	M	102	LMG	C18-C19-C20-C21
22	B	612	CLA	C2-C3-C5-C6
25	A	411	PL9	C4-C3-C7-C8
22	B	611	CLA	C14-C13-C15-C16
22	C	507	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	B	607	CLA	C13-C15-C16-C17
21	C	517	BCR	C36-C18-C19-C20
21	B	602	BCR	C7-C8-C9-C10
21	C	517	BCR	C17-C18-C19-C20
22	A	406	CLA	CBA-CGA-O2A-C1
21	C	517	BCR	C13-C14-C15-C16
23	A	409	LHG	C3-O3-P-O5
25	A	411	PL9	C3-C7-C8-C9
22	B	604	CLA	C16-C17-C18-C19
22	C	504	CLA	C10-C11-C12-C13
22	A	407	CLA	C3-C5-C6-C7
22	A	407	CLA	C16-C17-C18-C20
22	B	605	CLA	CAD-CBD-CGD-O1D
22	B	611	CLA	CAD-CBD-CGD-O1D
22	C	516	CLA	CAD-CBD-CGD-O1D
22	A	406	CLA	O1A-CGA-O2A-C1
24	A	410	PHO	C3-C5-C6-C7
22	B	612	CLA	CBA-CGA-O2A-C1
23	A	409	LHG	C24-C25-C26-C27
24	A	410	PHO	C4-C3-C5-C6
22	B	608	CLA	C11-C10-C8-C7
22	B	614	CLA	C11-C12-C13-C15
22	C	505	CLA	C12-C13-C15-C16
22	C	507	CLA	C6-C7-C8-C10
22	C	507	CLA	C12-C13-C15-C16
22	C	514	CLA	C6-C7-C8-C10
22	C	516	CLA	C12-C13-C15-C16
22	A	408	CLA	C2A-CAA-CBA-CGA
22	C	504	CLA	C2A-CAA-CBA-CGA
22	B	608	CLA	O1A-CGA-O2A-C1
22	C	512	CLA	C10-C11-C12-C13
24	D	407	PHO	O2A-C1-C2-C3
27	D	405	LMG	C8-C7-O1-C1
22	C	511	CLA	CBA-CGA-O2A-C1
22	B	609	CLA	C14-C13-C15-C16
22	B	616	CLA	C11-C12-C13-C14
22	C	516	CLA	C14-C13-C15-C16
22	D	403	CLA	C11-C10-C8-C9
22	A	406	CLA	C2C-C3C-CAC-CBC
22	B	612	CLA	O1A-CGA-O2A-C1
22	C	511	CLA	O1A-CGA-O2A-C1
23	A	412	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
22	B	611	CLA	C10-C11-C12-C13
27	C	515	LMG	C33-C34-C35-C36
27	L	101	LMG	C15-C16-C17-C18
23	A	409	LHG	O2-C2-C3-O3
24	A	410	PHO	C2-C3-C5-C6
22	D	403	CLA	C13-C15-C16-C17
23	A	409	LHG	C18-C19-C20-C21
22	C	511	CLA	C3-C5-C6-C7
27	D	401	LMG	C9-C8-O7-C10
27	D	401	LMG	C36-C37-C38-C39
25	A	411	PL9	C15-C14-C16-C17
21	B	601	BCR	C23-C24-C25-C30
21	J	102	BCR	C1-C6-C7-C8
22	C	507	CLA	C2C-C3C-CAC-CBC
23	A	409	LHG	C12-C13-C14-C15
25	D	408	PL9	C44-C46-C47-C48
24	D	407	PHO	C8-C10-C11-C12
22	A	407	CLA	CHA-CBD-CGD-O2D
22	B	609	CLA	CHA-CBD-CGD-O2D
22	B	612	CLA	CHA-CBD-CGD-O2D
22	B	613	CLA	CHA-CBD-CGD-O1D
22	B	613	CLA	CHA-CBD-CGD-O2D
22	C	503	CLA	CHA-CBD-CGD-O2D
22	C	504	CLA	CHA-CBD-CGD-O1D
22	C	504	CLA	CHA-CBD-CGD-O2D
22	C	507	CLA	CHA-CBD-CGD-O2D
22	C	510	CLA	CHA-CBD-CGD-O1D
22	C	510	CLA	CHA-CBD-CGD-O2D
22	D	403	CLA	CHA-CBD-CGD-O2D
22	B	611	CLA	C12-C13-C15-C16
27	L	101	LMG	C30-C31-C32-C33
22	C	503	CLA	C14-C13-C15-C16
21	A	404	BCR	C9-C10-C11-C12
22	A	407	CLA	C16-C17-C18-C19
22	C	503	CLA	C16-C17-C18-C20
27	L	101	LMG	C20-C21-C22-C23
27	C	515	LMG	C36-C37-C38-C39
21	C	501	BCR	C11-C12-C13-C35
27	I	101	LMG	C20-C21-C22-C23
21	C	501	BCR	C11-C12-C13-C14
22	B	604	CLA	C16-C17-C18-C20
21	B	601	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	B	604	CLA	C4-C3-C5-C6
22	C	510	CLA	C4-C3-C5-C6
22	A	408	CLA	C2-C3-C5-C6
22	B	604	CLA	C2-C3-C5-C6
27	L	101	LMG	C22-C23-C24-C25
22	A	408	CLA	C4-C3-C5-C6
27	M	102	LMG	C28-C29-C30-C31
22	B	609	CLA	C11-C10-C8-C9
23	A	409	LHG	C31-C32-C33-C34
22	A	408	CLA	O2A-C1-C2-C3
22	B	618	CLA	O2A-C1-C2-C3
24	A	410	PHO	O2A-C1-C2-C3
27	D	406	LMG	C36-C37-C38-C39
21	C	501	BCR	C36-C18-C19-C20
21	A	404	BCR	C7-C8-C9-C10
27	M	102	LMG	C29-C30-C31-C32
27	D	406	LMG	C9-C8-O7-C10
22	C	504	CLA	C12-C13-C15-C16
21	J	101	BCR	C15-C16-C17-C18
23	A	409	LHG	C28-C29-C30-C31
28	F	101	HEM	CAA-CBA-CGA-O1A
22	B	613	CLA	C2A-CAA-CBA-CGA
22	C	503	CLA	C2A-CAA-CBA-CGA
22	C	511	CLA	C8-C10-C11-C12
25	A	411	PL9	C17-C18-C19-C20
24	D	407	PHO	C2C-C3C-CAC-CBC
22	B	603	CLA	C13-C15-C16-C17
22	C	516	CLA	C13-C15-C16-C17
22	C	511	CLA	C10-C11-C12-C13
24	D	407	PHO	C10-C11-C12-C13
25	D	408	PL9	C39-C41-C42-C43
22	C	514	CLA	C3-C5-C6-C7
22	C	507	CLA	C4-C3-C5-C6
22	D	404	CLA	C2-C1-O2A-CGA
22	C	507	CLA	C11-C12-C13-C14
22	C	511	CLA	C6-C7-C8-C9
22	A	408	CLA	C3-C5-C6-C7
28	F	101	HEM	CAA-CBA-CGA-O2A
22	A	407	CLA	C1A-C2A-CAA-CBA
22	B	603	CLA	C1A-C2A-CAA-CBA
22	B	610	CLA	C1A-C2A-CAA-CBA
22	C	507	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	C	514	CLA	C1A-C2A-CAA-CBA
23	A	412	LHG	O2-C2-C3-O3
22	B	612	CLA	C2A-CAA-CBA-CGA
21	J	102	BCR	C23-C24-C25-C30
22	B	617	CLA	C4-C3-C5-C6
22	B	612	CLA	C3-C5-C6-C7
27	D	406	LMG	C8-C7-O1-C1
27	C	515	LMG	C23-C24-C25-C26
27	D	406	LMG	C24-C25-C26-C27
24	A	410	PHO	C10-C11-C12-C13
23	A	409	LHG	O6-C4-C5-C6
22	A	405	CLA	C4-C3-C5-C6
25	A	411	PL9	C24-C26-C27-C28
22	B	617	CLA	C2-C3-C5-C6
25	A	411	PL9	C18-C19-C21-C22
27	D	406	LMG	C31-C32-C33-C34
22	C	505	CLA	C4-C3-C5-C6
22	C	510	CLA	C2-C3-C5-C6
22	B	604	CLA	C11-C12-C13-C14
22	B	611	CLA	C11-C12-C13-C14
22	B	614	CLA	C11-C12-C13-C14
22	C	503	CLA	C11-C12-C13-C14
22	C	505	CLA	C14-C13-C15-C16
22	C	514	CLA	C6-C7-C8-C9
22	B	604	CLA	CAD-CBD-CGD-O2D
22	B	615	CLA	CAD-CBD-CGD-O2D
22	B	616	CLA	CAD-CBD-CGD-O2D
22	B	613	CLA	CAA-CBA-CGA-O2A
27	L	101	LMG	O7-C10-C11-C12
22	A	406	CLA	C4-C3-C5-C6
22	C	507	CLA	C2-C3-C5-C6
22	C	505	CLA	CAA-CBA-CGA-O2A
22	C	512	CLA	CAA-CBA-CGA-O2A
27	K	101	LMG	O8-C28-C29-C30
21	C	501	BCR	C17-C18-C19-C20
21	M	101	BCR	C17-C18-C19-C20
27	D	405	LMG	C7-C8-C9-O8
22	B	607	CLA	CAA-CBA-CGA-O1A
22	B	604	CLA	O2A-C1-C2-C3
22	D	404	CLA	O2A-C1-C2-C3
22	B	618	CLA	CAA-CBA-CGA-O2A
22	C	516	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	C	509	CLA	CAA-CBA-CGA-O2A
25	A	411	PL9	C13-C14-C16-C17
22	B	612	CLA	CAA-CBA-CGA-O2A
27	L	101	LMG	O8-C28-C29-C30
22	A	407	CLA	CHA-CBD-CGD-O1D
22	B	604	CLA	CHA-CBD-CGD-O1D
22	B	609	CLA	CHA-CBD-CGD-O1D
22	B	612	CLA	CHA-CBD-CGD-O1D
22	B	614	CLA	CHA-CBD-CGD-O1D
22	C	505	CLA	CHA-CBD-CGD-O1D
22	D	403	CLA	CHA-CBD-CGD-O1D
23	A	412	LHG	C28-C29-C30-C31
27	M	102	LMG	O7-C10-C11-C12
27	I	101	LMG	O6-C1-O1-C7
22	D	403	CLA	CAA-CBA-CGA-O2A
23	A	412	LHG	C29-C30-C31-C32
22	C	504	CLA	C11-C12-C13-C14
22	C	504	CLA	C14-C13-C15-C16
22	C	507	CLA	C14-C13-C15-C16
27	K	101	LMG	C12-C13-C14-C15
27	D	405	LMG	C40-C41-C42-C43
22	C	513	CLA	C16-C17-C18-C20
23	A	412	LHG	C17-C18-C19-C20
22	B	613	CLA	CAA-CBA-CGA-O1A
22	C	512	CLA	CAA-CBA-CGA-O1A
27	K	101	LMG	C37-C38-C39-C40
22	C	505	CLA	CAA-CBA-CGA-O1A
27	K	101	LMG	O10-C28-C29-C30
22	C	512	CLA	C3-C5-C6-C7
22	C	509	CLA	CAA-CBA-CGA-O1A
22	C	516	CLA	CAA-CBA-CGA-O1A
22	B	616	CLA	CAA-CBA-CGA-O2A
22	B	609	CLA	C10-C11-C12-C13
22	B	612	CLA	CAA-CBA-CGA-O1A
22	B	618	CLA	CAA-CBA-CGA-O1A
22	D	403	CLA	CAA-CBA-CGA-O1A
21	B	602	BCR	C23-C24-C25-C30
27	L	101	LMG	O10-C28-C29-C30
27	I	101	LMG	C29-C30-C31-C32
27	L	101	LMG	O9-C10-C11-C12
27	I	101	LMG	C30-C31-C32-C33
25	A	411	PL9	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
22	A	405	CLA	C2-C3-C5-C6
23	A	409	LHG	C32-C33-C34-C35
22	B	606	CLA	CAD-CBD-CGD-O1D
23	A	409	LHG	C4-C5-O7-C7
27	M	102	LMG	O9-C10-C11-C12
22	B	607	CLA	C11-C12-C13-C14
22	C	516	CLA	C11-C12-C13-C14
23	A	412	LHG	O8-C23-C24-C25
22	B	610	CLA	CAA-CBA-CGA-O2A
23	A	412	LHG	O7-C7-C8-C9
22	B	616	CLA	CAA-CBA-CGA-O1A
25	D	408	PL9	C37-C38-C39-C41
22	A	405	CLA	C6-C7-C8-C10
22	B	603	CLA	C3A-C2A-CAA-CBA
22	B	615	CLA	C12-C13-C15-C16
22	C	504	CLA	C11-C12-C13-C15
22	C	504	CLA	CAA-CBA-CGA-O1A
22	C	504	CLA	CAA-CBA-CGA-O2A
21	C	502	BCR	C11-C12-C13-C14
21	C	502	BCR	C9-C10-C11-C12
27	D	406	LMG	C14-C15-C16-C17
22	B	605	CLA	C10-C11-C12-C13
27	D	406	LMG	C23-C24-C25-C26
22	C	510	CLA	C13-C15-C16-C17
22	C	511	CLA	CAA-CBA-CGA-O2A
22	C	512	CLA	C5-C6-C7-C8

There are no ring outliers.

24 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	M	101	BCR	1	0
21	J	102	BCR	1	0
22	B	610	CLA	1	0
22	B	614	CLA	1	0
22	B	604	CLA	1	0
22	D	403	CLA	3	0
21	J	101	BCR	2	0
24	D	407	PHO	2	0
22	B	606	CLA	1	0
22	B	617	CLA	1	0
21	C	502	BCR	3	0

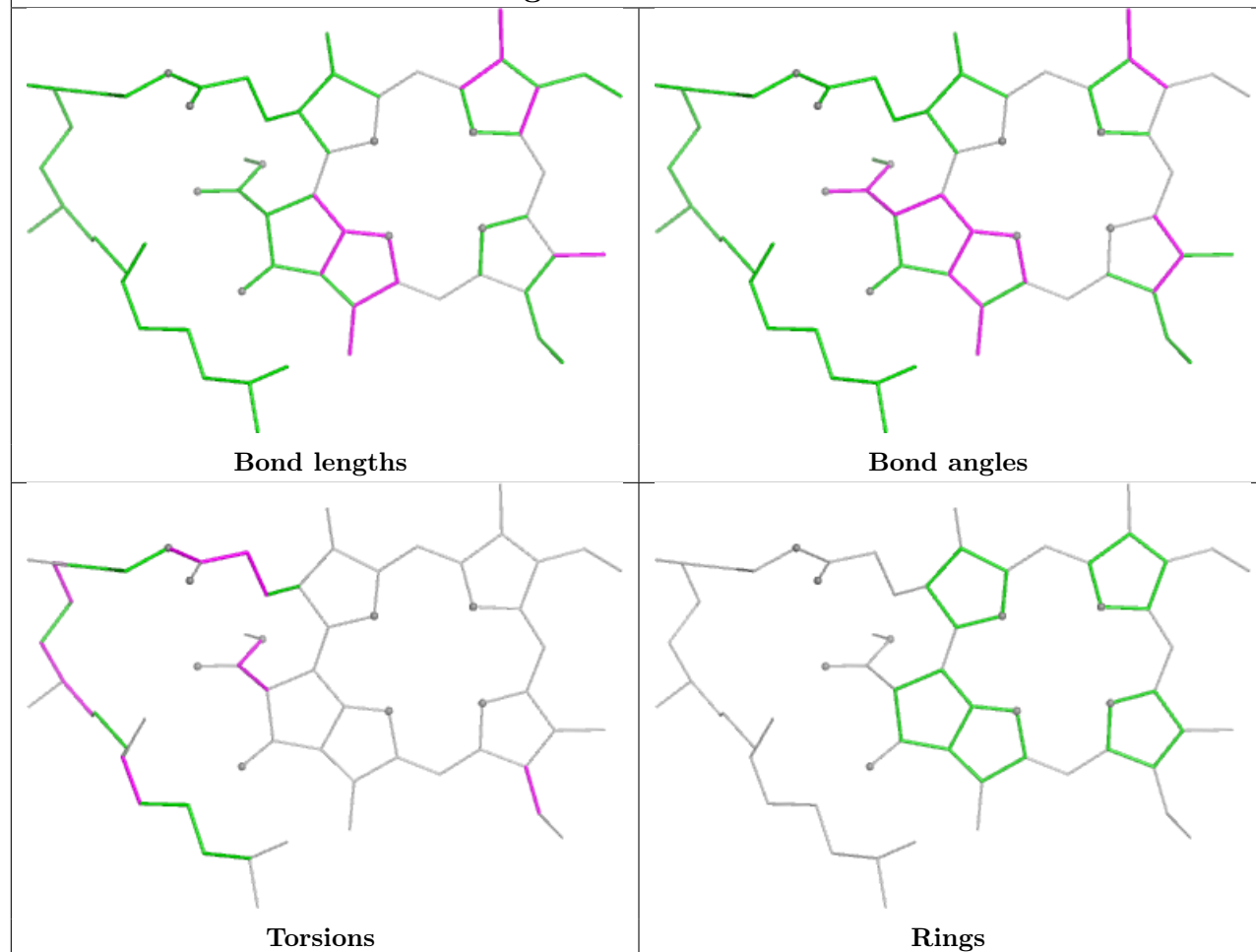
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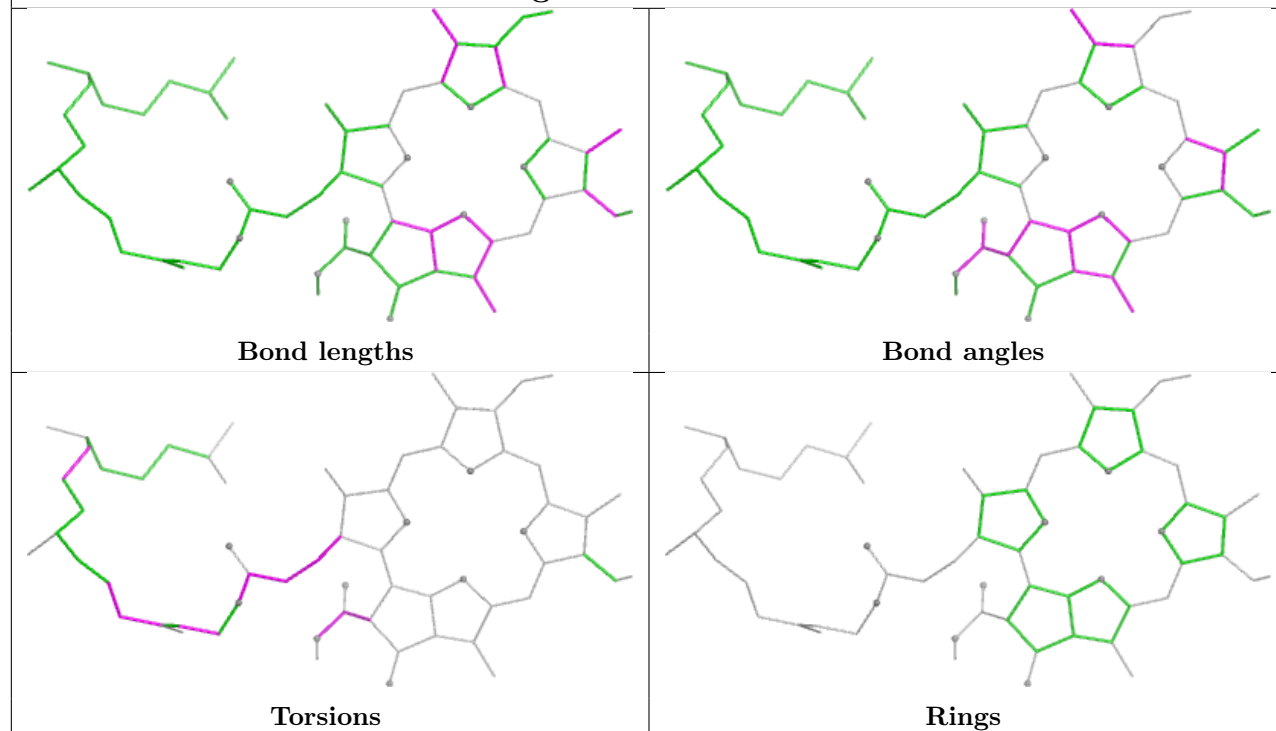
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	507	CLA	3	0
22	C	503	CLA	2	0
22	A	405	CLA	3	0
22	A	406	CLA	1	0
22	B	616	CLA	1	0
22	C	506	CLA	1	0
22	D	404	CLA	1	0
28	F	101	HEM	4	0
27	D	406	LMG	1	0
22	A	407	CLA	1	0
22	B	605	CLA	3	0
21	A	404	BCR	1	0
21	C	517	BCR	4	0

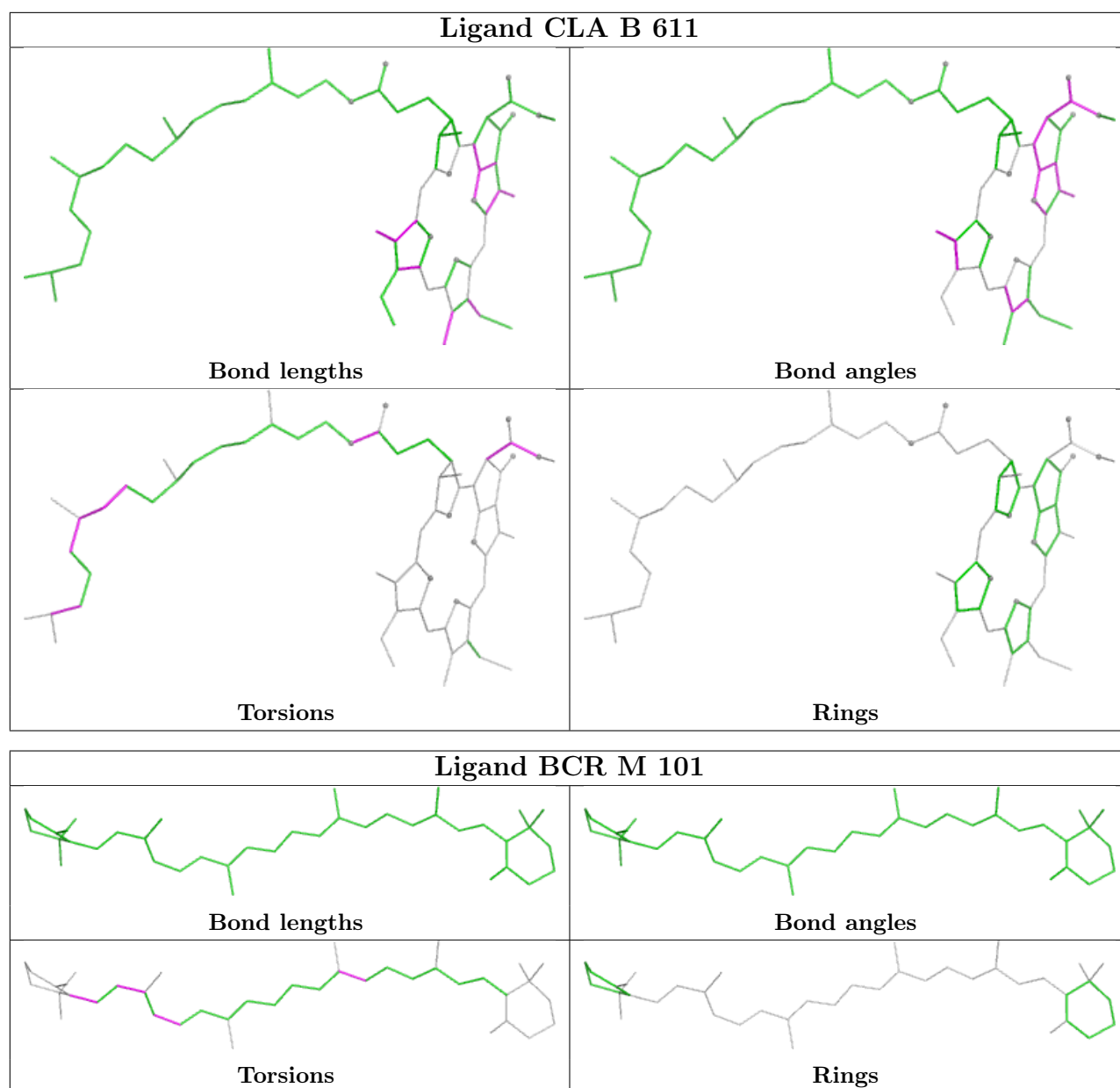
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

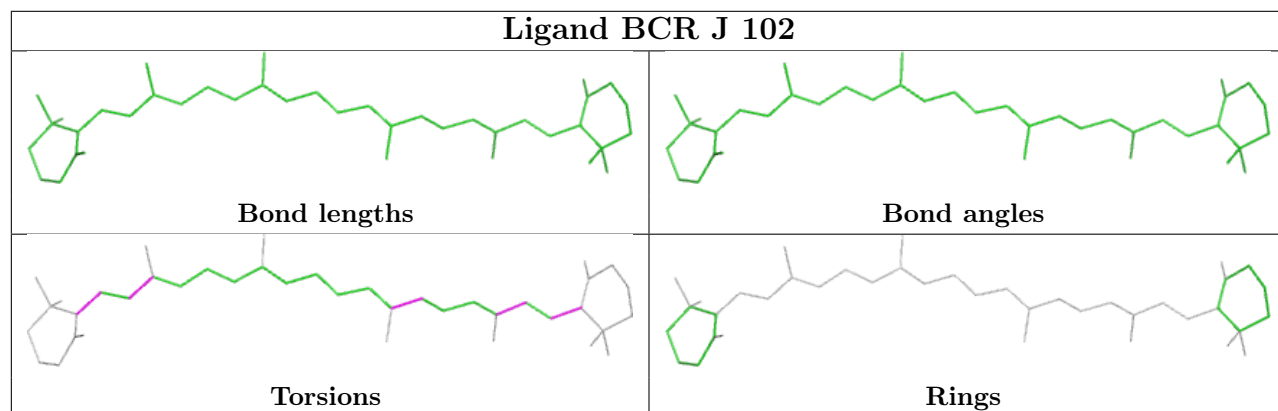
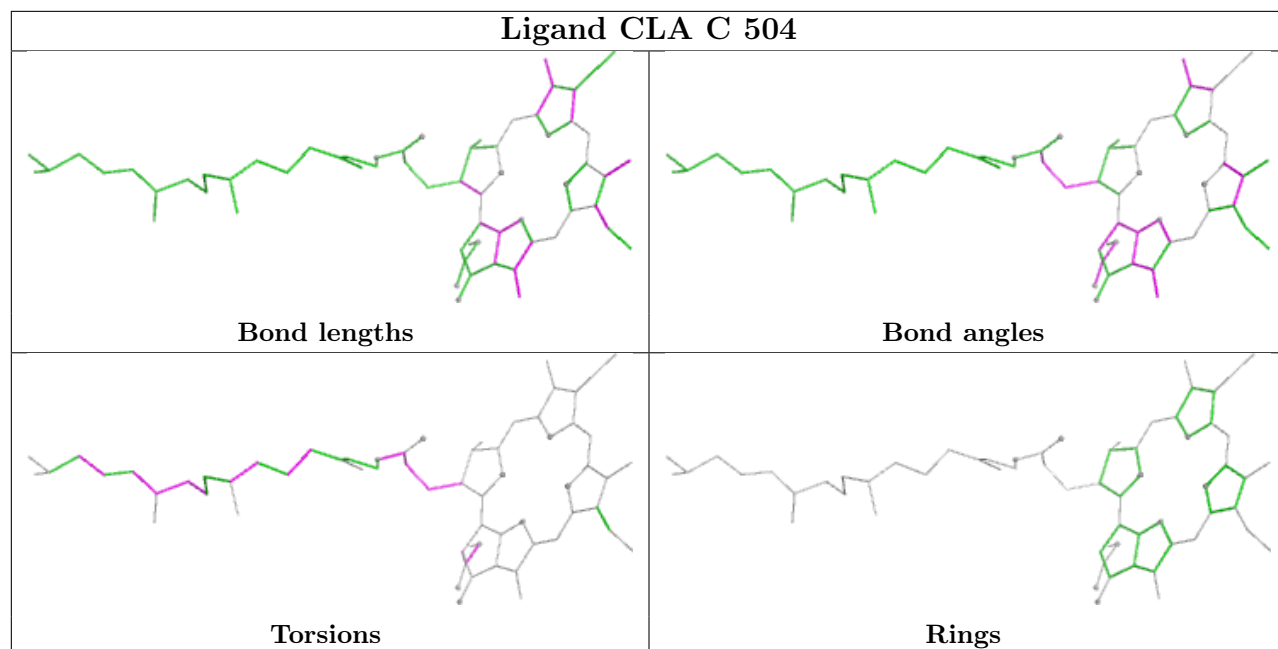
Ligand CLA B 612

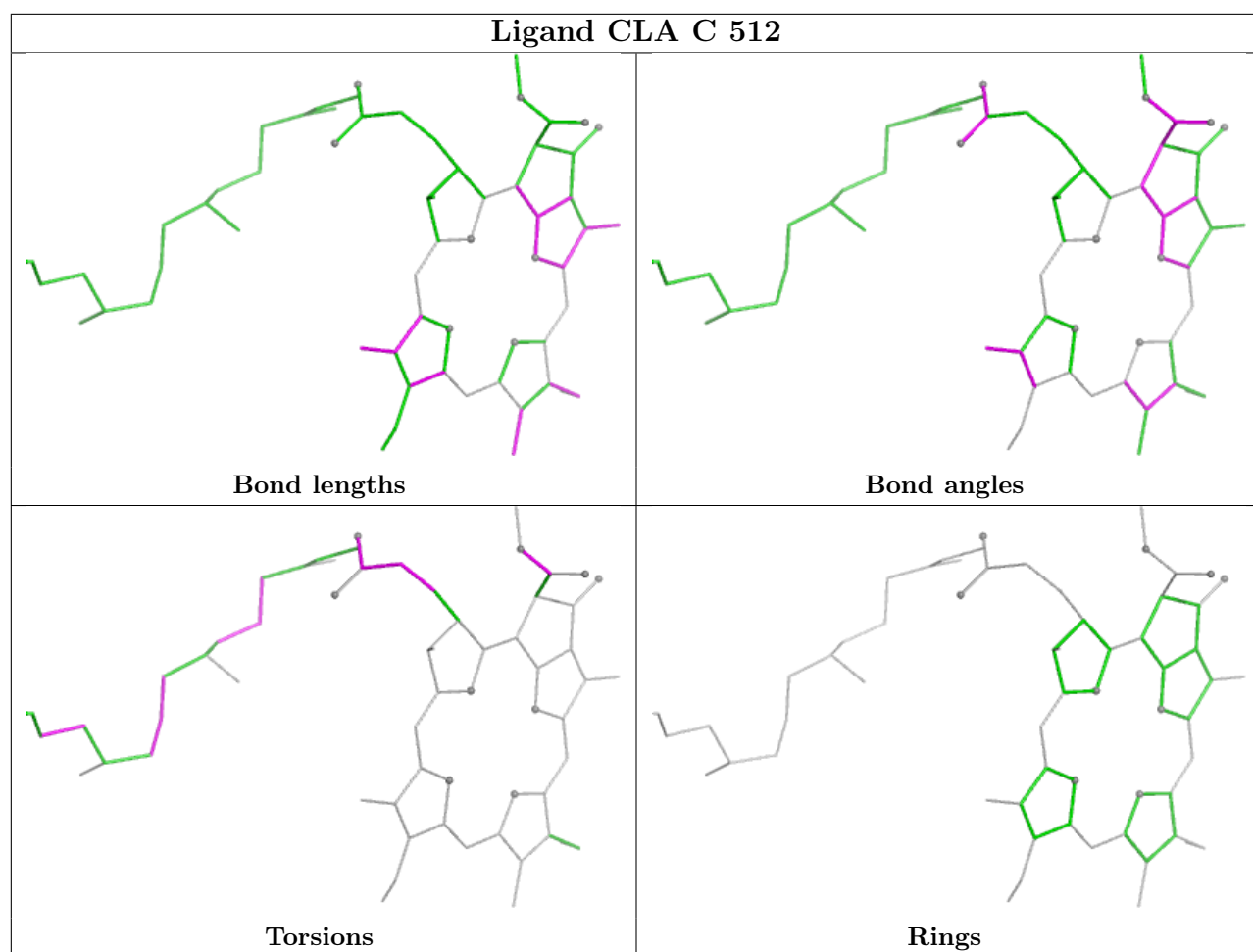


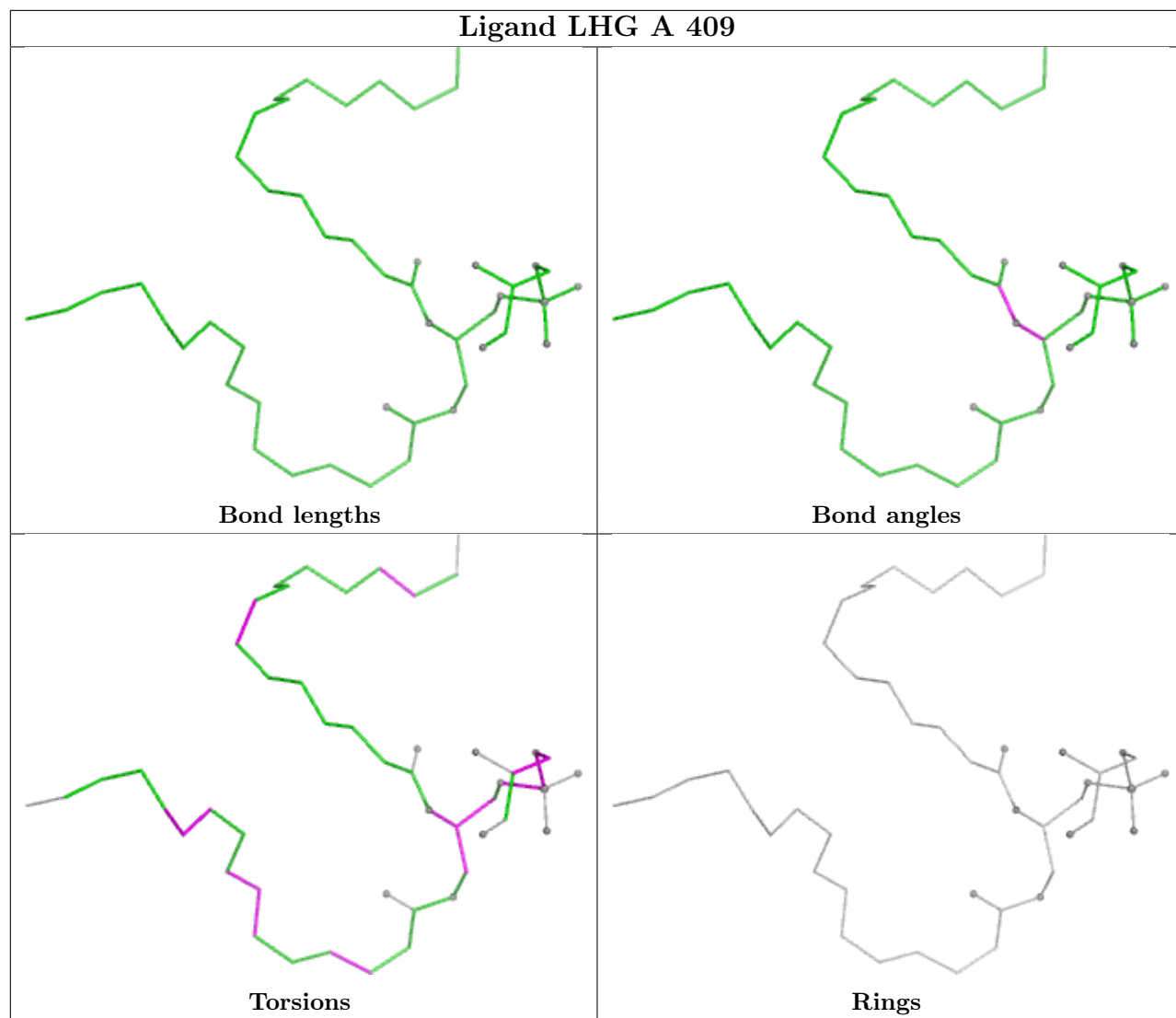
Ligand CLA B 618

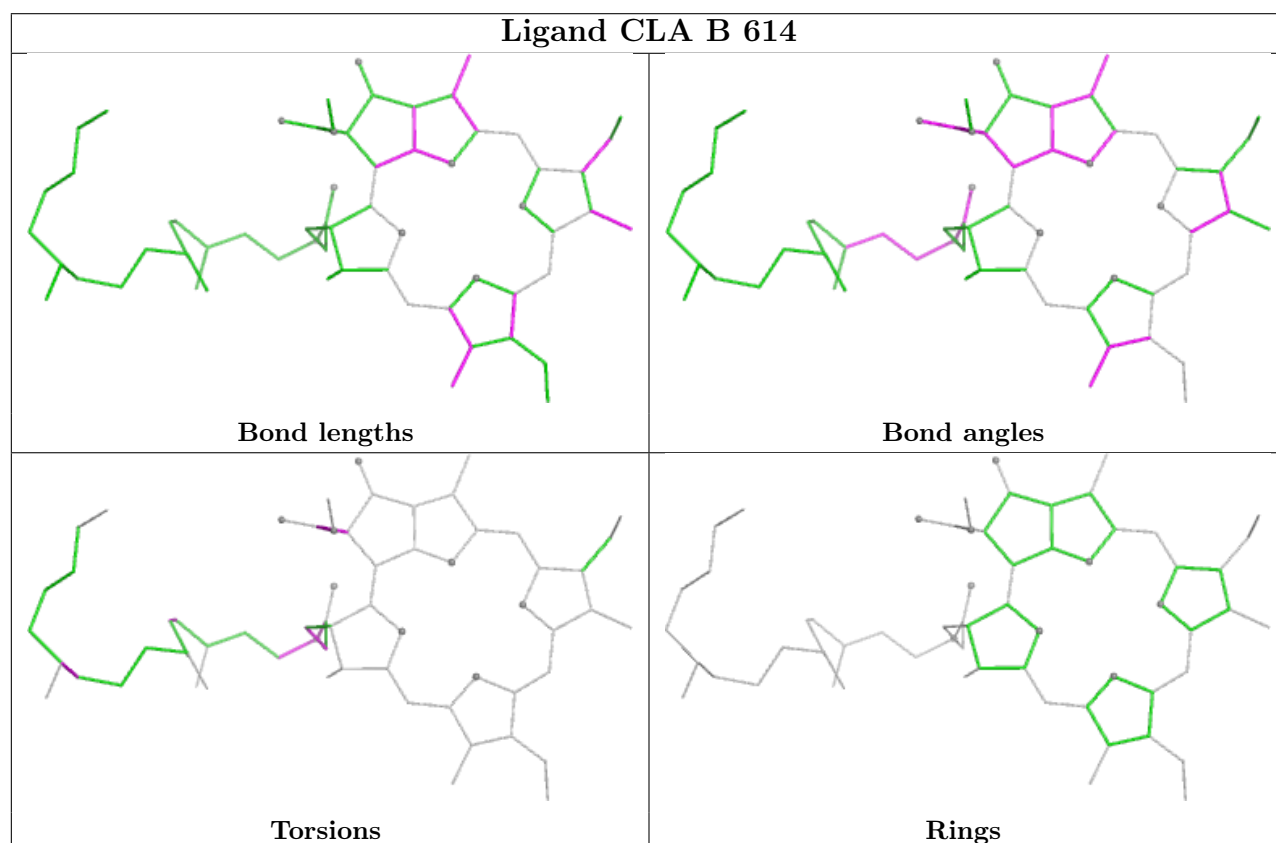
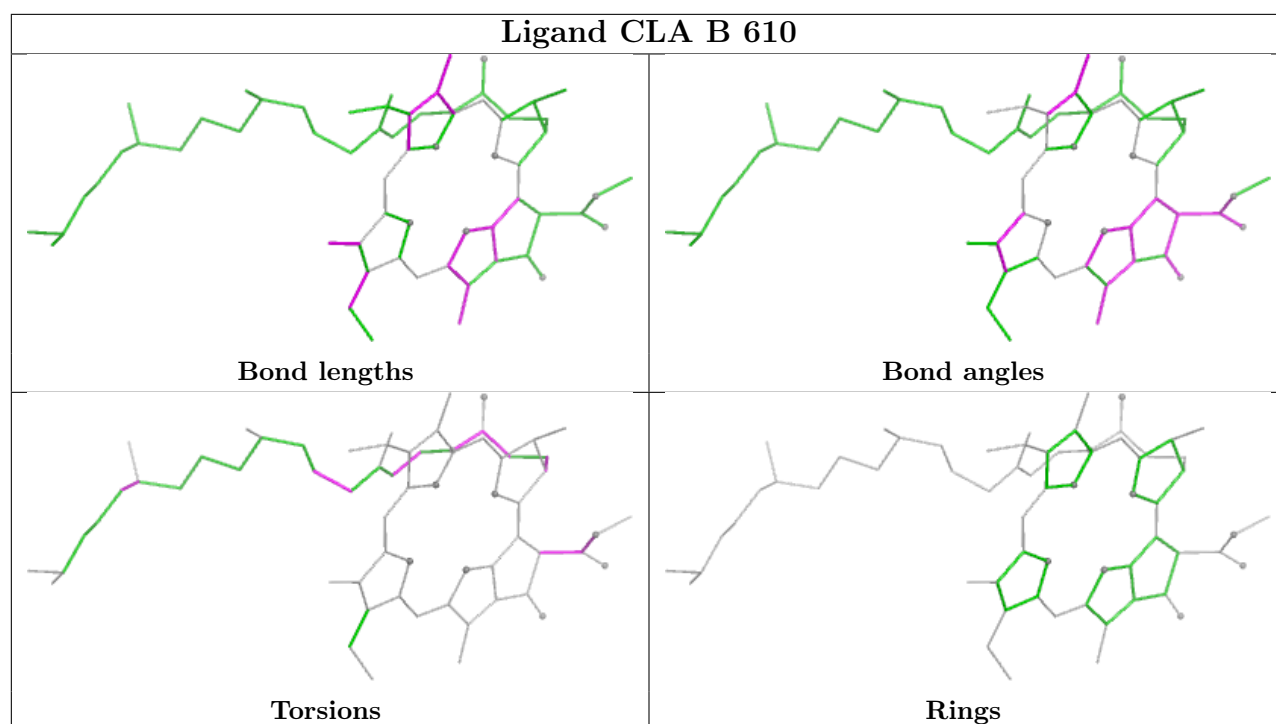


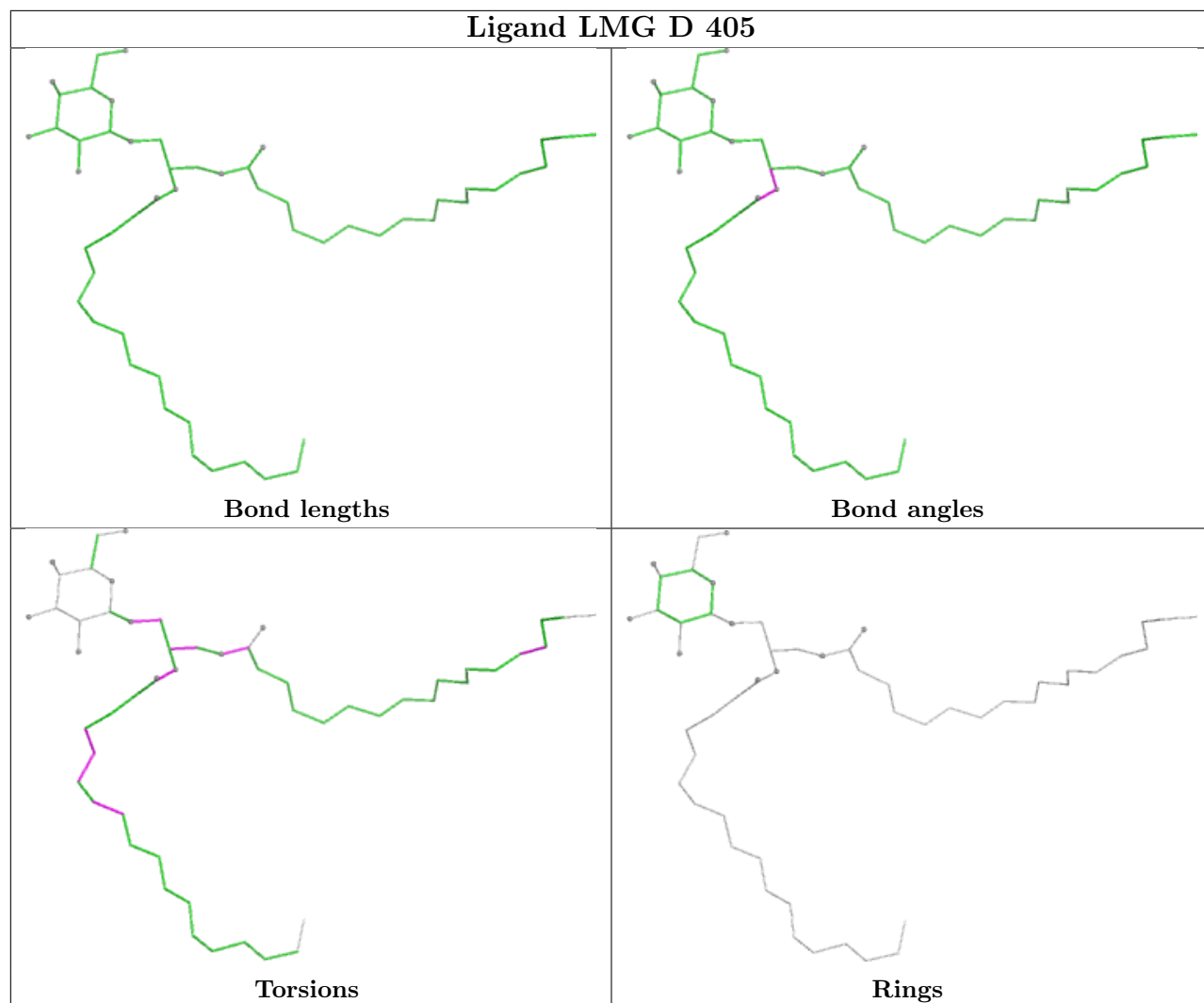


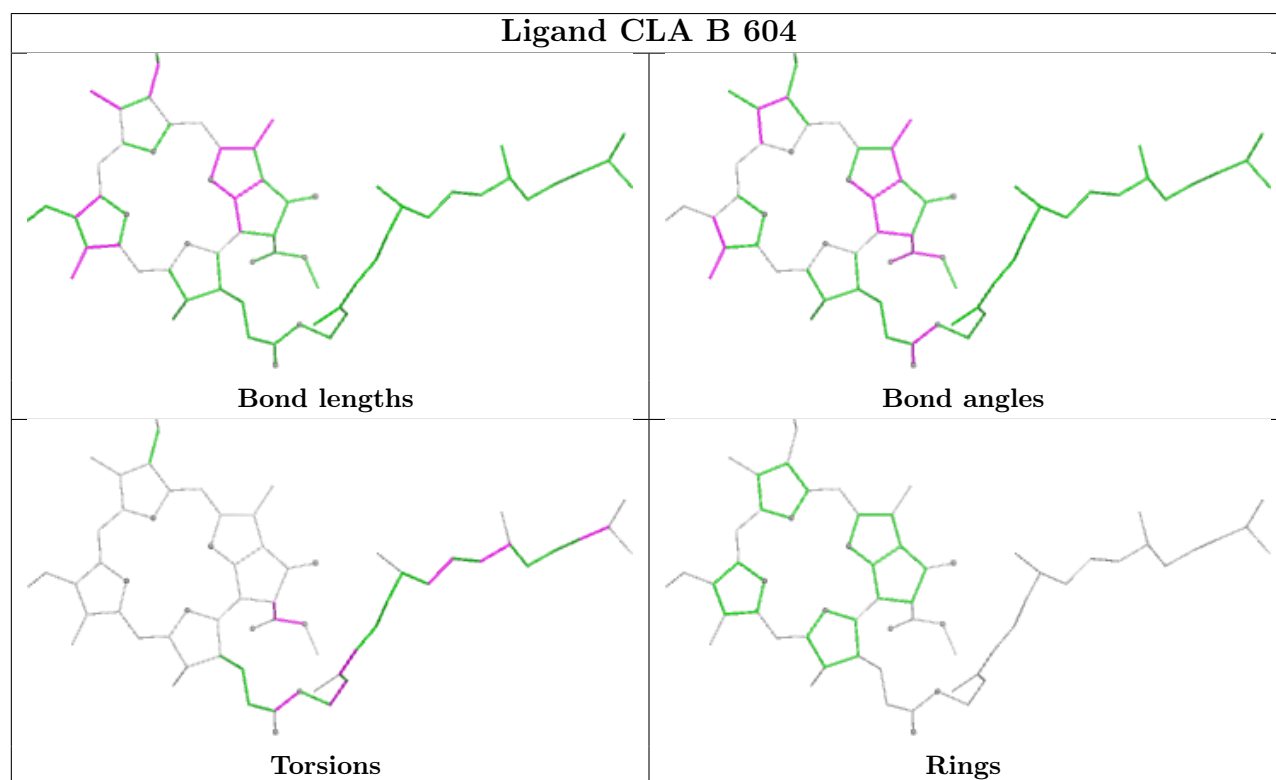
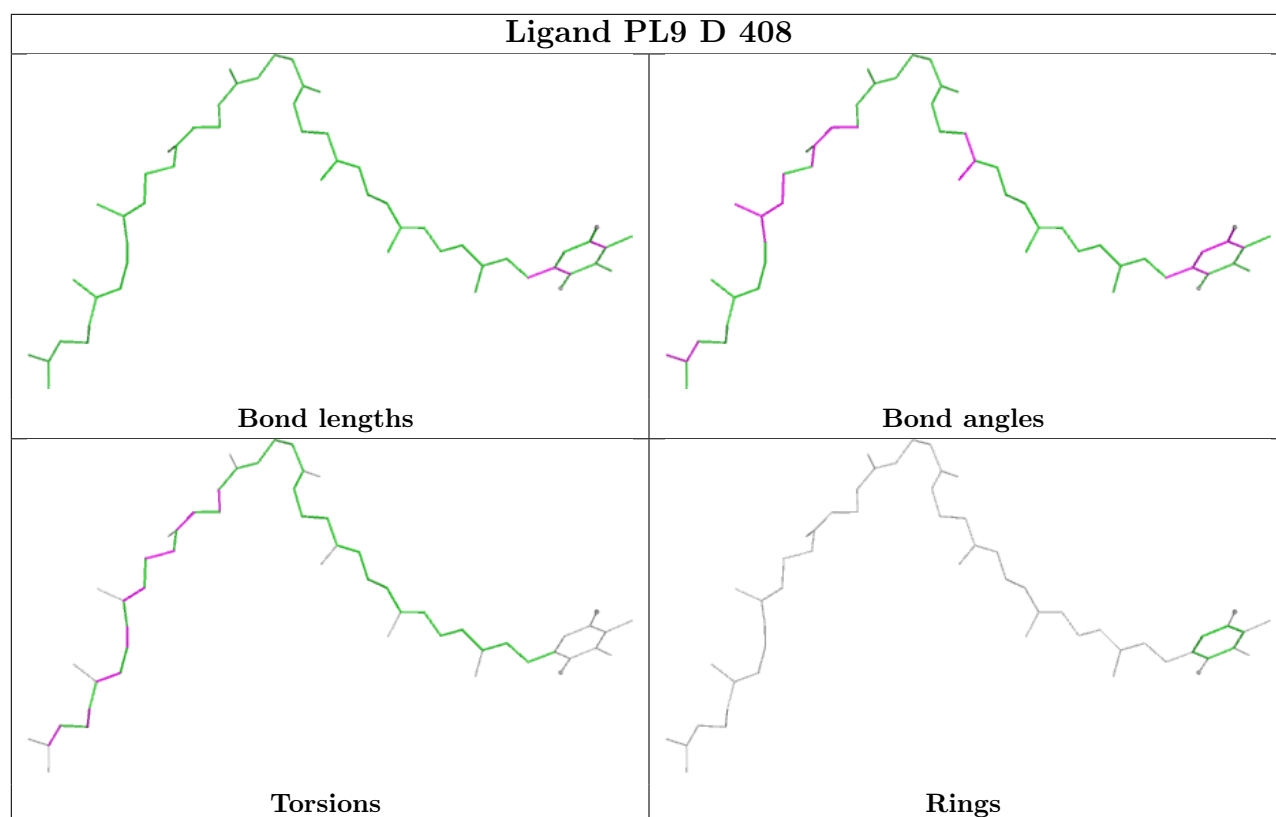


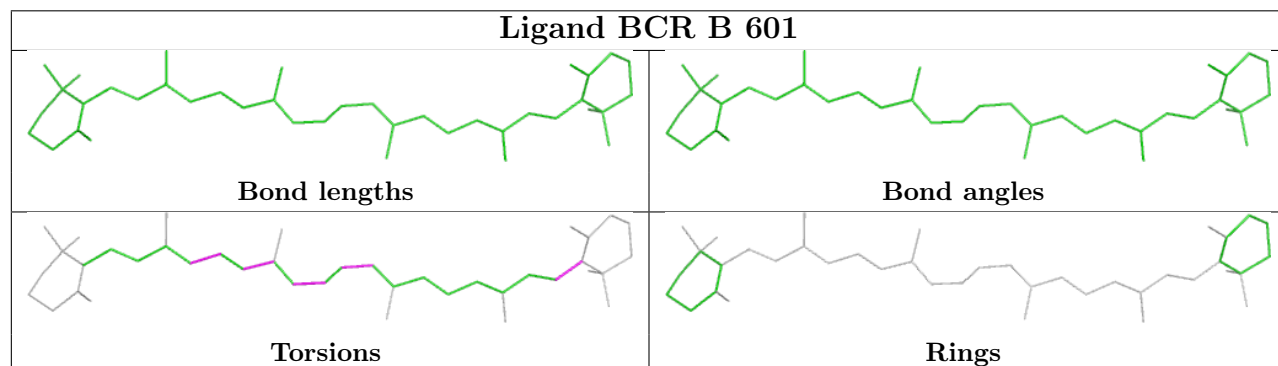
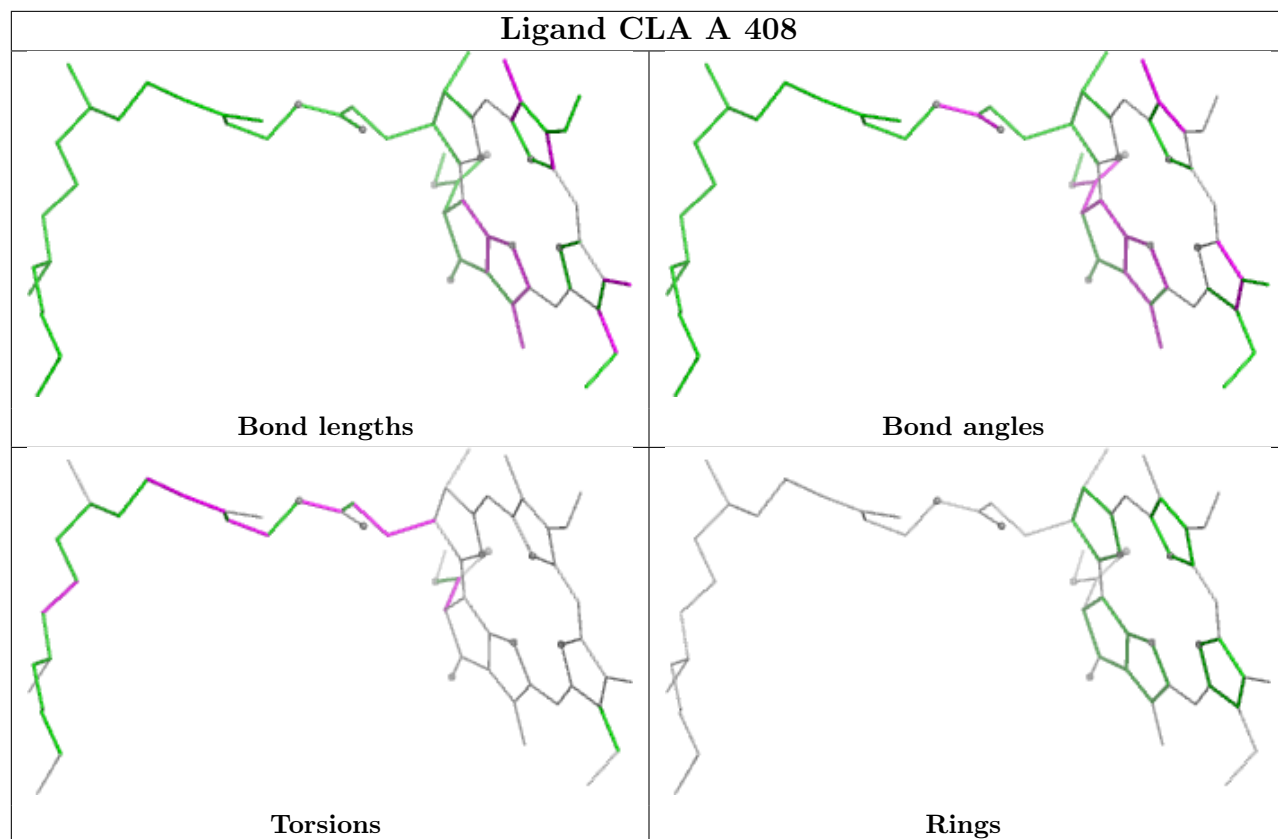


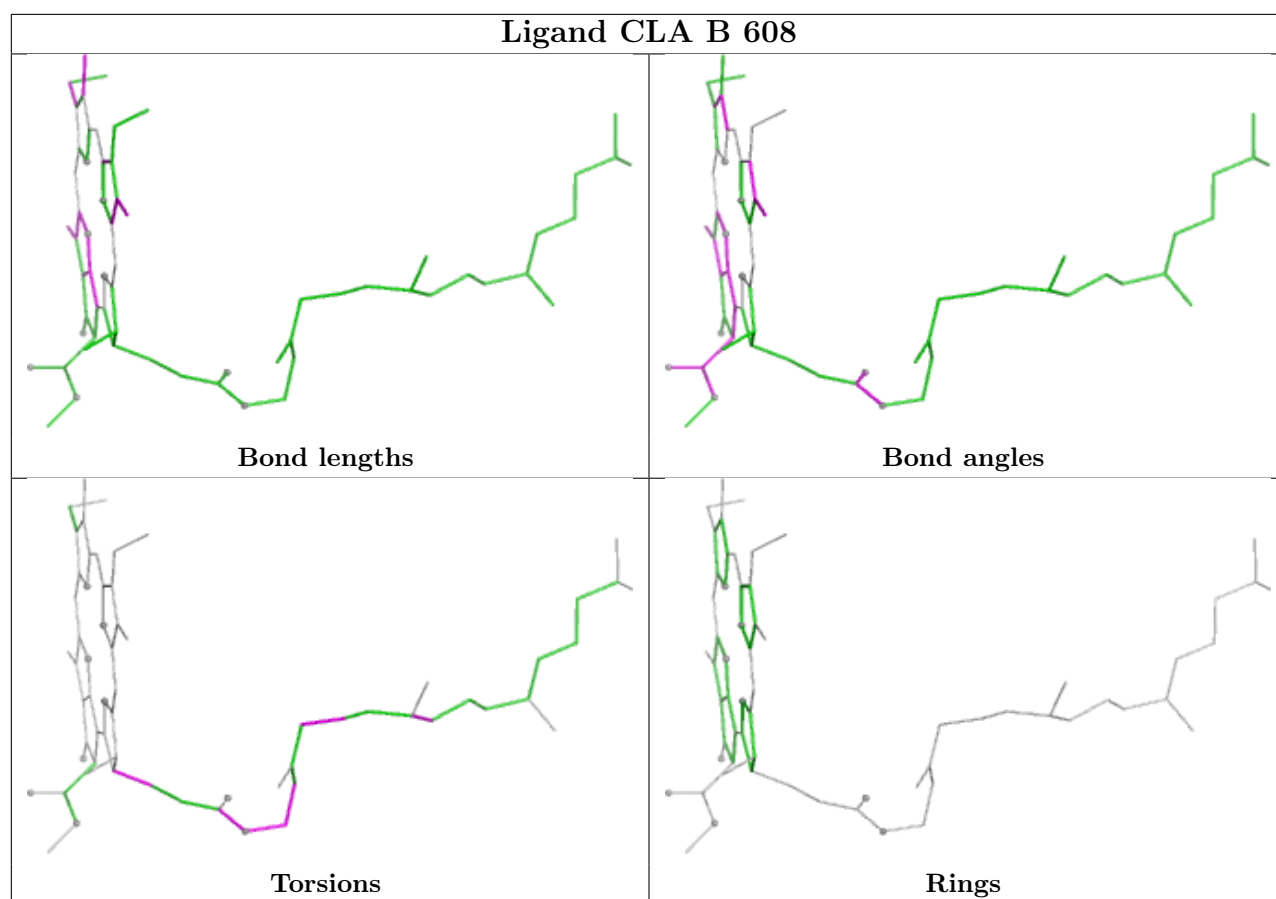


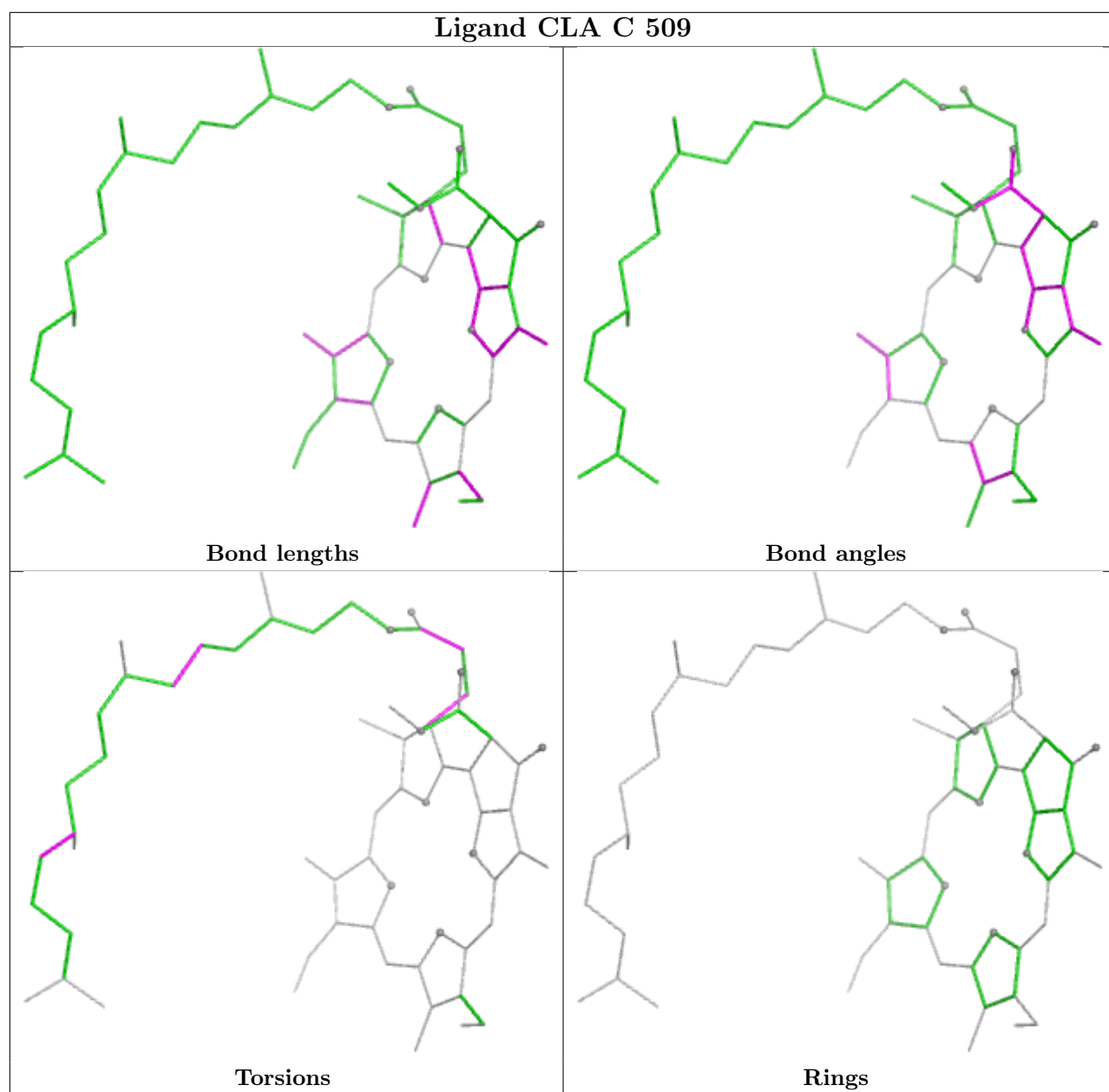


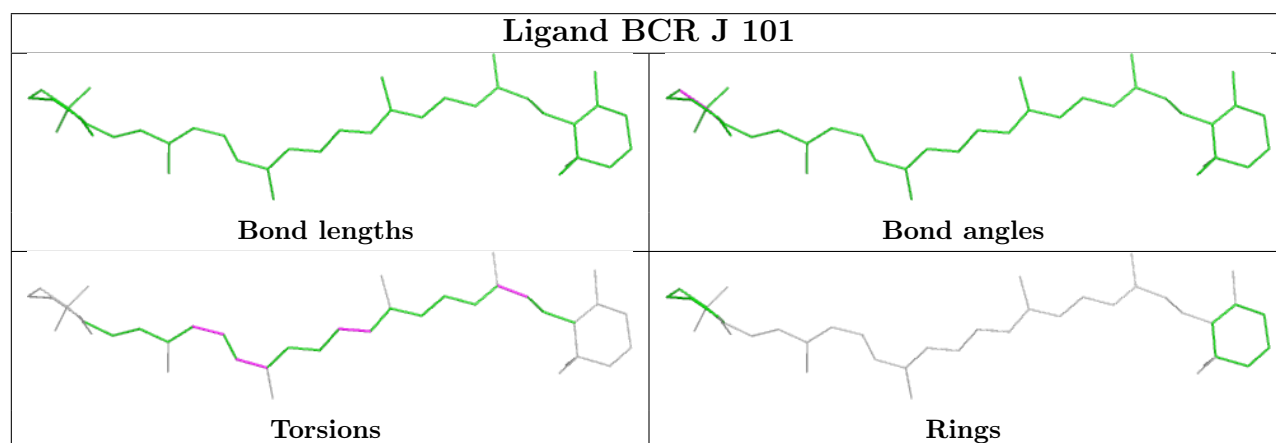
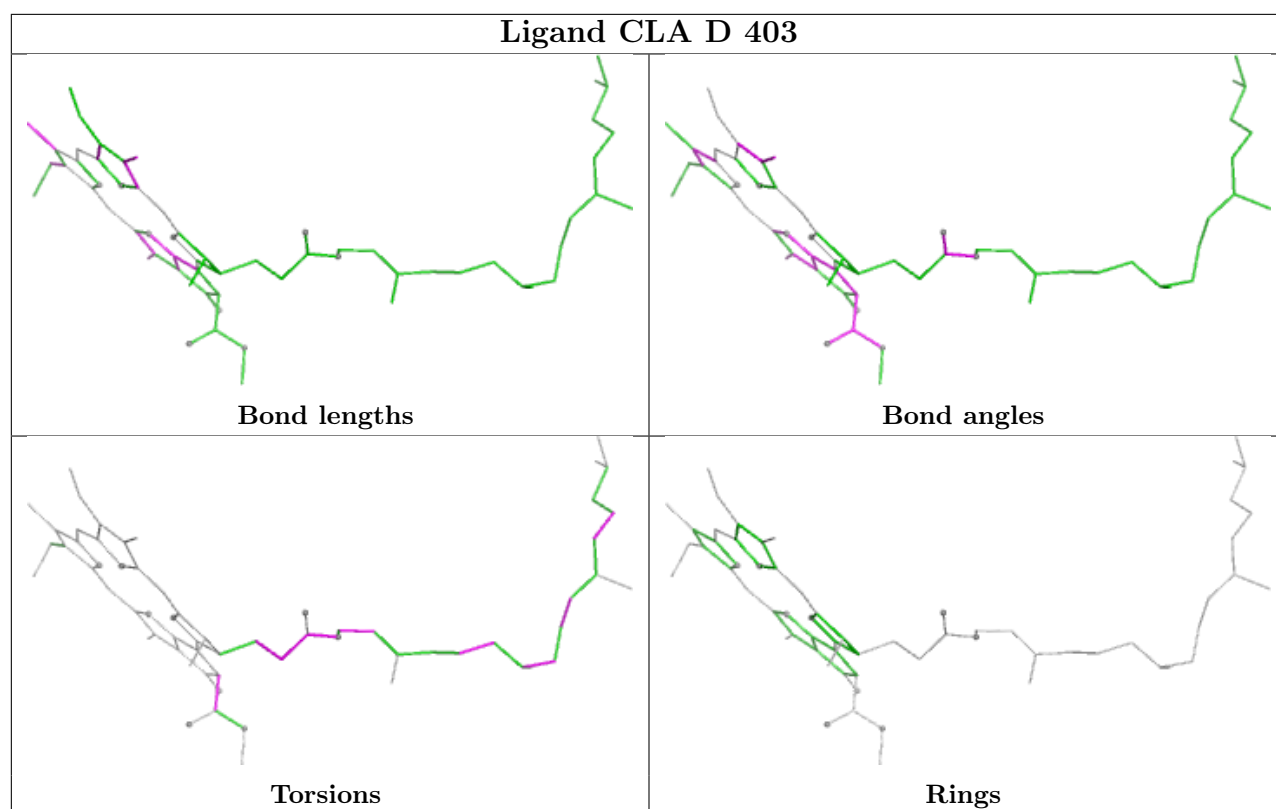


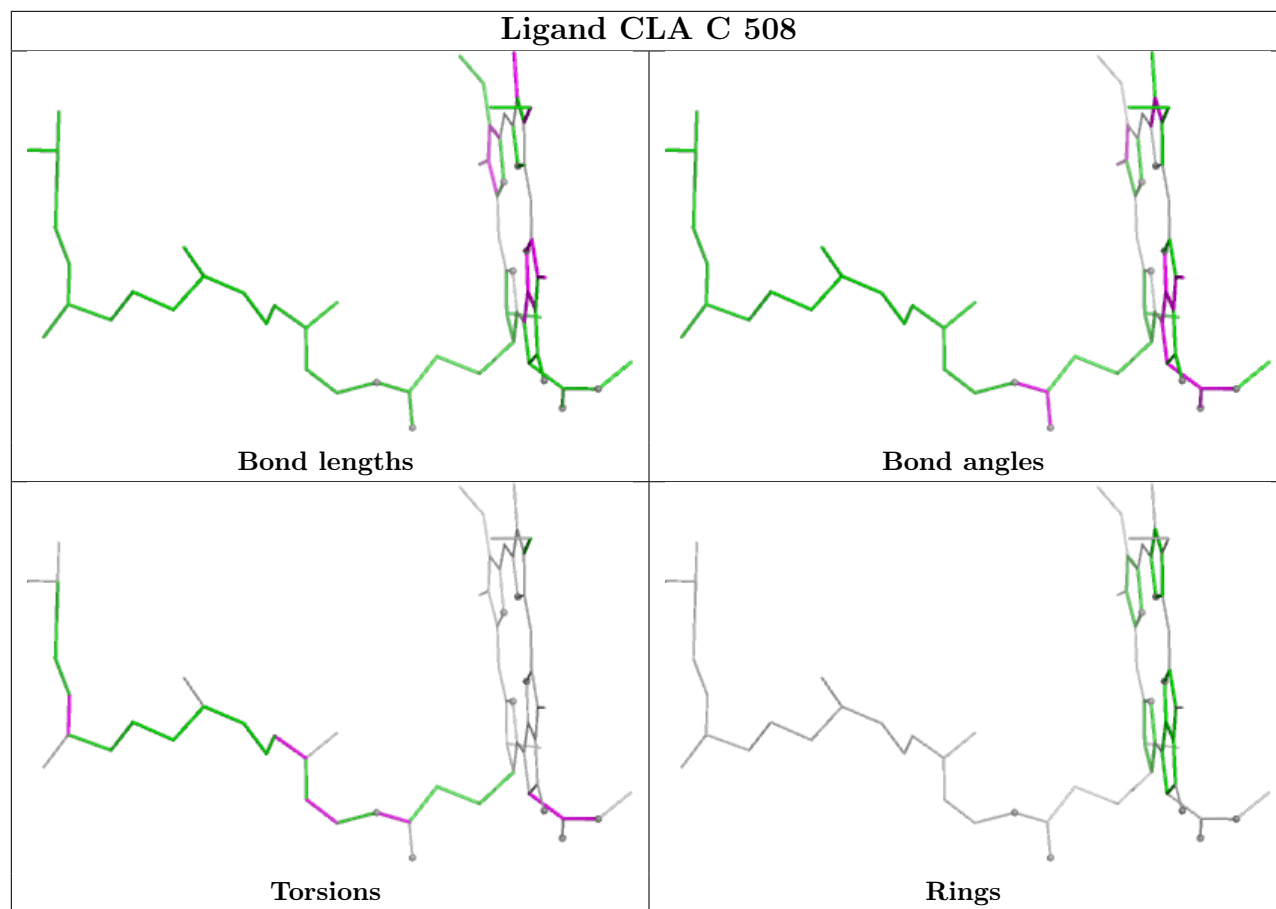


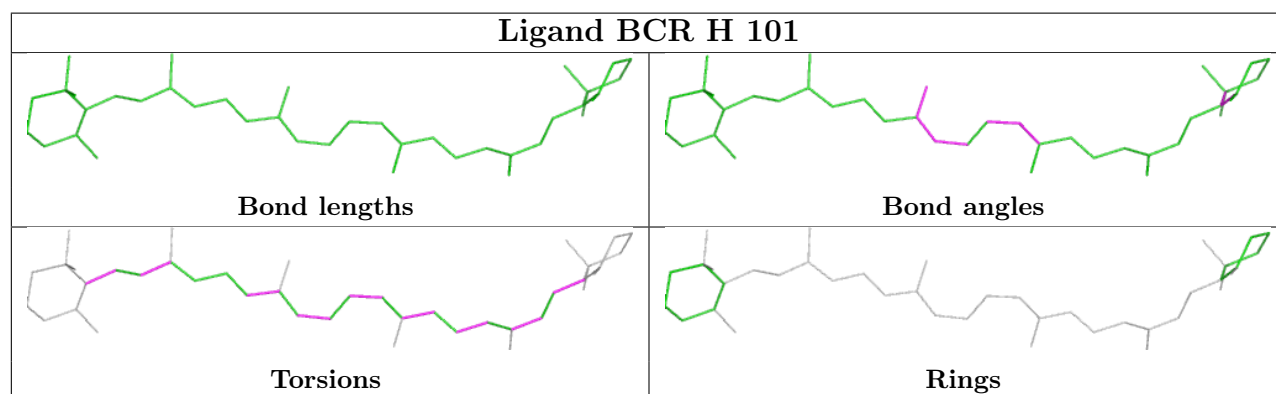
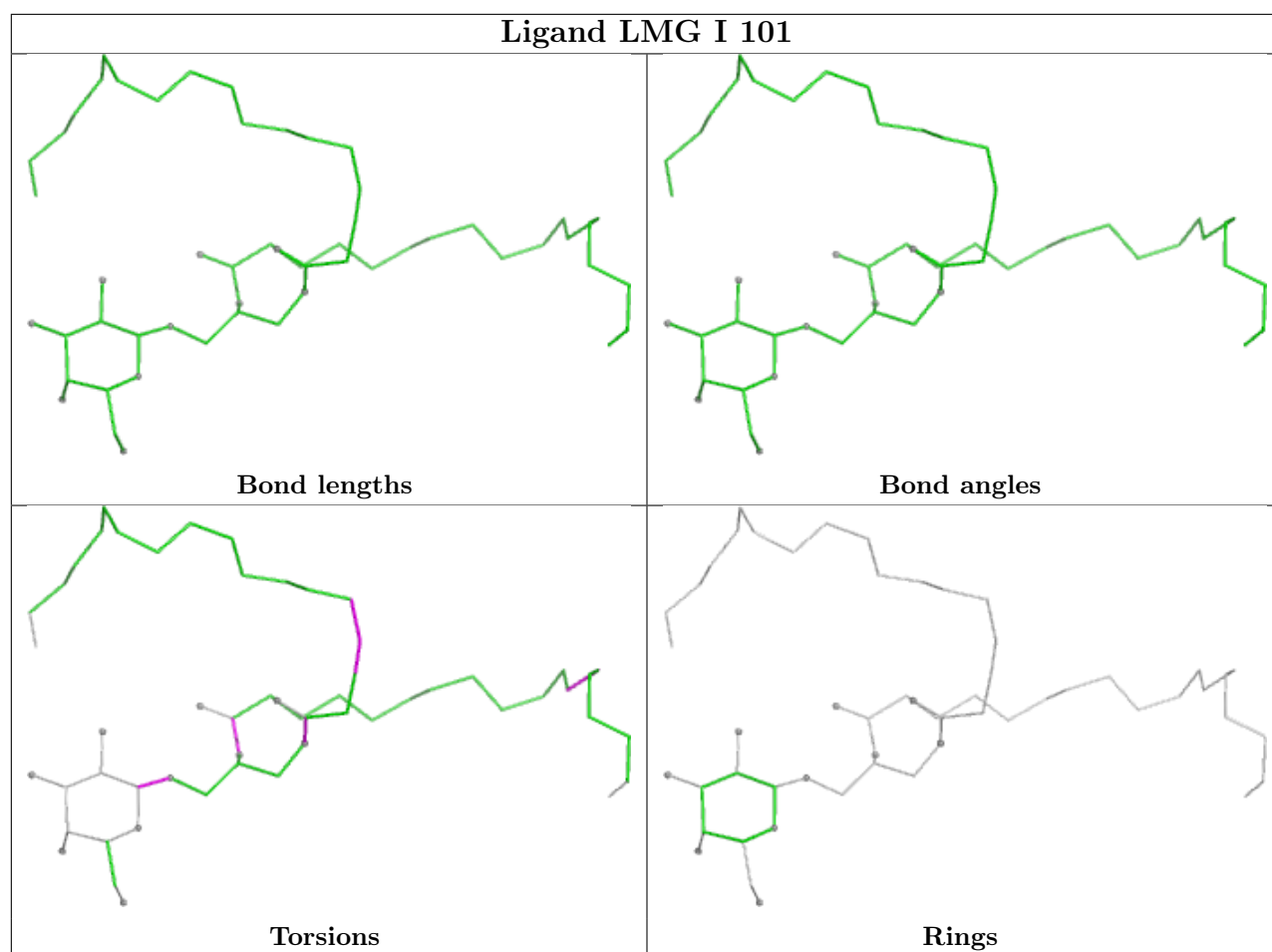


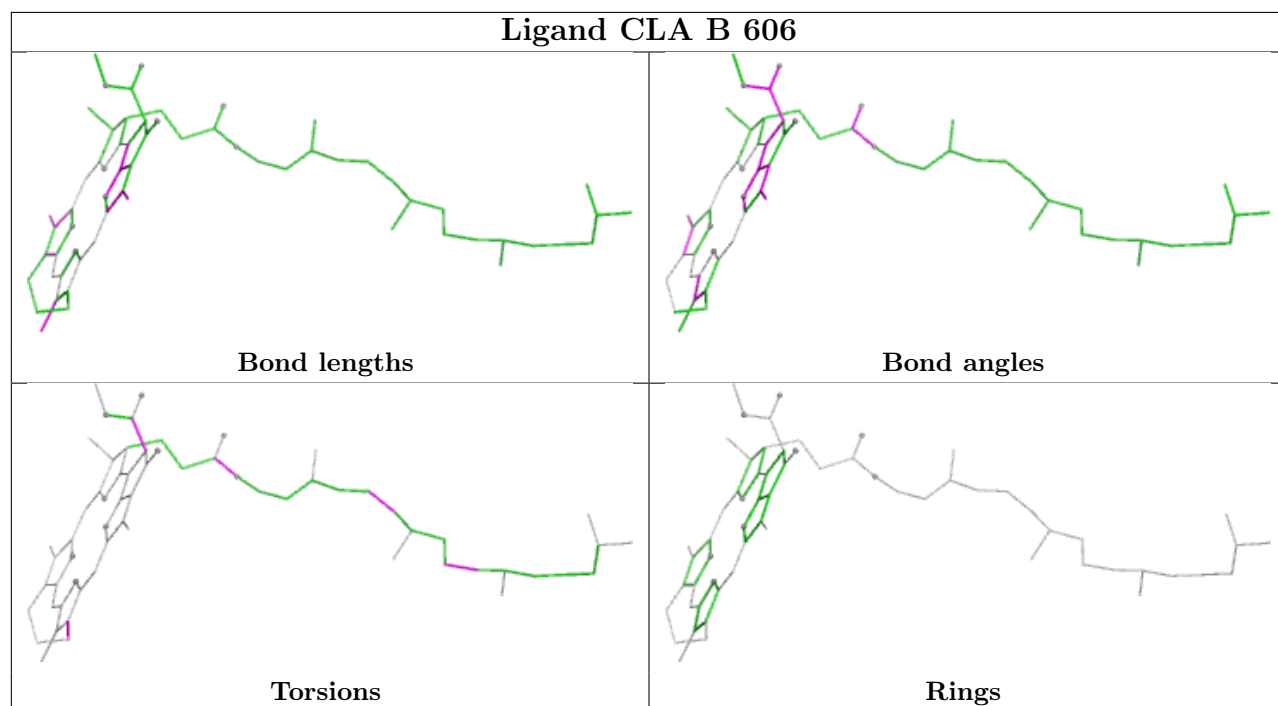
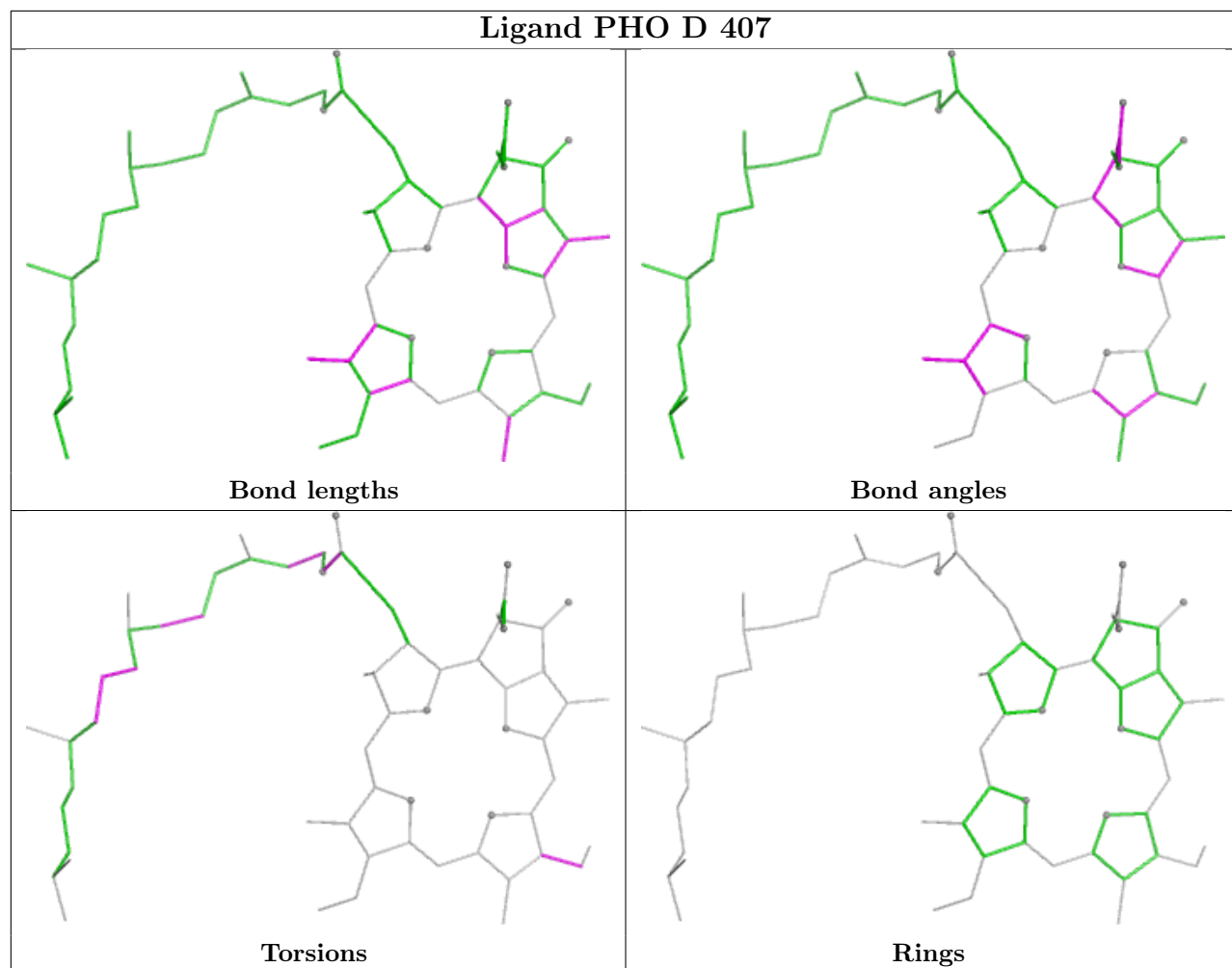


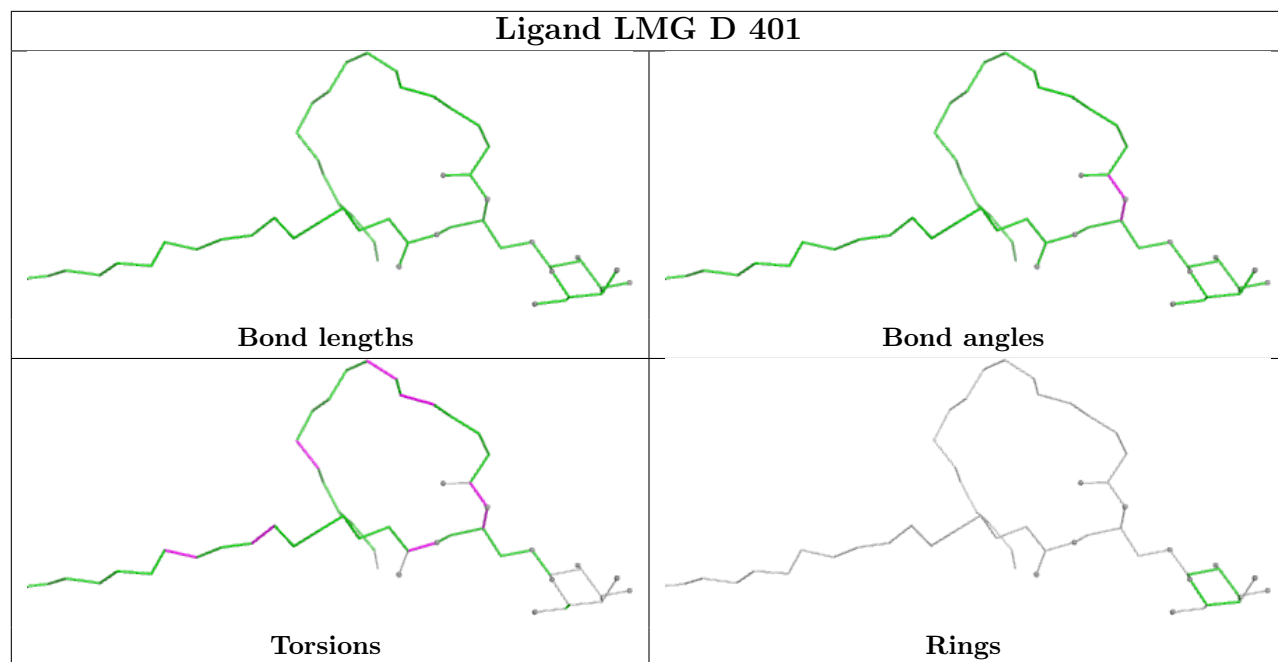


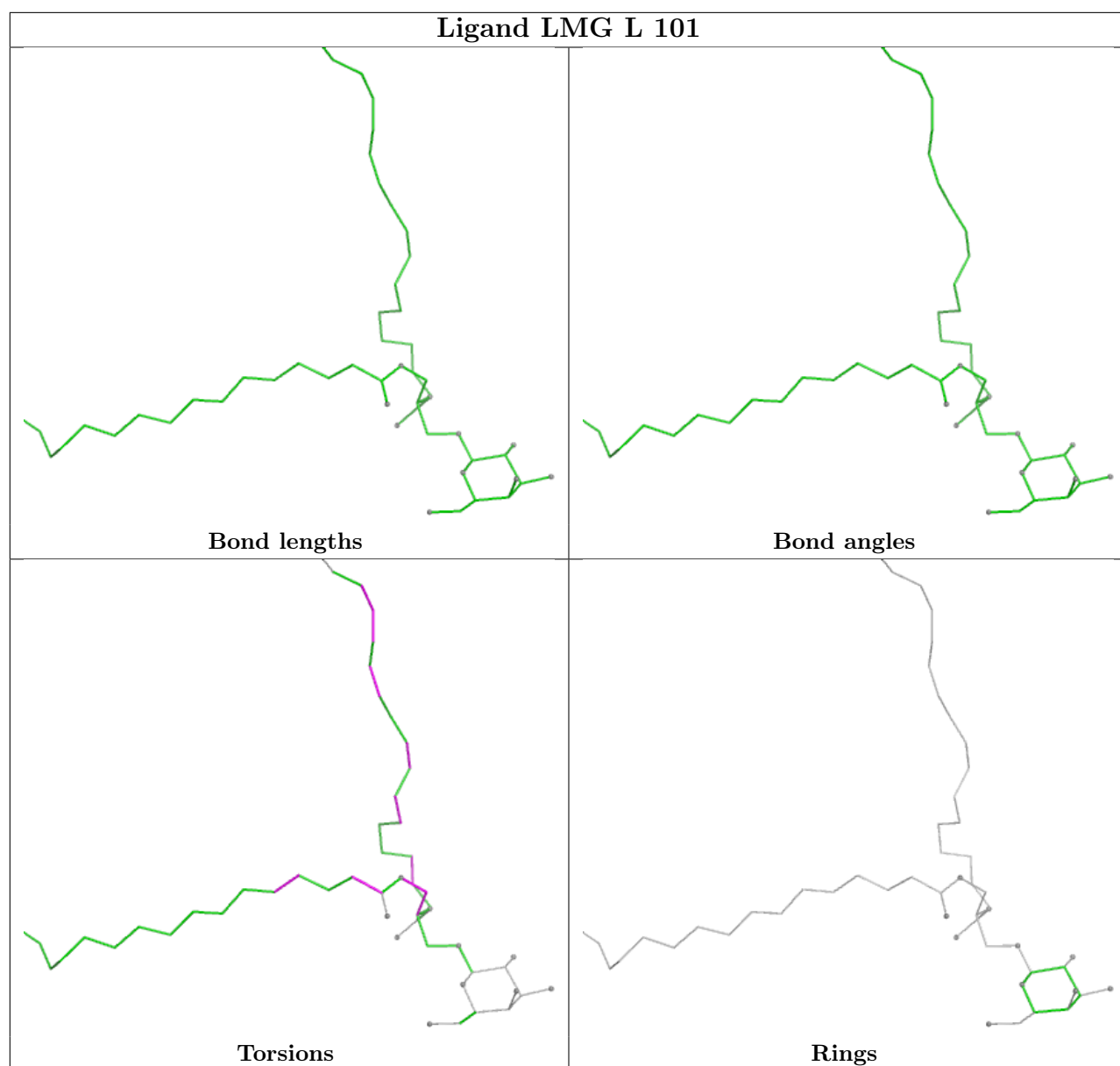




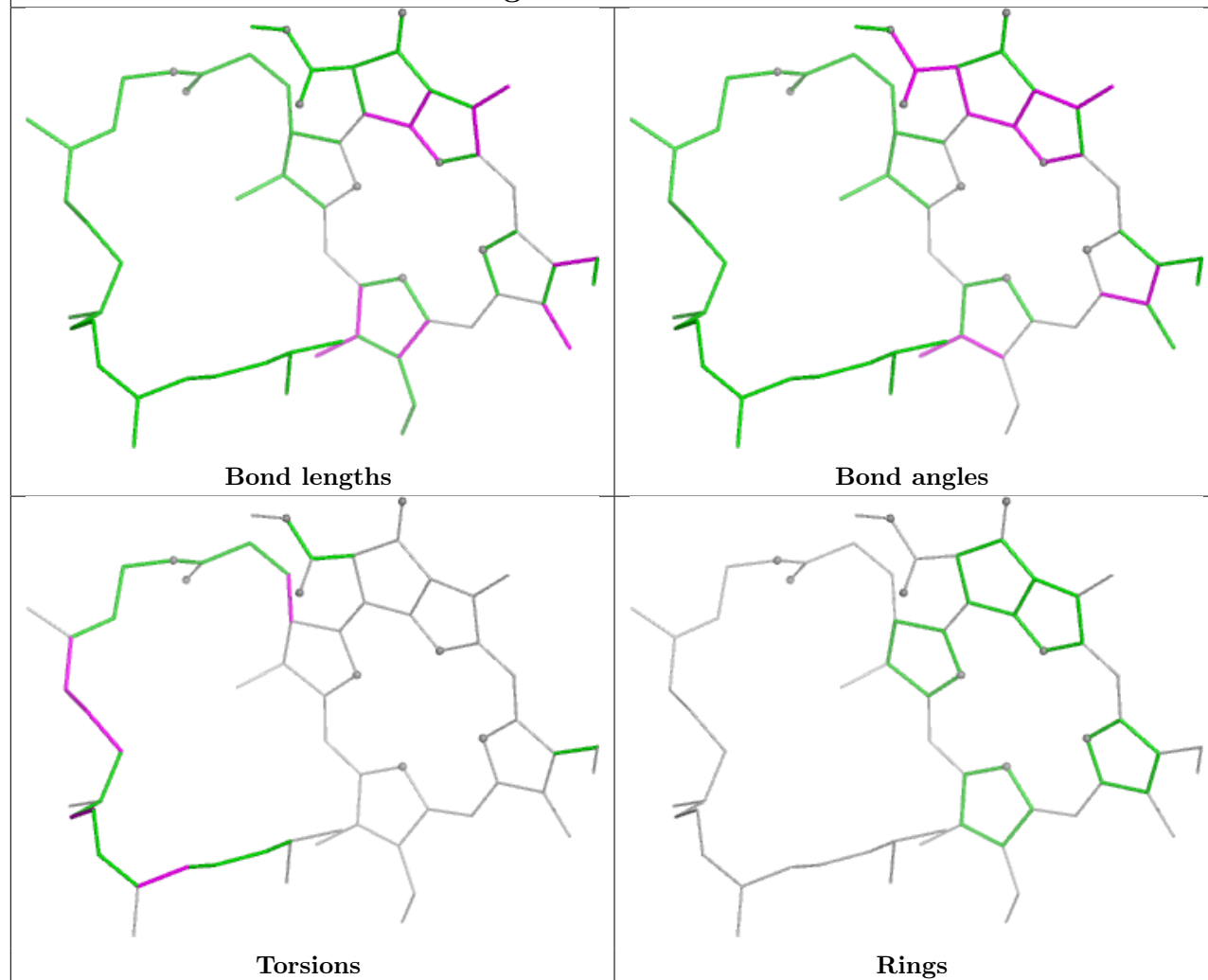




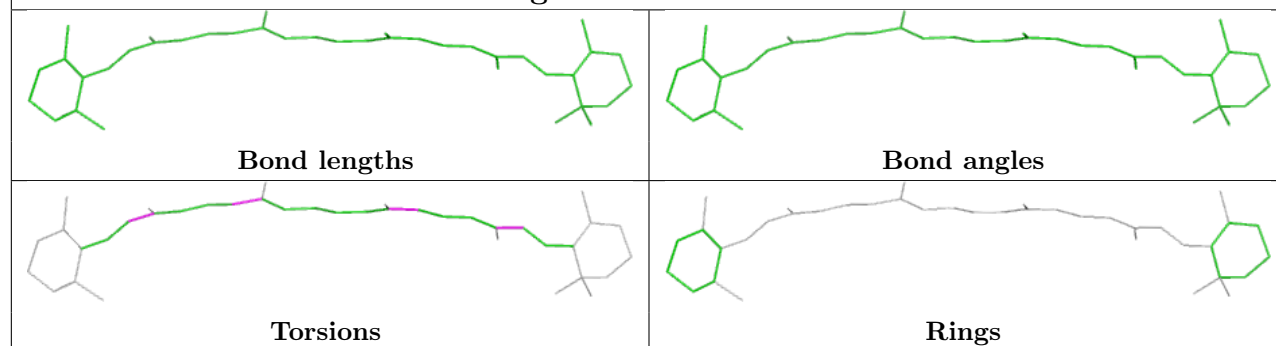


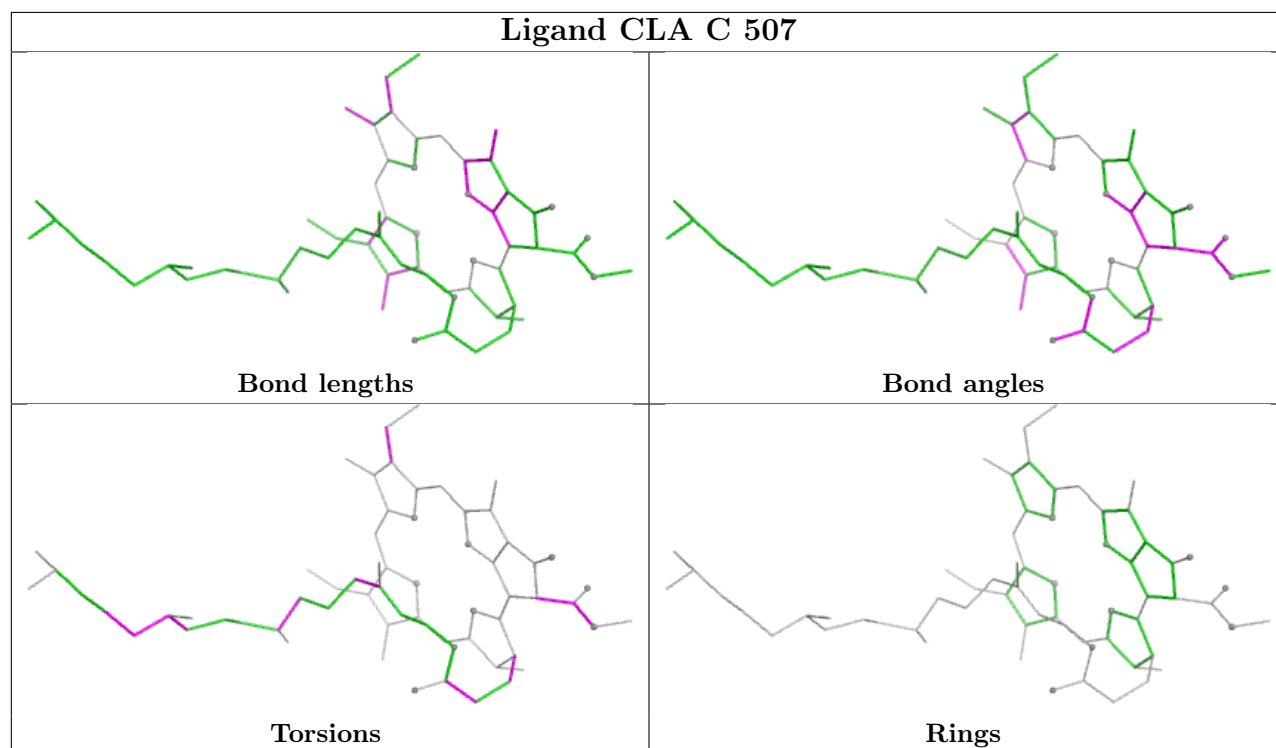
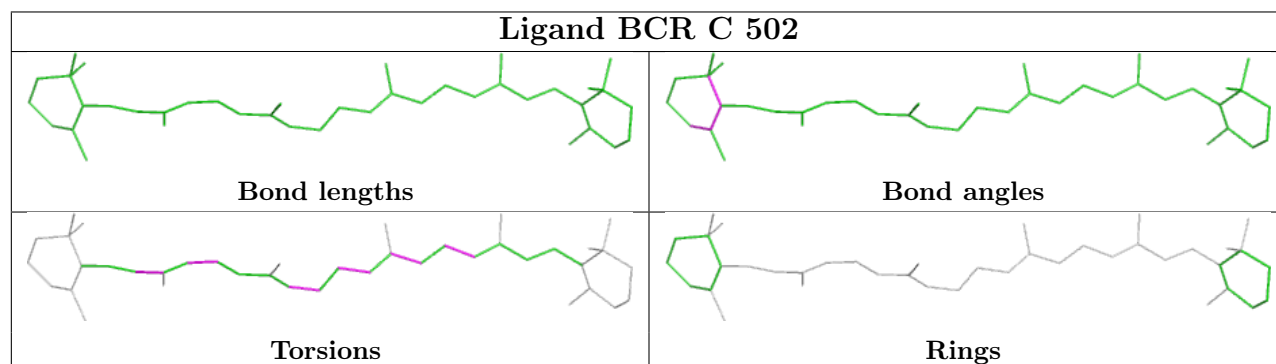
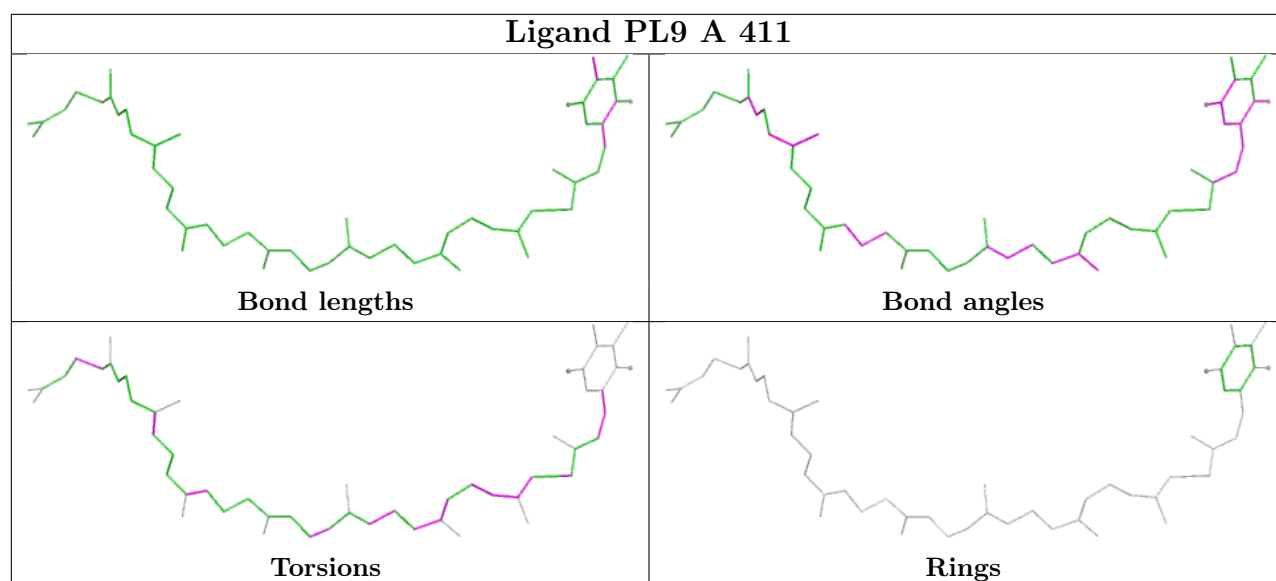


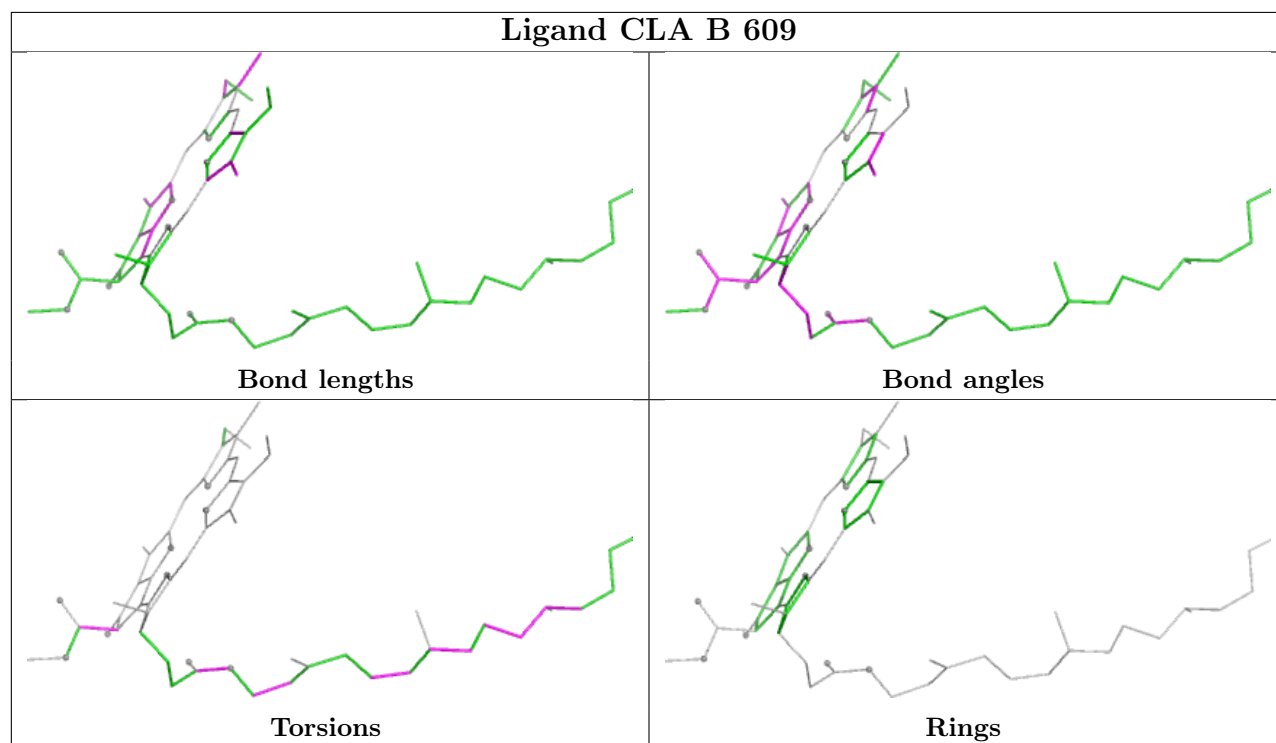
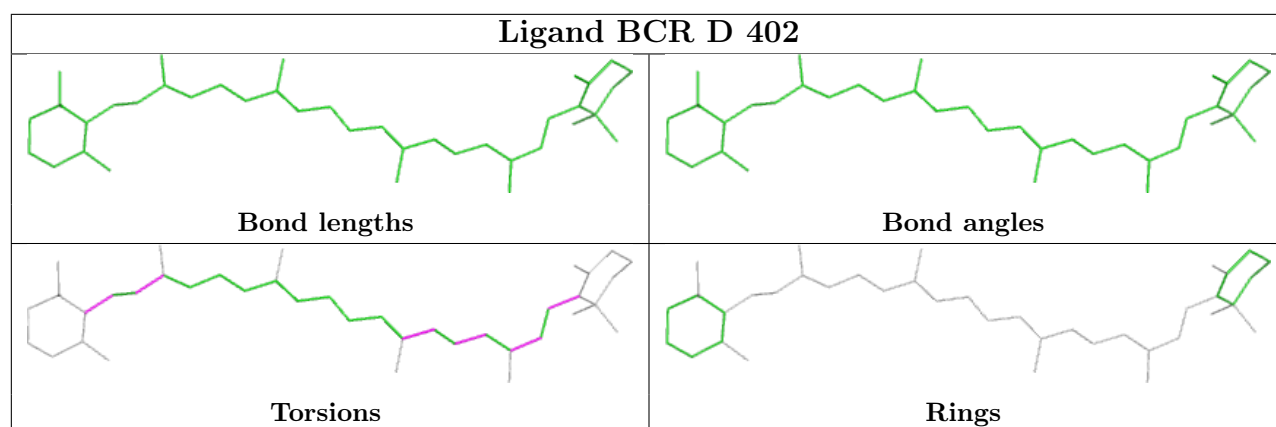
Ligand CLA B 617

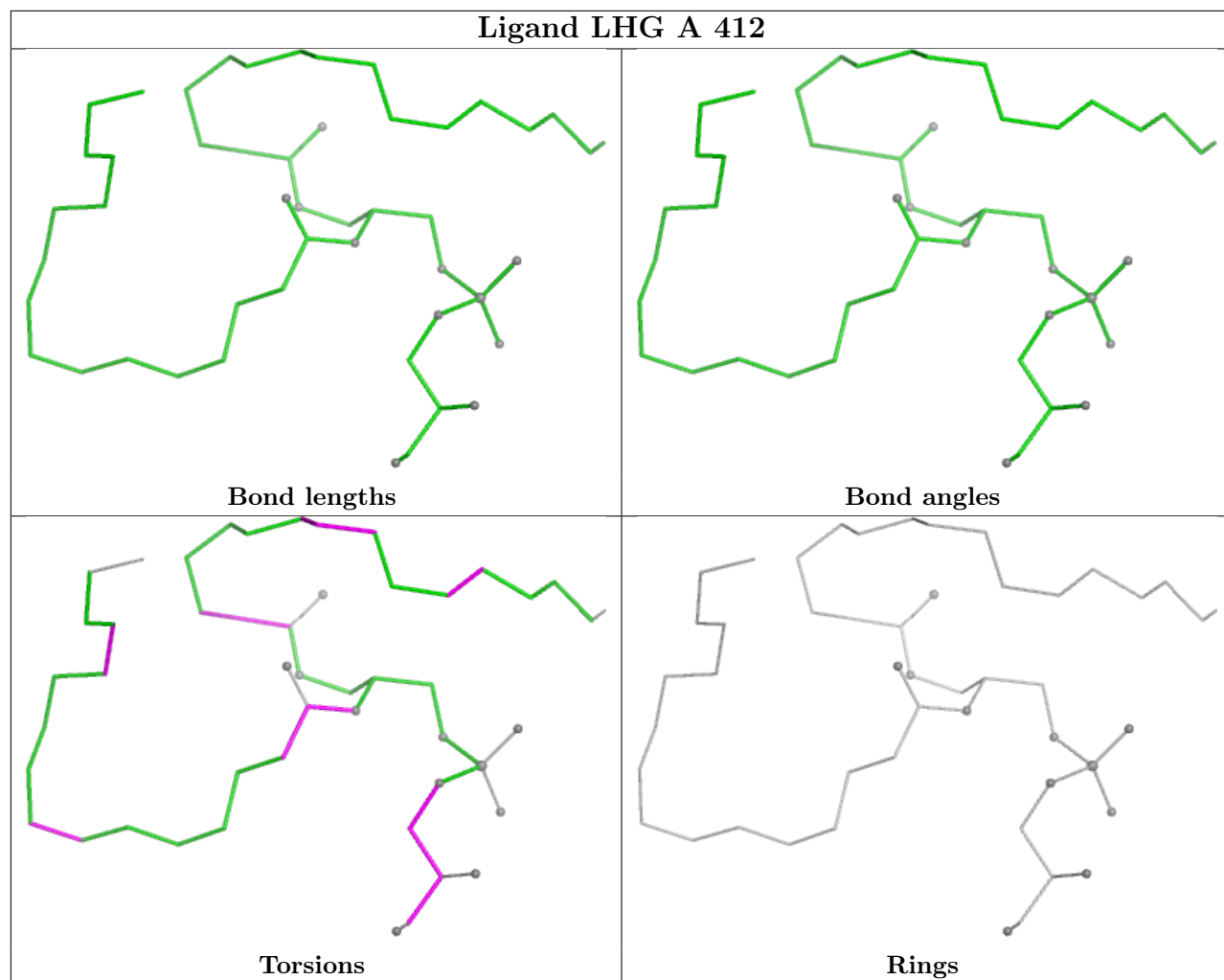


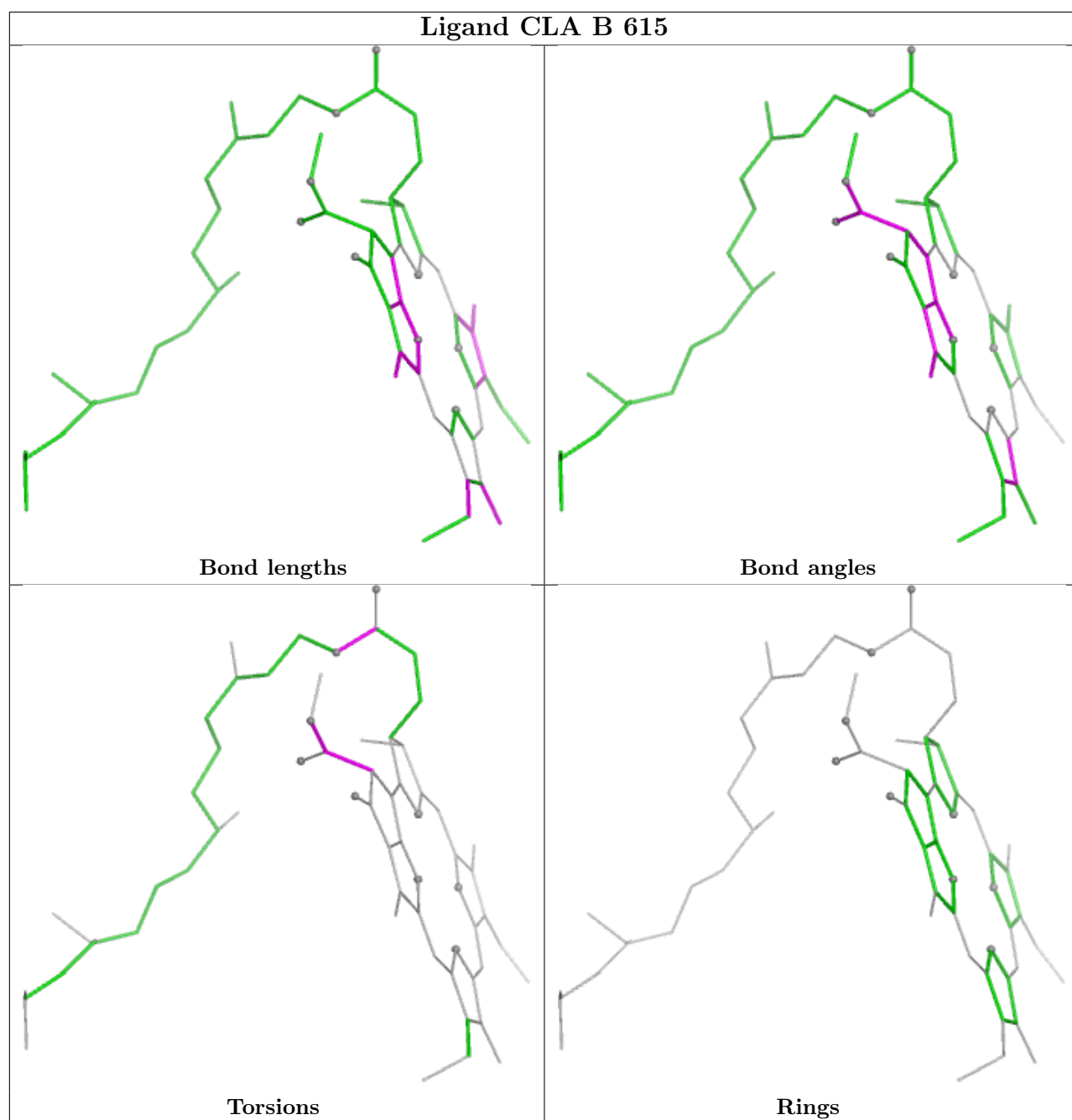
Ligand BCR C 501

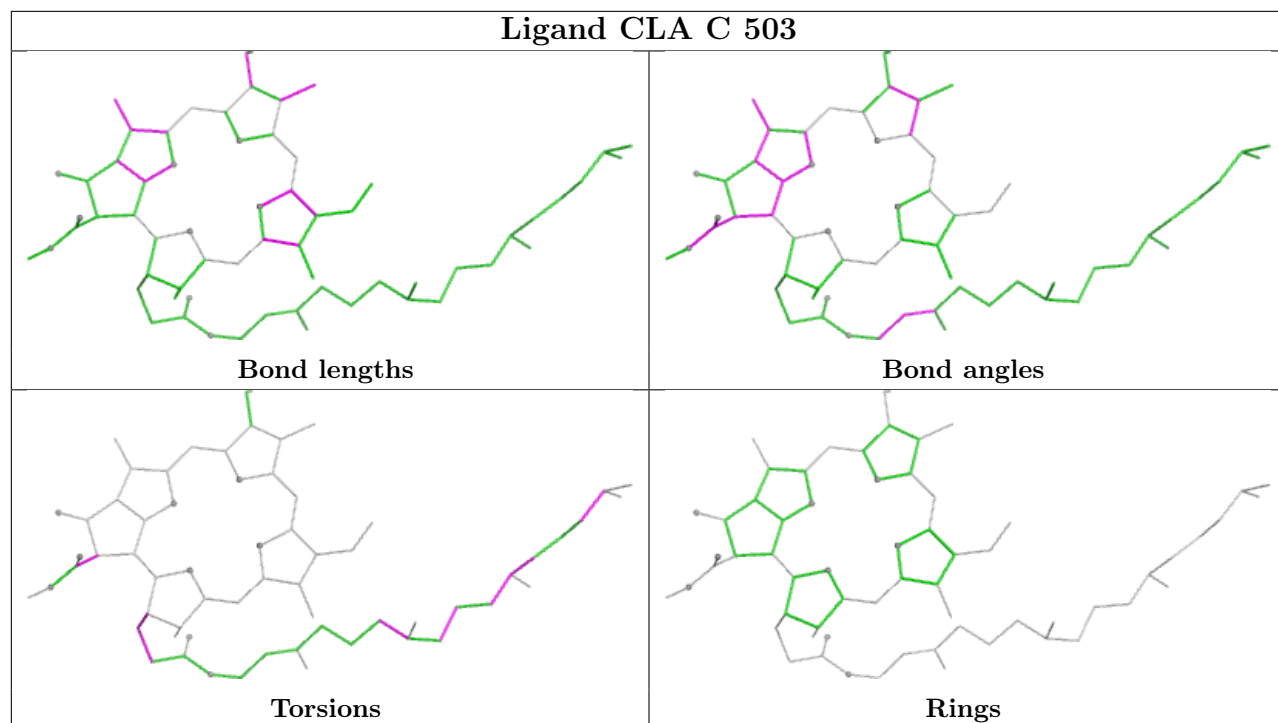
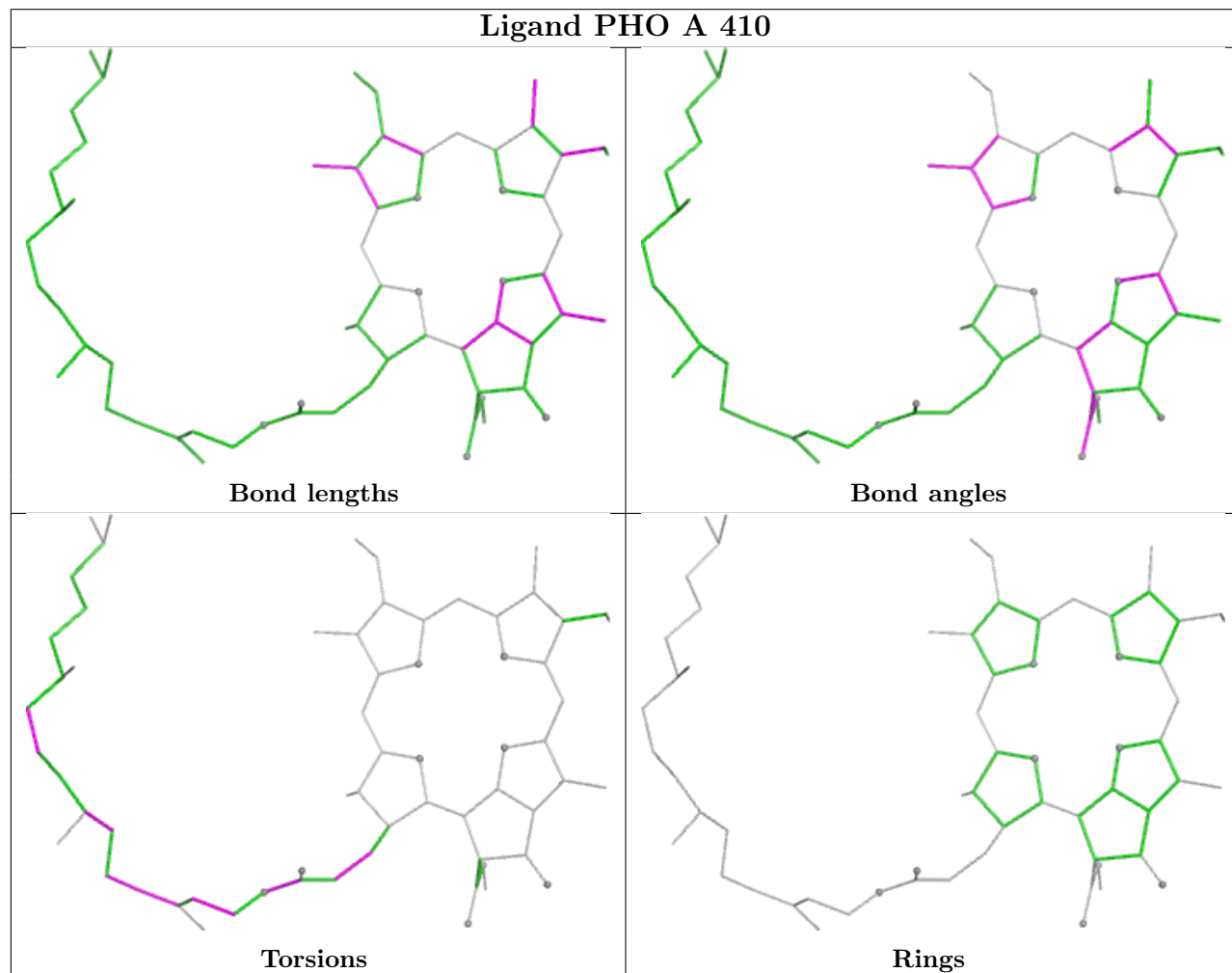


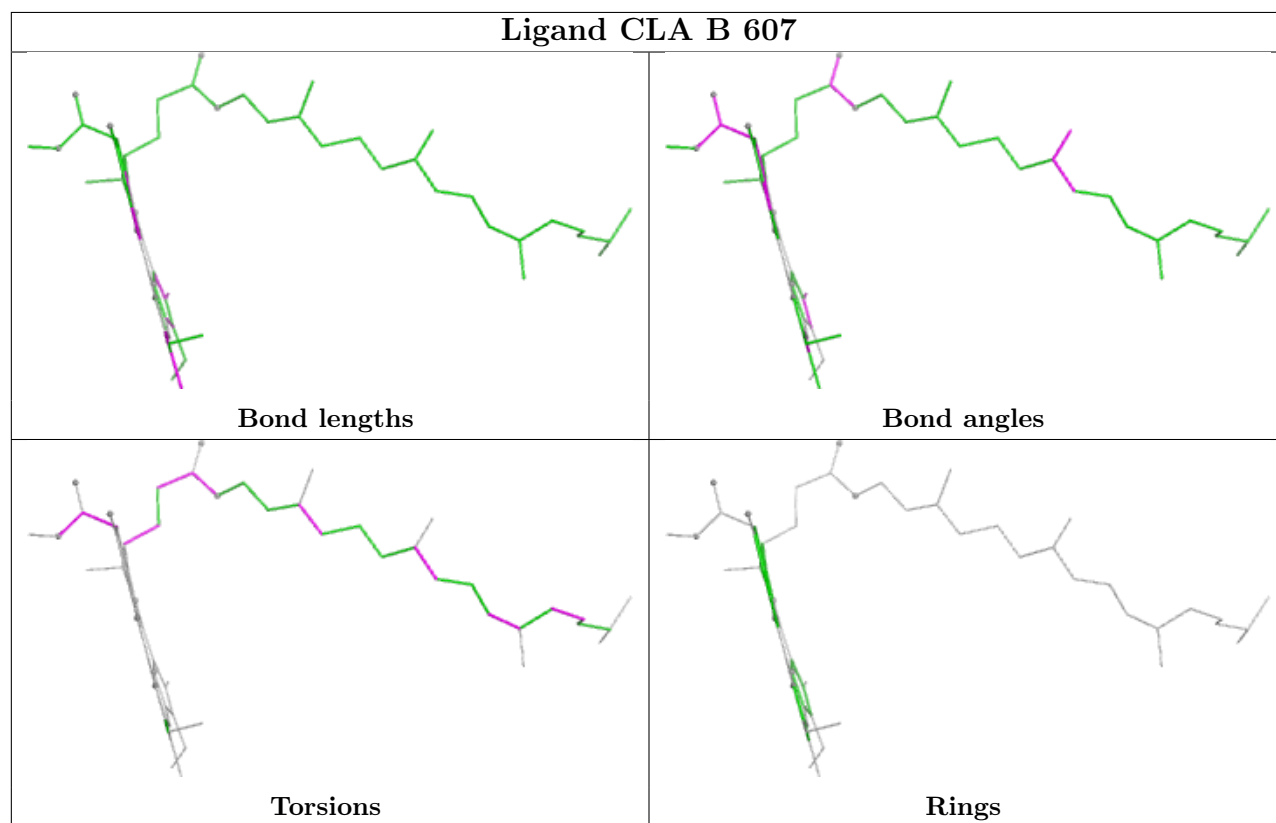
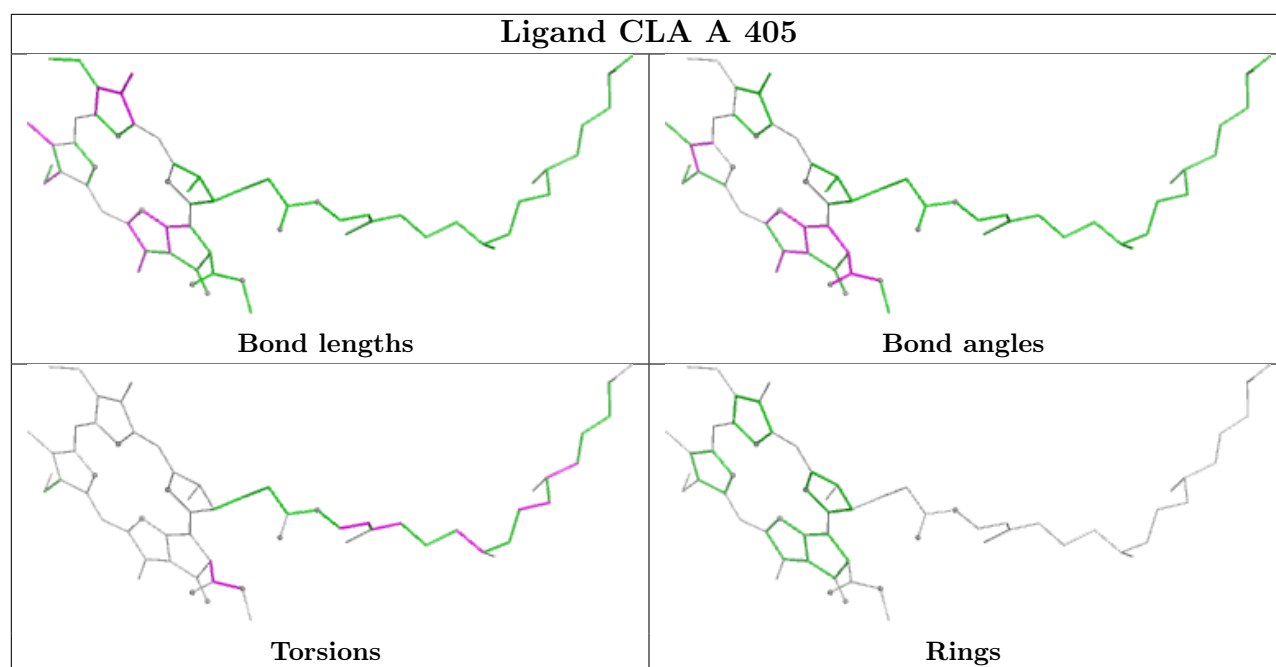


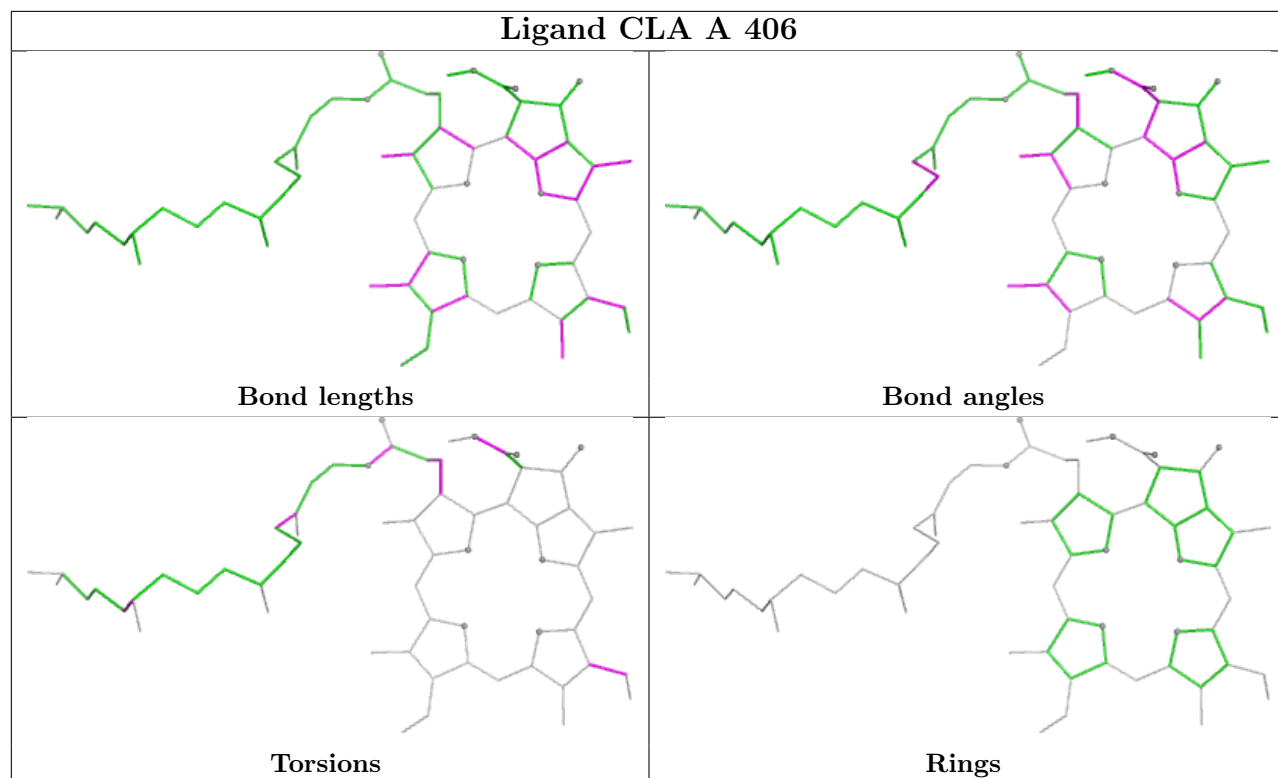


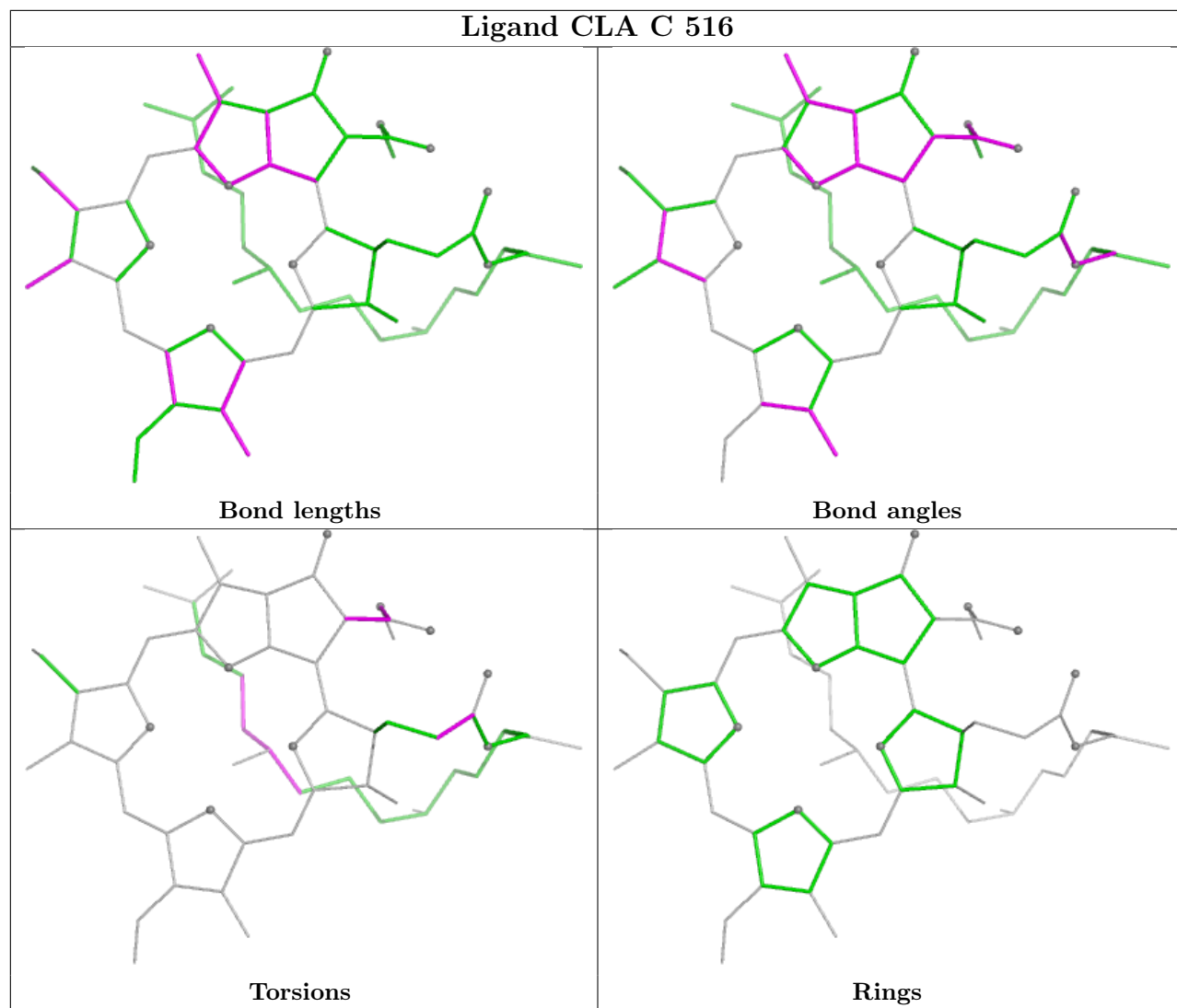


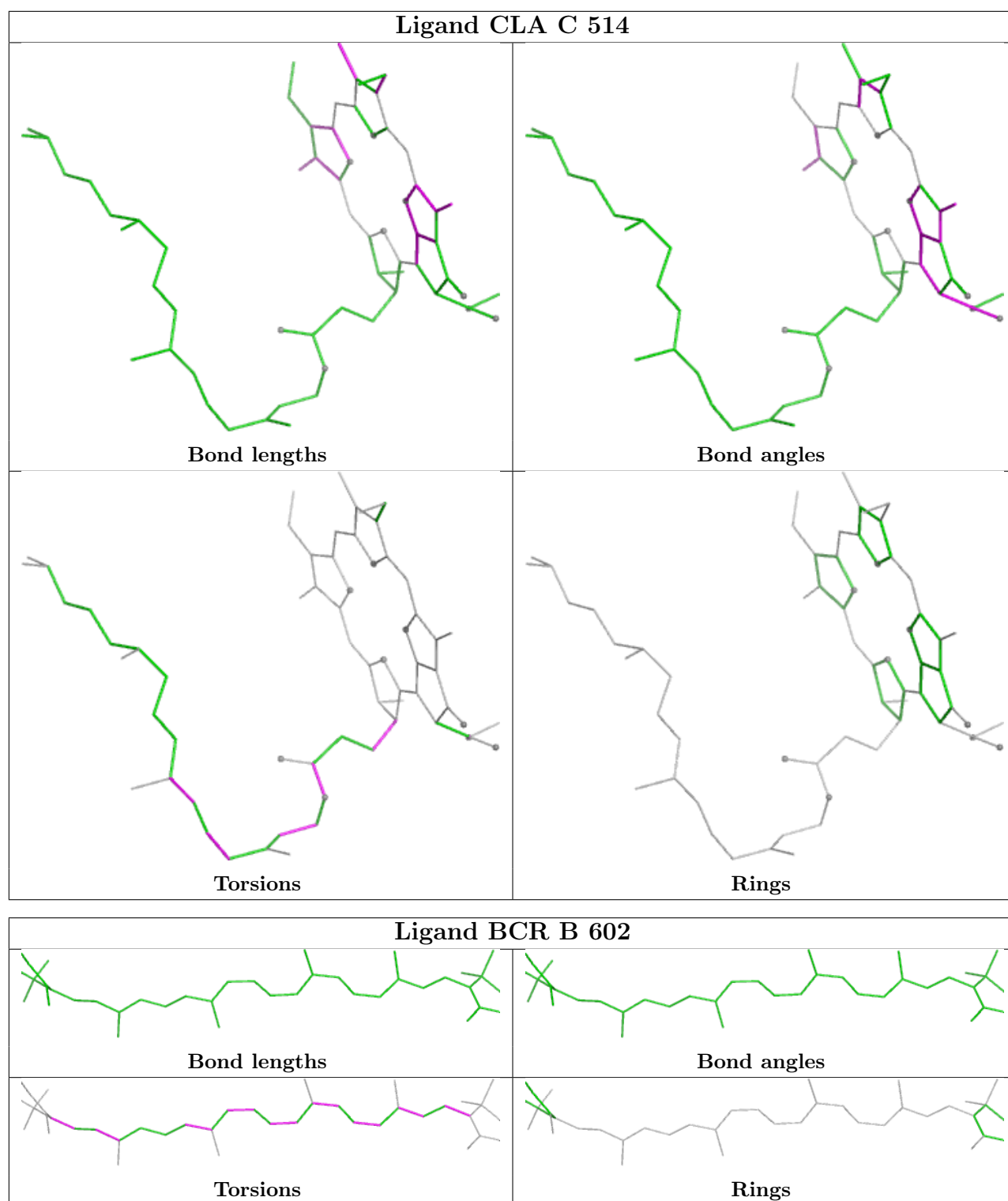


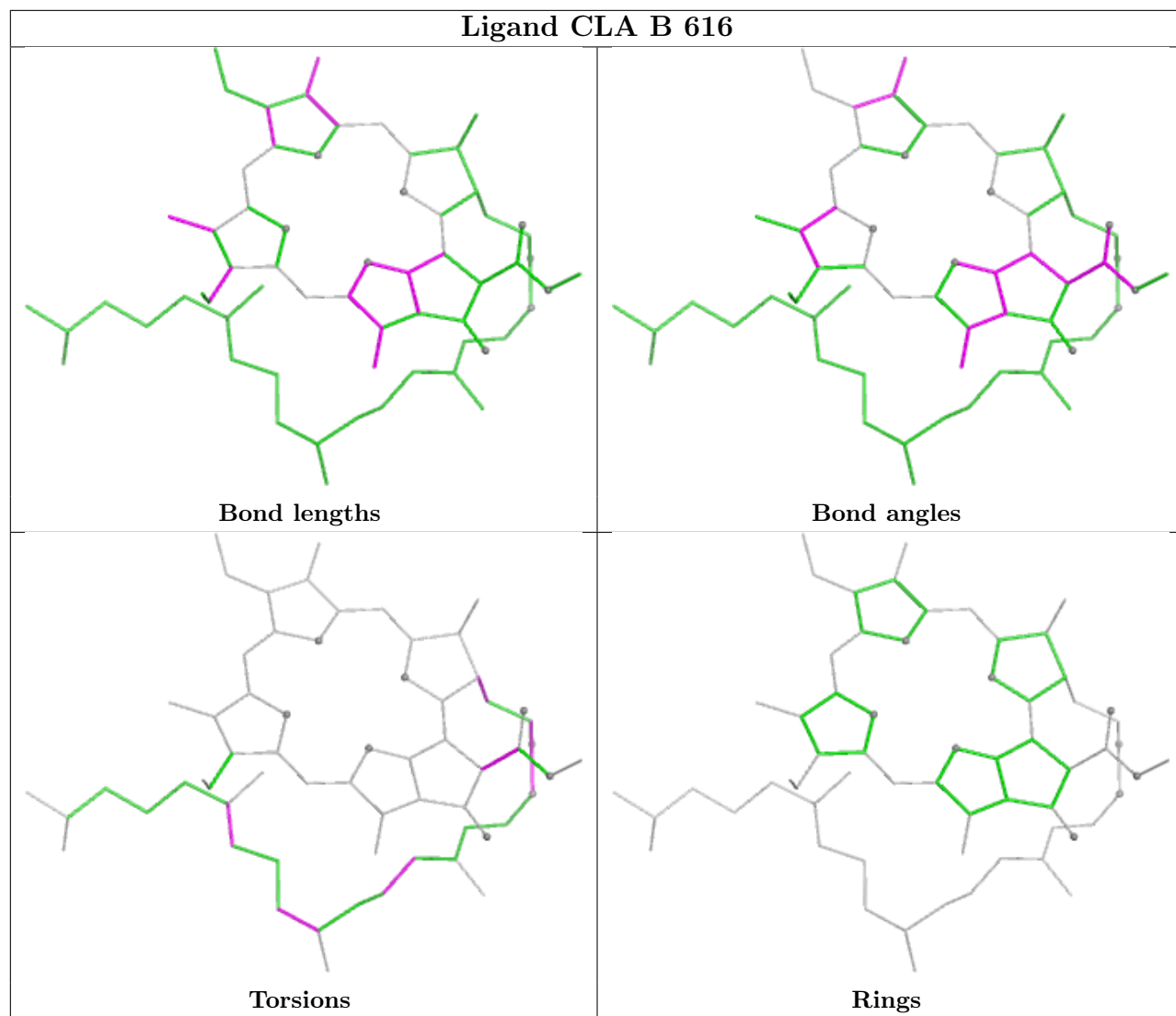
Ligand CLA C 503**Ligand PHO A 410**

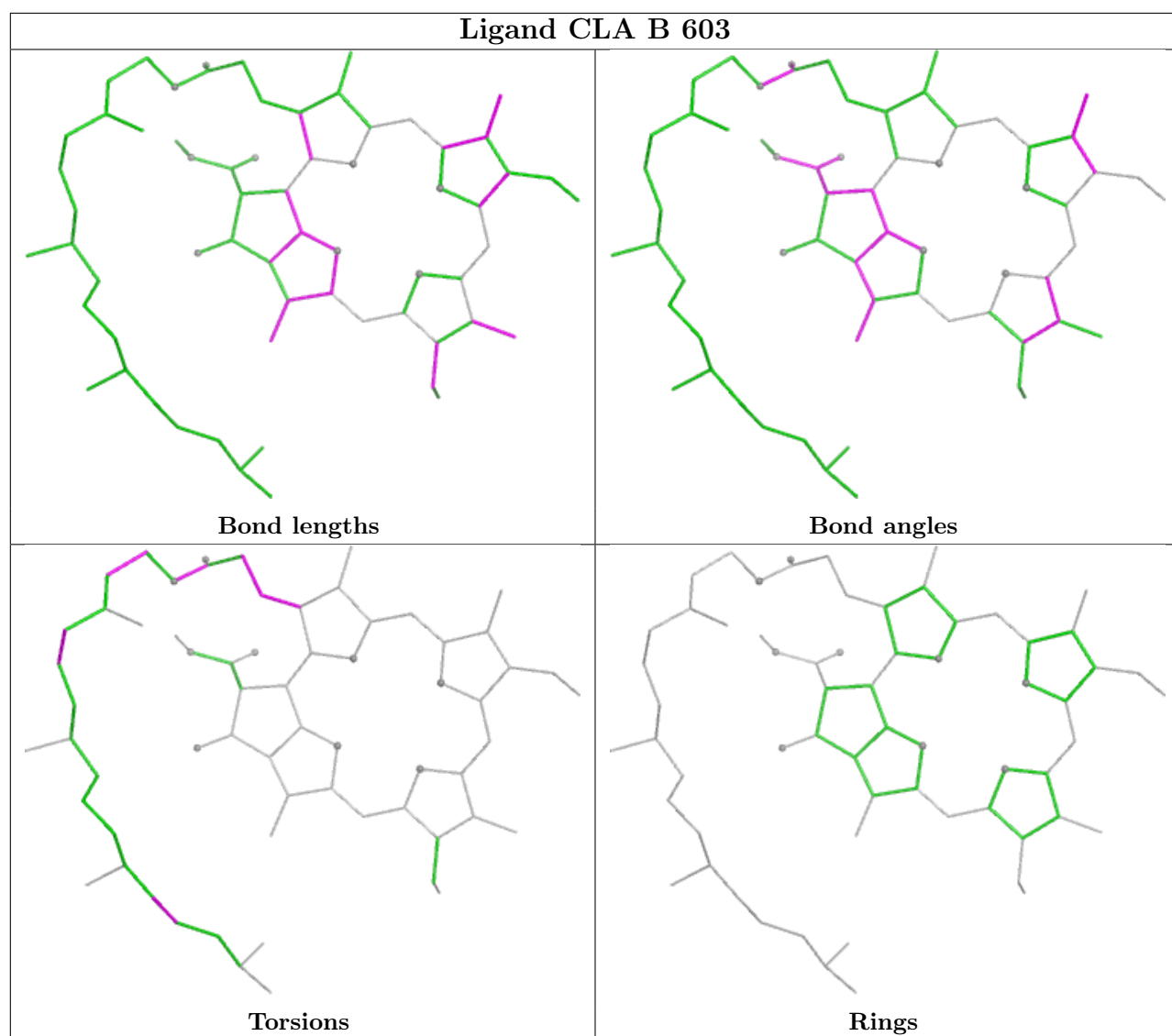


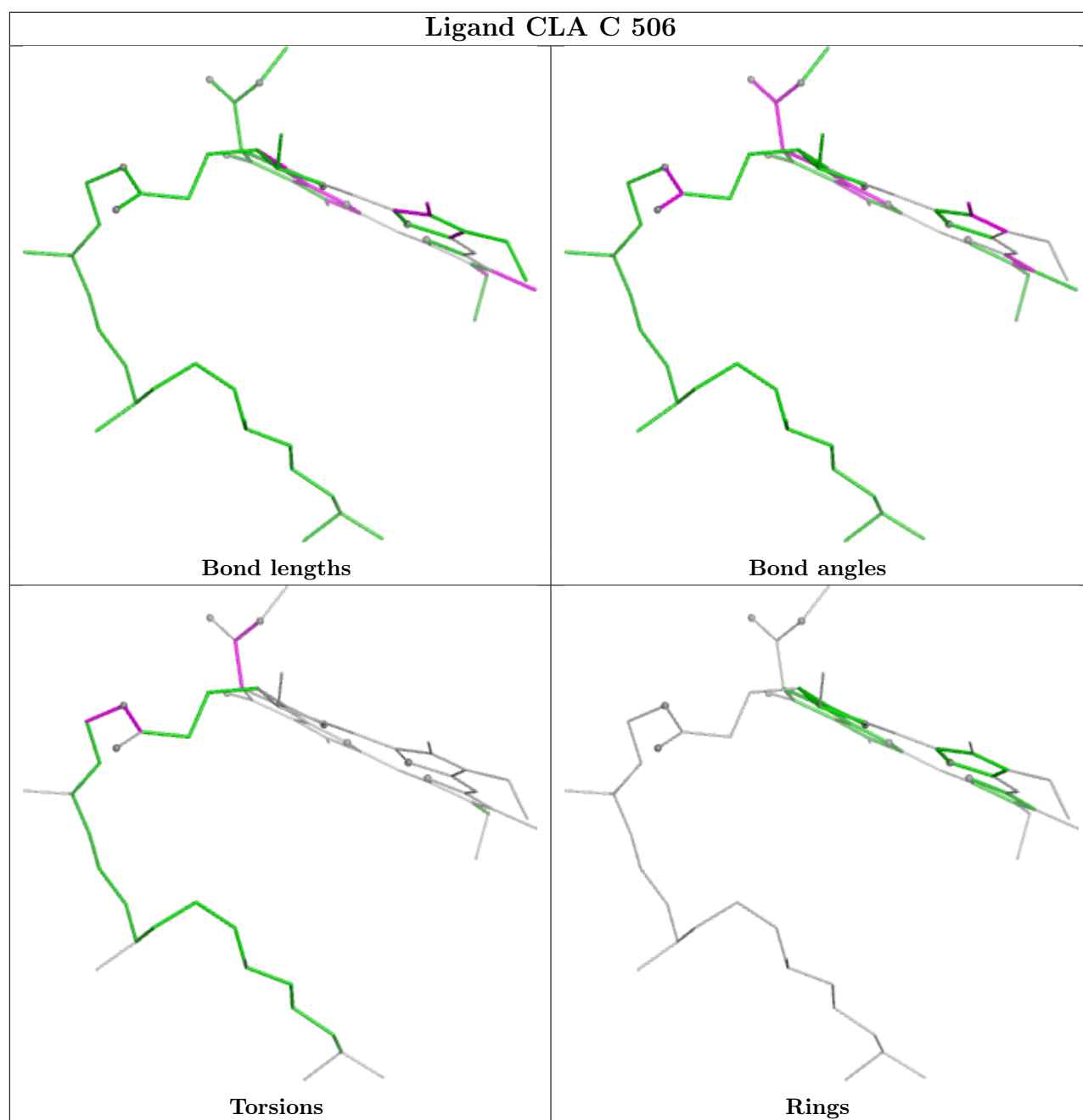


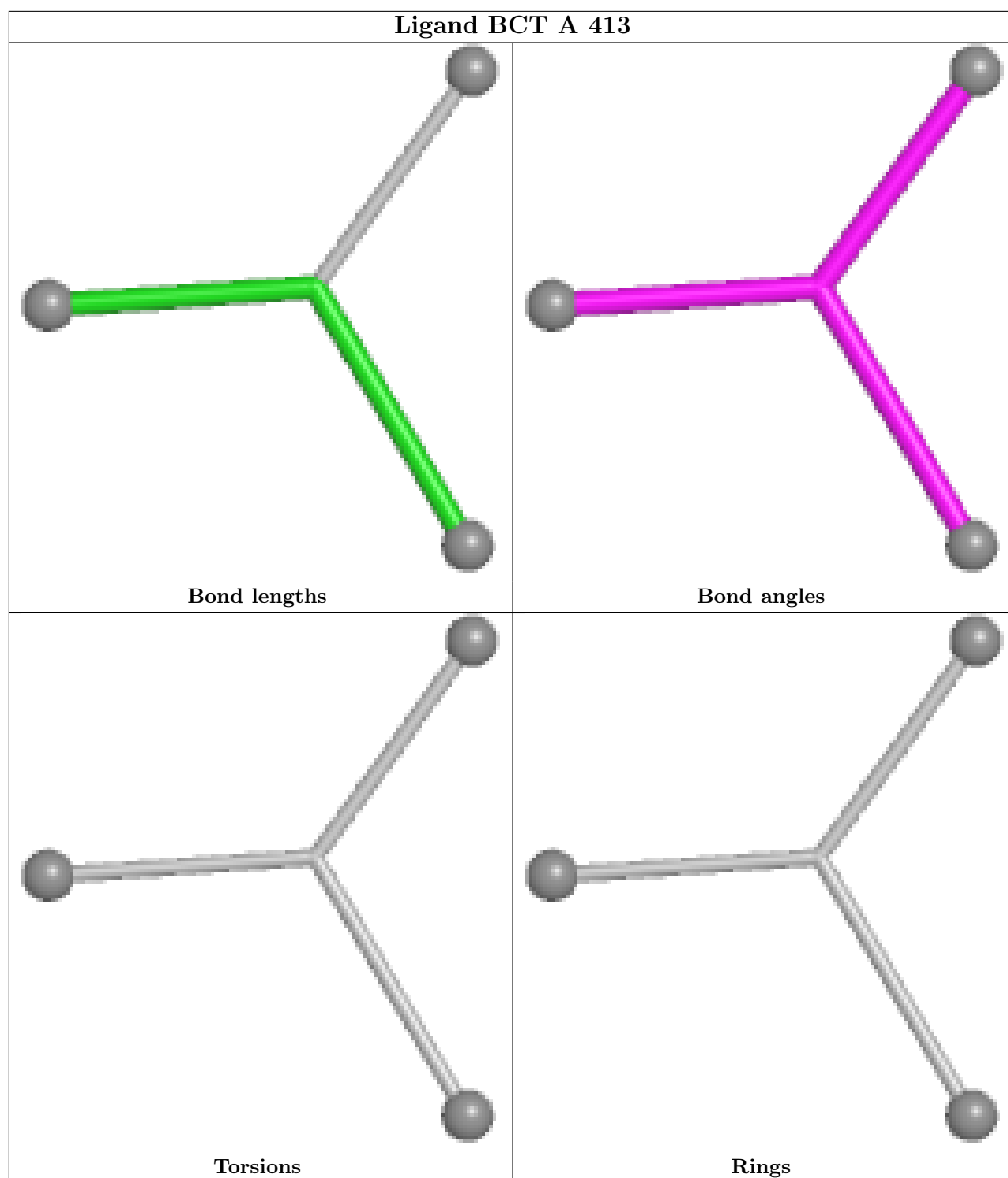


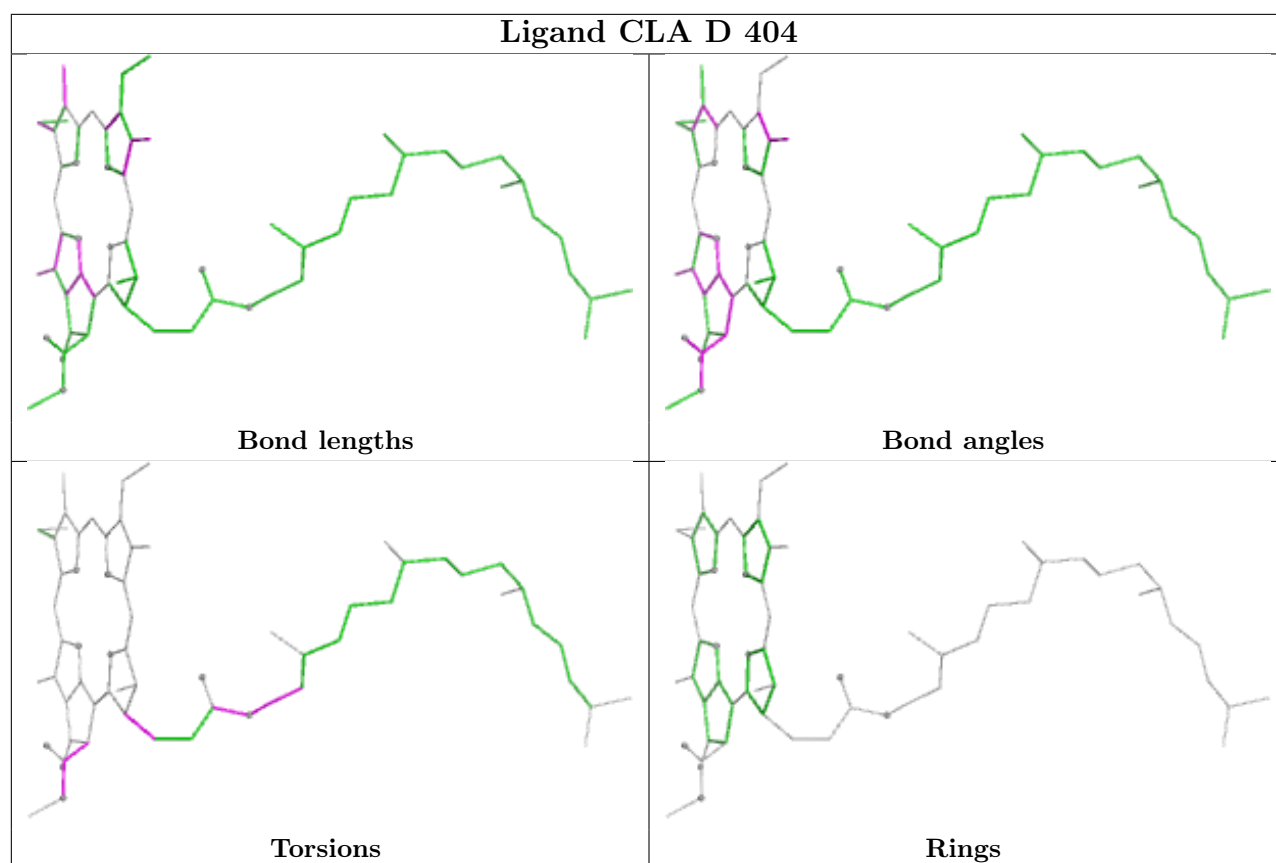


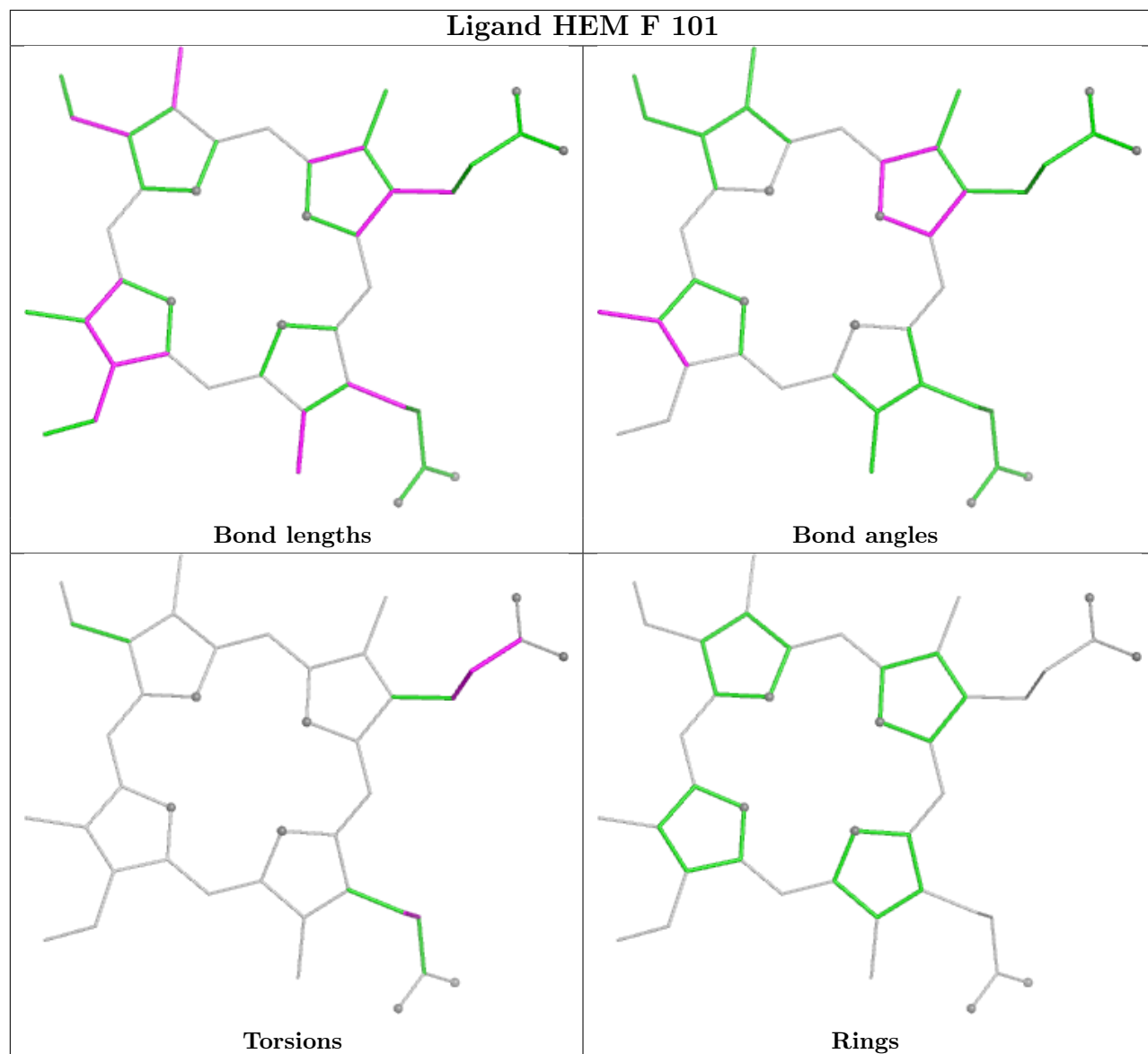


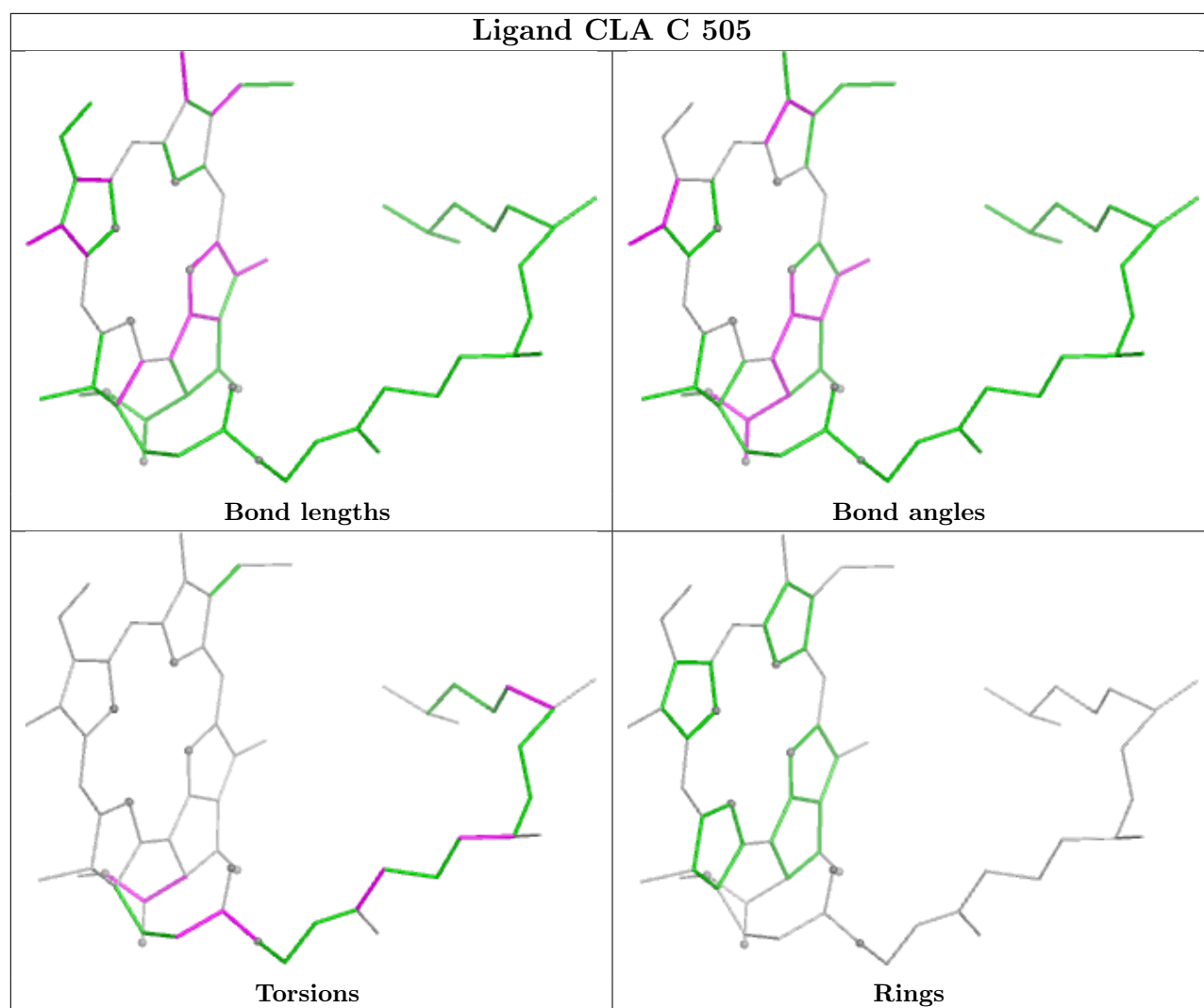


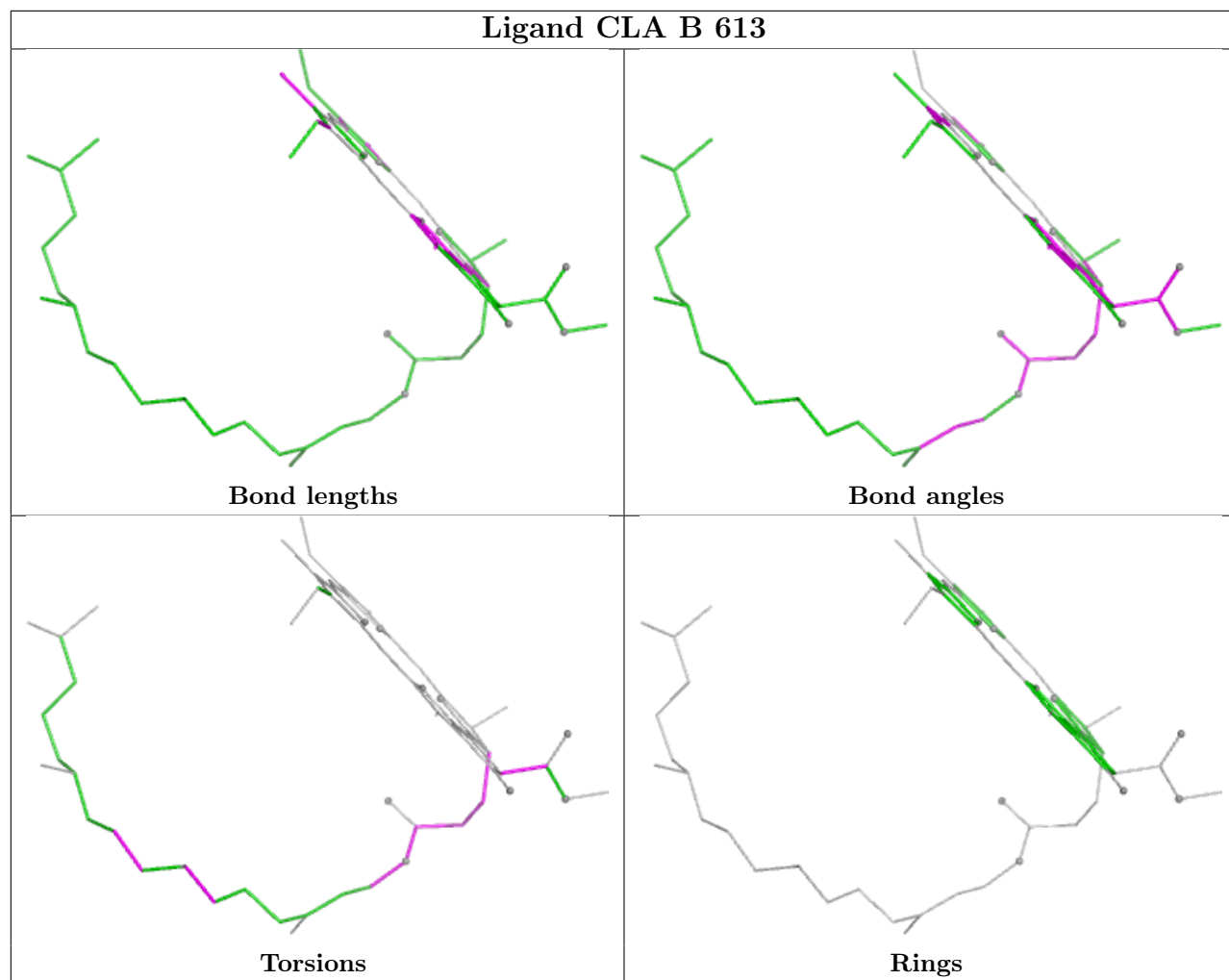


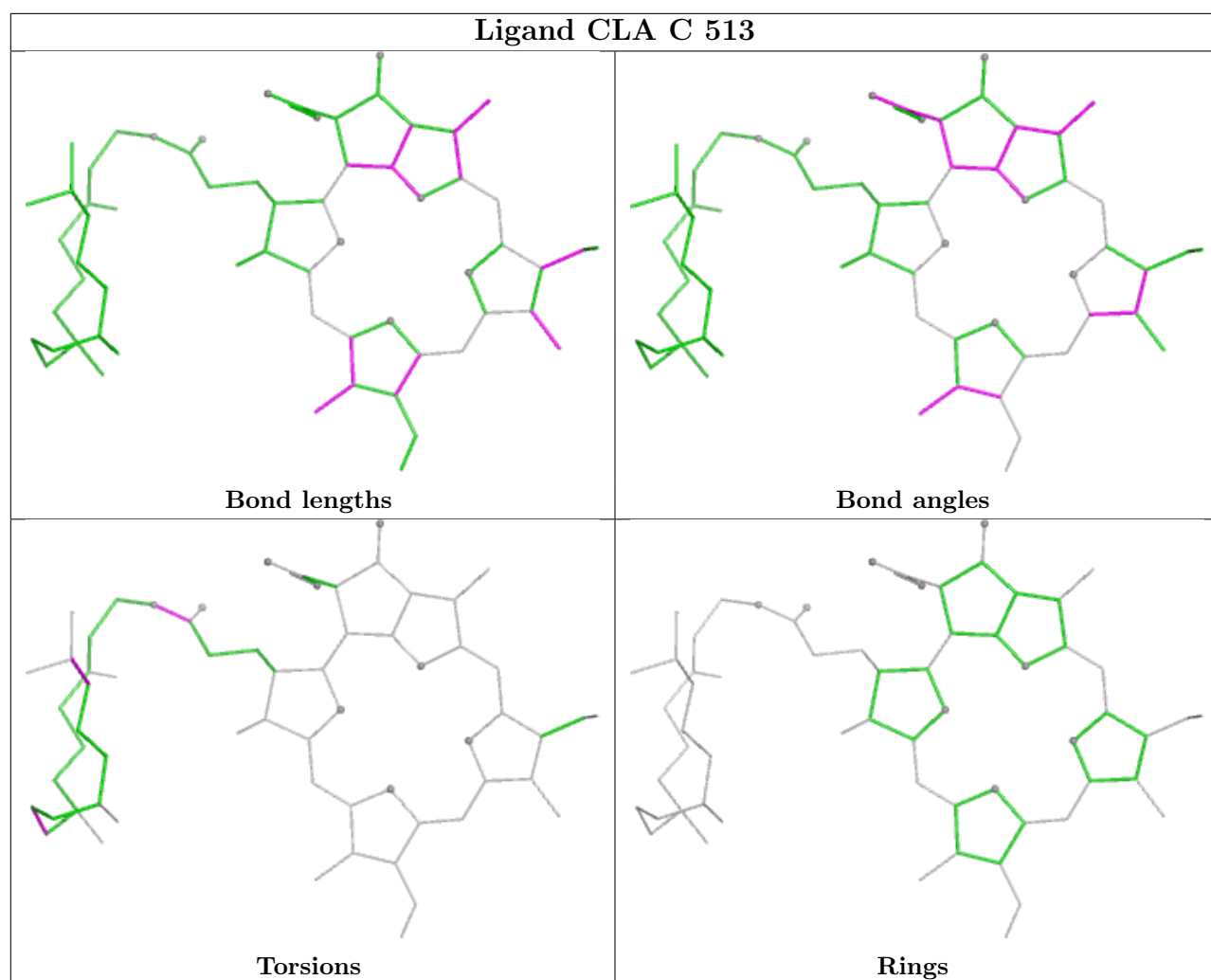


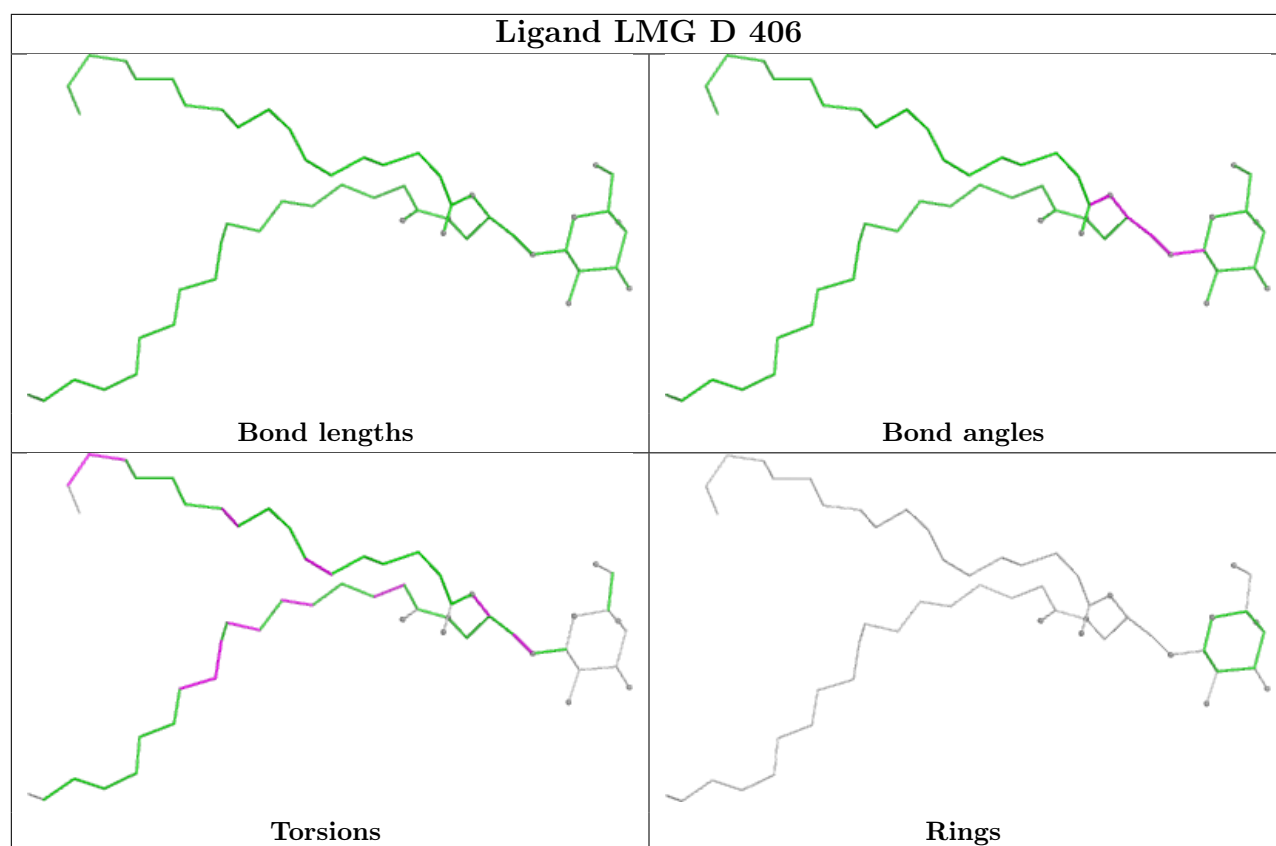


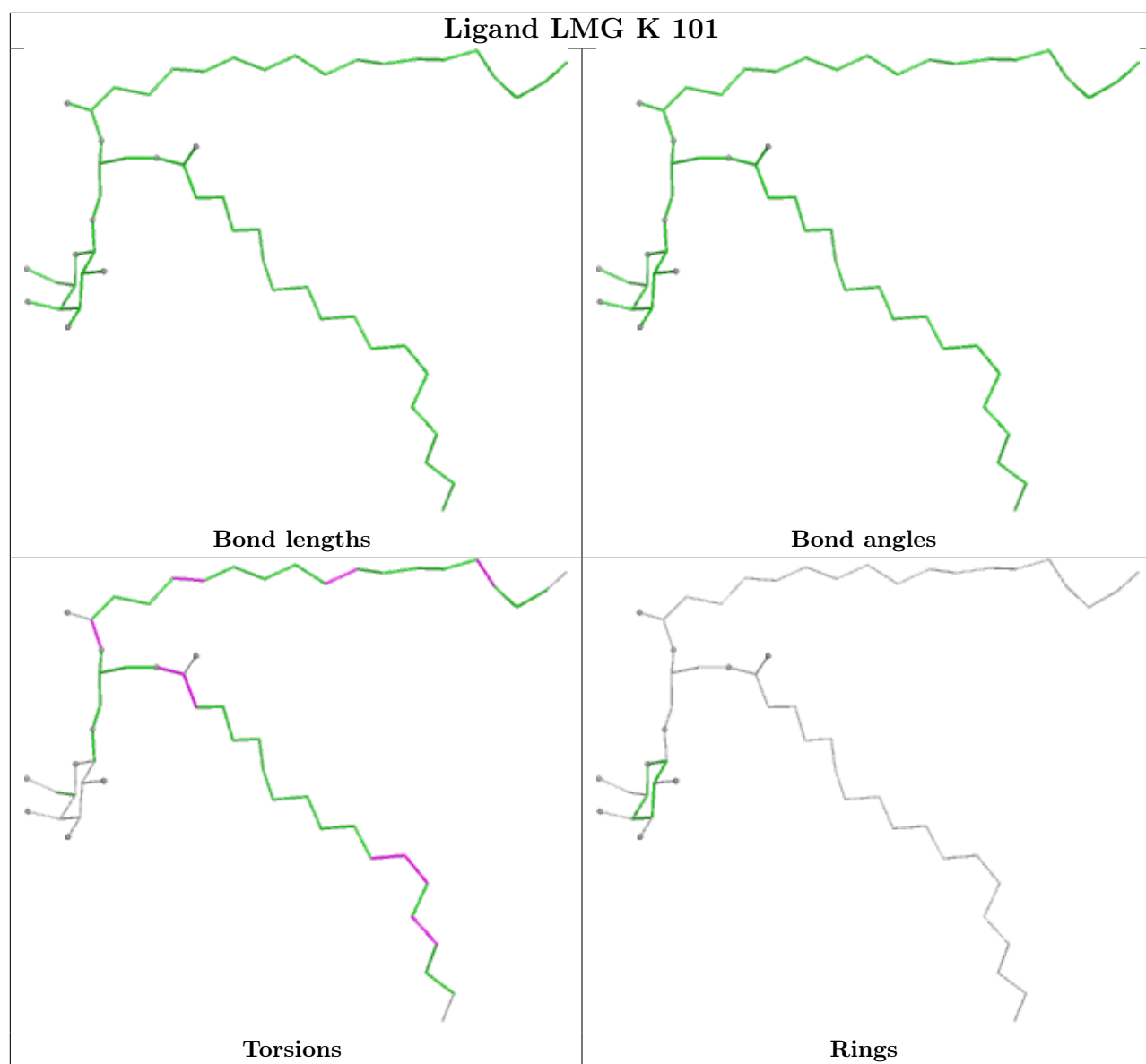


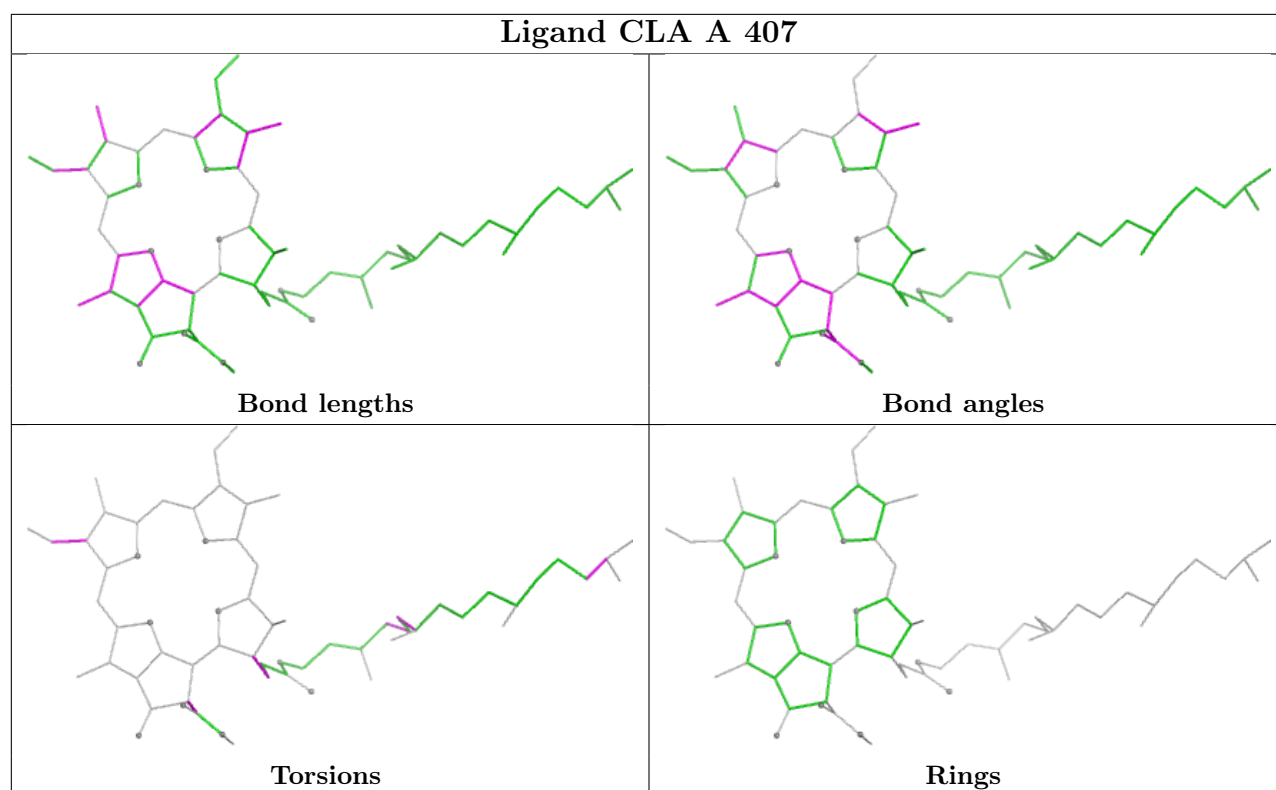


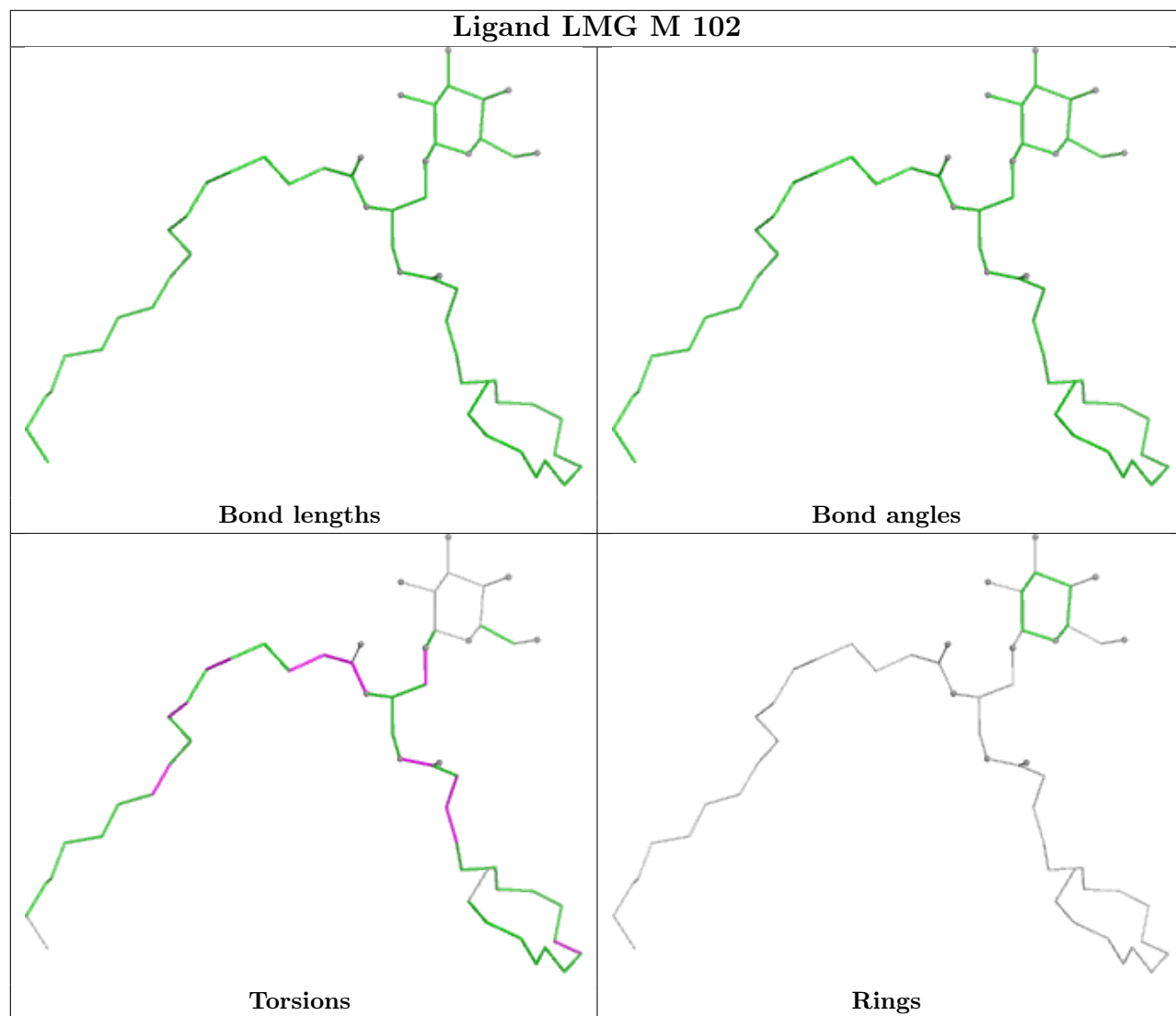


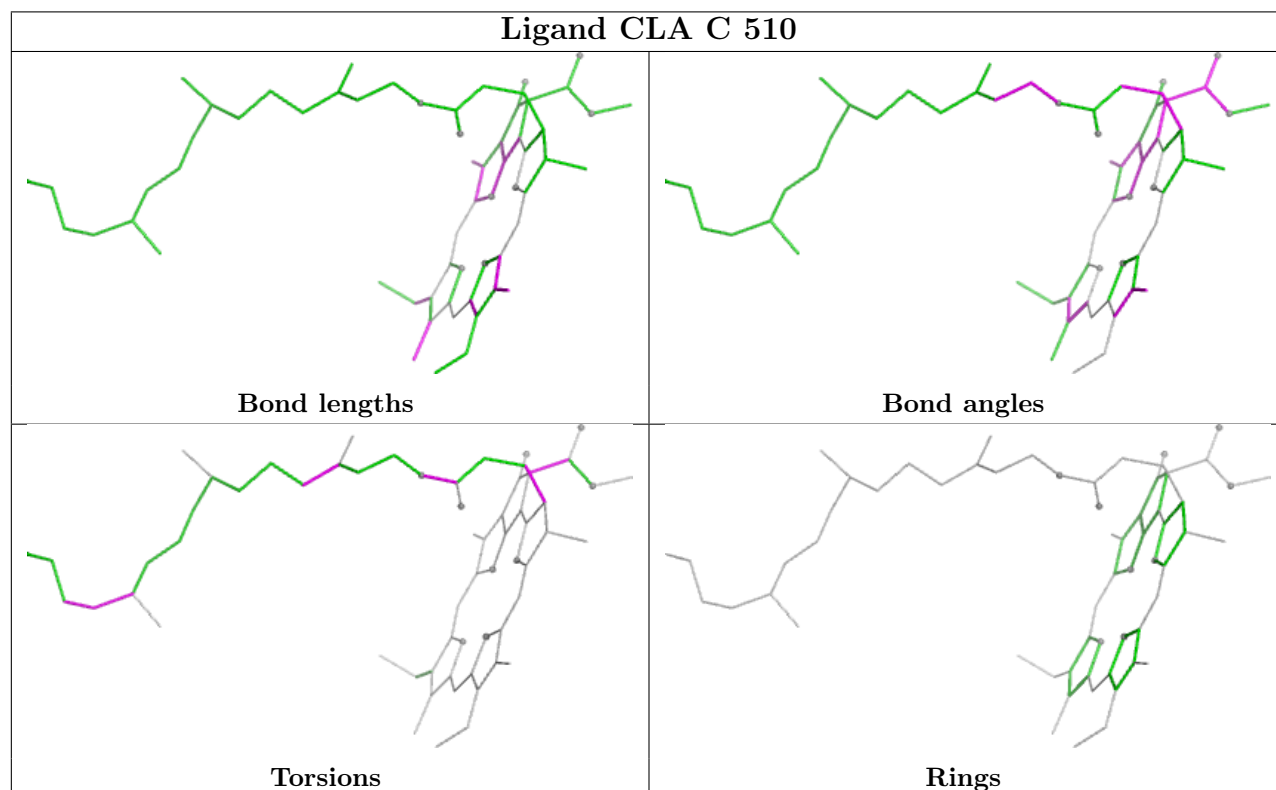
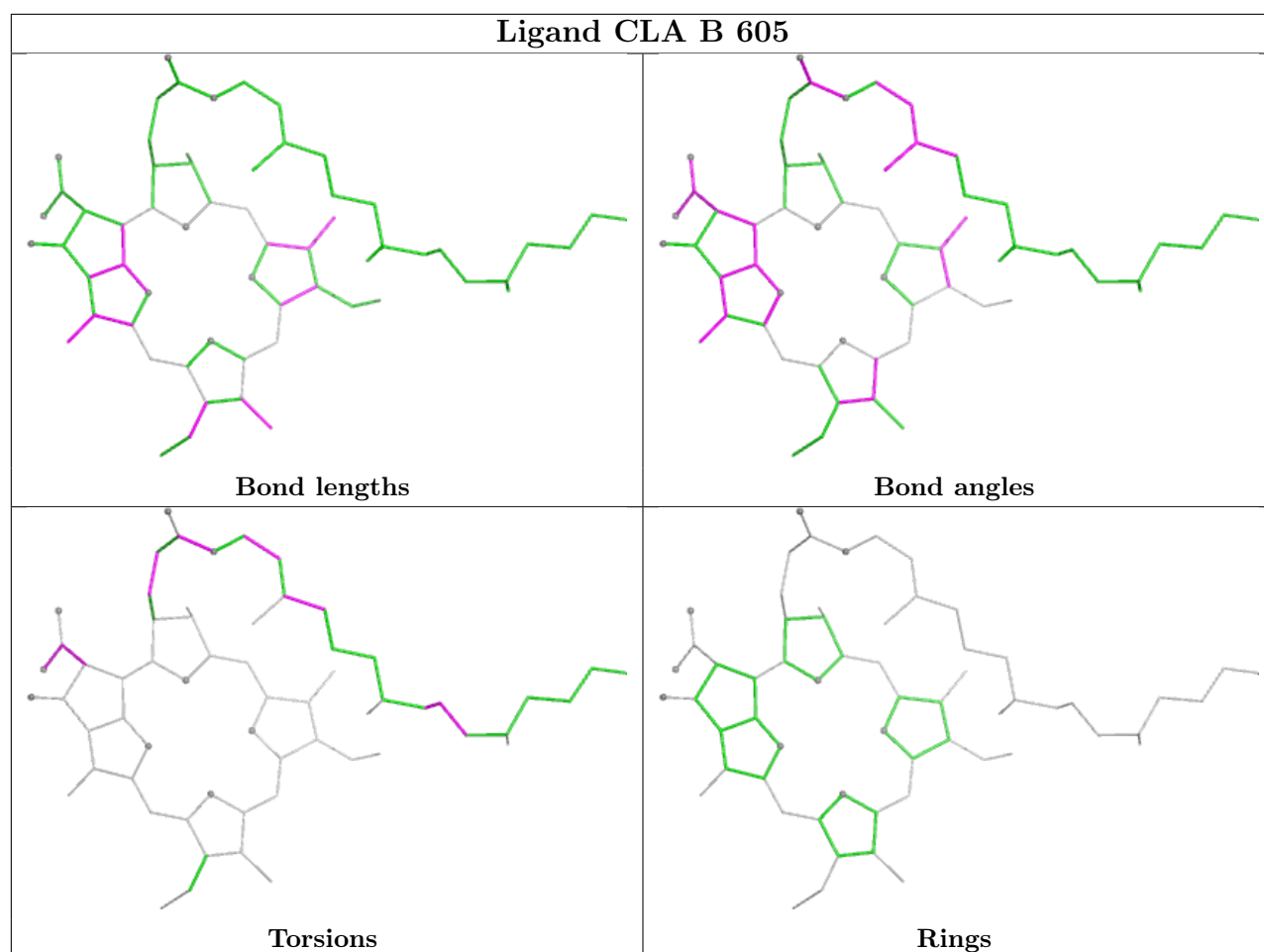


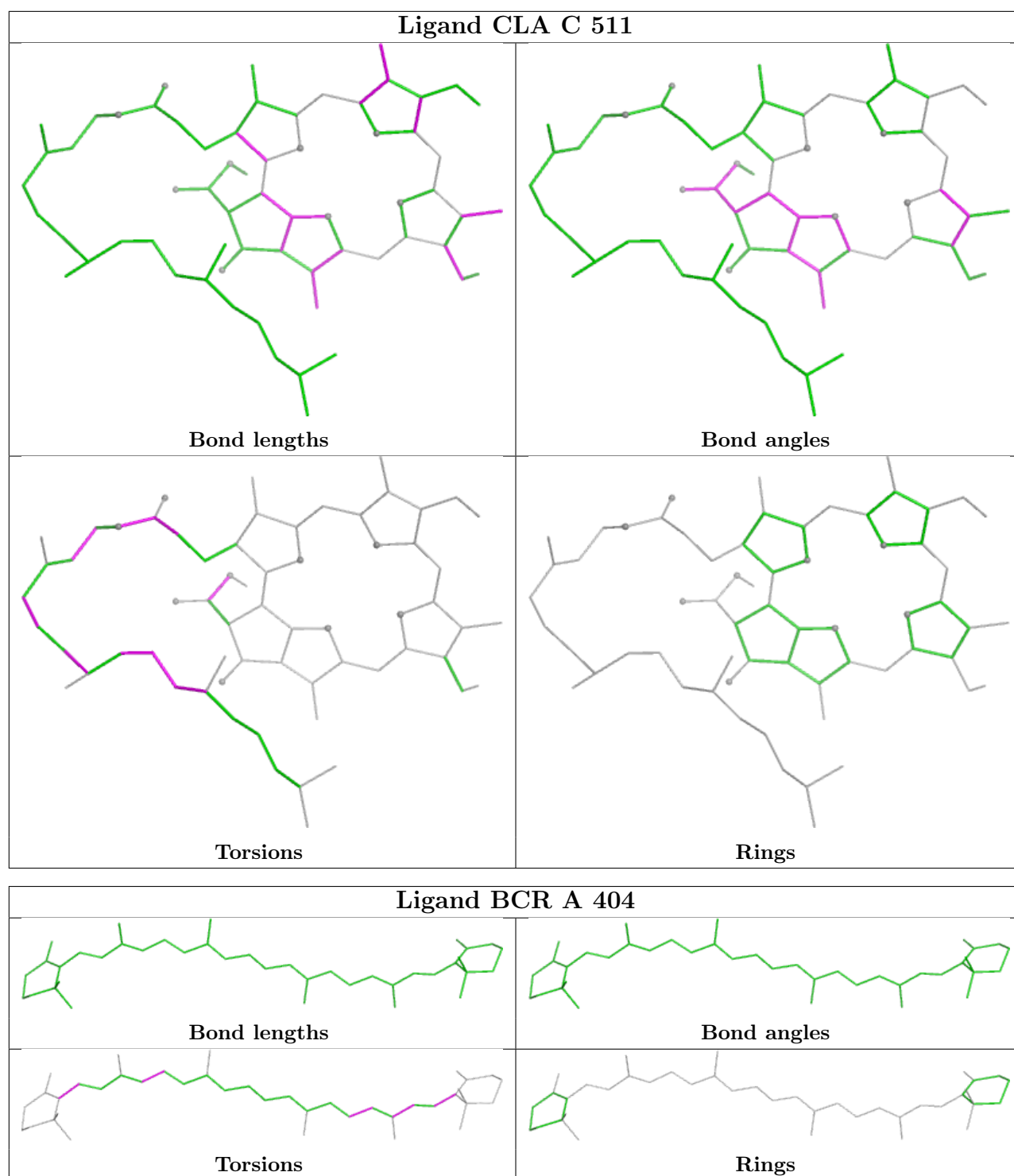


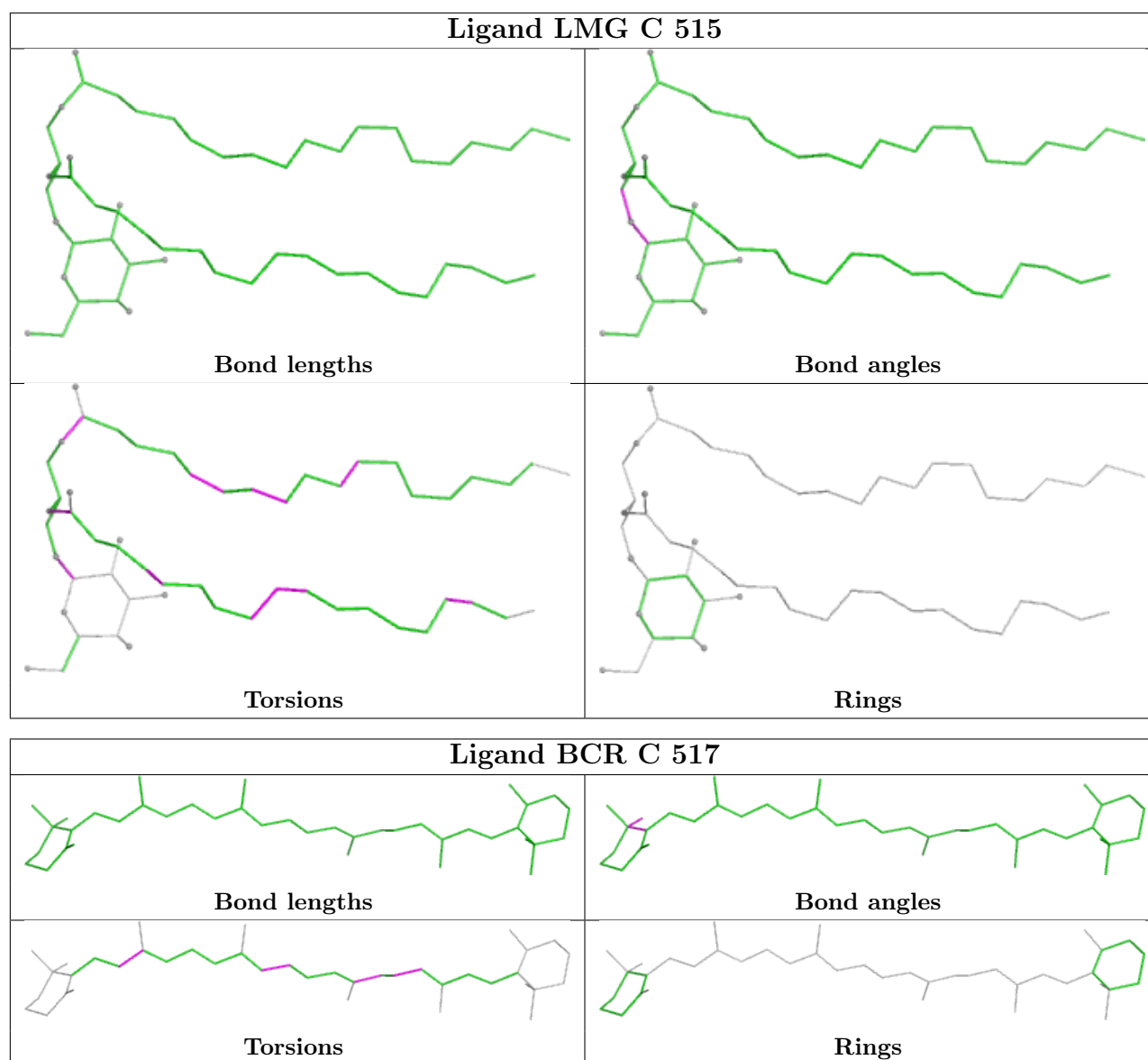












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

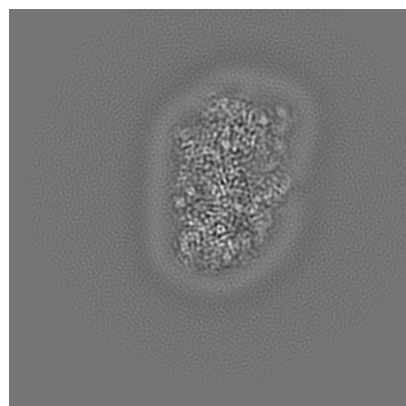
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52705. These allow visual inspection of the internal detail of the map and identification of artifacts.

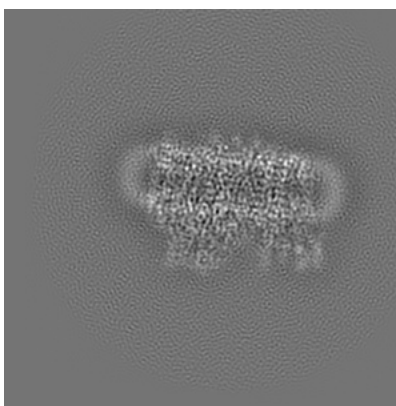
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

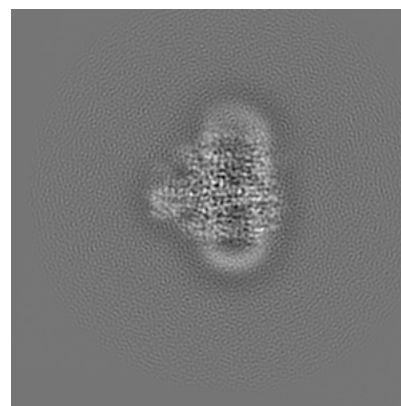
6.1.1 Primary map



X

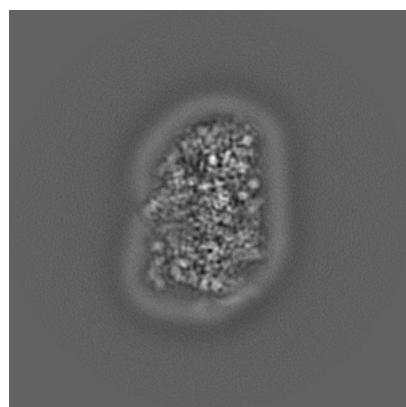


Y

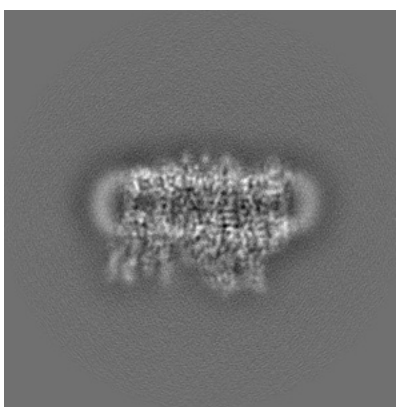


Z

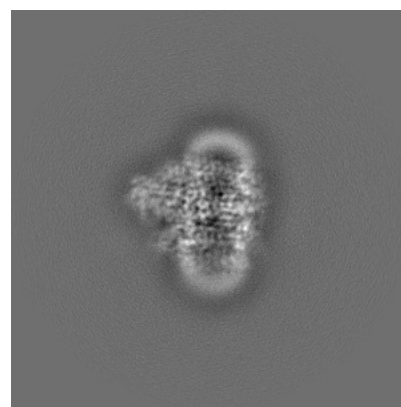
6.1.2 Raw map



X



Y

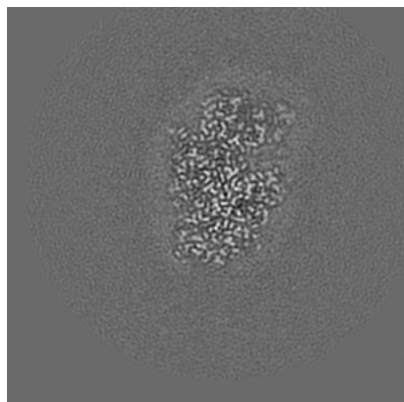


Z

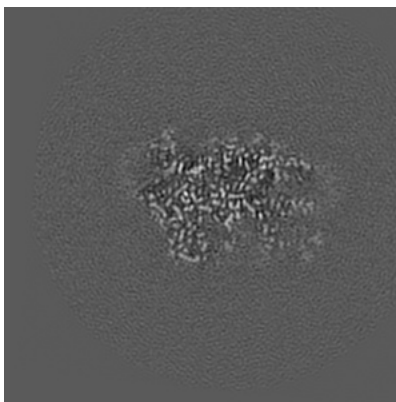
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

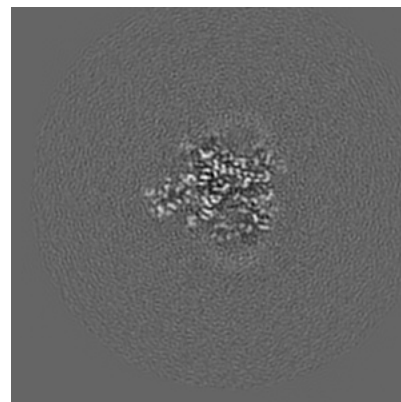
6.2.1 Primary map



X Index: 160

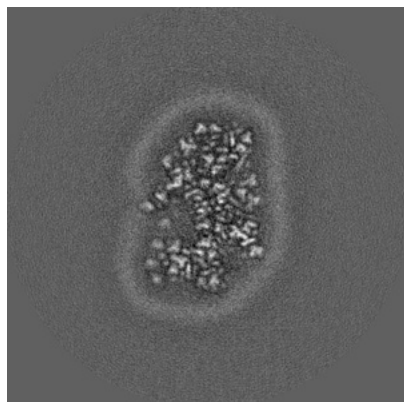


Y Index: 160

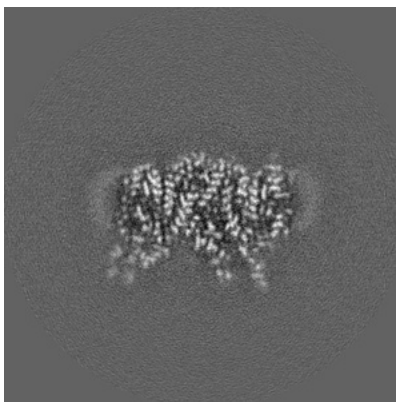


Z Index: 160

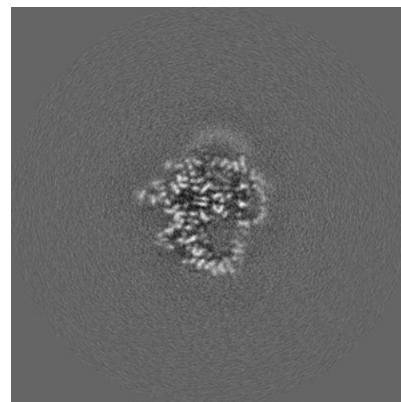
6.2.2 Raw map



X Index: 160



Y Index: 160

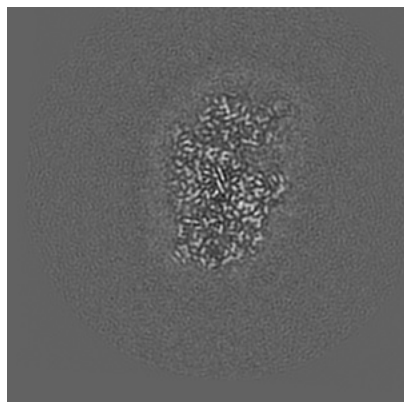


Z Index: 160

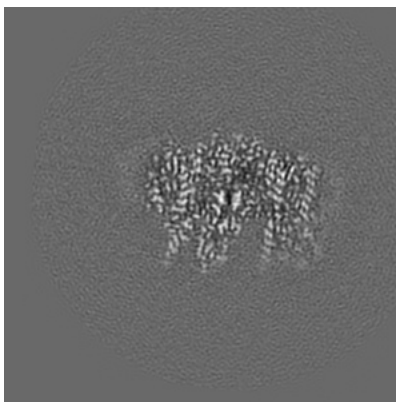
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

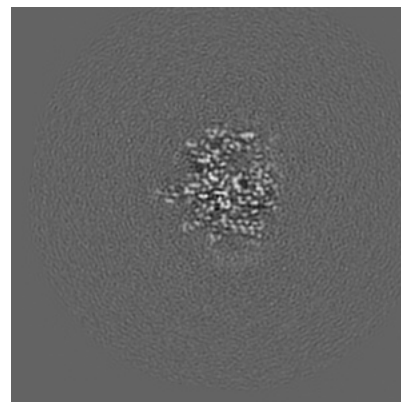
6.3.1 Primary map



X Index: 163

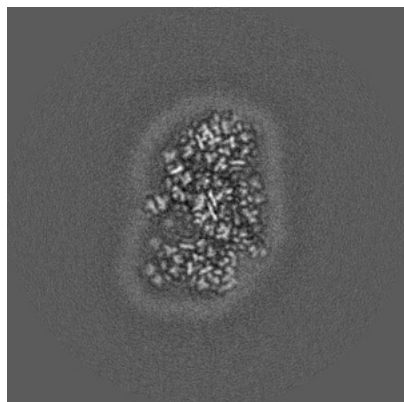


Y Index: 171

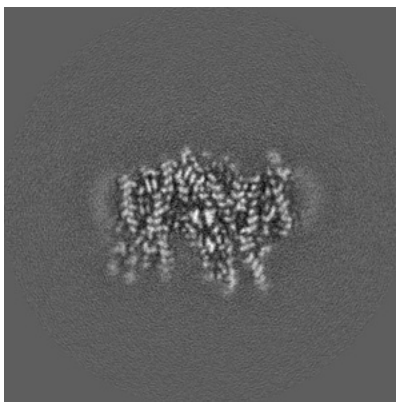


Z Index: 174

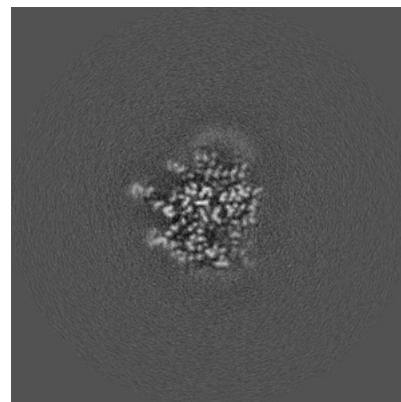
6.3.2 Raw map



X Index: 152



Y Index: 165

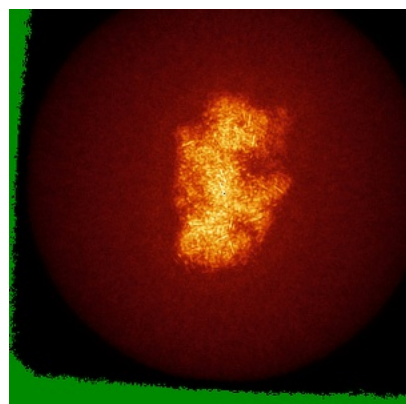


Z Index: 168

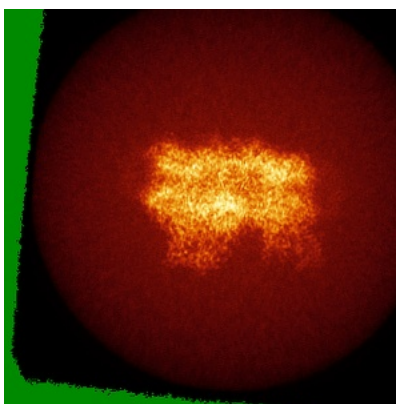
The images above show the largest variance slices of the map in three orthogonal directions.

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

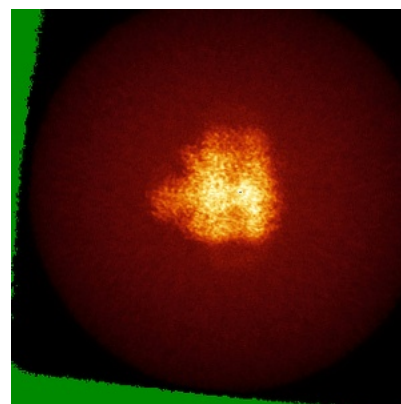
6.4.1 Primary map



X

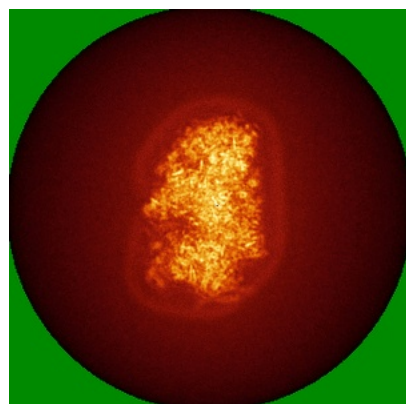


Y

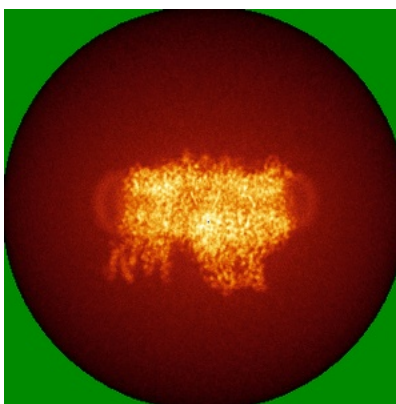


Z

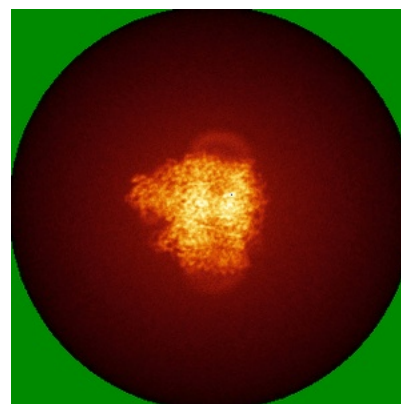
6.4.2 Raw map



X



Y



Z

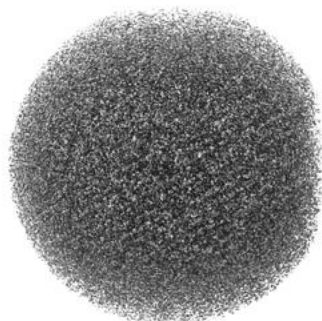
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

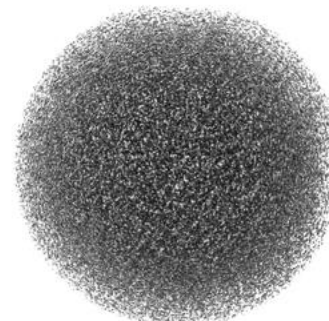
6.5.1 Primary map



X



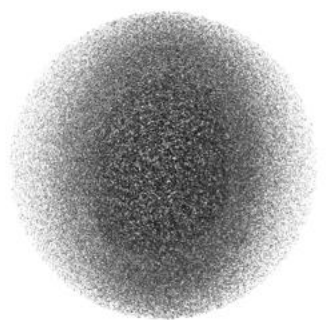
Y



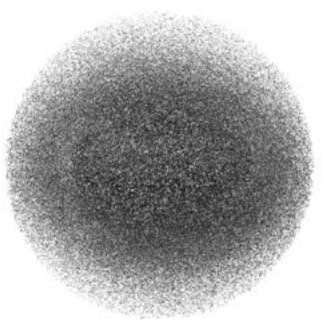
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0061. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

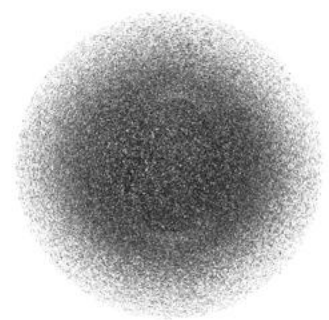
6.5.2 Raw map



X



Y



Z

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

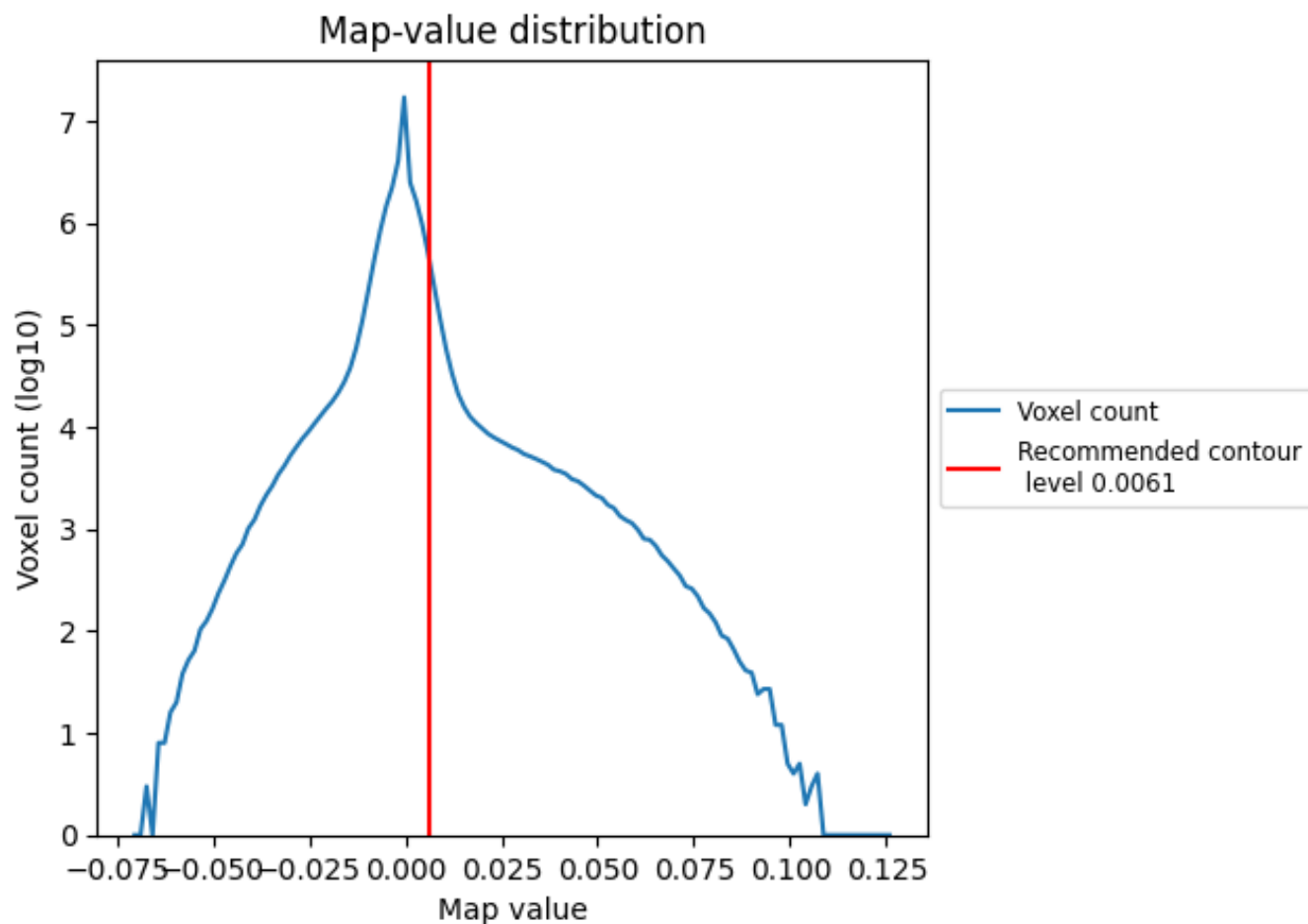
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

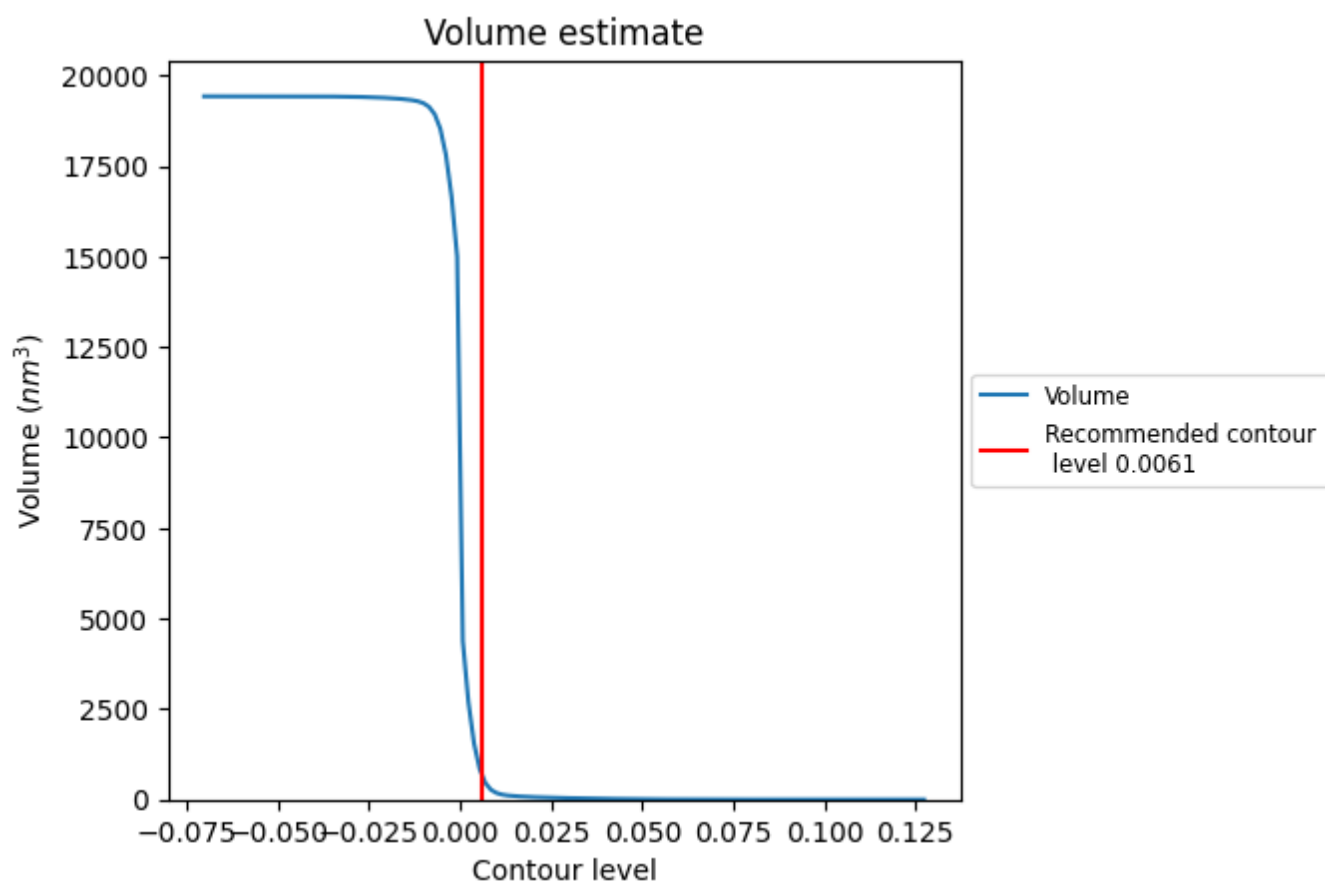
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

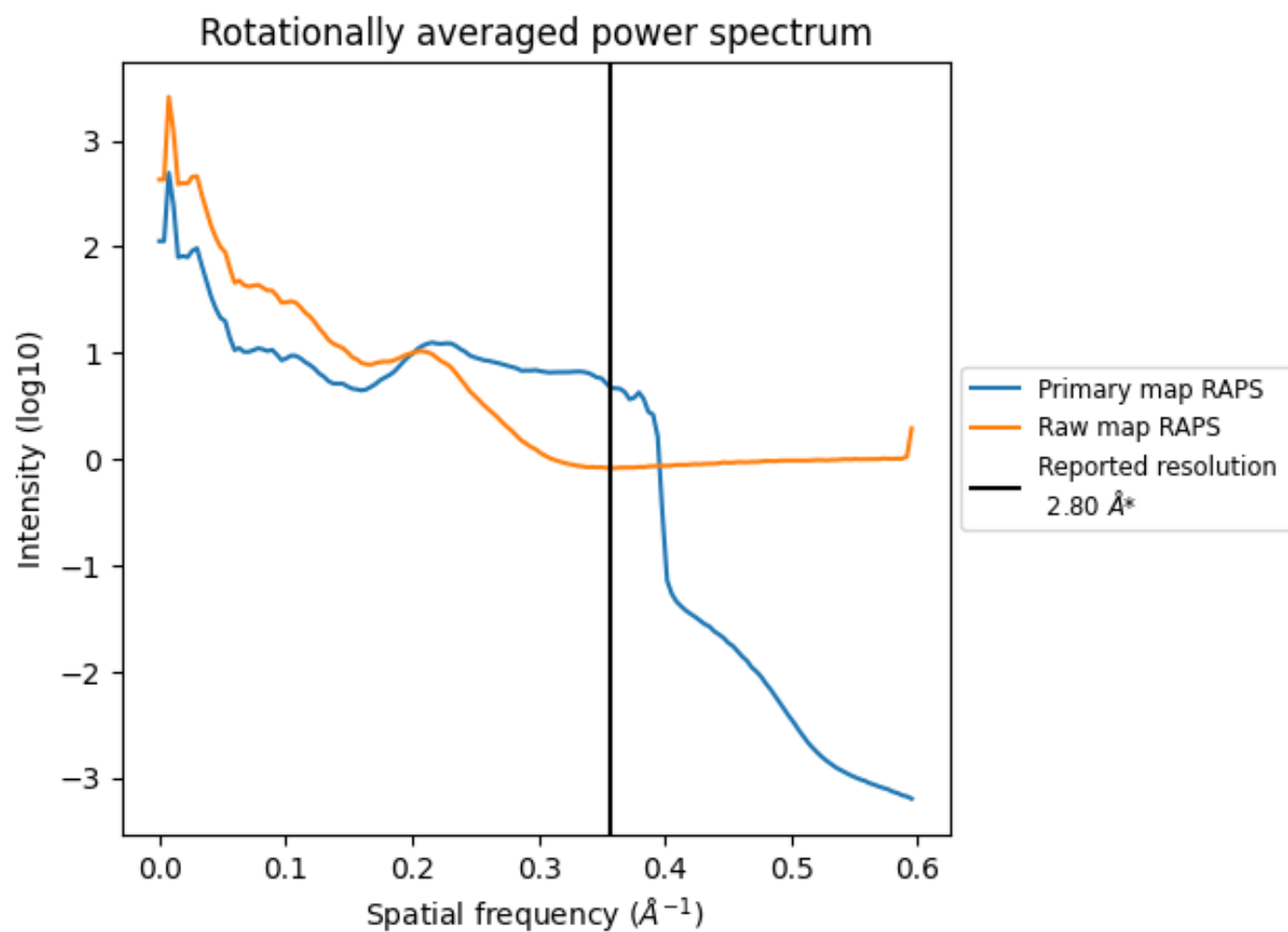
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 660 nm³; this corresponds to an approximate mass of 596 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 ⓘ

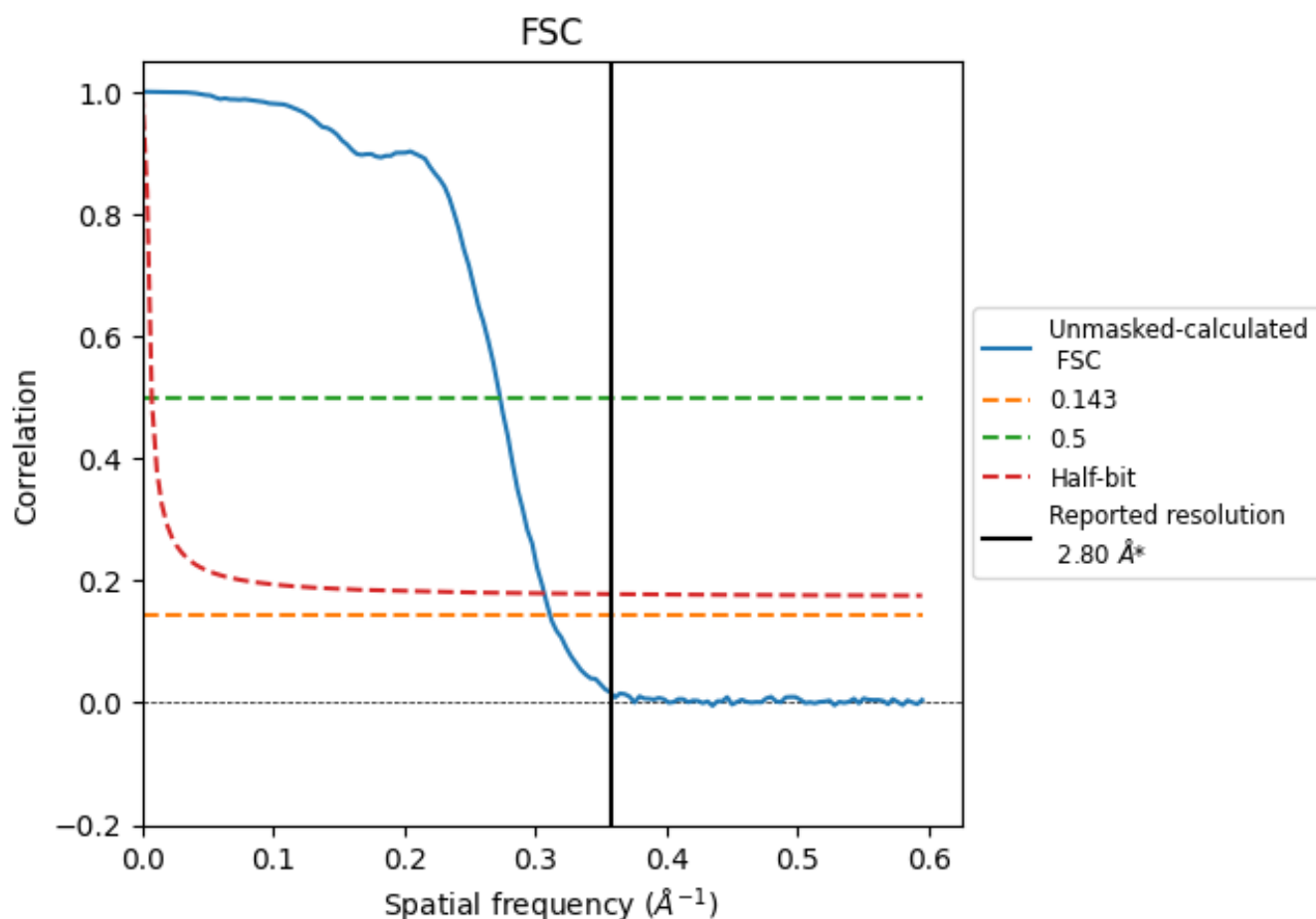


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.357 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

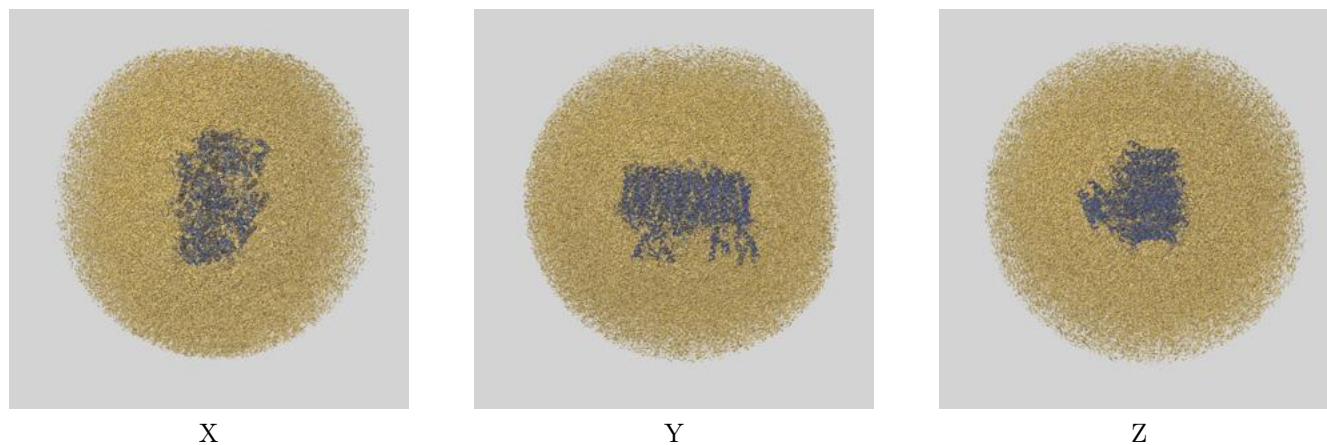
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.21	3.66	3.26

*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 3.21 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

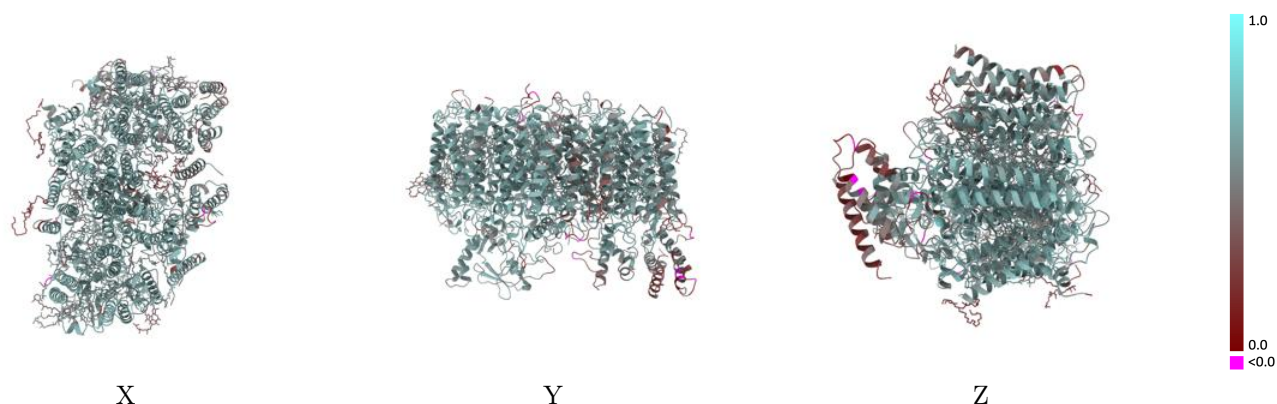
This section contains information regarding the fit between EMDB map EMD-52705 and PDB model 9I82. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



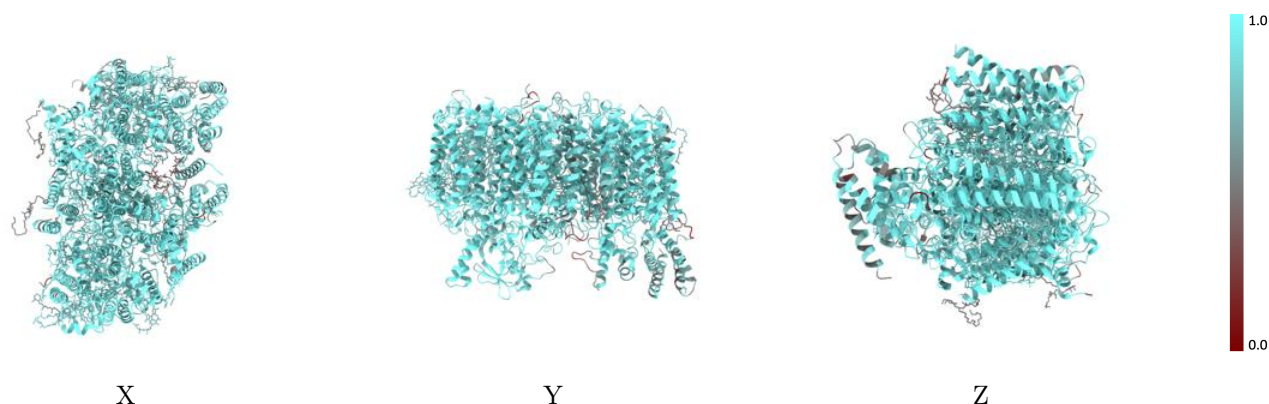
The images above show the 3D surface view of the map at the recommended contour level 0.0061 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



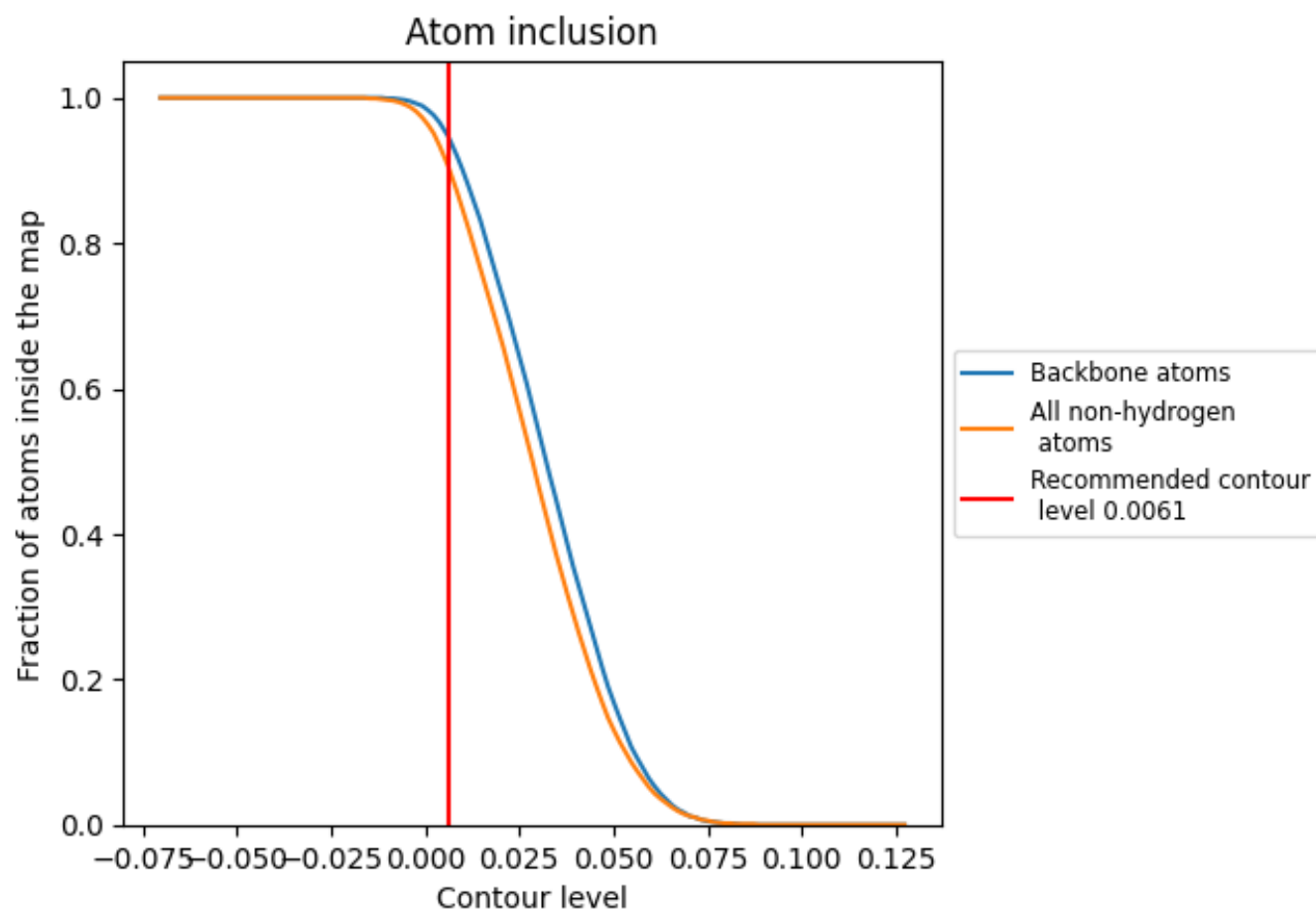
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0061).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.0061) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9060	 0.5710
1	 0.7180	 0.3610
A	 0.9350	 0.6050
B	 0.9390	 0.5950
C	 0.9000	 0.5720
D	 0.9550	 0.6180
E	 0.8850	 0.5330
F	 0.8110	 0.4870
H	 0.9480	 0.6030
I	 0.8780	 0.5370
J	 0.7440	 0.4520
K	 0.8370	 0.5320
L	 0.8780	 0.5660
M	 0.7780	 0.4830
T	 0.9600	 0.6120
X	 0.9130	 0.5600
Y	 0.7840	 0.4620
Z	 0.8350	 0.4890

