



Full wwPDB EM Validation Report ⓘ

Aug 10, 2026 – 06:26 pm BST

PDB ID : 9I83 / pdb_00009i83
EMDB ID : EMD-52706
Title : Cryo-EM structure of PSII intermediate Psb32-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 : 2.90 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

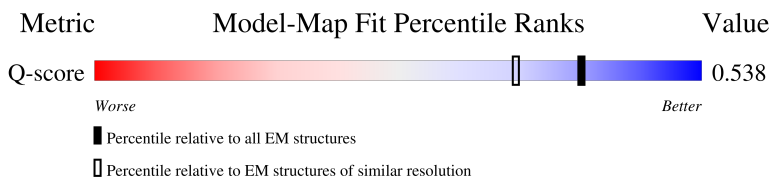
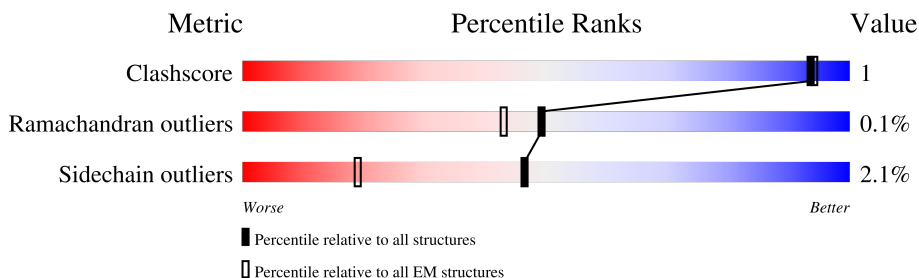
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

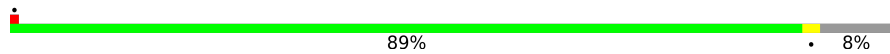
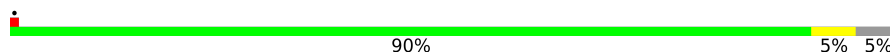
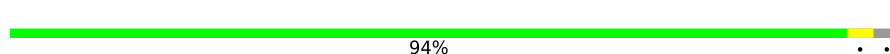
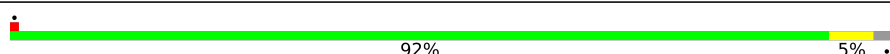
The reported resolution of this entry is 2.90 Å.

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.



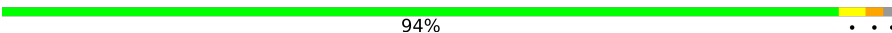
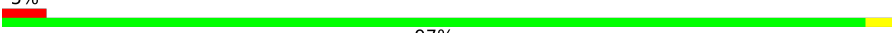
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	
2	B	510	
3	C	461	
4	D	352	

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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	V	163	
15	X	41	
16	Y	46	
17	Z	62	
18	1	134	
19	3	228	

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 23670 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	331	Total	C	N	O	S	0	0
			2598	1701	428	454	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 Cytochrome c-550.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	137	Total	C	N	O	S	0	0
			1064	675	177	208	4		

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

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

- Molecule 16 is a protein called Photosystem II reaction center protein Ycf12.

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

- Molecule 17 is a protein called Photosystem II reaction center protein Z.

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

- Molecule 18 is a protein called Photosystem II lipoprotein Psb27.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1	113	Total	C	N	O	S	0	0
			893	556	161	173	3		

- Molecule 19 is a protein called Tll0404 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	3	197	Total	C	N	O	S	0	0
			1499	941	249	306	3		

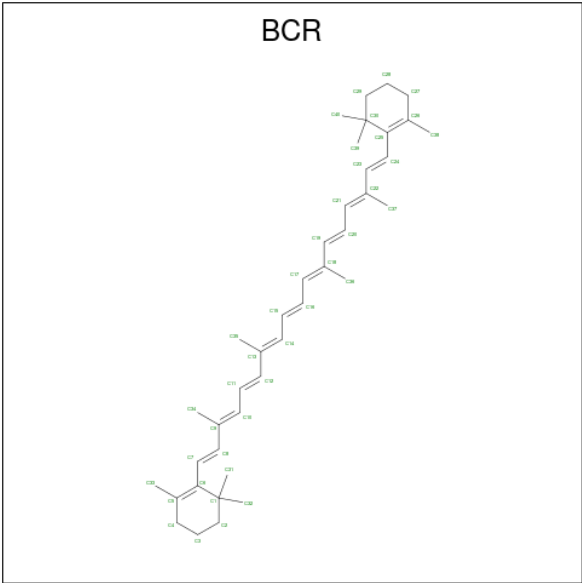
- Molecule 20 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 21 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



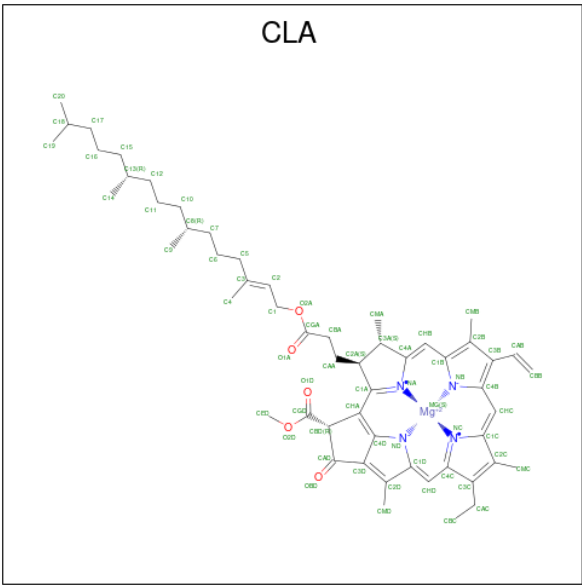
Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	C	1	Total	C	0
			40	40	
22	C	1	Total	C	0
			40	40	
22	C	1	Total	C	0
			40	40	
22	D	1	Total	C	0
			40	40	
22	H	1	Total	C	0
			40	40	
22	J	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms			AltConf
22	K	1	Total	C		0
			40	40		

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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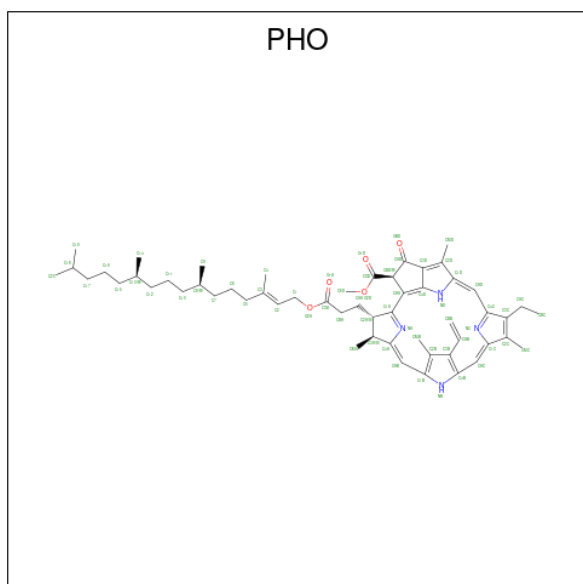
Mol	Chain	Residues	Atoms					AltConf
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

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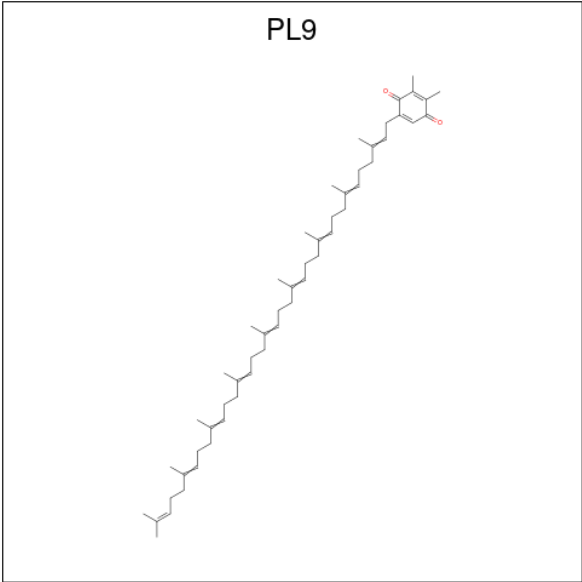
Mol	Chain	Residues	Atoms					AltConf
23	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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



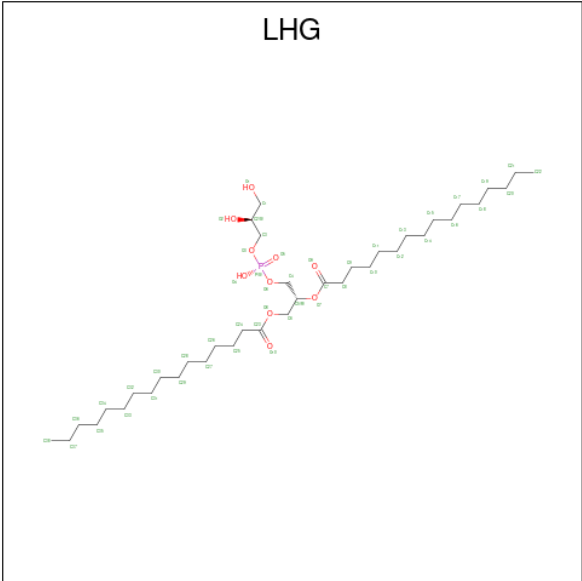
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	N	O	0
			64	55	4	5	
24	D	1	Total	C	N	O	0
			64	55	4	5	

- 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: $C_{53}H_{80}O_2$) (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 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



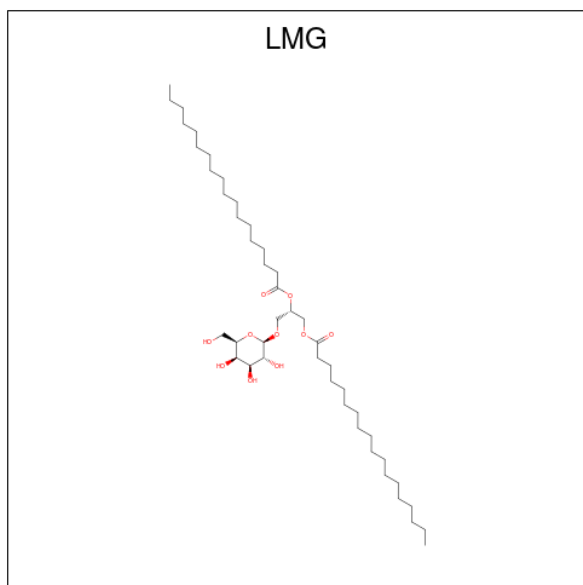
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	P	0
			49	38	10	1	

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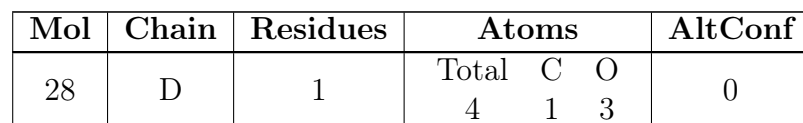
Mol	Chain	Residues	Atoms				AltConf
26	C	1	Total	C	O	P	0
			49	38	10	1	

- 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	D	1	Total	C	O		0
			55	45	10		
27	D	1	Total	C	O		0
			55	45	10		
27	D	1	Total	C	O		0
			55	45	10		
27	I	1	Total	C	O		0
			55	45	10		
27	K	1	Total	C	O		0
			55	45	10		
27	L	1	Total	C	O		0
			55	45	10		
27	M	1	Total	C	O		0
			55	45	10		
27	Z	1	Total	C	O		0
			55	45	10		

- Molecule 28 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



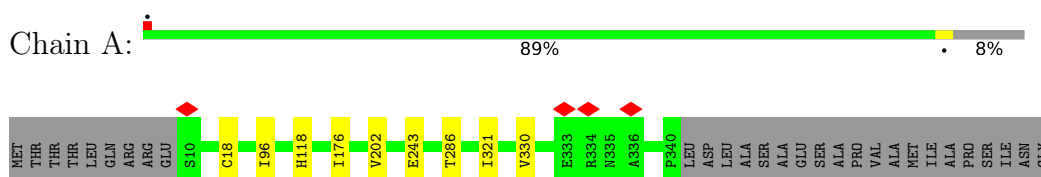
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Mol	Chain	Residues	Atoms					AltConf
29	F	1	Total 43	C 34	Fe 1	N 4	O 4	0
29	V	1	Total 43	C 34	Fe 1	N 4	O 4	0

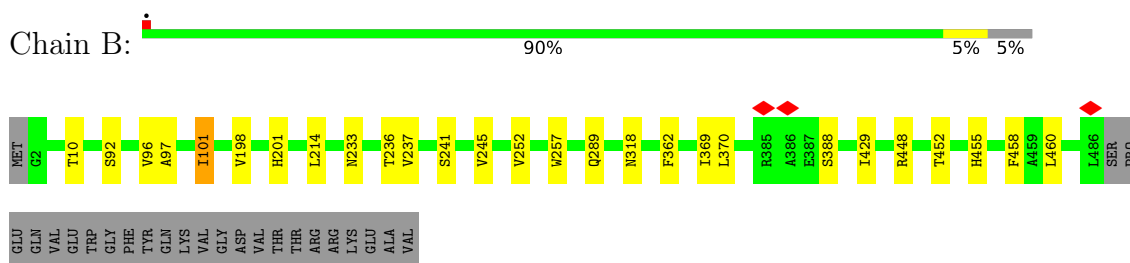
3 Residue-property plots [i](#)

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.

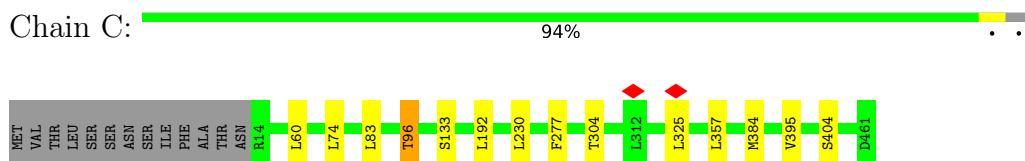
- Molecule 1: Photosystem II protein D1 1



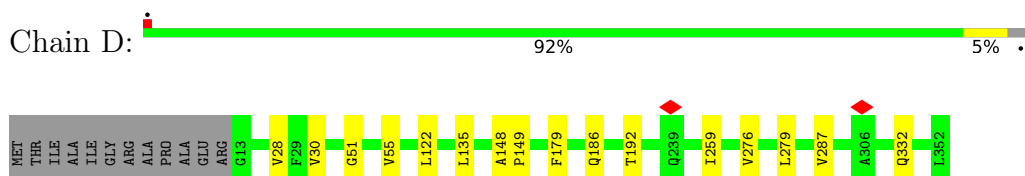
- Molecule 2: Photosystem II CP47 reaction center protein



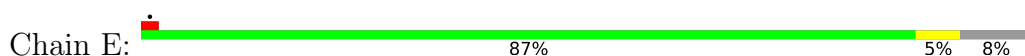
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 4: Photosystem II D2 protein

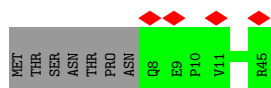
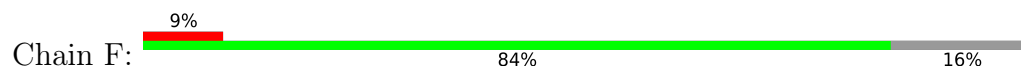


- Molecule 5: Cytochrome b559 subunit alpha

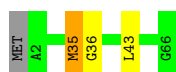




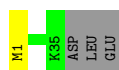
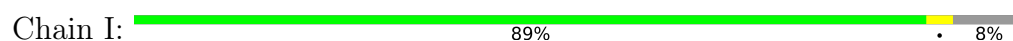
- Molecule 6: Cytochrome b559 subunit beta



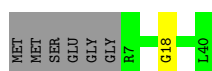
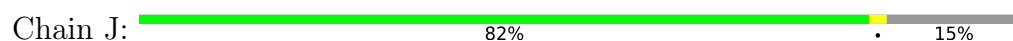
- Molecule 7: Photosystem II reaction center protein H



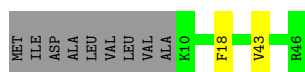
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



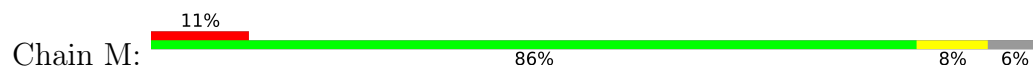
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



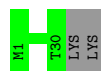
- Molecule 12: Photosystem II reaction center protein M





- Molecule 13: Photosystem II reaction center protein T

Chain T: 94% 6%



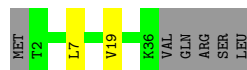
- Molecule 14: Cytochrome c-550

Chain V: 5% 80% 16%



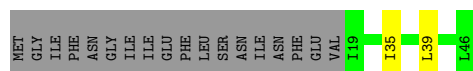
- Molecule 15: Photosystem II reaction center X protein

Chain X: 80% 5% 15%



- Molecule 16: Photosystem II reaction center protein Ycf12

Chain Y: 57% 39%



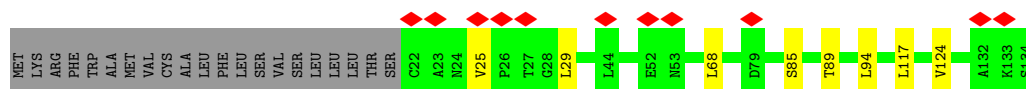
- Molecule 17: Photosystem II reaction center protein Z

Chain Z: 90% 10%

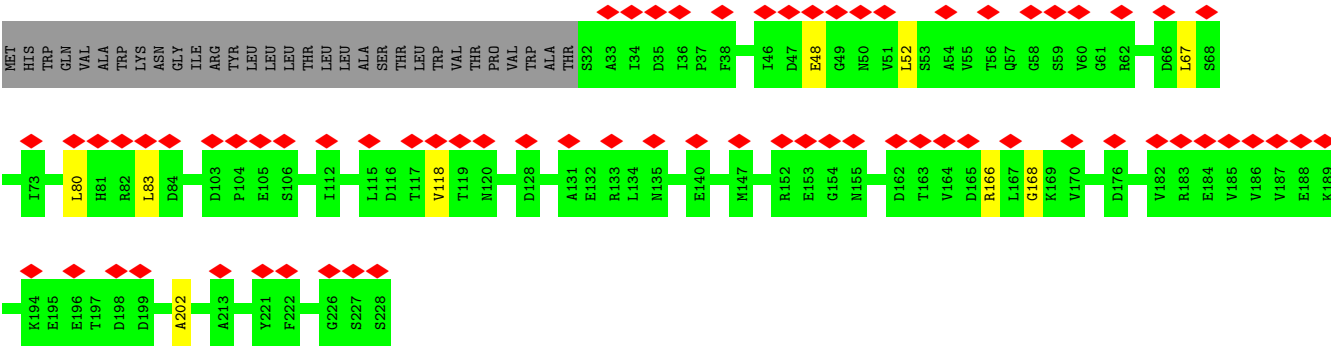
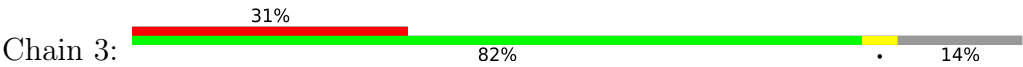


- Molecule 18: Photosystem II lipoprotein Psb27

Chain 1: 8% 78% 6% 16%



- Molecule 19: Tll0404 protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	199653	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	0.096	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.00634	Depositor
Map size ($\text{\AA}$)	268.8, 268.8, 268.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: CL, PHO, CLA, BCT, BCR, FE, PL9, LHG, HEM, LMG

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	0.20	0/2683	0.39	0/3660
2	B	0.20	0/3947	0.40	0/5379
3	C	0.20	0/3579	0.40	0/4872
4	D	0.18	0/2801	0.40	0/3818
5	E	0.19	0/654	0.42	0/891
6	F	0.18	0/317	0.44	0/433
7	H	0.20	0/524	0.45	0/713
8	I	0.25	0/293	0.43	0/395
9	J	0.19	0/255	0.41	0/346
10	K	0.23	0/303	0.46	0/416
11	L	0.20	0/311	0.38	0/422
12	M	0.25	0/270	0.53	0/367
13	T	0.21	0/265	0.36	0/359
14	V	0.19	0/1085	0.38	0/1473
15	X	0.19	0/257	0.38	0/348
16	Y	0.19	0/209	0.43	0/279
17	Z	0.21	0/490	0.42	0/669
18	1	0.22	0/907	0.48	0/1220
19	3	0.18	0/1526	0.36	0/2086
All	All	0.20	0/20676	0.40	0/28146

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	2598	0	2493	5	0
2	B	3812	0	3683	15	0
3	C	3466	0	3389	6	0
4	D	2706	0	2608	8	0
5	E	635	0	625	2	0
6	F	307	0	312	0	0
7	H	511	0	532	1	0
8	I	286	0	308	1	0
9	J	249	0	262	1	0
10	K	293	0	305	1	0
11	L	304	0	316	0	0
12	M	267	0	289	1	0
13	T	256	0	262	0	0
14	V	1064	0	1072	4	0
15	X	254	0	282	0	0
16	Y	208	0	237	1	0
17	Z	479	0	516	5	0
18	1	893	0	896	6	0
19	3	1499	0	1475	2	0
20	A	1	0	0	0	0
21	A	1	0	0	0	0
22	A	40	0	56	0	0
22	B	120	0	168	0	0
22	C	120	0	168	3	0
22	D	40	0	56	0	0
22	H	40	0	56	2	0
22	J	40	0	56	0	0
22	K	40	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	A	260	0	288	3	0
23	B	1040	0	1152	9	0
23	C	845	0	936	7	0
23	D	130	0	144	3	0
24	A	64	0	74	0	0
24	D	64	0	74	1	0
25	A	55	0	80	0	0
25	D	55	0	80	0	0
26	A	49	0	74	0	0
26	C	49	0	74	0	0
27	D	165	0	258	0	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
27	Z	55	0	86	0	0
28	D	4	0	1	0	0
29	F	43	0	30	1	0
29	V	43	0	30	3	0
All	All	23670	0	24203	62	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 (62) 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:304:THR:HG21	3:C:384:MET:HE1	1.67	0.75
4:D:279:LEU:HD22	24:D:408:PHO:HBC3	1.71	0.70
29:V:201:HEM:HMB1	29:V:201:HEM:HBB2	1.76	0.67
3:C:384:MET:HE3	14:V:74:THR:HG22	1.77	0.67
29:V:201:HEM:HBC2	29:V:201:HEM:HHH	1.78	0.65
2:B:241:SER:O	2:B:245:VAL:HG23	1.99	0.63
29:F:101:HEM:HMB1	29:F:101:HEM:HBB2	1.82	0.62
14:V:32:GLU:O	14:V:35:THR:HG22	2.00	0.61
18:1:68:LEU:CD2	18:1:94:LEU:HD22	2.31	0.60
2:B:237:VAL:HG22	23:B:613:CLA:HBC2	1.84	0.59
4:D:186:GLN:HB2	23:D:404:CLA:HBC1	1.83	0.58
4:D:192:THR:HG23	23:D:404:CLA:HBC2	1.84	0.58
18:1:89:THR:HG23	18:1:124:VAL:HG12	1.85	0.58
18:1:68:LEU:HD22	18:1:94:LEU:HD22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:TRP:CE3	2:B:452:THR:HG21	2.39	0.57
23:C:513:CLA:H141	17:Z:20:VAL:HG13	1.85	0.57
3:C:60:LEU:HD21	3:C:96:THR:HG22	1.86	0.56
18:1:85:SER:O	18:1:89:THR:HG22	2.05	0.56
2:B:458:PHE:HB3	23:B:607:CLA:HBC2	1.89	0.55
4:D:148:ALA:HB2	4:D:276:VAL:HG23	1.89	0.53
10:K:18:PHE:CE2	17:Z:9:LEU:HD23	2.44	0.53
18:1:25:VAL:HG21	18:1:29:LEU:HB2	1.91	0.52
9:J:18:GLY:HA3	22:K:101:BCR:H371	1.93	0.49
5:E:36:LEU:O	5:E:40:THR:HG22	2.12	0.49
22:H:101:BCR:H392	22:H:101:BCR:H23C	1.95	0.49
2:B:92:SER:O	2:B:96:VAL:HG23	2.11	0.48
2:B:97:ALA:O	2:B:101:ILE:HD12	2.14	0.48
23:B:614:CLA:H41	23:B:617:CLA:HBC3	1.94	0.48
5:E:40:THR:HG21	19:3:202:ALA:HB1	1.96	0.47
23:C:511:CLA:HBB1	23:C:516:CLA:HMA1	1.98	0.46
12:M:12:ALA:O	12:M:16:LEU:HD23	2.15	0.46
2:B:198:VAL:HG11	23:B:606:CLA:HED2	1.98	0.46
3:C:404:SER:HB2	14:V:68:VAL:HG23	1.97	0.46
17:Z:3:ILE:HD12	17:Z:4:LEU:N	2.31	0.46
1:A:118:HIS:NE2	23:A:407:CLA:NA	2.63	0.45
22:C:503:BCR:H362	23:C:510:CLA:H121	1.99	0.45
4:D:51:GLY:HA2	4:D:55:VAL:HG22	1.98	0.45
3:C:83:LEU:HD21	23:C:504:CLA:OBD	2.17	0.45
17:Z:50:LEU:O	17:Z:54:VAL:HG23	2.17	0.45
3:C:304:THR:HG21	3:C:384:MET:CE	2.42	0.45
2:B:10:THR:HG23	23:B:614:CLA:HAA2	1.97	0.45
2:B:448:ARG:O	2:B:452:THR:HG22	2.17	0.45
22:C:502:BCR:H312	17:Z:9:LEU:HD21	1.99	0.45
1:A:321:ILE:HD11	4:D:179:PHE:HB2	1.99	0.44
23:B:604:CLA:HMA1	22:H:101:BCR:H391	1.99	0.44
23:C:513:CLA:H143	16:Y:35:ILE:HD13	1.99	0.44
1:A:202:VAL:HG12	23:A:404:CLA:CHB	2.48	0.44
18:1:89:THR:HG23	18:1:124:VAL:CG1	2.46	0.43
2:B:369:ILE:C	2:B:370:LEU:HD12	2.44	0.43
1:A:96:ILE:HG22	8:I:1:MET:HE1	2.01	0.42
2:B:455:HIS:NE2	23:B:607:CLA:ND	2.67	0.42
23:D:405:CLA:C1	7:H:43:LEU:HD21	2.49	0.42
22:C:503:BCR:C40	23:C:504:CLA:HMB3	2.50	0.42
14:V:74:THR:HG21	29:V:201:HEM:HBC1	2.02	0.42
19:3:67:LEU:HD13	19:3:168:GLY:HA2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:ASN:O	2:B:236:THR:HG22	2.20	0.41
4:D:148:ALA:HB3	4:D:149:PRO:HD3	2.02	0.41
2:B:460:LEU:CD1	4:D:287:VAL:HG11	2.51	0.41
1:A:176:ILE:HD12	23:A:405:CLA:HED1	2.02	0.41
23:C:504:CLA:HBB1	23:C:504:CLA:HHC	2.04	0.40
2:B:201:HIS:HE2	23:B:606:CLA:C2B	2.34	0.40
2:B:252:VAL:HG12	23:B:606:CLA:H11	2.03	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	329/360 (91%)	320 (97%)	9 (3%)	0	100	100
2	B	483/510 (95%)	475 (98%)	7 (1%)	1 (0%)	43	72
3	C	446/461 (97%)	423 (95%)	23 (5%)	0	100	100
4	D	338/352 (96%)	324 (96%)	14 (4%)	0	100	100
5	E	75/84 (89%)	73 (97%)	2 (3%)	0	100	100
6	F	36/45 (80%)	33 (92%)	3 (8%)	0	100	100
7	H	63/66 (96%)	59 (94%)	3 (5%)	1 (2%)	7	27
8	I	33/38 (87%)	30 (91%)	3 (9%)	0	100	100
9	J	32/40 (80%)	30 (94%)	2 (6%)	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	V	135/163 (83%)	129 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	X	33/41 (80%)	32 (97%)	1 (3%)	0	100	100
16	Y	26/46 (56%)	25 (96%)	1 (4%)	0	100	100
17	Z	60/62 (97%)	60 (100%)	0	0	100	100
18	1	111/134 (83%)	110 (99%)	1 (1%)	0	100	100
19	3	195/228 (86%)	191 (98%)	4 (2%)	0	100	100
All	All	2525/2781 (91%)	2443 (97%)	80 (3%)	2 (0%)	49	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	H	36	GLY
2	B	388	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	268/291 (92%)	264 (98%)	4 (2%)	57	84
2	B	385/407 (95%)	379 (98%)	6 (2%)	55	83
3	C	350/362 (97%)	341 (97%)	9 (3%)	40	73
4	D	275/283 (97%)	269 (98%)	6 (2%)	45	77
5	E	69/73 (94%)	67 (97%)	2 (3%)	37	71
6	F	32/39 (82%)	32 (100%)	0	100	100
7	H	54/55 (98%)	53 (98%)	1 (2%)	50	79
8	I	32/35 (91%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
10	K	30/37 (81%)	29 (97%)	1 (3%)	33	67
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	71
12	M	31/33 (94%)	30 (97%)	1 (3%)	34	68
13	T	27/29 (93%)	27 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	V	117/138 (85%)	114 (97%)	3 (3%)	40	73
15	X	28/34 (82%)	26 (93%)	2 (7%)	13	40
16	Y	21/37 (57%)	20 (95%)	1 (5%)	23	55
17	Z	52/52 (100%)	52 (100%)	0	100	100
18	1	96/115 (84%)	95 (99%)	1 (1%)	68	89
19	3	168/195 (86%)	162 (96%)	6 (4%)	31	65
All	All	2094/2278 (92%)	2050 (98%)	44 (2%)	46	77

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	CYS
1	A	243	GLU
1	A	286	THR
1	A	330	VAL
2	B	101	ILE
2	B	214	LEU
2	B	289	GLN
2	B	318	ASN
2	B	362	PHE
2	B	429	ILE
3	C	74	LEU
3	C	96	THR
3	C	133	SER
3	C	192	LEU
3	C	230	LEU
3	C	277	PHE
3	C	325	LEU
3	C	357	LEU
3	C	395	VAL
4	D	28	VAL
4	D	30	VAL
4	D	122	LEU
4	D	135	LEU
4	D	259	ILE
4	D	332	GLN
5	E	62	SER
5	E	78	THR
7	H	35	MET
10	K	43	VAL

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Mol	Chain	Res	Type
11	L	1	MET
12	M	6	LEU
14	V	47	LEU
14	V	99	VAL
14	V	122	ARG
15	X	7	LEU
15	X	19	VAL
16	Y	39	LEU
18	1	117	LEU
19	3	48	GLU
19	3	52	LEU
19	3	80	LEU
19	3	83	LEU
19	3	118	VAL
19	3	166	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	ASN
1	A	198	HIS
2	B	285	ASN
3	C	418	HIS
4	D	338	ASN
18	1	95	ASN
19	3	81	HIS

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, 2 are monoatomic - leaving 63 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	511	3	69,73,73	1.25	7 (10%)	83,113,113	1.27	7 (8%)
27	LMG	D	407	-	55,55,55	0.48	0	63,63,63	0.73	1 (1%)
23	CLA	B	619	-	69,73,73	1.26	7 (10%)	83,113,113	1.22	6 (7%)
23	CLA	C	509	3	69,73,73	1.27	7 (10%)	83,113,113	1.29	6 (7%)
23	CLA	C	513	3	69,73,73	1.26	6 (8%)	83,113,113	1.36	8 (9%)
23	CLA	B	615	2	69,73,73	1.25	8 (11%)	83,113,113	1.25	6 (7%)
22	BCR	B	602	-	41,41,41	0.39	0	56,56,56	0.59	0
24	PHO	D	408	-	58,69,69	2.10	10 (17%)	56,99,99	1.75	8 (14%)
22	BCR	C	503	-	41,41,41	0.40	0	56,56,56	0.84	1 (1%)
22	BCR	C	502	-	41,41,41	0.37	0	56,56,56	0.81	0
23	CLA	C	515	3	69,73,73	1.25	6 (8%)	83,113,113	1.29	6 (7%)
23	CLA	B	612	-	69,73,73	1.25	6 (8%)	83,113,113	1.22	5 (6%)
27	LMG	K	102	-	55,55,55	0.45	0	63,63,63	0.68	1 (1%)
22	BCR	D	403	-	41,41,41	0.40	0	56,56,56	0.78	1 (1%)
27	LMG	I	101	-	55,55,55	0.48	0	63,63,63	0.61	0
29	HEM	F	101	6	50,50,50	1.45	8 (16%)	66,82,82	1.10	5 (7%)
23	CLA	A	404	-	69,73,73	1.23	8 (11%)	83,113,113	1.29	6 (7%)
23	CLA	B	611	2	69,73,73	1.26	8 (11%)	83,113,113	1.41	8 (9%)
27	LMG	D	401	-	55,55,55	0.48	0	63,63,63	0.54	0
22	BCR	H	101	-	41,41,41	0.44	0	56,56,56	1.01	1 (1%)
23	CLA	C	506	3	69,73,73	1.25	8 (11%)	83,113,113	1.32	9 (10%)
23	CLA	A	407	1	69,73,73	1.24	8 (11%)	83,113,113	1.30	4 (4%)
23	CLA	B	614	2	69,73,73	1.26	7 (10%)	83,113,113	1.32	7 (8%)
23	CLA	C	512	3	69,73,73	1.25	7 (10%)	83,113,113	1.24	4 (4%)
22	BCR	J	101	-	41,41,41	0.39	0	56,56,56	0.70	1 (1%)
23	CLA	B	606	2	69,73,73	1.25	8 (11%)	83,113,113	1.32	5 (6%)
23	CLA	B	607	2	69,73,73	1.25	8 (11%)	83,113,113	1.25	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PL9	D	409	-	55,55,55	0.90	2 (3%)	68,69,69	1.60	12 (17%)
23	CLA	B	605	2	69,73,73	1.25	8 (11%)	83,113,113	1.30	7 (8%)
23	CLA	B	616	2	69,73,73	1.28	7 (10%)	83,113,113	1.18	6 (7%)
28	BCT	D	402	20	2,3,3	0.87	0	2,3,3	3.12	2 (100%)
23	CLA	B	609	-	69,73,73	1.25	8 (11%)	83,113,113	1.28	6 (7%)
23	CLA	B	608	2	69,73,73	1.26	8 (11%)	83,113,113	1.31	6 (7%)
23	CLA	B	613	-	69,73,73	1.26	7 (10%)	83,113,113	1.26	6 (7%)
23	CLA	C	504	3	69,73,73	1.27	6 (8%)	83,113,113	1.37	6 (7%)
23	CLA	B	604	-	69,73,73	1.27	7 (10%)	83,113,113	1.30	7 (8%)
23	CLA	A	405	-	69,73,73	1.26	7 (10%)	83,113,113	1.23	7 (8%)
23	CLA	B	617	2	69,73,73	1.24	7 (10%)	83,113,113	1.34	8 (9%)
23	CLA	C	514	3	69,73,73	1.26	8 (11%)	83,113,113	1.29	6 (7%)
22	BCR	B	601	-	41,41,41	0.41	0	56,56,56	0.84	3 (5%)
23	CLA	B	618	2	69,73,73	1.25	7 (10%)	83,113,113	1.31	6 (7%)
23	CLA	C	505	3	69,73,73	1.26	10 (14%)	83,113,113	1.30	8 (9%)
27	LMG	M	101	-	55,55,55	0.45	0	63,63,63	0.66	1 (1%)
24	PHO	A	408	-	58,69,69	2.10	10 (17%)	56,99,99	1.69	6 (10%)
27	LMG	L	101	-	55,55,55	0.47	0	63,63,63	0.75	2 (3%)
29	HEM	V	201	14	50,50,50	1.50	8 (16%)	66,82,82	1.25	8 (12%)
22	BCR	K	101	-	41,41,41	0.42	0	56,56,56	0.92	3 (5%)
22	BCR	C	517	-	41,41,41	0.32	0	56,56,56	0.84	1 (1%)
23	CLA	C	516	3	69,73,73	1.25	7 (10%)	83,113,113	1.28	6 (7%)
23	CLA	B	610	-	69,73,73	1.24	7 (10%)	83,113,113	1.24	5 (6%)
23	CLA	A	406	-	69,73,73	1.27	9 (13%)	83,113,113	1.30	9 (10%)
25	PL9	A	409	-	55,55,55	0.81	1 (1%)	68,69,69	1.42	11 (16%)
23	CLA	C	508	3	69,73,73	1.28	7 (10%)	83,113,113	1.27	7 (8%)
23	CLA	D	405	4	69,73,73	1.24	8 (11%)	83,113,113	1.36	7 (8%)
27	LMG	Z	101	-	55,55,55	0.45	0	63,63,63	0.72	2 (3%)
26	LHG	A	410	-	48,48,48	0.52	0	51,54,54	0.52	0
23	CLA	D	404	4	69,73,73	1.26	7 (10%)	83,113,113	1.35	6 (7%)
22	BCR	B	603	-	41,41,41	0.38	0	56,56,56	0.62	0
23	CLA	C	507	-	69,73,73	1.25	7 (10%)	83,113,113	1.29	6 (7%)
23	CLA	C	510	-	69,73,73	1.25	8 (11%)	83,113,113	1.30	5 (6%)
26	LHG	C	501	-	48,48,48	0.51	0	51,54,54	0.56	0
22	BCR	A	403	-	41,41,41	0.48	0	56,56,56	0.51	0
27	LMG	D	406	-	55,55,55	0.49	0	63,63,63	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	511	3	-	10/39/115/115	-
27	LMG	D	407	-	-	11/50/70/70	0/1/1/1
23	CLA	B	619	-	-	9/39/115/115	-
23	CLA	C	509	3	-	10/39/115/115	-
23	CLA	C	513	3	-	9/39/115/115	-
23	CLA	B	615	2	-	11/39/115/115	-
22	BCR	B	602	-	-	9/29/63/63	0/2/2/2
24	PHO	D	408	-	-	8/37/103/103	0/5/6/6
22	BCR	C	503	-	-	12/29/63/63	0/2/2/2
22	BCR	C	502	-	-	8/29/63/63	0/2/2/2
23	CLA	C	515	3	-	9/39/115/115	-
23	CLA	B	612	-	-	20/39/115/115	-
27	LMG	K	102	-	-	13/50/70/70	0/1/1/1
22	BCR	D	403	-	-	11/29/63/63	0/2/2/2
27	LMG	I	101	-	-	9/50/70/70	0/1/1/1
29	HEM	F	101	6	-	0/14/54/54	-
23	CLA	A	404	-	-	8/39/115/115	-
23	CLA	B	611	2	-	9/39/115/115	-
27	LMG	D	401	-	-	14/50/70/70	0/1/1/1
22	BCR	H	101	-	-	12/29/63/63	0/2/2/2
23	CLA	C	506	3	-	17/39/115/115	-
23	CLA	A	407	1	-	10/39/115/115	-
23	CLA	B	614	2	-	11/39/115/115	-
23	CLA	C	512	3	-	14/39/115/115	-
22	BCR	J	101	-	-	12/29/63/63	0/2/2/2
23	CLA	B	606	2	-	17/39/115/115	-
23	CLA	B	607	2	-	10/39/115/115	-
25	PL9	D	409	-	-	12/53/73/73	0/1/1/1
23	CLA	B	605	2	-	11/39/115/115	-
23	CLA	B	616	2	-	5/39/115/115	-
23	CLA	B	609	-	-	8/39/115/115	-
23	CLA	B	608	2	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	613	-	-	12/39/115/115	-
23	CLA	C	504	3	-	12/39/115/115	-
23	CLA	B	604	-	-	9/39/115/115	-
23	CLA	A	405	-	-	14/39/115/115	-
23	CLA	B	617	2	-	13/39/115/115	-
23	CLA	C	514	3	-	7/39/115/115	-
22	BCR	B	601	-	-	10/29/63/63	0/2/2/2
23	CLA	B	618	2	-	14/39/115/115	-
23	CLA	C	505	3	-	11/39/115/115	-
27	LMG	M	101	-	-	13/50/70/70	0/1/1/1
24	PHO	A	408	-	-	11/37/103/103	0/5/6/6
27	LMG	L	101	-	-	15/50/70/70	0/1/1/1
29	HEM	V	201	14	-	4/14/54/54	-
22	BCR	K	101	-	-	10/29/63/63	0/2/2/2
22	BCR	C	517	-	-	15/29/63/63	0/2/2/2
23	CLA	C	516	3	-	16/39/115/115	-
23	CLA	B	610	-	-	8/39/115/115	-
23	CLA	A	406	-	-	2/39/115/115	-
25	PL9	A	409	-	-	17/53/73/73	0/1/1/1
23	CLA	C	508	3	-	6/39/115/115	-
23	CLA	D	405	4	-	11/39/115/115	-
27	LMG	Z	101	-	-	15/50/70/70	0/1/1/1
26	LHG	A	410	-	-	18/53/53/53	-
23	CLA	D	404	4	-	8/39/115/115	-
22	BCR	B	603	-	-	6/29/63/63	0/2/2/2
23	CLA	C	507	-	-	14/39/115/115	-
23	CLA	C	510	-	-	9/39/115/115	-
26	LHG	C	501	-	-	14/53/53/53	-
22	BCR	A	403	-	-	7/29/63/63	0/2/2/2
27	LMG	D	406	-	-	16/50/70/70	0/1/1/1

All (298) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	408	PHO	C1B-C2B	9.67	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	408	PHO	C1B-C2B	9.51	1.50	1.39
24	D	408	PHO	C3B-C4B	7.98	1.50	1.41
24	A	408	PHO	C3B-C4B	7.64	1.50	1.41
24	A	408	PHO	C1D-C2D	4.29	1.44	1.39
24	D	408	PHO	C1D-C2D	4.21	1.44	1.39
23	C	513	CLA	C1D-ND	3.94	1.42	1.37
23	B	605	CLA	C1D-ND	3.94	1.42	1.37
23	B	618	CLA	C1D-ND	3.89	1.42	1.37
23	B	612	CLA	C1D-ND	3.89	1.42	1.37
23	C	504	CLA	C4B-NB	3.88	1.42	1.37
23	C	508	CLA	C1D-ND	3.82	1.42	1.37
23	C	515	CLA	C1D-ND	3.81	1.42	1.37
23	B	607	CLA	C1D-ND	3.80	1.42	1.37
23	A	405	CLA	C1D-ND	3.80	1.42	1.37
29	V	201	HEM	FE-NC	3.79	2.08	1.95
23	B	611	CLA	C4B-NB	3.77	1.42	1.37
23	C	510	CLA	C1D-ND	3.77	1.42	1.37
23	D	405	CLA	C1D-ND	3.77	1.42	1.37
23	C	509	CLA	C1D-ND	3.77	1.42	1.37
29	F	101	HEM	FE-ND	3.77	2.06	1.94
23	B	611	CLA	C1D-ND	3.77	1.42	1.37
23	B	619	CLA	C1D-ND	3.77	1.42	1.37
23	B	609	CLA	C1D-ND	3.76	1.42	1.37
23	B	613	CLA	C1D-ND	3.76	1.42	1.37
23	C	514	CLA	C1D-ND	3.76	1.42	1.37
23	B	617	CLA	C1D-ND	3.75	1.42	1.37
23	A	407	CLA	C1D-ND	3.75	1.42	1.37
23	B	606	CLA	C1D-ND	3.74	1.42	1.37
24	D	408	PHO	C4D-CHA	3.73	1.45	1.39
23	B	604	CLA	C1D-ND	3.73	1.42	1.37
23	C	511	CLA	C4B-NB	3.72	1.42	1.37
23	B	616	CLA	C1D-ND	3.71	1.42	1.37
23	C	504	CLA	C1D-ND	3.71	1.42	1.37
23	A	406	CLA	C1D-ND	3.71	1.42	1.37
23	B	610	CLA	C1D-ND	3.71	1.42	1.37
23	B	614	CLA	C1D-ND	3.71	1.42	1.37
23	C	508	CLA	C4B-NB	3.70	1.42	1.37
23	C	511	CLA	C1D-ND	3.69	1.42	1.37
23	C	507	CLA	C1D-ND	3.69	1.42	1.37
23	C	516	CLA	C1D-ND	3.68	1.42	1.37
23	A	404	CLA	C1D-ND	3.67	1.42	1.37
23	B	616	CLA	C4B-NB	3.62	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	604	CLA	C4B-NB	3.62	1.42	1.37
23	B	614	CLA	C4B-NB	3.62	1.42	1.37
29	F	101	HEM	FE-NB	3.60	2.06	1.94
29	V	201	HEM	FE-ND	3.59	2.06	1.94
23	B	612	CLA	C4B-NB	3.59	1.42	1.37
23	C	512	CLA	C1D-ND	3.57	1.42	1.37
23	B	615	CLA	C1D-ND	3.56	1.42	1.37
24	A	408	PHO	C4D-CHA	3.55	1.45	1.39
23	B	608	CLA	C4B-NB	3.55	1.42	1.37
29	V	201	HEM	FE-NB	3.53	2.05	1.94
23	D	404	CLA	C1D-ND	3.53	1.42	1.37
23	D	404	CLA	C4B-NB	3.53	1.42	1.37
23	C	505	CLA	C1D-ND	3.49	1.42	1.37
23	C	507	CLA	C4B-NB	3.46	1.42	1.37
23	B	618	CLA	C4B-NB	3.46	1.42	1.37
23	C	506	CLA	C1D-ND	3.45	1.42	1.37
23	B	608	CLA	C1D-ND	3.44	1.42	1.37
23	B	616	CLA	C3B-C4B	3.42	1.50	1.42
23	C	504	CLA	C3B-C4B	3.42	1.50	1.42
23	C	515	CLA	C4B-NB	3.42	1.42	1.37
29	V	201	HEM	FE-NA	3.39	2.06	1.95
23	B	619	CLA	C4B-NB	3.35	1.41	1.37
23	B	614	CLA	C3B-C4B	3.33	1.50	1.42
23	C	512	CLA	C4B-NB	3.30	1.41	1.37
23	D	404	CLA	C3B-C4B	3.29	1.50	1.42
23	C	513	CLA	C4B-NB	3.29	1.41	1.37
23	C	505	CLA	C4B-NB	3.27	1.41	1.37
23	B	613	CLA	C4B-NB	3.27	1.41	1.37
23	C	511	CLA	C3B-C4B	3.25	1.50	1.42
23	A	406	CLA	C4B-NB	3.24	1.41	1.37
23	D	405	CLA	C4B-NB	3.23	1.41	1.37
23	C	514	CLA	C4B-NB	3.22	1.41	1.37
25	D	409	PL9	C7-C3	-3.21	1.48	1.51
23	A	407	CLA	C4B-NB	3.20	1.41	1.37
23	C	509	CLA	C4B-NB	3.20	1.41	1.37
23	B	618	CLA	C3B-C4B	3.18	1.50	1.42
23	B	606	CLA	C4B-NB	3.17	1.41	1.37
23	C	506	CLA	C4B-NB	3.17	1.41	1.37
29	F	101	HEM	FE-NC	3.17	2.05	1.95
23	B	604	CLA	C3B-C4B	3.17	1.50	1.42
23	B	610	CLA	C4B-NB	3.15	1.41	1.37
23	B	605	CLA	C4B-NB	3.15	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	615	CLA	C4D-ND	-3.15	1.33	1.37
23	A	406	CLA	C4D-ND	-3.14	1.33	1.37
23	B	611	CLA	C3B-C4B	3.14	1.50	1.42
23	B	615	CLA	C4B-NB	3.13	1.41	1.37
23	C	516	CLA	C4B-NB	3.13	1.41	1.37
23	B	609	CLA	C4B-NB	3.12	1.41	1.37
23	B	613	CLA	C3B-C4B	3.11	1.50	1.42
23	C	508	CLA	C3B-C4B	3.09	1.50	1.42
23	B	617	CLA	C4B-NB	3.09	1.41	1.37
23	C	515	CLA	C3B-C4B	3.09	1.50	1.42
23	B	607	CLA	C4B-NB	3.08	1.41	1.37
23	B	613	CLA	C4D-ND	-3.08	1.33	1.37
23	B	608	CLA	C3B-C4B	3.08	1.50	1.42
23	B	619	CLA	C3B-C4B	3.08	1.50	1.42
23	C	510	CLA	C4B-NB	3.08	1.41	1.37
29	V	201	HEM	CAC-C3C	3.07	1.55	1.47
23	B	610	CLA	C4D-ND	-3.07	1.33	1.37
23	A	405	CLA	C4D-ND	-3.06	1.33	1.37
29	V	201	HEM	CAB-C3B	3.06	1.55	1.47
23	C	505	CLA	C4D-ND	-3.05	1.33	1.37
23	C	512	CLA	C4D-ND	-3.04	1.33	1.37
23	A	405	CLA	C4B-NB	3.03	1.41	1.37
23	B	605	CLA	C3B-C4B	3.01	1.49	1.42
23	C	513	CLA	C4D-ND	-3.01	1.33	1.37
23	C	509	CLA	C4D-ND	-3.01	1.33	1.37
29	F	101	HEM	CAB-C3B	3.00	1.55	1.47
23	C	504	CLA	C1B-C2B	3.00	1.50	1.43
23	B	619	CLA	C4D-ND	-3.00	1.33	1.37
23	C	514	CLA	C4D-ND	-2.99	1.33	1.37
23	A	404	CLA	C4D-ND	-2.98	1.33	1.37
23	C	510	CLA	C4D-ND	-2.98	1.33	1.37
23	D	405	CLA	C4D-ND	-2.97	1.33	1.37
23	C	507	CLA	C3B-C4B	2.96	1.49	1.42
23	C	513	CLA	C3B-C4B	2.96	1.49	1.42
23	B	605	CLA	C4D-ND	-2.95	1.33	1.37
23	B	606	CLA	C4D-ND	-2.95	1.33	1.37
23	C	512	CLA	C3B-C4B	2.94	1.49	1.42
23	C	505	CLA	C3B-C4B	2.94	1.49	1.42
29	F	101	HEM	CAC-C3C	2.94	1.55	1.47
23	B	608	CLA	C4D-ND	-2.93	1.33	1.37
23	C	511	CLA	C4D-ND	-2.92	1.33	1.37
23	A	406	CLA	C3B-C4B	2.92	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	C4D-ND	-2.91	1.33	1.37
23	B	609	CLA	C4D-ND	-2.91	1.33	1.37
23	B	614	CLA	C4D-ND	-2.91	1.33	1.37
23	A	405	CLA	C3B-C4B	2.91	1.49	1.42
23	B	612	CLA	C3B-C4B	2.90	1.49	1.42
23	B	616	CLA	C4D-ND	-2.90	1.33	1.37
23	C	506	CLA	C4D-ND	-2.89	1.33	1.37
23	B	606	CLA	C3B-C4B	2.89	1.49	1.42
23	A	404	CLA	C3B-C4B	2.89	1.49	1.42
23	C	504	CLA	C4D-ND	-2.88	1.33	1.37
23	C	516	CLA	C4D-ND	-2.88	1.33	1.37
29	F	101	HEM	FE-NA	2.87	2.04	1.95
23	C	509	CLA	C3B-C4B	2.87	1.49	1.42
23	A	404	CLA	C4B-NB	2.87	1.41	1.37
23	A	407	CLA	C4D-ND	-2.87	1.33	1.37
23	B	617	CLA	C4D-ND	-2.86	1.33	1.37
23	C	510	CLA	C1B-C2B	2.86	1.50	1.43
23	C	508	CLA	C4D-ND	-2.86	1.33	1.37
23	B	607	CLA	C4D-ND	-2.86	1.33	1.37
23	B	615	CLA	C1B-C2B	2.85	1.50	1.43
23	C	515	CLA	C1B-C2B	2.85	1.50	1.43
23	B	609	CLA	C3B-C4B	2.83	1.49	1.42
23	B	617	CLA	C3B-C4B	2.83	1.49	1.42
23	B	615	CLA	C3B-C4B	2.82	1.49	1.42
23	D	404	CLA	C4D-ND	-2.81	1.33	1.37
23	C	514	CLA	C1B-C2B	2.81	1.49	1.43
23	C	513	CLA	C1B-C2B	2.80	1.49	1.43
23	B	604	CLA	C4D-ND	-2.80	1.33	1.37
23	C	507	CLA	C1B-C2B	2.79	1.49	1.43
23	B	607	CLA	C3B-C4B	2.79	1.49	1.42
23	C	506	CLA	C3B-C4B	2.78	1.49	1.42
23	A	407	CLA	C3B-C4B	2.77	1.49	1.42
23	C	514	CLA	C3B-C4B	2.76	1.49	1.42
23	B	617	CLA	C1B-C2B	2.76	1.49	1.43
23	C	515	CLA	C4D-ND	-2.74	1.33	1.37
23	B	610	CLA	C3B-C4B	2.74	1.49	1.42
23	C	516	CLA	C3B-C4B	2.73	1.49	1.42
23	D	405	CLA	C3B-C4B	2.72	1.49	1.42
23	A	405	CLA	C1B-C2B	2.72	1.49	1.43
23	C	506	CLA	C1B-C2B	2.71	1.49	1.43
23	C	512	CLA	C1B-C2B	2.71	1.49	1.43
23	B	612	CLA	C4D-ND	-2.69	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	606	CLA	C1B-C2B	2.68	1.49	1.43
23	A	407	CLA	C1B-C2B	2.67	1.49	1.43
23	C	508	CLA	C1B-C2B	2.67	1.49	1.43
23	C	510	CLA	C3B-C4B	2.67	1.49	1.42
23	B	610	CLA	C1B-C2B	2.66	1.49	1.43
23	B	604	CLA	C1B-C2B	2.65	1.49	1.43
23	D	405	CLA	C1B-C2B	2.65	1.49	1.43
23	B	607	CLA	C1B-C2B	2.64	1.49	1.43
23	B	608	CLA	C1B-C2B	2.64	1.49	1.43
23	C	516	CLA	C1B-C2B	2.63	1.49	1.43
23	B	609	CLA	C1B-C2B	2.62	1.49	1.43
23	C	505	CLA	C1B-C2B	2.62	1.49	1.43
23	B	618	CLA	C4D-ND	-2.61	1.34	1.37
23	A	404	CLA	C1B-C2B	2.60	1.49	1.43
23	B	616	CLA	C1B-C2B	2.59	1.49	1.43
23	B	612	CLA	C1B-C2B	2.58	1.49	1.43
23	B	605	CLA	C1B-C2B	2.58	1.49	1.43
25	D	409	PL9	C3-C4	-2.57	1.45	1.49
23	B	613	CLA	C1B-C2B	2.56	1.49	1.43
23	D	404	CLA	C1B-C2B	2.56	1.49	1.43
23	B	611	CLA	C4D-ND	-2.55	1.34	1.37
23	C	509	CLA	C1B-C2B	2.52	1.49	1.43
23	B	619	CLA	C1B-C2B	2.51	1.49	1.43
23	B	618	CLA	C1B-C2B	2.46	1.49	1.43
24	A	408	PHO	C4D-ND	-2.46	1.35	1.38
23	B	614	CLA	C1B-C2B	2.45	1.49	1.43
24	A	408	PHO	CMD-C2D	-2.44	1.46	1.51
25	A	409	PL9	C3-C4	-2.42	1.45	1.49
24	A	408	PHO	CMB-C2B	-2.41	1.46	1.51
24	D	408	PHO	CMD-C2D	-2.41	1.46	1.51
23	D	404	CLA	CMD-C2D	-2.40	1.45	1.50
23	A	406	CLA	C1B-C2B	2.37	1.48	1.43
23	B	611	CLA	C1B-C2B	2.35	1.48	1.43
23	C	511	CLA	C1B-C2B	2.34	1.48	1.43
23	C	504	CLA	CMD-C2D	-2.34	1.45	1.50
24	D	408	PHO	CMC-C2C	-2.31	1.46	1.50
23	B	605	CLA	CHC-C1C	2.30	1.43	1.38
23	C	513	CLA	CHC-C1C	2.28	1.43	1.38
24	D	408	PHO	C4D-ND	-2.28	1.35	1.38
23	C	511	CLA	CHC-C1C	2.28	1.43	1.38
24	A	408	PHO	CAC-C3C	-2.27	1.47	1.51
23	B	609	CLA	CHC-C1C	2.27	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	CMB-C2B	-2.27	1.46	1.50
23	D	404	CLA	CHC-C1C	2.26	1.43	1.38
23	C	512	CLA	CHC-C1C	2.26	1.43	1.38
23	C	505	CLA	CHC-C1C	2.26	1.43	1.38
23	A	406	CLA	CHC-C1C	2.24	1.43	1.38
24	D	408	PHO	CMB-C2B	-2.24	1.47	1.51
24	A	408	PHO	CMC-C2C	-2.23	1.47	1.50
23	B	610	CLA	CHC-C1C	2.22	1.43	1.38
23	B	607	CLA	CMD-C2D	-2.22	1.46	1.50
23	B	606	CLA	CHC-C1C	2.21	1.43	1.38
23	B	607	CLA	CHC-C1C	2.21	1.43	1.38
23	B	615	CLA	CMD-C2D	-2.20	1.46	1.50
23	B	613	CLA	CHC-C1C	2.20	1.43	1.38
23	B	615	CLA	CHC-C1C	2.19	1.43	1.38
23	B	619	CLA	CHC-C1C	2.19	1.43	1.38
23	B	611	CLA	CMB-C2B	-2.19	1.46	1.50
23	C	509	CLA	CHC-C1C	2.18	1.43	1.38
23	B	617	CLA	CHC-C1C	2.18	1.43	1.38
23	A	406	CLA	CMB-C2B	-2.18	1.46	1.50
23	C	508	CLA	CMD-C2D	-2.18	1.46	1.50
23	C	507	CLA	CHC-C1C	2.16	1.42	1.38
23	A	406	CLA	MG-NB	-2.16	2.01	2.05
23	A	407	CLA	CHC-C1C	2.16	1.42	1.38
23	C	506	CLA	CHC-C1C	2.15	1.42	1.38
23	B	618	CLA	CHC-C1C	2.15	1.42	1.38
23	B	614	CLA	CHC-C1C	2.15	1.42	1.38
23	B	615	CLA	MG-NB	-2.15	2.01	2.05
23	B	612	CLA	CHC-C1C	2.14	1.42	1.38
23	C	506	CLA	MG-NB	-2.14	2.01	2.05
23	B	608	CLA	CHC-C1C	2.14	1.42	1.38
23	C	516	CLA	CHC-C1C	2.13	1.42	1.38
23	D	405	CLA	CHC-C1C	2.13	1.42	1.38
24	A	408	PHO	C3B-C2B	-2.13	1.37	1.40
23	B	616	CLA	CHC-C1C	2.13	1.42	1.38
23	C	515	CLA	CHC-C1C	2.13	1.42	1.38
23	A	405	CLA	CHC-C1C	2.13	1.42	1.38
29	F	101	HEM	CMB-C2B	2.12	1.55	1.50
23	C	510	CLA	CHC-C1C	2.11	1.42	1.38
23	B	613	CLA	CMD-C2D	-2.11	1.46	1.50
23	D	405	CLA	CMD-C2D	-2.11	1.46	1.50
23	A	404	CLA	CMD-C2D	-2.11	1.46	1.50
23	B	610	CLA	MG-NB	-2.10	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	405	CLA	MG-NB	-2.10	2.01	2.05
23	A	405	CLA	CMD-C2D	-2.10	1.46	1.50
23	C	510	CLA	CMD-C2D	-2.10	1.46	1.50
23	B	608	CLA	CMD-C2D	-2.09	1.46	1.50
23	B	609	CLA	CMD-C2D	-2.09	1.46	1.50
23	B	604	CLA	CHC-C1C	2.09	1.42	1.38
23	C	505	CLA	MG-NB	-2.09	2.01	2.05
23	B	617	CLA	CMD-C2D	-2.08	1.46	1.50
23	C	511	CLA	CMD-C2D	-2.08	1.46	1.50
29	V	201	HEM	CMB-C2B	2.08	1.55	1.50
24	D	408	PHO	CAC-C3C	-2.07	1.47	1.51
23	B	606	CLA	MG-NB	-2.07	2.01	2.05
23	C	514	CLA	MG-NB	-2.07	2.01	2.05
23	C	505	CLA	CMD-C2D	-2.07	1.46	1.50
23	A	404	CLA	CHC-C1C	2.06	1.42	1.38
23	A	406	CLA	CMD-C2D	-2.06	1.46	1.50
23	A	407	CLA	MG-NB	-2.06	2.01	2.05
23	B	611	CLA	CMD-C2D	-2.06	1.46	1.50
23	A	404	CLA	MG-NB	-2.05	2.01	2.05
23	B	616	CLA	CMD-C2D	-2.05	1.46	1.50
23	B	608	CLA	CMB-C2B	-2.05	1.46	1.50
23	C	508	CLA	CHC-C1C	2.05	1.42	1.38
29	F	101	HEM	CMC-C2C	2.05	1.55	1.50
23	C	505	CLA	CMB-C2B	-2.05	1.46	1.50
23	C	516	CLA	CMD-C2D	-2.05	1.46	1.50
23	B	609	CLA	MG-NB	-2.04	2.01	2.05
23	B	619	CLA	CMD-C2D	-2.04	1.46	1.50
23	B	618	CLA	CMD-C2D	-2.04	1.46	1.50
24	D	408	PHO	C3D-C4D	2.04	1.44	1.41
23	C	514	CLA	CHC-C1C	2.04	1.42	1.38
23	C	505	CLA	CMC-C2C	-2.04	1.46	1.50
23	B	606	CLA	CMD-C2D	-2.04	1.46	1.50
23	B	605	CLA	MG-NB	-2.03	2.01	2.05
23	A	407	CLA	CMD-C2D	-2.03	1.46	1.50
23	C	506	CLA	CMD-C2D	-2.03	1.46	1.50
29	V	201	HEM	CMC-C2C	2.03	1.55	1.50
23	B	607	CLA	CMB-C2B	-2.03	1.46	1.50
23	B	611	CLA	CHC-C1C	2.02	1.42	1.38
23	B	605	CLA	CMD-C2D	-2.02	1.46	1.50
23	C	512	CLA	CMD-C2D	-2.02	1.46	1.50
23	C	514	CLA	CMD-C2D	-2.02	1.46	1.50
23	C	507	CLA	CMD-C2D	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	CMD-C2D	-2.01	1.46	1.50
23	C	510	CLA	MG-NB	-2.00	2.01	2.05
23	B	604	CLA	CMD-C2D	-2.00	1.46	1.50

All (294) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	408	PHO	C4D-CHA-CBD	-8.26	104.78	108.52
24	A	408	PHO	C4D-CHA-CBD	-7.76	105.01	108.52
23	C	510	CLA	C4A-NA-C1A	7.32	110.00	106.71
23	D	405	CLA	C4A-NA-C1A	7.27	109.97	106.71
23	D	404	CLA	C4A-NA-C1A	7.20	109.94	106.71
23	B	618	CLA	C4A-NA-C1A	7.09	109.89	106.71
23	B	608	CLA	C4A-NA-C1A	7.02	109.86	106.71
23	B	604	CLA	C4A-NA-C1A	7.00	109.85	106.71
23	B	614	CLA	C4A-NA-C1A	6.94	109.83	106.71
23	C	514	CLA	C4A-NA-C1A	6.89	109.80	106.71
23	B	617	CLA	C4A-NA-C1A	6.83	109.78	106.71
23	C	515	CLA	C4A-NA-C1A	6.76	109.75	106.71
23	C	504	CLA	C4A-NA-C1A	6.75	109.74	106.71
23	C	507	CLA	C4A-NA-C1A	6.74	109.74	106.71
23	B	611	CLA	C4A-NA-C1A	6.73	109.73	106.71
23	A	407	CLA	C4A-NA-C1A	6.72	109.72	106.71
23	B	610	CLA	C4A-NA-C1A	6.70	109.72	106.71
23	C	505	CLA	C4A-NA-C1A	6.66	109.70	106.71
23	B	606	CLA	C4A-NA-C1A	6.64	109.69	106.71
23	B	615	CLA	C4A-NA-C1A	6.62	109.68	106.71
23	C	509	CLA	C4A-NA-C1A	6.60	109.67	106.71
23	C	512	CLA	C4A-NA-C1A	6.59	109.67	106.71
23	B	609	CLA	C4A-NA-C1A	6.55	109.65	106.71
23	B	605	CLA	C4A-NA-C1A	6.53	109.64	106.71
23	C	508	CLA	C4A-NA-C1A	6.45	109.61	106.71
23	B	613	CLA	C4A-NA-C1A	6.33	109.55	106.71
23	C	506	CLA	C4A-NA-C1A	6.32	109.55	106.71
23	A	404	CLA	C4A-NA-C1A	6.29	109.53	106.71
23	B	619	CLA	C4A-NA-C1A	6.21	109.50	106.71
23	A	405	CLA	C4A-NA-C1A	6.20	109.49	106.71
23	B	612	CLA	C4A-NA-C1A	6.20	109.49	106.71
23	C	513	CLA	C4A-NA-C1A	6.19	109.49	106.71
25	D	409	PL9	C7-C3-C4	6.17	121.89	116.88
23	C	516	CLA	C4A-NA-C1A	6.14	109.47	106.71
23	B	607	CLA	C4A-NA-C1A	5.99	109.40	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	C4A-NA-C1A	5.96	109.39	106.71
23	B	616	CLA	C4A-NA-C1A	5.95	109.38	106.71
23	A	406	CLA	C4A-NA-C1A	5.86	109.34	106.71
24	A	408	PHO	C2B-C1B-NB	-5.03	106.05	109.53
25	A	409	PL9	C7-C3-C4	4.87	120.83	116.88
23	B	611	CLA	O2D-CGD-O1D	-4.48	115.08	123.84
24	D	408	PHO	C2B-C1B-NB	-4.38	106.50	109.53
25	D	409	PL9	C7-C3-C2	-4.00	118.05	123.30
23	B	611	CLA	O2D-CGD-CBD	3.90	118.20	111.27
28	D	402	BCT	O2-C-O1	3.80	129.39	119.55
23	C	511	CLA	O2D-CGD-O1D	-3.61	116.77	123.84
23	B	605	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
23	D	404	CLA	CAA-C2A-C3A	-3.42	103.42	112.78
23	D	405	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
23	C	513	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
23	C	508	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
23	B	617	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
23	C	513	CLA	CBA-CAA-C2A	3.25	123.46	113.86
23	B	614	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
23	C	510	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
23	C	511	CLA	C3B-C4B-NB	-3.16	107.59	110.52
23	A	406	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
23	B	617	CLA	C4-C3-C5	3.15	120.57	115.27
23	C	515	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
23	D	405	CLA	O2D-CGD-CBD	3.13	116.83	111.27
23	B	608	CLA	C4-C3-C5	3.13	120.53	115.27
23	B	604	CLA	CHB-C4A-NA	3.11	128.81	124.51
23	D	404	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
23	B	613	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
23	C	504	CLA	C4-C3-C5	3.05	120.40	115.27
23	B	613	CLA	C3B-C4B-NB	-3.04	107.69	110.52
23	C	512	CLA	C3B-C4B-NB	-3.03	107.70	110.52
22	K	101	BCR	C37-C22-C23	-3.00	113.34	118.08
23	C	504	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
24	A	408	PHO	C1C-C2C-C3C	-2.98	106.14	108.61
24	D	408	PHO	C2D-C1D-ND	-2.97	107.47	109.53
23	C	505	CLA	CBA-CAA-C2A	2.97	122.64	113.86
23	B	619	CLA	C3B-C4B-NB	-2.97	107.76	110.52
23	B	607	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
23	C	506	CLA	C3B-C4B-NB	-2.97	107.76	110.52
23	C	516	CLA	C3B-C4B-NB	-2.96	107.77	110.52
23	B	604	CLA	O2D-CGD-O1D	-2.95	118.07	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	V	201	HEM	C4D-ND-C1D	2.95	108.12	105.07
27	K	102	LMG	C7-O1-C1	2.93	119.46	113.74
23	C	514	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
23	B	614	CLA	C3B-C4B-NB	-2.92	107.80	110.52
23	B	606	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
23	C	504	CLA	CHB-C4A-NA	2.92	128.55	124.51
23	C	507	CLA	C3B-C4B-NB	-2.92	107.81	110.52
23	B	614	CLA	CBA-CAA-C2A	2.91	122.46	113.86
23	B	616	CLA	C3B-C4B-NB	-2.91	107.81	110.52
23	A	407	CLA	CHB-C4A-NA	2.91	128.53	124.51
23	C	512	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
23	A	406	CLA	CMB-C2B-C1B	-2.89	120.97	125.37
23	B	615	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
23	D	405	CLA	CHB-C4A-NA	2.88	128.49	124.51
23	C	511	CLA	O2D-CGD-CBD	2.88	116.38	111.27
29	V	201	HEM	C4A-NA-C1A	2.88	108.16	105.35
24	A	408	PHO	C2D-C1D-ND	-2.87	107.54	109.53
23	B	609	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
25	A	409	PL9	C7-C3-C2	-2.86	119.53	123.30
23	C	507	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
23	B	609	CLA	CHB-C4A-NA	2.85	128.45	124.51
23	D	404	CLA	CHB-C4A-NA	2.84	128.44	124.51
23	C	508	CLA	CBA-CAA-C2A	2.84	122.26	113.86
23	B	615	CLA	C3B-C4B-NB	-2.84	107.88	110.52
23	B	611	CLA	CHB-C4A-NA	2.84	128.44	124.51
23	B	605	CLA	CHB-C4A-NA	2.82	128.41	124.51
23	B	608	CLA	CHB-C4A-NA	2.82	128.41	124.51
22	H	101	BCR	C4-C5-C6	-2.82	118.64	122.73
29	V	201	HEM	C4C-NC-C1C	2.81	108.10	105.35
25	D	409	PL9	C40-C39-C41	2.81	119.99	115.27
23	C	513	CLA	CHB-C4A-NA	2.79	128.38	124.51
23	B	618	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
23	B	617	CLA	CHB-C4A-NA	2.78	128.36	124.51
23	B	604	CLA	C3B-C4B-NB	-2.78	107.94	110.52
23	C	511	CLA	CHB-C1B-NB	2.78	127.20	124.26
23	B	610	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
23	C	516	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
29	F	101	HEM	C1B-NB-C4B	2.77	107.93	105.07
24	D	408	PHO	O2D-CGD-O1D	-2.76	118.44	123.84
23	B	610	CLA	C3B-C4B-NB	-2.75	107.97	110.52
23	C	506	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
23	B	608	CLA	O2D-CGD-O1D	-2.75	118.47	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	CHB-C4A-NA	2.75	128.31	124.51
23	B	619	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
24	A	408	PHO	O1D-CGD-CBD	2.73	129.29	124.74
23	C	504	CLA	CBA-CAA-C2A	2.73	121.92	113.86
27	Z	101	LMG	C7-O1-C1	2.72	119.06	113.74
23	B	612	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
24	D	408	PHO	O1D-CGD-CBD	2.72	129.26	124.74
23	A	407	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
23	B	613	CLA	CHB-C4A-NA	2.70	128.24	124.51
22	C	517	BCR	C15-C16-C17	-2.69	117.96	123.47
23	B	608	CLA	C3B-C4B-NB	-2.69	108.02	110.52
23	B	614	CLA	CHB-C4A-NA	2.69	128.23	124.51
23	D	404	CLA	C3B-C4B-NB	-2.68	108.03	110.52
25	D	409	PL9	C50-C49-C48	-2.68	114.91	122.65
23	B	616	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
23	B	605	CLA	C3B-C4B-NB	-2.67	108.04	110.52
23	C	505	CLA	C3B-C4B-NB	-2.66	108.04	110.52
23	C	514	CLA	CHB-C4A-NA	2.65	128.18	124.51
23	C	509	CLA	C3B-C4B-NB	-2.65	108.06	110.52
23	A	404	CLA	CHB-C4A-NA	2.64	128.17	124.51
23	C	516	CLA	CHB-C4A-NA	2.64	128.16	124.51
23	C	514	CLA	C3B-C4B-NB	-2.63	108.08	110.52
23	C	513	CLA	C3B-C4B-NB	-2.62	108.08	110.52
24	D	408	PHO	C6-C5-C3	-2.62	106.59	113.45
23	C	513	CLA	CHD-C1D-ND	-2.62	122.05	124.45
29	F	101	HEM	C4A-NA-C1A	2.62	107.91	105.35
23	B	611	CLA	C3B-C4B-NB	-2.62	108.09	110.52
29	V	201	HEM	C1B-NB-C4B	2.62	107.78	105.07
23	C	513	CLA	O2D-CGD-CBD	2.61	115.91	111.27
24	D	408	PHO	C1C-C2C-C3C	-2.61	106.44	108.61
23	A	406	CLA	CHB-C1B-NB	2.61	127.02	124.26
23	B	609	CLA	C3B-C4B-NB	-2.61	108.10	110.52
23	A	406	CLA	C3B-C4B-NB	-2.61	108.10	110.52
23	C	515	CLA	CHB-C4A-NA	2.60	128.11	124.51
23	A	406	CLA	CHD-C1D-ND	-2.60	122.06	124.45
23	B	605	CLA	O2D-CGD-CBD	2.60	115.89	111.27
23	B	617	CLA	C3B-C4B-NB	-2.60	108.11	110.52
29	F	101	HEM	C4D-ND-C1D	2.59	107.75	105.07
23	A	405	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
23	C	505	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
27	D	407	LMG	C8-O7-C10	2.57	124.13	117.79
23	B	607	CLA	C3B-C4B-NB	-2.57	108.13	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	408	PHO	O2D-CGD-O1D	-2.56	118.84	123.84
25	D	409	PL9	C22-C23-C24	-2.55	121.52	127.66
23	C	507	CLA	O2A-CGA-O1A	-2.55	117.17	123.59
23	B	606	CLA	C3B-C4B-NB	-2.55	108.15	110.52
25	D	409	PL9	C36-C34-C33	-2.54	115.97	121.12
23	A	406	CLA	O2D-CGD-CBD	2.54	115.78	111.27
23	A	404	CLA	C3B-C4B-NB	-2.52	108.18	110.52
23	C	509	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
24	D	408	PHO	CMB-C2B-C3B	2.52	129.39	124.68
29	F	101	HEM	C4C-NC-C1C	2.51	107.81	105.35
23	C	509	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	A	407	CLA	C3B-C4B-NB	-2.51	108.19	110.52
23	A	404	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
23	B	619	CLA	CHB-C4A-NA	2.50	127.96	124.51
23	C	513	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
23	B	617	CLA	O2A-CGA-O1A	-2.49	117.32	123.59
23	C	507	CLA	C4-C3-C5	2.48	119.44	115.27
23	C	506	CLA	CHB-C4A-NA	2.48	127.94	124.51
23	C	507	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	A	409	PL9	C40-C39-C41	2.47	119.43	115.27
25	A	409	PL9	C22-C23-C24	-2.47	121.71	127.66
27	L	101	LMG	C1-O6-C5	2.47	118.54	113.69
25	D	409	PL9	C37-C38-C39	-2.46	121.73	127.66
25	D	409	PL9	C20-C19-C21	2.46	119.42	115.27
23	C	515	CLA	C3B-C4B-NB	-2.45	108.24	110.52
23	D	405	CLA	C3B-C4B-NB	-2.43	108.26	110.52
23	B	618	CLA	CHB-C4A-NA	2.42	127.86	124.51
27	M	101	LMG	C7-O1-C1	2.42	118.47	113.74
23	B	614	CLA	O2D-CGD-CBD	2.42	115.57	111.27
25	A	409	PL9	O2-C1-C2	-2.41	116.25	121.78
23	C	508	CLA	O2A-CGA-O1A	-2.41	117.51	123.59
23	C	508	CLA	CHB-C4A-NA	2.40	127.83	124.51
23	C	506	CLA	CBA-CAA-C2A	2.40	120.94	113.86
23	C	510	CLA	C3B-C4B-NB	-2.40	108.29	110.52
25	D	409	PL9	O2-C1-C2	-2.39	116.31	121.78
23	B	604	CLA	O2A-CGA-O1A	-2.38	117.57	123.59
23	A	405	CLA	CHB-C4A-NA	2.38	127.80	124.51
23	B	611	CLA	CHB-C1B-NB	2.38	126.77	124.26
23	C	508	CLA	O2D-CGD-CBD	2.37	115.48	111.27
23	B	615	CLA	CHB-C4A-NA	2.37	127.79	124.51
23	B	611	CLA	C3A-C2A-C1A	2.37	104.89	101.34
22	K	101	BCR	C23-C22-C21	2.36	122.57	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405	CLA	C3B-C4B-NB	-2.35	108.33	110.52
23	B	604	CLA	C2A-C1A-CHA	2.35	127.96	123.86
22	C	503	BCR	C30-C25-C26	-2.34	119.32	122.61
23	B	618	CLA	C3B-C4B-NB	-2.33	108.35	110.52
23	C	504	CLA	C3B-C4B-NB	-2.33	108.35	110.52
23	C	505	CLA	CHB-C4A-NA	2.33	127.74	124.51
25	D	409	PL9	O2-C1-C6	2.32	124.61	120.59
23	C	516	CLA	CHD-C1D-ND	-2.32	122.32	124.45
23	A	404	CLA	CAC-C3C-C4C	2.31	127.81	124.81
23	B	607	CLA	CHB-C4A-NA	2.31	127.70	124.51
23	B	618	CLA	C2A-C1A-CHA	2.31	127.89	123.86
25	A	409	PL9	C20-C19-C21	2.30	119.15	115.27
23	C	511	CLA	CHB-C4A-NA	2.30	127.69	124.51
25	A	409	PL9	O2-C1-C6	2.30	124.57	120.59
23	B	614	CLA	CHB-C1B-NB	2.29	126.69	124.26
23	B	612	CLA	C4-C3-C5	2.29	119.12	115.27
23	A	405	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
23	B	616	CLA	CHB-C4A-NA	2.28	127.67	124.51
23	C	512	CLA	CHB-C4A-NA	2.27	127.65	124.51
23	B	606	CLA	CHB-C4A-NA	2.26	127.64	124.51
28	D	402	BCT	O3-C-O1	-2.26	113.69	119.55
23	A	404	CLA	CHD-C1D-ND	-2.24	122.39	124.45
23	B	617	CLA	CAC-C3C-C4C	2.24	127.72	124.81
23	C	506	CLA	C4-C3-C5	2.24	119.03	115.27
29	V	201	HEM	C3D-C4D-ND	-2.24	107.68	110.17
23	C	505	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
23	B	612	CLA	CHB-C4A-NA	2.23	127.59	124.51
22	B	601	BCR	C29-C30-C25	2.21	113.88	110.48
22	D	403	BCR	C20-C21-C22	2.21	130.46	127.31
25	A	409	PL9	C37-C38-C39	-2.20	122.37	127.66
23	C	510	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
23	B	618	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
23	B	612	CLA	C3B-C4B-NB	-2.17	108.50	110.52
23	A	406	CLA	CMB-C2B-C3B	2.17	131.84	126.59
23	B	611	CLA	C2A-C1A-CHA	2.17	127.65	123.86
23	C	505	CLA	CHD-C1D-ND	-2.16	122.47	124.45
23	A	405	CLA	CAC-C3C-C4C	2.16	127.62	124.81
23	C	509	CLA	CHB-C1B-NB	2.16	126.54	124.26
22	J	101	BCR	C40-C30-C25	2.16	113.80	110.30
23	C	515	CLA	C4-C3-C5	2.16	118.90	115.27
23	B	610	CLA	CHB-C4A-NA	2.16	127.49	124.51
23	B	605	CLA	O2A-CGA-O1A	-2.15	118.16	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	619	CLA	CHB-C1B-NB	2.15	126.53	124.26
25	D	409	PL9	C12-C13-C14	-2.15	122.48	127.66
23	D	404	CLA	C2A-C1A-CHA	2.15	127.62	123.86
22	K	101	BCR	C24-C23-C22	2.15	129.48	126.23
23	C	515	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
23	B	617	CLA	O1D-CGD-CBD	2.14	128.87	124.48
25	A	409	PL9	C7-C8-C9	-2.14	123.23	126.79
23	C	506	CLA	CHC-C4B-NB	2.13	126.51	124.26
23	C	511	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
23	B	604	CLA	CHA-C1A-NA	-2.12	121.54	126.40
23	B	607	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
23	B	616	CLA	C1-O2A-CGA	2.11	121.99	116.44
23	C	506	CLA	C6-C5-C3	2.11	119.00	113.45
23	B	615	CLA	CHD-C1D-ND	-2.11	122.52	124.45
23	C	509	CLA	CAA-CBA-CGA	-2.11	107.10	113.25
23	D	405	CLA	CAA-CBA-CGA	-2.10	107.12	113.25
23	B	619	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
23	B	609	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	B	613	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	B	615	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
29	V	201	HEM	C2A-C1A-NA	-2.09	107.81	110.15
23	C	505	CLA	CHB-C1B-NB	2.08	126.46	124.26
23	B	616	CLA	O1D-CGD-CBD	2.08	128.74	124.48
23	D	405	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
23	B	608	CLA	CHD-C1D-ND	-2.08	122.55	124.45
25	A	409	PL9	C50-C49-C48	-2.06	116.68	122.65
23	B	613	CLA	CHB-C1B-NB	2.06	126.44	124.26
23	A	406	CLA	C2D-C1D-ND	-2.06	108.59	110.10
23	C	508	CLA	C3B-C4B-NB	-2.05	108.61	110.52
22	B	601	BCR	C11-C10-C9	2.05	130.24	127.31
23	B	605	CLA	C3A-C2A-C1A	2.05	104.41	101.34
23	A	405	CLA	CHD-C1D-ND	-2.05	122.57	124.45
27	L	101	LMG	C9-C8-C7	2.05	116.64	111.79
23	B	609	CLA	CHD-C1D-ND	-2.05	122.57	124.45
29	V	201	HEM	CHD-C4C-C3C	2.05	128.76	125.26
25	A	409	PL9	O1-C4-C3	-2.04	118.47	120.72
23	B	606	CLA	C6-C5-C3	-2.04	108.10	113.45
23	C	514	CLA	CHC-C4B-NB	2.04	126.41	124.26
22	B	601	BCR	C34-C9-C8	-2.03	114.88	118.08
29	V	201	HEM	CHC-C1C-NC	2.03	126.63	124.44
29	F	101	HEM	CBD-CAD-C3D	-2.03	106.99	112.63
23	B	610	CLA	CHD-C1D-ND	-2.02	122.59	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Z	101	LMG	C8-O7-C10	2.02	122.77	117.79
23	C	514	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
23	C	506	CLA	C2A-C1A-CHA	2.02	127.39	123.86
23	B	607	CLA	CAC-C3C-C4C	2.01	127.41	124.81
23	C	516	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
23	B	607	CLA	CHB-C1B-NB	2.00	126.38	124.26
25	D	409	PL9	C7-C8-C9	-2.00	123.46	126.79

There are no chirality outliers.

All (676) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	601	BCR	C17-C18-C19-C20
22	B	601	BCR	C36-C18-C19-C20
22	B	602	BCR	C11-C12-C13-C14
22	B	602	BCR	C11-C12-C13-C35
22	B	602	BCR	C17-C18-C19-C20
22	B	602	BCR	C36-C18-C19-C20
22	B	602	BCR	C19-C20-C21-C22
22	B	603	BCR	C19-C20-C21-C22
22	B	603	BCR	C21-C22-C23-C24
22	B	603	BCR	C37-C22-C23-C24
22	C	502	BCR	C7-C8-C9-C10
22	C	502	BCR	C7-C8-C9-C34
22	C	502	BCR	C11-C12-C13-C14
22	C	502	BCR	C11-C12-C13-C35
22	C	502	BCR	C17-C18-C19-C20
22	C	502	BCR	C36-C18-C19-C20
22	C	503	BCR	C9-C10-C11-C12
22	C	503	BCR	C11-C12-C13-C14
22	C	503	BCR	C11-C12-C13-C35
22	C	503	BCR	C17-C18-C19-C20
22	C	503	BCR	C36-C18-C19-C20
22	C	517	BCR	C9-C10-C11-C12
22	C	517	BCR	C17-C18-C19-C20
22	C	517	BCR	C36-C18-C19-C20
22	C	517	BCR	C37-C22-C23-C24
22	D	403	BCR	C17-C18-C19-C20
22	H	101	BCR	C11-C12-C13-C35
22	H	101	BCR	C17-C18-C19-C20
22	H	101	BCR	C36-C18-C19-C20
22	H	101	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
22	H	101	BCR	C37-C22-C23-C24
22	H	101	BCR	C23-C24-C25-C30
22	J	101	BCR	C9-C10-C11-C12
22	J	101	BCR	C13-C14-C15-C16
22	J	101	BCR	C15-C16-C17-C18
22	J	101	BCR	C17-C18-C19-C20
22	J	101	BCR	C36-C18-C19-C20
22	K	101	BCR	C7-C8-C9-C10
22	K	101	BCR	C7-C8-C9-C34
22	K	101	BCR	C9-C10-C11-C12
22	K	101	BCR	C11-C12-C13-C14
22	K	101	BCR	C11-C12-C13-C35
23	A	404	CLA	CBD-CGD-O2D-CED
23	A	405	CLA	C1A-C2A-CAA-CBA
23	A	405	CLA	CBD-CGD-O2D-CED
23	B	604	CLA	CBD-CGD-O2D-CED
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	609	CLA	C3A-C2A-CAA-CBA
23	B	609	CLA	C2B-C3B-CAB-CBB
23	B	609	CLA	C4B-C3B-CAB-CBB
23	B	609	CLA	CHA-CBD-CGD-O1D
23	B	609	CLA	CHA-CBD-CGD-O2D
23	B	610	CLA	CHA-CBD-CGD-O1D
23	B	610	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	C1A-C2A-CAA-CBA
23	B	614	CLA	C3A-C2A-CAA-CBA
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	C	504	CLA	C1A-C2A-CAA-CBA
23	C	504	CLA	C3A-C2A-CAA-CBA
23	C	505	CLA	C1A-C2A-CAA-CBA
23	C	506	CLA	CBD-CGD-O2D-CED
23	C	508	CLA	C1A-C2A-CAA-CBA
23	C	508	CLA	C3A-C2A-CAA-CBA
23	C	511	CLA	C11-C10-C8-C9
23	C	512	CLA	CBD-CGD-O2D-CED
23	C	513	CLA	C1A-C2A-CAA-CBA
23	C	513	CLA	C3A-C2A-CAA-CBA
23	C	513	CLA	CHA-CBD-CGD-O1D
23	C	513	CLA	CBD-CGD-O2D-CED
23	C	515	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	C	515	CLA	CHA-CBD-CGD-O2D
23	C	516	CLA	CBD-CGD-O2D-CED
23	D	405	CLA	CHA-CBD-CGD-O1D
23	D	405	CLA	CHA-CBD-CGD-O2D
24	A	408	PHO	C6-C7-C8-C9
25	A	409	PL9	C22-C23-C24-C26
25	A	409	PL9	C32-C33-C34-C35
25	A	409	PL9	C32-C33-C34-C36
25	D	409	PL9	C29-C31-C32-C33
25	D	409	PL9	C39-C41-C42-C43
26	A	410	LHG	C3-O3-P-O5
26	A	410	LHG	C4-O6-P-O4
26	A	410	LHG	C4-O6-P-O5
27	D	406	LMG	O9-C10-O7-C8
27	D	406	LMG	C11-C10-O7-C8
27	K	102	LMG	C2-C1-O1-C7
27	K	102	LMG	O6-C1-O1-C7
27	L	101	LMG	C2-C1-O1-C7
27	L	101	LMG	O6-C1-O1-C7
27	M	101	LMG	O6-C1-O1-C7
27	M	101	LMG	C11-C10-O7-C8
27	Z	101	LMG	O9-C10-O7-C8
23	C	513	CLA	O1D-CGD-O2D-CED
23	B	606	CLA	CBD-CGD-O2D-CED
23	B	608	CLA	CBD-CGD-O2D-CED
23	B	611	CLA	CBD-CGD-O2D-CED
23	B	619	CLA	CBD-CGD-O2D-CED
23	C	514	CLA	CBD-CGD-O2D-CED
23	C	515	CLA	CBD-CGD-O2D-CED
27	I	101	LMG	O10-C28-O8-C9
27	M	101	LMG	O10-C28-O8-C9
23	B	611	CLA	O1D-CGD-O2D-CED
23	B	619	CLA	O1D-CGD-O2D-CED
23	C	514	CLA	O1D-CGD-O2D-CED
23	A	404	CLA	O1D-CGD-O2D-CED
23	C	506	CLA	O1D-CGD-O2D-CED
23	C	512	CLA	O1D-CGD-O2D-CED
23	B	618	CLA	O1A-CGA-O2A-C1
23	C	505	CLA	O1A-CGA-O2A-C1
23	C	507	CLA	O1A-CGA-O2A-C1
23	C	510	CLA	O1A-CGA-O2A-C1
27	D	406	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
23	B	604	CLA	O1D-CGD-O2D-CED
23	A	405	CLA	O1D-CGD-O2D-CED
23	C	516	CLA	O1D-CGD-O2D-CED
23	B	619	CLA	C3-C5-C6-C7
23	C	515	CLA	C3-C5-C6-C7
23	B	604	CLA	CBA-CGA-O2A-C1
23	B	606	CLA	CBA-CGA-O2A-C1
23	B	619	CLA	CBA-CGA-O2A-C1
23	C	505	CLA	CBA-CGA-O2A-C1
27	D	406	LMG	C29-C28-O8-C9
27	I	101	LMG	C29-C28-O8-C9
27	M	101	LMG	C29-C28-O8-C9
27	Z	101	LMG	C11-C10-O7-C8
23	B	608	CLA	O1D-CGD-O2D-CED
23	B	612	CLA	CBD-CGD-O2D-CED
23	C	506	CLA	O1A-CGA-O2A-C1
23	B	617	CLA	C4-C3-C5-C6
23	C	506	CLA	C4-C3-C5-C6
23	B	618	CLA	C2A-CAA-CBA-CGA
23	C	513	CLA	C2A-CAA-CBA-CGA
27	Z	101	LMG	O10-C28-O8-C9
23	D	404	CLA	C3-C5-C6-C7
23	A	405	CLA	CBA-CGA-O2A-C1
23	B	610	CLA	CBA-CGA-O2A-C1
23	B	618	CLA	CBA-CGA-O2A-C1
23	C	506	CLA	CBA-CGA-O2A-C1
23	C	507	CLA	CBA-CGA-O2A-C1
23	C	510	CLA	CBA-CGA-O2A-C1
27	D	401	LMG	C29-C28-O8-C9
27	Z	101	LMG	C29-C28-O8-C9
25	D	409	PL9	C32-C33-C34-C35
23	B	606	CLA	O1D-CGD-O2D-CED
23	C	515	CLA	O1D-CGD-O2D-CED
27	M	101	LMG	O9-C10-O7-C8
25	D	409	PL9	C32-C33-C34-C36
23	A	405	CLA	O1A-CGA-O2A-C1
23	B	604	CLA	O1A-CGA-O2A-C1
23	B	611	CLA	O1A-CGA-O2A-C1
23	C	504	CLA	O1A-CGA-O2A-C1
27	D	401	LMG	O10-C28-O8-C9
22	C	517	BCR	C13-C14-C15-C16
22	C	517	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	C	517	BCR	C19-C20-C21-C22
22	H	101	BCR	C9-C10-C11-C12
23	C	504	CLA	CBA-CGA-O2A-C1
26	A	410	LHG	C24-C23-O8-C6
23	B	606	CLA	O1A-CGA-O2A-C1
23	B	619	CLA	O1A-CGA-O2A-C1
26	A	410	LHG	O10-C23-O8-C6
23	B	607	CLA	CBD-CGD-O2D-CED
24	A	408	PHO	C3-C5-C6-C7
23	B	611	CLA	CBA-CGA-O2A-C1
23	B	610	CLA	O1A-CGA-O2A-C1
23	C	507	CLA	C2A-CAA-CBA-CGA
25	A	409	PL9	C14-C16-C17-C18
25	A	409	PL9	C29-C31-C32-C33
25	A	409	PL9	C44-C46-C47-C48
23	B	607	CLA	CBA-CGA-O2A-C1
23	B	607	CLA	O1A-CGA-O2A-C1
25	D	409	PL9	C7-C8-C9-C10
23	B	605	CLA	CBA-CGA-O2A-C1
23	B	609	CLA	CBA-CGA-O2A-C1
23	B	613	CLA	CBA-CGA-O2A-C1
23	B	614	CLA	CBA-CGA-O2A-C1
23	B	617	CLA	CBA-CGA-O2A-C1
23	C	514	CLA	CBA-CGA-O2A-C1
23	C	516	CLA	CBA-CGA-O2A-C1
23	D	405	CLA	CBA-CGA-O2A-C1
23	B	615	CLA	CBD-CGD-O2D-CED
23	D	404	CLA	CBD-CGD-O2D-CED
27	M	101	LMG	C2-C1-O1-C7
27	Z	101	LMG	C2-C1-O1-C7
23	B	613	CLA	O1A-CGA-O2A-C1
23	B	617	CLA	C2-C3-C5-C6
23	C	506	CLA	C2-C3-C5-C6
23	B	618	CLA	C6-C7-C8-C9
23	B	619	CLA	C11-C10-C8-C9
24	D	408	PHO	C6-C7-C8-C9
26	A	410	LHG	C28-C29-C30-C31
22	A	403	BCR	C7-C8-C9-C34
22	A	403	BCR	C37-C22-C23-C24
22	B	601	BCR	C11-C12-C13-C35
22	C	503	BCR	C37-C22-C23-C24
22	C	517	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
22	D	403	BCR	C36-C18-C19-C20
22	K	101	BCR	C37-C22-C23-C24
22	B	601	BCR	C7-C8-C9-C10
22	C	517	BCR	C11-C12-C13-C14
22	C	517	BCR	C21-C22-C23-C24
22	J	101	BCR	C7-C8-C9-C10
23	B	605	CLA	O1A-CGA-O2A-C1
23	B	614	CLA	O1A-CGA-O2A-C1
23	B	617	CLA	O1A-CGA-O2A-C1
23	C	514	CLA	O1A-CGA-O2A-C1
23	C	516	CLA	O1A-CGA-O2A-C1
23	D	405	CLA	O1A-CGA-O2A-C1
23	B	606	CLA	C3-C5-C6-C7
23	C	509	CLA	CBA-CGA-O2A-C1
23	B	617	CLA	C8-C10-C11-C12
23	B	608	CLA	C10-C11-C12-C13
23	B	608	CLA	C13-C15-C16-C17
23	B	610	CLA	C5-C6-C7-C8
25	D	409	PL9	C42-C43-C44-C45
26	A	410	LHG	C7-C8-C9-C10
23	C	507	CLA	C2-C1-O2A-CGA
26	C	501	LHG	C2-C3-O3-P
23	A	405	CLA	C8-C10-C11-C12
23	C	504	CLA	C8-C10-C11-C12
23	C	513	CLA	C10-C11-C12-C13
23	A	406	CLA	C6-C7-C8-C10
23	B	618	CLA	C6-C7-C8-C10
23	B	619	CLA	C11-C10-C8-C7
22	C	503	BCR	C19-C20-C21-C22
22	D	403	BCR	C9-C10-C11-C12
22	H	101	BCR	C19-C20-C21-C22
22	J	101	BCR	C19-C20-C21-C22
22	K	101	BCR	C15-C16-C17-C18
23	B	611	CLA	C2A-CAA-CBA-CGA
23	D	405	CLA	C2A-CAA-CBA-CGA
23	B	612	CLA	C8-C10-C11-C12
23	B	609	CLA	O1A-CGA-O2A-C1
25	D	409	PL9	C34-C36-C37-C38
23	A	404	CLA	C15-C16-C17-C18
23	B	613	CLA	C5-C6-C7-C8
23	C	506	CLA	C5-C6-C7-C8
23	C	506	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	C	509	CLA	O1A-CGA-O2A-C1
27	D	406	LMG	C10-C11-C12-C13
23	B	606	CLA	C13-C15-C16-C17
23	C	505	CLA	C15-C16-C17-C18
23	C	511	CLA	C5-C6-C7-C8
23	B	612	CLA	O1D-CGD-O2D-CED
26	C	501	LHG	C9-C10-C11-C12
26	A	410	LHG	C4-O6-P-O3
23	A	407	CLA	CBA-CGA-O2A-C1
23	B	616	CLA	C3-C5-C6-C7
23	B	618	CLA	C3-C5-C6-C7
22	B	602	BCR	C9-C10-C11-C12
27	L	101	LMG	C30-C31-C32-C33
27	D	406	LMG	C12-C13-C14-C15
27	L	101	LMG	C11-C12-C13-C14
27	M	101	LMG	C32-C33-C34-C35
27	D	401	LMG	C15-C16-C17-C18
27	D	401	LMG	C23-C24-C25-C26
24	A	408	PHO	C4-C3-C5-C6
25	A	409	PL9	C22-C23-C24-C25
23	B	612	CLA	C14-C13-C15-C16
23	C	506	CLA	C11-C10-C8-C9
23	B	614	CLA	C5-C6-C7-C8
22	B	601	BCR	C7-C8-C9-C34
22	C	517	BCR	C7-C8-C9-C34
22	D	403	BCR	C7-C8-C9-C34
22	J	101	BCR	C7-C8-C9-C34
22	C	517	BCR	C7-C8-C9-C10
22	K	101	BCR	C21-C22-C23-C24
23	B	606	CLA	C10-C11-C12-C13
27	D	407	LMG	C39-C40-C41-C42
23	C	512	CLA	C4B-C3B-CAB-CBB
23	C	507	CLA	CBD-CGD-O2D-CED
23	A	407	CLA	O1A-CGA-O2A-C1
23	A	405	CLA	C3A-C2A-CAA-CBA
23	B	618	CLA	C3A-C2A-CAA-CBA
23	C	510	CLA	C3A-C2A-CAA-CBA
23	D	405	CLA	C3A-C2A-CAA-CBA
23	B	613	CLA	C4-C3-C5-C6
25	D	409	PL9	C13-C14-C16-C17
26	A	410	LHG	C33-C34-C35-C36
23	B	613	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	D	408	PHO	CBA-CGA-O2A-C1
26	C	501	LHG	C28-C29-C30-C31
23	B	617	CLA	C5-C6-C7-C8
24	D	408	PHO	O1A-CGA-O2A-C1
22	C	503	BCR	C23-C24-C25-C26
22	C	503	BCR	C23-C24-C25-C30
22	C	517	BCR	C23-C24-C25-C26
22	H	101	BCR	C1-C6-C7-C8
22	H	101	BCR	C5-C6-C7-C8
22	H	101	BCR	C23-C24-C25-C26
22	J	101	BCR	C1-C6-C7-C8
22	J	101	BCR	C5-C6-C7-C8
27	D	407	LMG	C11-C10-O7-C8
27	K	102	LMG	C11-C10-O7-C8
27	D	406	LMG	C11-C12-C13-C14
27	Z	101	LMG	C41-C42-C43-C44
27	L	101	LMG	C32-C33-C34-C35
25	D	409	PL9	C47-C48-C49-C51
23	C	512	CLA	C10-C11-C12-C13
23	B	612	CLA	C12-C13-C15-C16
23	B	613	CLA	C2-C3-C5-C6
23	C	506	CLA	C11-C10-C8-C7
24	A	408	PHO	C2-C3-C5-C6
23	B	607	CLA	O1D-CGD-O2D-CED
27	Z	101	LMG	C39-C40-C41-C42
23	B	614	CLA	C2A-CAA-CBA-CGA
23	A	407	CLA	C5-C6-C7-C8
27	D	401	LMG	C31-C32-C33-C34
25	D	409	PL9	C19-C21-C22-C23
29	V	201	HEM	C4C-C3C-CAC-CBC
27	D	407	LMG	O9-C10-O7-C8
23	D	404	CLA	O1D-CGD-O2D-CED
23	C	516	CLA	C4-C3-C5-C6
25	D	409	PL9	C33-C34-C36-C37
23	A	406	CLA	C6-C7-C8-C9
22	B	602	BCR	C37-C22-C23-C24
22	B	603	BCR	C36-C18-C19-C20
22	D	403	BCR	C37-C22-C23-C24
22	B	603	BCR	C17-C18-C19-C20
22	D	403	BCR	C21-C22-C23-C24
23	B	609	CLA	C1A-C2A-CAA-CBA
23	B	618	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	C	510	CLA	C1A-C2A-CAA-CBA
23	C	511	CLA	C1A-C2A-CAA-CBA
23	D	405	CLA	C1A-C2A-CAA-CBA
27	K	102	LMG	O9-C10-O7-C8
27	K	102	LMG	C29-C28-O8-C9
27	K	102	LMG	C28-C29-C30-C31
23	B	615	CLA	O1D-CGD-O2D-CED
27	K	102	LMG	C17-C18-C19-C20
23	D	405	CLA	C8-C10-C11-C12
23	B	606	CLA	C16-C17-C18-C20
27	I	101	LMG	O1-C7-C8-C9
23	A	407	CLA	C15-C16-C17-C18
27	D	401	LMG	C11-C12-C13-C14
27	D	406	LMG	C31-C32-C33-C34
27	I	101	LMG	C41-C42-C43-C44
27	Z	101	LMG	C29-C30-C31-C32
25	A	409	PL9	C24-C26-C27-C28
23	A	404	CLA	CBA-CGA-O2A-C1
23	B	605	CLA	C4-C3-C5-C6
23	B	610	CLA	C4-C3-C5-C6
27	L	101	LMG	C40-C41-C42-C43
23	B	610	CLA	C2-C3-C5-C6
23	B	606	CLA	C16-C17-C18-C19
23	C	512	CLA	C13-C15-C16-C17
26	C	501	LHG	C15-C16-C17-C18
27	K	102	LMG	O10-C28-O8-C9
26	A	410	LHG	C24-C25-C26-C27
23	A	405	CLA	C6-C7-C8-C10
23	B	605	CLA	C2-C3-C5-C6
23	B	615	CLA	C6-C7-C8-C10
23	B	618	CLA	C12-C13-C15-C16
23	C	510	CLA	C11-C10-C8-C7
23	C	511	CLA	C11-C10-C8-C7
23	C	515	CLA	C11-C10-C8-C7
23	C	516	CLA	C12-C13-C15-C16
23	A	405	CLA	C6-C7-C8-C9
23	A	407	CLA	C14-C13-C15-C16
23	B	615	CLA	C6-C7-C8-C9
23	B	618	CLA	C14-C13-C15-C16
23	C	504	CLA	C6-C7-C8-C9
23	C	509	CLA	C6-C7-C8-C9
23	C	513	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	C	516	CLA	C14-C13-C15-C16
23	A	404	CLA	O1A-CGA-O2A-C1
23	C	516	CLA	C16-C17-C18-C19
27	M	101	LMG	C23-C24-C25-C26
23	C	511	CLA	CBA-CGA-O2A-C1
23	C	506	CLA	C8-C10-C11-C12
23	C	516	CLA	C2-C3-C5-C6
26	C	501	LHG	C12-C13-C14-C15
26	C	501	LHG	C24-C23-O8-C6
23	B	604	CLA	O2A-C1-C2-C3
23	B	611	CLA	O2A-C1-C2-C3
23	C	514	CLA	O2A-C1-C2-C3
27	D	406	LMG	C15-C16-C17-C18
23	C	507	CLA	O1D-CGD-O2D-CED
23	C	511	CLA	C3-C5-C6-C7
25	A	409	PL9	C7-C8-C9-C10
27	K	102	LMG	C24-C25-C26-C27
23	C	512	CLA	C2B-C3B-CAB-CBB
27	L	101	LMG	O1-C7-C8-O7
23	C	508	CLA	C5-C6-C7-C8
27	M	101	LMG	C41-C42-C43-C44
22	D	403	BCR	C19-C20-C21-C22
27	Z	101	LMG	O6-C1-O1-C7
23	B	606	CLA	C5-C6-C7-C8
24	A	408	PHO	C2-C1-O2A-CGA
23	B	605	CLA	C11-C12-C13-C14
23	C	510	CLA	C5-C6-C7-C8
22	A	403	BCR	C23-C24-C25-C26
22	C	503	BCR	C5-C6-C7-C8
22	C	517	BCR	C1-C6-C7-C8
22	C	517	BCR	C23-C24-C25-C30
22	D	403	BCR	C1-C6-C7-C8
22	D	403	BCR	C23-C24-C25-C30
22	K	101	BCR	C5-C6-C7-C8
22	B	601	BCR	C37-C22-C23-C24
22	A	403	BCR	C7-C8-C9-C10
22	H	101	BCR	C11-C12-C13-C14
23	C	516	CLA	C16-C17-C18-C20
23	B	605	CLA	C15-C16-C17-C18
23	A	407	CLA	C12-C13-C15-C16
23	C	504	CLA	C6-C7-C8-C10
23	C	509	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
23	C	511	CLA	C12-C13-C15-C16
23	C	516	CLA	C6-C7-C8-C10
23	C	511	CLA	C15-C16-C17-C18
22	A	403	BCR	C9-C10-C11-C12
22	B	601	BCR	C9-C10-C11-C12
22	B	601	BCR	C13-C14-C15-C16
22	B	602	BCR	C15-C16-C17-C18
23	C	508	CLA	C16-C17-C18-C20
27	L	101	LMG	C15-C16-C17-C18
23	A	404	CLA	C3-C5-C6-C7
23	B	612	CLA	C3-C5-C6-C7
23	B	605	CLA	CBD-CGD-O2D-CED
23	A	407	CLA	CAD-CBD-CGD-O2D
23	B	613	CLA	CAD-CBD-CGD-O2D
23	C	514	CLA	CAD-CBD-CGD-O2D
23	D	404	CLA	CAD-CBD-CGD-O2D
26	C	501	LHG	C4-C5-C6-O8
26	A	410	LHG	C11-C12-C13-C14
27	L	101	LMG	C17-C18-C19-C20
23	B	612	CLA	CHA-CBD-CGD-O1D
23	B	612	CLA	CHA-CBD-CGD-O2D
23	C	513	CLA	CHA-CBD-CGD-O2D
23	C	516	CLA	CHA-CBD-CGD-O1D
23	C	511	CLA	O1A-CGA-O2A-C1
26	C	501	LHG	O7-C5-C6-O8
27	D	401	LMG	C32-C33-C34-C35
23	B	612	CLA	C4-C3-C5-C6
25	D	409	PL9	C15-C14-C16-C17
26	C	501	LHG	O10-C23-O8-C6
23	B	612	CLA	C2-C3-C5-C6
25	A	409	PL9	C4-C3-C7-C8
23	C	512	CLA	C11-C10-C8-C9
26	A	410	LHG	C30-C31-C32-C33
23	B	607	CLA	C13-C15-C16-C17
23	B	618	CLA	C5-C6-C7-C8
23	C	514	CLA	C2A-CAA-CBA-CGA
22	J	101	BCR	C37-C22-C23-C24
22	A	403	BCR	C21-C22-C23-C24
22	B	601	BCR	C11-C12-C13-C14
22	J	101	BCR	C21-C22-C23-C24
23	C	507	CLA	C15-C16-C17-C18
27	M	101	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
23	B	605	CLA	O1D-CGD-O2D-CED
23	B	612	CLA	C4B-C3B-CAB-CBB
23	C	507	CLA	C4B-C3B-CAB-CBB
23	C	509	CLA	C4B-C3B-CAB-CBB
23	C	506	CLA	C15-C16-C17-C18
27	K	102	LMG	C42-C43-C44-C45
23	B	606	CLA	CAD-CBD-CGD-O1D
23	B	612	CLA	CAD-CBD-CGD-O1D
23	B	617	CLA	CAD-CBD-CGD-O1D
23	C	516	CLA	CAD-CBD-CGD-O1D
27	D	407	LMG	C29-C28-O8-C9
23	B	607	CLA	C16-C17-C18-C19
23	B	607	CLA	C11-C12-C13-C15
23	B	612	CLA	C11-C12-C13-C15
24	A	408	PHO	C6-C7-C8-C10
26	A	410	LHG	C13-C14-C15-C16
23	C	510	CLA	C2A-CAA-CBA-CGA
27	I	101	LMG	O1-C7-C8-O7
27	D	406	LMG	C42-C43-C44-C45
23	D	404	CLA	C13-C15-C16-C17
27	D	406	LMG	C30-C31-C32-C33
27	D	406	LMG	C8-C7-O1-C1
23	B	605	CLA	C5-C6-C7-C8
27	D	407	LMG	O10-C28-O8-C9
23	C	516	CLA	C6-C7-C8-C9
25	A	409	PL9	C9-C11-C12-C13
27	D	406	LMG	C24-C25-C26-C27
27	D	406	LMG	C29-C30-C31-C32
23	B	613	CLA	C10-C11-C12-C13
23	C	505	CLA	C10-C11-C12-C13
27	D	407	LMG	C9-C8-O7-C10
27	Z	101	LMG	C7-C8-O7-C10
23	B	606	CLA	C2A-CAA-CBA-CGA
23	B	610	CLA	C2A-CAA-CBA-CGA
23	C	512	CLA	O1A-CGA-O2A-C1
23	B	617	CLA	C2-C1-O2A-CGA
23	C	508	CLA	CAA-CBA-CGA-O2A
22	D	403	BCR	C5-C6-C7-C8
24	A	408	PHO	C15-C16-C17-C18
26	A	410	LHG	C3-O3-P-O6
26	C	501	LHG	C3-O3-P-O6
26	C	501	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
27	I	101	LMG	C34-C35-C36-C37
23	C	506	CLA	C16-C17-C18-C20
23	C	507	CLA	C6-C7-C8-C10
23	B	612	CLA	C11-C12-C13-C14
22	A	403	BCR	C19-C20-C21-C22
27	D	401	LMG	C40-C41-C42-C43
27	D	401	LMG	C16-C17-C18-C19
23	C	512	CLA	CBA-CGA-O2A-C1
26	C	501	LHG	O1-C1-C2-C3
27	D	407	LMG	C11-C12-C13-C14
22	D	403	BCR	C7-C8-C9-C10
25	A	409	PL9	C47-C48-C49-C50
27	D	407	LMG	C17-C18-C19-C20
25	A	409	PL9	C37-C38-C39-C41
27	Z	101	LMG	C13-C14-C15-C16
23	B	612	CLA	CBA-CGA-O2A-C1
23	B	604	CLA	C10-C11-C12-C13
23	B	612	CLA	O1A-CGA-O2A-C1
27	K	102	LMG	C13-C14-C15-C16
23	C	510	CLA	C4B-C3B-CAB-CBB
23	B	608	CLA	C4-C3-C5-C6
23	B	615	CLA	C4-C3-C5-C6
27	I	101	LMG	C30-C31-C32-C33
23	B	619	CLA	C2-C1-O2A-CGA
23	C	512	CLA	C2-C1-O2A-CGA
23	C	505	CLA	C3A-C2A-CAA-CBA
23	B	614	CLA	C14-C13-C15-C16
23	B	617	CLA	C11-C12-C13-C14
29	V	201	HEM	C2A-CAA-CBA-CGA
26	C	501	LHG	C33-C34-C35-C36
27	L	101	LMG	C14-C15-C16-C17
23	B	617	CLA	C2A-CAA-CBA-CGA
23	A	404	CLA	O2A-C1-C2-C3
23	B	605	CLA	O2A-C1-C2-C3
23	C	505	CLA	O2A-C1-C2-C3
23	C	507	CLA	O2A-C1-C2-C3
23	C	512	CLA	O2A-C1-C2-C3
23	D	405	CLA	O2A-C1-C2-C3
24	D	408	PHO	O2A-C1-C2-C3
22	C	502	BCR	C37-C22-C23-C24
27	Z	101	LMG	C9-C8-O7-C10
23	C	507	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	B	615	CLA	C1A-C2A-CAA-CBA
26	A	410	LHG	C17-C18-C19-C20
23	B	605	CLA	C11-C12-C13-C15
23	C	504	CLA	C11-C12-C13-C15
23	D	404	CLA	C12-C13-C15-C16
23	C	509	CLA	C8-C10-C11-C12
23	C	506	CLA	C16-C17-C18-C19
23	C	505	CLA	C2A-CAA-CBA-CGA
27	D	406	LMG	C23-C24-C25-C26
23	B	613	CLA	C8-C10-C11-C12
23	B	612	CLA	C2B-C3B-CAB-CBB
23	B	617	CLA	C2B-C3B-CAB-CBB
23	C	507	CLA	C2B-C3B-CAB-CBB
23	C	509	CLA	C2B-C3B-CAB-CBB
23	C	510	CLA	C2B-C3B-CAB-CBB
23	B	616	CLA	C13-C15-C16-C17
27	K	102	LMG	C41-C42-C43-C44
27	L	101	LMG	C13-C14-C15-C16
23	A	407	CLA	C4-C3-C5-C6
23	C	515	CLA	C4-C3-C5-C6
25	A	409	PL9	C35-C34-C36-C37
23	B	615	CLA	CAA-CBA-CGA-O2A
23	B	611	CLA	C11-C10-C8-C9
27	M	101	LMG	C24-C25-C26-C27
23	B	608	CLA	C2A-CAA-CBA-CGA
23	C	508	CLA	C16-C17-C18-C19
27	L	101	LMG	O1-C7-C8-C9
22	B	602	BCR	C21-C22-C23-C24
23	B	615	CLA	C15-C16-C17-C18
24	D	408	PHO	C8-C10-C11-C12
23	B	615	CLA	C2-C3-C5-C6
27	D	407	LMG	C13-C14-C15-C16
27	D	401	LMG	C21-C22-C23-C24
27	L	101	LMG	C20-C21-C22-C23
26	A	410	LHG	O6-C4-C5-O7
27	K	102	LMG	C35-C36-C37-C38
23	B	617	CLA	C4B-C3B-CAB-CBB
23	B	611	CLA	C4-C3-C5-C6
24	D	408	PHO	C4-C3-C5-C6
23	C	512	CLA	C11-C10-C8-C7
29	V	201	HEM	CAA-CBA-CGA-O2A
27	I	101	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	B	618	CLA	CAA-CBA-CGA-O2A
23	C	506	CLA	CAA-CBA-CGA-O2A
25	A	409	PL9	C20-C19-C21-C22
23	C	507	CLA	C2-C3-C5-C6
23	B	612	CLA	C15-C16-C17-C18
23	B	607	CLA	C11-C12-C13-C14
23	C	509	CLA	C11-C12-C13-C14
23	C	511	CLA	C14-C13-C15-C16
26	A	410	LHG	C16-C17-C18-C19
23	A	405	CLA	CAD-CBD-CGD-O2D
23	B	607	CLA	CAD-CBD-CGD-O2D
23	B	615	CLA	CAD-CBD-CGD-O2D
23	C	505	CLA	CAD-CBD-CGD-O2D
27	Z	101	LMG	C28-C29-C30-C31
23	B	608	CLA	C3-C5-C6-C7
23	A	405	CLA	C2C-C3C-CAC-CBC
23	B	618	CLA	C4-C3-C5-C6
23	C	509	CLA	C4-C3-C5-C6
23	C	515	CLA	C2-C3-C5-C6
23	B	604	CLA	CAA-CBA-CGA-O2A
23	B	613	CLA	CAA-CBA-CGA-O2A
23	B	616	CLA	CAA-CBA-CGA-O2A
23	C	504	CLA	CAA-CBA-CGA-O2A
22	B	601	BCR	C21-C22-C23-C24
22	C	503	BCR	C21-C22-C23-C24
27	I	101	LMG	C35-C36-C37-C38
29	V	201	HEM	CAA-CBA-CGA-O1A
24	D	408	PHO	CBD-CGD-O2D-CED
23	C	515	CLA	O2A-C1-C2-C3
23	D	404	CLA	O2A-C1-C2-C3
24	A	408	PHO	O2A-C1-C2-C3
27	L	101	LMG	C4-C5-C6-O5
23	A	407	CLA	CAA-CBA-CGA-O2A
22	B	603	BCR	C9-C10-C11-C12
23	B	608	CLA	CHA-CBD-CGD-O1D
23	C	506	CLA	CHA-CBD-CGD-O2D
23	C	512	CLA	CHA-CBD-CGD-O1D
23	C	512	CLA	CHA-CBD-CGD-O2D
23	C	516	CLA	CHA-CBD-CGD-O2D
23	C	516	CLA	C8-C10-C11-C12
23	B	606	CLA	CAA-CBA-CGA-O2A
23	B	615	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	B	607	CLA	C11-C10-C8-C7
23	B	617	CLA	C12-C13-C15-C16
23	C	505	CLA	C12-C13-C15-C16
23	A	404	CLA	C14-C13-C15-C16
23	B	613	CLA	C6-C7-C8-C9
23	C	507	CLA	C6-C7-C8-C9
22	C	503	BCR	C13-C14-C15-C16
22	K	101	BCR	C13-C14-C15-C16
23	C	505	CLA	C2B-C3B-CAB-CBB
23	B	612	CLA	C16-C17-C18-C19
23	C	509	CLA	C2A-CAA-CBA-CGA
25	A	409	PL9	C36-C37-C38-C39
23	B	613	CLA	CAA-CBA-CGA-O1A
23	B	616	CLA	CAA-CBA-CGA-O1A
23	A	407	CLA	CAA-CBA-CGA-O1A
23	B	612	CLA	C16-C17-C18-C20
25	A	409	PL9	C15-C14-C16-C17
23	B	611	CLA	C2-C3-C5-C6
22	C	502	BCR	C21-C22-C23-C24
23	B	618	CLA	CAA-CBA-CGA-O1A
23	C	506	CLA	CAA-CBA-CGA-O1A
27	Z	101	LMG	C24-C25-C26-C27
27	D	401	LMG	C12-C13-C14-C15
23	B	604	CLA	CAA-CBA-CGA-O1A
23	C	504	CLA	CAA-CBA-CGA-O1A
27	D	401	LMG	C41-C42-C43-C44
23	B	619	CLA	C4B-C3B-CAB-CBB
26	C	501	LHG	C3-O3-P-O5
24	A	408	PHO	C16-C17-C18-C19
27	D	406	LMG	C37-C38-C39-C40
23	A	405	CLA	C4C-C3C-CAC-CBC
23	B	614	CLA	C10-C11-C12-C13
23	D	405	CLA	CAA-CBA-CGA-O2A
27	L	101	LMG	O9-C10-O7-C8
26	A	410	LHG	C26-C27-C28-C29
27	M	101	LMG	C37-C38-C39-C40
23	B	604	CLA	CAD-CBD-CGD-O1D
23	B	608	CLA	CAD-CBD-CGD-O1D
23	C	504	CLA	CAD-CBD-CGD-O1D
23	C	504	CLA	C11-C12-C13-C14
27	D	401	LMG	C30-C31-C32-C33
24	A	408	PHO	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	A	405	CLA	CAA-CBA-CGA-O2A
27	D	407	LMG	O8-C28-C29-C30
23	B	606	CLA	CAA-CBA-CGA-O1A
23	B	606	CLA	C6-C7-C8-C10
23	B	608	CLA	C2-C3-C5-C6
23	D	404	CLA	C3A-C2A-CAA-CBA
24	D	408	PHO	C6-C7-C8-C10
23	B	614	CLA	CAA-CBA-CGA-O2A
27	D	401	LMG	O7-C10-C11-C12
24	A	408	PHO	C16-C17-C18-C20
23	B	616	CLA	C10-C11-C12-C13
23	D	405	CLA	CAA-CBA-CGA-O1A
27	M	101	LMG	O8-C28-C29-C30
27	D	407	LMG	O10-C28-C29-C30
23	A	405	CLA	CAA-CBA-CGA-O1A
27	Z	101	LMG	O8-C28-C29-C30

There are no ring outliers.

23 monomers are involved in 30 short contacts:

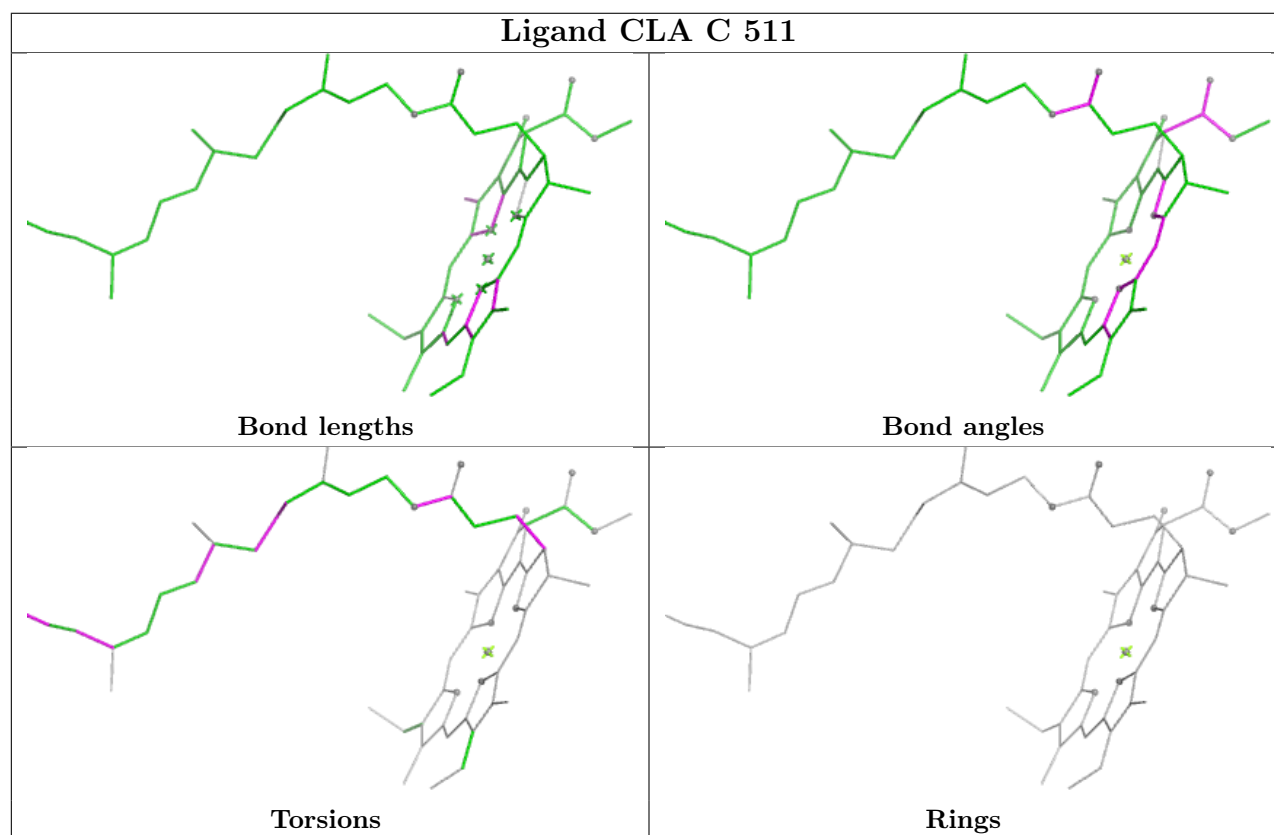
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	511	CLA	1	0
23	C	513	CLA	2	0
24	D	408	PHO	1	0
22	C	503	BCR	2	0
22	C	502	BCR	1	0
29	F	101	HEM	1	0
23	A	404	CLA	1	0
22	H	101	BCR	2	0
23	A	407	CLA	1	0
23	B	614	CLA	2	0
23	B	606	CLA	3	0
23	B	607	CLA	2	0
23	B	613	CLA	1	0
23	C	504	CLA	3	0
23	B	604	CLA	1	0
23	A	405	CLA	1	0
23	B	617	CLA	1	0
29	V	201	HEM	3	0
22	K	101	BCR	1	0
23	C	516	CLA	1	0
23	D	405	CLA	1	0

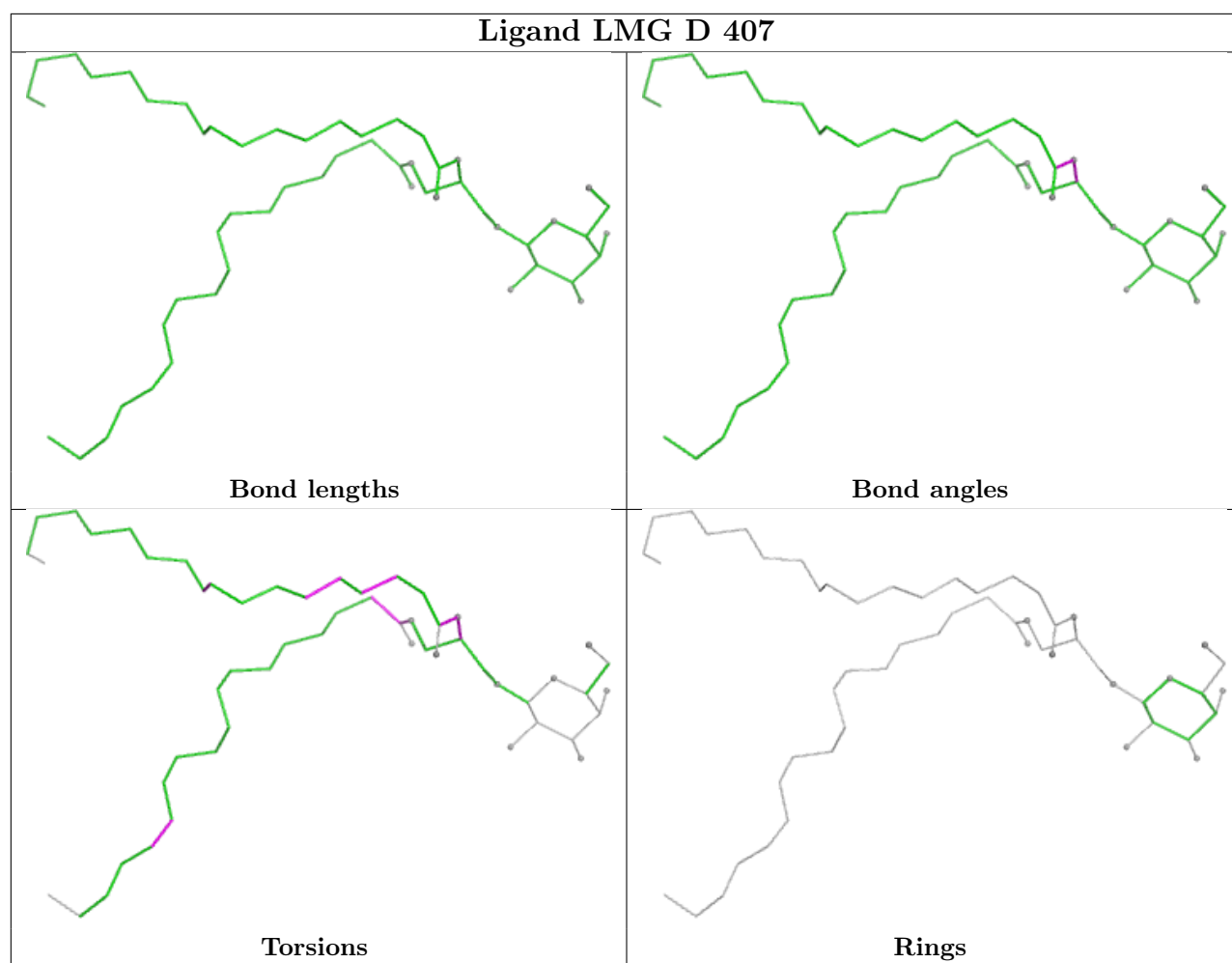
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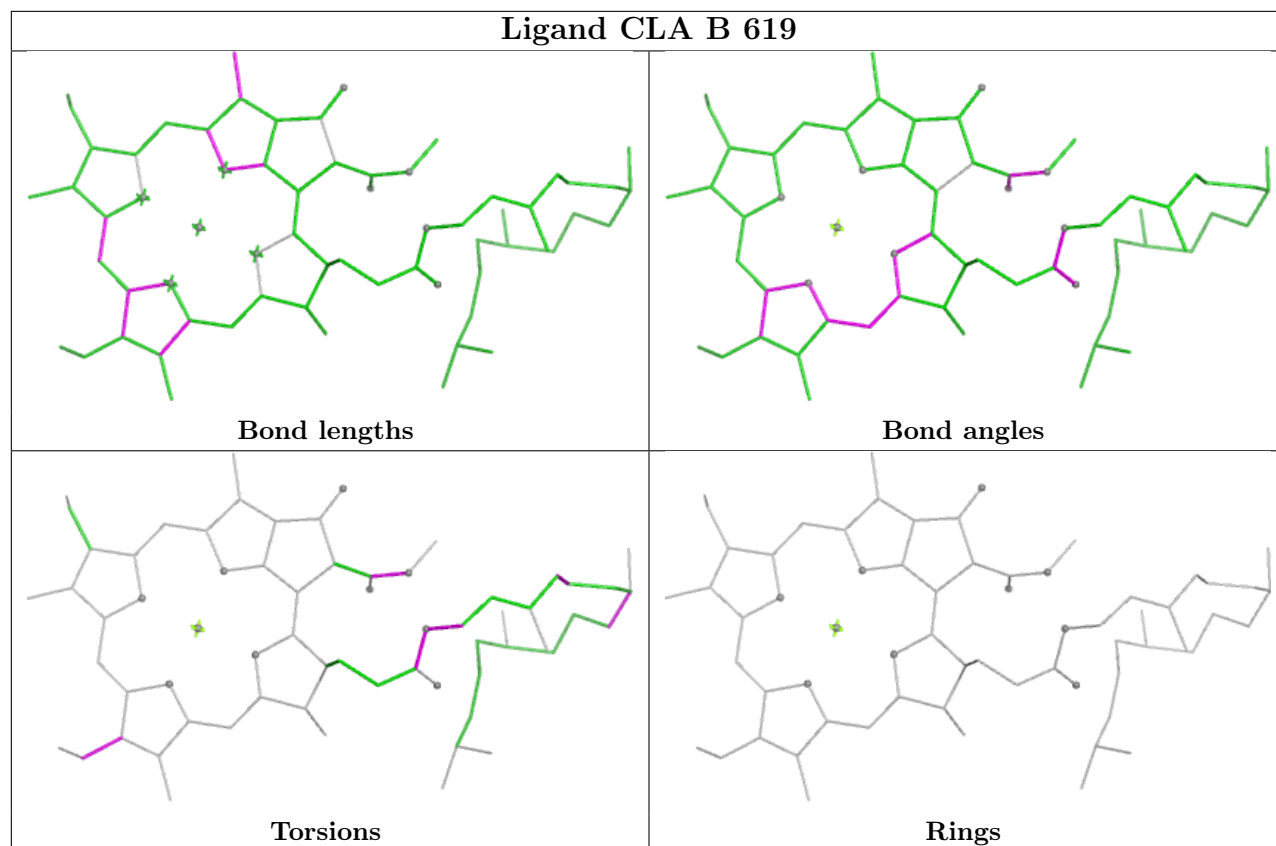
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	D	404	CLA	2	0
23	C	510	CLA	1	0

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.

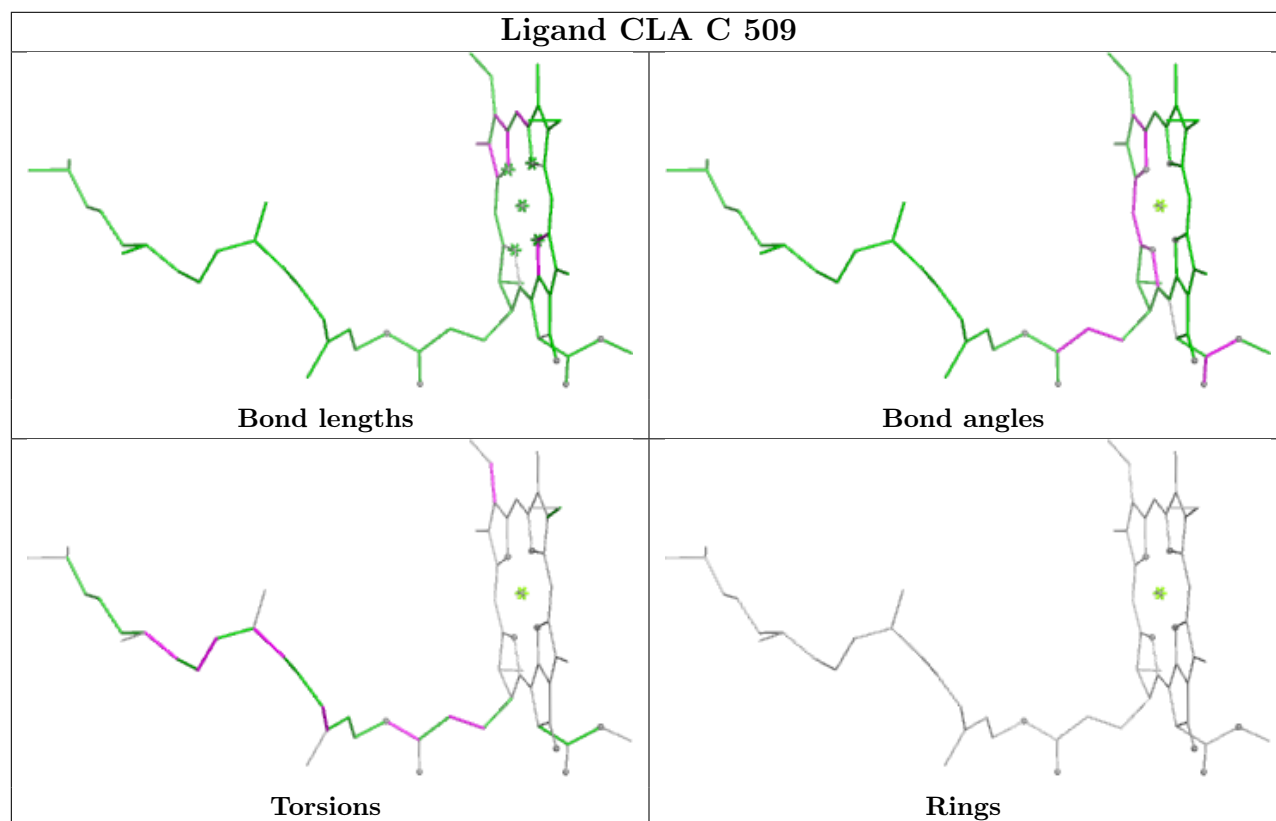


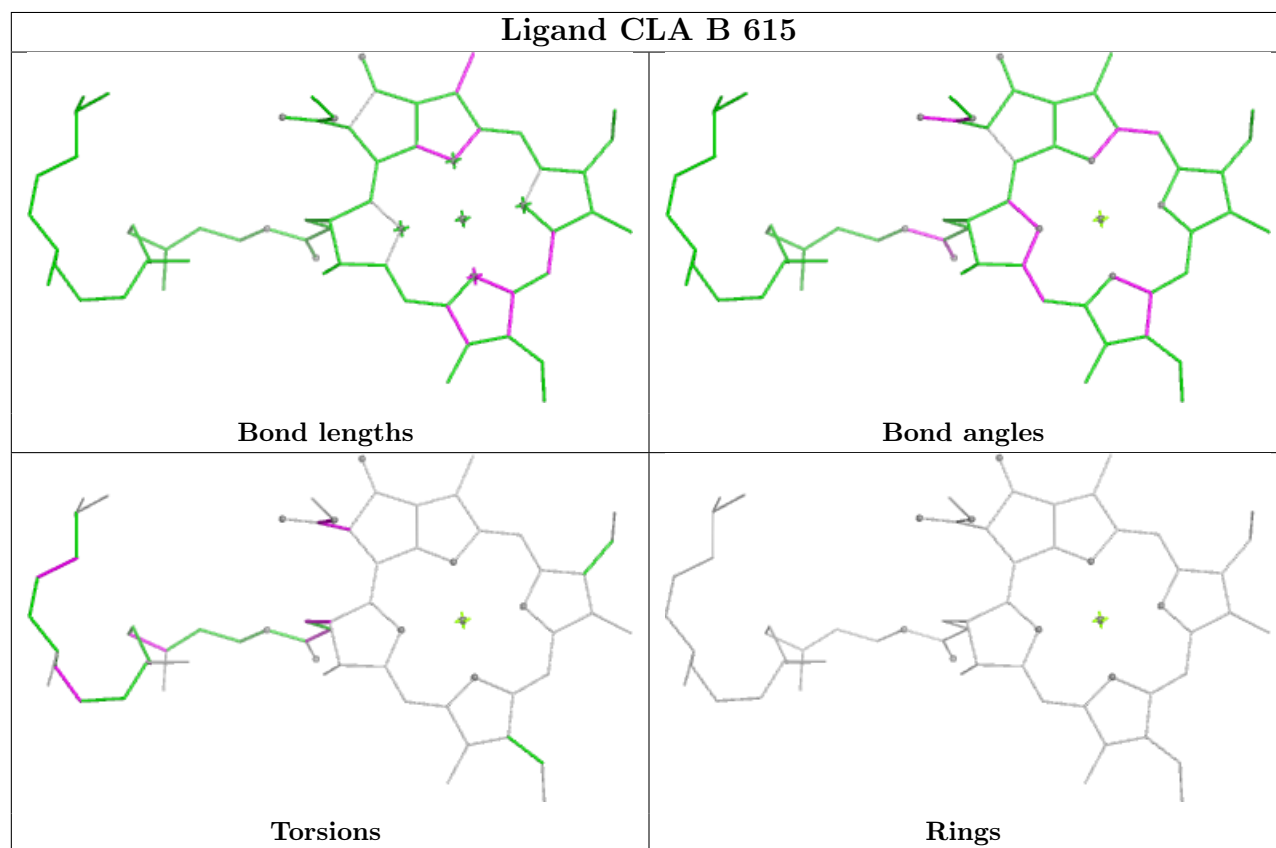
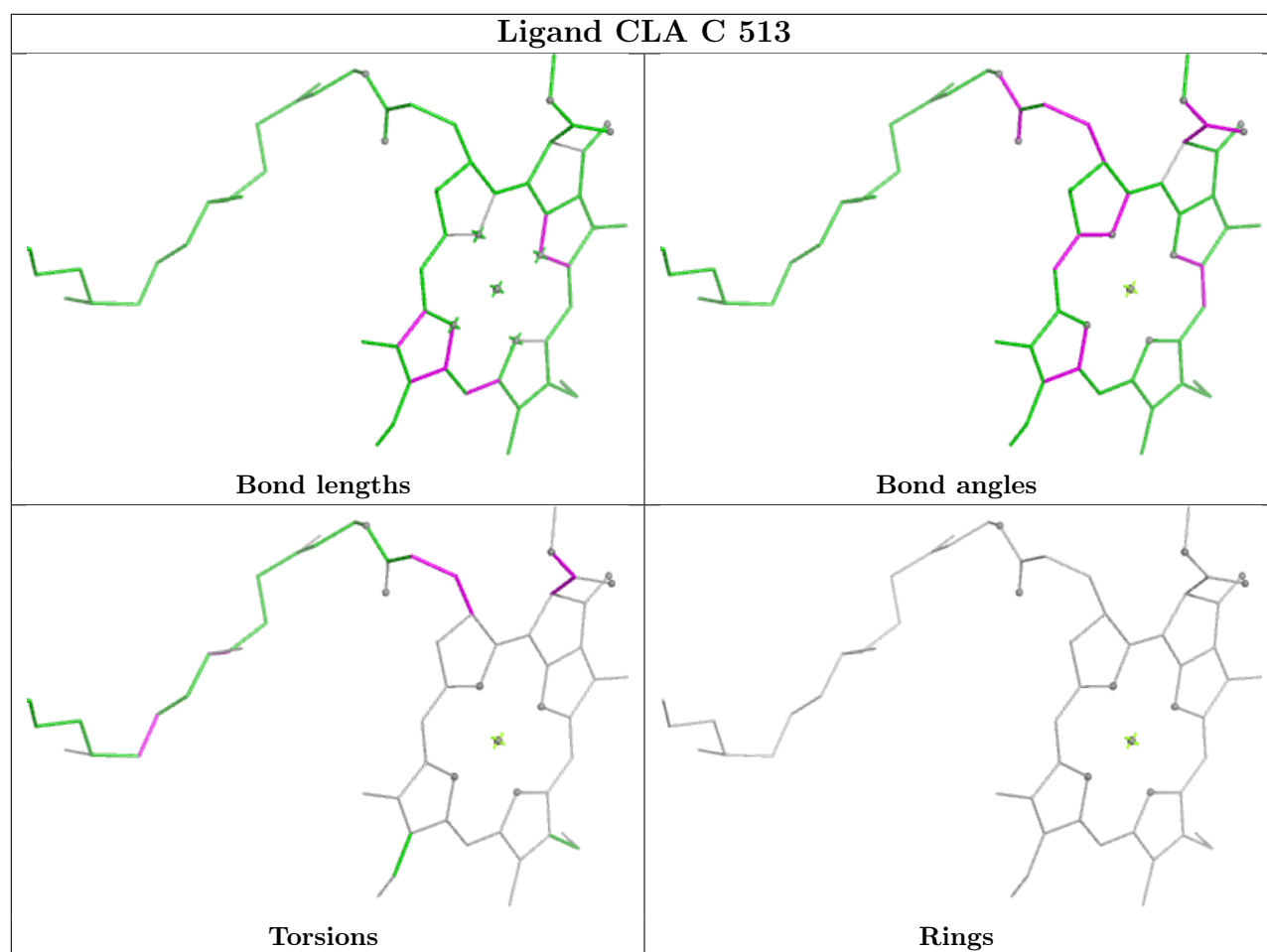


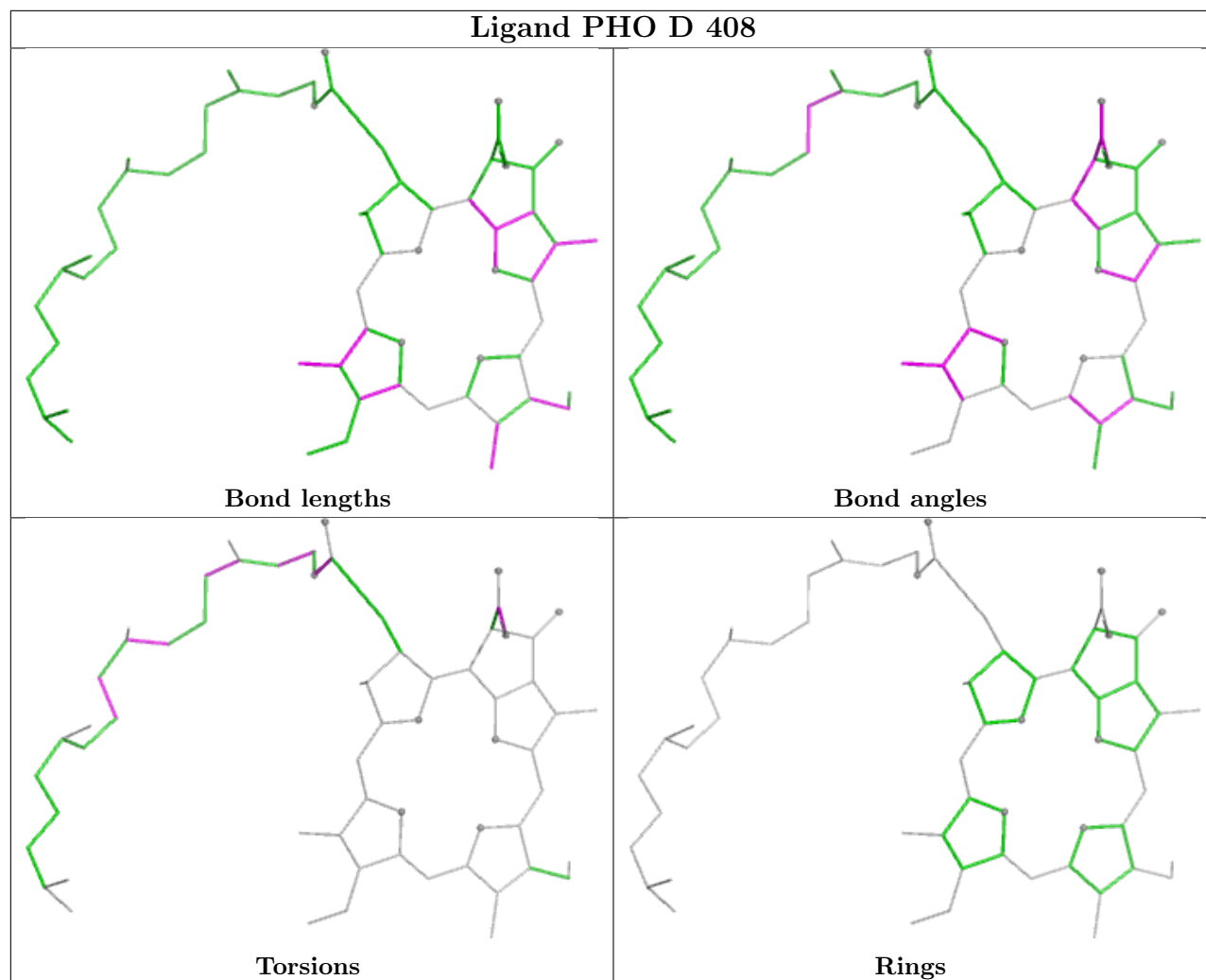
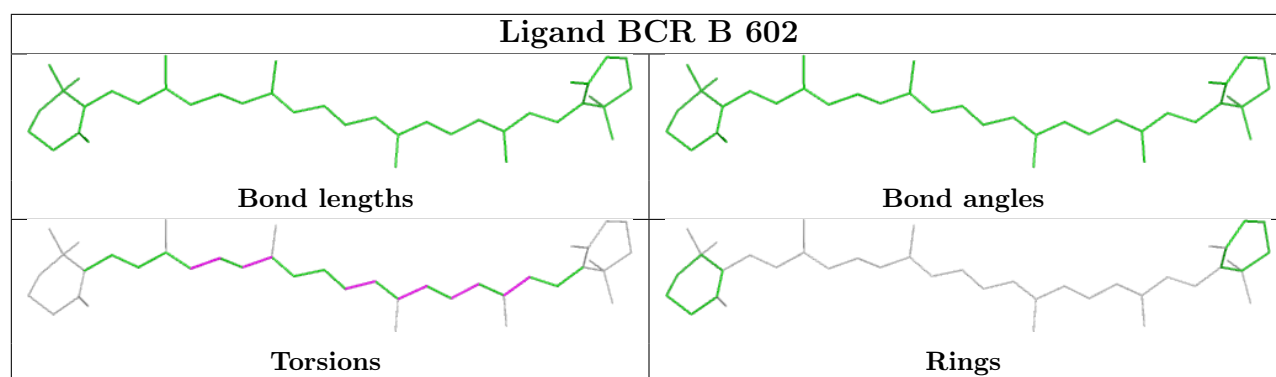
Ligand CLA B 619

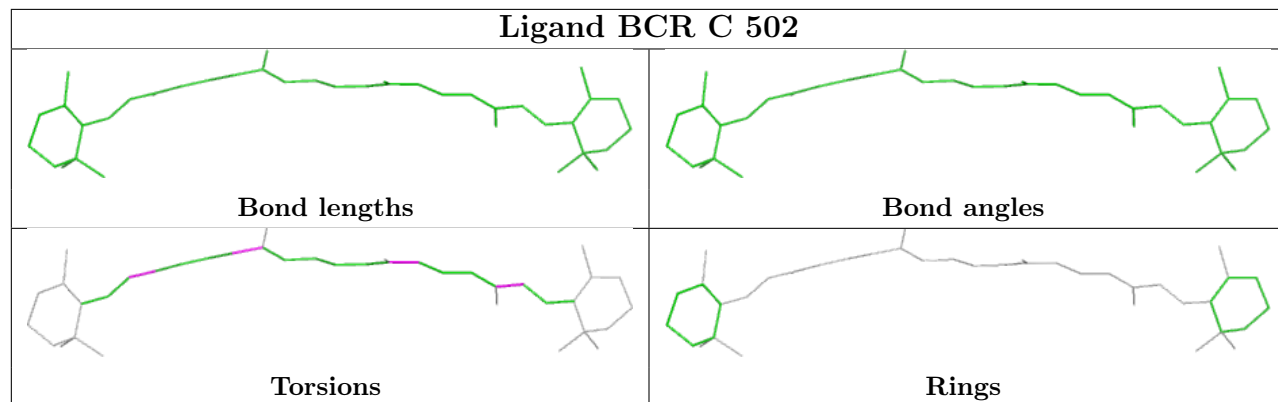
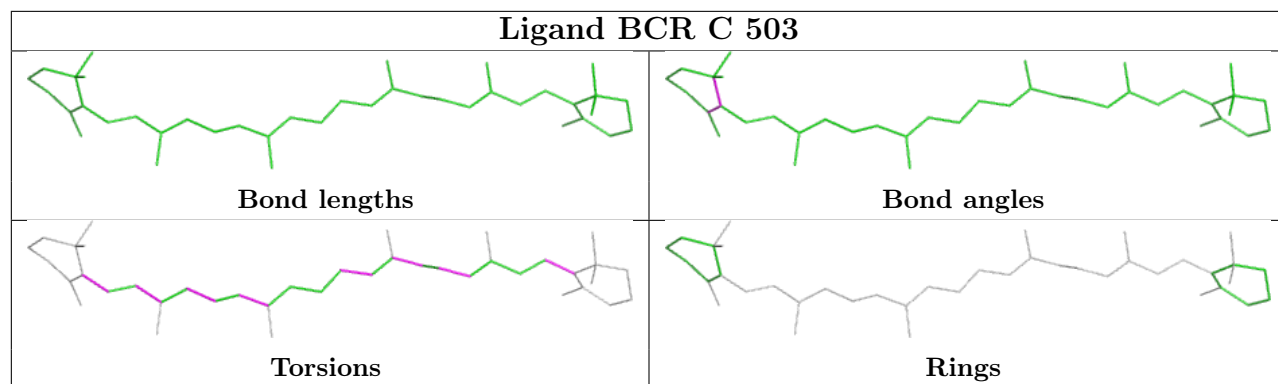


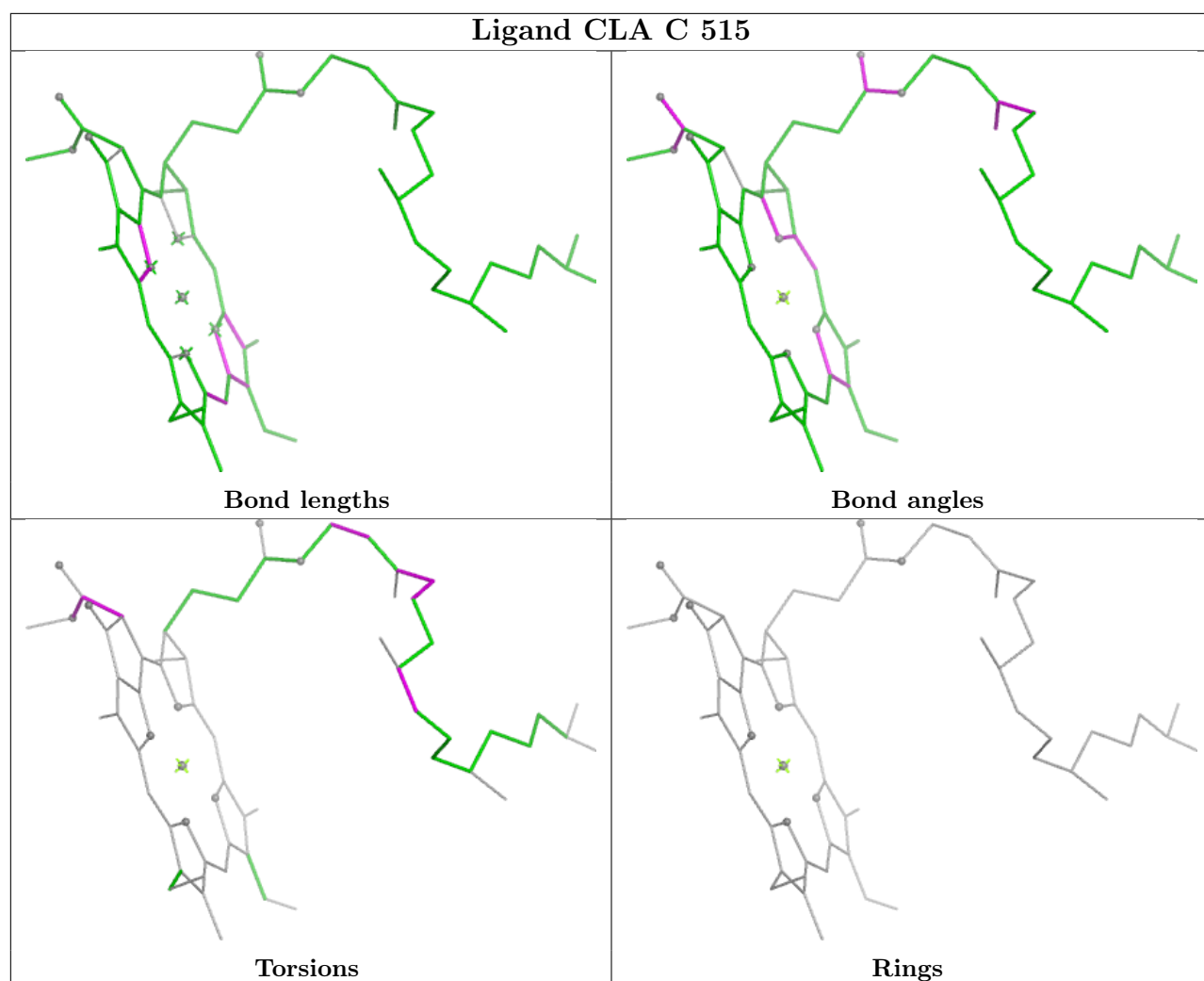
Ligand CLA C 509

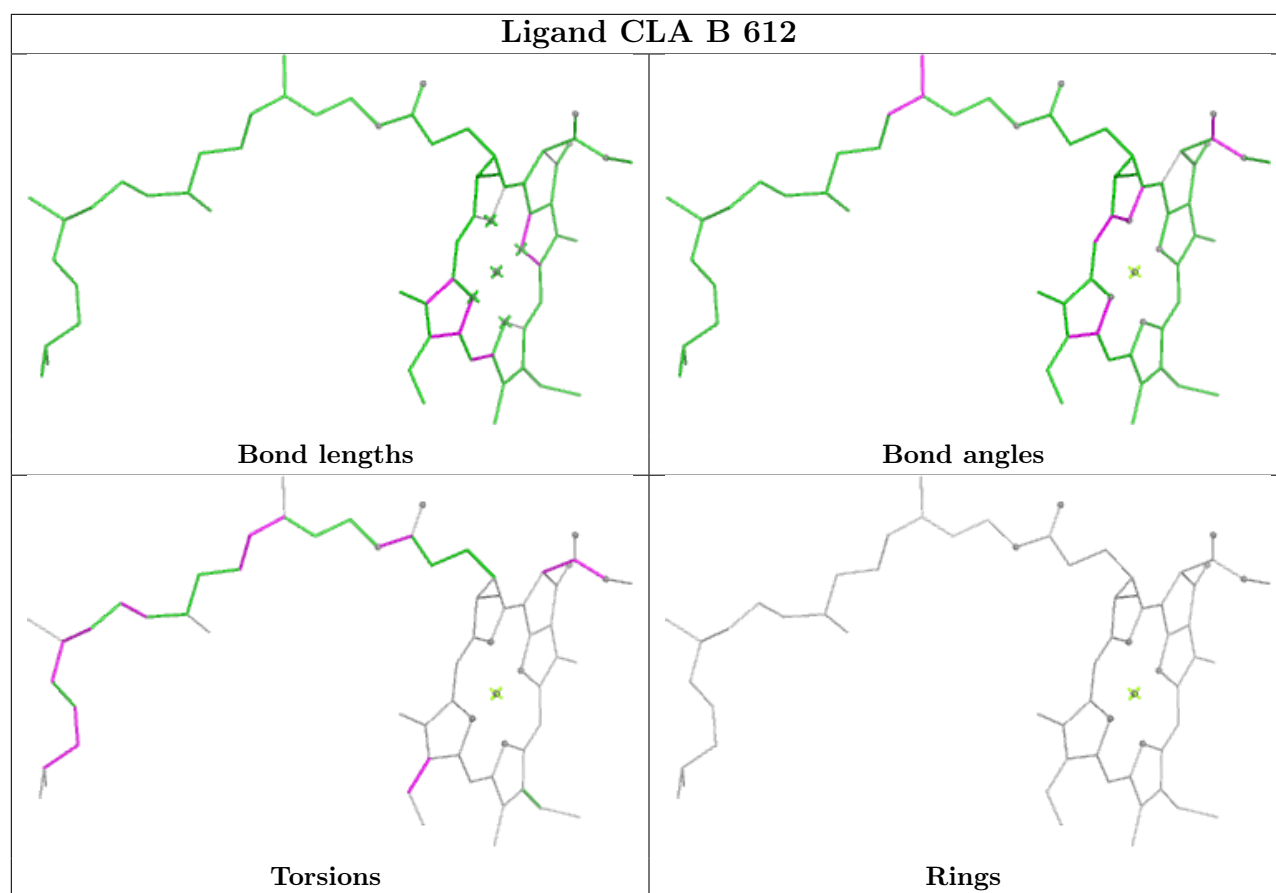


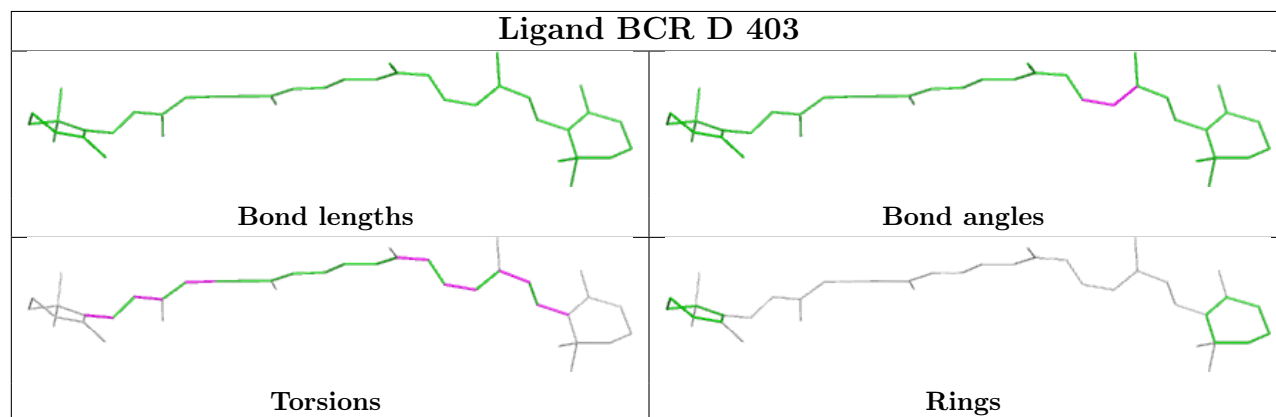
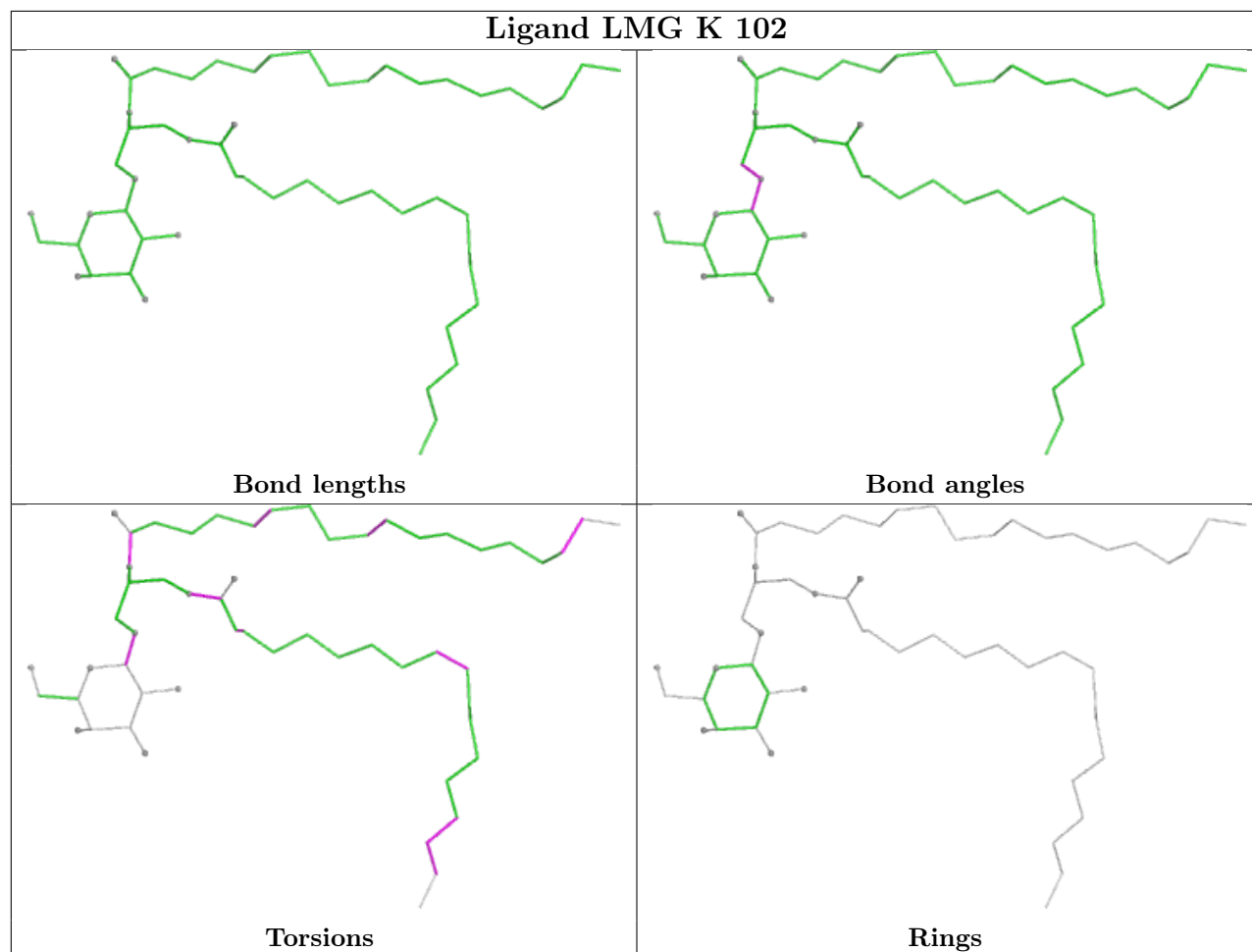


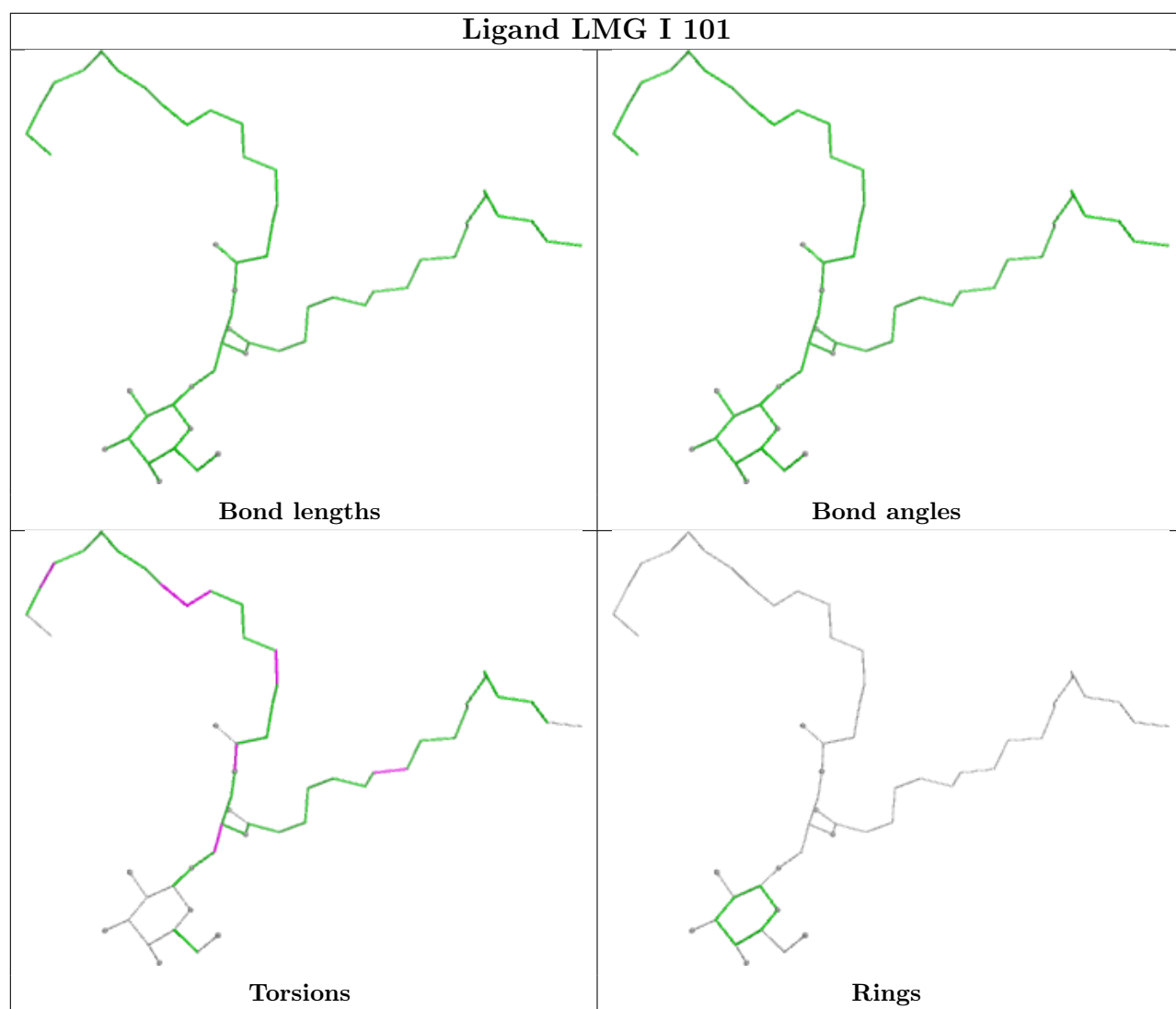


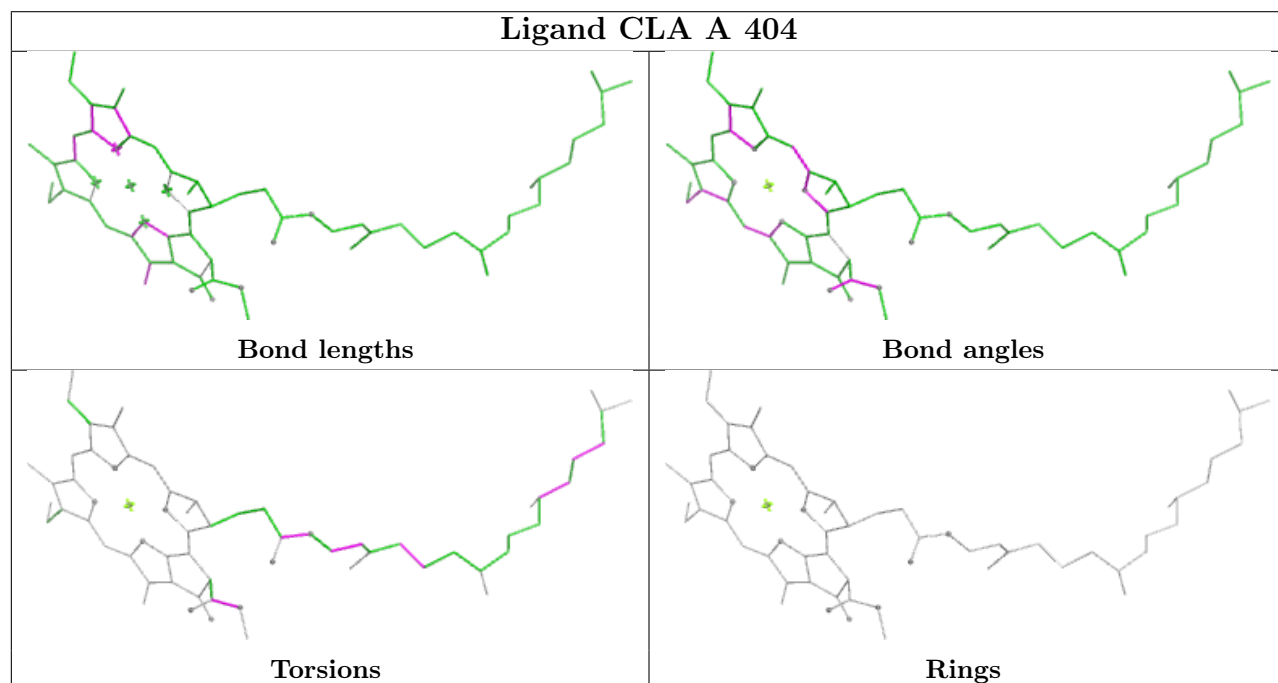
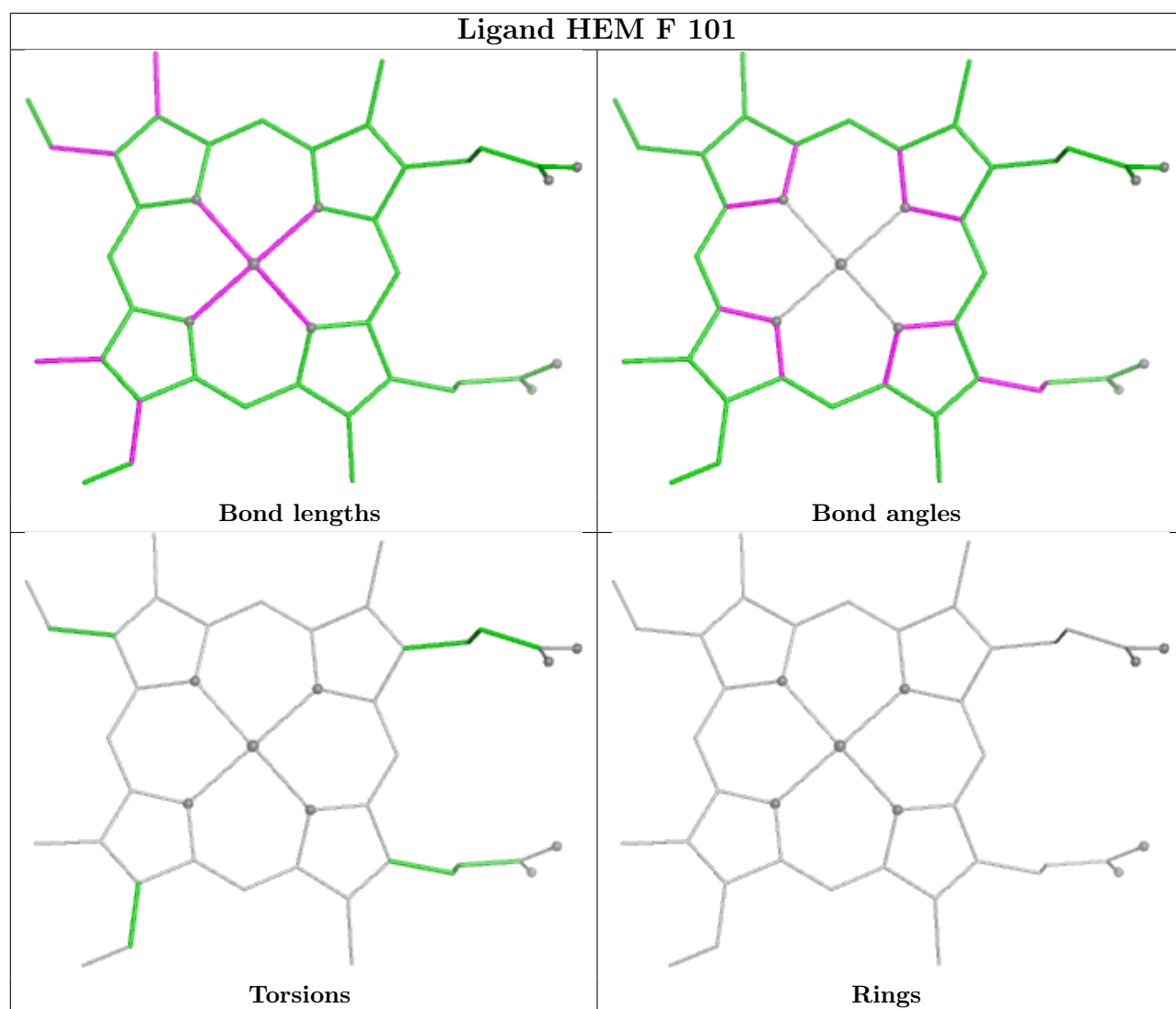


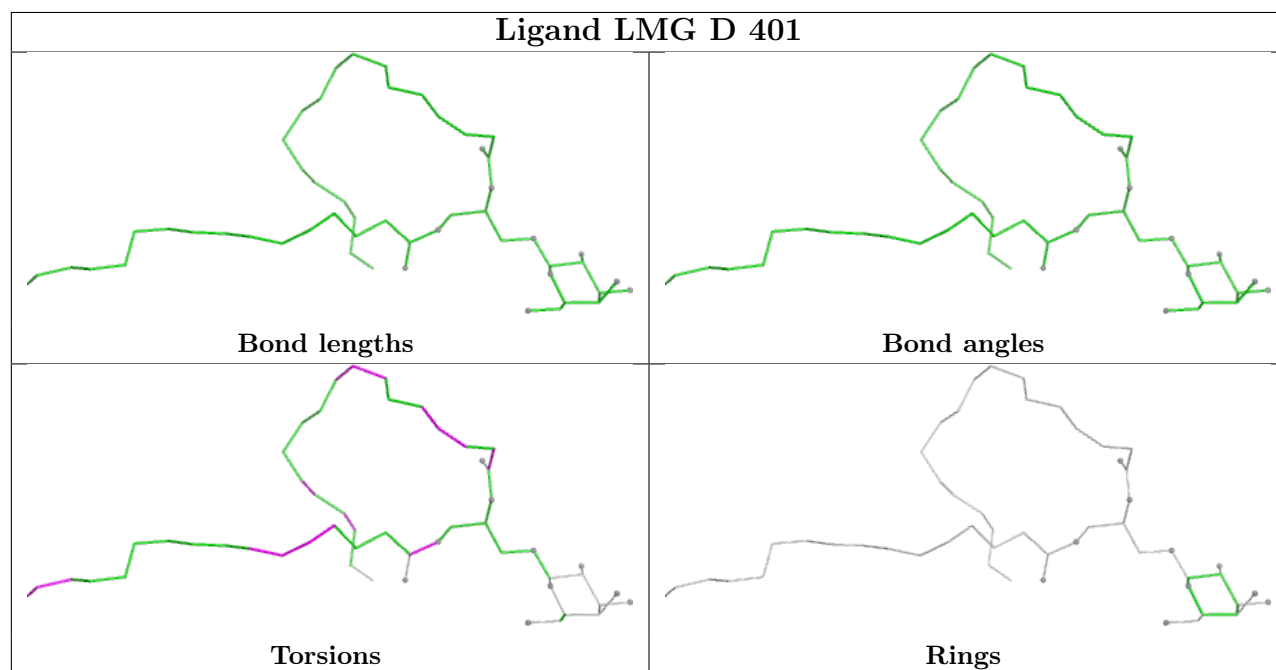
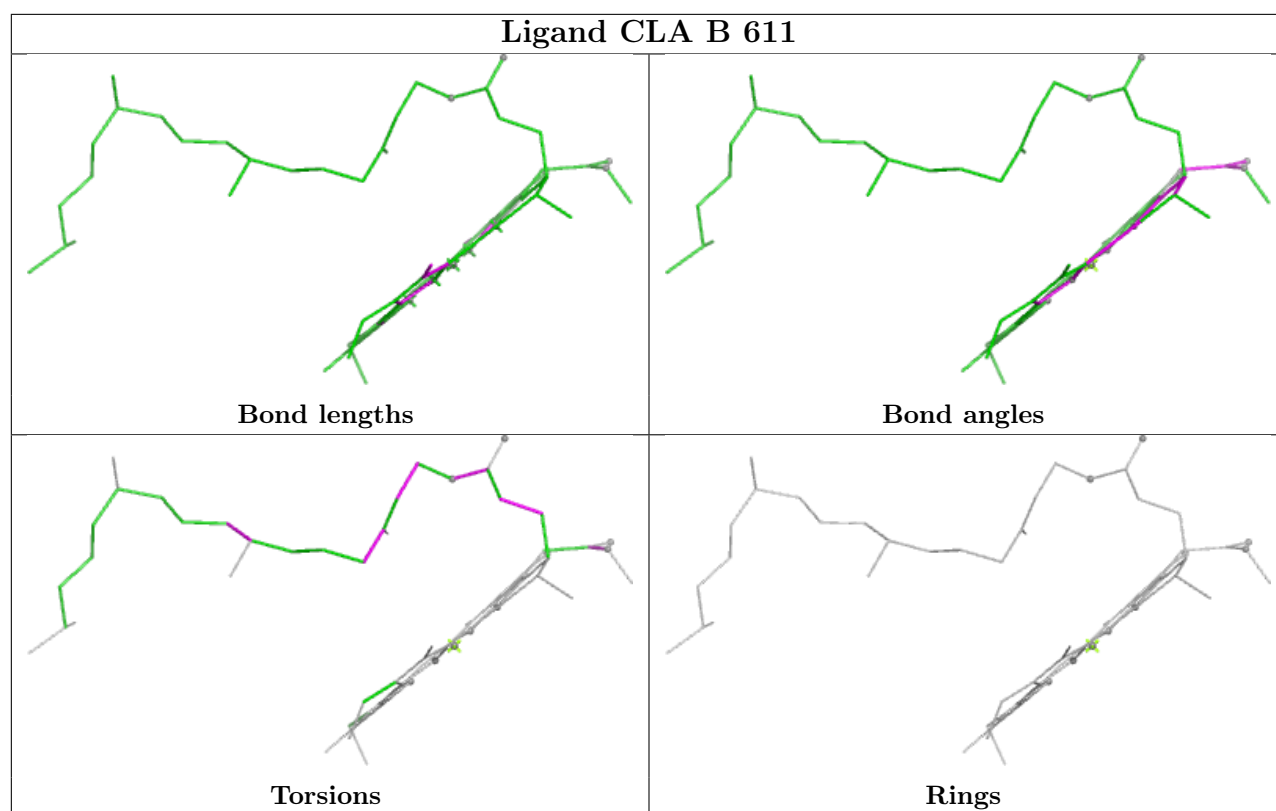


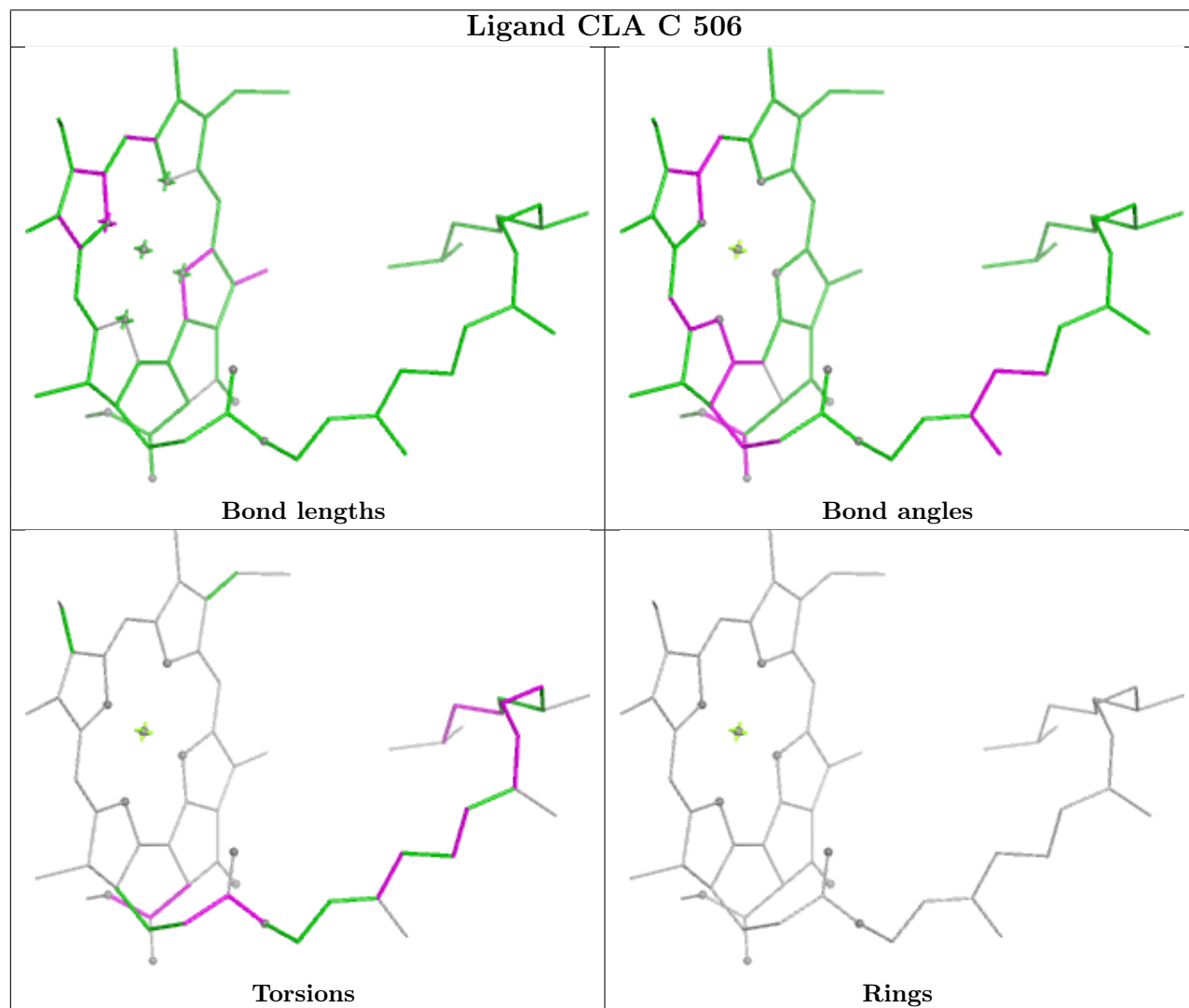
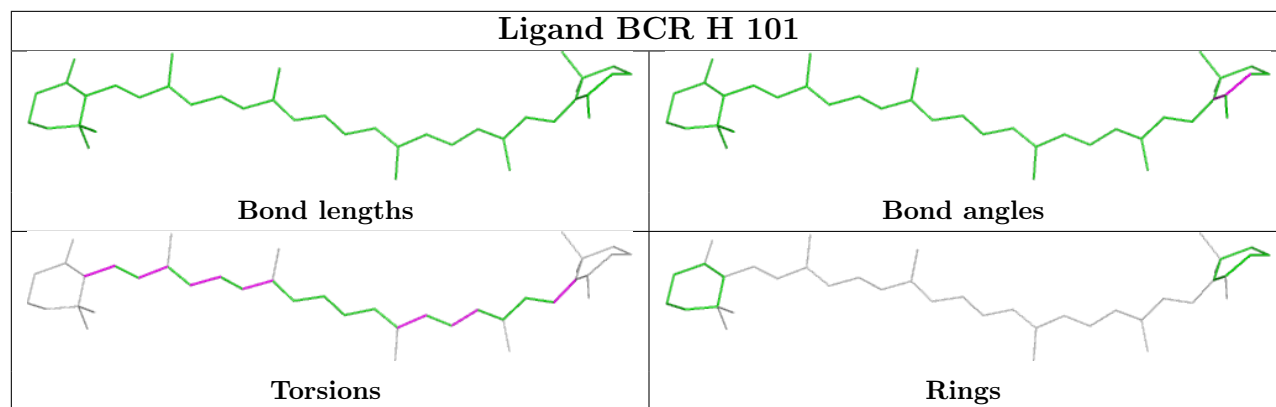


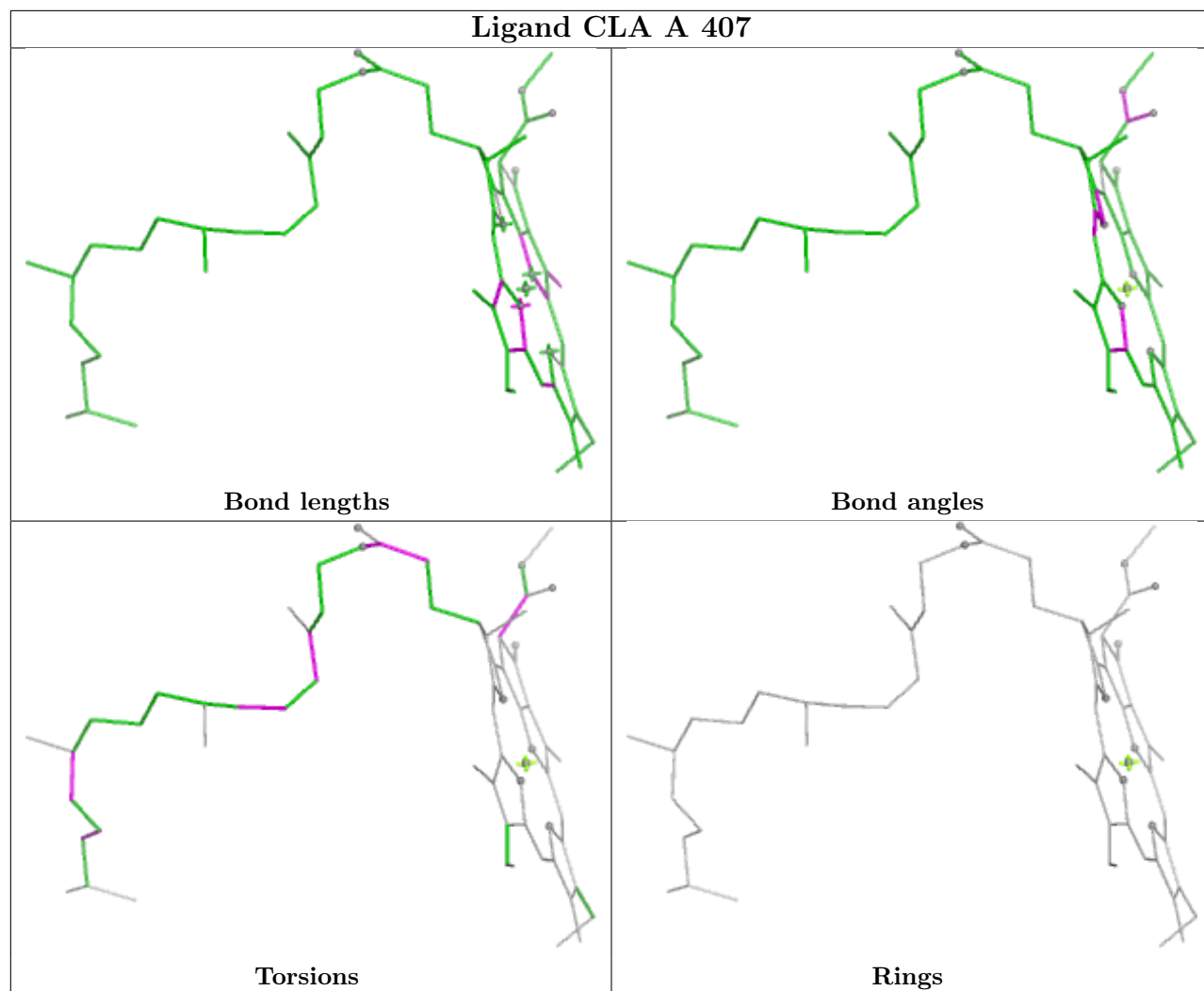


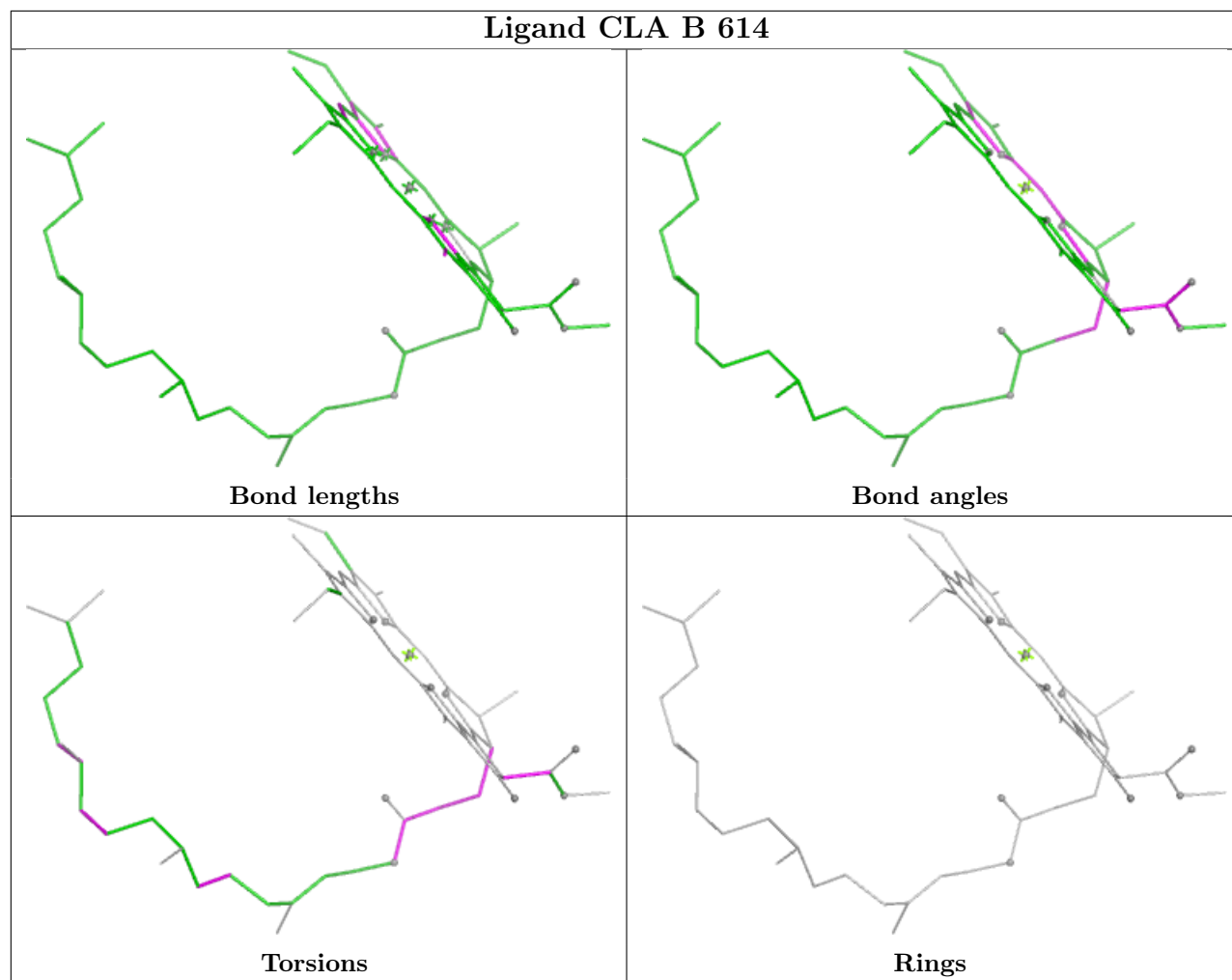




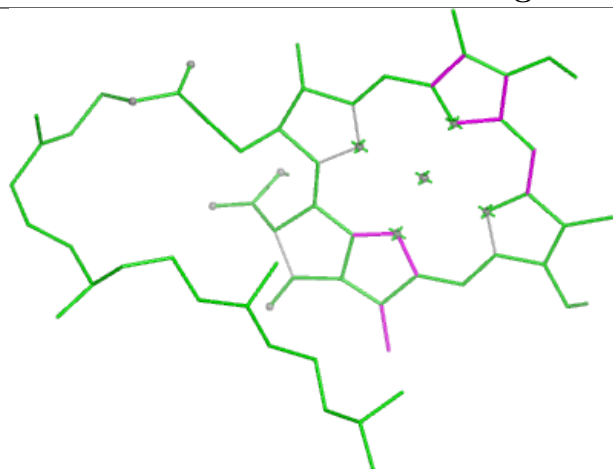




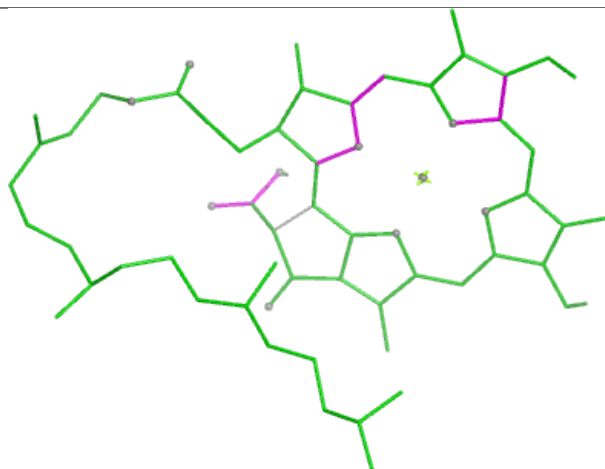




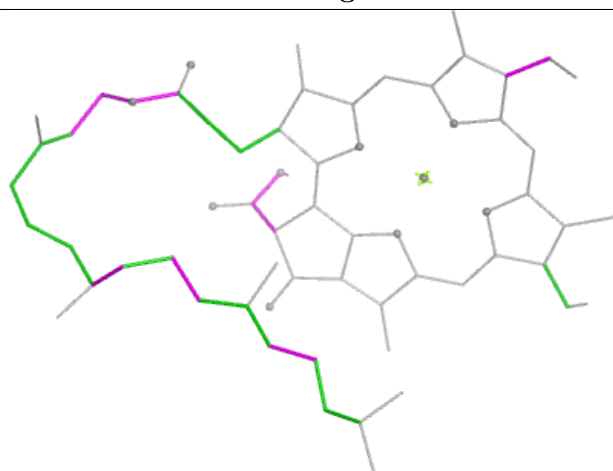
Ligand CLA C 512



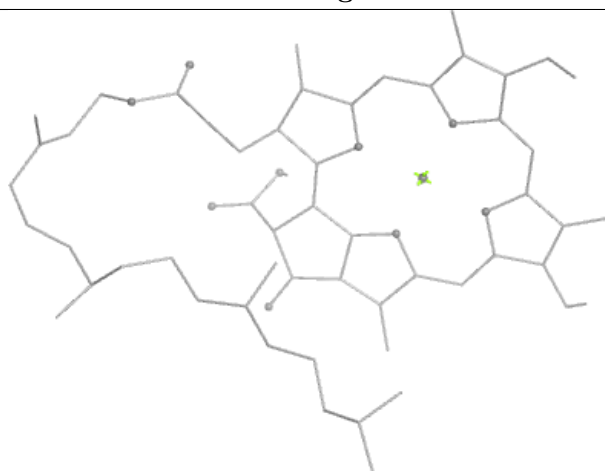
Bond lengths



Bond angles

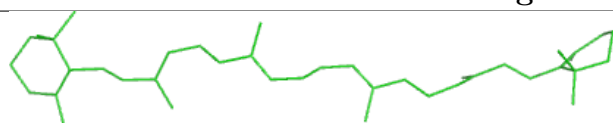


Torsions

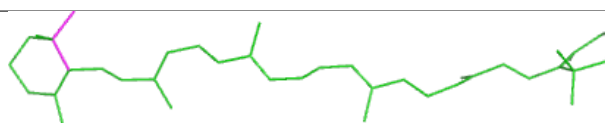


Rings

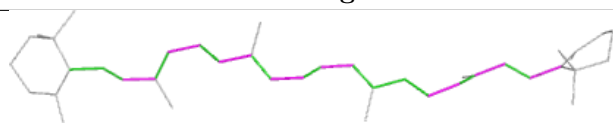
Ligand BCR J 101



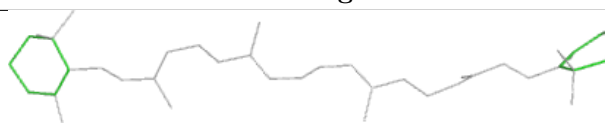
Bond lengths



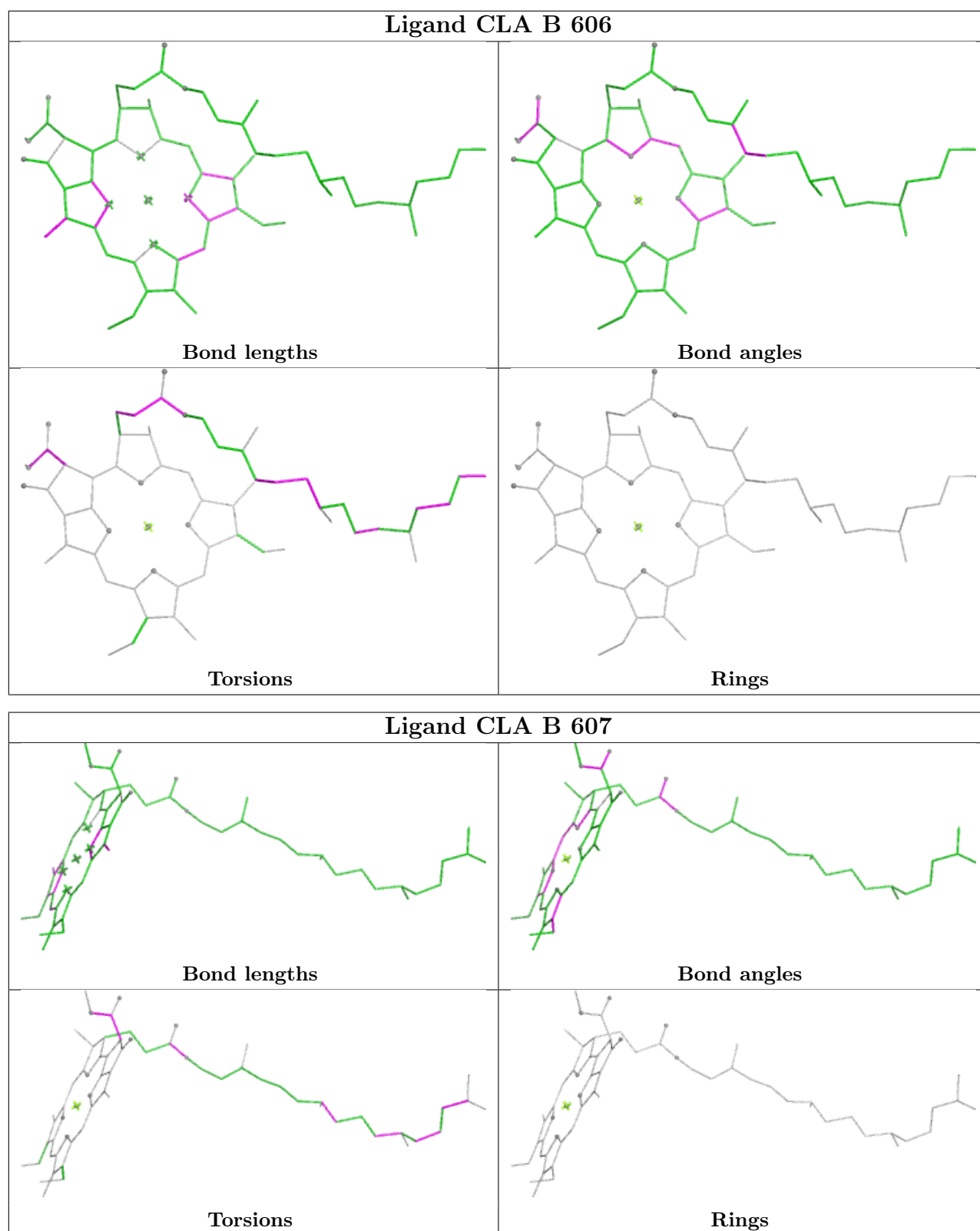
Bond angles

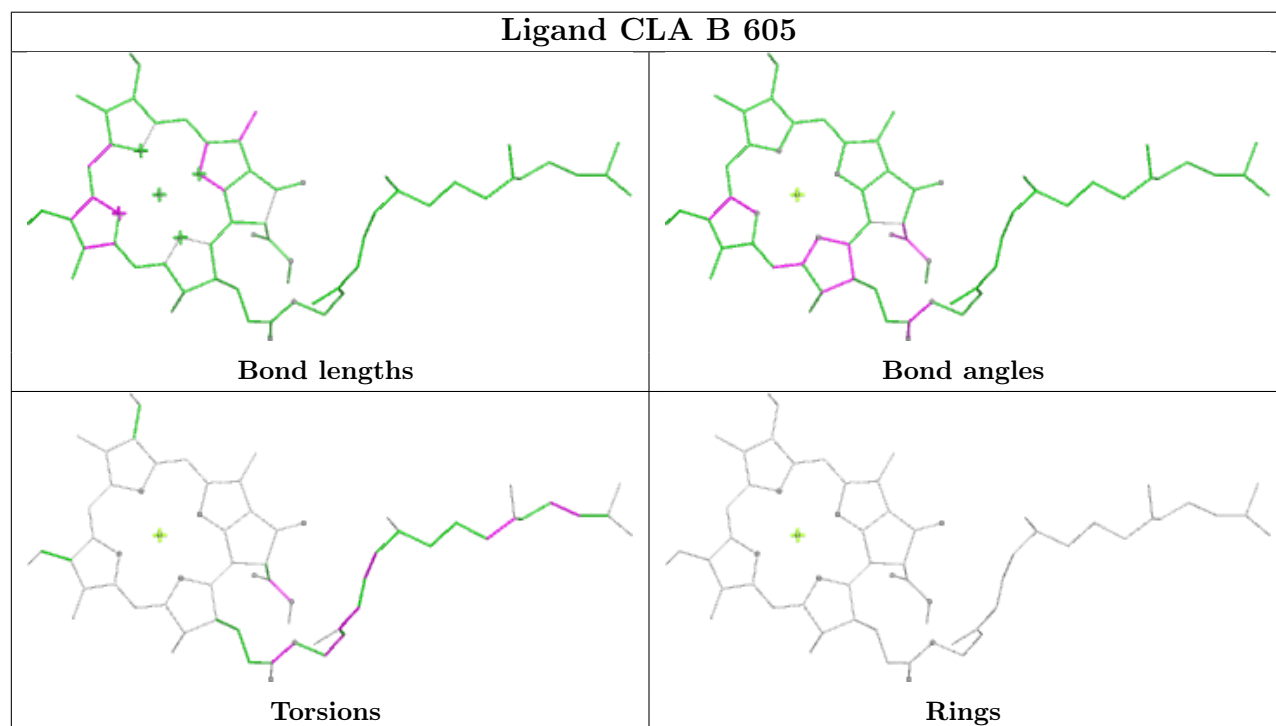
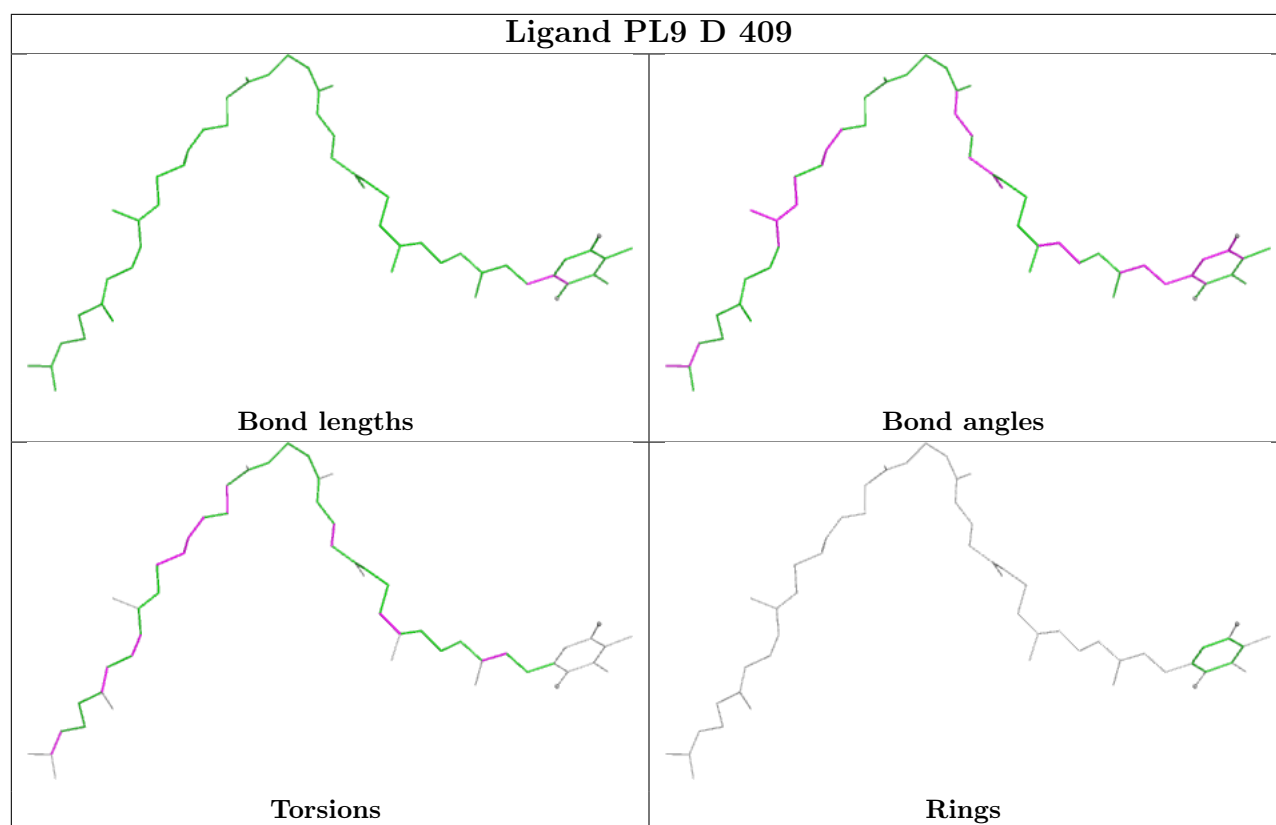


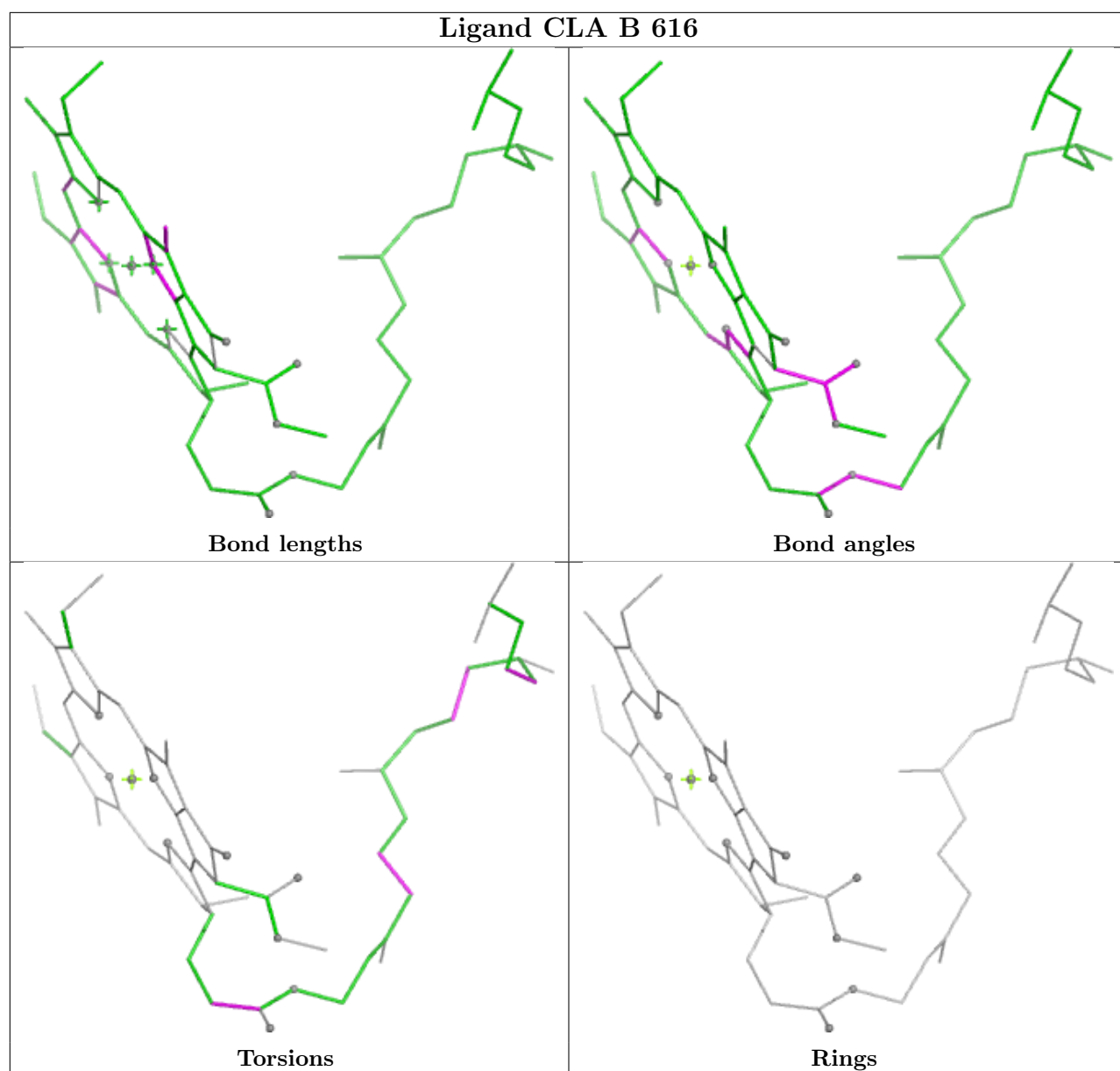
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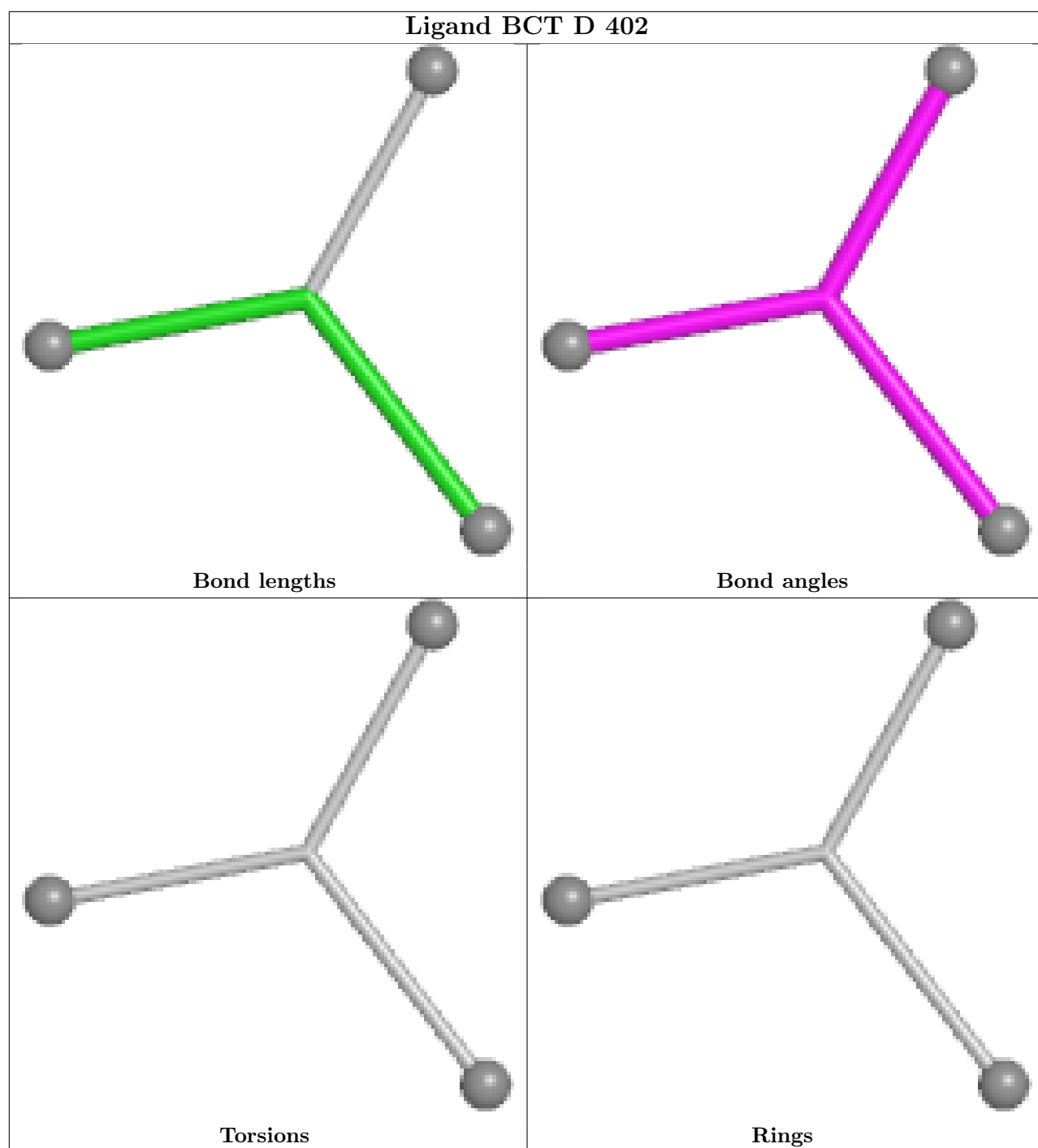


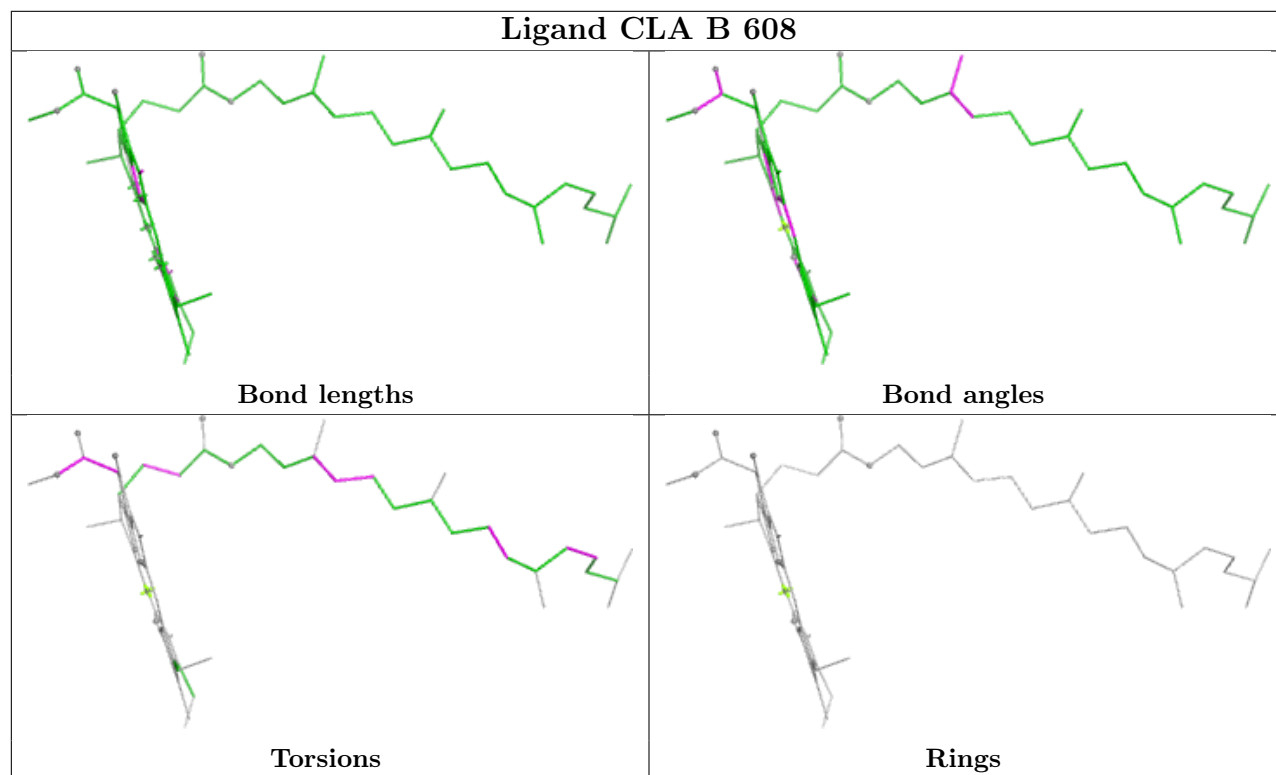
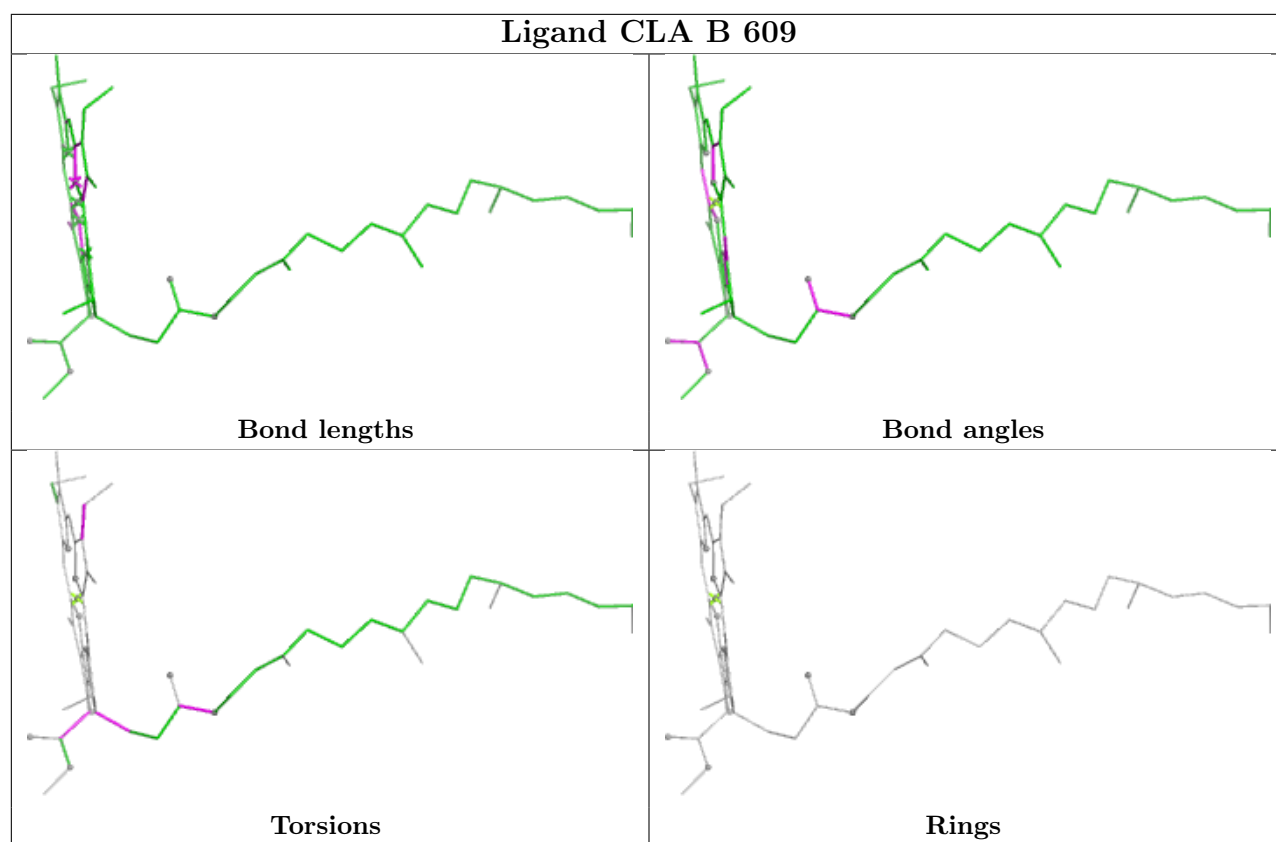
Rings



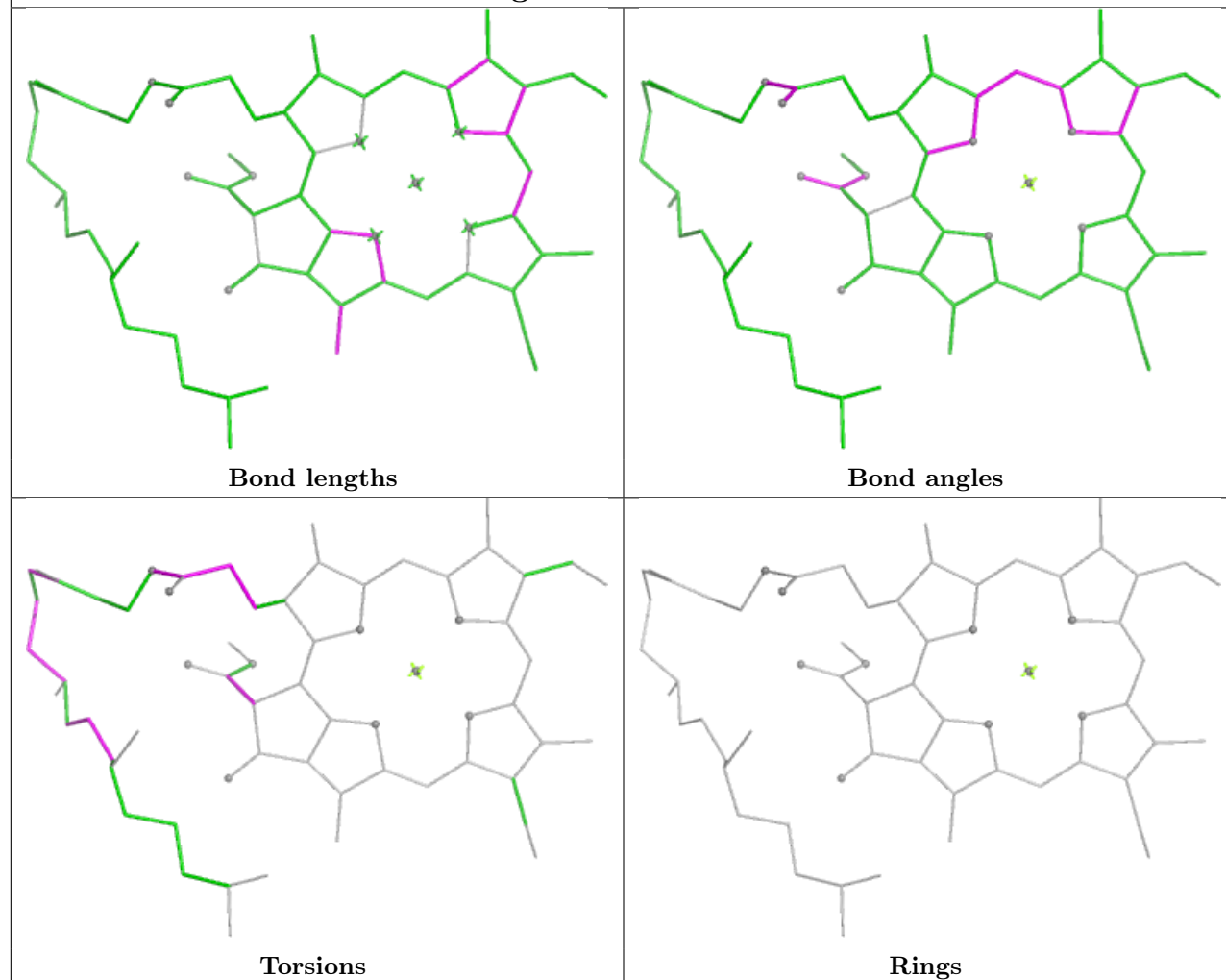




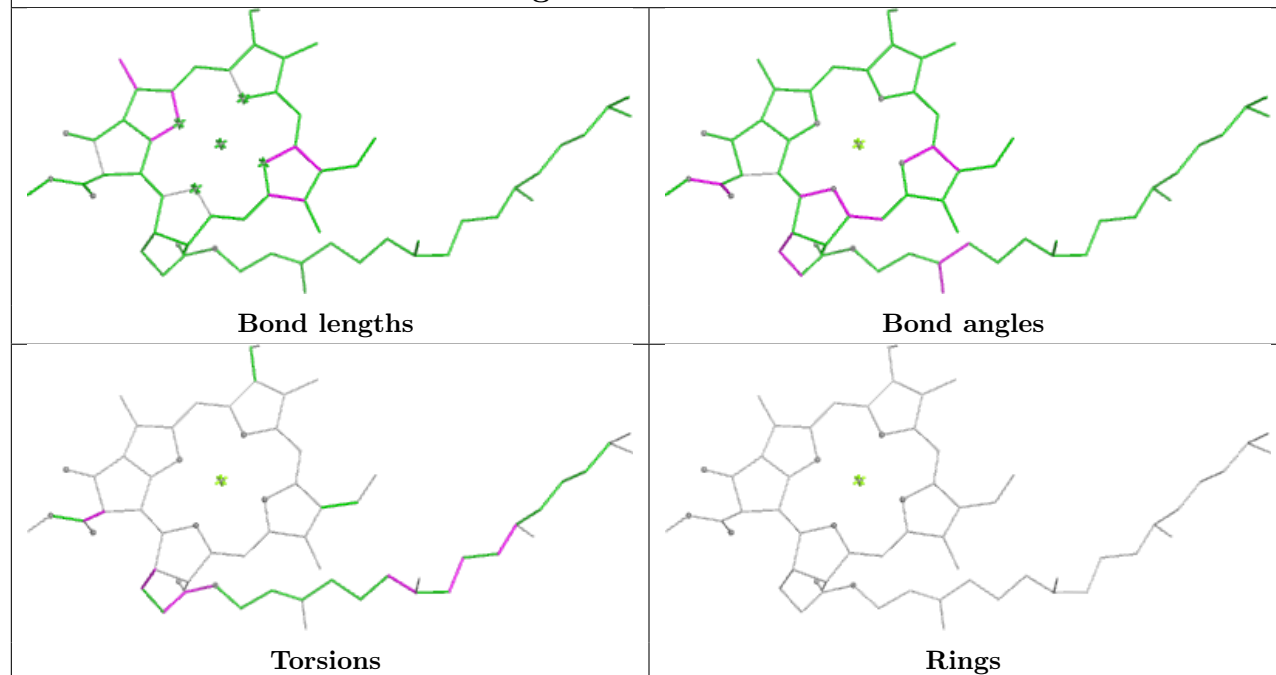


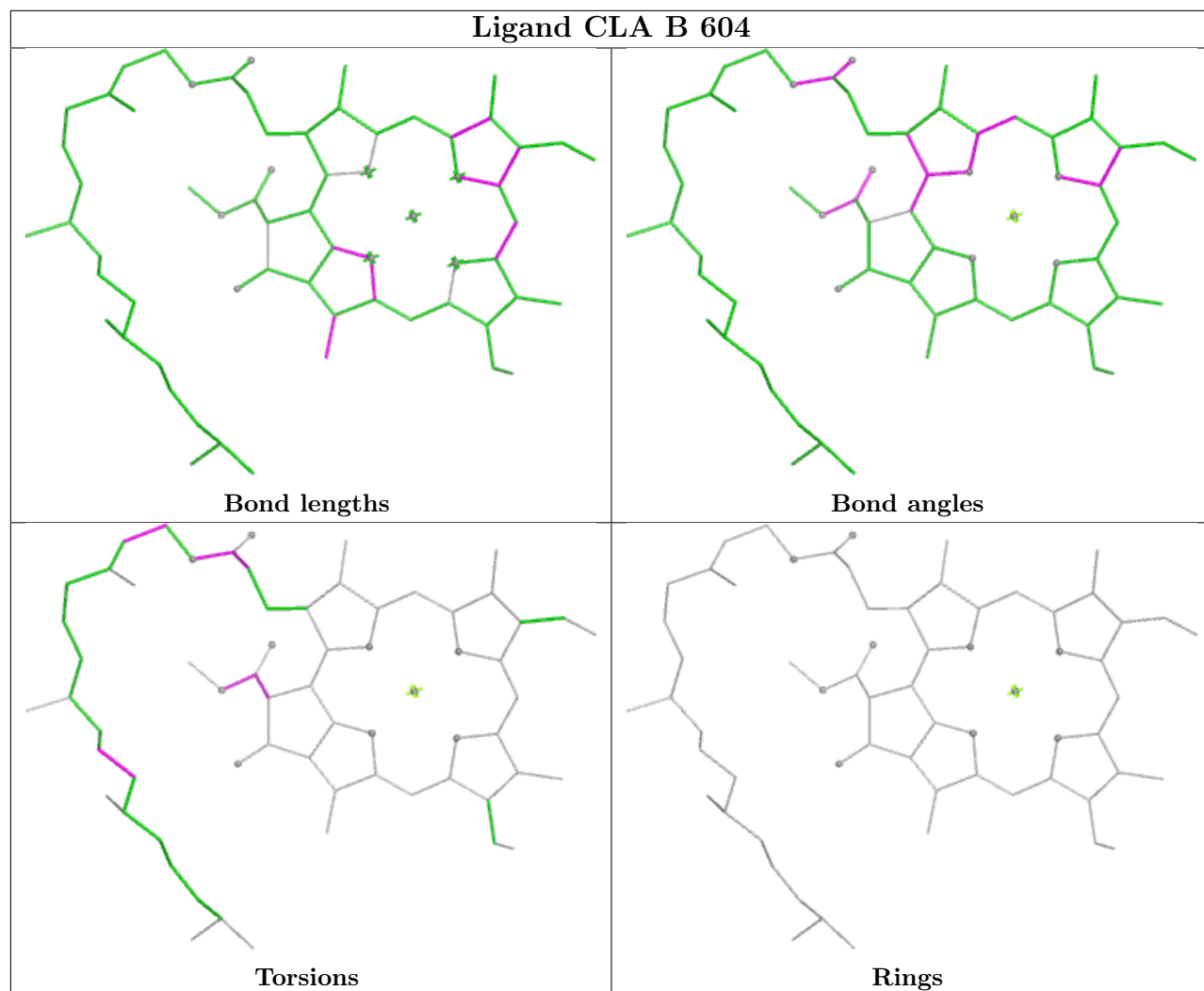


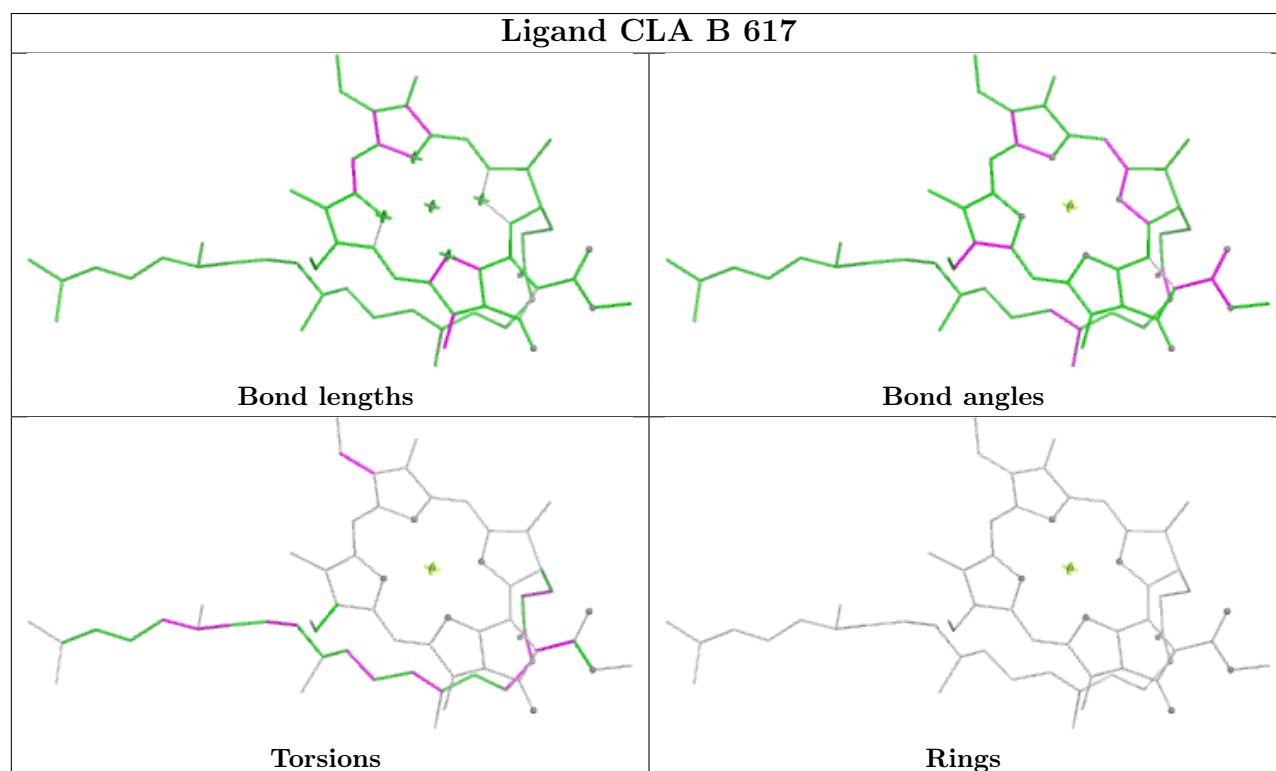
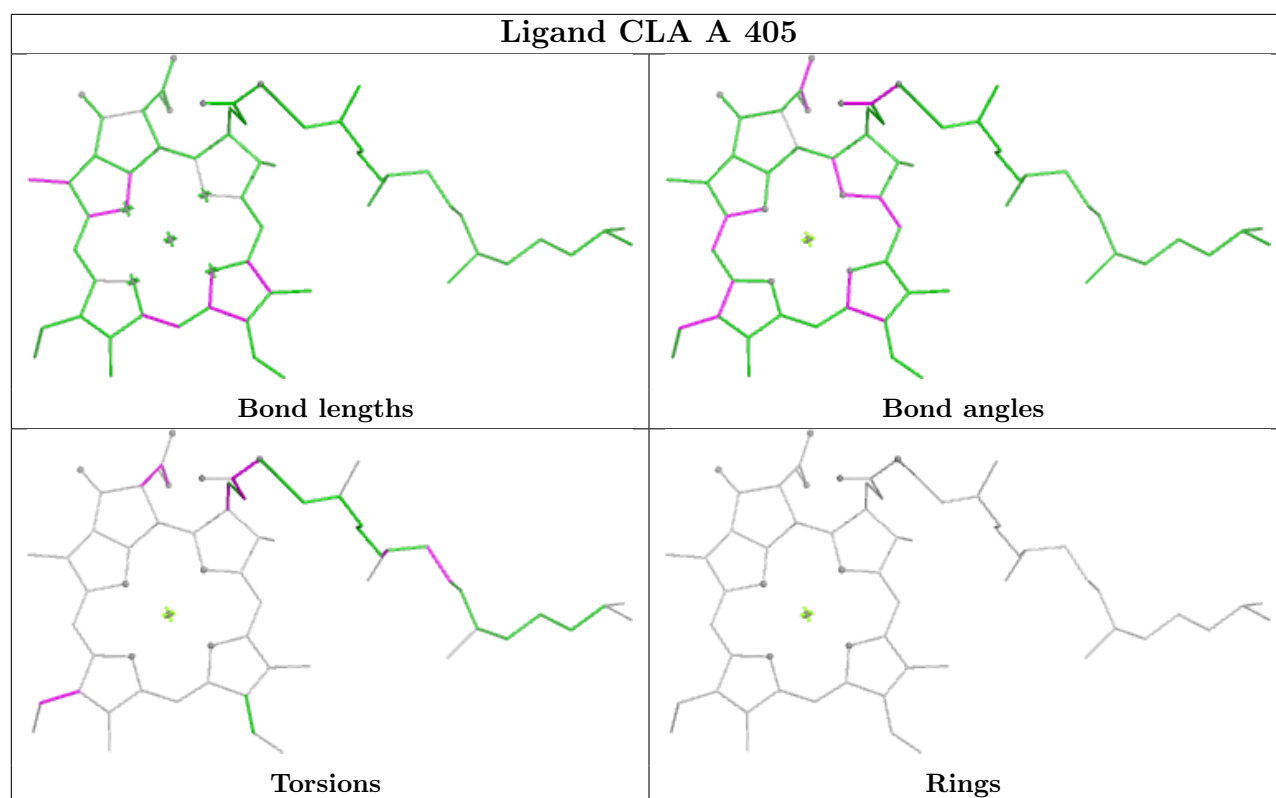
Ligand CLA B 613

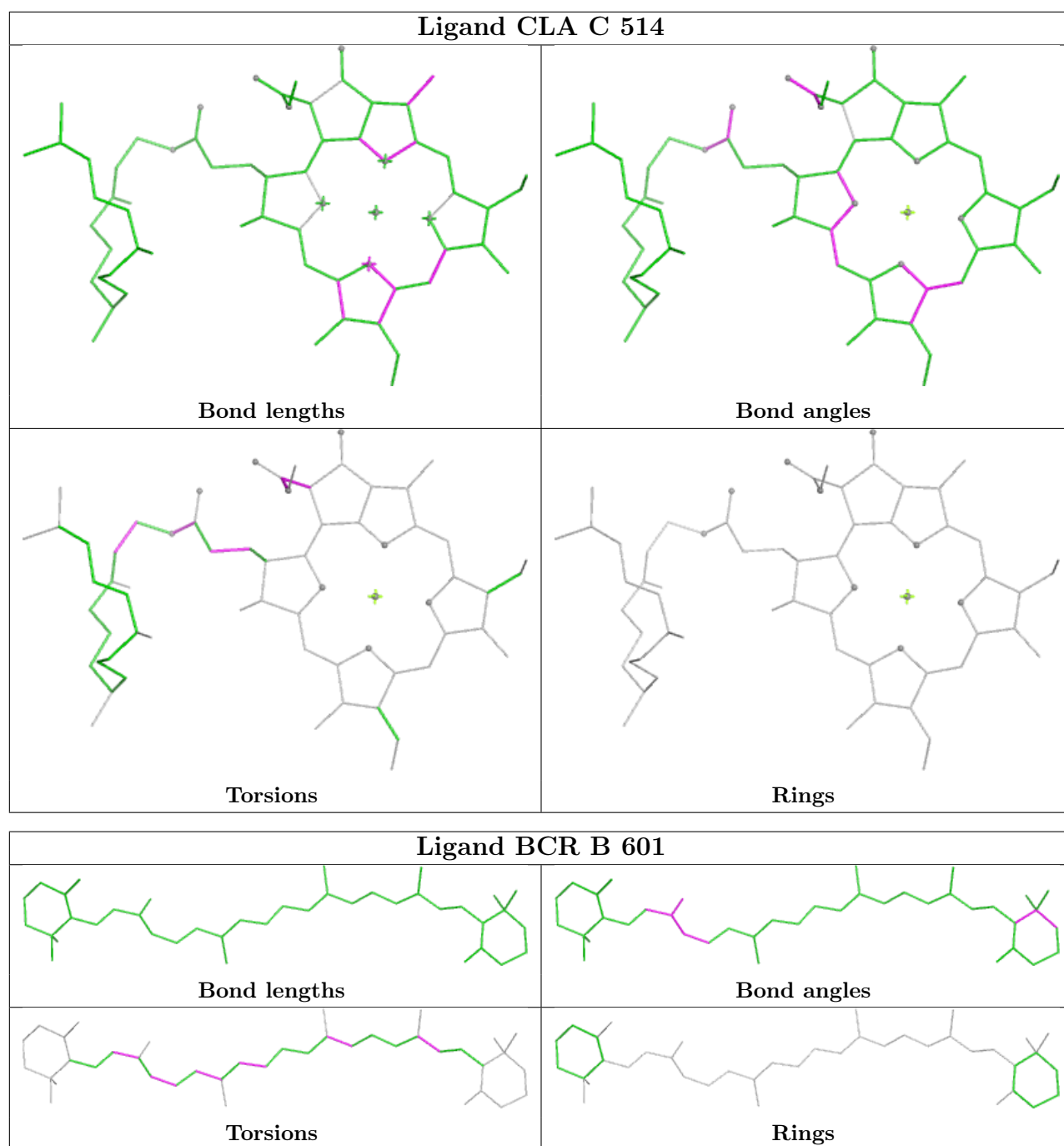


Ligand CLA C 504

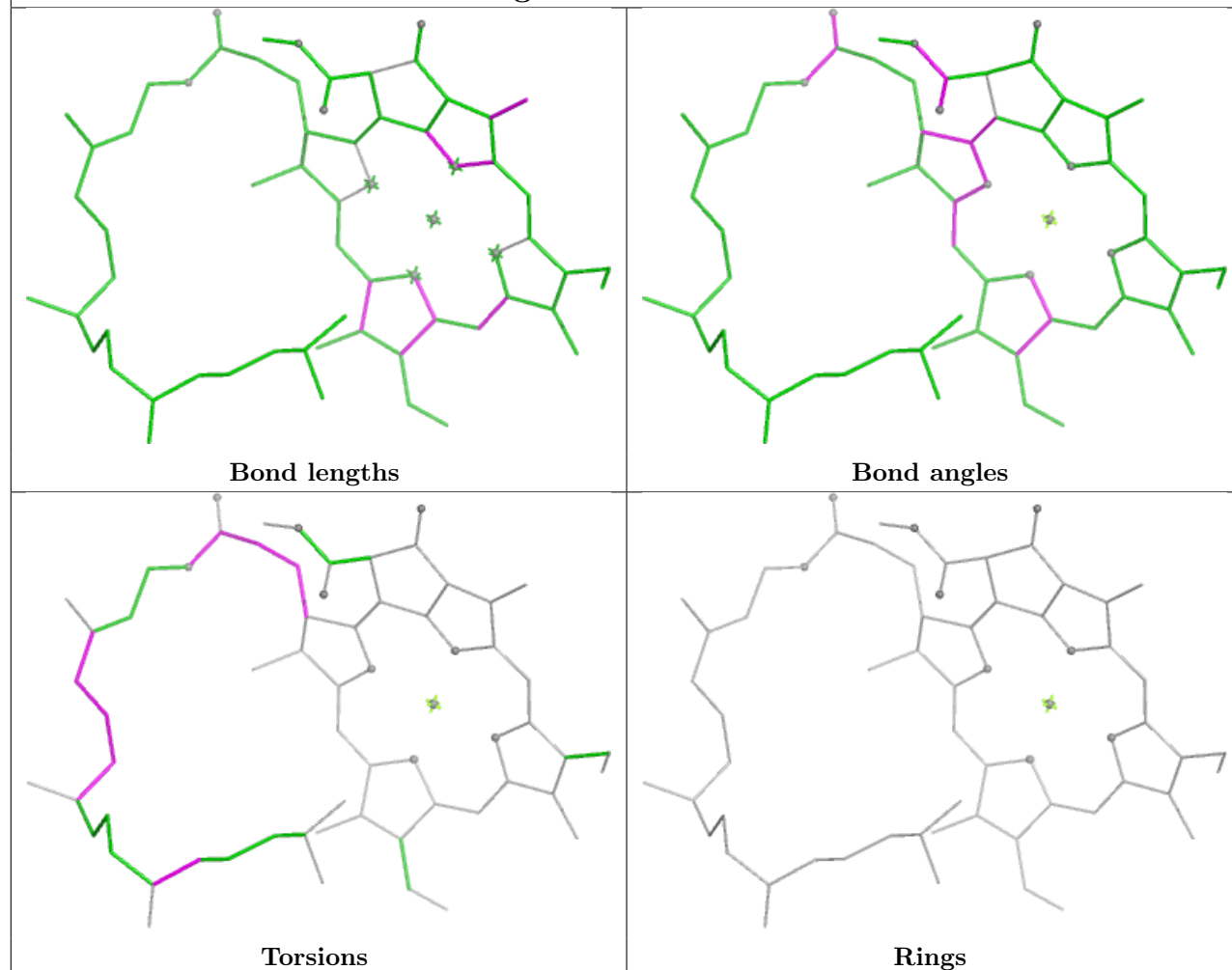




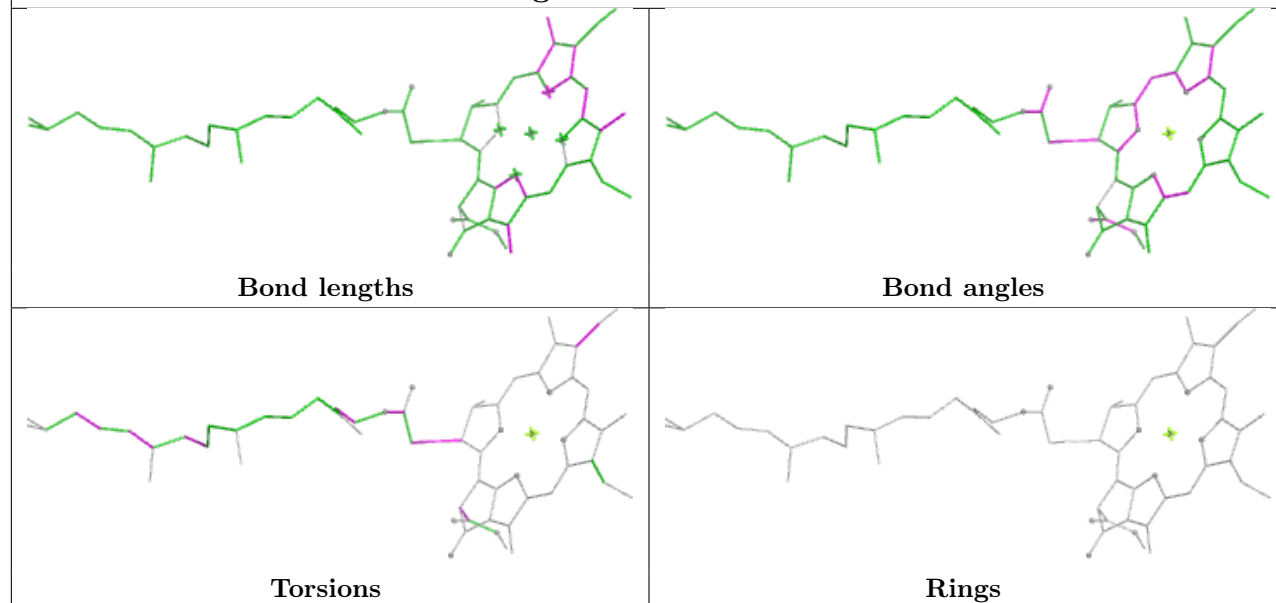


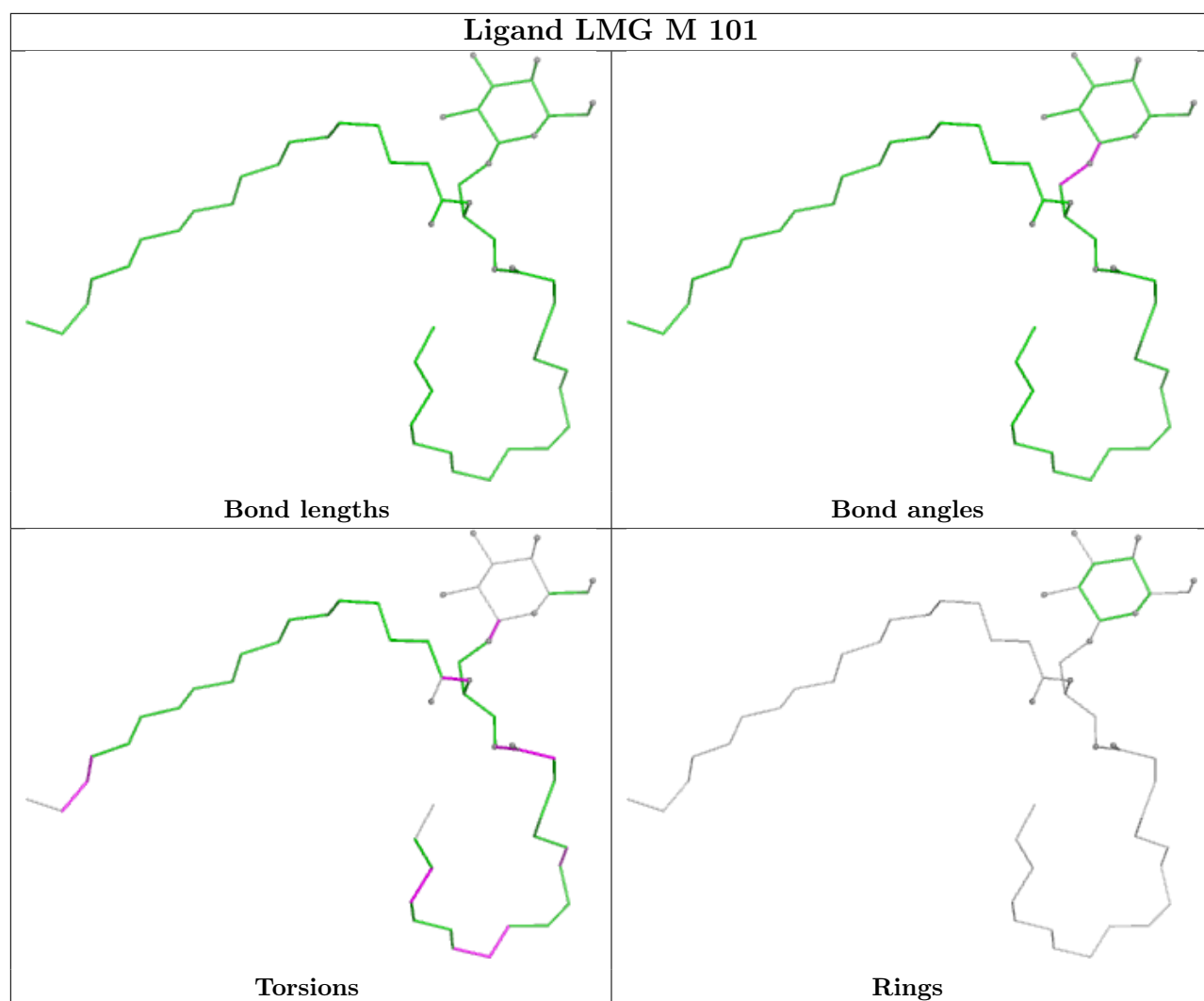


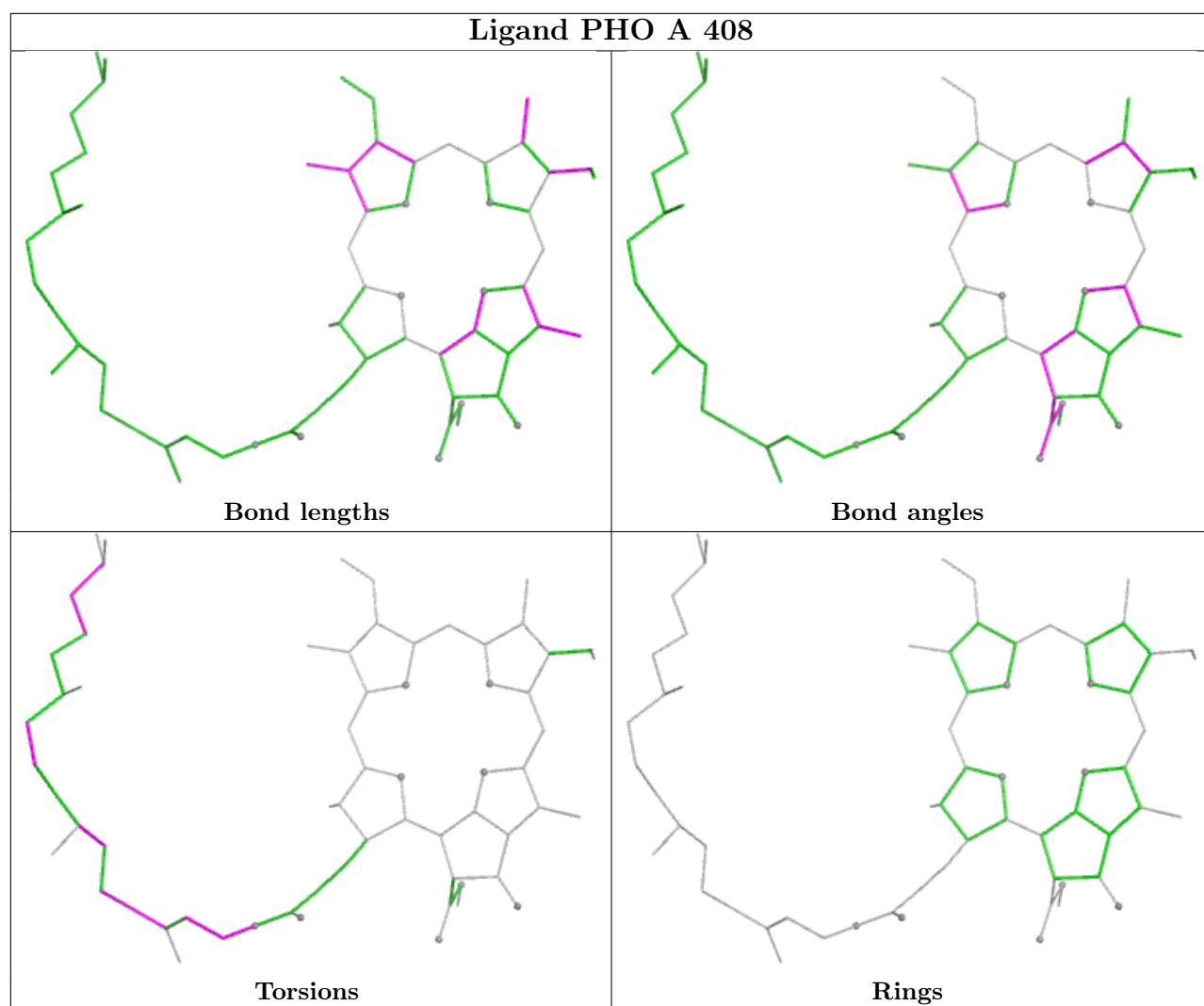
Ligand CLA B 618

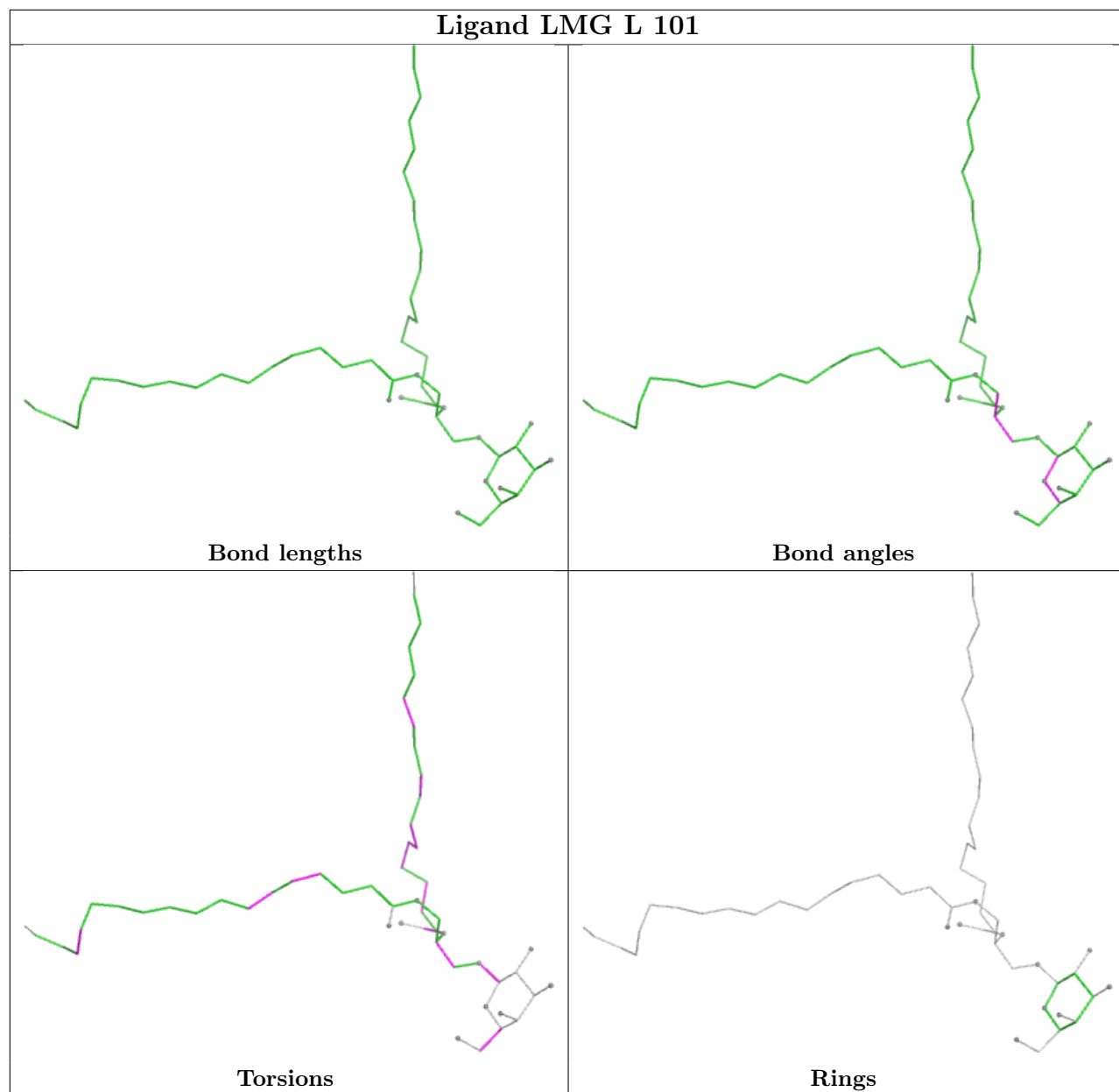


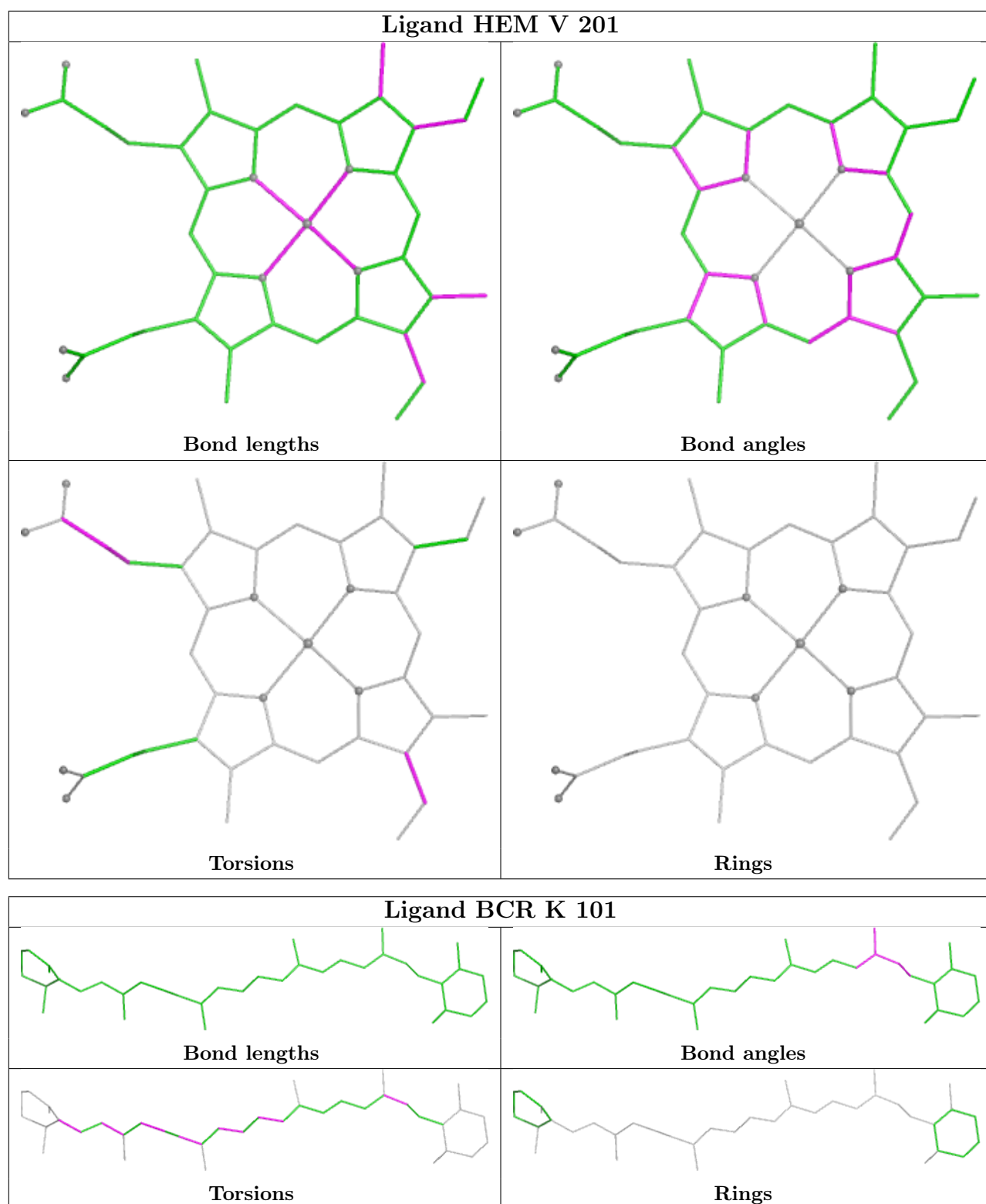
Ligand CLA C 505

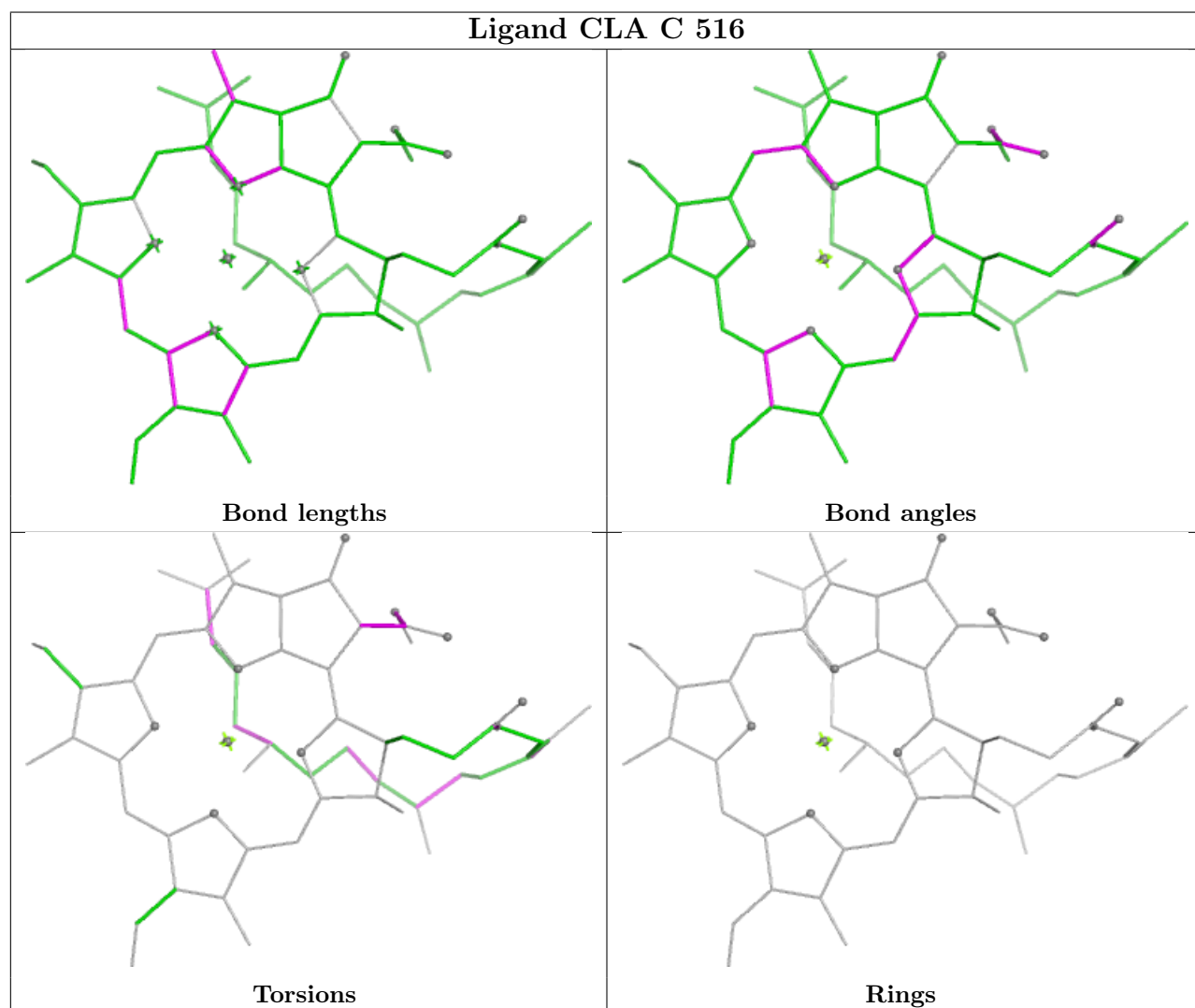
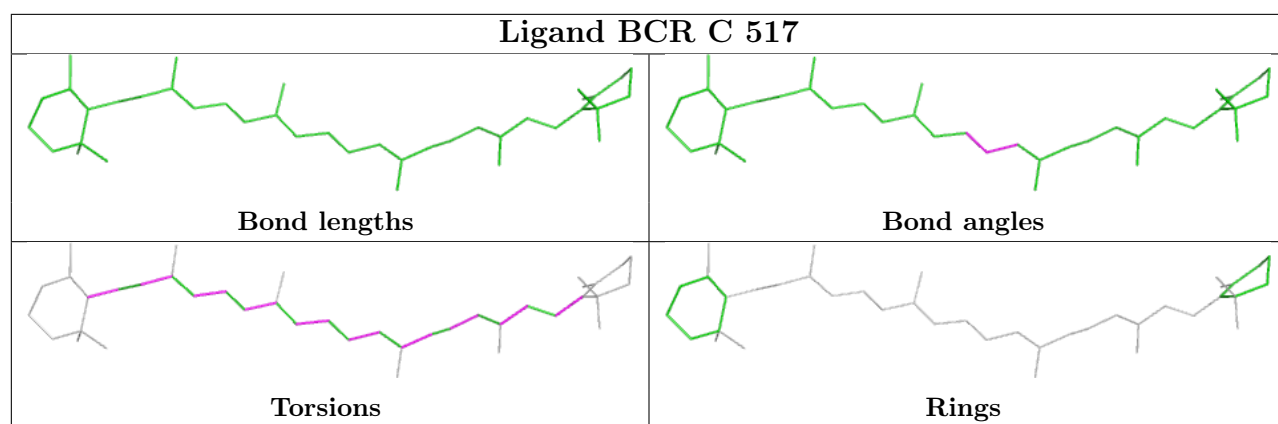


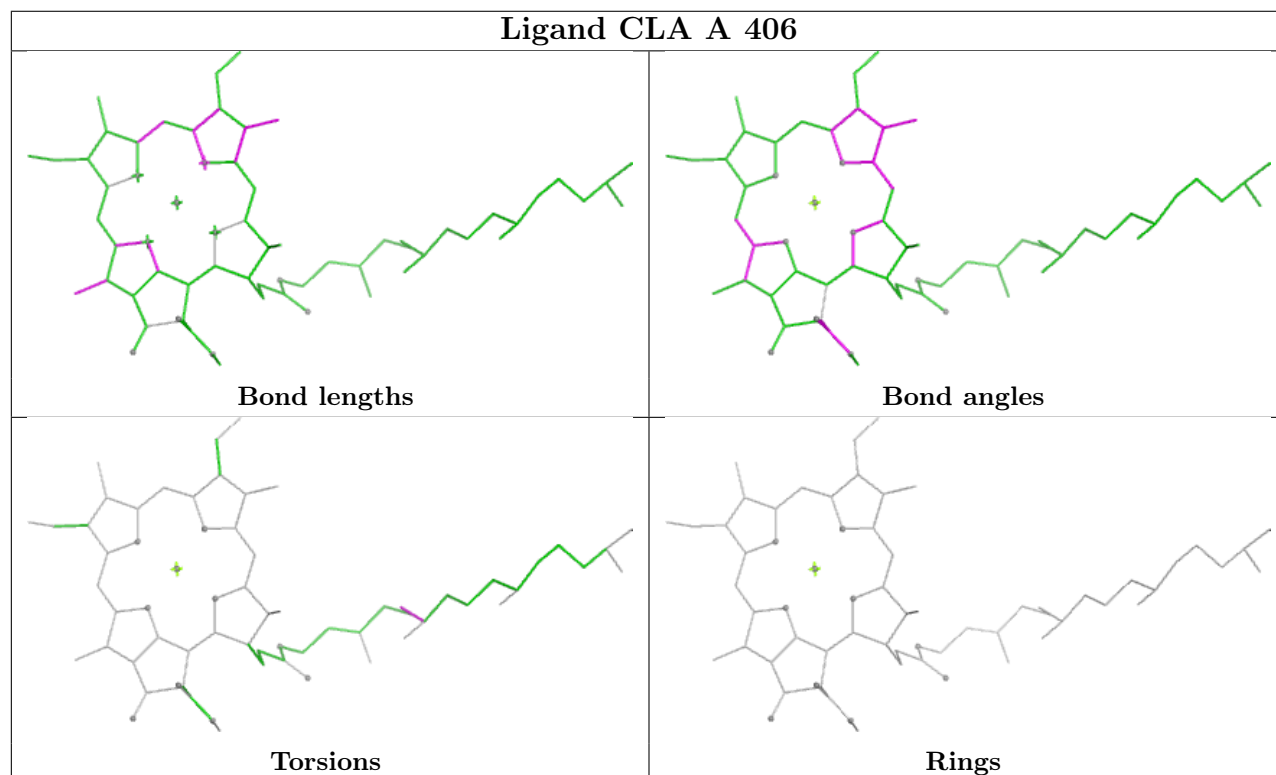
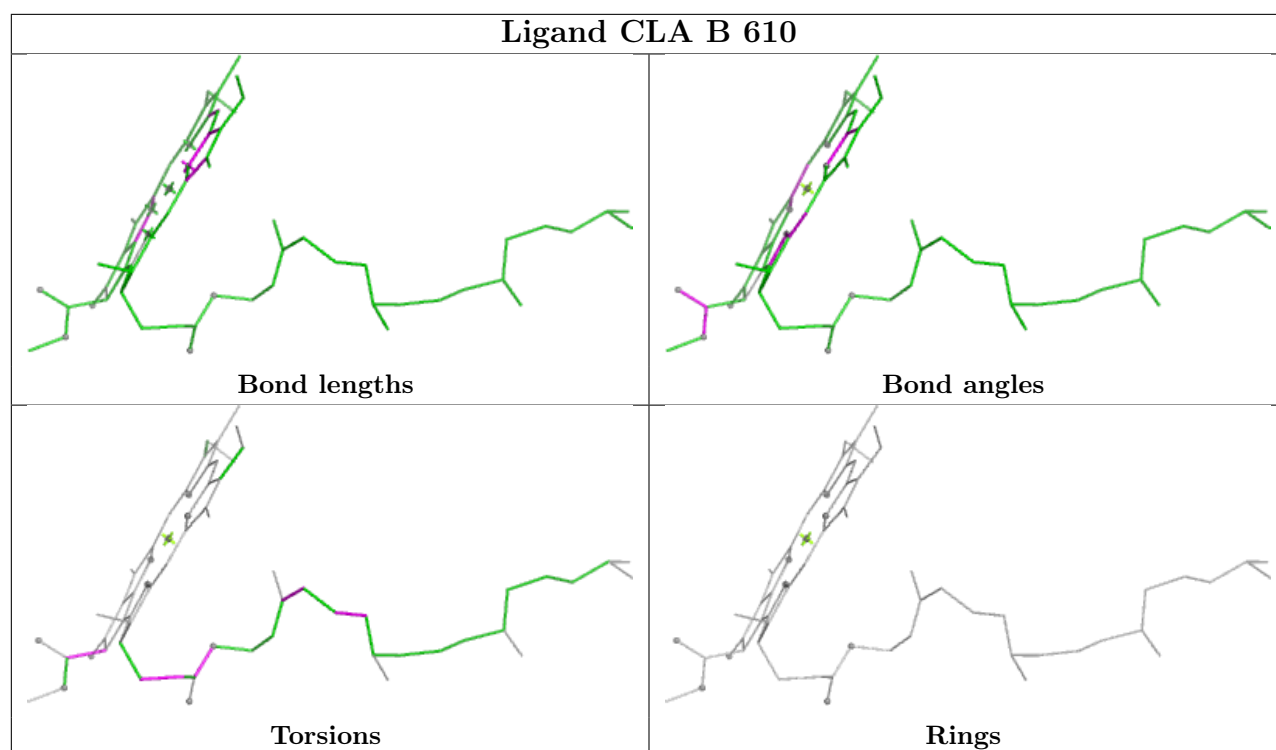


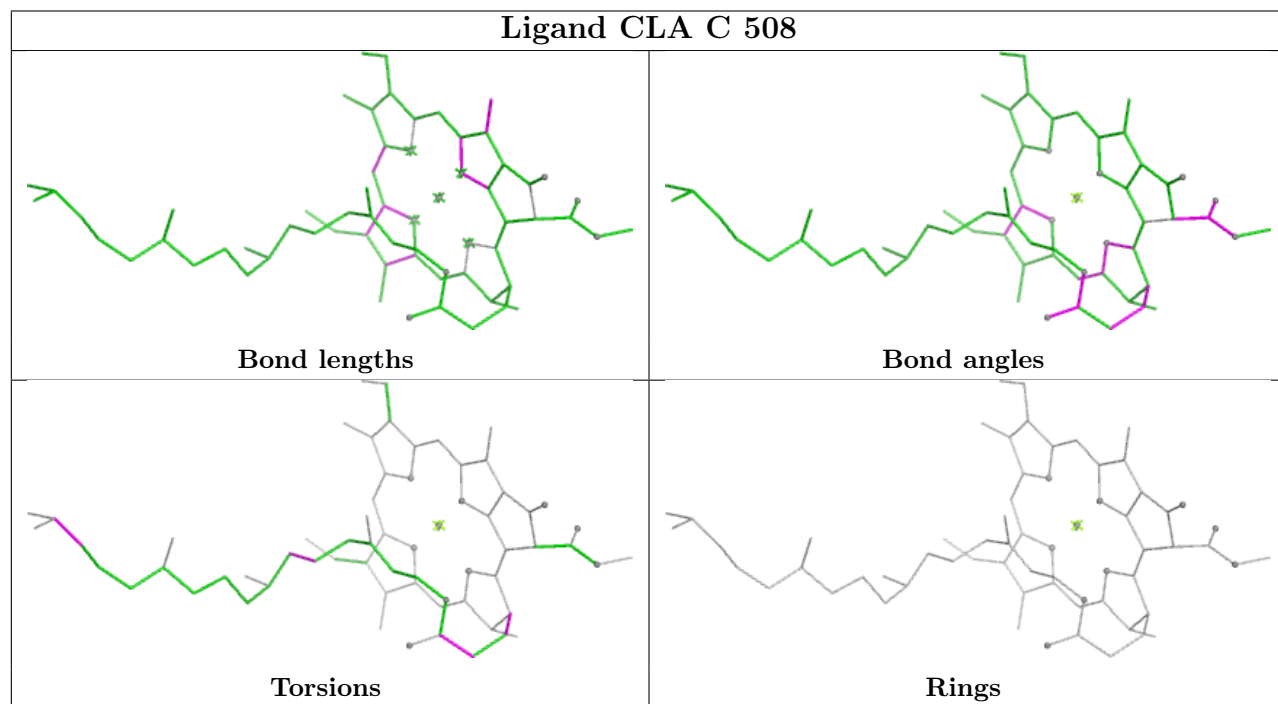
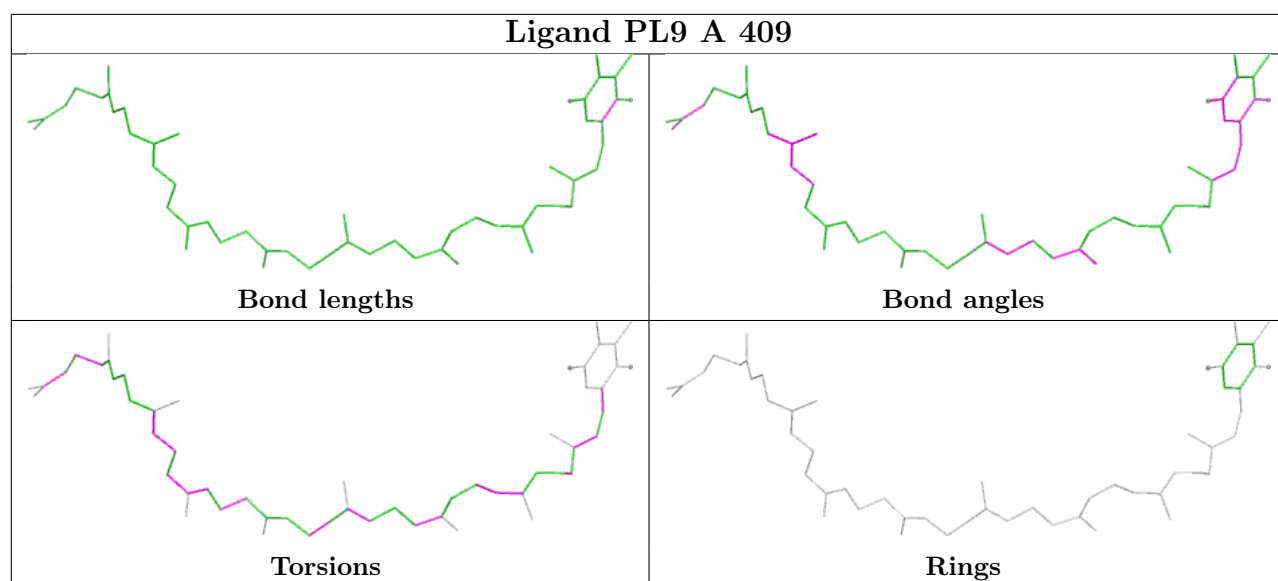


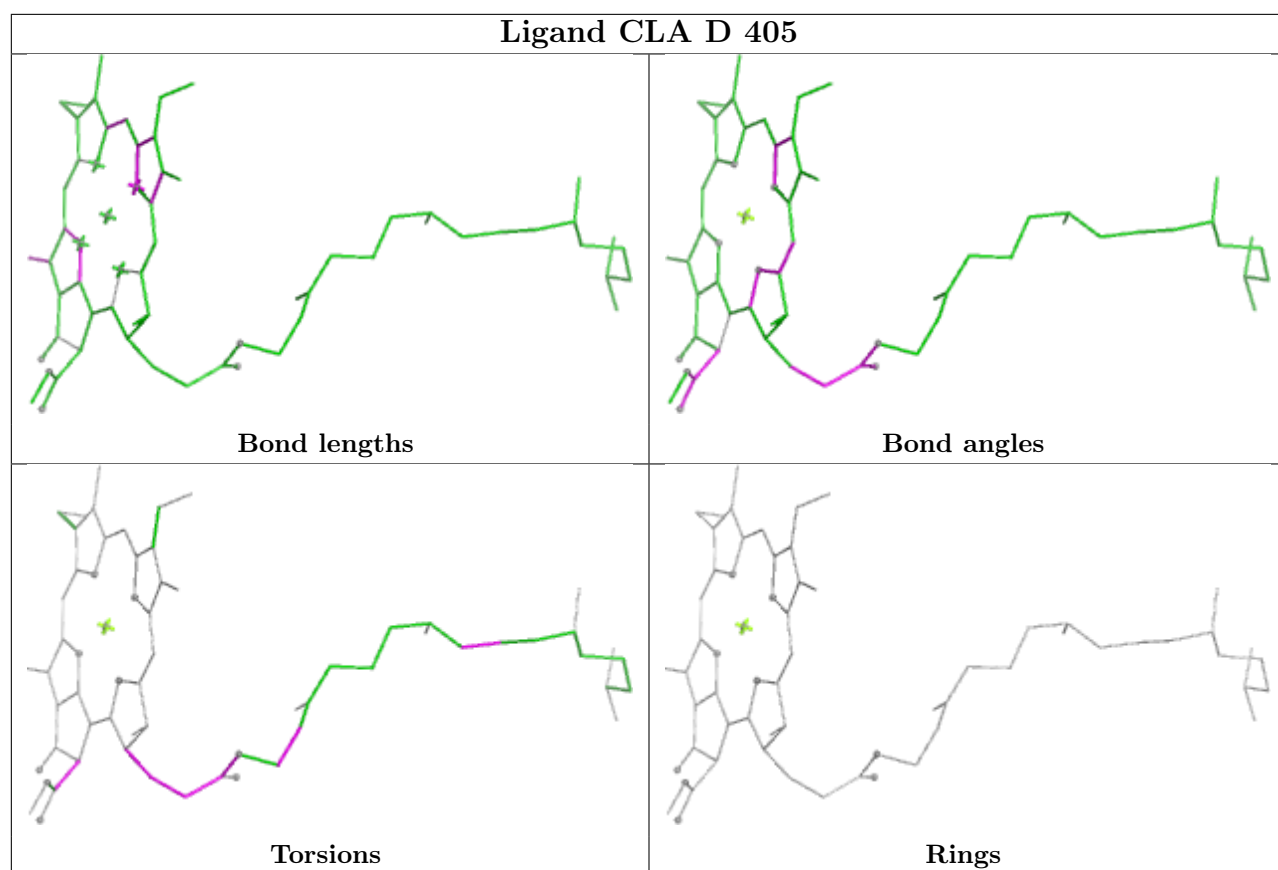


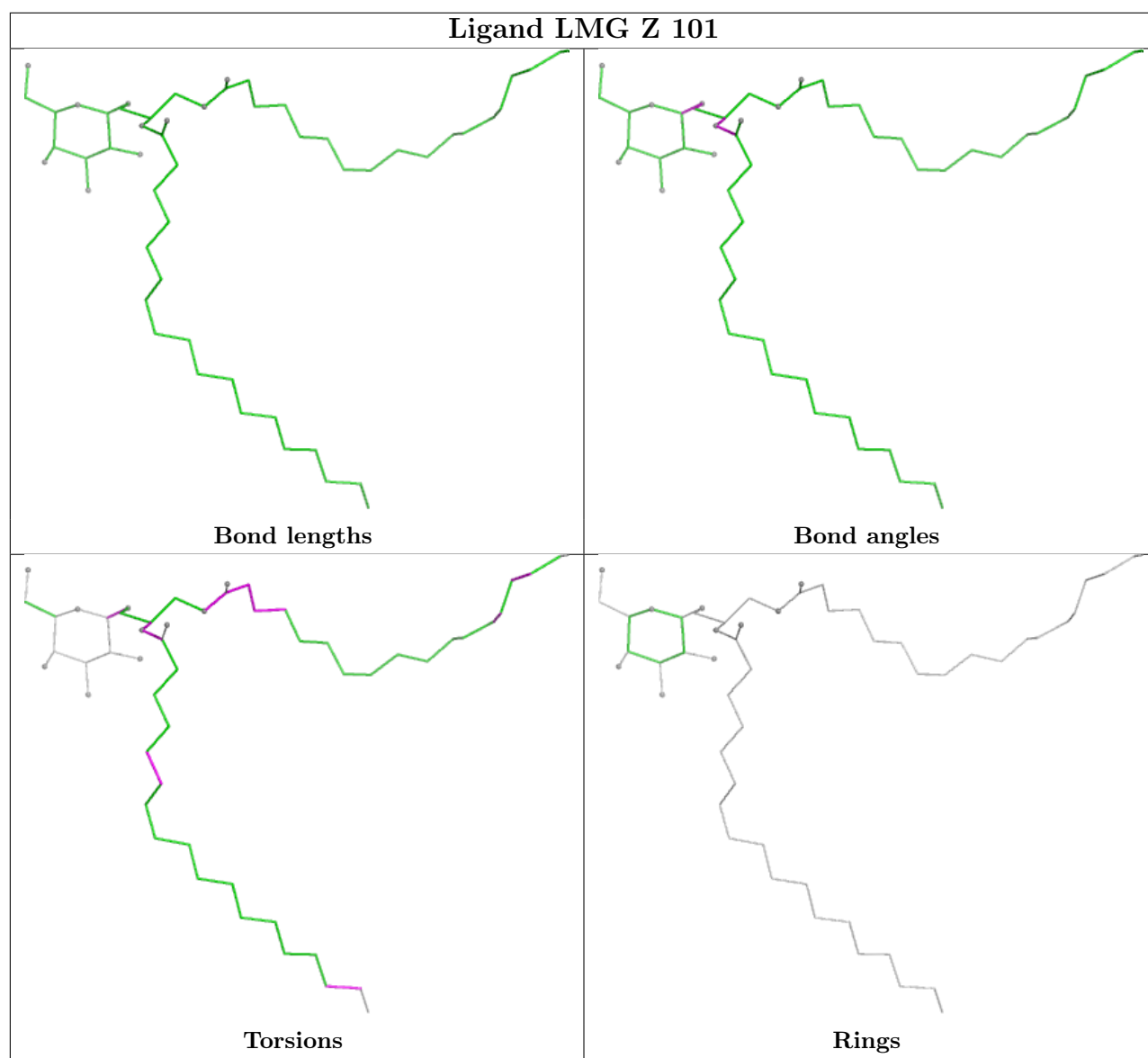


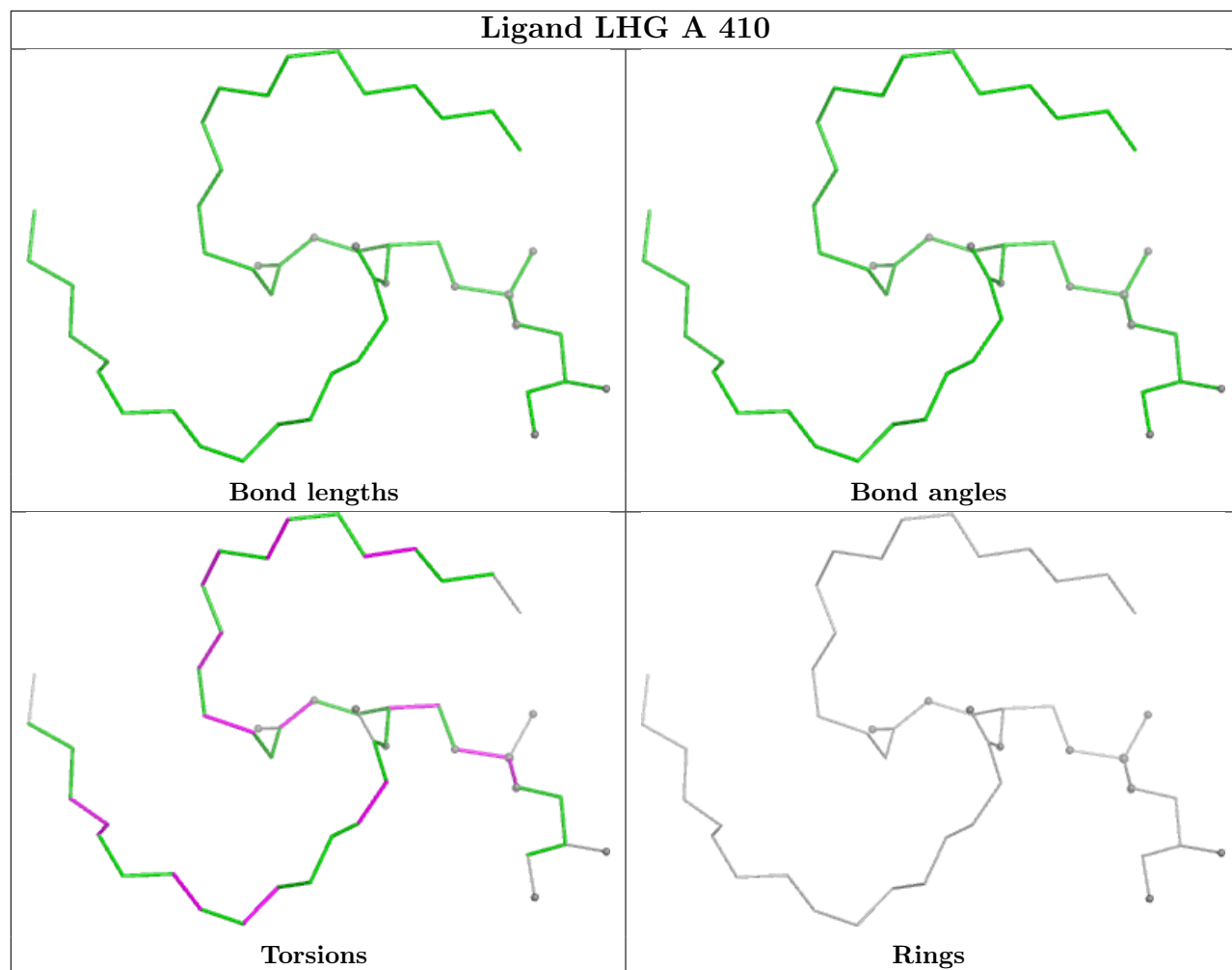


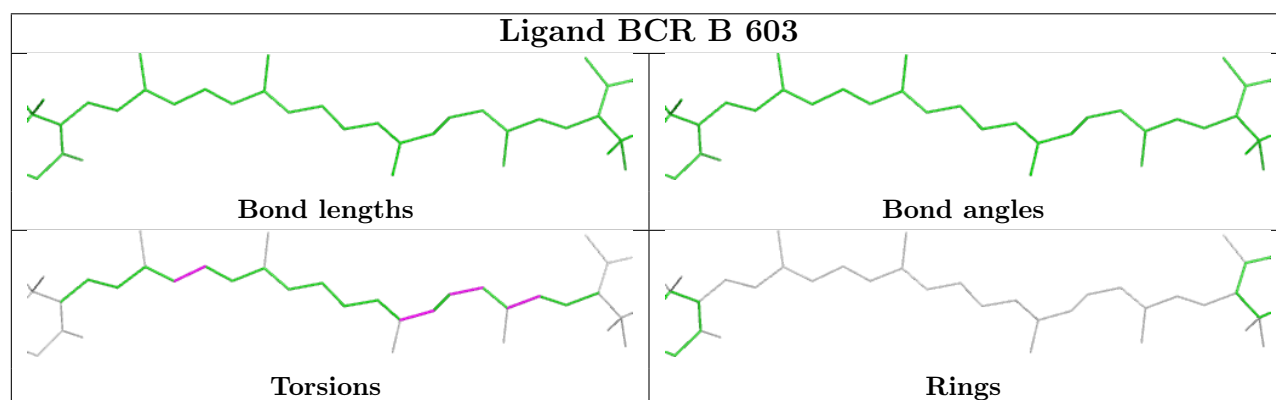
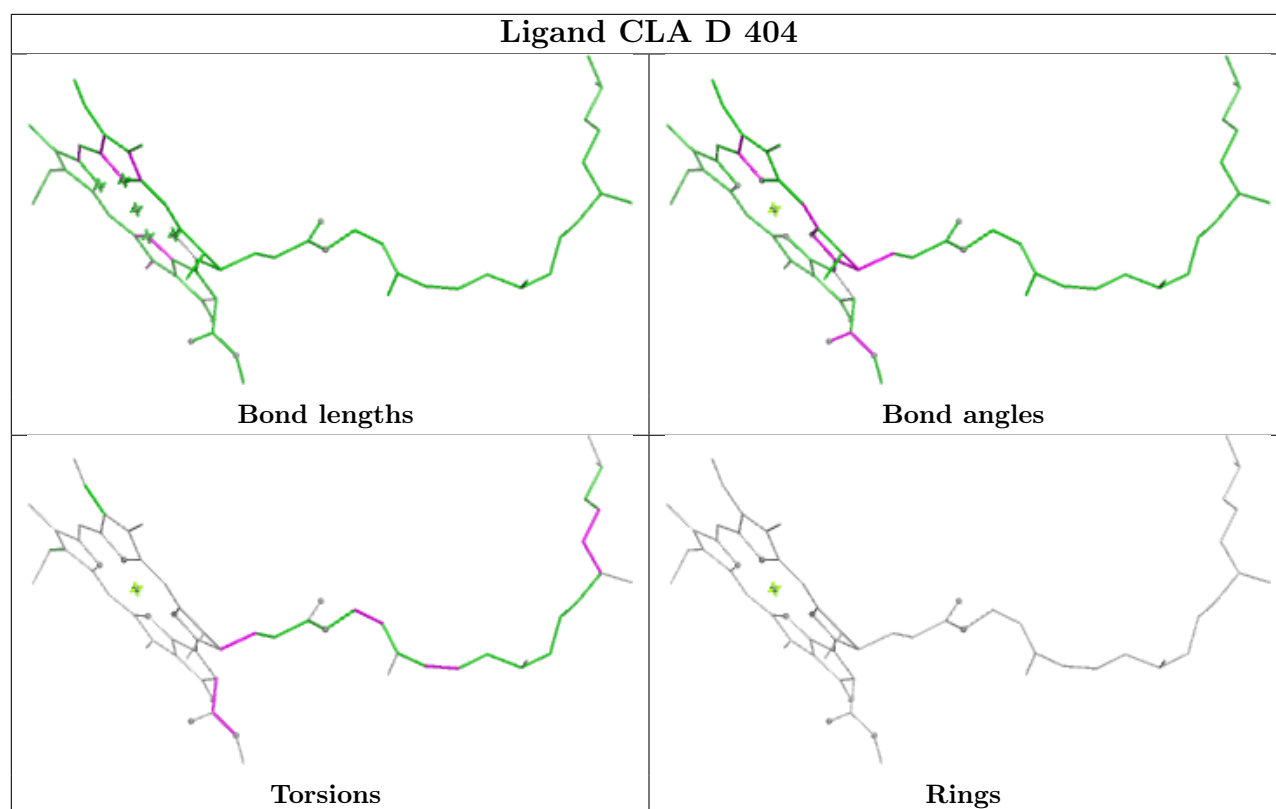


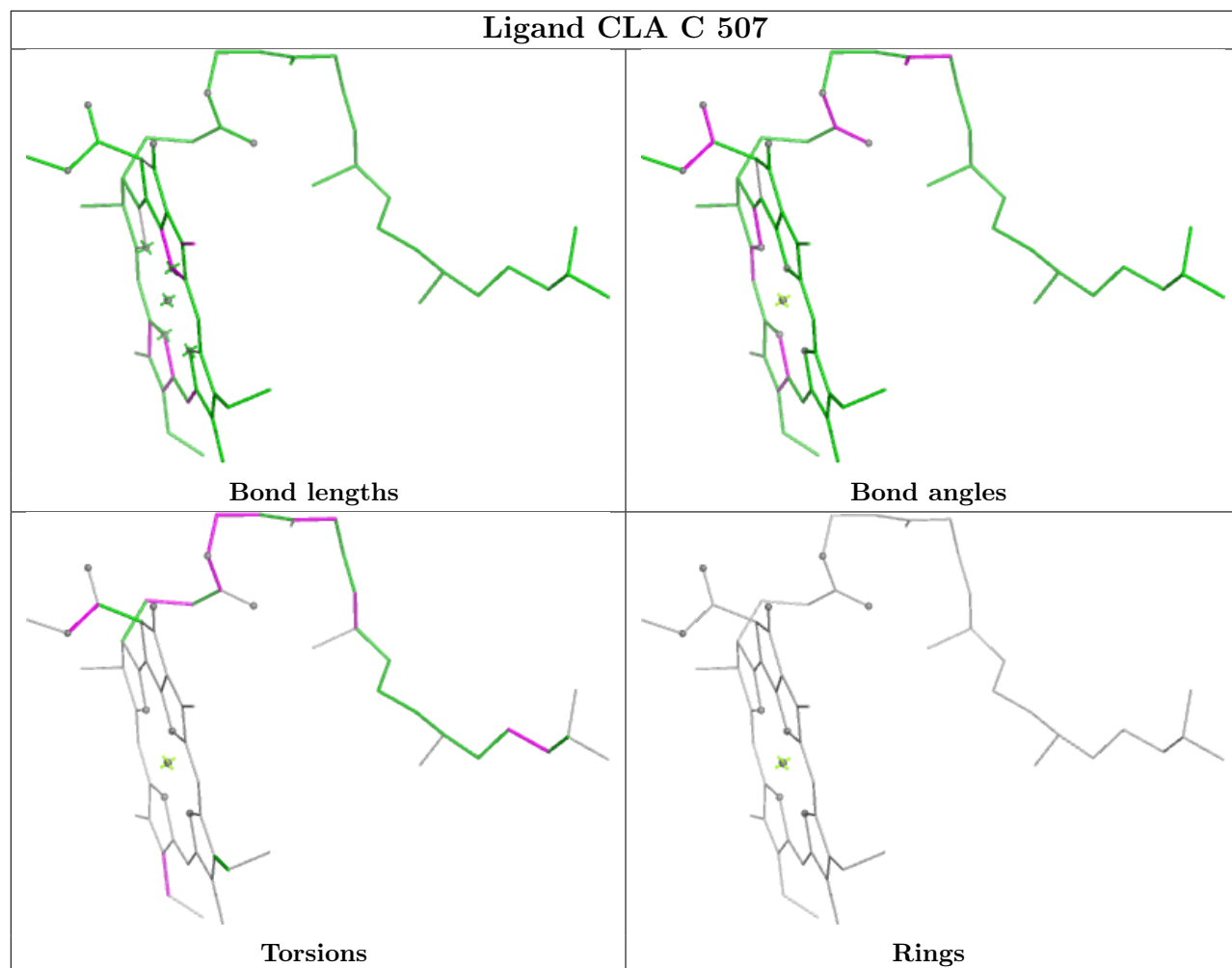


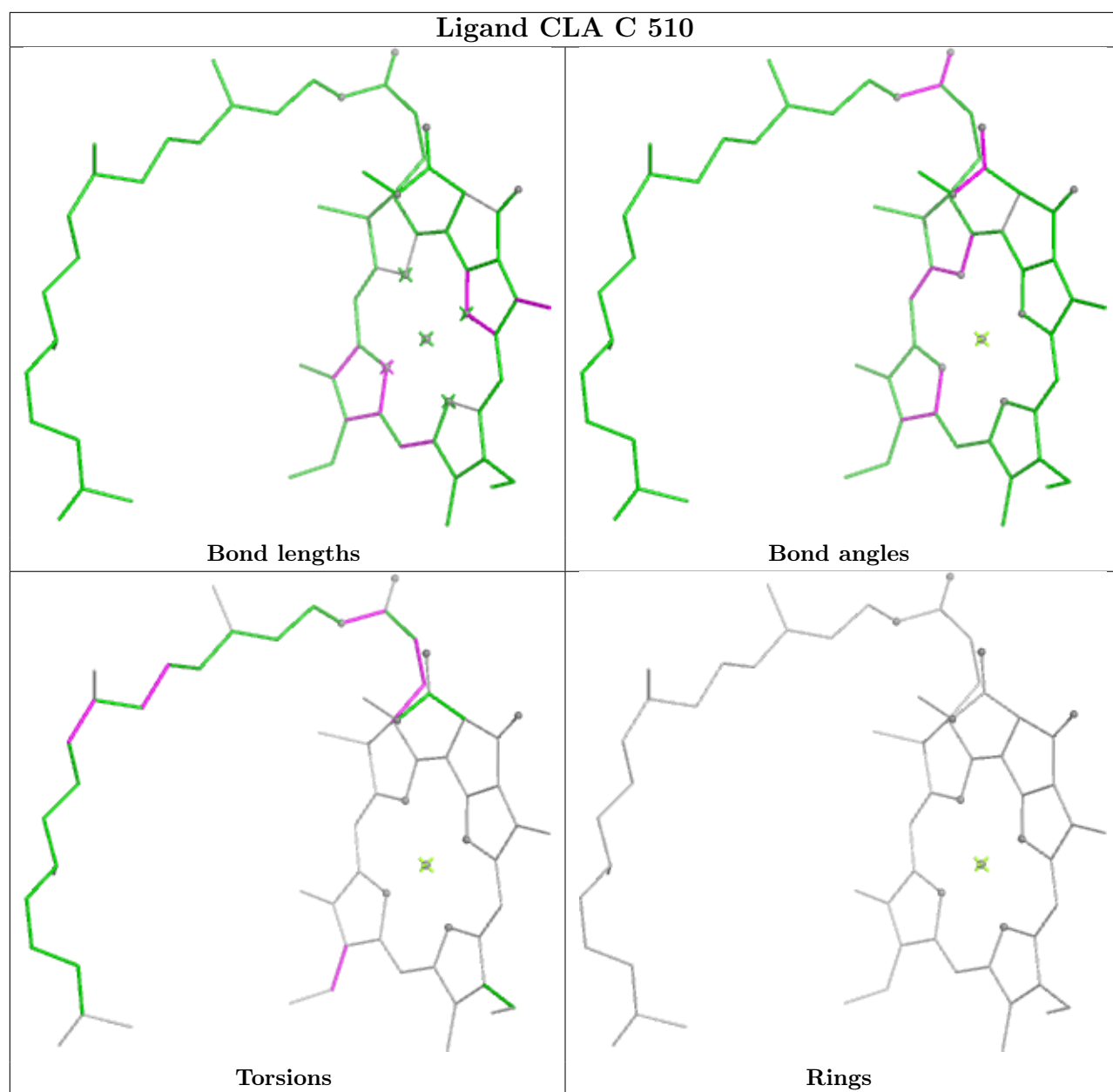


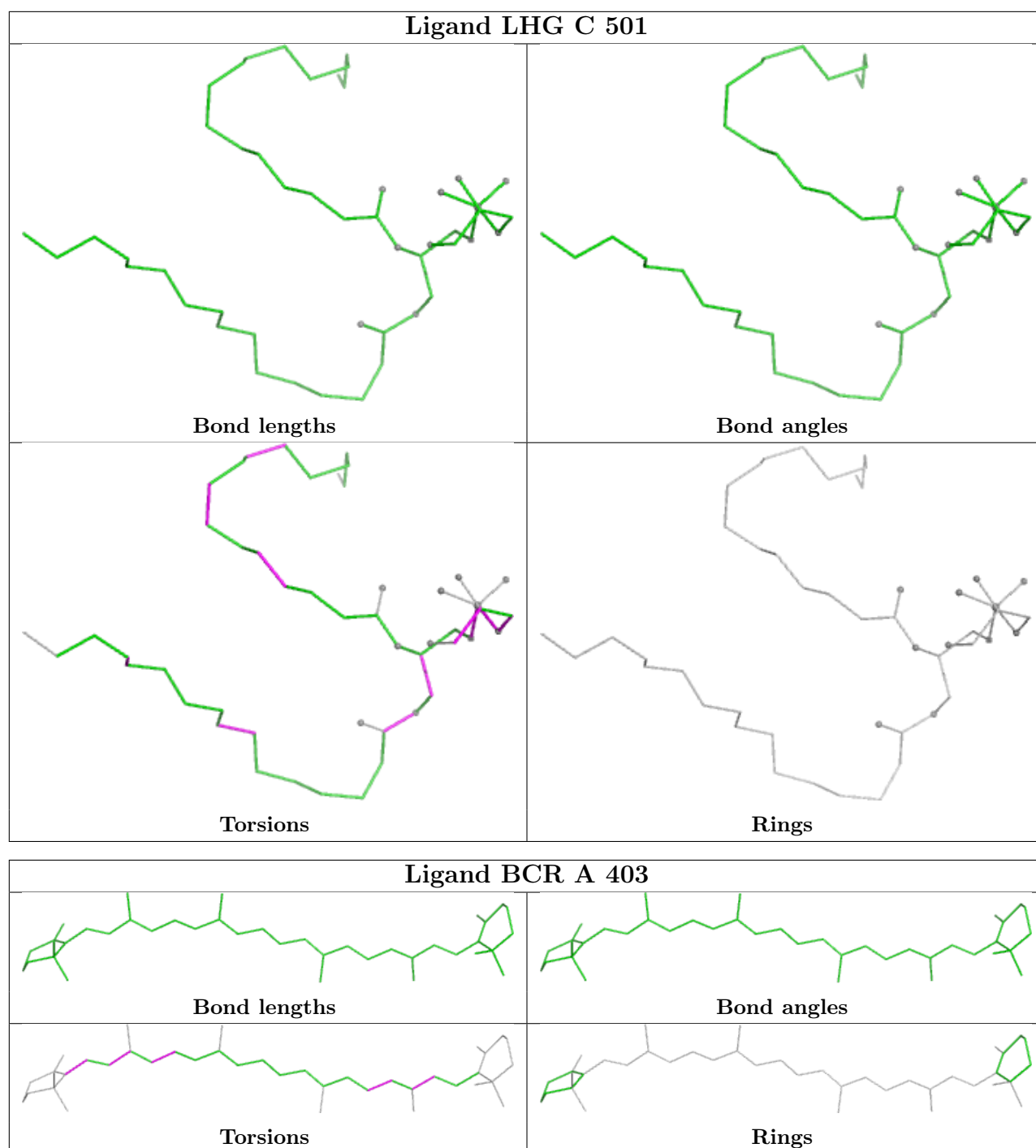


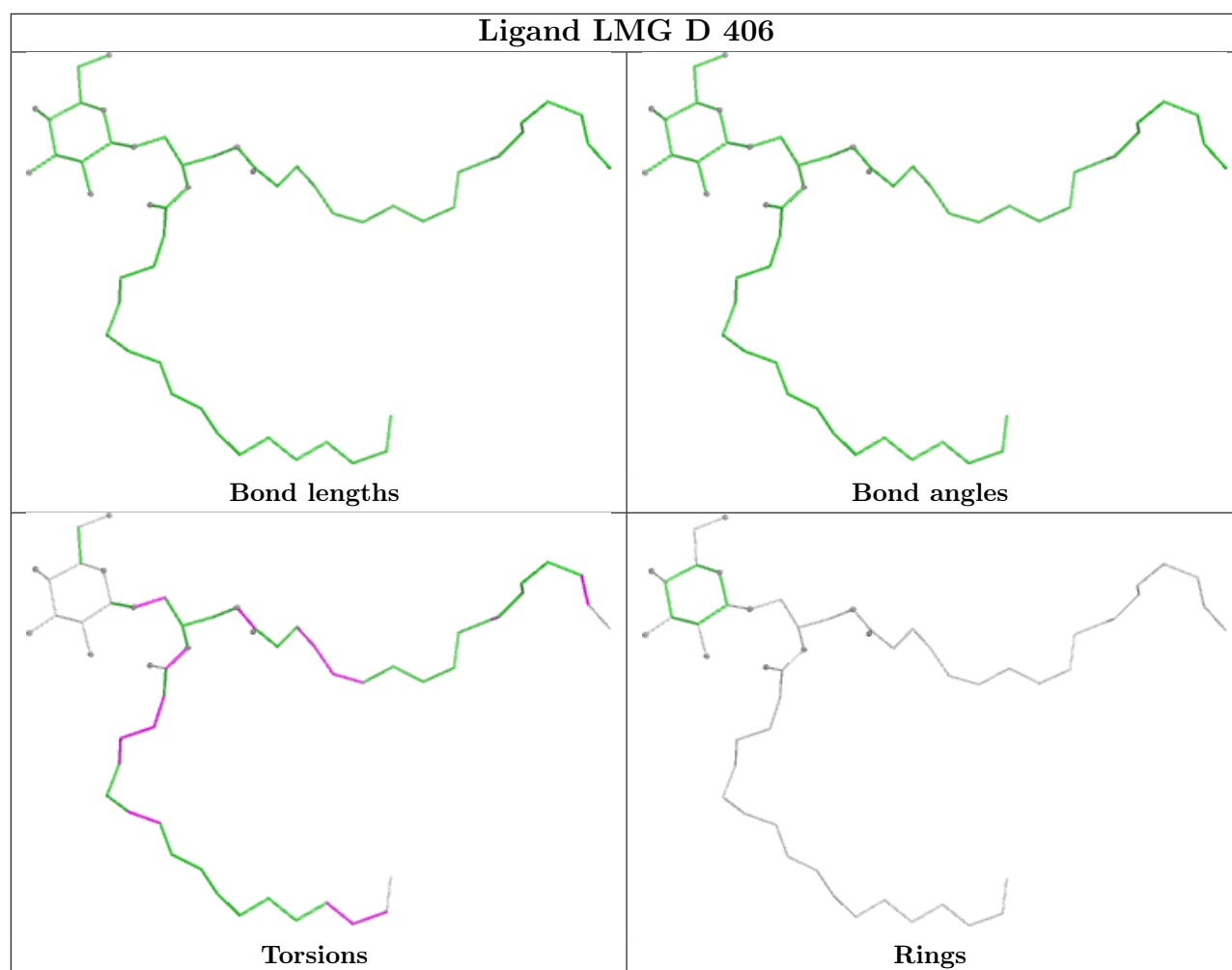












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

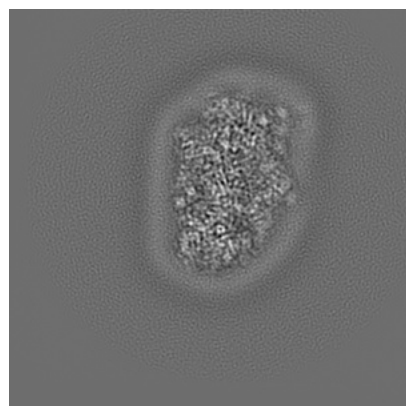
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52706. These allow visual inspection of the internal detail of the map and identification of artifacts.

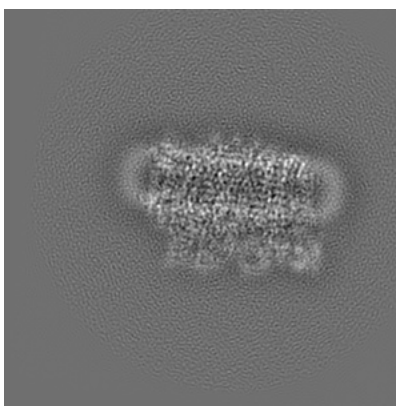
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

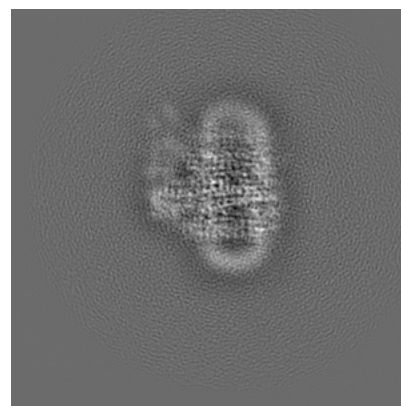
6.1.1 Primary map



X

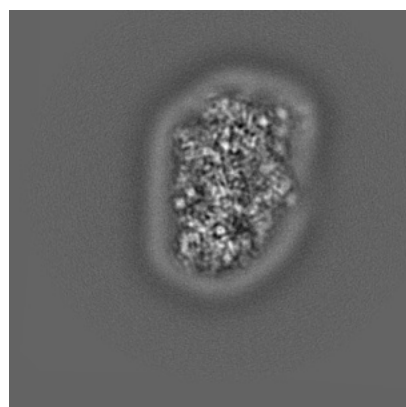


Y

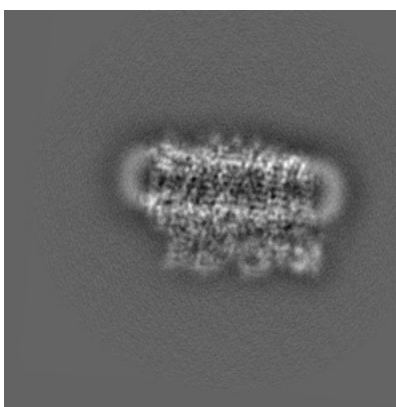


Z

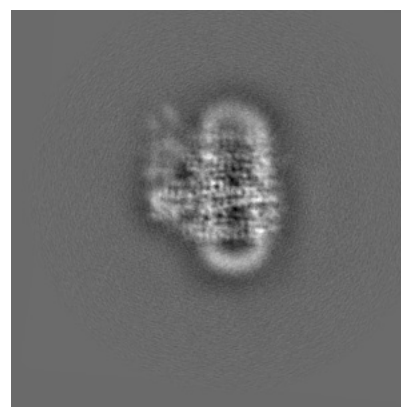
6.1.2 Raw map



X



Y

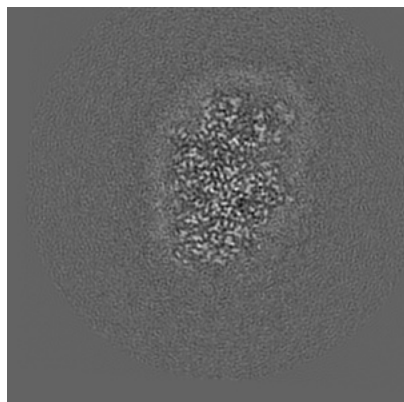


Z

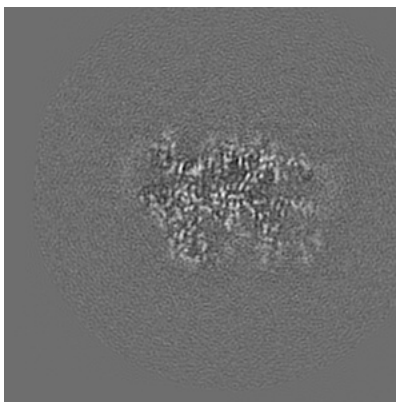
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

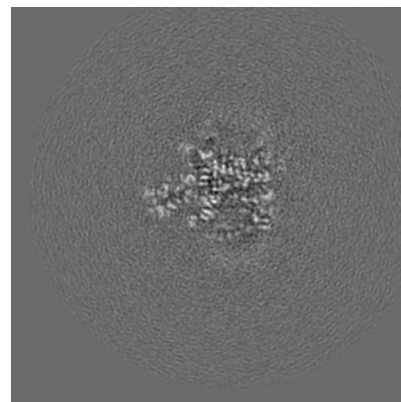
6.2.1 Primary map



X Index: 160

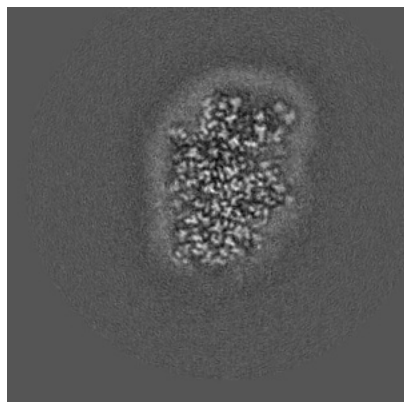


Y Index: 160

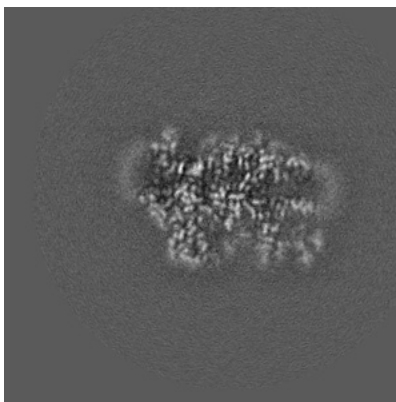


Z Index: 160

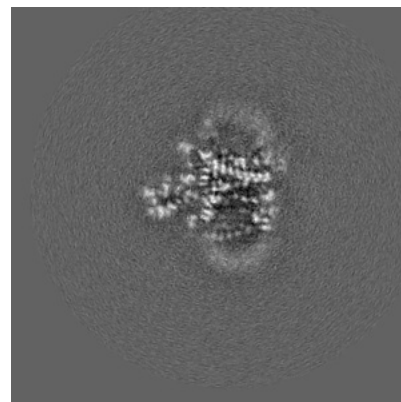
6.2.2 Raw map



X Index: 160



Y Index: 160

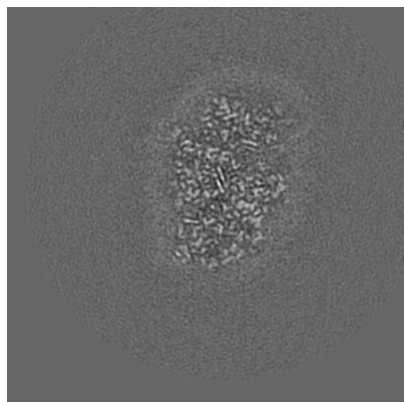


Z Index: 160

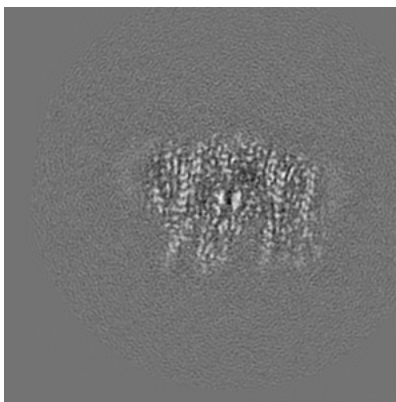
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

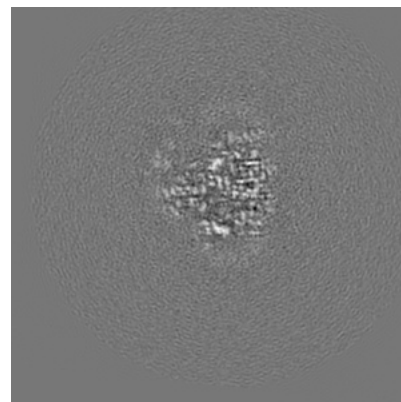
6.3.1 Primary map



X Index: 163

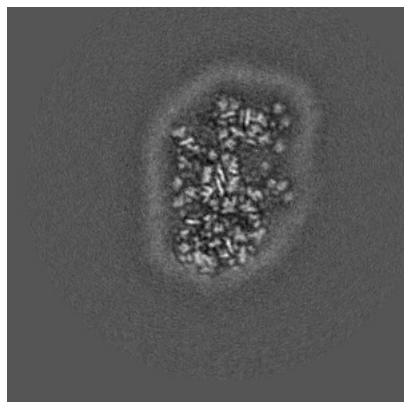


Y Index: 171

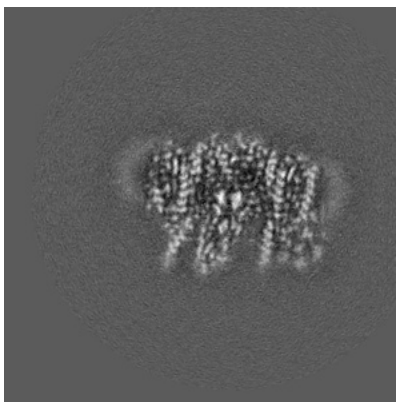


Z Index: 211

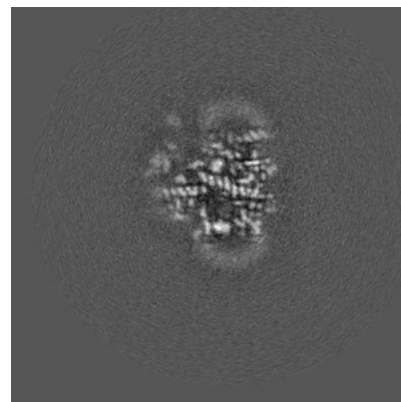
6.3.2 Raw map



X Index: 168



Y Index: 171

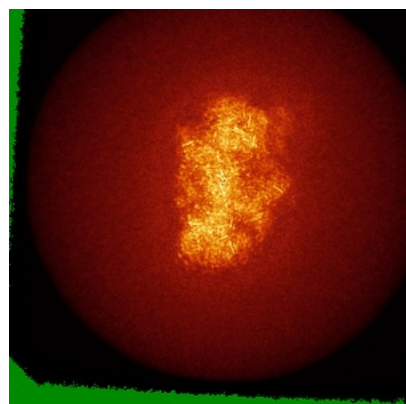


Z Index: 212

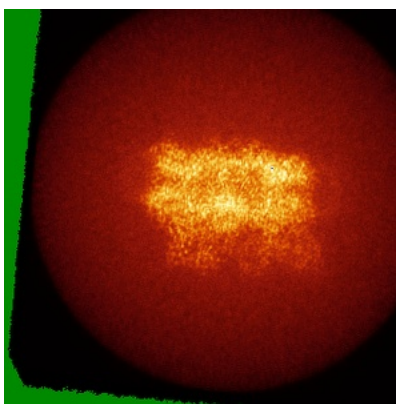
The images above show the largest variance slices of the map in three orthogonal directions.

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

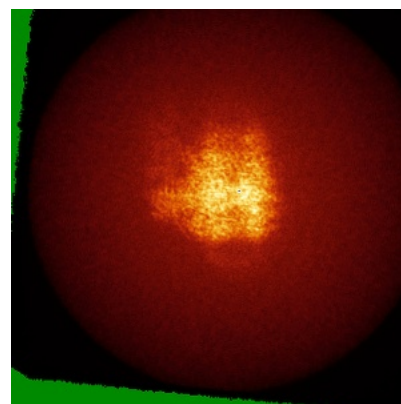
6.4.1 Primary map



X

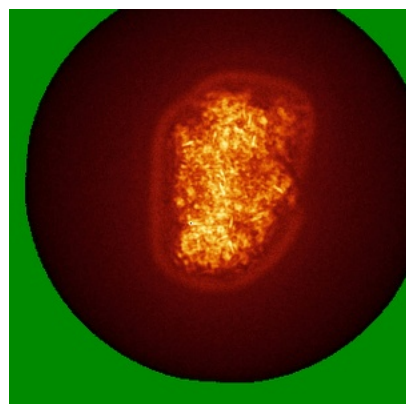


Y

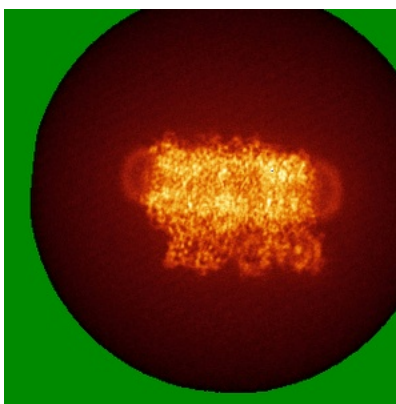


Z

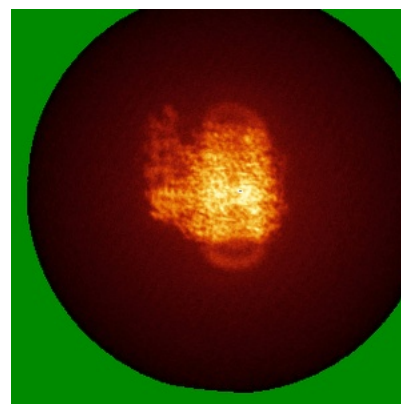
6.4.2 Raw map



X



Y

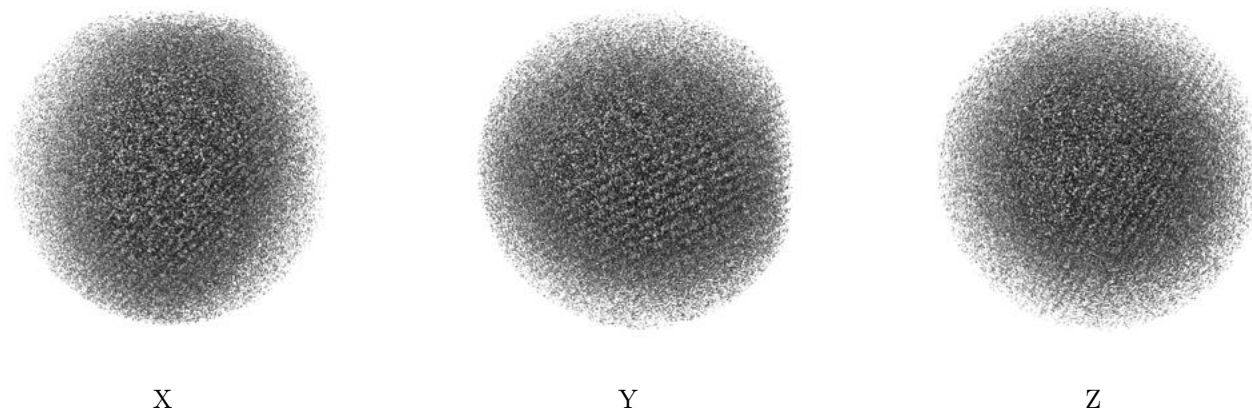


Z

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

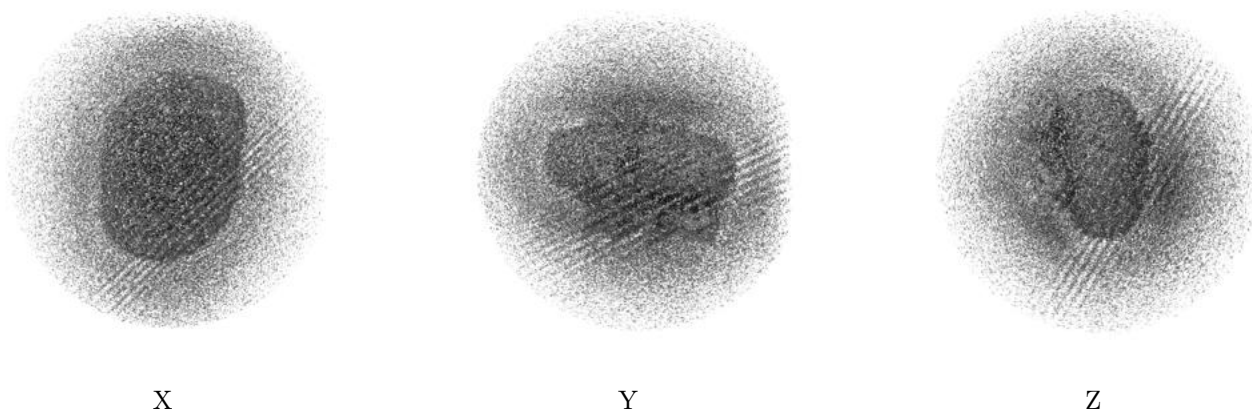
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00634. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

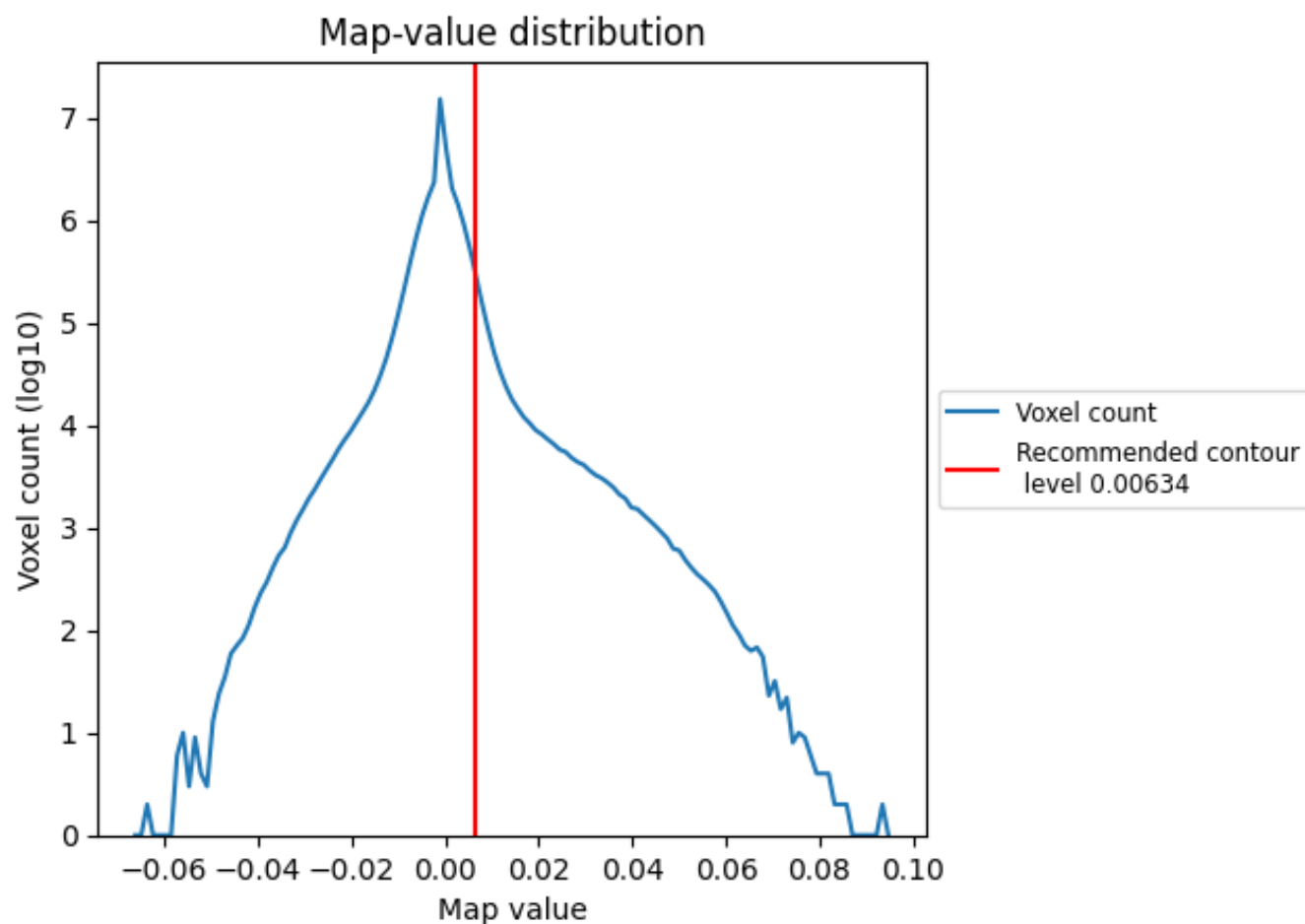
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

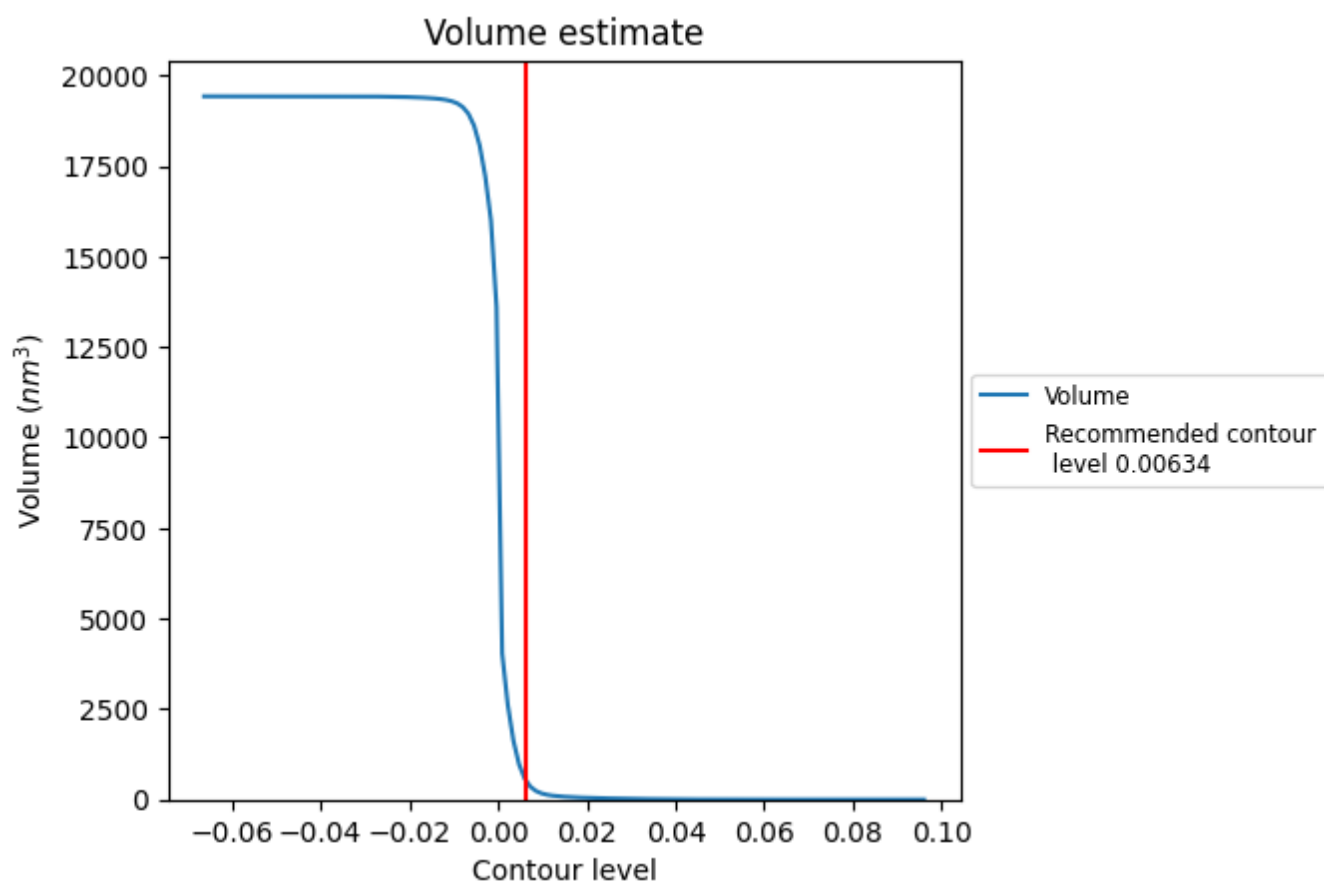
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

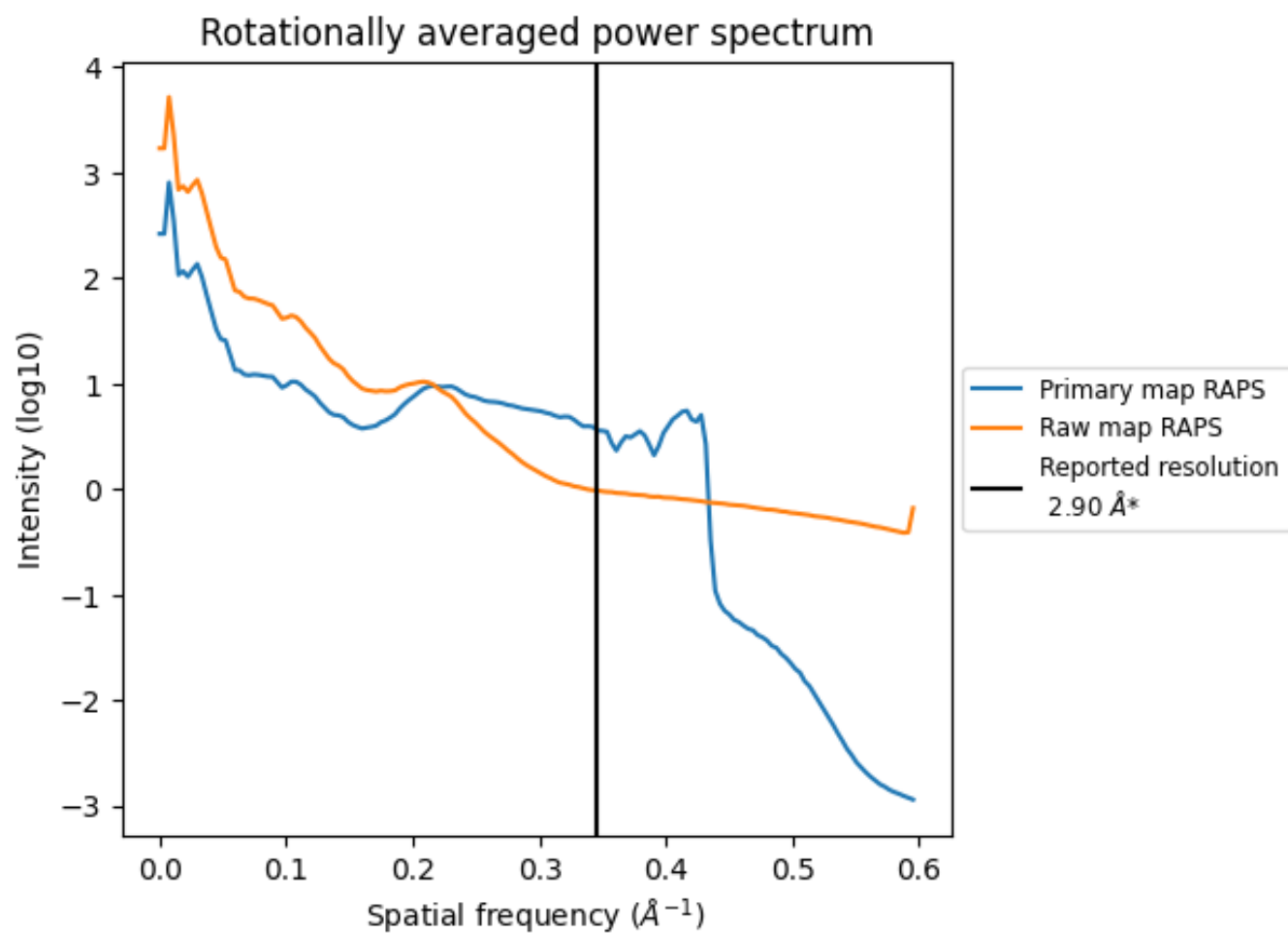
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 526 nm³; this corresponds to an approximate mass of 475 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 ⓘ

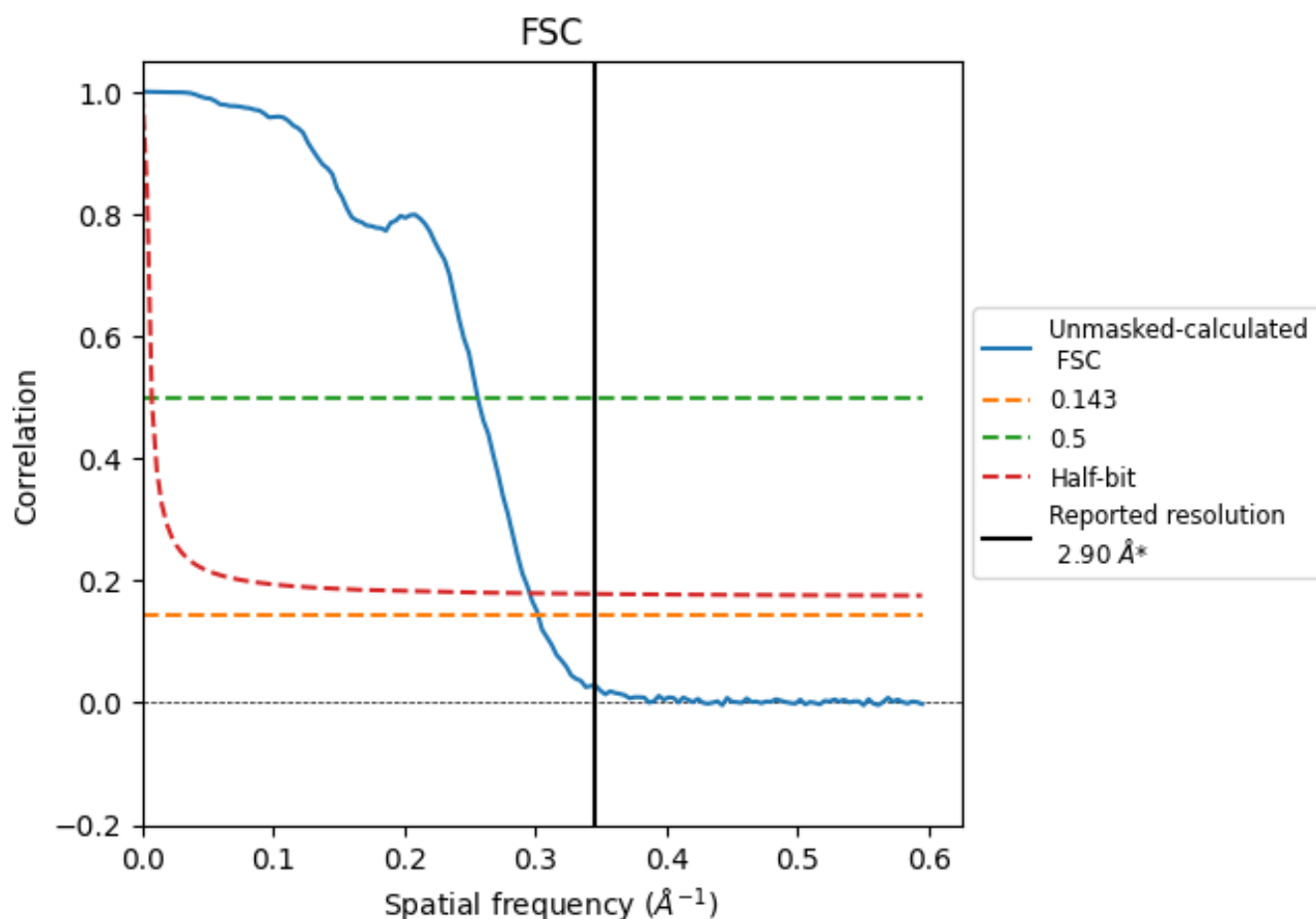


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 $0.345 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

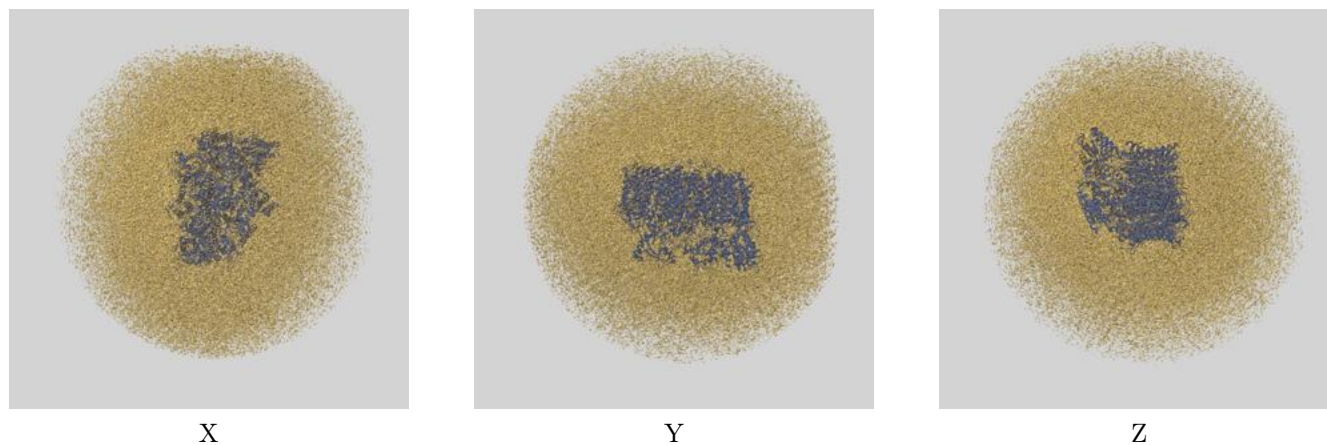
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.31	3.91	3.38

*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 3.31 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

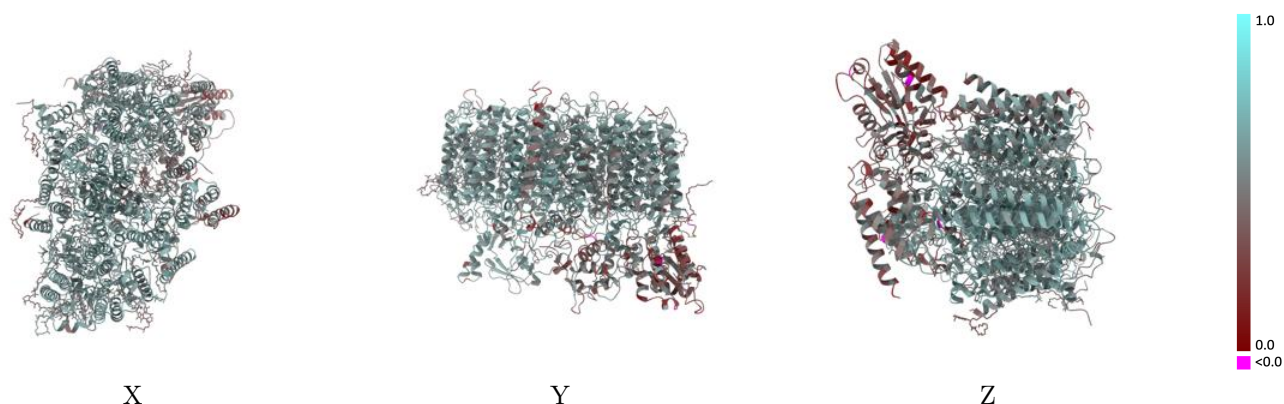
This section contains information regarding the fit between EMDB map EMD-52706 and PDB model 9I83. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



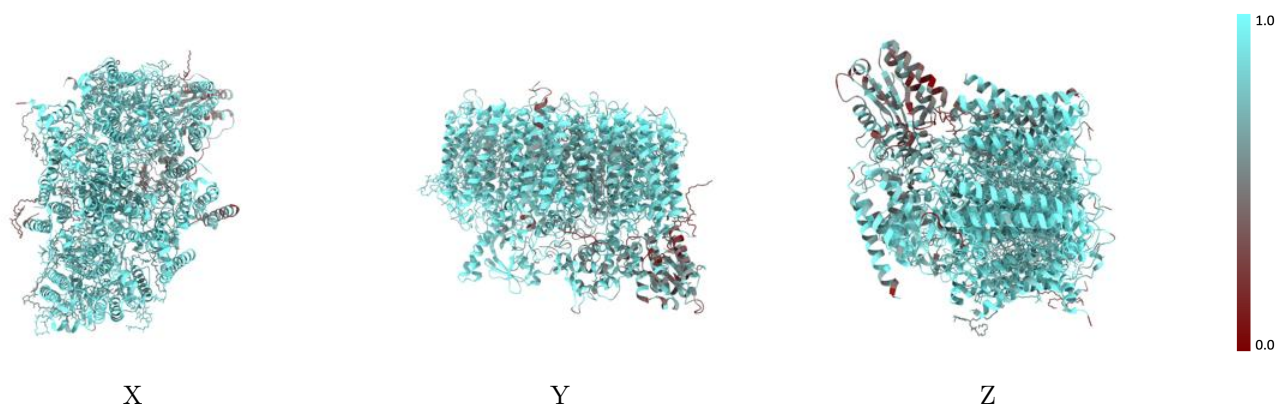
The images above show the 3D surface view of the map at the recommended contour level 0.00634 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



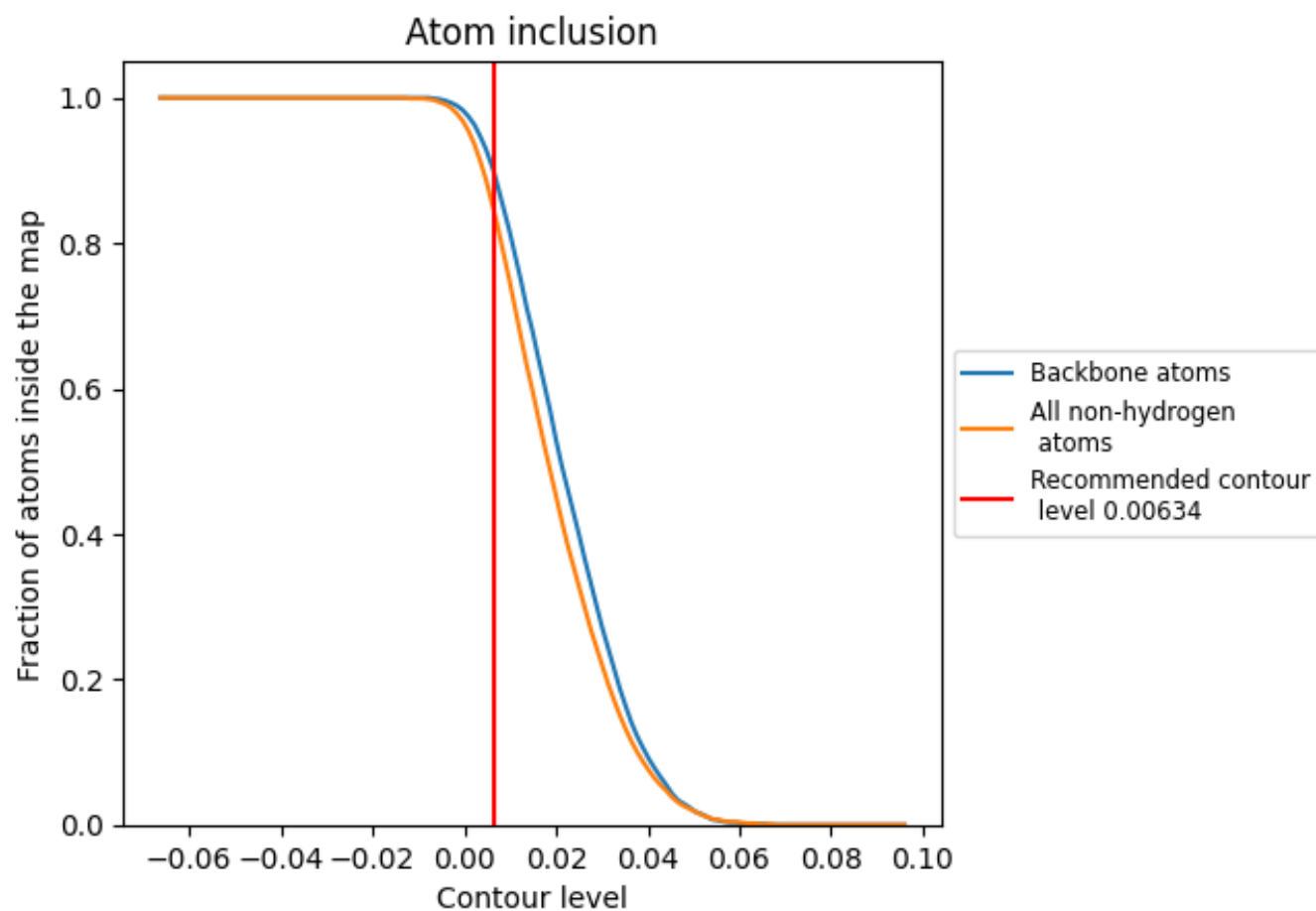
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00634).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 85% 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 (0.00634) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8480	 0.5380
1	 0.7320	 0.4060
3	 0.4970	 0.3280
A	 0.9020	 0.5820
B	 0.9070	 0.5710
C	 0.8980	 0.5710
D	 0.9120	 0.5930
E	 0.8820	 0.5330
F	 0.8440	 0.5260
H	 0.9020	 0.5670
I	 0.8040	 0.4930
J	 0.7710	 0.4890
K	 0.8100	 0.5190
L	 0.8560	 0.5620
M	 0.7100	 0.4740
T	 0.8760	 0.5560
V	 0.7040	 0.4260
X	 0.8660	 0.5540
Y	 0.7940	 0.4920
Z	 0.7770	 0.4780

