



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:57 PM UTC

PDB ID : 8KDE / pdb_00008kde
EMDB ID : EMD-37133
Title : Cryo-EM structure of an intermediate-state complex during the process of photosystem II repair
Authors : Li, A.; Wang, Y.; Liu, Z.
Deposited on : 2023-08-09
Resolution : 2.60 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:

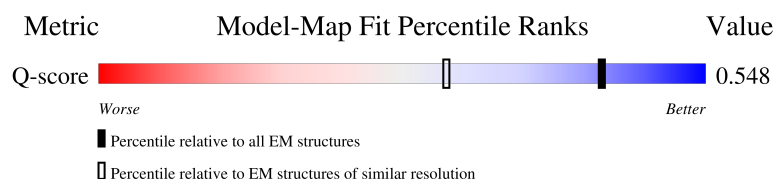
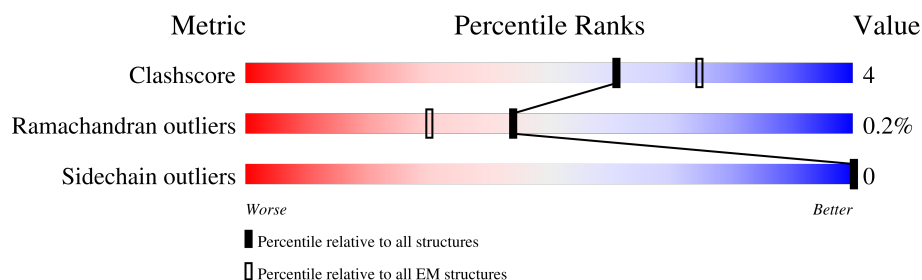
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 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	8728 (2.10 - 3.10)

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	B	508	 87% 8% 5%
2	D	352	 89% 10%
3	E	82	 83% 12% 5%
4	F	44	 61% 16% 23%

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Mol	Chain	Length	Quality of chain
5	H	88	
6	I	37	
7	K	46	
8	L	38	
9	M	34	
10	T	31	
11	V	33	
12	X	101	
13	Z	62	
14	G	196	
15	3	131	
16	C	461	
17	A	352	
18	1	117	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	403	X	-	-	-
19	CLA	A	404	X	-	-	-
19	CLA	A	405	X	-	-	-
19	CLA	B	601	X	-	-	-
19	CLA	B	602	X	-	-	-
19	CLA	B	603	X	-	-	-
19	CLA	B	604	X	-	-	-
19	CLA	B	605	X	-	-	-
19	CLA	B	606	X	-	-	-
19	CLA	B	607	X	-	-	-
19	CLA	B	608	X	-	-	-
19	CLA	B	609	X	-	-	-
19	CLA	B	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	611	X	-	-	-
19	CLA	B	612	X	-	-	-
19	CLA	B	613	X	-	-	-
19	CLA	B	614	X	-	-	-
19	CLA	B	615	X	-	-	-
19	CLA	B	616	X	-	-	-
19	CLA	C	602	X	-	-	-
19	CLA	C	603	X	-	-	-
19	CLA	C	604	X	-	-	-
19	CLA	C	605	X	-	-	-
19	CLA	C	606	X	-	-	-
19	CLA	C	607	X	-	-	-
19	CLA	C	608	X	-	-	-
19	CLA	C	609	X	-	-	-
19	CLA	C	610	X	-	-	-
19	CLA	C	611	X	-	-	-
19	CLA	C	612	X	-	-	-
19	CLA	C	613	X	-	-	-
19	CLA	C	614	X	-	-	-
19	CLA	D	401	X	-	-	-
19	CLA	D	402	X	-	-	-
19	CLA	D	409	X	-	-	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 22087 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 CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	482	Total	C	N	O	S	0	0
			3766	2469	629	656	12		

- Molecule 2 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	351	Total	C	N	O	S	0	0
			2791	1841	459	479	12		

- Molecule 3 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	78	Total	C	N	O	0	0
			633	414	104	115		

- Molecule 4 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	34	Total	C	N	O	S	0	0
			277	190	45	41	1		

- Molecule 5 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	73	Total	C	N	O	S	0	0
			561	372	84	103	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	35	Total	C	N	O	S	0	0
			283	193	43	45	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	K	37	Total	C	N	O	0	0
			297	209	43	45		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	38	Total	C	N	O	S	0	0
			314	210	51	52	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	M	31	Total	C	N	O	0	0
			239	163	33	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	T	31	Total	C	N	O	S	0	0
			256	177	38	39	2		

- Molecule 11 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	V	32	Total	C	N	O	0	0
			224	147	37	40		

- Molecule 12 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	X	35	Total	C	N	O	0	0
			242	159	39	44		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Z	61	Total	C	N	O	S	0	0
			458	314	68	75	1		

- Molecule 14 is a protein called Thylakoid enriched factor 14 (TEF14).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	145	Total	C	N	O	S	0	0
			1070	656	191	222	1		

- Molecule 15 is a protein called Photosystem II repair factor 1 (PRF1).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3	97	Total	C	N	O	S	0	0
			694	429	121	144			

- Molecule 16 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	C	430	Total	C	N	O	S	0	0
			3368	2209	561	581	17		

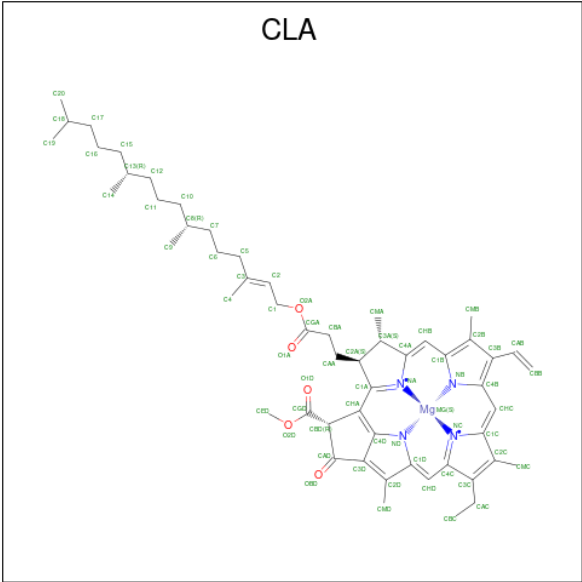
- Molecule 17 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	A	309	Total	C	N	O	S	0	0
			2418	1587	401	415	15		

- Molecule 18 is a protein called Photosystem II repair factor 2 (PRF2).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1	45	Total	C	N	O	S	0	0
			320	201	59	58	2		

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



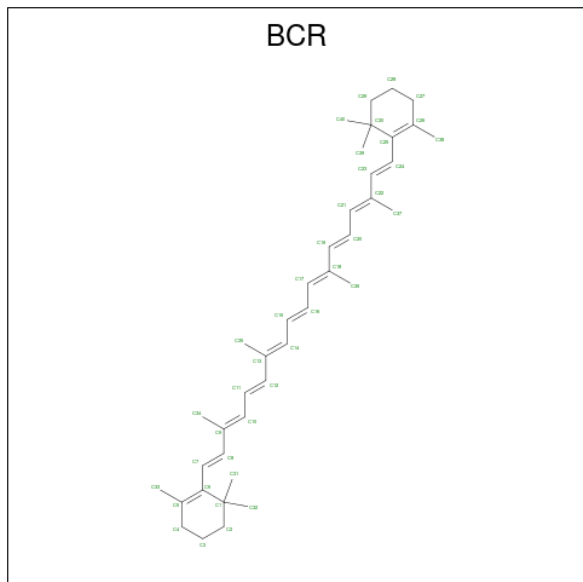
Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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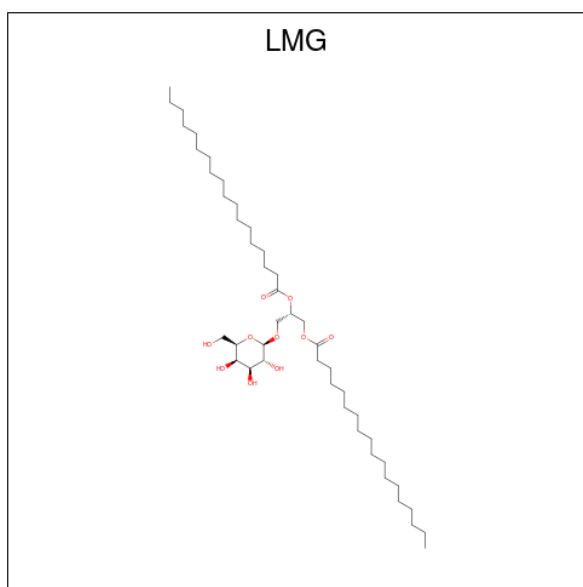
Mol	Chain	Residues	Atoms					AltConf
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19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
19	A	1	Total 60	C 50	Mg 1	N 4	O 5	0

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



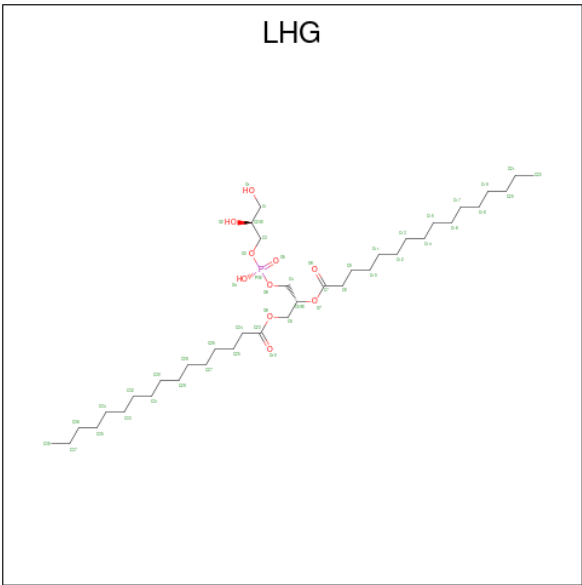
Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	D	1	Total C 40 40	0
20	H	1	Total C 40 40	0
20	K	1	Total C 40 40	0
20	Z	1	Total C 40 40	0
20	C	1	Total C 40 40	0
20	C	1	Total C 40 40	0
20	A	1	Total C 40 40	0

- Molecule 21 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



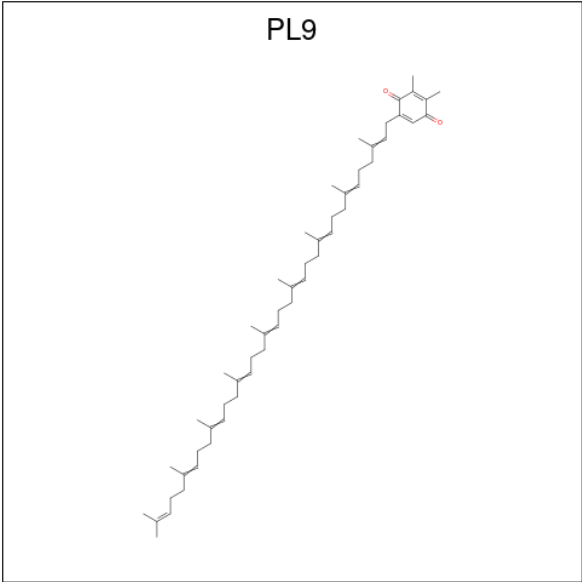
Mol	Chain	Residues	Atoms			AltConf
21	B	1	Total	C	O	0
			46	36	10	
21	B	1	Total	C	O	0
			48	38	10	
21	D	1	Total	C	O	0
			46	36	10	
21	K	1	Total	C	O	0
			51	41	10	
21	C	1	Total	C	O	0
			49	39	10	
21	A	1	Total	C	O	0
			48	38	10	

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



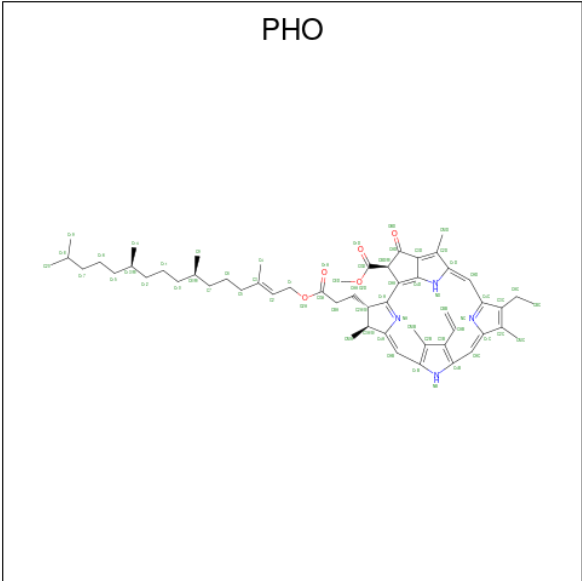
Mol	Chain	Residues	Atoms				AltConf
22	B	1	Total	C	O	P	0
			47	36	10	1	
22	B	1	Total	C	O	P	0
			49	38	10	1	
22	B	1	Total	C	O	P	0
			49	38	10	1	
22	D	1	Total	C	O	P	0
			44	33	10	1	
22	D	1	Total	C	O	P	0
			49	38	10	1	
22	D	1	Total	C	O	P	0
			43	32	10	1	
22	K	1	Total	C	O	P	0
			41	30	10	1	
22	L	1	Total	C	O	P	0
			49	38	10	1	
22	X	1	Total	C	O	P	0
			49	38	10	1	
22	A	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 23 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



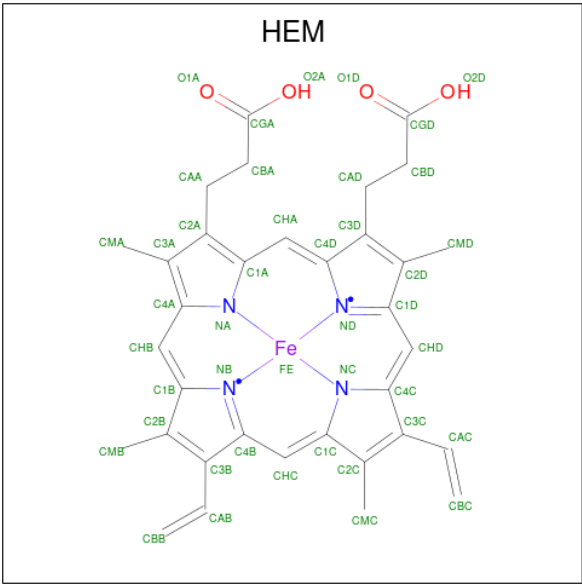
Mol	Chain	Residues	Atoms			AltConf
23	D	1	Total	C	O	0
			55	53	2	

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅) (labeled as "Ligand of Interest" by depositor).



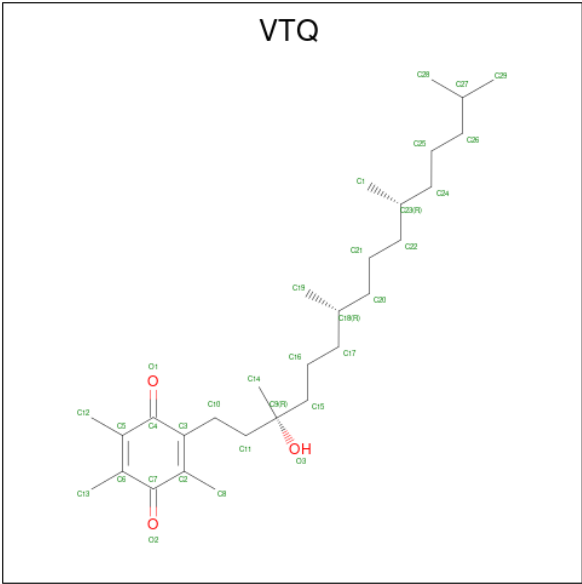
Mol	Chain	Residues	Atoms				AltConf
24	D	1	Total	C	N	O	0
			64	55	4	5	
24	D	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 25 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



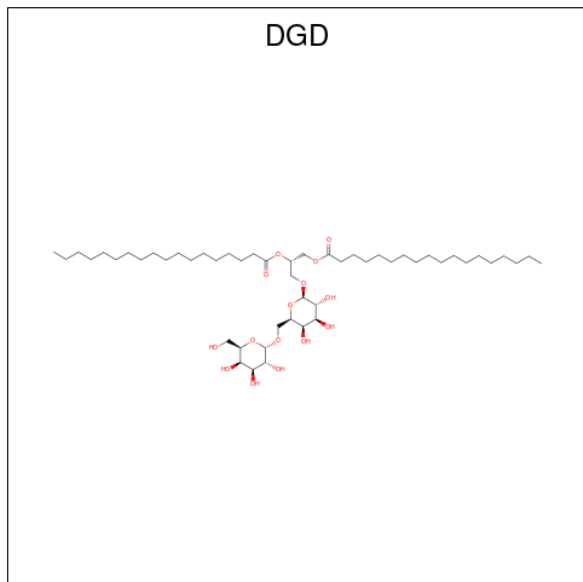
Mol	Chain	Residues	Atoms					AltConf
25	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 26 is RRR-ALPHA-TOCOPHERYLQUINONE (CCD ID: VTQ) (formula: $C_{29}H_{50}O_3$) (labeled as "Ligand of Interest" by depositor).



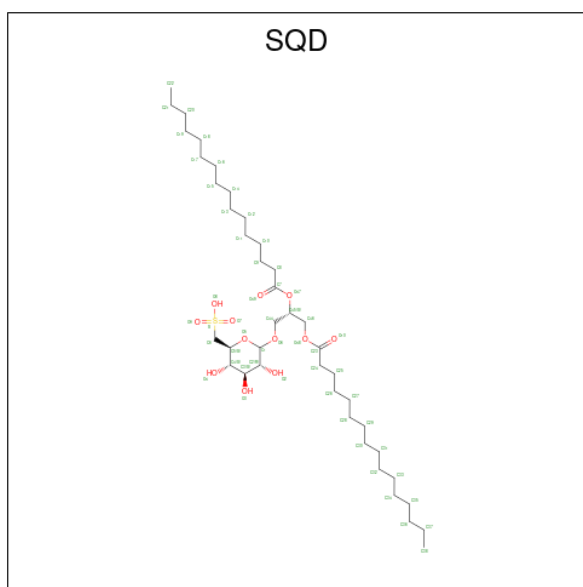
Mol	Chain	Residues	Atoms			AltConf
26	X	1	Total	C	O	0
			32	29	3	

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



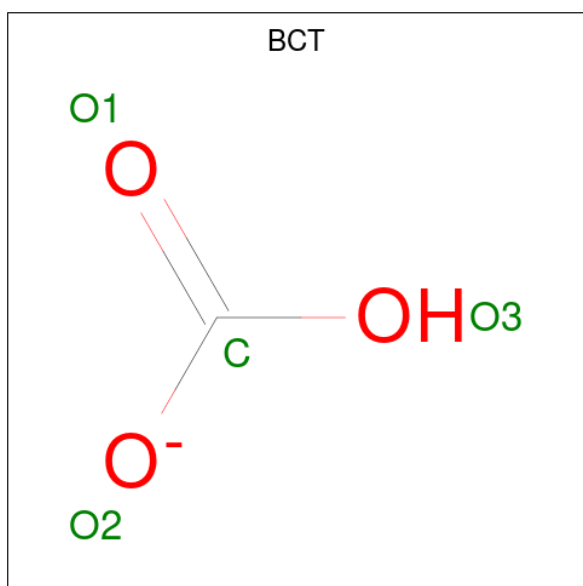
Mol	Chain	Residues	Atoms			AltConf
27	C	1	Total	C	O	0
			55	40	15	
27	C	1	Total	C	O	0
			57	42	15	
27	C	1	Total	C	O	0
			59	44	15	

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



Mol	Chain	Residues	Atoms				AltConf
28	C	1	Total	C	O	S	0
			51	38	12	1	

- Molecule 29 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 30 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

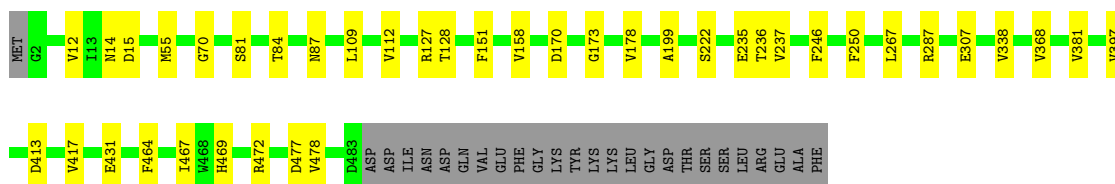
Mol	Chain	Residues	Atoms		AltConf
30	A	1	Total 1	Fe 1	0

3 Residue-property plots

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

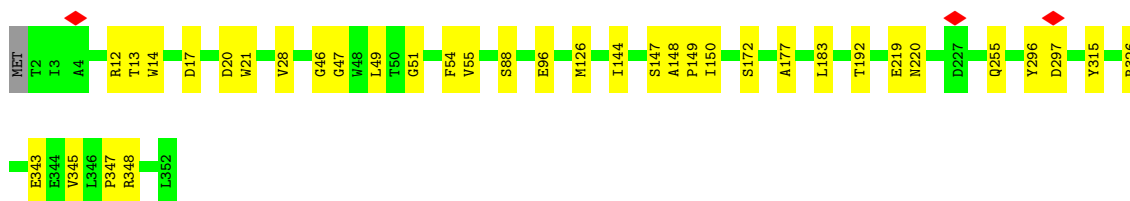
- Molecule 1: Photosystem II CP47 reaction center protein

Chain B: 



- Molecule 2: Photosystem II D2 protein

Chain D: 



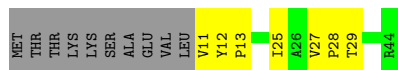
- Molecule 3: Cytochrome b559 subunit alpha

Chain E: 



- Molecule 4: Cytochrome b559 subunit beta

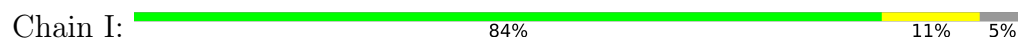
Chain F: 



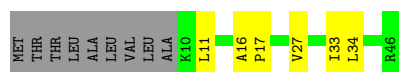
- Molecule 5: Photosystem II reaction center protein H



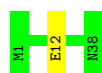
- Molecule 6: Photosystem II reaction center protein I



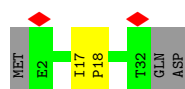
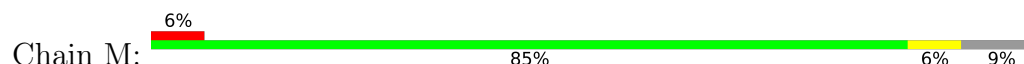
- Molecule 7: Photosystem II reaction center protein K



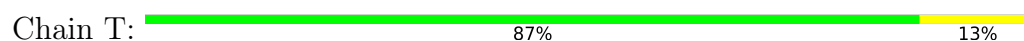
- Molecule 8: Photosystem II reaction center protein L



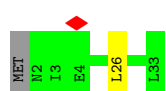
- Molecule 9: Photosystem II reaction center protein M



- Molecule 10: Photosystem II reaction center protein T

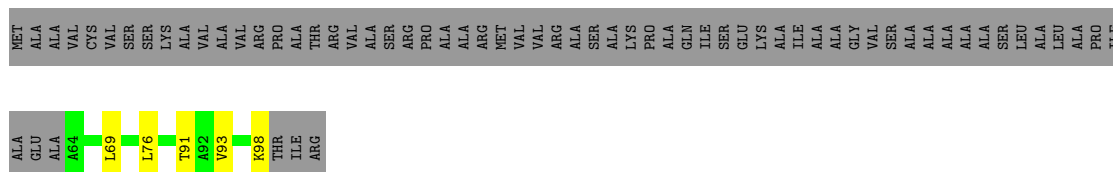


- Molecule 11: Photosystem II reaction center protein Ycf12



- Molecule 12: Uncharacterized protein

Chain X:  30% 5% 65%



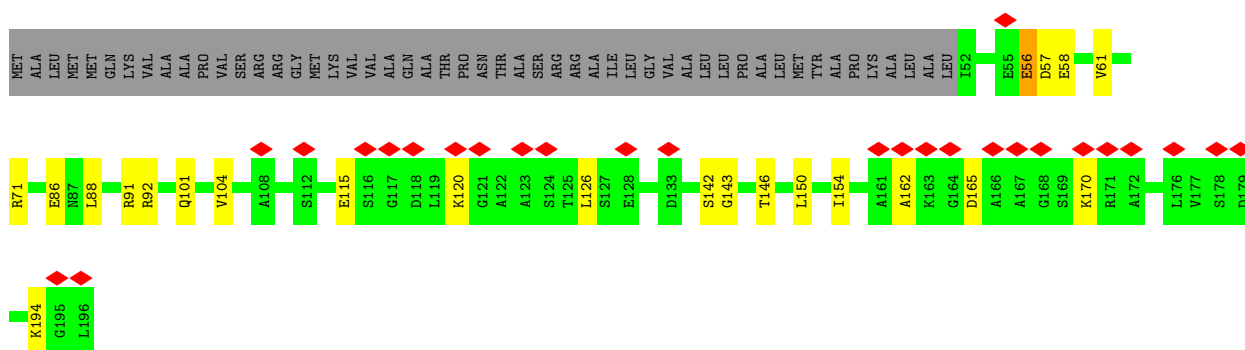
- Molecule 13: Photosystem II reaction center protein Z

Chain Z:  82% 16% .



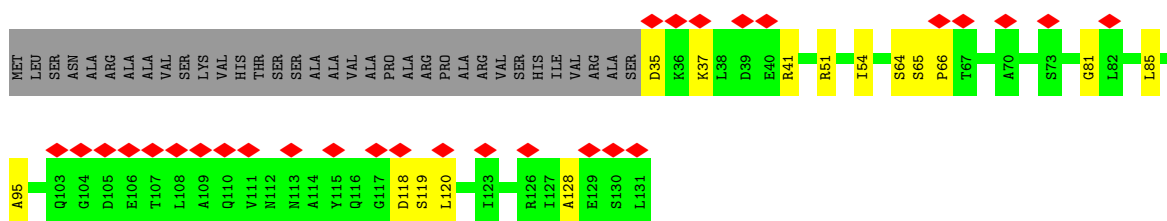
- Molecule 14: Thylakoid enriched factor 14 (TEF14)

Chain G:  14% 62% 11% . 26%



- Molecule 15: Photosystem II repair factor 1 (PRF1)

Chain 3:  22% 63% 11% 26%



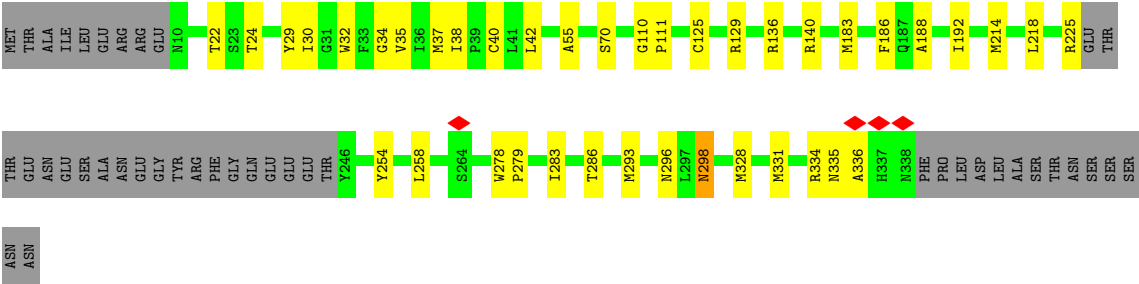
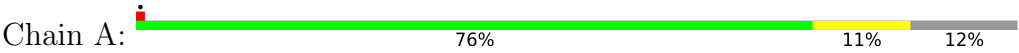
- Molecule 16: Photosystem II CP43 reaction center protein

Chain C:  85% 8% 7%

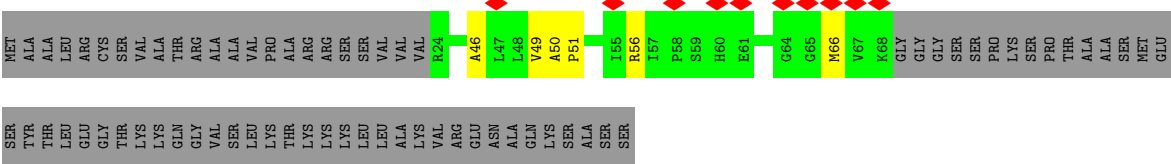




• Molecule 17: Photosystem II protein D1



• Molecule 18: Photosystem II repair factor 2 (PRF2)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	510932	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	61.421	Depositor
Minimum map value	-0.960	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.995	Depositor
Recommended contour level	3.9	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, VTQ, PHO, SQD, LHG, BCT, CLA, BCR, LMG, HEM, PL9, DGD

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	B	0.15	0/3894	0.26	0/5302
2	D	0.15	0/2886	0.27	0/3937
3	E	0.13	0/652	0.31	0/890
4	F	0.13	0/286	0.27	0/389
5	H	0.12	0/573	0.25	0/783
6	I	0.19	0/291	0.37	0/394
7	K	0.11	0/309	0.29	0/425
8	L	0.16	0/322	0.22	0/437
9	M	0.09	0/243	0.21	0/333
10	T	0.15	0/263	0.23	0/354
11	V	0.06	0/224	0.17	0/307
12	X	0.12	0/244	0.23	0/330
13	Z	0.14	0/469	0.24	0/644
14	G	0.11	0/1079	0.28	0/1454
15	3	0.11	0/700	0.29	0/947
16	C	0.13	0/3486	0.26	0/4743
17	A	0.15	0/2495	0.31	0/3402
18	1	0.16	0/323	0.28	0/435
All	All	0.14	0/18739	0.27	0/25506

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	B	3766	0	3649	30	0
2	D	2791	0	2678	26	0
3	E	633	0	622	9	0
4	F	277	0	288	4	0
5	H	561	0	581	10	0
6	I	283	0	293	3	0
7	K	297	0	308	3	0
8	L	314	0	327	1	0
9	M	239	0	258	1	0
10	T	256	0	273	4	0
11	V	224	0	256	1	0
12	X	242	0	266	7	0
13	Z	458	0	490	8	0
14	G	1070	0	1077	19	0
15	3	694	0	698	14	0
16	C	3368	0	3240	28	0
17	A	2418	0	2349	32	0
18	1	320	0	340	4	0
19	A	174	0	170	2	0
19	B	1020	0	1113	4	0
19	C	845	0	936	5	0
19	D	195	0	216	4	0
20	A	40	0	56	3	0
20	B	120	0	168	2	0
20	C	80	0	112	6	0
20	D	40	0	56	1	0
20	H	40	0	56	6	0
20	K	40	0	56	1	0
20	Z	40	0	56	7	0
21	A	48	0	66	0	0
21	B	94	0	128	1	0
21	C	49	0	68	0	0
21	D	46	0	62	0	0
21	K	51	0	72	0	0
22	A	49	0	74	0	0
22	B	145	0	215	0	0
22	D	136	0	191	2	0
22	K	41	0	52	0	0
22	L	49	0	74	0	0
22	X	49	0	74	0	0
23	D	55	0	80	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	D	128	0	148	1	0
25	E	43	0	30	4	0
26	X	32	0	50	0	0
27	C	171	0	216	2	0
28	C	51	0	69	0	0
29	A	4	0	0	0	0
30	A	1	0	0	0	0
All	All	22087	0	22657	198	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 4.

All (198) 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)
16:C:185:ARG:NH2	16:C:219:GLU:OE2	2.13	0.81
8:L:12:GLU:OE2	15:3:51:ARG:NH2	2.14	0.80
19:D:409:CLA:HMD3	17:A:183:MET:HE1	1.66	0.77
1:B:235:GLU:OE2	1:B:469:HIS:ND1	2.20	0.73
20:C:616:BCR:H383	20:C:616:BCR:H23C	1.71	0.72
22:D:407:LHG:O3	22:D:407:LHG:O1	2.08	0.70
25:E:101:HEM:HHC	25:E:101:HEM:HBB2	1.74	0.70
1:B:368:VAL:HG22	1:B:381:VAL:HG22	1.72	0.70
1:B:222:SER:OG	5:H:43:GLY:O	2.10	0.70
3:E:7:GLU:OE1	18:1:56:ARG:NH2	2.25	0.69
2:D:343:GLU:OE1	2:D:348:ARG:NH2	2.25	0.68
5:H:68:TYR:CD1	5:H:79:MET:HE1	2.31	0.65
15:3:64:SER:O	15:3:65:SER:OG	2.10	0.65
2:D:297:ASP:O	2:D:315:TYR:OH	2.07	0.65
15:3:35:ASP:O	17:A:225:ARG:NH2	2.30	0.65
16:C:44:HIS:CE1	19:C:610:CLA:HMA3	2.33	0.64
1:B:14:ASN:ND2	15:3:41:ARG:O	2.31	0.63
2:D:192:THR:HG23	19:D:401:CLA:HBC2	1.80	0.63
20:Z:101:BCR:H333	16:C:104:VAL:HG11	1.80	0.62
16:C:71:GLU:OE2	16:C:386:HIS:NE2	2.32	0.62
1:B:307:GLU:OE2	14:G:71:ARG:NH1	2.32	0.62
25:E:101:HEM:HBC2	25:E:101:HEM:HMC2	1.81	0.61
14:G:165:ASP:O	14:G:170:LYS:NZ	2.34	0.60
16:C:285:TYR:OH	19:C:603:CLA:HED3	2.00	0.60
14:G:120:LYS:NZ	14:G:162:ALA:O	2.34	0.60
17:A:334:ARG:O	17:A:336:ALA:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:8:ARG:NH2	3:E:12:ASP:OD2	2.36	0.59
16:C:15:ASP:OD1	16:C:16:GLN:N	2.35	0.59
1:B:464:PHE:HE1	2:D:144:ILE:HG23	1.66	0.59
5:H:54:ILE:HG13	20:H:101:BCR:H333	1.85	0.58
1:B:81:SER:OG	14:G:92:ARG:NH2	2.36	0.58
27:C:619:DGD:O5D	27:C:619:DGD:O4D	2.17	0.58
16:C:285:TYR:O	16:C:411:ARG:NH2	2.37	0.57
19:D:402:CLA:H43	12:X:76:LEU:HD23	1.86	0.57
6:I:27:ASP:OD1	17:A:136:ARG:NH2	2.38	0.57
10:T:30:ILE:HG23	10:T:30:ILE:O	2.05	0.57
16:C:391:SER:HA	17:A:298:ASN:HB2	1.86	0.57
1:B:12:VAL:HG12	1:B:12:VAL:O	2.04	0.57
15:3:118:ASP:OD1	15:3:119:SER:N	2.37	0.56
5:H:74:LEU:HB2	5:H:77:VAL:HG22	1.86	0.56
17:A:188:ALA:HB2	17:A:328:MET:HB3	1.88	0.56
15:3:37:LYS:HD2	15:3:37:LYS:O	2.05	0.56
20:C:615:BCR:H311	20:C:615:BCR:HC8	1.89	0.55
17:A:32:TRP:O	17:A:35:VAL:HG22	2.07	0.55
20:H:101:BCR:H393	12:X:69:LEU:HD21	1.89	0.54
20:B:617:BCR:H382	20:B:617:BCR:H23C	1.88	0.54
6:I:32:PRO:HD2	6:I:33:GLY:H	1.73	0.53
20:Z:101:BCR:C38	20:Z:101:BCR:H23C	2.39	0.53
17:A:22:THR:HG22	17:A:22:THR:O	2.09	0.52
1:B:70:GLY:HA2	1:B:178:VAL:HG11	1.90	0.52
20:Z:101:BCR:H23C	20:Z:101:BCR:H382	1.91	0.52
1:B:237:VAL:HG13	19:B:612:CLA:CMD	2.39	0.52
17:A:42:LEU:HB3	20:A:406:BCR:H353	1.92	0.52
16:C:50:PHE:HB2	16:C:110:SER:OG	2.09	0.52
2:D:51:GLY:HA2	2:D:55:VAL:HG22	1.92	0.51
2:D:14:TRP:NE1	12:X:91:THR:OG1	2.39	0.51
20:H:101:BCR:HC8	20:H:101:BCR:H331	1.93	0.51
19:D:402:CLA:H43	12:X:76:LEU:HA	1.93	0.51
3:E:57:THR:HG22	3:E:58:GLU:N	2.26	0.51
20:H:101:BCR:H23C	20:H:101:BCR:H383	1.93	0.51
17:A:283:ILE:HA	17:A:286:THR:HG22	1.92	0.51
1:B:472:ARG:NH2	15:3:54:ILE:O	2.42	0.51
2:D:172:SER:HB2	2:D:177:ALA:HB1	1.92	0.51
13:Z:50:LEU:HA	13:Z:53:VAL:HG12	1.93	0.50
16:C:364:ASP:OD2	16:C:367:LYS:NZ	2.43	0.50
2:D:13:THR:HG22	2:D:14:TRP:N	2.27	0.50
25:E:101:HEM:HBC2	25:E:101:HEM:CMC	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:146:THR:O	14:G:150:LEU:HD23	2.11	0.49
21:B:623:LMG:O5	21:B:623:LMG:O4	2.25	0.49
20:B:618:BCR:H383	20:B:618:BCR:H23C	1.94	0.49
17:A:186:PHE:HE2	17:A:192:ILE:HD12	1.78	0.49
17:A:29:TYR:O	17:A:129:ARG:NH2	2.36	0.48
1:B:109:LEU:O	1:B:112:VAL:HG12	2.13	0.48
2:D:255:GLN:NE2	17:A:24:THR:O	2.42	0.48
20:A:406:BCR:H382	20:A:406:BCR:H23C	1.94	0.48
17:A:110:GLY:N	17:A:111:PRO:HD2	2.28	0.48
2:D:347:PRO:HB2	17:A:331:MET:HE3	1.94	0.48
16:C:274:ALA:HB2	19:C:603:CLA:HMD2	1.96	0.48
17:A:214:MET:O	17:A:218:LEU:HD13	2.14	0.47
3:E:8:ARG:CB	4:F:11:VAL:HG23	2.44	0.47
15:3:81:GLY:O	15:3:85:LEU:HD12	2.14	0.47
1:B:413:ASP:OD1	1:B:413:ASP:N	2.48	0.47
17:A:37:MET:HG3	17:A:38:ILE:N	2.29	0.47
20:Z:101:BCR:H333	16:C:104:VAL:CG1	2.45	0.47
19:B:602:CLA:H43	5:H:65:LEU:HA	1.97	0.47
18:1:66:MET:O	18:1:66:MET:HG3	2.15	0.47
2:D:297:ASP:OD1	2:D:297:ASP:N	2.47	0.47
5:H:18:GLN:O	5:H:19:GLU:HG2	2.15	0.47
6:I:30:ARG:HD3	17:A:22:THR:HG21	1.97	0.47
13:Z:55:GLY:CA	20:Z:101:BCR:H323	2.45	0.47
20:C:615:BCR:H311	20:C:615:BCR:C8	2.45	0.46
17:A:278:TRP:HB3	17:A:279:PRO:HD3	1.96	0.46
18:1:50:ALA:HB3	18:1:51:PRO:HD3	1.97	0.46
16:C:278:SER:O	16:C:411:ARG:NH1	2.46	0.46
14:G:126:LEU:HD21	14:G:154:ILE:HG13	1.97	0.46
20:K:101:BCR:H343	13:Z:20:VAL:HG11	1.98	0.46
14:G:101:GLN:O	14:G:104:VAL:HG12	2.16	0.46
20:C:615:BCR:H382	20:C:615:BCR:H23C	1.98	0.46
5:H:80:SER:O	5:H:83:THR:HG22	2.16	0.46
2:D:345:VAL:HG22	2:D:345:VAL:O	2.15	0.46
3:E:59:ASP:OD1	3:E:60:ARG:N	2.49	0.46
17:A:34:GLY:HA2	17:A:37:MET:HG2	1.98	0.45
2:D:183:LEU:HD22	17:A:328:MET:HE1	1.97	0.45
17:A:37:MET:SD	17:A:129:ARG:HD2	2.57	0.45
1:B:87:ASN:O	1:B:87:ASN:OD1	2.35	0.45
1:B:287:ARG:NH1	14:G:86:GLU:OE1	2.50	0.45
5:H:85:ALA:HB1	14:G:88:LEU:HD22	1.98	0.45
20:C:616:BCR:H383	20:C:616:BCR:C23	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:25:ILE:O	4:F:29:THR:OG1	2.32	0.45
17:A:30:ILE:O	17:A:34:GLY:HA3	2.16	0.45
15:3:65:SER:HB2	15:3:66:PRO:HD2	1.97	0.45
1:B:55:MET:HE1	1:B:267:LEU:HD22	1.97	0.45
7:K:27:VAL:O	7:K:27:VAL:HG12	2.17	0.45
16:C:216:ASP:OD1	16:C:216:ASP:N	2.49	0.45
1:B:246:PHE:CE1	1:B:250:PHE:HE2	2.36	0.44
1:B:431:GLU:OE2	14:G:61:VAL:HA	2.17	0.44
2:D:20:ASP:OD2	12:X:98:LYS:NZ	2.49	0.44
1:B:127:ARG:O	1:B:128:THR:OG1	2.28	0.44
16:C:393:ASN:ND2	27:C:619:DGD:O1B	2.47	0.44
14:G:56:GLU:HG2	14:G:57:ASP:N	2.32	0.44
16:C:242:THR:HG22	16:C:243:THR:N	2.33	0.44
14:G:194:LYS:HD2	15:3:120:LEU:HD11	2.00	0.44
19:B:604:CLA:HAA2	19:B:612:CLA:H141	1.99	0.44
2:D:219:GLU:C	2:D:220:ASN:HD22	2.26	0.44
16:C:98:PRO:HA	16:C:101:VAL:HG12	1.99	0.44
9:M:17:ILE:HB	9:M:18:PRO:HD3	2.00	0.43
16:C:189:ASN:O	16:C:189:ASN:OD1	2.36	0.43
17:A:186:PHE:CE2	17:A:192:ILE:HD12	2.53	0.43
5:H:36:GLU:HG3	5:H:36:GLU:O	2.16	0.43
13:Z:19:LEU:HD21	13:Z:44:LEU:HD23	2.00	0.43
17:A:37:MET:O	17:A:40:CYS:N	2.52	0.43
16:C:287:SER:O	16:C:291:GLY:N	2.50	0.43
22:D:407:LHG:O5	17:A:140:ARG:NH2	2.36	0.43
16:C:49:VAL:HG23	16:C:110:SER:HB2	1.99	0.43
17:A:254:TYR:CE1	17:A:258:LEU:HD22	2.54	0.43
2:D:12:ARG:NH2	2:D:17:ASP:OD1	2.51	0.43
20:H:101:BCR:H393	12:X:69:LEU:CD2	2.49	0.43
14:G:115:GLU:OE1	15:3:128:ALA:HB2	2.18	0.43
17:A:188:ALA:HB2	17:A:328:MET:CB	2.48	0.43
2:D:296:TYR:OH	2:D:326:ARG:NH1	2.48	0.43
19:C:603:CLA:HED2	19:C:604:CLA:H43	1.99	0.43
1:B:467:ILE:HD12	2:D:126:MET:HE2	2.00	0.43
17:A:37:MET:HB3	17:A:125:CYS:HB2	2.00	0.43
2:D:54:PHE:O	3:E:49:THR:OG1	2.32	0.42
4:F:12:TYR:N	4:F:13:PRO:HD2	2.34	0.42
16:C:95:ASP:OD1	16:C:95:ASP:N	2.50	0.42
16:C:210:GLY:O	16:C:211:TRP:C	2.62	0.42
1:B:84:THR:HG21	14:G:143:GLY:HA3	2.01	0.42
1:B:477:ASP:OD1	1:B:478:VAL:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:TRP:NE1	12:X:93:VAL:HG12	2.34	0.42
1:B:397:VAL:HG23	1:B:417:VAL:HG11	2.01	0.42
16:C:361:ASN:OD1	16:C:361:ASN:N	2.53	0.42
17:A:55:ALA:O	17:A:70:SER:OG	2.34	0.42
2:D:148:ALA:HB3	2:D:149:PRO:CD	2.48	0.42
3:E:6:VAL:HG22	3:E:6:VAL:O	2.19	0.42
7:K:33:ILE:HG23	7:K:34:LEU:N	2.34	0.42
15:3:64:SER:C	15:3:65:SER:HG	2.17	0.42
1:B:338:VAL:HG21	14:G:61:VAL:HG23	2.01	0.42
13:Z:1:MET:O	13:Z:1:MET:HG3	2.19	0.42
20:Z:101:BCR:C33	16:C:104:VAL:HG11	2.47	0.42
14:G:57:ASP:C	14:G:58:GLU:OE1	2.63	0.42
13:Z:11:ALA:O	13:Z:15:VAL:HG23	2.20	0.42
16:C:395:VAL:HG23	16:C:396:GLY:N	2.34	0.41
10:T:25:ASP:O	10:T:25:ASP:OD1	2.38	0.41
16:C:97:PHE:N	16:C:98:PRO:CD	2.84	0.41
17:A:286:THR:OG1	19:A:403:CLA:O1D	2.36	0.41
2:D:28:VAL:HG23	2:D:28:VAL:O	2.20	0.41
4:F:27:VAL:HB	4:F:28:PRO:HD3	2.03	0.41
14:G:92:ARG:C	14:G:92:ARG:HD3	2.45	0.41
2:D:147:SER:HA	2:D:150:ILE:HG22	2.03	0.41
16:C:87:VAL:HG21	16:C:289:PHE:HZ	1.85	0.41
1:B:151:PHE:CZ	15:3:95:ALA:HB3	2.55	0.41
2:D:88:SER:OG	2:D:96:GLU:OE2	2.32	0.41
24:D:411:PHO:H151	19:A:404:CLA:HMB1	2.03	0.41
1:B:15:ASP:N	1:B:15:ASP:OD1	2.53	0.41
10:T:26:PRO:HB2	10:T:28:ARG:CD	2.51	0.41
11:V:26:LEU:HD21	13:Z:25:VAL:HA	2.03	0.41
13:Z:55:GLY:HA2	20:Z:101:BCR:H323	2.02	0.41
14:G:142:SER:OG	14:G:146:THR:OG1	2.21	0.41
16:C:200:TYR:CD2	20:C:615:BCR:H391	2.56	0.41
20:A:406:BCR:C33	20:A:406:BCR:HC8	2.51	0.41
1:B:236:THR:HG23	1:B:237:VAL:N	2.35	0.41
2:D:46:GLY:O	2:D:47:GLY:C	2.63	0.41
3:E:59:ASP:OD1	3:E:59:ASP:C	2.64	0.41
5:H:68:TYR:CE1	5:H:79:MET:HE1	2.56	0.41
19:C:602:CLA:H141	19:C:602:CLA:H162	1.88	0.41
18:1:46:ALA:HA	18:1:49:VAL:HG22	2.03	0.41
20:H:101:BCR:H331	20:H:101:BCR:C8	2.51	0.40
10:T:30:ILE:O	10:T:30:ILE:CG2	2.69	0.40
19:B:614:CLA:H2A	19:B:614:CLA:O1D	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:LEU:HD13	20:D:403:BCR:C15	2.51	0.40
14:G:91:ARG:HG2	14:G:91:ARG:O	2.21	0.40
1:B:158:VAL:HG21	1:B:199:ALA:HA	2.04	0.40
3:E:30:LEU:HD11	25:E:101:HEM:CBB	2.51	0.40
1:B:170:ASP:OD1	1:B:173:GLY:N	2.54	0.40
17:A:293:MET:C	17:A:296:ASN:H	2.29	0.40
1:B:151:PHE:CE2	15:3:95:ALA:HB3	2.57	0.40
7:K:16:ALA:N	7:K:17:PRO:HD2	2.37	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	B	480/508 (94%)	465 (97%)	15 (3%)	0	100	100
2	D	349/352 (99%)	331 (95%)	18 (5%)	0	100	100
3	E	76/82 (93%)	71 (93%)	5 (7%)	0	100	100
4	F	32/44 (73%)	29 (91%)	3 (9%)	0	100	100
5	H	71/88 (81%)	68 (96%)	3 (4%)	0	100	100
6	I	33/37 (89%)	33 (100%)	0	0	100	100
7	K	35/46 (76%)	34 (97%)	0	1 (3%)	3	6
8	L	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
9	M	29/34 (85%)	28 (97%)	1 (3%)	0	100	100
10	T	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
11	V	30/33 (91%)	29 (97%)	1 (3%)	0	100	100
12	X	33/101 (33%)	33 (100%)	0	0	100	100
13	Z	59/62 (95%)	59 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	G	143/196 (73%)	134 (94%)	8 (6%)	1 (1%)	18	38
15	3	95/131 (72%)	84 (88%)	11 (12%)	0	100	100
16	C	424/461 (92%)	415 (98%)	9 (2%)	0	100	100
17	A	305/352 (87%)	294 (96%)	9 (3%)	2 (1%)	18	38
18	1	43/117 (37%)	40 (93%)	3 (7%)	0	100	100
All	All	2302/2713 (85%)	2210 (96%)	88 (4%)	4 (0%)	44	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	A	335	ASN
17	A	298	ASN
14	G	56	GLU
7	K	11	LEU

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	B	384/407 (94%)	384 (100%)	0	100	100
2	D	280/281 (100%)	280 (100%)	0	100	100
3	E	69/71 (97%)	69 (100%)	0	100	100
4	F	28/37 (76%)	28 (100%)	0	100	100
5	H	63/75 (84%)	63 (100%)	0	100	100
6	I	32/34 (94%)	32 (100%)	0	100	100
7	K	31/38 (82%)	31 (100%)	0	100	100
8	L	35/35 (100%)	35 (100%)	0	100	100
9	M	27/30 (90%)	27 (100%)	0	100	100
10	T	28/28 (100%)	28 (100%)	0	100	100
11	V	26/27 (96%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	X	25/67 (37%)	25 (100%)	0	100	100
13	Z	51/52 (98%)	51 (100%)	0	100	100
14	G	112/149 (75%)	112 (100%)	0	100	100
15	3	73/98 (74%)	73 (100%)	0	100	100
16	C	338/362 (93%)	338 (100%)	0	100	100
17	A	251/289 (87%)	251 (100%)	0	100	100
18	1	31/87 (36%)	31 (100%)	0	100	100
All	All	1884/2167 (87%)	1884 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	317	ASN
1	B	343	HIS
2	D	186	GLN
2	D	220	ASN
3	E	53	ASN
7	K	40	GLN
14	G	95	GLN
17	A	75	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 72 ligands modelled in this entry, 1 is monoatomic - leaving 71 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$
26	VTQ	X	202	-	30,32,32	1.51	5 (16%)	39,44,44	0.95	1 (2%)
19	CLA	B	608	-	69,73,73	1.15	6 (8%)	82,113,113	1.09	4 (4%)
19	CLA	C	602	-	69,73,73	1.17	7 (10%)	82,113,113	1.09	4 (4%)
20	BCR	B	619	-	41,41,41	0.79	1 (2%)	56,56,56	2.05	20 (35%)
20	BCR	A	406	-	41,41,41	0.80	1 (2%)	56,56,56	1.92	18 (32%)
22	LHG	B	621	-	46,46,48	0.97	2 (4%)	49,52,54	0.96	2 (4%)
22	LHG	A	408	-	48,48,48	0.95	2 (4%)	51,54,54	0.95	2 (3%)
27	DGD	C	617	-	56,56,67	0.94	2 (3%)	70,70,81	0.98	4 (5%)
20	BCR	B	618	-	41,41,41	0.76	1 (2%)	56,56,56	2.01	20 (35%)
19	CLA	B	601	-	69,73,73	1.18	8 (11%)	82,113,113	1.10	6 (7%)
19	CLA	B	607	-	69,73,73	1.17	7 (10%)	82,113,113	1.08	5 (6%)
22	LHG	D	406	-	48,48,48	0.92	2 (4%)	51,54,54	0.98	2 (3%)
22	LHG	D	407	-	42,42,48	0.99	2 (4%)	45,48,54	1.07	3 (6%)
27	DGD	C	619	-	60,60,67	0.90	2 (3%)	74,74,81	0.88	2 (2%)
19	CLA	C	614	-	69,73,73	1.16	6 (8%)	82,113,113	1.12	5 (6%)
22	LHG	B	624	-	48,48,48	0.93	2 (4%)	51,54,54	0.99	3 (5%)
20	BCR	D	403	-	41,41,41	0.78	1 (2%)	56,56,56	2.17	22 (39%)
23	PL9	D	404	-	55,55,55	1.19	4 (7%)	68,69,69	1.51	12 (17%)
20	BCR	B	617	-	41,41,41	0.79	1 (2%)	56,56,56	1.98	20 (35%)
19	CLA	C	611	-	69,73,73	1.18	8 (11%)	82,113,113	1.09	3 (3%)
19	CLA	C	608	-	69,73,73	1.17	7 (10%)	82,113,113	1.20	5 (6%)
19	CLA	B	610	-	69,73,73	1.15	7 (10%)	82,113,113	1.16	5 (6%)
19	CLA	C	604	-	69,73,73	1.17	6 (8%)	82,113,113	1.14	7 (8%)
22	LHG	X	201	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	3 (5%)
28	SQD	C	620	-	49,51,54	1.16	3 (6%)	59,62,65	1.11	6 (10%)
24	PHO	D	410	-	58,69,69	2.12	11 (18%)	55,99,99	1.47	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	C	610	-	69,73,73	1.16	7 (10%)	82,113,113	1.14	3 (3%)
19	CLA	B	614	-	49,53,73	1.37	7 (14%)	58,89,113	1.26	4 (6%)
19	CLA	D	402	-	69,73,73	1.17	7 (10%)	82,113,113	1.10	4 (4%)
19	CLA	C	609	-	69,73,73	1.17	8 (11%)	82,113,113	1.05	5 (6%)
22	LHG	K	103	-	40,40,48	1.03	2 (5%)	43,46,54	1.01	3 (6%)
20	BCR	H	101	-	41,41,41	0.68	0	56,56,56	2.26	21 (37%)
29	BCT	A	401	30	3,3,3	1.12	0	2,3,3	4.18	1 (50%)
19	CLA	B	611	-	69,73,73	1.16	6 (8%)	82,113,113	1.10	5 (6%)
19	CLA	D	409	-	69,73,73	1.16	8 (11%)	82,113,113	1.07	6 (7%)
20	BCR	K	101	-	41,41,41	0.74	0	56,56,56	2.22	20 (35%)
27	DGD	C	618	-	58,58,67	0.92	2 (3%)	72,72,81	1.00	4 (5%)
19	CLA	A	403	-	69,73,73	1.17	8 (11%)	82,113,113	1.10	5 (6%)
19	CLA	C	606	-	69,73,73	1.15	8 (11%)	82,113,113	1.04	4 (4%)
19	CLA	B	605	-	69,73,73	1.16	7 (10%)	82,113,113	1.08	4 (4%)
24	PHO	D	411	-	58,69,69	2.13	11 (18%)	55,99,99	1.42	6 (10%)
21	LMG	C	601	-	49,49,55	0.97	2 (4%)	57,57,63	0.95	2 (3%)
19	CLA	B	616	-	69,73,73	1.15	8 (11%)	82,113,113	1.12	5 (6%)
19	CLA	C	605	-	69,73,73	1.17	7 (10%)	82,113,113	1.09	4 (4%)
21	LMG	D	408	-	46,46,55	1.00	2 (4%)	54,54,63	0.91	2 (3%)
19	CLA	B	615	-	69,73,73	1.16	7 (10%)	82,113,113	1.15	4 (4%)
19	CLA	B	609	-	69,73,73	1.16	6 (8%)	82,113,113	1.13	7 (8%)
19	CLA	B	603	-	69,73,73	1.16	7 (10%)	82,113,113	1.11	6 (7%)
21	LMG	B	623	-	48,48,55	0.98	2 (4%)	56,56,63	0.98	2 (3%)
22	LHG	L	101	-	48,48,48	0.95	2 (4%)	51,54,54	0.94	2 (3%)
19	CLA	B	612	-	69,73,73	1.17	8 (11%)	82,113,113	1.18	5 (6%)
19	CLA	B	613	-	69,73,73	1.17	7 (10%)	82,113,113	1.15	6 (7%)
19	CLA	C	613	-	69,73,73	1.16	6 (8%)	82,113,113	1.11	5 (6%)
19	CLA	A	404	-	53,57,73	1.31	7 (13%)	61,93,113	1.20	4 (6%)
20	BCR	C	616	-	41,41,41	0.80	1 (2%)	56,56,56	2.00	17 (30%)
19	CLA	B	604	-	69,73,73	1.16	7 (10%)	82,113,113	1.14	5 (6%)
21	LMG	B	620	-	46,46,55	1.00	2 (4%)	54,54,63	0.93	2 (3%)
21	LMG	K	102	-	51,51,55	0.96	3 (5%)	59,59,63	0.93	3 (5%)
19	CLA	A	405	-	64,68,73	1.21	7 (10%)	76,107,113	1.15	5 (6%)
22	LHG	D	405	-	43,43,48	1.00	2 (4%)	46,49,54	1.00	2 (4%)
19	CLA	C	603	-	69,73,73	1.16	8 (11%)	82,113,113	1.19	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	C	612	16	69,73,73	1.18	7 (10%)	82,113,113	1.08	4 (4%)
19	CLA	B	606	-	69,73,73	1.17	7 (10%)	82,113,113	1.06	6 (7%)
19	CLA	C	607	-	69,73,73	1.18	7 (10%)	82,113,113	1.11	6 (7%)
20	BCR	C	615	-	41,41,41	0.80	1 (2%)	56,56,56	2.31	23 (41%)
22	LHG	B	622	-	48,48,48	0.92	2 (4%)	51,54,54	0.94	2 (3%)
20	BCR	Z	101	-	41,41,41	0.83	1 (2%)	56,56,56	1.94	18 (32%)
21	LMG	A	407	-	48,48,55	1.00	3 (6%)	56,56,63	1.13	5 (8%)
19	CLA	D	401	-	69,73,73	1.17	7 (10%)	82,113,113	1.21	6 (7%)
19	CLA	B	602	-	69,73,73	1.16	8 (11%)	82,113,113	1.11	6 (7%)
25	HEM	E	101	3,4	50,50,50	1.45	8 (16%)	67,82,82	1.14	4 (5%)

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
26	VTQ	X	202	-	-	7/25/49/49	0/1/1/1
19	CLA	B	608	-	1/1/15/20	14/39/115/115	-
19	CLA	C	602	-	1/1/15/20	13/39/115/115	-
20	BCR	B	619	-	-	4/29/63/63	0/2/2/2
20	BCR	A	406	-	-	4/29/63/63	0/2/2/2
22	LHG	B	621	-	-	8/51/51/53	-
22	LHG	A	408	-	-	8/53/53/53	-
27	DGD	C	617	-	-	10/44/84/95	0/2/2/2
20	BCR	B	618	-	-	4/29/63/63	0/2/2/2
19	CLA	B	601	-	1/1/15/20	10/39/115/115	-
19	CLA	B	607	-	1/1/15/20	12/39/115/115	-
22	LHG	D	406	-	-	11/53/53/53	-
22	LHG	D	407	-	-	17/47/47/53	-
27	DGD	C	619	-	-	6/48/88/95	0/2/2/2
19	CLA	C	614	-	1/1/15/20	15/39/115/115	-
22	LHG	B	624	-	-	12/53/53/53	-
20	BCR	D	403	-	-	4/29/63/63	0/2/2/2
23	PL9	D	404	-	-	8/53/73/73	0/1/1/1
20	BCR	B	617	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	C	611	-	1/1/15/20	14/39/115/115	-
19	CLA	C	608	-	1/1/15/20	6/39/115/115	-
19	CLA	B	610	-	1/1/15/20	17/39/115/115	-
19	CLA	C	604	-	1/1/15/20	16/39/115/115	-
22	LHG	X	201	-	-	11/53/53/53	-
28	SQD	C	620	-	-	12/46/66/69	0/1/1/1
24	PHO	D	410	-	-	10/37/103/103	0/5/6/6
19	CLA	C	610	-	1/1/15/20	16/39/115/115	-
19	CLA	B	614	-	1/1/11/20	3/15/91/115	-
19	CLA	D	402	-	1/1/15/20	15/39/115/115	-
19	CLA	C	609	-	1/1/15/20	17/39/115/115	-
22	LHG	K	103	-	-	8/45/45/53	-
20	BCR	H	101	-	-	5/29/63/63	0/2/2/2
19	CLA	B	611	-	1/1/15/20	14/39/115/115	-
19	CLA	D	409	-	1/1/15/20	8/39/115/115	-
20	BCR	K	101	-	-	4/29/63/63	0/2/2/2
27	DGD	C	618	-	-	8/46/86/95	0/2/2/2
19	CLA	A	403	-	1/1/15/20	10/39/115/115	-
19	CLA	C	606	-	1/1/15/20	16/39/115/115	-
19	CLA	B	605	-	1/1/15/20	16/39/115/115	-
24	PHO	D	411	-	-	10/37/103/103	0/5/6/6
21	LMG	C	601	-	-	3/44/64/70	0/1/1/1
19	CLA	B	616	-	1/1/15/20	10/39/115/115	-
19	CLA	C	605	-	1/1/15/20	8/39/115/115	-
21	LMG	D	408	-	-	6/41/61/70	0/1/1/1
19	CLA	B	615	-	1/1/15/20	3/39/115/115	-
19	CLA	B	609	-	1/1/15/20	15/39/115/115	-
19	CLA	B	603	-	1/1/15/20	11/39/115/115	-
21	LMG	B	623	-	-	9/43/63/70	0/1/1/1
22	LHG	L	101	-	-	8/53/53/53	-
19	CLA	B	612	-	1/1/15/20	11/39/115/115	-
19	CLA	B	613	-	1/1/15/20	11/39/115/115	-
19	CLA	C	613	-	1/1/15/20	16/39/115/115	-
19	CLA	A	404	-	1/1/11/20	3/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	BCR	C	616	-	-	4/29/63/63	0/2/2/2
19	CLA	B	604	-	1/1/15/20	16/39/115/115	-
21	LMG	B	620	-	-	5/41/61/70	0/1/1/1
21	LMG	K	102	-	-	7/46/66/70	0/1/1/1
19	CLA	A	405	-	1/1/14/20	6/33/109/115	-
22	LHG	D	405	-	-	10/48/48/53	-
19	CLA	C	603	-	1/1/15/20	14/39/115/115	-
19	CLA	C	612	16	1/1/15/20	14/39/115/115	-
19	CLA	B	606	-	1/1/15/20	11/39/115/115	-
19	CLA	C	607	-	1/1/15/20	18/39/115/115	-
20	BCR	C	615	-	-	3/29/63/63	0/2/2/2
22	LHG	B	622	-	-	11/53/53/53	-
20	BCR	Z	101	-	-	4/29/63/63	0/2/2/2
21	LMG	A	407	-	-	10/43/63/70	0/1/1/1
19	CLA	D	401	-	1/1/15/20	16/39/115/115	-
19	CLA	B	602	-	1/1/15/20	7/39/115/115	-
25	HEM	E	101	3,4	-	3/14/54/54	-

All (339) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	411	PHO	C1B-C2B	9.53	1.50	1.39
24	D	410	PHO	C1B-C2B	9.29	1.49	1.39
24	D	411	PHO	C3B-C4B	8.29	1.49	1.41
24	D	410	PHO	C3B-C4B	8.28	1.49	1.41
28	C	620	SQD	O8-S	4.51	1.64	1.47
21	C	601	LMG	O8-C28	4.37	1.46	1.33
21	D	408	LMG	O8-C28	4.36	1.46	1.33
21	A	407	LMG	O8-C28	4.31	1.45	1.33
27	C	619	DGD	O1G-C1A	4.30	1.45	1.33
21	B	623	LMG	O8-C28	4.30	1.45	1.33
22	L	101	LHG	O8-C23	4.29	1.45	1.33
27	C	617	DGD	O1G-C1A	4.29	1.45	1.33
21	K	102	LMG	O7-C10	4.28	1.46	1.34
28	C	620	SQD	O48-C23	4.28	1.45	1.33
21	K	102	LMG	O8-C28	4.27	1.45	1.33
22	B	621	LHG	O8-C23	4.26	1.45	1.33
22	A	408	LHG	O8-C23	4.25	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	620	LMG	O7-C10	4.24	1.46	1.34
21	D	408	LMG	O7-C10	4.23	1.46	1.34
21	B	620	LMG	O8-C28	4.23	1.45	1.33
22	X	201	LHG	O8-C23	4.23	1.45	1.33
22	B	624	LHG	O8-C23	4.23	1.45	1.33
22	B	621	LHG	O7-C7	4.23	1.46	1.34
27	C	618	DGD	O2G-C1B	4.22	1.46	1.34
22	K	103	LHG	O8-C23	4.22	1.45	1.33
27	C	618	DGD	O1G-C1A	4.20	1.45	1.33
22	D	405	LHG	O8-C23	4.20	1.45	1.33
22	D	407	LHG	O8-C23	4.20	1.45	1.33
21	B	623	LMG	O7-C10	4.19	1.46	1.34
22	K	103	LHG	O7-C7	4.19	1.46	1.34
22	A	408	LHG	O7-C7	4.16	1.46	1.34
22	D	405	LHG	O7-C7	4.16	1.46	1.34
21	A	407	LMG	O7-C10	4.16	1.46	1.34
22	B	622	LHG	O8-C23	4.14	1.45	1.33
22	X	201	LHG	O7-C7	4.13	1.45	1.34
27	C	617	DGD	O2G-C1B	4.12	1.45	1.34
27	C	619	DGD	O2G-C1B	4.11	1.45	1.34
22	L	101	LHG	O7-C7	4.11	1.45	1.34
22	B	624	LHG	O7-C7	4.09	1.45	1.34
28	C	620	SQD	O47-C7	4.08	1.45	1.34
22	D	406	LHG	O7-C7	4.07	1.45	1.34
22	D	407	LHG	O7-C7	4.07	1.45	1.34
22	D	406	LHG	O8-C23	4.07	1.45	1.33
24	D	410	PHO	C1D-C2D	4.06	1.44	1.39
21	C	601	LMG	O7-C10	4.05	1.45	1.34
22	B	622	LHG	O7-C7	4.04	1.45	1.34
25	E	101	HEM	FE-NB	4.01	2.07	1.94
24	D	411	PHO	C1D-C2D	3.89	1.43	1.39
19	C	614	CLA	C1D-ND	3.63	1.42	1.37
19	A	405	CLA	C1D-ND	3.62	1.42	1.37
19	C	605	CLA	C1D-ND	3.62	1.42	1.37
19	B	601	CLA	C1D-ND	3.60	1.42	1.37
19	C	611	CLA	C1D-ND	3.60	1.42	1.37
23	D	404	PL9	C3-C4	-3.60	1.43	1.49
19	D	402	CLA	C1D-ND	3.59	1.42	1.37
19	C	608	CLA	C1D-ND	3.57	1.42	1.37
19	C	612	CLA	C1D-ND	3.57	1.42	1.37
19	B	614	CLA	C1D-ND	3.57	1.42	1.37
19	B	615	CLA	C1D-ND	3.56	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	607	CLA	C1D-ND	3.55	1.42	1.37
24	D	410	PHO	C4D-CHA	3.54	1.44	1.39
19	B	604	CLA	C1D-ND	3.54	1.42	1.37
19	B	606	CLA	C1D-ND	3.53	1.42	1.37
19	C	609	CLA	C1D-ND	3.51	1.42	1.37
19	C	607	CLA	C1D-ND	3.50	1.42	1.37
19	A	404	CLA	C1D-ND	3.49	1.42	1.37
19	C	610	CLA	C1D-ND	3.49	1.42	1.37
19	C	604	CLA	C1D-ND	3.48	1.42	1.37
19	D	409	CLA	C1D-ND	3.48	1.42	1.37
19	B	609	CLA	C1D-ND	3.48	1.42	1.37
19	C	606	CLA	C1D-ND	3.48	1.42	1.37
24	D	411	PHO	C4D-CHA	3.47	1.44	1.39
19	B	616	CLA	C1D-ND	3.47	1.42	1.37
19	C	613	CLA	C1D-ND	3.47	1.42	1.37
25	E	101	HEM	FE-NA	3.47	2.06	1.95
19	C	602	CLA	C1D-ND	3.44	1.42	1.37
19	B	610	CLA	C1D-ND	3.44	1.42	1.37
19	A	403	CLA	C1D-ND	3.43	1.42	1.37
19	B	613	CLA	C1D-ND	3.43	1.42	1.37
19	B	611	CLA	C1D-ND	3.43	1.42	1.37
19	B	608	CLA	C1D-ND	3.41	1.42	1.37
19	C	609	CLA	C4B-NB	3.41	1.42	1.37
19	C	604	CLA	C4B-NB	3.40	1.42	1.37
19	B	612	CLA	C1D-ND	3.39	1.42	1.37
19	B	603	CLA	C1D-ND	3.38	1.42	1.37
19	B	602	CLA	C1D-ND	3.38	1.42	1.37
19	D	401	CLA	C1D-ND	3.36	1.42	1.37
19	C	603	CLA	C1D-ND	3.36	1.42	1.37
19	C	607	CLA	C4B-NB	3.35	1.42	1.37
19	C	612	CLA	C4B-NB	3.35	1.42	1.37
19	B	605	CLA	C1D-ND	3.35	1.42	1.37
19	C	611	CLA	C4B-NB	3.35	1.42	1.37
19	D	409	CLA	C4B-NB	3.34	1.42	1.37
19	C	605	CLA	C4B-NB	3.33	1.42	1.37
19	A	404	CLA	C4B-NB	3.32	1.42	1.37
19	B	603	CLA	C4B-NB	3.28	1.42	1.37
19	C	614	CLA	C4B-NB	3.27	1.42	1.37
19	B	601	CLA	C4B-NB	3.26	1.42	1.37
26	X	202	VTQ	O3-C9	-3.26	1.39	1.44
19	B	607	CLA	C4B-NB	3.25	1.42	1.37
19	C	606	CLA	C4B-NB	3.23	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	609	CLA	C4B-NB	3.22	1.42	1.37
19	A	405	CLA	C4B-NB	3.22	1.42	1.37
19	D	402	CLA	C4B-NB	3.21	1.42	1.37
19	B	606	CLA	C4B-NB	3.19	1.42	1.37
19	C	613	CLA	C4B-NB	3.17	1.42	1.37
19	B	605	CLA	C4B-NB	3.16	1.42	1.37
19	B	611	CLA	C4B-NB	3.16	1.42	1.37
19	A	403	CLA	C4B-NB	3.16	1.42	1.37
19	B	604	CLA	C4B-NB	3.14	1.42	1.37
19	B	613	CLA	C4B-NB	3.14	1.42	1.37
19	C	610	CLA	C4B-NB	3.13	1.42	1.37
23	D	404	PL9	C7-C3	-3.12	1.47	1.51
19	B	612	CLA	C4B-NB	3.12	1.42	1.37
19	C	602	CLA	C4B-NB	3.10	1.41	1.37
19	B	616	CLA	C4B-NB	3.09	1.41	1.37
19	B	602	CLA	C4B-NB	3.07	1.41	1.37
19	C	608	CLA	C4B-NB	3.07	1.41	1.37
19	D	401	CLA	C4B-NB	3.07	1.41	1.37
25	E	101	HEM	FE-ND	3.06	2.04	1.94
19	B	615	CLA	C4B-NB	3.05	1.41	1.37
19	C	603	CLA	C4B-NB	3.05	1.41	1.37
19	B	614	CLA	C4B-NB	3.04	1.41	1.37
19	B	608	CLA	C4B-NB	2.99	1.41	1.37
25	E	101	HEM	CAB-C3B	2.97	1.55	1.47
25	E	101	HEM	CAC-C3C	2.93	1.55	1.47
19	B	610	CLA	C4B-NB	2.91	1.41	1.37
23	D	404	PL9	C6-C1	-2.89	1.43	1.48
19	B	605	CLA	C1B-C2B	2.83	1.49	1.43
24	D	411	PHO	CMD-C2D	-2.80	1.46	1.51
19	B	607	CLA	C1B-C2B	2.79	1.49	1.43
19	B	608	CLA	C1B-C2B	2.78	1.49	1.43
19	A	405	CLA	C1B-C2B	2.73	1.49	1.43
19	C	612	CLA	C1B-C2B	2.72	1.49	1.43
19	C	614	CLA	C1B-C2B	2.72	1.49	1.43
19	C	602	CLA	C1B-C2B	2.72	1.49	1.43
19	C	605	CLA	C1B-C2B	2.72	1.49	1.43
19	B	610	CLA	C1B-C2B	2.72	1.49	1.43
19	C	606	CLA	C1B-C2B	2.72	1.49	1.43
19	C	604	CLA	C1B-C2B	2.71	1.49	1.43
19	B	614	CLA	C1B-C2B	2.71	1.49	1.43
19	B	612	CLA	C1B-C2B	2.70	1.49	1.43
19	B	615	CLA	C1B-C2B	2.70	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	610	CLA	C1B-C2B	2.70	1.49	1.43
19	C	611	CLA	C1B-C2B	2.69	1.49	1.43
19	B	616	CLA	C1B-C2B	2.68	1.49	1.43
19	B	611	CLA	C1B-C2B	2.68	1.49	1.43
19	C	608	CLA	C1B-C2B	2.67	1.49	1.43
19	A	403	CLA	C1B-C2B	2.67	1.49	1.43
19	D	402	CLA	C1B-C2B	2.66	1.49	1.43
19	B	604	CLA	C1B-C2B	2.66	1.49	1.43
25	E	101	HEM	FE-NC	2.66	2.03	1.95
19	B	601	CLA	C1B-C2B	2.65	1.49	1.43
19	B	606	CLA	C1B-C2B	2.64	1.49	1.43
19	B	613	CLA	C1B-C2B	2.64	1.49	1.43
19	C	609	CLA	C1B-C2B	2.63	1.49	1.43
19	B	602	CLA	C1B-C2B	2.61	1.49	1.43
24	D	410	PHO	CMC-C2C	-2.61	1.46	1.50
24	D	410	PHO	CMD-C2D	-2.60	1.46	1.51
24	D	410	PHO	CMB-C2B	-2.60	1.46	1.51
19	B	609	CLA	C1B-C2B	2.60	1.49	1.43
24	D	411	PHO	CMC-C2C	-2.59	1.46	1.50
19	C	613	CLA	C1B-C2B	2.58	1.49	1.43
19	C	603	CLA	C1B-C2B	2.58	1.49	1.43
19	A	404	CLA	C1B-C2B	2.57	1.49	1.43
19	D	401	CLA	C1B-C2B	2.55	1.49	1.43
26	X	202	VTQ	C10-C3	2.54	1.57	1.51
19	B	603	CLA	C1B-C2B	2.51	1.49	1.43
24	D	410	PHO	CAC-C3C	-2.51	1.47	1.51
26	X	202	VTQ	C3-C4	2.48	1.53	1.46
20	C	616	BCR	C1-C6	-2.47	1.50	1.53
19	C	607	CLA	C1B-C2B	2.45	1.48	1.43
24	D	411	PHO	CMB-C2B	-2.44	1.46	1.51
19	D	409	CLA	C1B-C2B	2.42	1.48	1.43
19	D	409	CLA	C3B-C4B	2.42	1.49	1.42
19	B	613	CLA	C3B-C4B	2.40	1.49	1.42
19	C	609	CLA	C3B-C4B	2.38	1.49	1.42
19	C	607	CLA	CMB-C2B	-2.37	1.45	1.50
19	B	612	CLA	CMD-C2D	-2.37	1.45	1.50
24	D	411	PHO	CAC-C3C	-2.36	1.47	1.51
19	C	614	CLA	C3B-C4B	2.35	1.49	1.42
19	C	613	CLA	C3B-C4B	2.34	1.49	1.42
19	D	409	CLA	CMD-C2D	-2.33	1.46	1.50
19	D	401	CLA	CHC-C1C	2.33	1.43	1.38
19	B	614	CLA	C3B-C4B	2.33	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	610	CLA	C3B-C4B	2.32	1.49	1.42
19	B	602	CLA	C3B-C4B	2.31	1.49	1.42
19	A	403	CLA	C3B-C4B	2.31	1.49	1.42
19	D	401	CLA	C3B-C4B	2.30	1.49	1.42
19	C	607	CLA	C3B-C4B	2.30	1.49	1.42
19	B	603	CLA	C3B-C4B	2.29	1.49	1.42
19	C	606	CLA	C3B-C4B	2.29	1.49	1.42
19	C	611	CLA	C3B-C4B	2.27	1.49	1.42
19	B	607	CLA	C3B-C4B	2.27	1.49	1.42
19	C	612	CLA	C3B-C4B	2.26	1.49	1.42
19	B	613	CLA	CHC-C1C	2.26	1.43	1.38
20	A	406	BCR	C30-C25	-2.26	1.50	1.53
19	C	605	CLA	C3B-C4B	2.26	1.49	1.42
24	D	410	PHO	C3D-C4D	2.25	1.44	1.41
19	C	602	CLA	CMD-C2D	-2.25	1.46	1.50
23	D	404	PL9	C53-C6	-2.25	1.46	1.50
19	C	608	CLA	C3B-C4B	2.25	1.49	1.42
19	B	616	CLA	C3B-C4B	2.25	1.49	1.42
19	B	602	CLA	CMD-C2D	-2.24	1.46	1.50
19	B	601	CLA	C3B-C4B	2.24	1.49	1.42
19	A	403	CLA	CMD-C2D	-2.24	1.46	1.50
21	A	407	LMG	O1-C1	2.24	1.43	1.40
19	B	608	CLA	CMD-C2D	-2.23	1.46	1.50
19	B	609	CLA	C3B-C4B	2.23	1.49	1.42
19	A	404	CLA	C3B-C4B	2.23	1.49	1.42
19	C	603	CLA	CMD-C2D	-2.23	1.46	1.50
19	C	603	CLA	C3B-C4B	2.22	1.49	1.42
20	Z	101	BCR	C1-C6	-2.22	1.50	1.53
19	B	604	CLA	C3B-C4B	2.22	1.49	1.42
19	B	603	CLA	CMB-C2B	-2.21	1.46	1.50
19	B	601	CLA	CMD-C2D	-2.21	1.46	1.50
19	B	612	CLA	C3B-C4B	2.21	1.49	1.42
19	B	603	CLA	CMD-C2D	-2.21	1.46	1.50
19	D	409	CLA	CMB-C2B	-2.20	1.46	1.50
19	C	604	CLA	C3B-C4B	2.20	1.49	1.42
24	D	411	PHO	C3D-C4D	2.20	1.44	1.41
19	B	612	CLA	CMB-C2B	-2.20	1.46	1.50
19	B	605	CLA	CMB-C2B	-2.20	1.46	1.50
19	D	401	CLA	CMD-C2D	-2.20	1.46	1.50
19	A	405	CLA	C3B-C4B	2.19	1.49	1.42
19	B	606	CLA	CMD-C2D	-2.19	1.46	1.50
19	B	605	CLA	CMD-C2D	-2.18	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	612	CLA	CMB-C2B	-2.18	1.46	1.50
19	C	611	CLA	CHC-C1C	2.18	1.42	1.38
19	B	613	CLA	CMD-C2D	-2.17	1.46	1.50
19	A	404	CLA	CMD-C2D	-2.17	1.46	1.50
19	B	615	CLA	C3B-C4B	2.17	1.49	1.42
19	C	606	CLA	CMD-C2D	-2.17	1.46	1.50
19	B	611	CLA	CMD-C2D	-2.16	1.46	1.50
19	A	404	CLA	CMB-C2B	-2.16	1.46	1.50
24	D	411	PHO	C4D-ND	-2.16	1.35	1.38
19	B	602	CLA	CHC-C1C	2.16	1.42	1.38
19	B	610	CLA	CMD-C2D	-2.16	1.46	1.50
19	C	602	CLA	CMB-C2B	-2.16	1.46	1.50
19	B	614	CLA	CMD-C2D	-2.15	1.46	1.50
19	D	402	CLA	C3B-C4B	2.15	1.49	1.42
19	B	611	CLA	C3B-C4B	2.15	1.49	1.42
19	C	602	CLA	C3B-C4B	2.15	1.49	1.42
19	C	611	CLA	CMD-C2D	-2.15	1.46	1.50
19	B	606	CLA	C3B-C4B	2.15	1.49	1.42
20	B	619	BCR	C1-C6	-2.15	1.51	1.53
24	D	410	PHO	C4D-ND	-2.14	1.35	1.38
19	B	606	CLA	CMB-C2B	-2.14	1.46	1.50
20	B	618	BCR	C1-C6	-2.14	1.51	1.53
19	C	613	CLA	CMD-C2D	-2.14	1.46	1.50
26	X	202	VTQ	C5-C4	2.14	1.54	1.47
19	A	403	CLA	CMC-C2C	-2.14	1.46	1.50
19	B	604	CLA	CMC-C2C	-2.14	1.46	1.50
19	C	612	CLA	CMC-C2C	-2.13	1.46	1.50
19	D	402	CLA	CMD-C2D	-2.13	1.46	1.50
19	B	610	CLA	C3B-C4B	2.12	1.48	1.42
19	B	615	CLA	CMB-C2B	-2.12	1.46	1.50
19	C	610	CLA	CMD-C2D	-2.12	1.46	1.50
19	B	616	CLA	CMD-C2D	-2.12	1.46	1.50
19	B	607	CLA	CMD-C2D	-2.12	1.46	1.50
19	B	608	CLA	C3B-C4B	2.11	1.48	1.42
19	C	608	CLA	CHC-C1C	2.11	1.42	1.38
19	B	611	CLA	CMB-C2B	-2.11	1.46	1.50
19	B	610	CLA	CMB-C2B	-2.11	1.46	1.50
19	B	610	CLA	CMC-C2C	-2.11	1.46	1.50
19	B	615	CLA	CMD-C2D	-2.10	1.46	1.50
19	C	609	CLA	CMB-C2B	-2.10	1.46	1.50
19	D	409	CLA	CHC-C1C	2.10	1.42	1.38
19	B	616	CLA	CMB-C2B	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	405	CLA	CMB-C2B	-2.10	1.46	1.50
19	A	405	CLA	CMD-C2D	-2.10	1.46	1.50
19	D	402	CLA	CMB-C2B	-2.09	1.46	1.50
19	B	607	CLA	CHC-C1C	2.09	1.42	1.38
20	D	403	BCR	C30-C25	-2.09	1.51	1.53
19	C	607	CLA	CHC-C1C	2.09	1.42	1.38
19	C	609	CLA	CMD-C2D	-2.09	1.46	1.50
24	D	410	PHO	C3B-C2B	-2.09	1.37	1.40
19	C	614	CLA	CMD-C2D	-2.08	1.46	1.50
19	C	610	CLA	CMC-C2C	-2.08	1.46	1.50
19	C	603	CLA	CMB-C2B	-2.08	1.46	1.50
19	B	614	CLA	CHC-C1C	2.08	1.42	1.38
19	C	607	CLA	CMD-C2D	-2.08	1.46	1.50
19	B	603	CLA	CHC-C1C	2.08	1.42	1.38
19	B	608	CLA	CMB-C2B	-2.08	1.46	1.50
21	K	102	LMG	O1-C1	2.08	1.43	1.40
26	X	202	VTQ	O1-C4	-2.08	1.18	1.23
20	C	615	BCR	C30-C25	-2.07	1.51	1.53
19	B	601	CLA	CHC-C1C	2.07	1.42	1.38
19	C	603	CLA	CHC-C1C	2.07	1.42	1.38
19	B	604	CLA	CMD-C2D	-2.07	1.46	1.50
19	B	616	CLA	CHC-C1C	2.07	1.42	1.38
19	C	608	CLA	CMD-C2D	-2.07	1.46	1.50
20	B	617	BCR	C30-C25	-2.07	1.51	1.53
19	C	609	CLA	CHC-C1C	2.07	1.42	1.38
19	A	403	CLA	CHC-C1C	2.07	1.42	1.38
19	C	605	CLA	CMB-C2B	-2.07	1.46	1.50
19	B	615	CLA	CMC-C2C	-2.06	1.46	1.50
19	A	404	CLA	CMC-C2C	-2.06	1.46	1.50
19	B	609	CLA	CMD-C2D	-2.06	1.46	1.50
19	B	609	CLA	CMB-C2B	-2.06	1.46	1.50
19	D	401	CLA	CMB-C2B	-2.06	1.46	1.50
19	C	605	CLA	CMC-C2C	-2.06	1.46	1.50
19	C	603	CLA	CMC-C2C	-2.06	1.46	1.50
19	C	605	CLA	CMD-C2D	-2.06	1.46	1.50
19	C	614	CLA	CHC-C1C	2.06	1.42	1.38
19	B	604	CLA	CMB-C2B	-2.06	1.46	1.50
19	C	612	CLA	CMD-C2D	-2.05	1.46	1.50
19	C	613	CLA	CHC-C1C	2.05	1.42	1.38
24	D	411	PHO	C3B-C2B	-2.05	1.37	1.40
19	C	611	CLA	CMB-C2B	-2.05	1.46	1.50
19	B	613	CLA	CMB-C2B	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	606	CLA	CMC-C2C	-2.04	1.46	1.50
19	C	606	CLA	CHC-C1C	2.04	1.42	1.38
19	C	604	CLA	CHC-C1C	2.04	1.42	1.38
19	B	614	CLA	CMB-C2B	-2.04	1.46	1.50
19	C	609	CLA	CMC-C2C	-2.04	1.46	1.50
19	B	612	CLA	CHC-C1C	2.04	1.42	1.38
19	B	602	CLA	CMB-C2B	-2.04	1.46	1.50
19	A	403	CLA	CMB-C2B	-2.04	1.46	1.50
19	C	604	CLA	CMD-C2D	-2.03	1.46	1.50
19	B	601	CLA	CMB-C2B	-2.03	1.46	1.50
19	B	607	CLA	CMC-C2C	-2.03	1.46	1.50
19	D	402	CLA	CMC-C2C	-2.03	1.46	1.50
19	B	602	CLA	CMC-C2C	-2.02	1.46	1.50
19	C	608	CLA	CMB-C2B	-2.02	1.46	1.50
19	B	616	CLA	CMC-C2C	-2.02	1.46	1.50
19	C	610	CLA	CMB-C2B	-2.02	1.46	1.50
19	C	602	CLA	CHC-C1C	2.02	1.42	1.38
19	B	601	CLA	CMC-C2C	-2.02	1.46	1.50
19	B	606	CLA	CMC-C2C	-2.02	1.46	1.50
19	B	605	CLA	C3B-C4B	2.02	1.48	1.42
19	C	611	CLA	CMC-C2C	-2.01	1.46	1.50
19	B	605	CLA	CMC-C2C	-2.01	1.46	1.50
19	A	405	CLA	CMC-C2C	-2.01	1.46	1.50
19	C	606	CLA	CMB-C2B	-2.01	1.46	1.50
19	D	409	CLA	CMC-C2C	-2.01	1.46	1.50
25	E	101	HEM	CMC-C2C	2.01	1.54	1.50
19	B	612	CLA	CMC-C2C	-2.01	1.46	1.50
25	E	101	HEM	CMB-C2B	2.00	1.54	1.50

All (460) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	615	BCR	C30-C25-C26	-6.12	114.27	122.64
20	C	615	BCR	C3-C4-C5	-5.86	103.60	114.06
19	B	612	CLA	C4A-NA-C1A	5.86	109.35	106.68
19	C	608	CLA	C4A-NA-C1A	5.63	109.25	106.68
29	A	401	BCT	O2-C-O1	5.58	133.94	119.68
24	D	410	PHO	C4D-CHA-CBD	-5.52	105.81	108.45
24	D	411	PHO	C4D-CHA-CBD	-5.39	105.87	108.45
20	K	101	BCR	C3-C4-C5	-5.36	104.49	114.06
20	H	101	BCR	C28-C27-C26	-5.34	104.53	114.06
20	K	101	BCR	C28-C27-C26	-5.28	104.63	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	101	BCR	C3-C4-C5	-5.27	104.67	114.06
20	H	101	BCR	C7-C8-C9	-5.26	118.45	126.23
19	C	603	CLA	C4A-NA-C1A	5.25	109.07	106.68
19	B	610	CLA	C4A-NA-C1A	5.23	109.06	106.68
20	B	618	BCR	C28-C27-C26	-5.21	104.77	114.06
19	C	610	CLA	C4A-NA-C1A	5.16	109.03	106.68
23	D	404	PL9	C7-C3-C4	5.09	121.10	116.91
19	D	401	CLA	C4A-NA-C1A	5.03	108.97	106.68
20	D	403	BCR	C30-C25-C26	-5.02	115.78	122.64
19	C	602	CLA	C4A-NA-C1A	4.98	108.95	106.68
20	D	403	BCR	C1-C6-C5	-4.92	115.92	122.64
19	B	605	CLA	C4A-NA-C1A	4.91	108.92	106.68
19	C	614	CLA	C4A-NA-C1A	4.86	108.90	106.68
19	B	613	CLA	C4A-NA-C1A	4.82	108.88	106.68
19	B	616	CLA	C4A-NA-C1A	4.81	108.87	106.68
20	B	619	BCR	C28-C27-C26	-4.66	105.74	114.06
19	B	615	CLA	C4A-NA-C1A	4.63	108.79	106.68
19	C	605	CLA	C4A-NA-C1A	4.57	108.76	106.68
20	Z	101	BCR	C1-C6-C5	-4.55	116.41	122.64
19	C	611	CLA	C4A-NA-C1A	4.53	108.75	106.68
21	A	407	LMG	O7-C10-C11	4.52	121.26	111.48
19	B	614	CLA	C4A-NA-C1A	4.44	108.70	106.68
20	B	619	BCR	C30-C25-C26	-4.42	116.60	122.64
19	B	607	CLA	C4A-NA-C1A	4.40	108.69	106.68
19	A	405	CLA	C4A-NA-C1A	4.38	108.68	106.68
20	Z	101	BCR	C33-C5-C6	-4.37	119.72	124.48
19	C	613	CLA	C4A-NA-C1A	4.28	108.63	106.68
19	B	611	CLA	C4A-NA-C1A	4.26	108.62	106.68
20	K	101	BCR	C30-C25-C26	-4.26	116.82	122.64
20	C	616	BCR	C28-C27-C26	-4.24	106.50	114.06
20	B	617	BCR	C1-C6-C5	-4.23	116.86	122.64
20	C	615	BCR	C33-C5-C6	-4.17	119.94	124.48
19	A	403	CLA	C4A-NA-C1A	4.16	108.58	106.68
20	D	403	BCR	C3-C4-C5	-4.13	106.69	114.06
22	X	201	LHG	O7-C7-C8	4.13	120.41	111.48
20	C	615	BCR	C1-C6-C5	-4.12	117.00	122.64
19	B	601	CLA	C4A-NA-C1A	4.12	108.56	106.68
19	B	608	CLA	C4A-NA-C1A	4.12	108.56	106.68
19	B	604	CLA	C4A-NA-C1A	4.11	108.56	106.68
19	C	609	CLA	C4A-NA-C1A	4.06	108.53	106.68
19	C	612	CLA	C4A-NA-C1A	4.04	108.52	106.68
20	B	617	BCR	C36-C18-C19	4.01	124.21	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	602	CLA	C4A-NA-C1A	4.00	108.50	106.68
20	H	101	BCR	C20-C21-C22	-3.98	121.69	127.28
20	C	616	BCR	C33-C5-C6	-3.98	120.14	124.48
20	K	101	BCR	C37-C22-C23	3.95	124.13	118.09
23	D	404	PL9	C7-C3-C2	-3.95	118.73	123.39
21	B	623	LMG	O7-C10-C11	3.95	120.03	111.48
22	D	407	LHG	O7-C7-C8	3.93	119.99	111.48
24	D	411	PHO	C2B-C1B-NB	-3.92	106.60	109.43
22	B	624	LHG	O7-C7-C8	3.90	119.92	111.48
19	C	607	CLA	C4A-NA-C1A	3.89	108.45	106.68
20	H	101	BCR	C27-C26-C25	-3.89	117.45	122.70
20	K	101	BCR	C16-C17-C18	-3.86	121.86	127.28
20	A	406	BCR	C20-C21-C22	-3.86	121.87	127.28
19	B	603	CLA	C4A-NA-C1A	3.85	108.44	106.68
20	H	101	BCR	C4-C5-C6	-3.84	117.52	122.70
19	B	606	CLA	C4A-NA-C1A	3.83	108.43	106.68
22	K	103	LHG	O7-C7-C8	3.83	119.77	111.48
19	D	402	CLA	C4A-NA-C1A	3.82	108.42	106.68
22	D	405	LHG	O7-C7-C8	3.81	119.72	111.48
20	C	616	BCR	C20-C21-C22	-3.81	121.94	127.28
19	A	404	CLA	C4A-NA-C1A	3.79	108.41	106.68
20	A	406	BCR	C38-C26-C25	-3.79	120.35	124.48
27	C	617	DGD	O2G-C1B-C2B	3.77	119.64	111.48
20	B	618	BCR	C36-C18-C19	3.77	123.84	118.09
20	B	618	BCR	C33-C5-C6	-3.77	120.37	124.48
20	B	619	BCR	C20-C21-C22	-3.77	122.00	127.28
28	C	620	SQD	O47-C7-C8	3.74	119.58	111.48
24	D	410	PHO	C2B-C1B-NB	-3.73	106.73	109.43
19	D	401	CLA	O2D-CGD-O1D	-3.73	116.59	123.85
20	D	403	BCR	C4-C5-C6	-3.73	117.66	122.70
20	A	406	BCR	C3-C4-C5	-3.73	107.41	114.06
22	B	621	LHG	O7-C7-C8	3.73	119.54	111.48
22	A	408	LHG	O7-C7-C8	3.72	119.54	111.48
21	K	102	LMG	O7-C10-C11	3.71	119.50	111.48
20	D	403	BCR	C20-C21-C22	-3.71	122.08	127.28
20	D	403	BCR	C16-C17-C18	-3.70	122.09	127.28
27	C	618	DGD	O2G-C1B-C2B	3.70	119.49	111.48
20	Z	101	BCR	C37-C22-C23	3.69	123.72	118.09
20	H	101	BCR	C16-C17-C18	-3.69	122.11	127.28
20	B	617	BCR	C37-C22-C23	3.66	123.68	118.09
19	C	604	CLA	C4A-NA-C1A	3.64	108.34	106.68
20	B	619	BCR	C16-C17-C18	-3.62	122.20	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	406	BCR	C30-C25-C26	-3.61	117.71	122.64
20	C	615	BCR	C1-C6-C7	3.60	125.42	115.65
20	A	406	BCR	C16-C17-C18	-3.59	122.24	127.28
21	C	601	LMG	O7-C10-C11	3.57	119.19	111.48
20	H	101	BCR	C36-C18-C19	3.57	123.53	118.09
21	D	408	LMG	O7-C10-C11	3.57	119.19	111.48
20	B	619	BCR	C36-C18-C19	3.56	123.53	118.09
22	D	406	LHG	O7-C7-C8	3.56	119.18	111.48
20	H	101	BCR	C37-C22-C23	3.56	123.53	118.09
20	B	619	BCR	C7-C8-C9	-3.55	120.98	126.23
20	B	618	BCR	C37-C22-C23	3.55	123.51	118.09
20	A	406	BCR	C7-C8-C9	-3.54	121.00	126.23
20	H	101	BCR	C11-C10-C9	-3.53	122.33	127.28
20	B	618	BCR	C20-C21-C22	-3.52	122.35	127.28
20	B	619	BCR	C33-C5-C6	-3.51	120.65	124.48
20	C	616	BCR	C24-C23-C22	-3.51	121.04	126.23
20	C	615	BCR	C38-C26-C25	-3.51	120.66	124.48
19	D	409	CLA	C4A-NA-C1A	3.51	108.28	106.68
19	A	405	CLA	O2D-CGD-O1D	-3.50	117.04	123.85
20	B	617	BCR	C38-C26-C25	-3.49	120.67	124.48
20	K	101	BCR	C7-C8-C9	-3.49	121.07	126.23
20	C	616	BCR	C29-C30-C25	3.48	115.50	110.44
21	B	620	LMG	O7-C10-C11	3.48	119.00	111.48
20	B	617	BCR	C20-C21-C22	-3.46	122.42	127.28
20	B	619	BCR	C37-C22-C23	3.45	123.36	118.09
20	C	615	BCR	C28-C27-C26	-3.44	107.92	114.06
19	B	614	CLA	O2D-CGD-O1D	-3.43	117.17	123.85
20	C	616	BCR	C1-C6-C5	-3.43	117.95	122.64
20	K	101	BCR	C36-C18-C19	3.43	123.32	118.09
20	H	101	BCR	C2-C1-C6	3.43	115.42	110.44
20	B	619	BCR	C1-C6-C5	-3.41	117.98	122.64
20	A	406	BCR	C24-C23-C22	-3.40	121.20	126.23
20	C	615	BCR	C33-C5-C4	3.40	120.85	113.60
20	D	403	BCR	C37-C22-C23	3.39	123.27	118.09
19	B	608	CLA	O2D-CGD-O1D	-3.38	117.28	123.85
19	A	404	CLA	O2D-CGD-O1D	-3.37	117.28	123.85
20	D	403	BCR	C36-C18-C19	3.37	123.23	118.09
27	C	619	DGD	O2G-C1B-C2B	3.37	118.77	111.48
19	B	611	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
19	C	613	CLA	O2D-CGD-O1D	-3.34	117.34	123.85
20	A	406	BCR	C11-C10-C9	-3.34	122.59	127.28
20	B	618	BCR	C30-C25-C26	-3.34	118.07	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	406	BCR	C36-C18-C19	3.34	123.19	118.09
19	B	602	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
22	L	101	LHG	O7-C7-C8	3.32	118.66	111.48
20	C	616	BCR	C16-C17-C18	-3.31	122.63	127.28
20	Z	101	BCR	C36-C18-C19	3.31	123.14	118.09
20	Z	101	BCR	C33-C5-C4	3.31	120.64	113.60
20	D	403	BCR	C28-C27-C26	-3.30	108.17	114.06
19	C	610	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
22	B	622	LHG	O7-C7-C8	3.30	118.62	111.48
20	B	617	BCR	C15-C16-C17	-3.29	116.79	123.52
20	C	616	BCR	C36-C18-C19	3.29	123.11	118.09
20	B	618	BCR	C7-C8-C9	-3.29	121.37	126.23
19	B	609	CLA	C4A-NA-C1A	3.29	108.18	106.68
20	B	617	BCR	C3-C4-C5	-3.27	108.22	114.06
20	K	101	BCR	C27-C26-C25	-3.26	118.29	122.70
19	B	606	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
19	B	612	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
19	B	615	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
20	C	616	BCR	C7-C8-C9	-3.25	121.43	126.23
19	B	603	CLA	O2D-CGD-O1D	-3.25	117.53	123.85
24	D	410	PHO	O1D-CGD-CBD	3.24	129.64	124.72
20	C	615	BCR	C37-C22-C23	3.24	123.03	118.09
20	D	403	BCR	C27-C26-C25	-3.23	118.34	122.70
24	D	411	PHO	O1D-CGD-CBD	3.22	129.61	124.72
19	C	612	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
19	D	402	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
19	B	610	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
20	C	615	BCR	C36-C18-C19	3.17	122.93	118.09
19	C	608	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
19	C	603	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
19	B	604	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
19	C	606	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
20	K	101	BCR	C1-C6-C5	-3.10	118.40	122.64
20	D	403	BCR	C38-C26-C27	3.10	120.20	113.60
28	C	620	SQD	O48-C23-C24	3.09	121.27	111.83
20	B	618	BCR	C1-C6-C5	-3.09	118.41	122.64
19	C	605	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
20	B	617	BCR	C4-C5-C6	-3.07	118.55	122.70
20	B	619	BCR	C38-C26-C25	-3.07	121.13	124.48
20	K	101	BCR	C20-C21-C22	-3.07	122.98	127.28
19	B	607	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
19	C	609	CLA	O2D-CGD-O1D	-3.05	117.91	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	617	BCR	C30-C25-C26	-3.03	118.49	122.64
26	X	202	VTQ	C10-C11-C9	-3.03	110.53	118.08
21	A	407	LMG	O8-C28-C29	3.02	121.06	111.83
20	Z	101	BCR	C20-C21-C22	-3.02	123.04	127.28
20	Z	101	BCR	C3-C4-C5	-3.01	108.69	114.06
24	D	410	PHO	C1-C2-C3	-3.00	121.28	126.20
20	D	403	BCR	C33-C5-C4	3.00	119.99	113.60
19	C	611	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
20	B	618	BCR	C16-C17-C18	-2.97	123.11	127.28
19	B	616	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
20	B	619	BCR	C38-C26-C27	2.96	119.90	113.60
20	Z	101	BCR	C16-C17-C18	-2.95	123.14	127.28
20	C	616	BCR	C37-C22-C23	2.95	122.59	118.09
19	C	602	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
20	C	615	BCR	C7-C8-C9	-2.94	121.88	126.23
20	B	619	BCR	C27-C26-C25	-2.94	118.73	122.70
20	Z	101	BCR	C29-C30-C25	2.94	114.70	110.44
19	C	606	CLA	C4A-NA-C1A	2.93	108.02	106.68
20	A	406	BCR	C1-C6-C5	-2.93	118.63	122.64
20	D	403	BCR	C38-C26-C25	-2.93	121.29	124.48
19	D	409	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
21	C	601	LMG	O8-C28-C29	2.91	120.71	111.83
19	C	604	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
23	D	404	PL9	C22-C23-C24	-2.90	120.98	127.62
25	E	101	HEM	C3B-C2B-C1B	2.89	108.58	106.41
20	K	101	BCR	C16-C15-C14	-2.89	117.61	123.52
19	B	601	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
20	C	615	BCR	C38-C26-C27	2.88	119.74	113.60
20	K	101	BCR	C38-C26-C27	2.88	119.74	113.60
20	B	617	BCR	C33-C5-C4	2.88	119.73	113.60
20	B	617	BCR	C7-C8-C9	-2.87	122.00	126.23
20	B	618	BCR	C15-C16-C17	-2.85	117.68	123.52
19	B	613	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
24	D	410	PHO	O2D-CGD-O1D	-2.84	118.31	123.85
20	B	618	BCR	C27-C26-C25	-2.84	118.87	122.70
20	A	406	BCR	C37-C22-C23	2.83	122.41	118.09
19	C	614	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
20	K	101	BCR	C33-C5-C6	-2.82	121.40	124.48
19	C	607	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
24	D	411	PHO	O2D-CGD-O1D	-2.82	118.36	123.85
20	C	615	BCR	C15-C16-C17	-2.82	117.75	123.52
21	A	407	LMG	C8-O7-C10	-2.82	111.05	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	616	BCR	C33-C5-C4	2.80	119.57	113.60
20	D	403	BCR	C16-C15-C14	-2.79	117.80	123.52
19	B	605	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
22	B	621	LHG	O8-C23-C24	2.79	120.34	111.83
19	A	403	CLA	O2D-CGD-O1D	-2.79	118.43	123.85
20	H	101	BCR	C30-C25-C26	-2.78	118.84	122.64
19	B	613	CLA	CHB-C4A-NA	2.77	128.40	124.40
22	X	201	LHG	C5-O7-C7	-2.76	111.18	117.80
22	D	405	LHG	O8-C23-C24	2.75	120.21	111.83
20	C	615	BCR	C20-C21-C22	-2.75	123.43	127.28
22	D	407	LHG	O8-C23-C24	2.74	120.20	111.83
27	C	617	DGD	O1G-C1A-C2A	2.73	120.15	111.83
20	H	101	BCR	C24-C23-C22	-2.72	122.21	126.23
23	D	404	PL9	C7-C8-C9	-2.71	122.17	126.83
21	B	620	LMG	O8-C28-C29	2.71	120.08	111.83
20	B	617	BCR	C15-C14-C13	-2.71	123.48	127.28
22	L	101	LHG	O8-C23-C24	2.70	120.06	111.83
20	C	615	BCR	C4-C5-C6	-2.69	119.07	122.70
20	K	101	BCR	C2-C1-C6	2.66	114.31	110.44
20	A	406	BCR	C33-C5-C6	-2.65	121.59	124.48
20	B	618	BCR	C33-C5-C4	2.65	119.24	113.60
20	C	615	BCR	C30-C25-C24	2.65	122.83	115.65
19	D	401	CLA	C3B-C4B-NB	-2.64	108.17	110.53
20	B	619	BCR	C33-C5-C4	2.63	119.21	113.60
20	H	101	BCR	C1-C6-C5	-2.63	119.04	122.64
19	B	609	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
22	B	622	LHG	O8-C23-C24	2.63	119.86	111.83
27	C	618	DGD	O1G-C1A-C2A	2.63	119.85	111.83
20	Z	101	BCR	C7-C8-C9	-2.63	122.35	126.23
19	B	615	CLA	CHB-C4A-NA	2.62	128.19	124.40
19	D	401	CLA	O2D-CGD-CBD	2.62	115.81	111.23
20	H	101	BCR	C38-C26-C27	2.62	119.18	113.60
20	B	617	BCR	C37-C22-C21	-2.60	118.60	122.82
23	D	404	PL9	C40-C39-C41	2.60	119.74	115.23
19	B	604	CLA	CAA-CBA-CGA	-2.59	105.85	113.21
25	E	101	HEM	C3B-C4B-NB	-2.59	107.61	109.47
20	B	617	BCR	C16-C17-C18	-2.59	123.65	127.28
19	B	602	CLA	C3B-C4B-NB	-2.58	108.22	110.53
20	C	615	BCR	C27-C26-C25	-2.58	119.22	122.70
20	C	616	BCR	C11-C10-C9	-2.58	123.67	127.28
20	B	617	BCR	C33-C5-C6	-2.56	121.69	124.48
20	K	101	BCR	C33-C5-C4	2.55	119.04	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	623	LMG	O8-C28-C29	2.54	119.59	111.83
24	D	410	PHO	CMB-C2B-C3B	2.54	129.76	124.68
20	B	618	BCR	C37-C22-C21	-2.54	118.71	122.82
27	C	617	DGD	O6D-C5D-C6D	2.52	111.70	106.69
20	K	101	BCR	C38-C26-C25	-2.52	121.73	124.48
25	E	101	HEM	C1B-NB-C4B	2.52	108.19	105.21
20	B	618	BCR	C29-C30-C25	2.52	114.10	110.44
20	K	101	BCR	C4-C5-C6	-2.52	119.30	122.70
19	C	606	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
28	C	620	SQD	O8-S-C6	2.52	110.84	105.97
19	B	616	CLA	CHB-C4A-NA	2.51	128.03	124.40
19	B	609	CLA	CAA-CBA-CGA	-2.51	106.07	113.21
21	D	408	LMG	O8-C28-C29	2.51	119.50	111.83
20	B	618	BCR	C15-C14-C13	-2.51	123.75	127.28
27	C	618	DGD	C4E-C3E-C2E	-2.51	106.43	110.83
19	C	608	CLA	C3B-C4B-NB	-2.50	108.30	110.53
20	A	406	BCR	C38-C26-C27	2.49	118.91	113.60
19	C	603	CLA	C1-C2-C3	-2.49	122.12	126.20
20	B	619	BCR	C11-C10-C9	-2.48	123.80	127.28
20	Z	101	BCR	C8-C7-C6	-2.48	120.37	127.00
22	B	624	LHG	O8-C23-C24	2.48	119.40	111.83
20	B	618	BCR	C3-C4-C5	-2.48	109.64	114.06
20	C	615	BCR	C23-C24-C25	-2.47	120.39	127.00
23	D	404	PL9	O2-C1-C6	2.47	124.41	120.48
20	C	615	BCR	C16-C17-C18	-2.47	123.82	127.28
22	D	406	LHG	O8-C23-C24	2.46	119.32	111.83
20	H	101	BCR	C29-C30-C25	2.45	114.00	110.44
19	B	608	CLA	O2A-CGA-O1A	-2.45	117.51	123.63
19	C	603	CLA	C3B-C4B-NB	-2.44	108.35	110.53
20	B	619	BCR	C3-C4-C5	-2.43	109.72	114.06
20	C	615	BCR	C15-C14-C13	-2.43	123.87	127.28
19	A	405	CLA	C1-C2-C3	-2.43	122.22	126.20
19	C	610	CLA	CHB-C4A-NA	2.42	127.90	124.40
20	B	617	BCR	C24-C23-C22	-2.42	122.65	126.23
20	Z	101	BCR	C15-C16-C17	-2.42	118.56	123.52
20	Z	101	BCR	C39-C30-C25	-2.41	106.46	110.24
27	C	619	DGD	O1G-C1A-C2A	2.41	119.18	111.83
19	C	604	CLA	CHB-C4A-NA	2.41	127.87	124.40
20	B	617	BCR	C28-C27-C26	-2.39	109.80	114.06
19	C	613	CLA	CHB-C4A-NA	2.38	127.83	124.40
20	C	615	BCR	C11-C10-C9	-2.38	123.94	127.28
21	K	102	LMG	O8-C28-C29	2.38	119.08	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	617	BCR	C19-C18-C17	-2.38	115.27	119.01
23	D	404	PL9	C27-C28-C29	-2.37	122.20	127.62
22	X	201	LHG	O8-C23-C24	2.37	119.06	111.83
19	B	612	CLA	CHB-C4A-NA	2.37	127.81	124.40
27	C	618	DGD	O5D-C1E-C2E	2.37	111.86	108.27
19	B	615	CLA	O2A-CGA-O1A	-2.36	117.71	123.63
19	B	613	CLA	C1-C2-C3	-2.36	122.34	126.20
19	D	402	CLA	C1-C2-C3	-2.35	122.34	126.20
19	C	605	CLA	O2A-CGA-O1A	-2.35	117.74	123.63
20	Z	101	BCR	C4-C5-C6	-2.35	119.53	122.70
20	D	403	BCR	C7-C8-C9	-2.35	122.76	126.23
19	C	607	CLA	CMB-C2B-C1B	-2.35	121.84	125.42
19	B	603	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
20	D	403	BCR	C10-C11-C12	-2.34	116.41	123.20
22	A	408	LHG	O8-C23-C24	2.34	118.97	111.83
19	C	611	CLA	CHB-C4A-NA	2.34	127.78	124.40
20	D	403	BCR	C1-C6-C7	2.34	121.99	115.65
24	D	411	PHO	CMB-C2B-C3B	2.34	129.35	124.68
23	D	404	PL9	O1-C4-C3	-2.34	118.27	120.73
19	B	616	CLA	C3B-C4B-NB	-2.34	108.44	110.53
20	B	618	BCR	C38-C26-C27	2.33	118.57	113.60
20	B	618	BCR	C11-C10-C9	-2.33	124.01	127.28
20	Z	101	BCR	C15-C14-C13	-2.33	124.01	127.28
19	B	614	CLA	CHB-C4A-NA	2.33	127.76	124.40
19	B	613	CLA	C3B-C4B-NB	-2.32	108.46	110.53
19	C	604	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
19	B	610	CLA	CHB-C4A-NA	2.32	127.75	124.40
19	D	402	CLA	C4-C3-C5	2.32	119.25	115.23
20	C	616	BCR	C15-C16-C17	-2.31	118.79	123.52
19	B	603	CLA	C3B-C4B-NB	-2.30	108.48	110.53
19	C	609	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
20	B	619	BCR	C36-C18-C17	-2.29	119.10	122.82
19	B	604	CLA	CHB-C4A-NA	2.29	127.70	124.40
19	C	607	CLA	C1-C2-C3	-2.29	122.45	126.20
19	C	607	CLA	C3B-C4B-NB	-2.29	108.49	110.53
19	C	614	CLA	CHB-C4A-NA	2.29	127.70	124.40
20	H	101	BCR	C16-C15-C14	-2.28	118.85	123.52
20	B	618	BCR	C24-C23-C22	-2.28	122.87	126.23
22	K	103	LHG	O8-C23-C24	2.27	118.77	111.83
28	C	620	SQD	C45-O47-C7	-2.27	112.36	117.80
19	D	409	CLA	C3B-C4B-NB	-2.27	108.51	110.53
19	A	403	CLA	CHB-C4A-NA	2.26	127.67	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	619	BCR	C16-C15-C14	-2.26	118.89	123.52
20	A	406	BCR	C36-C18-C17	-2.26	119.16	122.82
20	Z	101	BCR	C1-C6-C7	2.26	121.77	115.65
19	B	601	CLA	C3B-C4B-NB	-2.25	108.52	110.53
19	C	604	CLA	CAA-CBA-CGA	-2.25	106.81	113.21
19	B	607	CLA	C3B-C4B-NB	-2.25	108.52	110.53
19	A	404	CLA	O2D-CGD-CBD	2.25	115.16	111.23
19	D	409	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
20	D	403	BCR	C8-C9-C10	-2.25	115.47	119.01
20	C	616	BCR	C8-C7-C6	-2.24	121.01	127.00
19	C	602	CLA	CHB-C4A-NA	2.24	127.64	124.40
19	A	405	CLA	O2D-CGD-CBD	2.24	115.14	111.23
19	B	609	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
19	B	603	CLA	CHB-C4A-NA	2.24	127.63	124.40
19	A	405	CLA	CHB-C4A-NA	2.23	127.62	124.40
19	B	602	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
19	C	608	CLA	CHB-C4A-NA	2.23	127.62	124.40
19	C	603	CLA	CHB-C4A-NA	2.23	127.61	124.40
19	C	604	CLA	CAA-C2A-C3A	-2.22	107.00	113.00
24	D	410	PHO	O2A-CGA-O1A	-2.22	118.08	123.63
19	C	603	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
19	B	611	CLA	O1D-CGD-CBD	2.21	128.87	124.52
19	C	613	CLA	C3B-C4B-NB	-2.21	108.56	110.53
19	C	614	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
19	B	601	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
19	B	611	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
19	B	601	CLA	CHB-C4A-NA	2.20	127.58	124.40
19	B	606	CLA	CHB-C4A-NA	2.20	127.57	124.40
19	A	403	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
19	B	607	CLA	CHB-C4A-NA	2.19	127.56	124.40
23	D	404	PL9	C32-C33-C34	-2.19	122.62	127.62
19	B	601	CLA	CHD-C1D-ND	-2.19	121.73	124.80
19	B	605	CLA	CHB-C4A-NA	2.18	127.55	124.40
20	H	101	BCR	C15-C14-C13	-2.18	124.21	127.28
20	C	616	BCR	C15-C14-C13	-2.18	124.22	127.28
19	B	609	CLA	CAA-C2A-C1A	-2.18	104.83	111.97
20	A	406	BCR	C37-C22-C21	-2.17	119.29	122.82
23	D	404	PL9	O2-C1-C2	-2.17	116.89	121.83
19	B	610	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
19	C	608	CLA	C1-C2-C3	-2.17	122.64	126.20
25	E	101	HEM	C4D-ND-C1D	2.17	107.78	105.21
20	B	619	BCR	C37-C22-C21	-2.17	119.30	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	612	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
28	C	620	SQD	O48-C23-O10	-2.17	118.20	123.63
23	D	404	PL9	C12-C13-C14	-2.17	122.66	127.62
20	K	101	BCR	C31-C1-C6	-2.17	106.84	110.24
19	B	612	CLA	C3B-C4B-NB	-2.17	108.60	110.53
20	K	101	BCR	C10-C11-C12	-2.17	116.92	123.20
19	B	611	CLA	CHB-C4A-NA	2.17	127.53	124.40
19	C	613	CLA	O2D-CGD-CBD	2.16	115.01	111.23
20	A	406	BCR	C15-C14-C13	-2.16	124.25	127.28
20	D	403	BCR	C36-C18-C17	-2.16	119.31	122.82
19	D	409	CLA	O2D-CGD-CBD	2.16	115.01	111.23
19	B	616	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
19	A	403	CLA	C3B-C4B-NB	-2.15	108.61	110.53
20	B	617	BCR	C11-C10-C9	-2.15	124.26	127.28
24	D	411	PHO	C3B-C4B-NB	-2.15	106.06	107.46
21	K	102	LMG	C4-C3-C2	-2.15	107.06	110.83
20	H	101	BCR	C37-C22-C21	-2.15	119.34	122.82
19	C	606	CLA	C3B-C4B-NB	-2.15	108.61	110.53
19	B	602	CLA	O2D-CGD-CBD	2.14	114.98	111.23
20	A	406	BCR	C16-C15-C14	-2.14	119.14	123.52
21	A	407	LMG	O7-C10-O9	-2.14	118.70	123.70
19	B	608	CLA	CHB-C4A-NA	2.14	127.49	124.40
20	C	615	BCR	C21-C20-C19	-2.13	117.02	123.20
19	B	606	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
19	C	614	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
19	D	409	CLA	CHB-C4A-NA	2.12	127.46	124.40
19	B	609	CLA	CHB-C4A-NA	2.12	127.46	124.40
20	A	406	BCR	C33-C5-C4	2.12	118.11	113.60
23	D	404	PL9	C20-C19-C21	2.12	118.91	115.23
28	C	620	SQD	O9-S-C6	2.12	109.91	106.76
19	C	612	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
20	D	403	BCR	C37-C22-C21	-2.11	119.40	122.82
19	C	609	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
20	K	101	BCR	C12-C13-C14	-2.10	115.70	119.01
19	C	612	CLA	C1-C2-C3	-2.10	122.76	126.20
20	Z	101	BCR	C30-C25-C26	-2.09	119.77	122.64
19	B	610	CLA	C3B-C4B-NB	-2.09	108.66	110.53
20	B	619	BCR	C30-C25-C24	2.09	121.32	115.65
19	A	404	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
19	B	614	CLA	O1D-CGD-CBD	2.09	128.64	124.52
19	D	401	CLA	CHB-C4A-NA	2.08	127.40	124.40
19	D	401	CLA	O2A-CGA-O1A	-2.08	118.43	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	101	BCR	C36-C18-C17	-2.07	119.46	122.82
22	B	624	LHG	C5-O7-C7	-2.07	112.85	117.80
19	C	605	CLA	CHB-C4A-NA	2.07	127.38	124.40
20	H	101	BCR	C15-C16-C17	-2.06	119.30	123.52
20	C	616	BCR	C16-C15-C14	-2.06	119.30	123.52
20	B	617	BCR	C1-C6-C7	2.06	121.24	115.65
20	B	618	BCR	C38-C26-C25	-2.05	122.24	124.48
20	D	403	BCR	C12-C13-C14	-2.05	115.78	119.01
19	B	609	CLA	O1D-CGD-CBD	2.05	128.56	124.52
20	C	615	BCR	C24-C23-C22	-2.05	123.21	126.23
19	B	606	CLA	C3B-C4B-NB	-2.05	108.70	110.53
20	D	403	BCR	C33-C5-C6	-2.05	122.25	124.48
20	B	619	BCR	C24-C23-C22	-2.04	123.21	126.23
19	B	604	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
20	Z	101	BCR	C40-C30-C25	2.04	113.44	110.24
19	C	607	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
19	B	613	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
22	D	407	LHG	C5-O7-C7	-2.03	112.93	117.80
19	B	607	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
19	C	604	CLA	C3B-C4B-NB	-2.03	108.72	110.53
20	C	616	BCR	C37-C22-C21	-2.03	119.53	122.82
21	A	407	LMG	O8-C28-O10	-2.03	118.56	123.63
22	K	103	LHG	C5-O7-C7	-2.03	112.94	117.80
19	B	603	CLA	O1D-CGD-CBD	2.02	128.50	124.52
27	C	617	DGD	C2G-O2G-C1B	-2.01	112.97	117.80
19	C	602	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
19	B	605	CLA	CHC-C4B-NB	2.01	127.07	124.05
19	C	609	CLA	CHB-C4A-NA	2.01	127.30	124.40
19	B	606	CLA	O1D-CGD-CBD	2.01	128.48	124.52
19	B	602	CLA	CHB-C4A-NA	2.00	127.29	124.40

All (35) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	B	601	CLA	ND
19	B	602	CLA	ND
19	B	603	CLA	ND
19	B	604	CLA	ND
19	B	605	CLA	ND
19	B	606	CLA	ND
19	B	607	CLA	ND
19	B	608	CLA	ND

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Mol	Chain	Res	Type	Atom
19	B	609	CLA	ND
19	B	610	CLA	ND
19	B	611	CLA	ND
19	B	612	CLA	ND
19	B	613	CLA	ND
19	B	614	CLA	ND
19	B	615	CLA	ND
19	B	616	CLA	ND
19	D	401	CLA	ND
19	D	402	CLA	ND
19	D	409	CLA	ND
19	C	602	CLA	ND
19	C	603	CLA	ND
19	C	604	CLA	ND
19	C	605	CLA	ND
19	C	606	CLA	ND
19	C	607	CLA	ND
19	C	608	CLA	ND
19	C	609	CLA	ND
19	C	610	CLA	ND
19	C	611	CLA	ND
19	C	612	CLA	ND
19	C	613	CLA	ND
19	C	614	CLA	ND
19	A	403	CLA	ND
19	A	404	CLA	ND
19	A	405	CLA	ND

All (680) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	B	603	CLA	C1A-C2A-CAA-CBA
19	B	603	CLA	C3A-C2A-CAA-CBA
19	B	603	CLA	CAD-CBD-CGD-O1D
19	B	603	CLA	CAD-CBD-CGD-O2D
19	B	606	CLA	C1A-C2A-CAA-CBA
19	B	606	CLA	CAD-CBD-CGD-O1D
19	B	606	CLA	CAD-CBD-CGD-O2D
19	B	606	CLA	CBD-CGD-O2D-CED
19	B	607	CLA	C1A-C2A-CAA-CBA
19	B	607	CLA	C3A-C2A-CAA-CBA
19	B	608	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	B	608	CLA	C3A-C2A-CAA-CBA
19	B	608	CLA	CAD-CBD-CGD-O1D
19	B	608	CLA	CAD-CBD-CGD-O2D
19	B	609	CLA	CAD-CBD-CGD-O1D
19	B	609	CLA	CAD-CBD-CGD-O2D
19	B	609	CLA	CBD-CGD-O2D-CED
19	B	610	CLA	CHA-CBD-CGD-O2D
19	B	611	CLA	CAD-CBD-CGD-O1D
19	B	611	CLA	CAD-CBD-CGD-O2D
19	B	611	CLA	CBD-CGD-O2D-CED
19	B	613	CLA	CHA-CBD-CGD-O1D
19	B	613	CLA	CHA-CBD-CGD-O2D
19	B	614	CLA	CAD-CBD-CGD-O1D
19	B	614	CLA	CAD-CBD-CGD-O2D
19	D	401	CLA	CAD-CBD-CGD-O1D
19	D	401	CLA	CAD-CBD-CGD-O2D
19	D	402	CLA	C1A-C2A-CAA-CBA
19	D	402	CLA	C3A-C2A-CAA-CBA
19	D	402	CLA	CAD-CBD-CGD-O1D
19	D	402	CLA	CAD-CBD-CGD-O2D
19	C	602	CLA	C4B-C3B-CAB-CBB
19	C	602	CLA	CAD-CBD-CGD-O1D
19	C	602	CLA	CAD-CBD-CGD-O2D
19	C	603	CLA	CBD-CGD-O2D-CED
19	C	603	CLA	O1D-CGD-O2D-CED
19	C	604	CLA	C1A-C2A-CAA-CBA
19	C	604	CLA	CAD-CBD-CGD-O2D
19	C	607	CLA	CAD-CBD-CGD-O2D
19	C	608	CLA	C1A-C2A-CAA-CBA
19	C	608	CLA	C3A-C2A-CAA-CBA
19	C	612	CLA	CAD-CBD-CGD-O1D
19	C	612	CLA	CAD-CBD-CGD-O2D
19	C	613	CLA	C2-C1-O2A-CGA
19	C	613	CLA	CHA-CBD-CGD-O1D
19	C	613	CLA	CHA-CBD-CGD-O2D
19	A	403	CLA	CBD-CGD-O2D-CED
19	A	405	CLA	CHA-CBD-CGD-O1D
19	A	405	CLA	CHA-CBD-CGD-O2D
20	B	617	BCR	C1-C6-C7-C8
20	B	617	BCR	C5-C6-C7-C8
20	B	617	BCR	C23-C24-C25-C26
20	B	618	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	B	618	BCR	C23-C24-C25-C26
20	B	619	BCR	C1-C6-C7-C8
20	B	619	BCR	C5-C6-C7-C8
20	B	619	BCR	C23-C24-C25-C26
20	D	403	BCR	C1-C6-C7-C8
20	D	403	BCR	C5-C6-C7-C8
20	D	403	BCR	C23-C24-C25-C26
20	D	403	BCR	C23-C24-C25-C30
20	H	101	BCR	C1-C6-C7-C8
20	H	101	BCR	C5-C6-C7-C8
20	H	101	BCR	C23-C24-C25-C26
20	K	101	BCR	C23-C24-C25-C26
20	Z	101	BCR	C5-C6-C7-C8
20	Z	101	BCR	C23-C24-C25-C26
20	A	406	BCR	C5-C6-C7-C8
20	A	406	BCR	C23-C24-C25-C26
21	B	623	LMG	O7-C8-C9-O8
21	A	407	LMG	O6-C1-O1-C7
22	B	621	LHG	C4-O6-P-O3
22	B	621	LHG	C4-O6-P-O4
22	B	622	LHG	C4-O6-P-O3
22	B	622	LHG	C4-O6-P-O4
22	B	624	LHG	C4-O6-P-O4
22	D	405	LHG	C3-O3-P-O4
22	D	405	LHG	C3-O3-P-O6
22	D	405	LHG	C4-O6-P-O3
22	D	405	LHG	C4-O6-P-O4
22	D	406	LHG	C3-O3-P-O4
22	D	406	LHG	C4-O6-P-O3
22	D	406	LHG	C4-O6-P-O4
22	D	407	LHG	C3-O3-P-O4
22	D	407	LHG	C3-O3-P-O6
22	D	407	LHG	C4-O6-P-O3
22	D	407	LHG	C4-O6-P-O4
22	K	103	LHG	C3-O3-P-O5
22	K	103	LHG	C4-O6-P-O3
22	K	103	LHG	C4-O6-P-O4
22	L	101	LHG	C3-O3-P-O5
22	L	101	LHG	C4-O6-P-O5
22	X	201	LHG	C4-O6-P-O3
22	A	408	LHG	C4-O6-P-O3
22	A	408	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
22	A	408	LHG	C4-O6-P-O5
23	D	404	PL9	C42-C43-C44-C46
26	X	202	VTQ	C16-C15-C9-C14
26	X	202	VTQ	C16-C15-C9-C11
19	C	604	CLA	O1D-CGD-O2D-CED
19	C	607	CLA	O1D-CGD-O2D-CED
19	C	604	CLA	CBD-CGD-O2D-CED
19	C	607	CLA	CBD-CGD-O2D-CED
19	C	614	CLA	CBD-CGD-O2D-CED
19	B	607	CLA	O1A-CGA-O2A-C1
27	C	618	DGD	C4D-C5D-C6D-O5D
23	D	404	PL9	C47-C48-C49-C51
19	B	607	CLA	CBA-CGA-O2A-C1
19	B	605	CLA	O1A-CGA-O2A-C1
19	B	616	CLA	O1A-CGA-O2A-C1
19	D	409	CLA	O1A-CGA-O2A-C1
19	C	607	CLA	O1A-CGA-O2A-C1
24	D	410	PHO	O1A-CGA-O2A-C1
19	B	606	CLA	O1D-CGD-O2D-CED
19	C	614	CLA	O1D-CGD-O2D-CED
19	B	609	CLA	O1D-CGD-O2D-CED
19	B	611	CLA	O1D-CGD-O2D-CED
19	A	403	CLA	O1D-CGD-O2D-CED
19	B	607	CLA	CBD-CGD-O2D-CED
19	D	401	CLA	C3-C5-C6-C7
19	C	605	CLA	C3-C5-C6-C7
19	A	405	CLA	C3-C5-C6-C7
19	B	605	CLA	CBA-CGA-O2A-C1
19	B	616	CLA	CBA-CGA-O2A-C1
19	C	607	CLA	CBA-CGA-O2A-C1
24	D	410	PHO	CBA-CGA-O2A-C1
19	B	603	CLA	CBD-CGD-O2D-CED
19	D	402	CLA	C4-C3-C5-C6
19	C	604	CLA	C4-C3-C5-C6
19	D	402	CLA	C2-C3-C5-C6
19	C	604	CLA	C2-C3-C5-C6
19	B	606	CLA	CBA-CGA-O2A-C1
19	D	409	CLA	CBA-CGA-O2A-C1
19	C	606	CLA	CBA-CGA-O2A-C1
19	C	609	CLA	CBA-CGA-O2A-C1
19	B	606	CLA	O1A-CGA-O2A-C1
19	B	611	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	C	609	CLA	O1A-CGA-O2A-C1
19	C	612	CLA	O1A-CGA-O2A-C1
19	B	603	CLA	C3-C5-C6-C7
24	D	411	PHO	C3-C5-C6-C7
19	B	602	CLA	CBA-CGA-O2A-C1
19	C	613	CLA	CBA-CGA-O2A-C1
19	C	611	CLA	CBD-CGD-O2D-CED
19	C	603	CLA	C3-C5-C6-C7
19	B	605	CLA	CBD-CGD-O2D-CED
19	B	615	CLA	CBD-CGD-O2D-CED
19	C	605	CLA	CBD-CGD-O2D-CED
19	B	611	CLA	CBA-CGA-O2A-C1
19	C	612	CLA	CBA-CGA-O2A-C1
19	C	606	CLA	O1A-CGA-O2A-C1
19	C	613	CLA	O1A-CGA-O2A-C1
19	B	602	CLA	O1A-CGA-O2A-C1
19	C	612	CLA	CBD-CGD-O2D-CED
22	X	201	LHG	C8-C7-O7-C5
19	B	601	CLA	CBA-CGA-O2A-C1
19	C	614	CLA	CBA-CGA-O2A-C1
24	D	411	PHO	CBA-CGA-O2A-C1
19	B	607	CLA	O1D-CGD-O2D-CED
19	B	603	CLA	O1D-CGD-O2D-CED
19	C	602	CLA	C14-C13-C15-C16
19	C	608	CLA	C14-C13-C15-C16
19	B	604	CLA	CBD-CGD-O2D-CED
22	D	407	LHG	O6-C4-C5-O7
28	C	620	SQD	O6-C44-C45-O47
19	B	612	CLA	C13-C15-C16-C17
19	B	608	CLA	CBD-CGD-O2D-CED
19	B	608	CLA	C3-C5-C6-C7
27	C	618	DGD	O6D-C5D-C6D-O5D
23	D	404	PL9	C34-C36-C37-C38
19	B	601	CLA	O1A-CGA-O2A-C1
19	C	610	CLA	CBA-CGA-O2A-C1
19	C	602	CLA	C13-C15-C16-C17
19	C	609	CLA	C8-C10-C11-C12
19	C	612	CLA	C15-C16-C17-C18
19	B	611	CLA	C2A-CAA-CBA-CGA
19	B	616	CLA	C2A-CAA-CBA-CGA
19	D	409	CLA	C2A-CAA-CBA-CGA
19	C	603	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	C	609	CLA	C2A-CAA-CBA-CGA
19	C	612	CLA	C2A-CAA-CBA-CGA
19	C	614	CLA	O1A-CGA-O2A-C1
24	D	411	PHO	O1A-CGA-O2A-C1
19	B	602	CLA	C3-C5-C6-C7
19	D	402	CLA	C10-C11-C12-C13
19	C	606	CLA	C8-C10-C11-C12
19	C	611	CLA	C10-C11-C12-C13
19	C	602	CLA	CBA-CGA-O2A-C1
19	C	605	CLA	CBA-CGA-O2A-C1
19	B	611	CLA	C5-C6-C7-C8
19	C	611	CLA	C15-C16-C17-C18
22	X	201	LHG	O9-C7-O7-C5
23	D	404	PL9	C47-C48-C49-C50
19	B	602	CLA	C10-C11-C12-C13
26	X	202	VTQ	C15-C16-C17-C18
19	D	401	CLA	C13-C15-C16-C17
19	B	601	CLA	C10-C11-C12-C13
19	B	604	CLA	C15-C16-C17-C18
19	B	616	CLA	C10-C11-C12-C13
19	C	611	CLA	O1D-CGD-O2D-CED
19	B	601	CLA	C5-C6-C7-C8
19	C	602	CLA	C10-C11-C12-C13
19	B	605	CLA	C13-C15-C16-C17
19	D	402	CLA	C15-C16-C17-C18
19	D	401	CLA	CBD-CGD-O2D-CED
21	A	407	LMG	C2-C1-O1-C7
19	B	615	CLA	O1D-CGD-O2D-CED
19	C	605	CLA	O1A-CGA-O2A-C1
19	B	604	CLA	C2A-CAA-CBA-CGA
19	C	607	CLA	C2A-CAA-CBA-CGA
19	C	610	CLA	O1A-CGA-O2A-C1
19	B	605	CLA	O1D-CGD-O2D-CED
19	C	614	CLA	C10-C11-C12-C13
19	C	605	CLA	O1D-CGD-O2D-CED
19	B	613	CLA	CBA-CGA-O2A-C1
19	C	606	CLA	C2-C1-O2A-CGA
19	C	609	CLA	C2-C1-O2A-CGA
19	C	612	CLA	C2-C1-O2A-CGA
19	D	401	CLA	C10-C11-C12-C13
22	D	405	LHG	C30-C31-C32-C33
19	C	602	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	B	624	LHG	C11-C12-C13-C14
19	C	609	CLA	C16-C17-C18-C19
19	C	609	CLA	C16-C17-C18-C20
19	C	614	CLA	C2A-CAA-CBA-CGA
27	C	619	DGD	C6B-C7B-C8B-C9B
21	A	407	LMG	C11-C10-O7-C8
28	C	620	SQD	C8-C7-O47-C45
19	A	403	CLA	CBA-CGA-O2A-C1
21	B	623	LMG	C15-C16-C17-C18
19	B	604	CLA	C3A-C2A-CAA-CBA
19	B	606	CLA	C3A-C2A-CAA-CBA
19	B	609	CLA	C3A-C2A-CAA-CBA
28	C	620	SQD	C27-C28-C29-C30
19	B	602	CLA	C5-C6-C7-C8
19	B	607	CLA	C5-C6-C7-C8
27	C	619	DGD	C3B-C4B-C5B-C6B
22	B	624	LHG	C23-C24-C25-C26
22	A	408	LHG	C13-C14-C15-C16
19	C	612	CLA	O1D-CGD-O2D-CED
19	C	602	CLA	C2B-C3B-CAB-CBB
20	B	617	BCR	C23-C24-C25-C30
20	B	618	BCR	C1-C6-C7-C8
20	B	618	BCR	C23-C24-C25-C30
20	B	619	BCR	C23-C24-C25-C30
20	H	101	BCR	C23-C24-C25-C30
20	K	101	BCR	C1-C6-C7-C8
20	K	101	BCR	C5-C6-C7-C8
20	K	101	BCR	C23-C24-C25-C30
20	Z	101	BCR	C1-C6-C7-C8
20	Z	101	BCR	C23-C24-C25-C30
20	C	615	BCR	C23-C24-C25-C26
20	C	615	BCR	C23-C24-C25-C30
20	C	616	BCR	C1-C6-C7-C8
20	C	616	BCR	C5-C6-C7-C8
20	C	616	BCR	C23-C24-C25-C26
20	C	616	BCR	C23-C24-C25-C30
20	A	406	BCR	C1-C6-C7-C8
20	A	406	BCR	C23-C24-C25-C30
21	K	102	LMG	C15-C16-C17-C18
19	B	613	CLA	O1A-CGA-O2A-C1
19	A	403	CLA	O1A-CGA-O2A-C1
22	B	624	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
21	A	407	LMG	O9-C10-O7-C8
19	C	613	CLA	C6-C7-C8-C9
27	C	617	DGD	O6E-C5E-C6E-O5E
22	D	406	LHG	C11-C10-C9-C8
19	B	604	CLA	C8-C10-C11-C12
27	C	618	DGD	C2A-C1A-O1G-C1G
22	L	101	LHG	C8-C7-O7-C5
27	C	617	DGD	C1B-C2B-C3B-C4B
28	C	620	SQD	O49-C7-O47-C45
22	D	405	LHG	C11-C12-C13-C14
19	B	602	CLA	C2A-CAA-CBA-CGA
19	B	609	CLA	C16-C17-C18-C20
27	C	618	DGD	C6B-C7B-C8B-C9B
25	E	101	HEM	C4B-C3B-CAB-CBB
21	D	408	LMG	O6-C5-C6-O5
19	D	402	CLA	C3-C5-C6-C7
22	A	408	LHG	C17-C18-C19-C20
21	D	408	LMG	C33-C34-C35-C36
21	C	601	LMG	C11-C12-C13-C14
24	D	410	PHO	C8-C10-C11-C12
22	B	622	LHG	C11-C12-C13-C14
19	C	611	CLA	C2-C3-C5-C6
22	L	101	LHG	O9-C7-O7-C5
19	C	604	CLA	C8-C10-C11-C12
22	B	622	LHG	C8-C7-O7-C5
19	B	604	CLA	C1A-C2A-CAA-CBA
19	B	609	CLA	C1A-C2A-CAA-CBA
19	B	612	CLA	C1A-C2A-CAA-CBA
19	B	614	CLA	C1A-C2A-CAA-CBA
19	C	602	CLA	C1A-C2A-CAA-CBA
19	C	606	CLA	C1A-C2A-CAA-CBA
22	D	407	LHG	O6-C4-C5-C6
21	B	620	LMG	O6-C5-C6-O5
19	B	608	CLA	C11-C12-C13-C15
19	B	612	CLA	C11-C10-C8-C7
19	B	613	CLA	C6-C7-C8-C10
19	C	614	CLA	C6-C7-C8-C10
19	C	614	CLA	C12-C13-C15-C16
19	C	610	CLA	C5-C6-C7-C8
21	K	102	LMG	C28-C29-C30-C31
23	D	404	PL9	C45-C44-C46-C47
19	B	612	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
19	B	616	CLA	C11-C10-C8-C9
19	C	603	CLA	C14-C13-C15-C16
19	C	614	CLA	C11-C10-C8-C9
19	C	614	CLA	C14-C13-C15-C16
26	X	202	VTQ	C21-C22-C23-C1
19	A	404	CLA	CBA-CGA-O2A-C1
23	D	404	PL9	C7-C8-C9-C10
28	C	620	SQD	O6-C44-C45-C46
21	B	623	LMG	C38-C39-C40-C41
19	B	604	CLA	O1D-CGD-O2D-CED
22	K	103	LHG	C24-C23-O8-C6
21	K	102	LMG	O6-C5-C6-O5
27	C	618	DGD	O1A-C1A-O1G-C1G
24	D	411	PHO	CHA-CBD-CGD-O2D
21	D	408	LMG	C10-C11-C12-C13
27	C	617	DGD	C4B-C5B-C6B-C7B
19	C	611	CLA	C4-C3-C5-C6
19	B	615	CLA	O2A-C1-C2-C3
19	C	607	CLA	O2A-C1-C2-C3
22	D	405	LHG	C11-C10-C9-C8
22	X	201	LHG	C23-C24-C25-C26
19	C	603	CLA	CBA-CGA-O2A-C1
22	B	622	LHG	C25-C26-C27-C28
22	X	201	LHG	C26-C27-C28-C29
28	C	620	SQD	C9-C10-C11-C12
19	C	612	CLA	C3-C5-C6-C7
19	B	616	CLA	C13-C15-C16-C17
19	B	608	CLA	O1D-CGD-O2D-CED
19	B	604	CLA	CBA-CGA-O2A-C1
19	D	402	CLA	CBA-CGA-O2A-C1
19	C	604	CLA	CBA-CGA-O2A-C1
22	B	624	LHG	C8-C7-O7-C5
19	C	608	CLA	C8-C10-C11-C12
22	D	405	LHG	C23-C24-C25-C26
19	C	606	CLA	C4-C3-C5-C6
19	C	607	CLA	C2-C3-C5-C6
24	D	410	PHO	C2-C3-C5-C6
21	D	408	LMG	C29-C30-C31-C32
19	B	601	CLA	C11-C10-C8-C9
19	B	605	CLA	C11-C12-C13-C14
19	B	608	CLA	C11-C12-C13-C14
19	C	609	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	A	405	CLA	C11-C10-C8-C9
22	B	624	LHG	C13-C14-C15-C16
19	C	611	CLA	C8-C10-C11-C12
21	B	623	LMG	C11-C10-O7-C8
19	B	601	CLA	C11-C10-C8-C7
19	B	605	CLA	C11-C12-C13-C15
19	B	611	CLA	C6-C7-C8-C10
19	B	612	CLA	C6-C7-C8-C10
19	B	616	CLA	C11-C10-C8-C7
19	D	401	CLA	C11-C12-C13-C15
19	C	603	CLA	C12-C13-C15-C16
19	C	606	CLA	C12-C13-C15-C16
19	C	609	CLA	C6-C7-C8-C10
19	C	609	CLA	C12-C13-C15-C16
19	C	614	CLA	C11-C10-C8-C7
19	A	405	CLA	C11-C10-C8-C7
24	D	411	PHO	C11-C10-C8-C7
19	A	403	CLA	C5-C6-C7-C8
19	A	404	CLA	O1A-CGA-O2A-C1
19	B	612	CLA	C3A-C2A-CAA-CBA
19	C	606	CLA	C3A-C2A-CAA-CBA
19	C	613	CLA	C3A-C2A-CAA-CBA
19	B	609	CLA	C8-C10-C11-C12
21	B	623	LMG	C7-C8-C9-O8
27	C	617	DGD	O6D-C5D-C6D-O5D
21	A	407	LMG	C34-C35-C36-C37
21	B	620	LMG	C11-C12-C13-C14
19	C	607	CLA	C4-C3-C5-C6
24	D	410	PHO	C4-C3-C5-C6
23	D	404	PL9	C43-C44-C46-C47
22	K	103	LHG	O10-C23-O8-C6
19	C	614	CLA	C16-C17-C18-C20
27	C	617	DGD	C4D-C5D-C6D-O5D
21	A	407	LMG	O1-C7-C8-O7
19	C	606	CLA	C2-C3-C5-C6
21	D	408	LMG	C14-C15-C16-C17
21	A	407	LMG	C15-C16-C17-C18
24	D	411	PHO	C11-C10-C8-C9
26	X	202	VTQ	C16-C17-C18-C19
19	B	609	CLA	C16-C17-C18-C19
19	B	606	CLA	C5-C6-C7-C8
19	C	603	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	L	101	LHG	C11-C12-C13-C14
22	A	408	LHG	C18-C19-C20-C21
19	C	604	CLA	C15-C16-C17-C18
19	C	614	CLA	C5-C6-C7-C8
22	B	622	LHG	O9-C7-O7-C5
22	L	101	LHG	C14-C15-C16-C17
19	B	610	CLA	C15-C16-C17-C18
19	C	605	CLA	C11-C10-C8-C7
24	D	410	PHO	C11-C12-C13-C15
26	X	202	VTQ	C16-C17-C18-C20
22	X	201	LHG	C11-C12-C13-C14
21	B	623	LMG	C33-C34-C35-C36
19	B	604	CLA	C10-C11-C12-C13
19	C	614	CLA	C16-C17-C18-C19
22	B	624	LHG	O9-C7-O7-C5
19	B	604	CLA	O1A-CGA-O2A-C1
19	D	402	CLA	O1A-CGA-O2A-C1
19	C	604	CLA	O1A-CGA-O2A-C1
19	B	612	CLA	O2A-C1-C2-C3
22	D	407	LHG	C33-C34-C35-C36
28	C	620	SQD	C25-C26-C27-C28
19	B	613	CLA	C3-C5-C6-C7
22	D	406	LHG	C9-C10-C11-C12
22	B	622	LHG	O6-C4-C5-O7
27	C	619	DGD	O6D-C5D-C6D-O5D
22	B	624	LHG	C11-C10-C9-C8
19	B	603	CLA	C8-C10-C11-C12
19	B	610	CLA	C4-C3-C5-C6
19	C	603	CLA	C5-C6-C7-C8
19	C	605	CLA	C11-C10-C8-C9
19	C	610	CLA	C14-C13-C15-C16
24	D	411	PHO	C14-C13-C15-C16
22	A	408	LHG	C28-C29-C30-C31
22	B	621	LHG	C30-C31-C32-C33
19	B	609	CLA	CBA-CGA-O2A-C1
19	B	605	CLA	C16-C17-C18-C19
19	B	613	CLA	C10-C11-C12-C13
19	B	609	CLA	O1A-CGA-O2A-C1
22	B	622	LHG	C31-C32-C33-C34
19	C	613	CLA	C1A-C2A-CAA-CBA
19	D	401	CLA	O1D-CGD-O2D-CED
20	H	101	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
22	B	622	LHG	O6-C4-C5-C6
21	B	623	LMG	O9-C10-O7-C8
19	B	606	CLA	C12-C13-C15-C16
19	B	610	CLA	C12-C13-C15-C16
19	C	602	CLA	C6-C7-C8-C10
19	C	604	CLA	C11-C10-C8-C7
19	C	608	CLA	C12-C13-C15-C16
19	C	610	CLA	C6-C7-C8-C10
19	C	610	CLA	C16-C17-C18-C20
19	B	610	CLA	CBA-CGA-O2A-C1
28	C	620	SQD	C33-C34-C35-C36
22	X	201	LHG	C10-C11-C12-C13
19	B	611	CLA	C6-C7-C8-C9
19	B	612	CLA	C6-C7-C8-C9
19	D	401	CLA	C11-C12-C13-C14
19	D	402	CLA	C11-C10-C8-C9
19	C	606	CLA	C14-C13-C15-C16
19	C	614	CLA	C6-C7-C8-C9
24	D	410	PHO	C11-C12-C13-C14
21	B	623	LMG	C11-C12-C13-C14
27	C	618	DGD	O1G-C1G-C2G-O2G
19	B	605	CLA	C16-C17-C18-C20
27	C	618	DGD	O1G-C1G-C2G-C3G
19	B	601	CLA	CAD-CBD-CGD-O2D
19	B	604	CLA	CAD-CBD-CGD-O2D
19	B	605	CLA	CAD-CBD-CGD-O2D
19	C	606	CLA	CAD-CBD-CGD-O2D
21	B	620	LMG	O6-C1-O1-C7
19	B	610	CLA	O1A-CGA-O2A-C1
21	B	623	LMG	C35-C36-C37-C38
19	B	601	CLA	CAD-CBD-CGD-O1D
19	B	604	CLA	CAD-CBD-CGD-O1D
19	B	605	CLA	CAD-CBD-CGD-O1D
19	B	610	CLA	CHA-CBD-CGD-O1D
19	C	604	CLA	CAD-CBD-CGD-O1D
19	C	606	CLA	CAD-CBD-CGD-O1D
19	C	607	CLA	CAD-CBD-CGD-O1D
19	C	610	CLA	CHA-CBD-CGD-O1D
19	C	610	CLA	CHA-CBD-CGD-O2D
22	B	624	LHG	C4-O6-P-O3
22	D	406	LHG	C3-O3-P-O6
22	X	201	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
24	D	411	PHO	CHA-CBD-CGD-O1D
21	K	102	LMG	C14-C15-C16-C17
19	B	609	CLA	C4-C3-C5-C6
19	B	610	CLA	C2-C3-C5-C6
25	E	101	HEM	C3D-CAD-CBD-CGD
21	B	620	LMG	C10-C11-C12-C13
28	C	620	SQD	C32-C33-C34-C35
19	C	607	CLA	C16-C17-C18-C20
19	B	608	CLA	C14-C13-C15-C16
19	C	609	CLA	C6-C7-C8-C9
19	C	610	CLA	C6-C7-C8-C9
19	C	611	CLA	C14-C13-C15-C16
19	C	610	CLA	C12-C13-C15-C16
19	C	611	CLA	C6-C7-C8-C10
19	A	403	CLA	C4C-C3C-CAC-CBC
19	C	613	CLA	C4-C3-C5-C6
22	D	406	LHG	C28-C29-C30-C31
27	C	617	DGD	C2B-C1B-O2G-C2G
19	B	601	CLA	CAA-CBA-CGA-O2A
22	B	621	LHG	C9-C10-C11-C12
19	C	603	CLA	C4-C3-C5-C6
19	B	611	CLA	C16-C17-C18-C19
19	A	405	CLA	C11-C12-C13-C15
22	D	406	LHG	C23-C24-C25-C26
19	D	402	CLA	CBD-CGD-O2D-CED
19	C	607	CLA	C13-C15-C16-C17
19	B	613	CLA	C16-C17-C18-C20
19	B	603	CLA	C11-C12-C13-C14
19	C	604	CLA	C11-C10-C8-C9
19	C	611	CLA	C6-C7-C8-C9
22	B	624	LHG	C14-C15-C16-C17
19	C	607	CLA	C15-C16-C17-C18
19	C	613	CLA	C2-C3-C5-C6
22	B	624	LHG	O6-C4-C5-O7
22	D	406	LHG	C32-C33-C34-C35
19	B	610	CLA	C11-C10-C8-C7
19	D	409	CLA	C11-C12-C13-C15
19	C	604	CLA	C6-C7-C8-C10
19	B	611	CLA	C16-C17-C18-C20
19	C	607	CLA	C16-C17-C18-C19
22	D	406	LHG	C25-C26-C27-C28
28	C	620	SQD	O47-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
19	B	610	CLA	C3A-C2A-CAA-CBA
19	C	604	CLA	C3A-C2A-CAA-CBA
19	C	610	CLA	C3A-C2A-CAA-CBA
19	C	609	CLA	C5-C6-C7-C8
23	D	404	PL9	C30-C29-C31-C32
19	C	606	CLA	C16-C17-C18-C20
22	B	622	LHG	C11-C10-C9-C8
21	A	407	LMG	O1-C7-C8-C9
22	B	624	LHG	C16-C17-C18-C19
22	D	407	LHG	C24-C25-C26-C27
19	B	607	CLA	C6-C7-C8-C9
19	B	610	CLA	C11-C10-C8-C9
19	C	603	CLA	C11-C10-C8-C9
19	C	604	CLA	C6-C7-C8-C9
19	C	606	CLA	C6-C7-C8-C9
19	C	613	CLA	C14-C13-C15-C16
22	D	405	LHG	C32-C33-C34-C35
19	C	613	CLA	C16-C17-C18-C19
22	L	101	LHG	C12-C13-C14-C15
27	C	619	DGD	C4B-C5B-C6B-C7B
22	D	405	LHG	C35-C36-C37-C38
19	C	603	CLA	C2-C3-C5-C6
19	B	610	CLA	C1A-C2A-CAA-CBA
19	C	612	CLA	C1A-C2A-CAA-CBA
19	D	401	CLA	C16-C17-C18-C19
21	K	102	LMG	C17-C18-C19-C20
28	C	620	SQD	C10-C11-C12-C13
27	C	617	DGD	O1B-C1B-O2G-C2G
19	B	603	CLA	C11-C12-C13-C15
19	D	401	CLA	C11-C10-C8-C7
19	D	402	CLA	C12-C13-C15-C16
19	C	602	CLA	C11-C12-C13-C15
22	K	103	LHG	C10-C11-C12-C13
21	C	601	LMG	O7-C8-C9-O8
22	D	406	LHG	C30-C31-C32-C33
22	B	621	LHG	C31-C32-C33-C34
19	B	604	CLA	C16-C17-C18-C20
19	B	607	CLA	C3-C5-C6-C7
19	B	613	CLA	C16-C17-C18-C19
19	B	605	CLA	C4-C3-C5-C6
19	B	609	CLA	C2-C3-C5-C6
22	D	407	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
19	D	409	CLA	C13-C15-C16-C17
22	X	201	LHG	C30-C31-C32-C33
19	A	404	CLA	O2A-C1-C2-C3
19	C	612	CLA	C8-C10-C11-C12
19	B	604	CLA	C16-C17-C18-C19
19	D	401	CLA	C16-C17-C18-C20
19	C	606	CLA	C16-C17-C18-C19
22	D	407	LHG	O9-C7-O7-C5
19	D	409	CLA	C16-C17-C18-C19
22	L	101	LHG	O7-C5-C6-O8
19	B	616	CLA	C11-C12-C13-C15
19	C	603	CLA	C11-C12-C13-C15
21	B	620	LMG	C32-C33-C34-C35
19	C	607	CLA	C5-C6-C7-C8
27	C	617	DGD	C5D-C6D-O5D-C1E
22	D	407	LHG	C23-C24-C25-C26
19	C	607	CLA	C3A-C2A-CAA-CBA
19	C	612	CLA	C3A-C2A-CAA-CBA
19	D	401	CLA	C2C-C3C-CAC-CBC
19	B	610	CLA	C13-C15-C16-C17
19	C	613	CLA	C16-C17-C18-C20
19	D	402	CLA	O1D-CGD-O2D-CED
19	C	609	CLA	O1D-CGD-O2D-CED
19	B	608	CLA	C4-C3-C5-C6
19	B	611	CLA	CAA-CBA-CGA-O2A
22	X	201	LHG	C15-C16-C17-C18
19	B	606	CLA	C14-C13-C15-C16
19	C	610	CLA	C11-C12-C13-C14
19	C	613	CLA	CAA-CBA-CGA-O2A
22	D	407	LHG	O8-C23-C24-C25
19	C	610	CLA	C13-C15-C16-C17
19	B	607	CLA	C6-C7-C8-C10
19	C	606	CLA	C6-C7-C8-C10
19	C	612	CLA	C12-C13-C15-C16
19	C	613	CLA	C12-C13-C15-C16
24	D	411	PHO	C11-C12-C13-C15
19	C	603	CLA	C2B-C3B-CAB-CBB
20	C	615	BCR	C5-C6-C7-C8
21	C	601	LMG	C12-C13-C14-C15
19	B	613	CLA	C2-C1-O2A-CGA
27	C	619	DGD	C8B-C9B-CAB-CBB
21	K	102	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
19	C	611	CLA	C2A-CAA-CBA-CGA
22	D	407	LHG	C8-C7-O7-C5
19	B	604	CLA	CAA-CBA-CGA-O2A
22	D	407	LHG	C25-C26-C27-C28
19	B	610	CLA	CAA-CBA-CGA-O2A
19	C	609	CLA	CBD-CGD-O2D-CED
19	C	609	CLA	CAA-CBA-CGA-O2A
19	C	610	CLA	CAA-CBA-CGA-O2A
24	D	410	PHO	C10-C11-C12-C13
19	A	403	CLA	C2C-C3C-CAC-CBC
19	D	401	CLA	C11-C10-C8-C9
19	C	602	CLA	C6-C7-C8-C9
19	B	613	CLA	C2C-C3C-CAC-CBC
27	C	619	DGD	C2B-C3B-C4B-C5B
19	B	605	CLA	CAA-CBA-CGA-O2A
19	B	607	CLA	CAA-CBA-CGA-O2A
19	B	616	CLA	C4B-C3B-CAB-CBB
19	D	401	CLA	C1A-C2A-CAA-CBA
19	C	607	CLA	C1A-C2A-CAA-CBA
19	C	610	CLA	C1A-C2A-CAA-CBA
19	B	609	CLA	CAA-CBA-CGA-O2A
22	K	103	LHG	O7-C7-C8-C9
21	K	102	LMG	C12-C13-C14-C15
22	D	407	LHG	C29-C30-C31-C32
27	C	618	DGD	C2A-C3A-C4A-C5A
19	C	611	CLA	CAA-CBA-CGA-O2A
19	B	605	CLA	C2A-CAA-CBA-CGA
21	A	407	LMG	C33-C34-C35-C36
19	C	611	CLA	C2-C1-O2A-CGA
19	B	612	CLA	CAA-CBA-CGA-O2A
19	C	608	CLA	C11-C12-C13-C15
19	C	605	CLA	C15-C16-C17-C18
19	A	403	CLA	O2A-C1-C2-C3
21	D	408	LMG	C19-C20-C21-C22
19	C	609	CLA	C10-C11-C12-C13
19	D	401	CLA	C3A-C2A-CAA-CBA
19	C	610	CLA	CAA-CBA-CGA-O1A
26	X	202	VTQ	C18-C20-C21-C22
19	B	608	CLA	C16-C17-C18-C20
19	B	605	CLA	C2-C3-C5-C6
19	C	613	CLA	CAA-CBA-CGA-O1A
19	C	607	CLA	CAA-CBA-CGA-O2A

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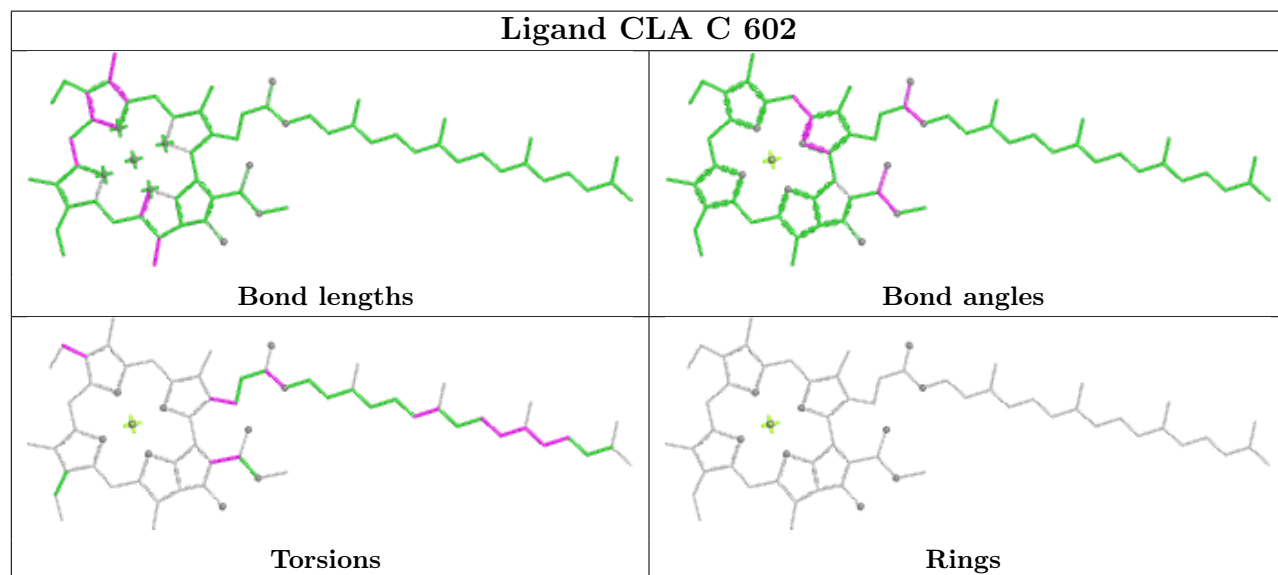
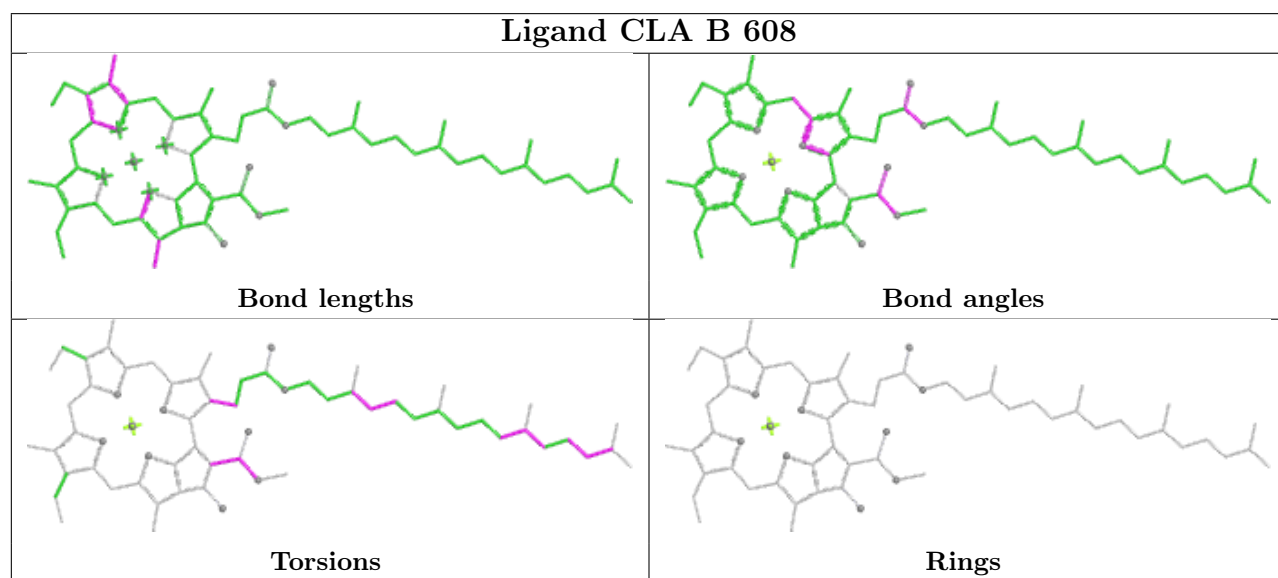
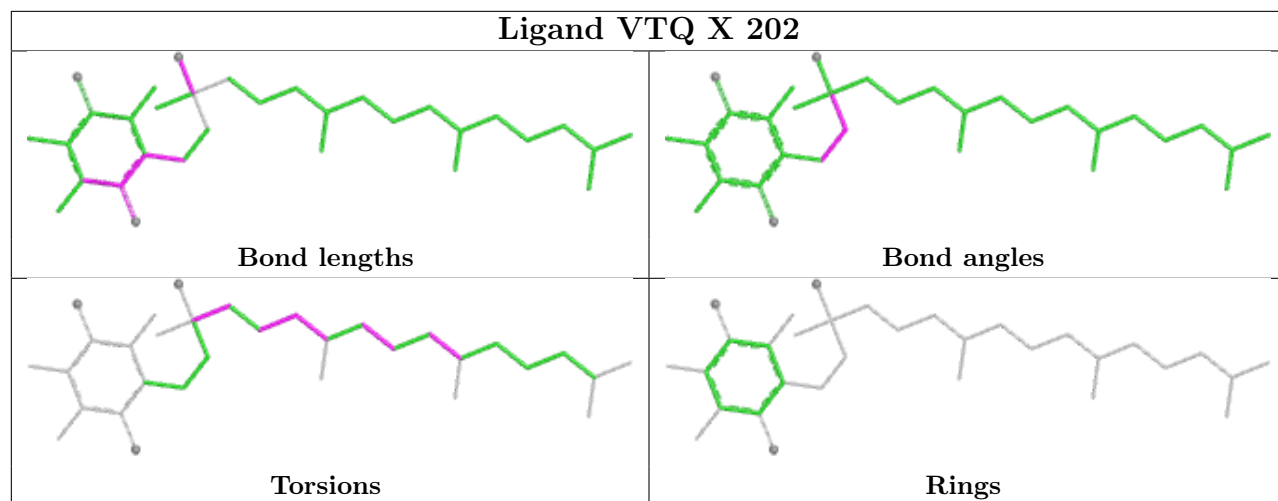
Mol	Chain	Res	Type	Atoms
19	B	610	CLA	C14-C13-C15-C16
19	D	409	CLA	C11-C12-C13-C14
19	B	610	CLA	CAA-CBA-CGA-O1A
19	C	609	CLA	CAA-CBA-CGA-O1A
22	D	407	LHG	O10-C23-C24-C25
24	D	410	PHO	C15-C16-C17-C18
19	B	603	CLA	C4-C3-C5-C6
21	A	407	LMG	C16-C17-C18-C19
19	B	604	CLA	CAA-CBA-CGA-O1A
19	C	611	CLA	CAA-CBA-CGA-O1A
19	B	601	CLA	C2C-C3C-CAC-CBC
22	B	621	LHG	C34-C35-C36-C37
22	B	621	LHG	C12-C13-C14-C15
27	C	617	DGD	C3A-C4A-C5A-C6A
19	B	608	CLA	C16-C17-C18-C19
19	B	605	CLA	CAA-CBA-CGA-O1A
19	B	609	CLA	CAA-CBA-CGA-O1A
19	B	612	CLA	CAA-CBA-CGA-O1A
19	B	608	CLA	C15-C16-C17-C18
19	A	403	CLA	C15-C16-C17-C18
22	D	407	LHG	C1-C2-C3-O3
19	B	607	CLA	CAA-CBA-CGA-O1A
19	B	611	CLA	CAA-CBA-CGA-O1A
22	B	622	LHG	O8-C23-C24-C25
28	C	620	SQD	O47-C7-C8-C9
22	X	201	LHG	C12-C13-C14-C15
22	A	408	LHG	C25-C26-C27-C28
19	B	616	CLA	C16-C17-C18-C20
19	D	409	CLA	CAD-CBD-CGD-O2D
24	D	410	PHO	CAD-CBD-CGD-O2D
22	B	621	LHG	O8-C23-C24-C25
27	C	617	DGD	C4A-C5A-C6A-C7A
19	B	612	CLA	C8-C10-C11-C12
25	E	101	HEM	CAA-CBA-CGA-O2A
19	B	602	CLA	CAA-CBA-CGA-O2A
19	B	610	CLA	C5-C6-C7-C8
19	A	403	CLA	CAA-CBA-CGA-O2A
24	D	411	PHO	CAA-CBA-CGA-O2A
22	K	103	LHG	O9-C7-C8-C9

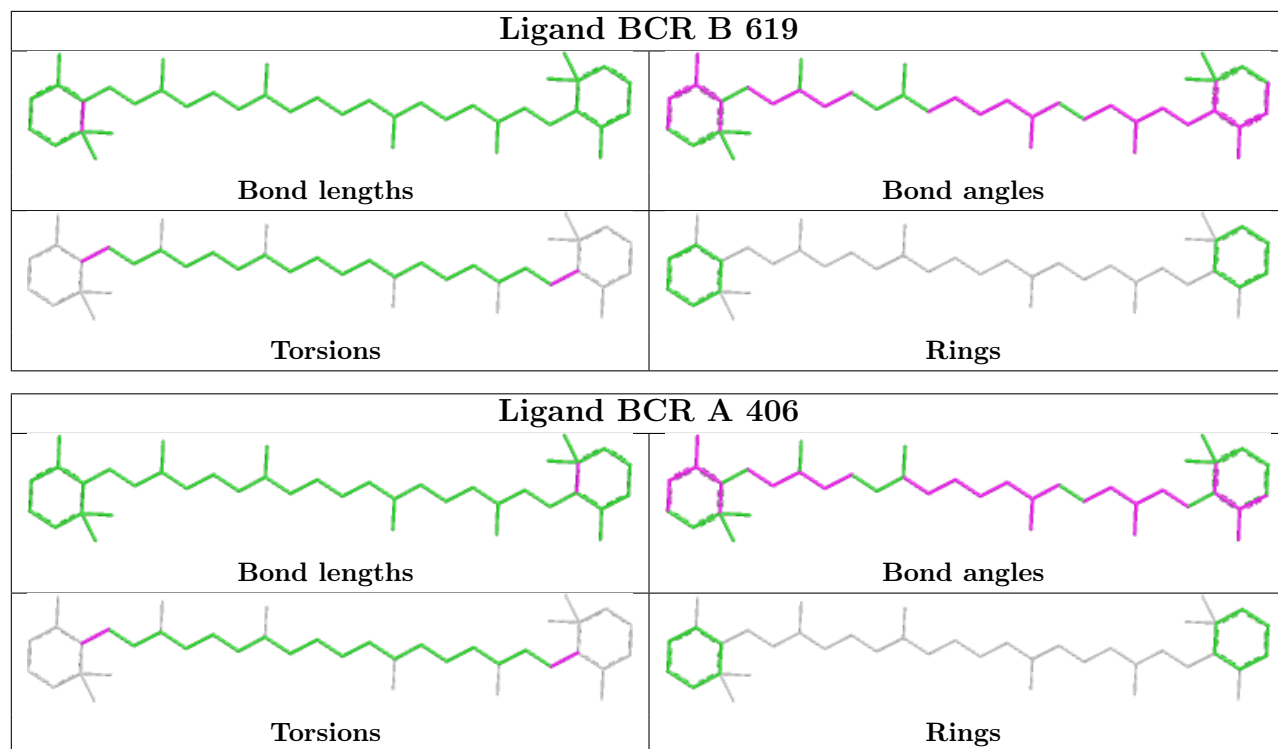
There are no ring outliers.

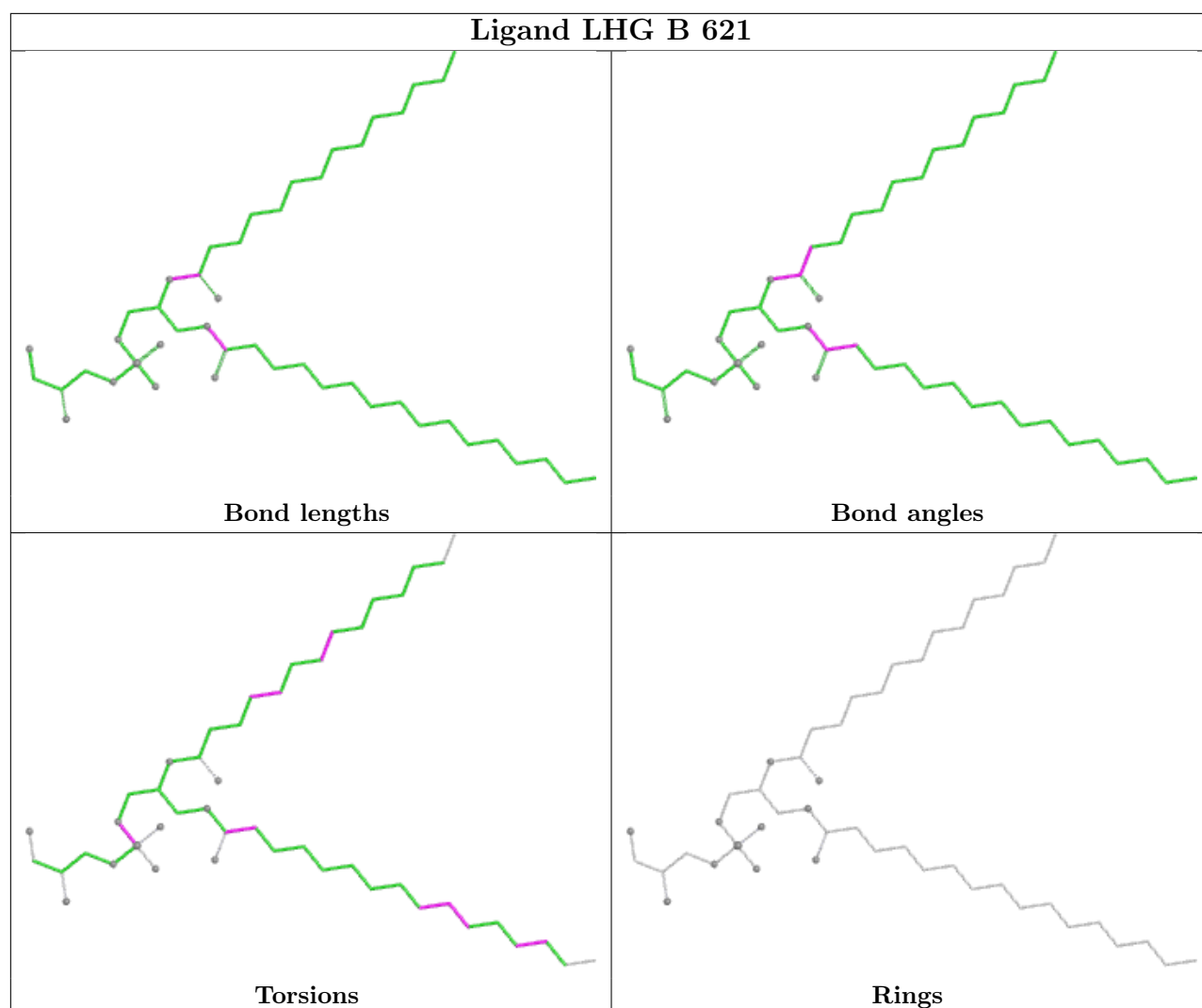
27 monomers are involved in 50 short contacts:

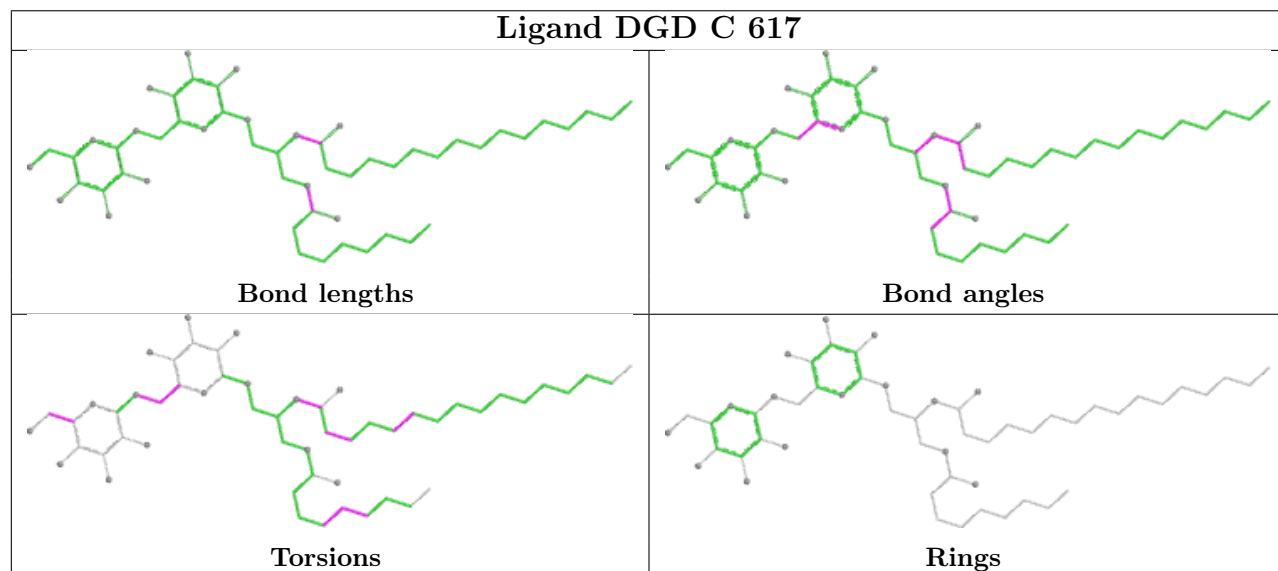
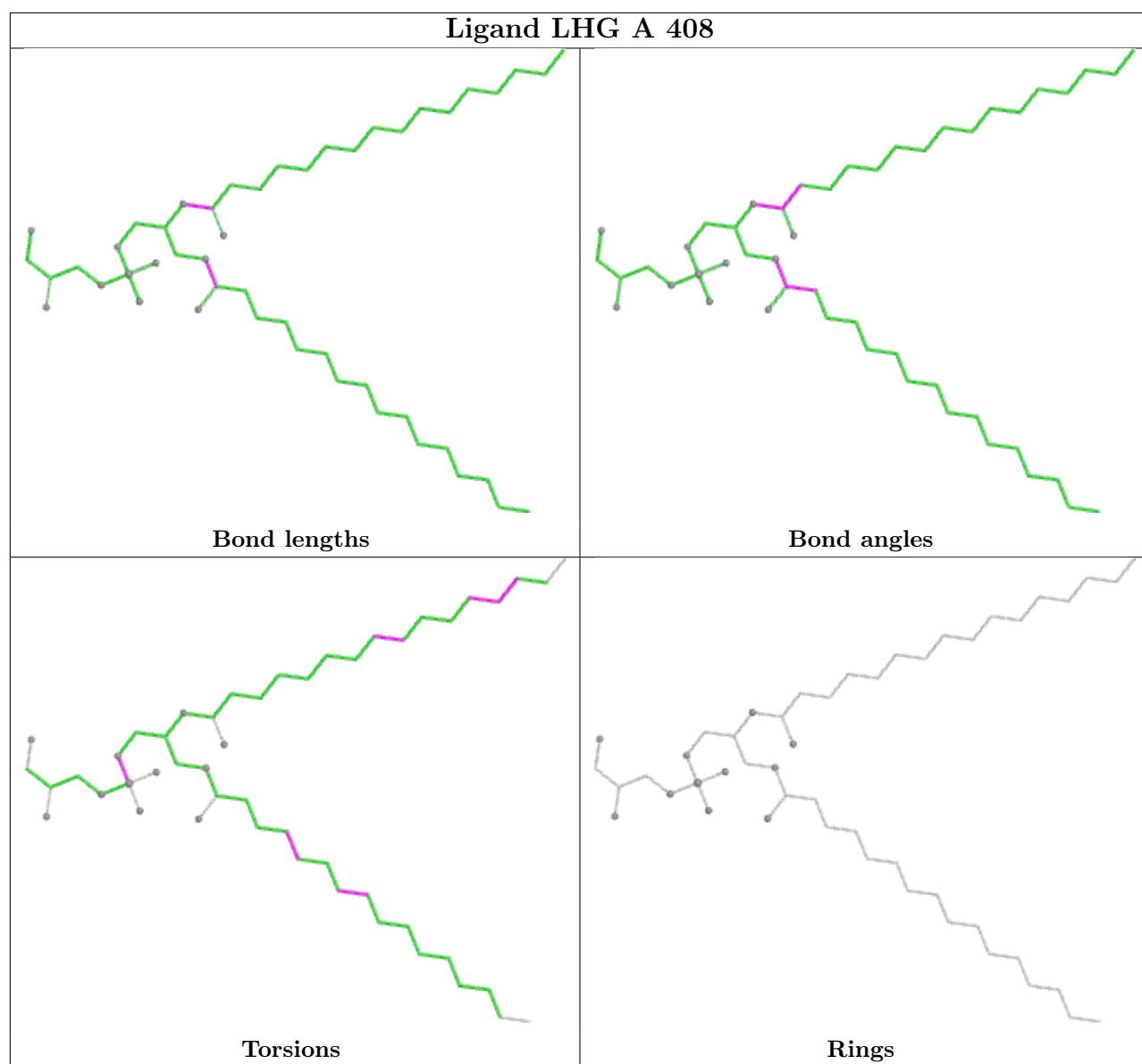
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	C	602	CLA	1	0
20	A	406	BCR	3	0
20	B	618	BCR	1	0
22	D	407	LHG	2	0
27	C	619	DGD	2	0
20	D	403	BCR	1	0
20	B	617	BCR	1	0
19	C	604	CLA	1	0
19	C	610	CLA	1	0
19	B	614	CLA	1	0
19	D	402	CLA	2	0
20	H	101	BCR	6	0
19	D	409	CLA	1	0
20	K	101	BCR	1	0
19	A	403	CLA	1	0
24	D	411	PHO	1	0
21	B	623	LMG	1	0
19	B	612	CLA	2	0
19	A	404	CLA	1	0
20	C	616	BCR	2	0
19	B	604	CLA	1	0
19	C	603	CLA	3	0
20	C	615	BCR	4	0
20	Z	101	BCR	7	0
19	D	401	CLA	1	0
19	B	602	CLA	1	0
25	E	101	HEM	4	0

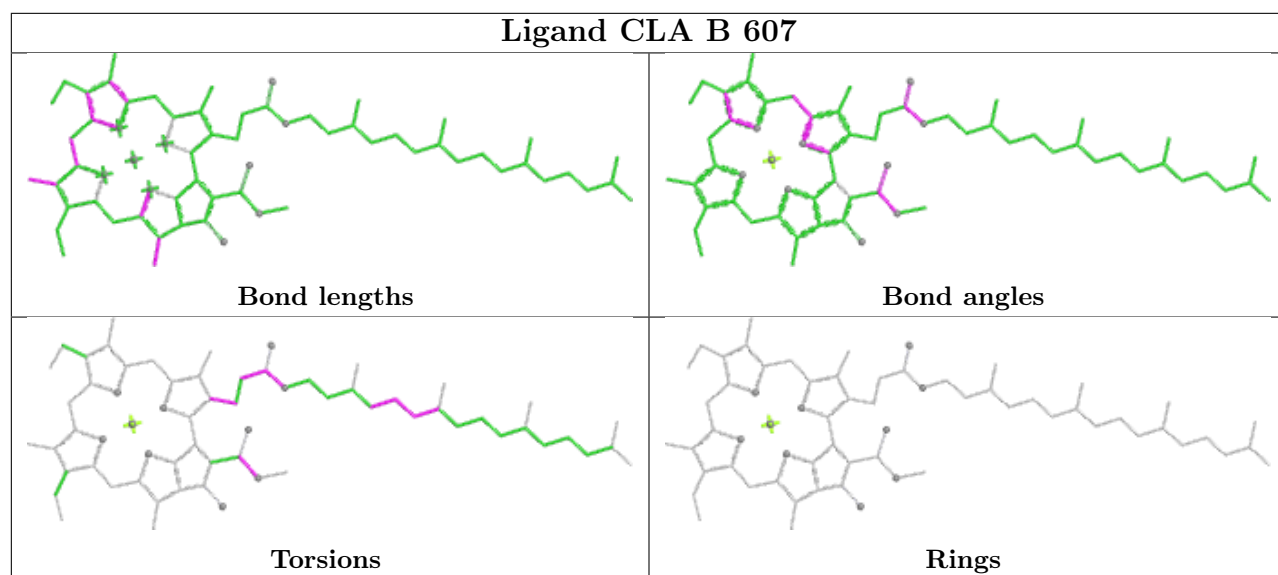
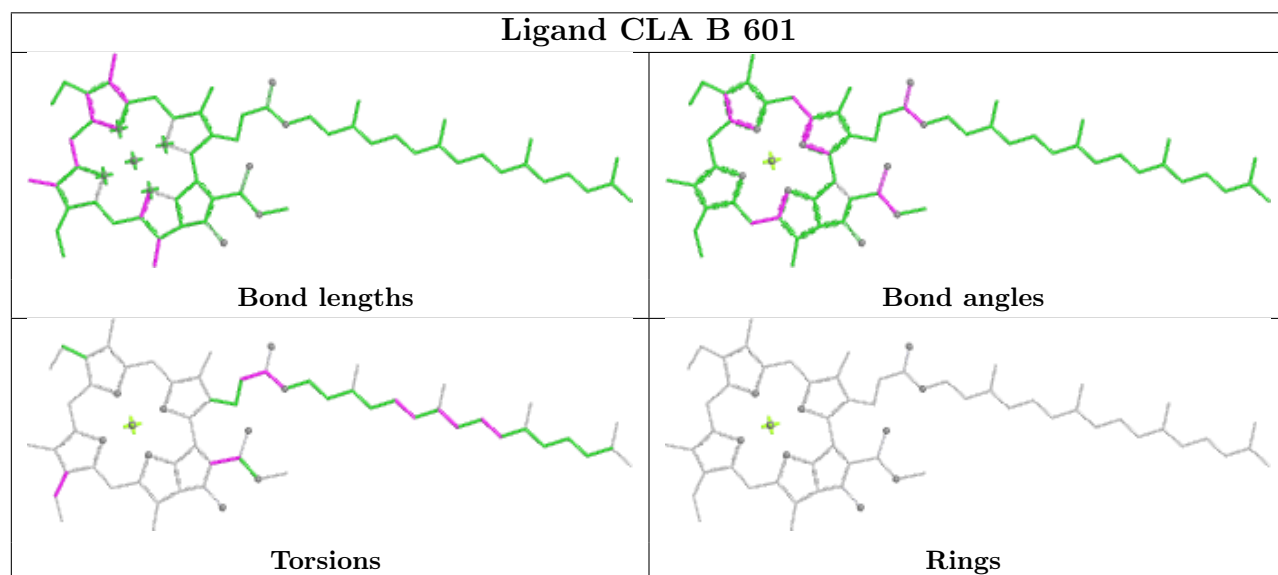
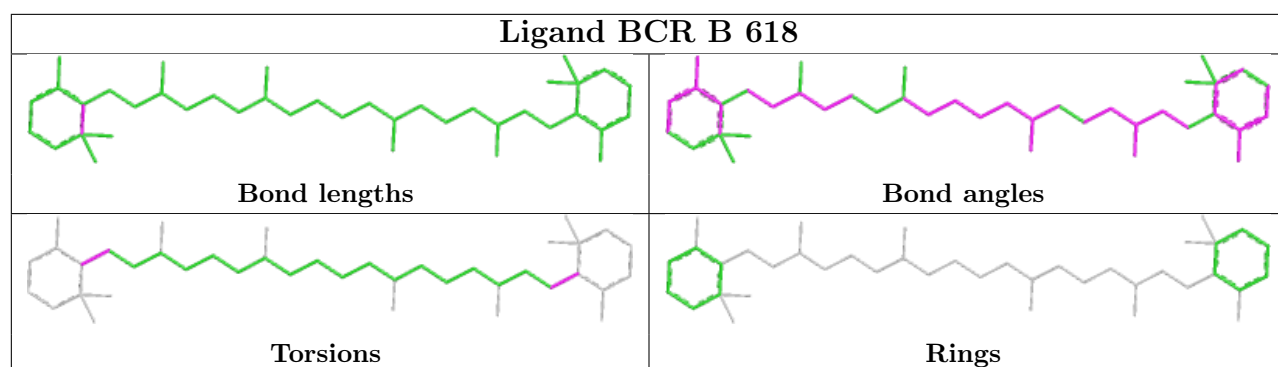
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

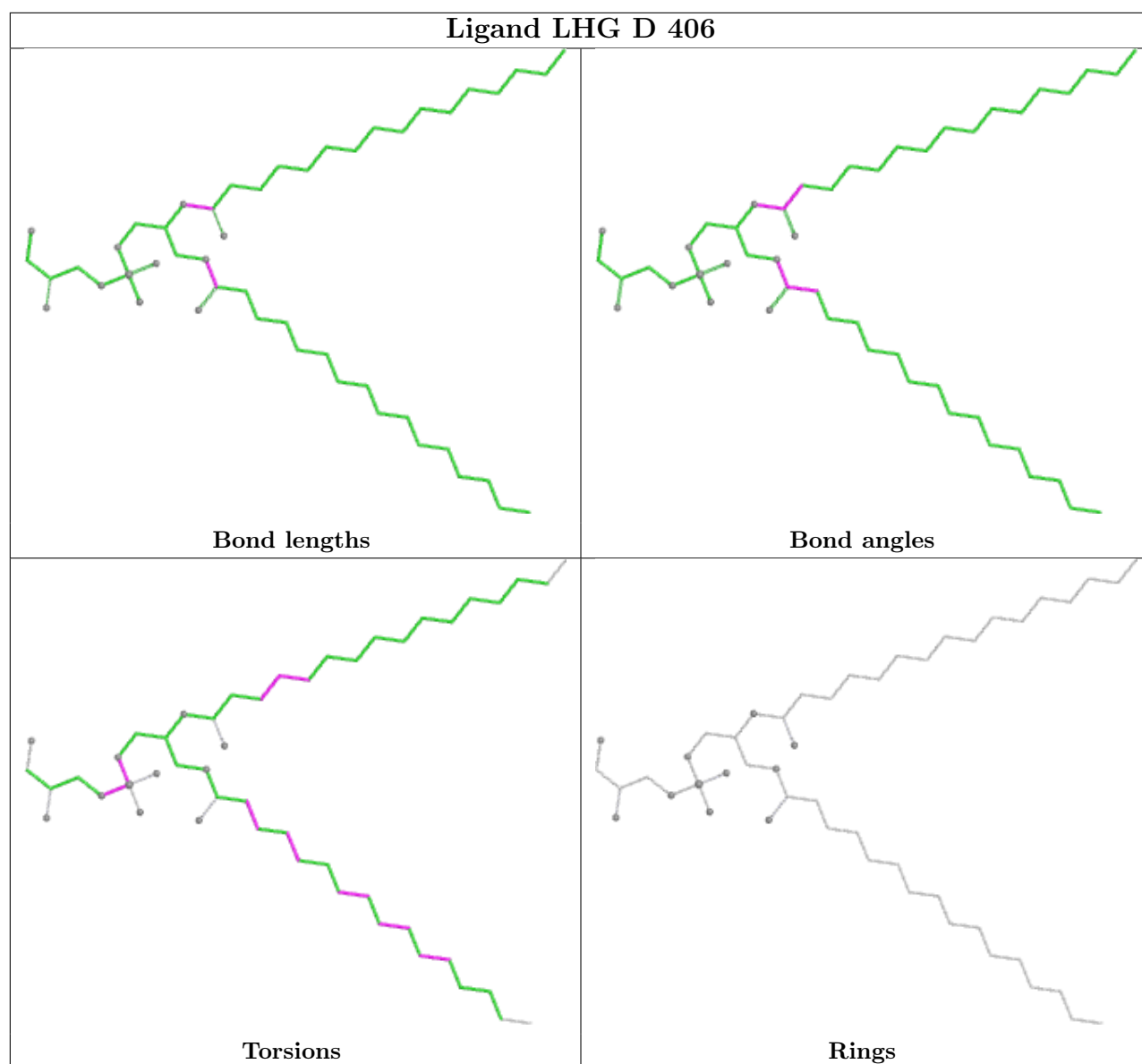


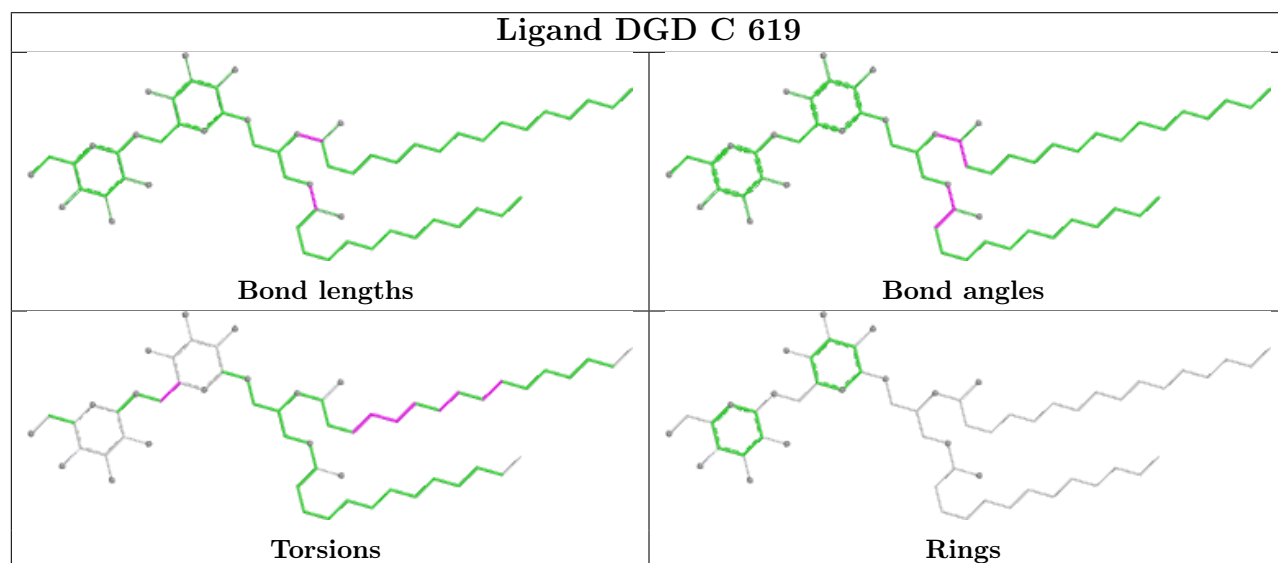
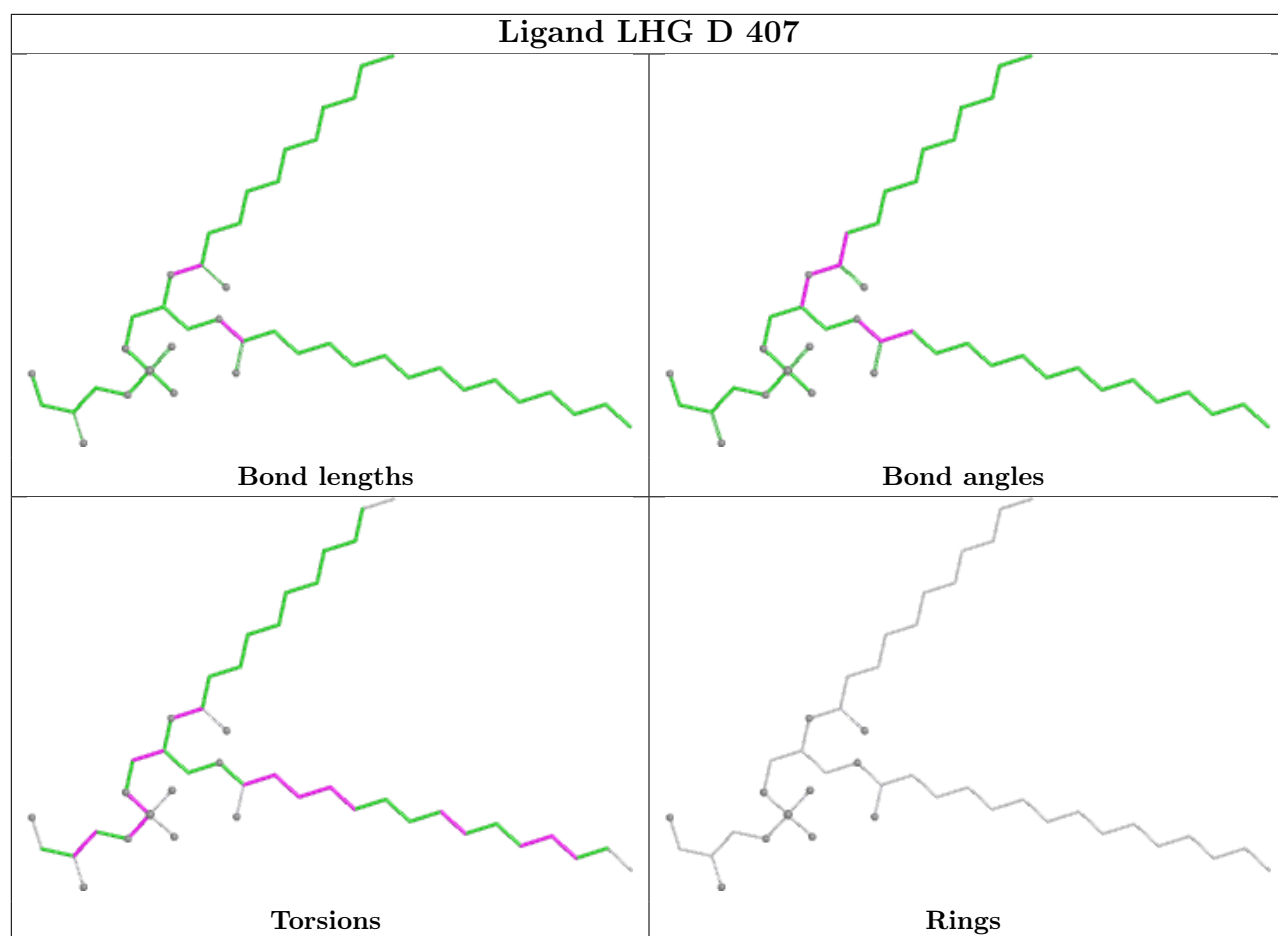


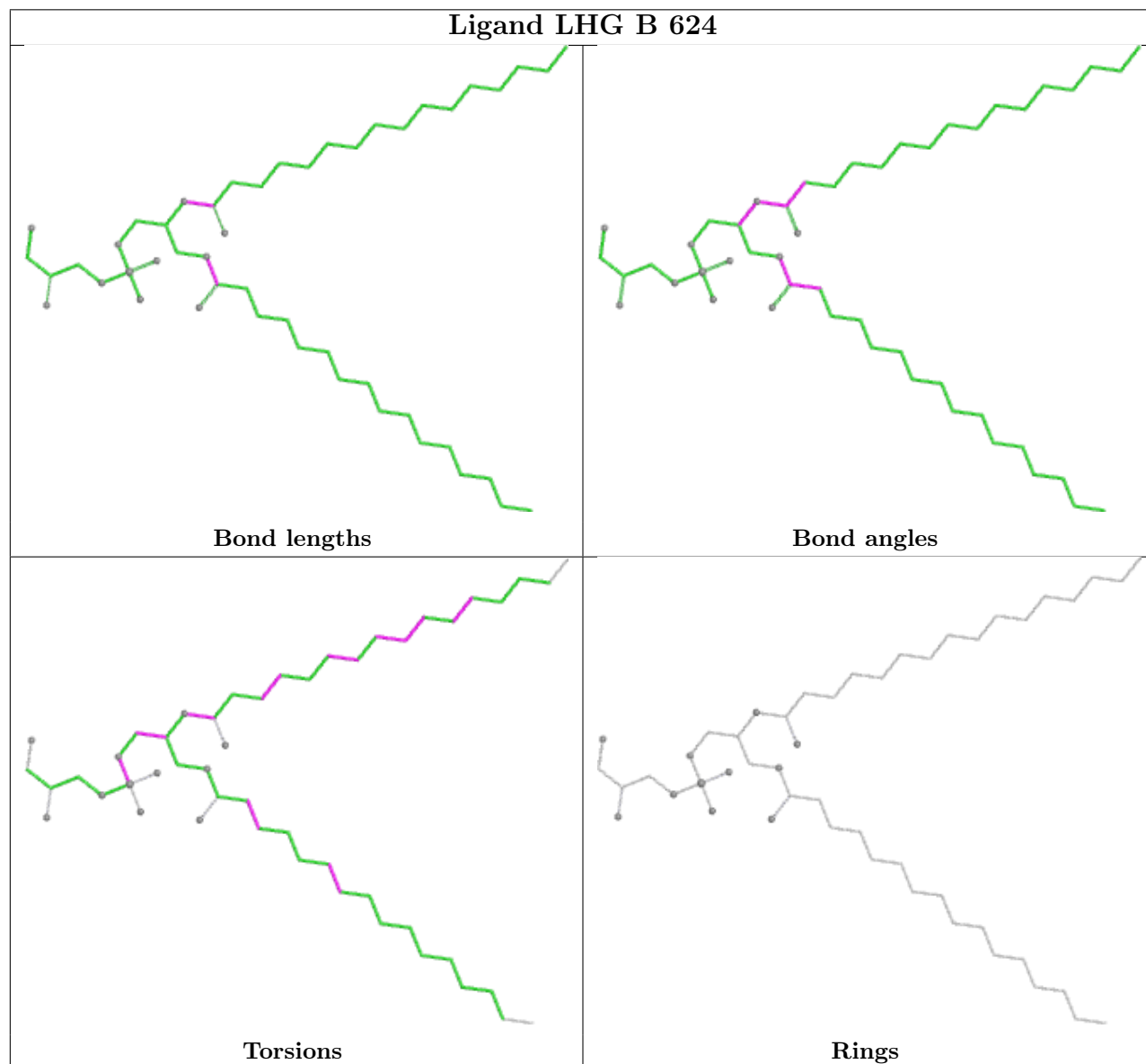
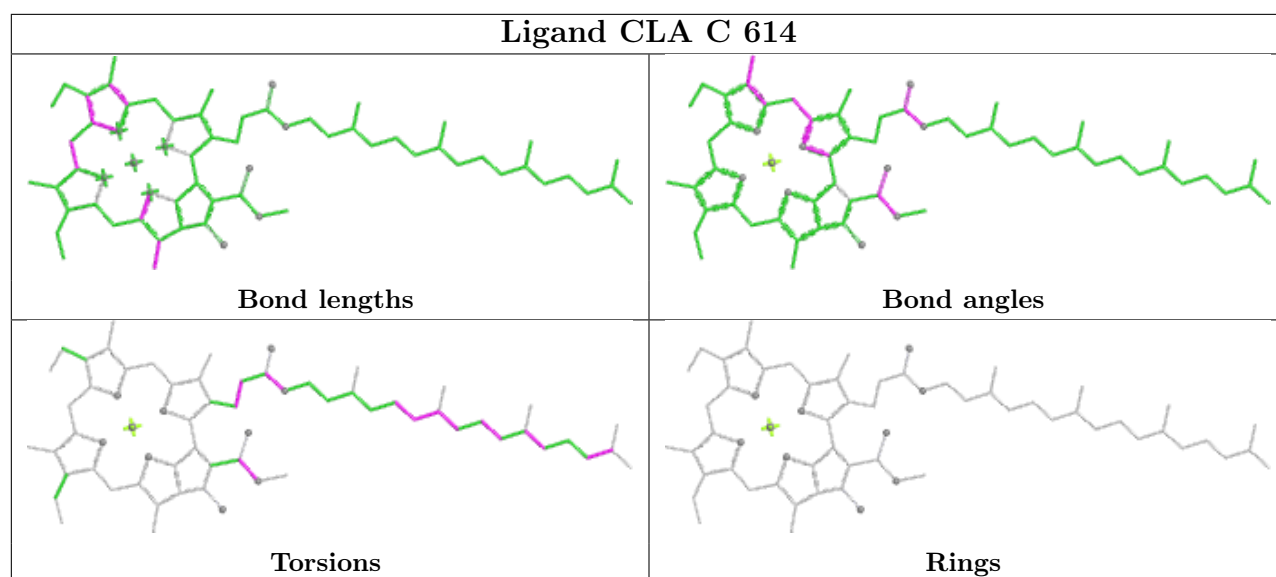


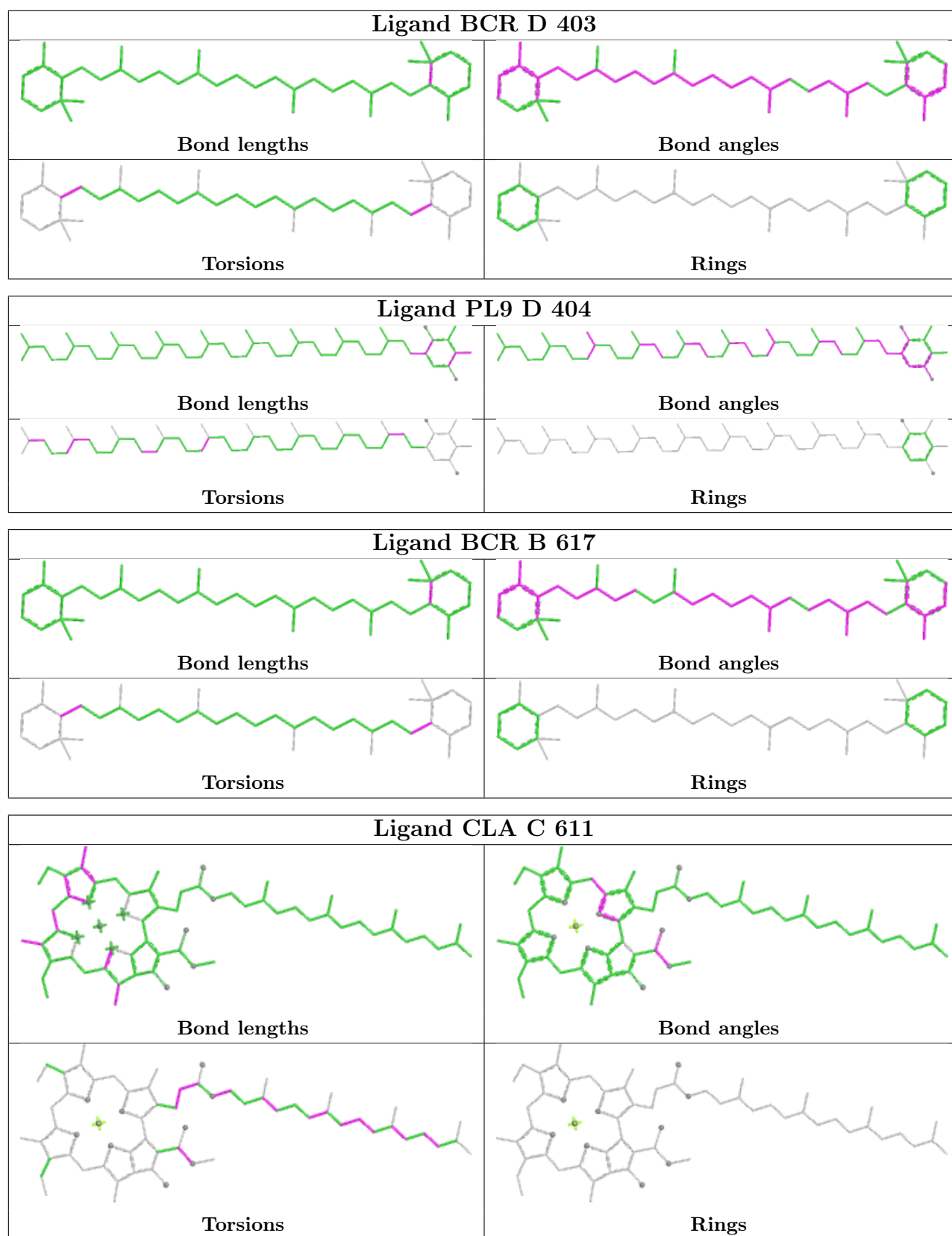


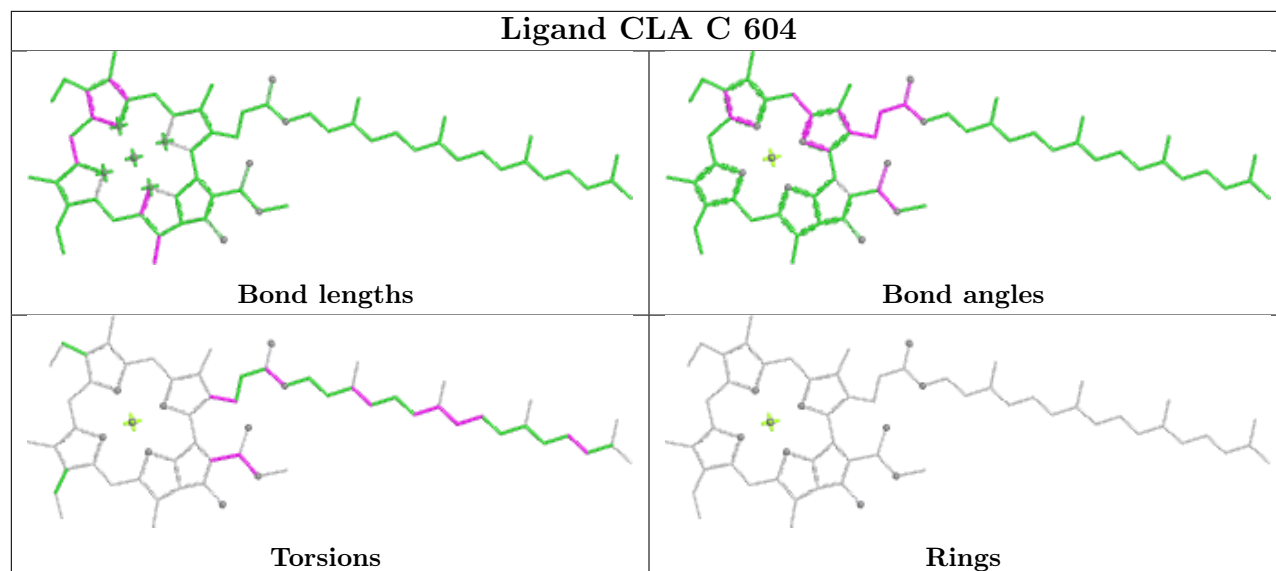
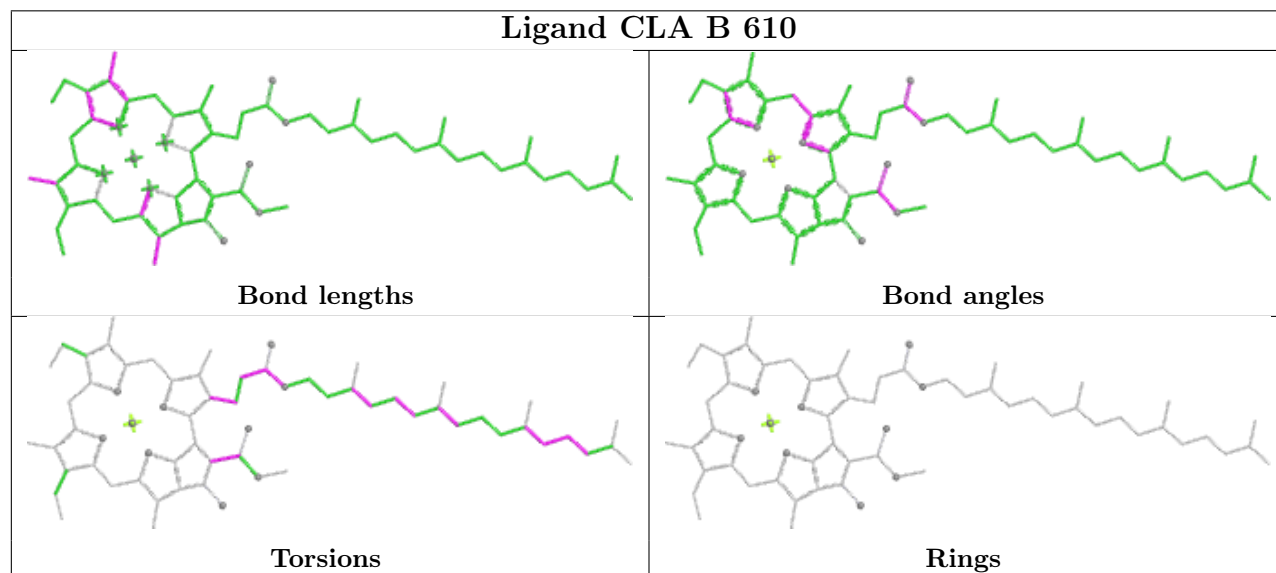
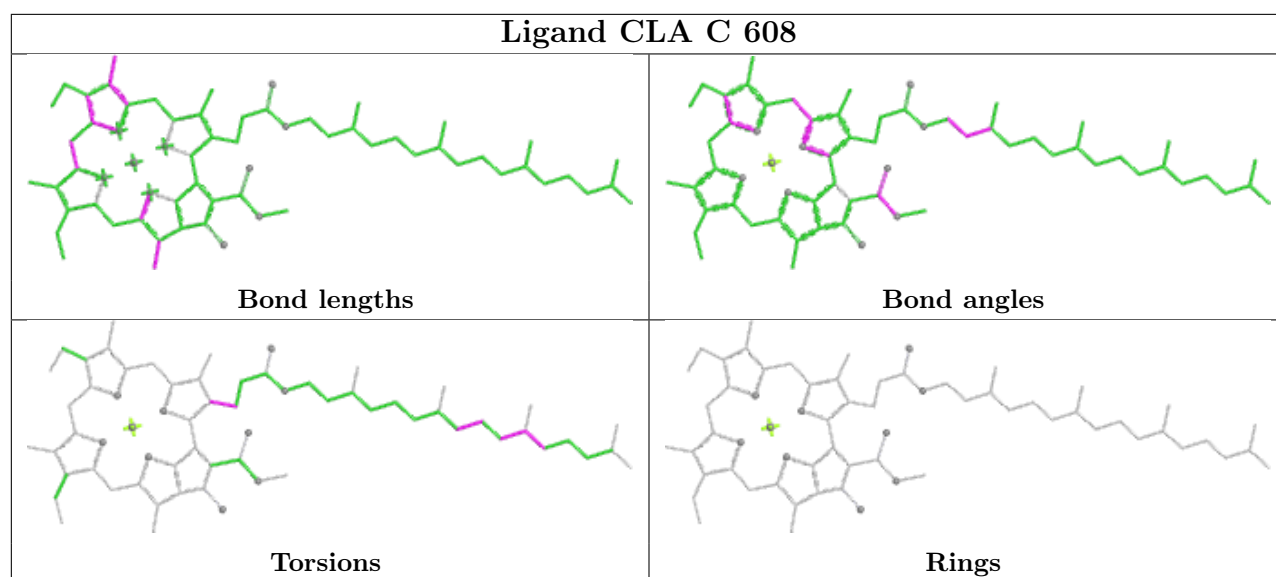


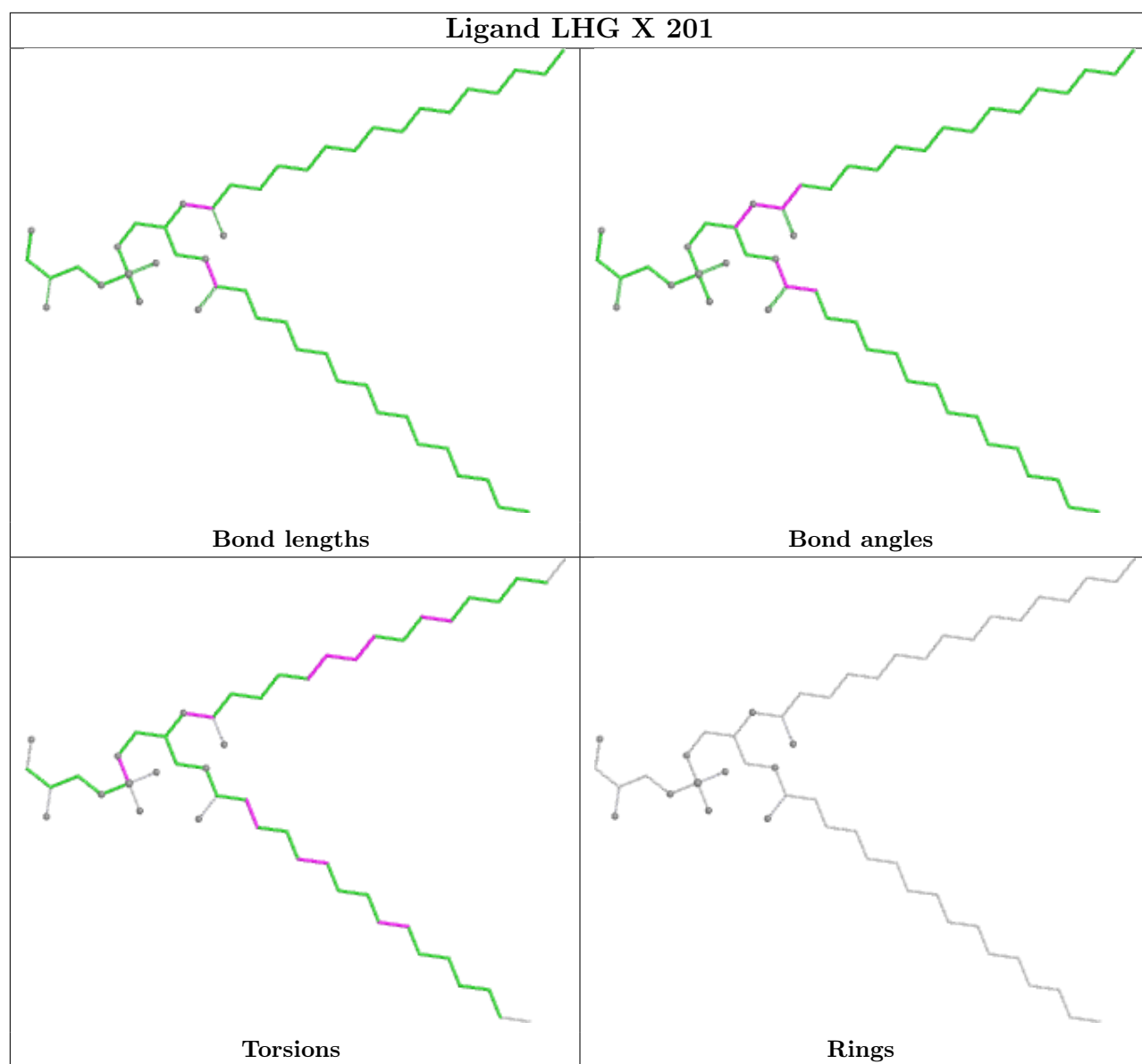


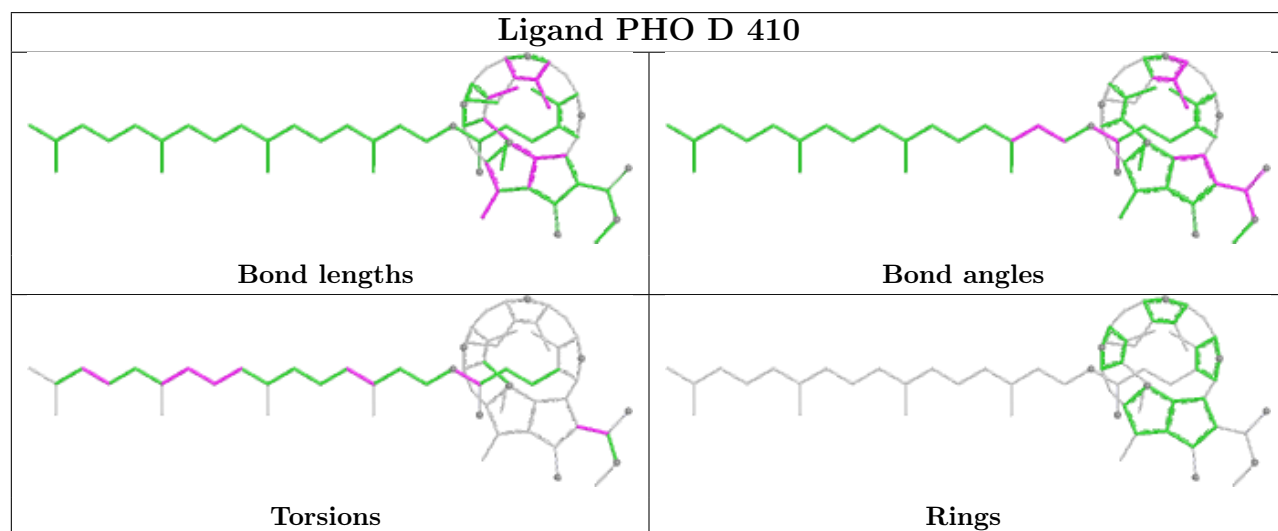
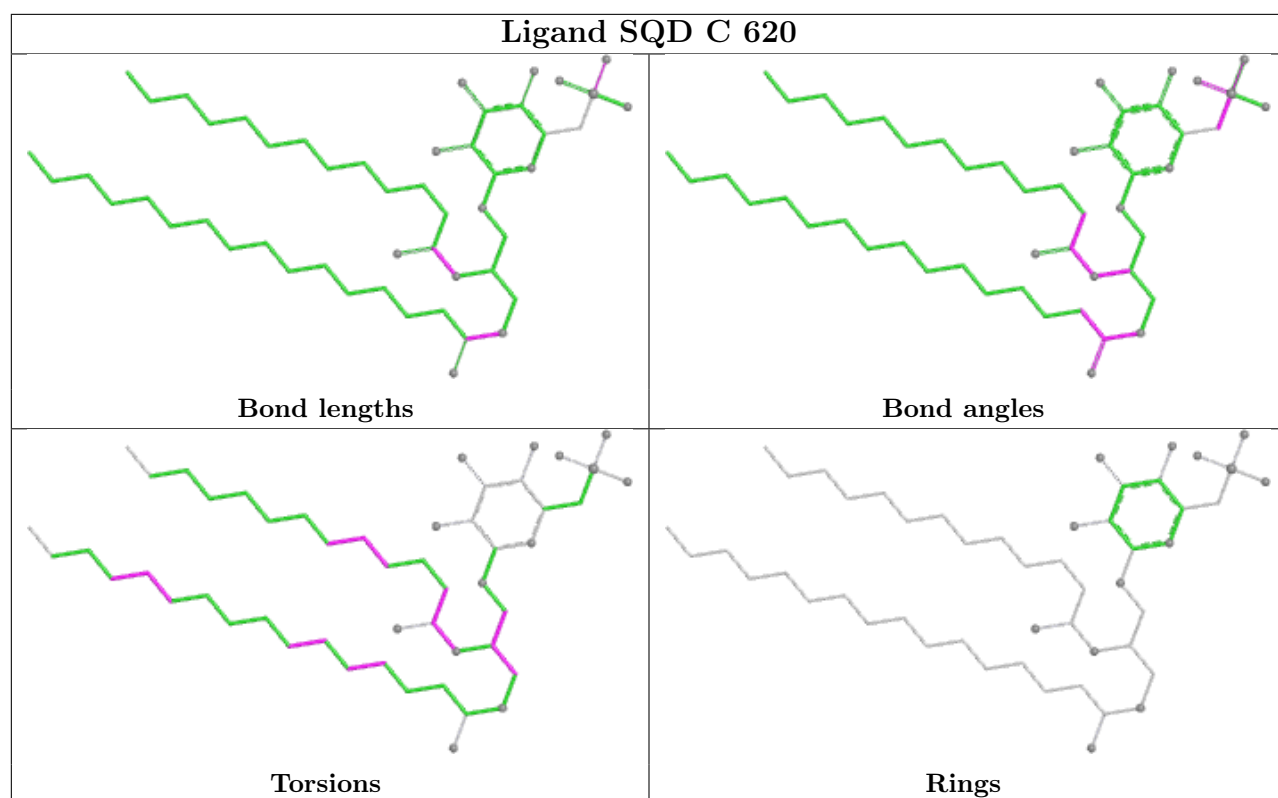


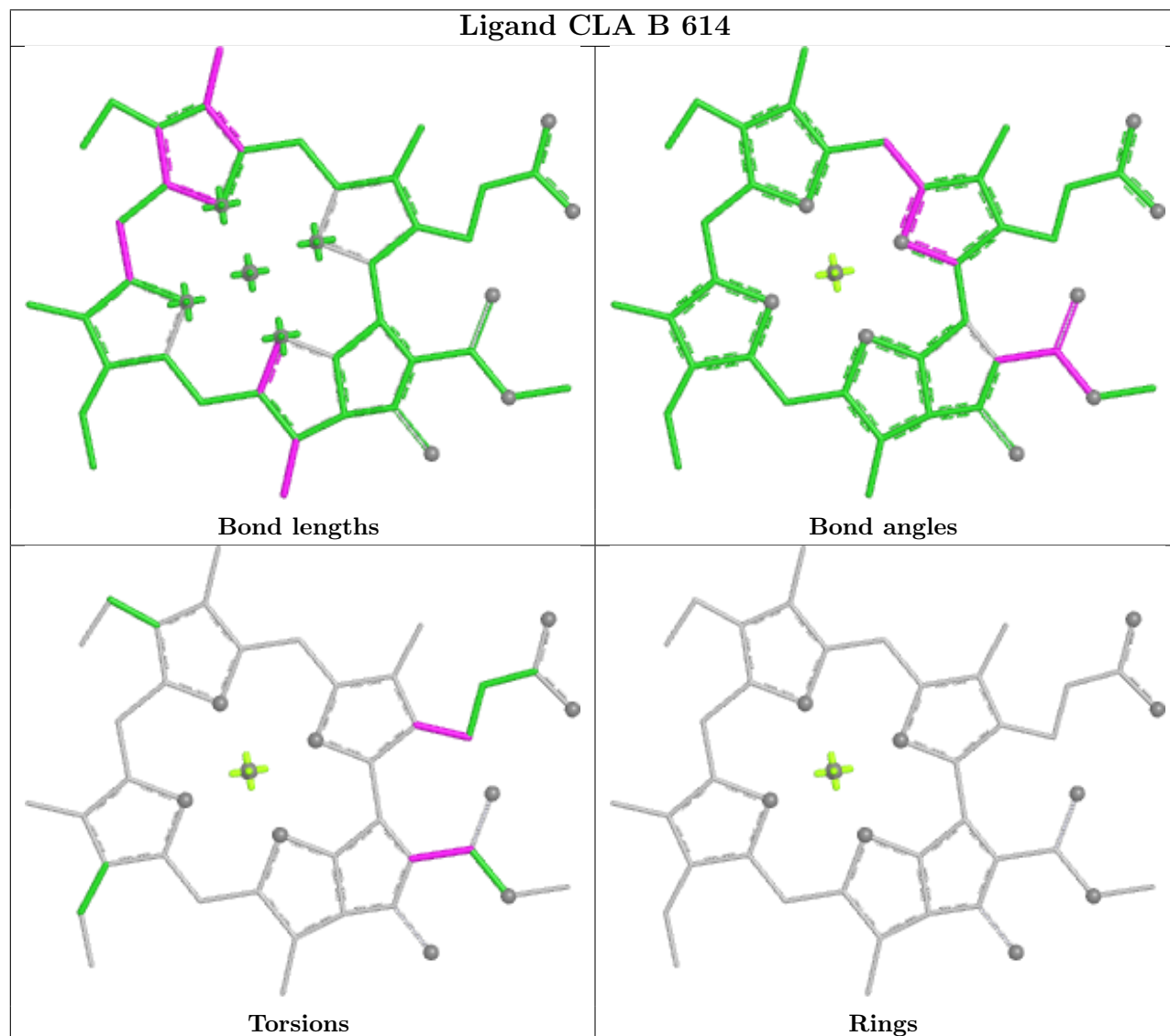
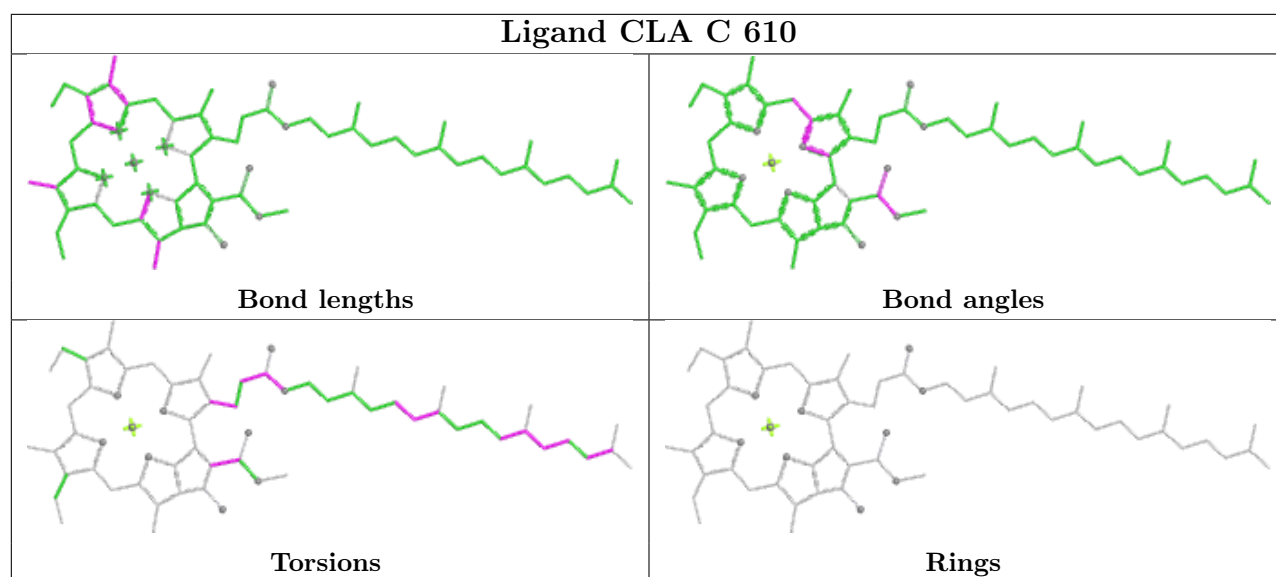


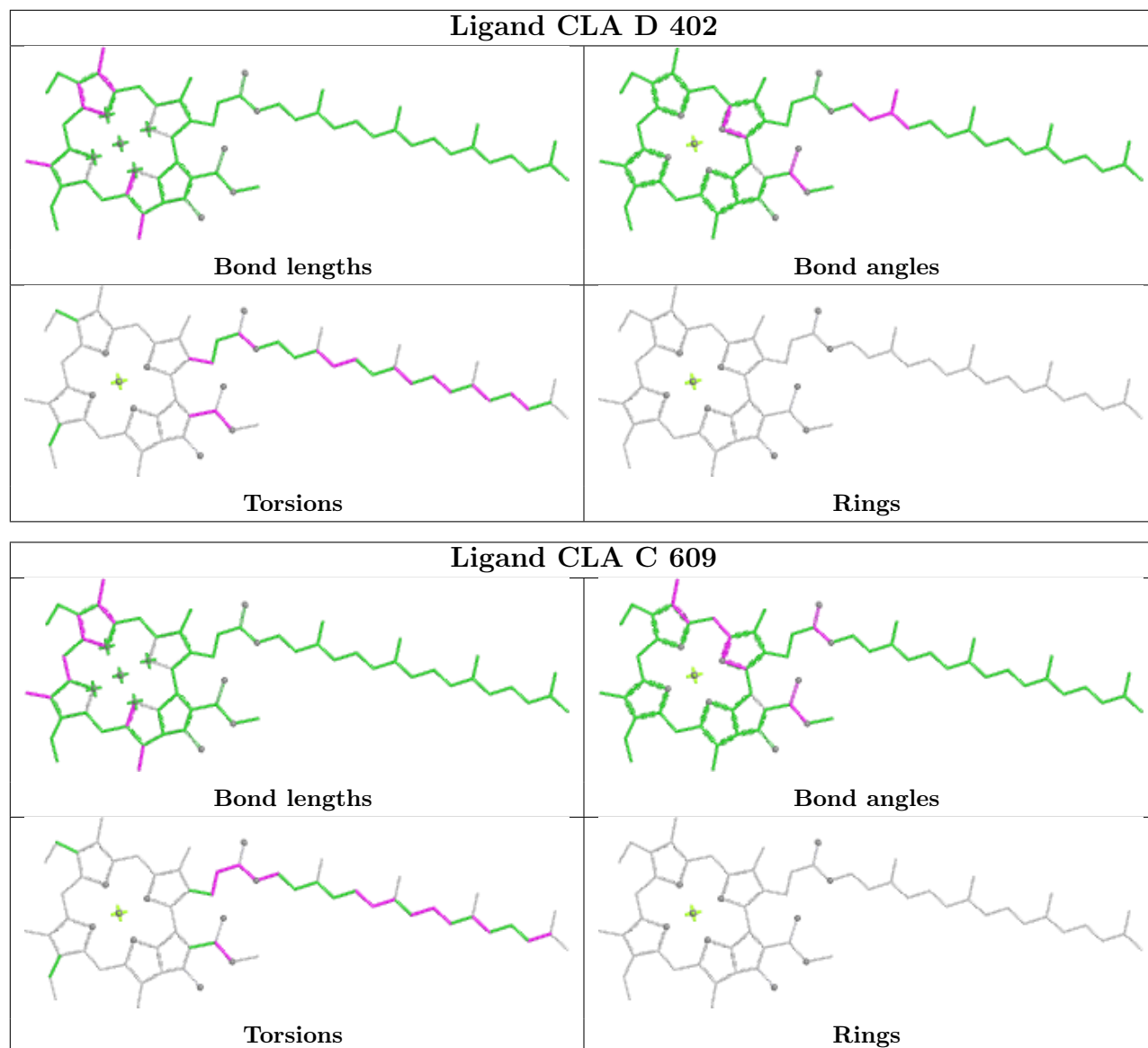


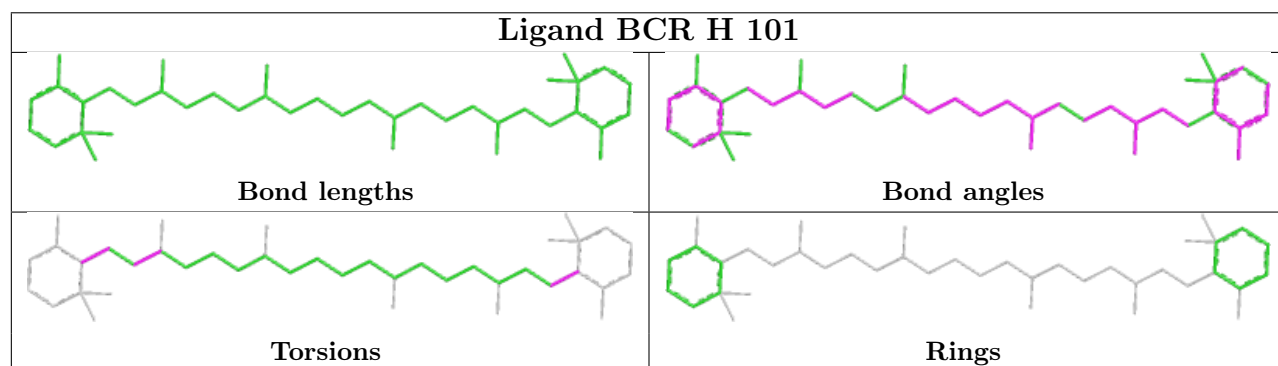
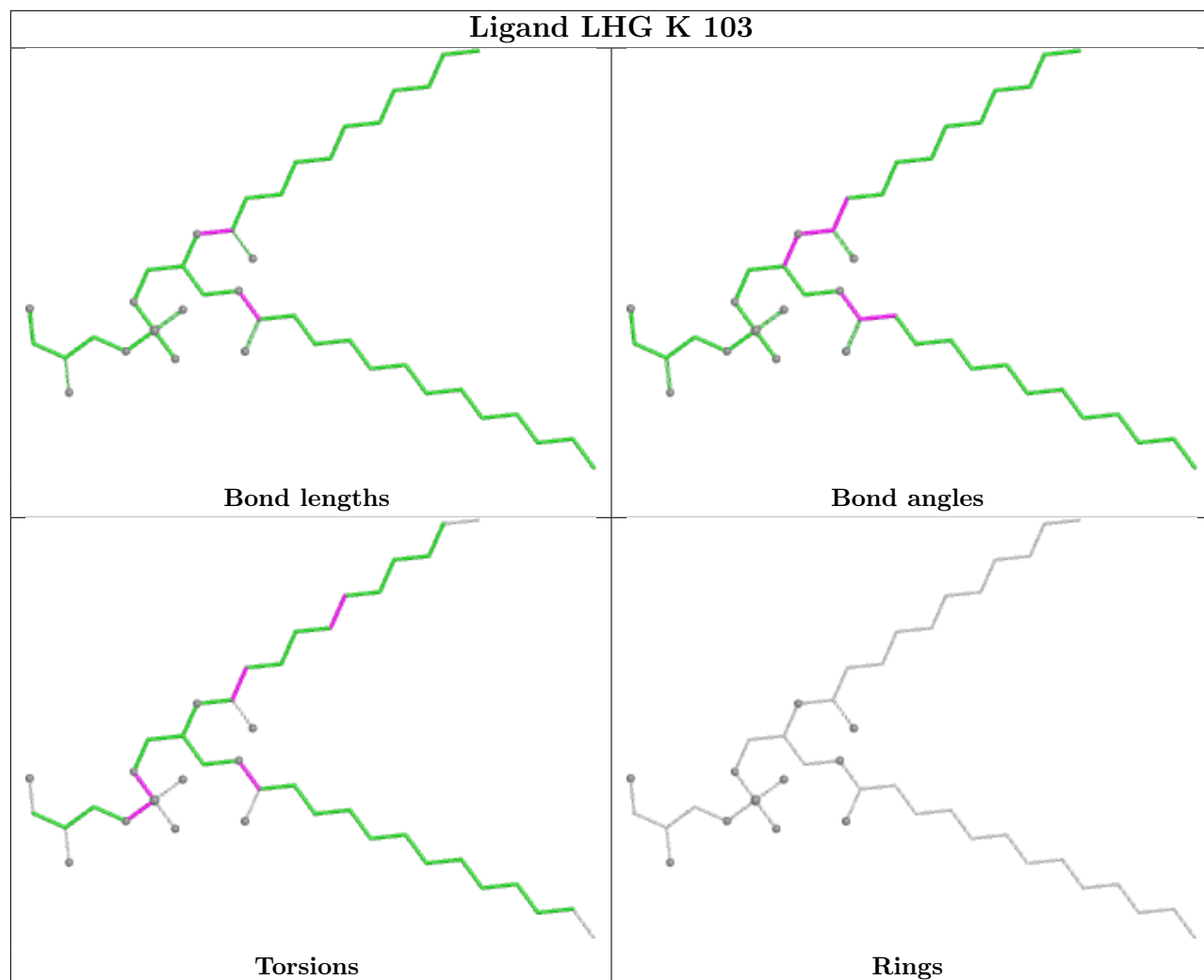


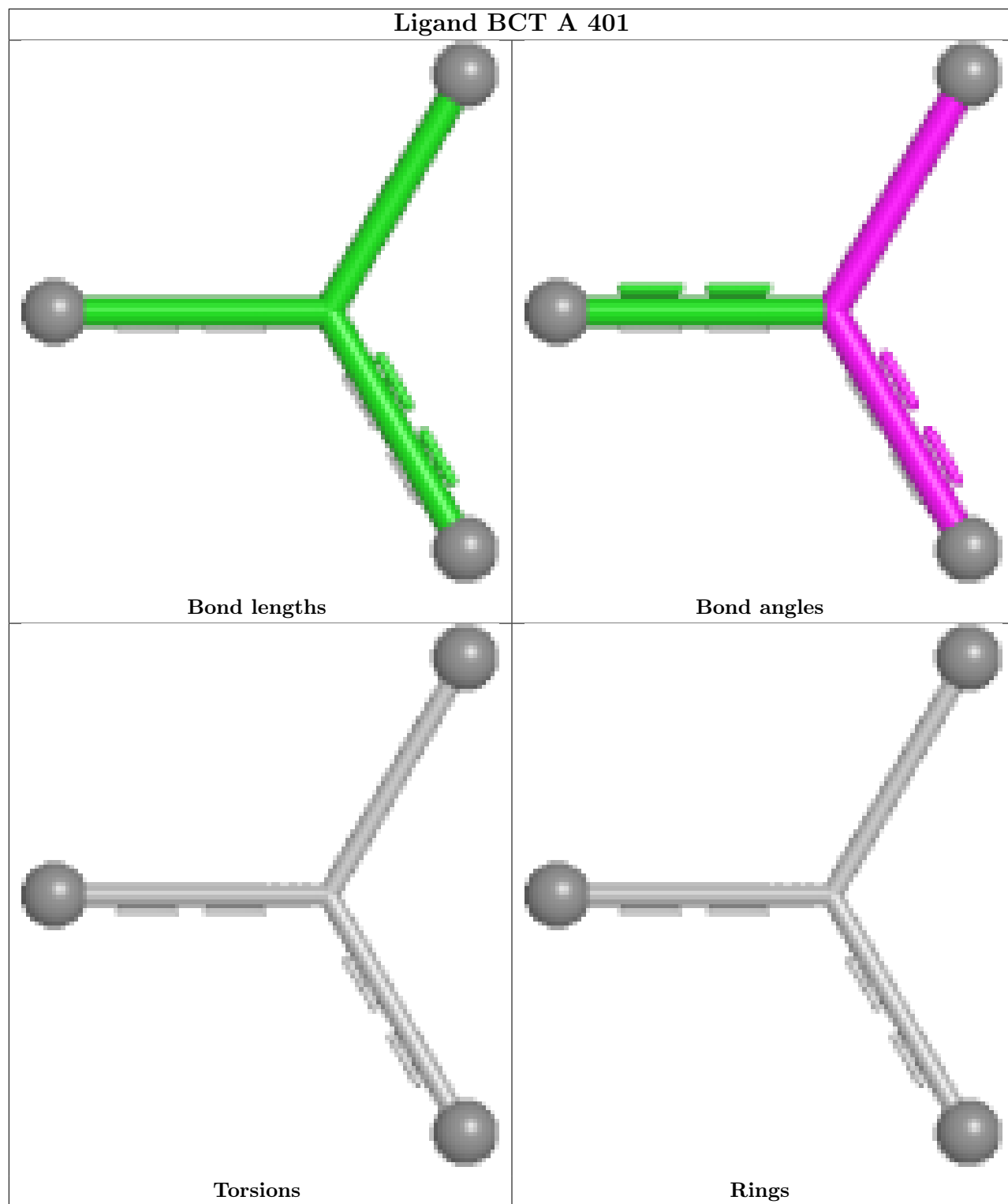


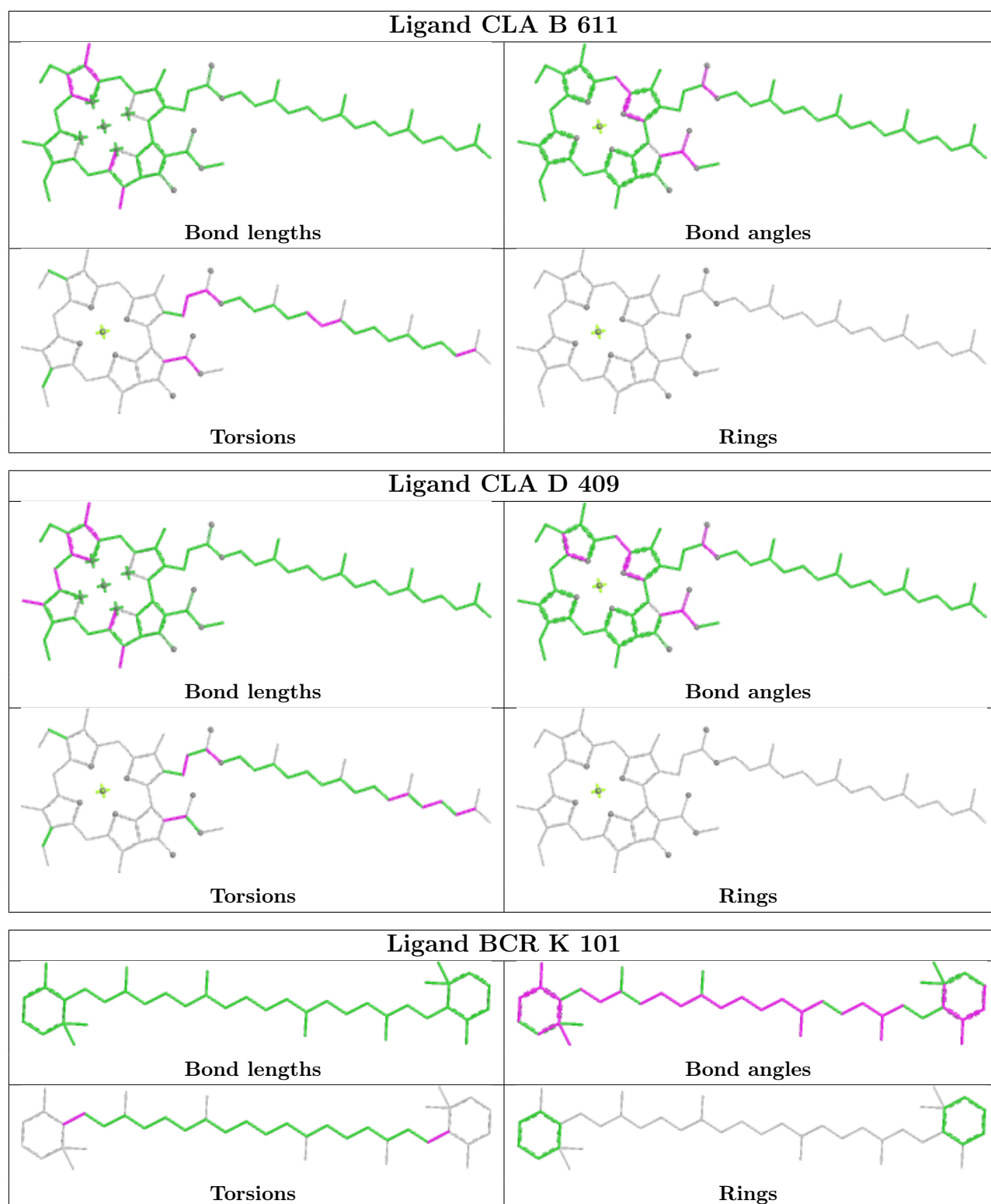


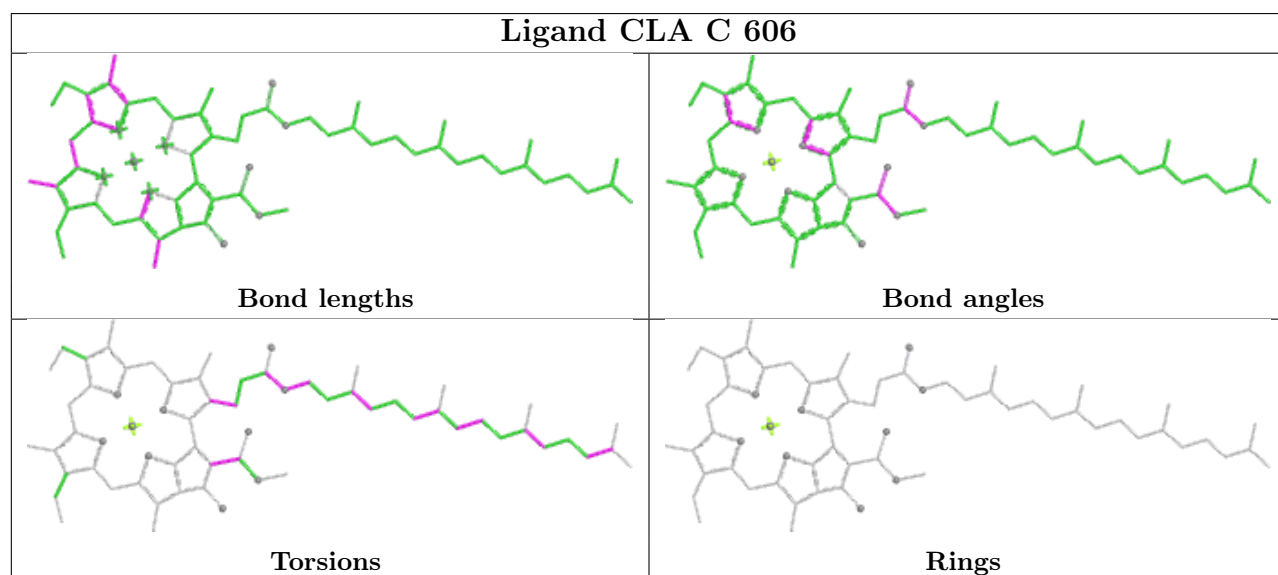
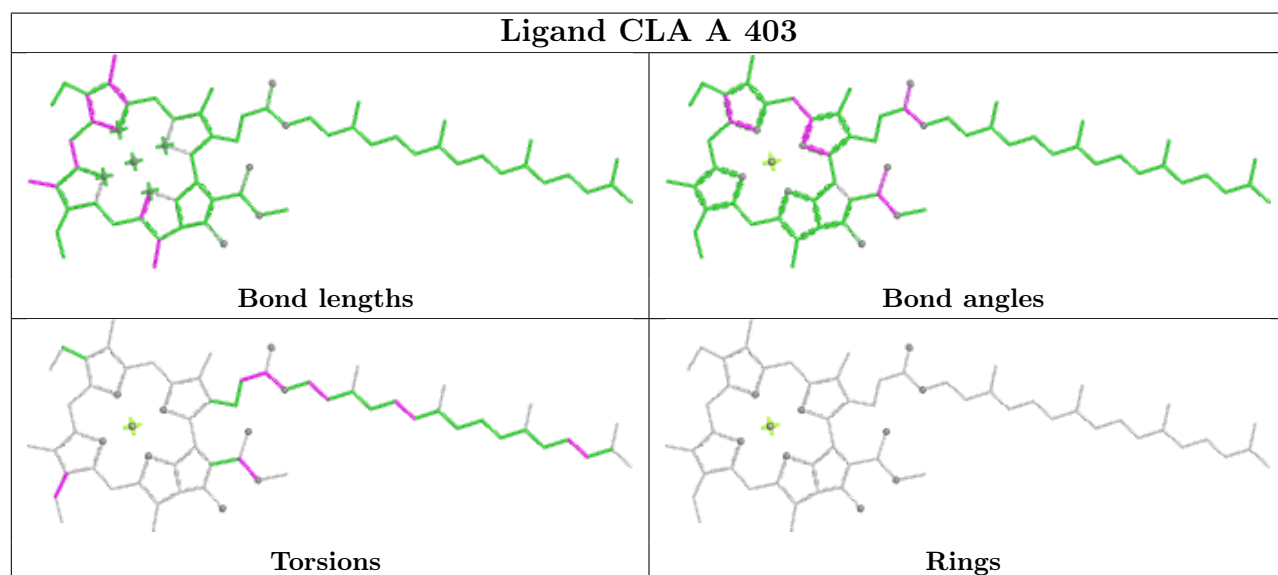
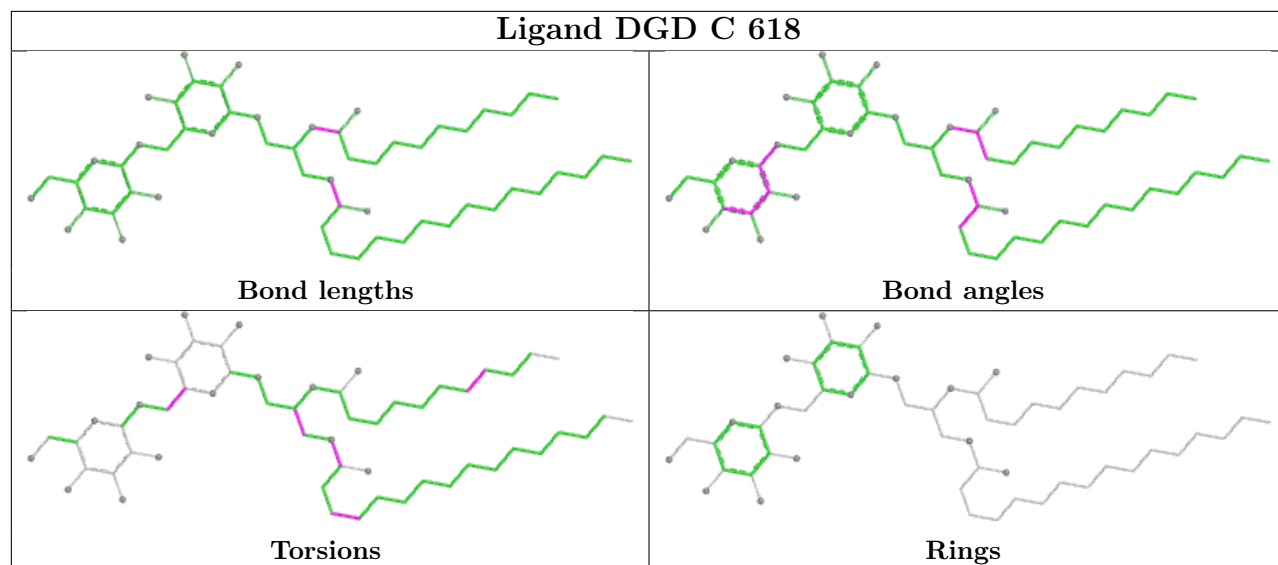


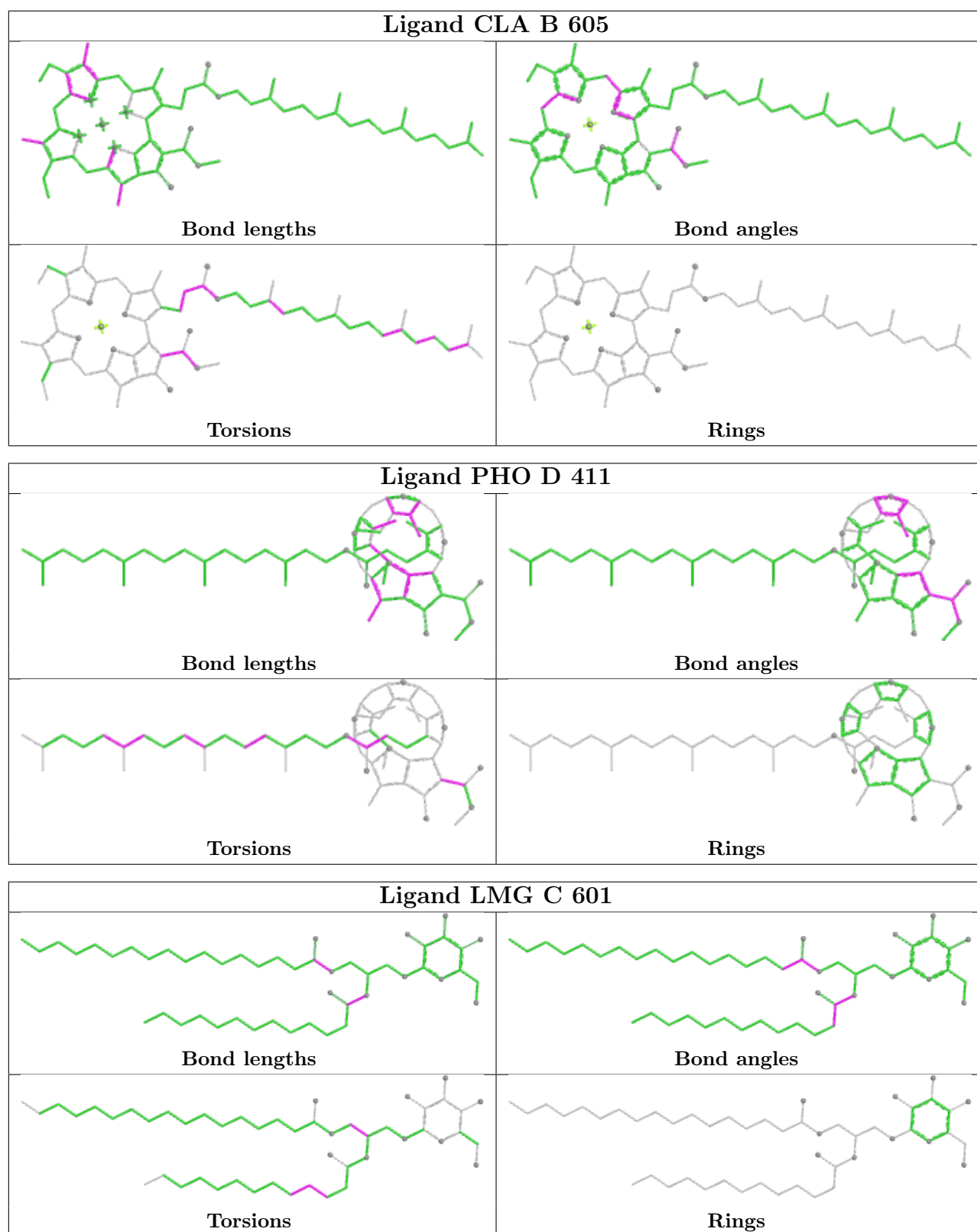


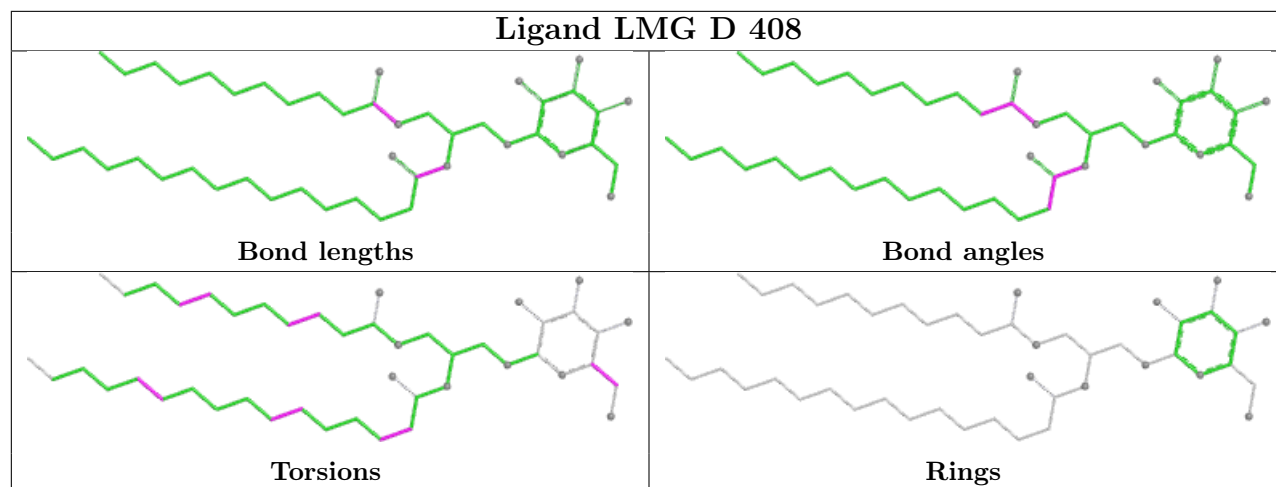
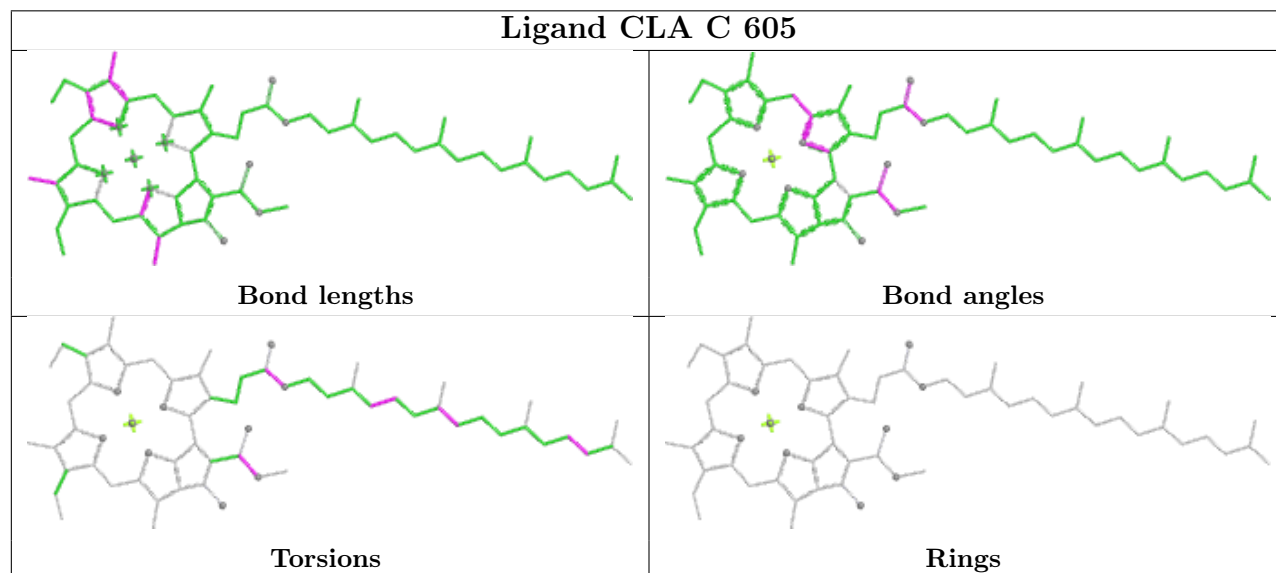
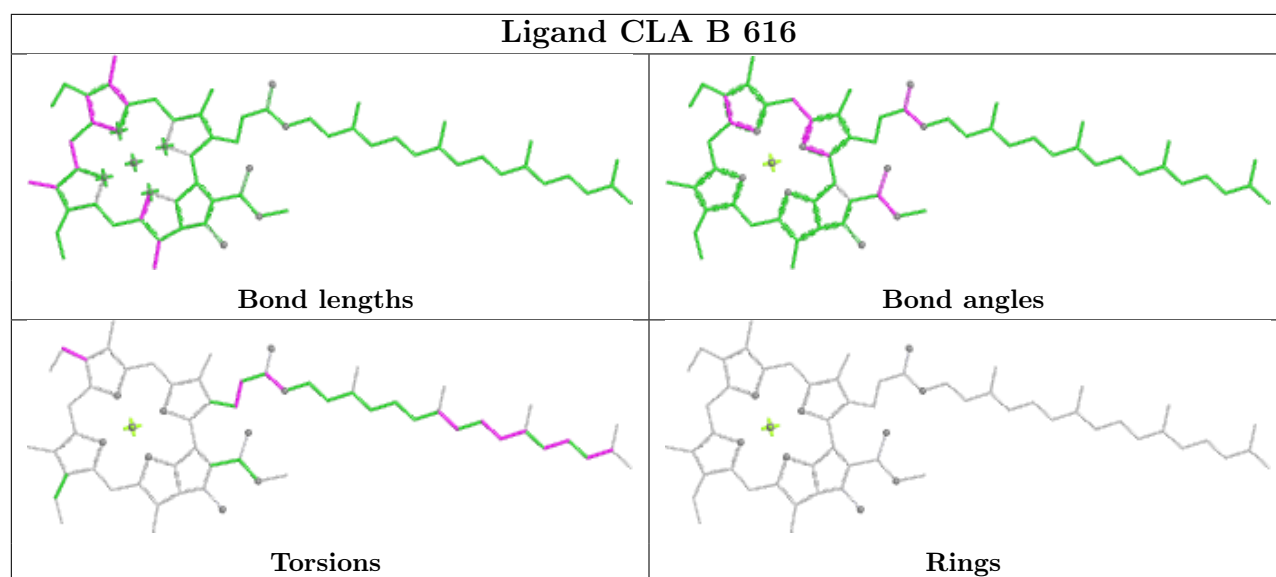


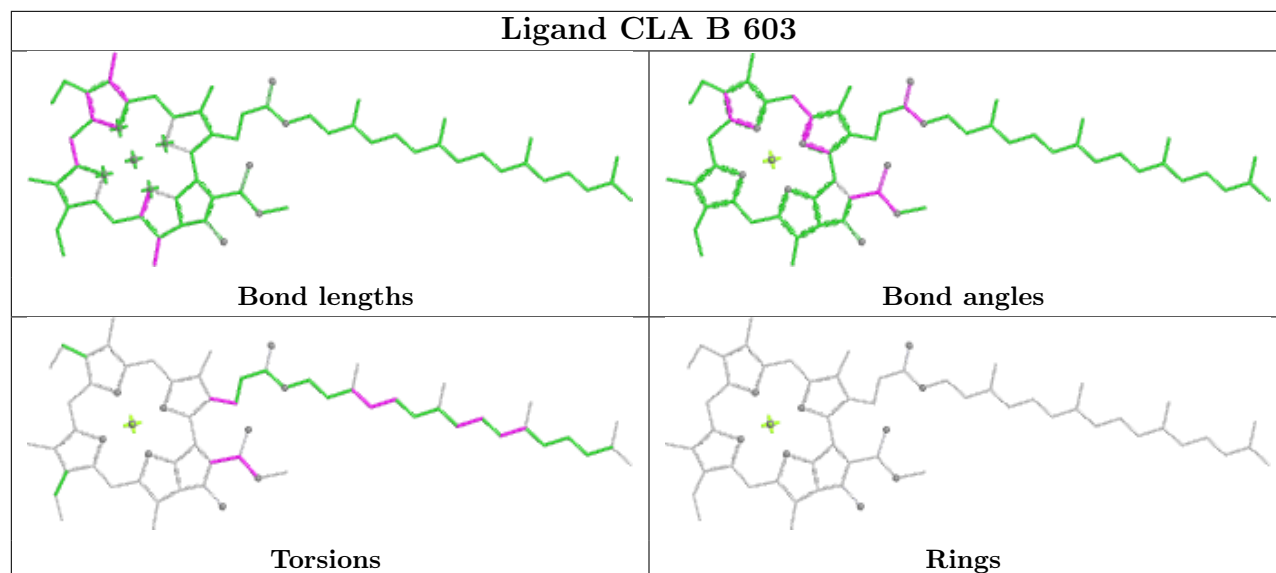
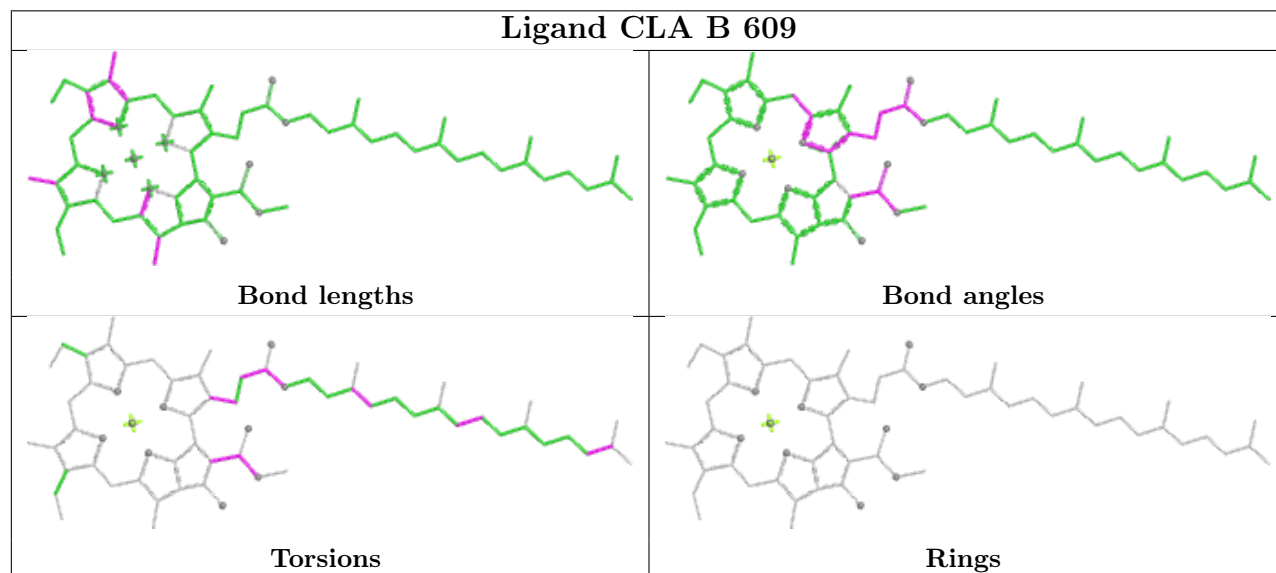
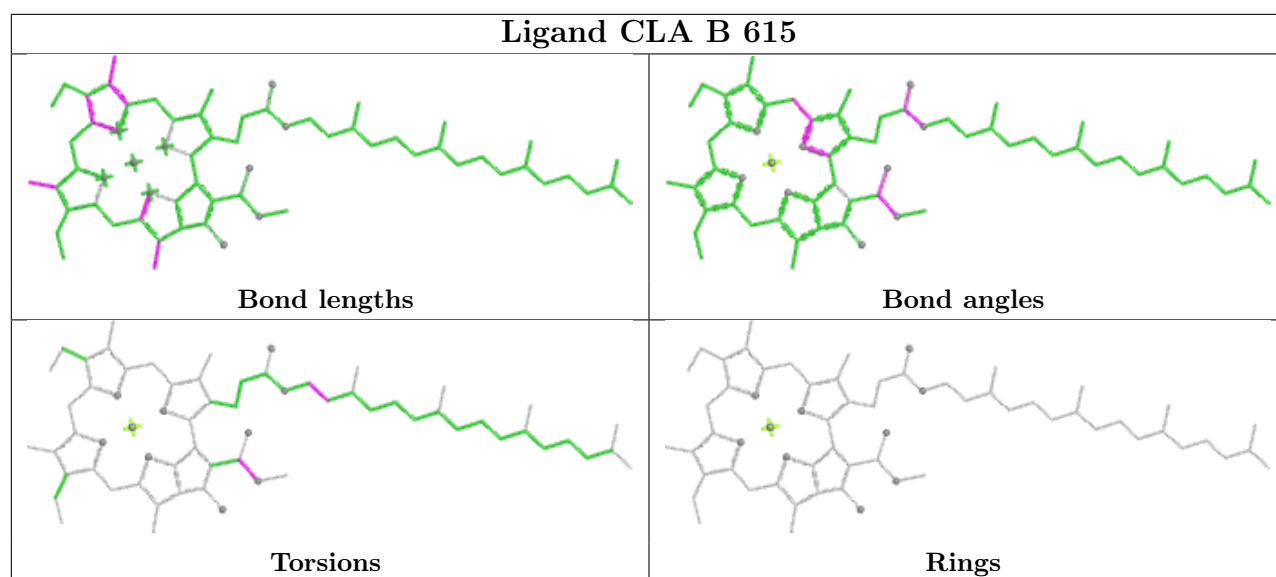


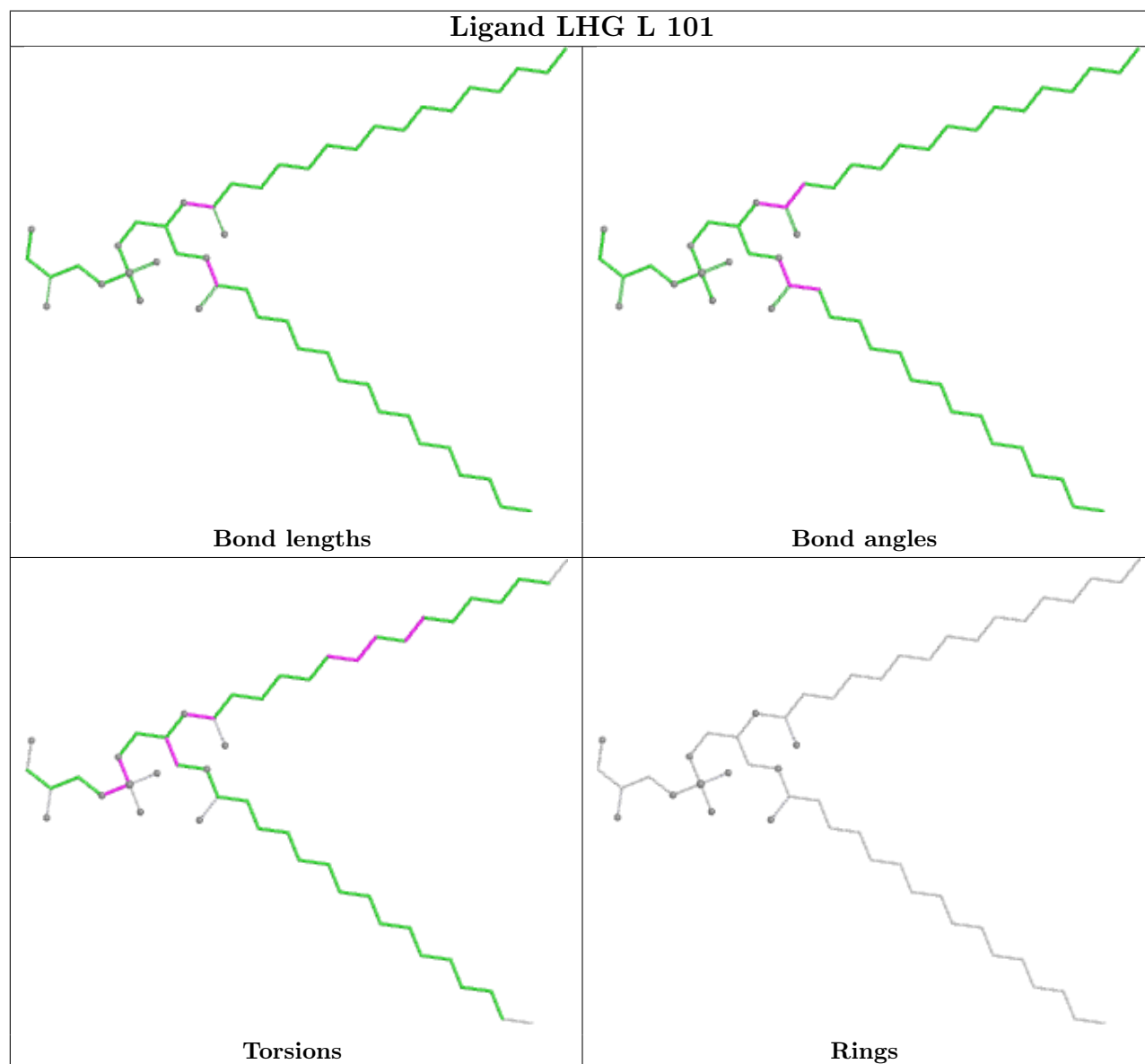
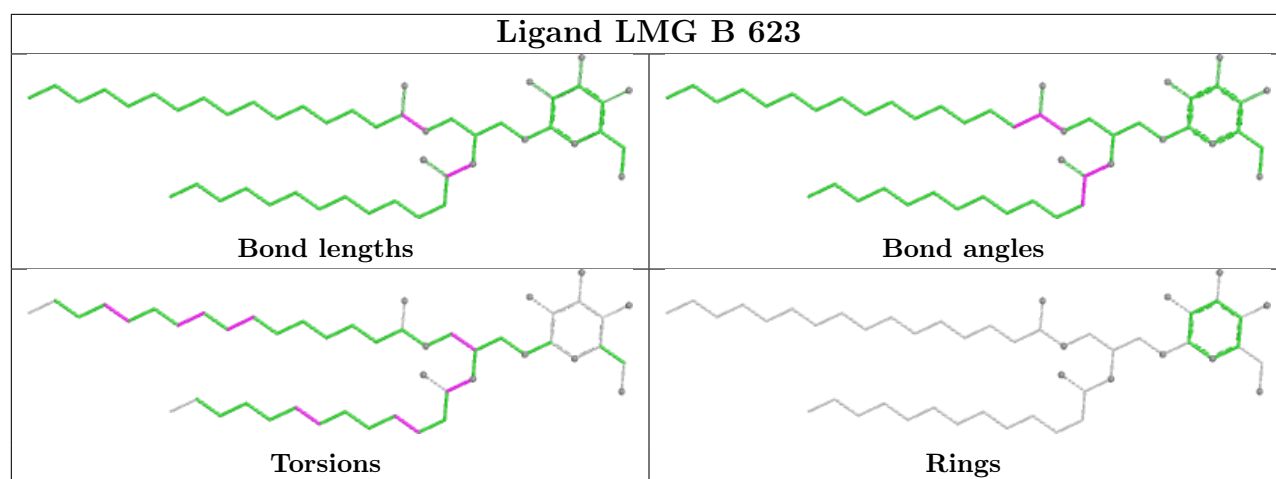


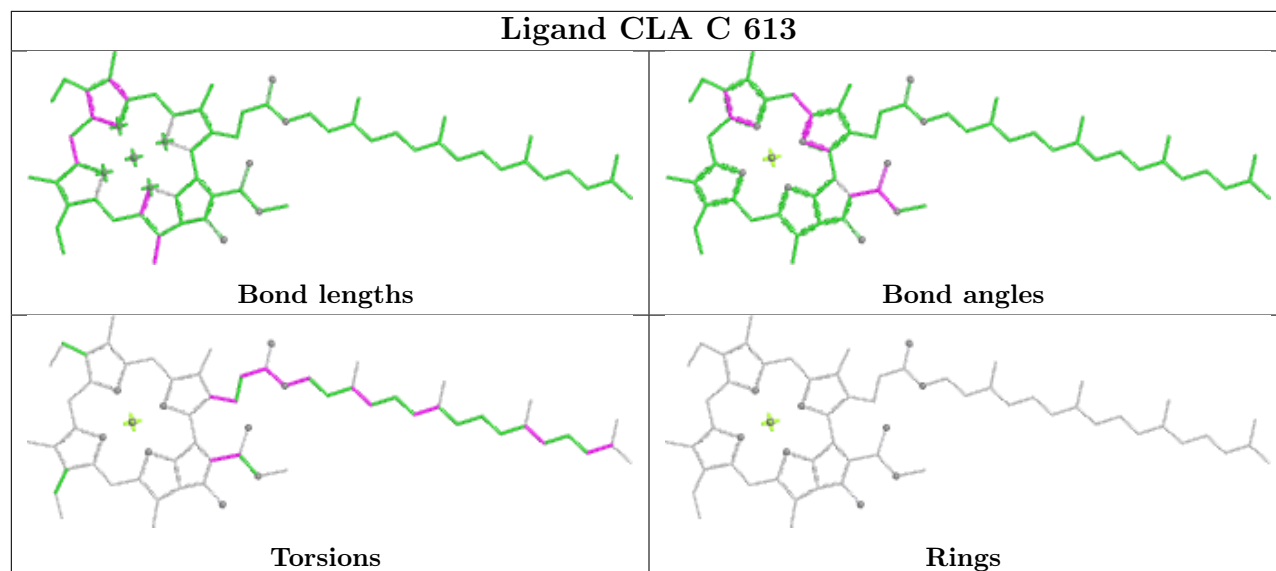
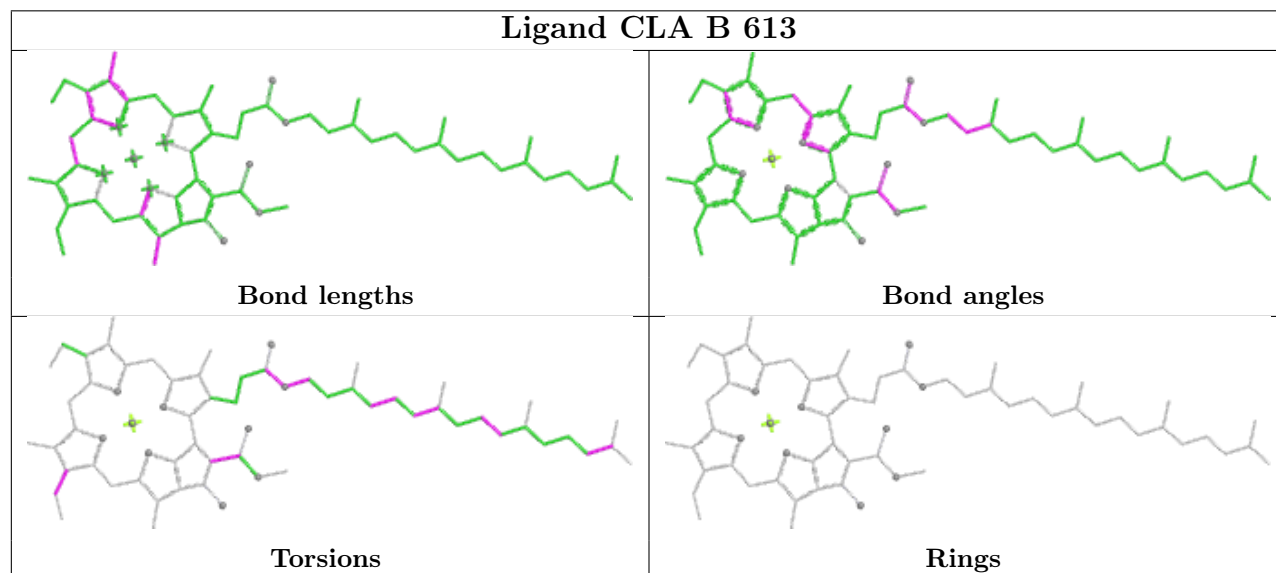
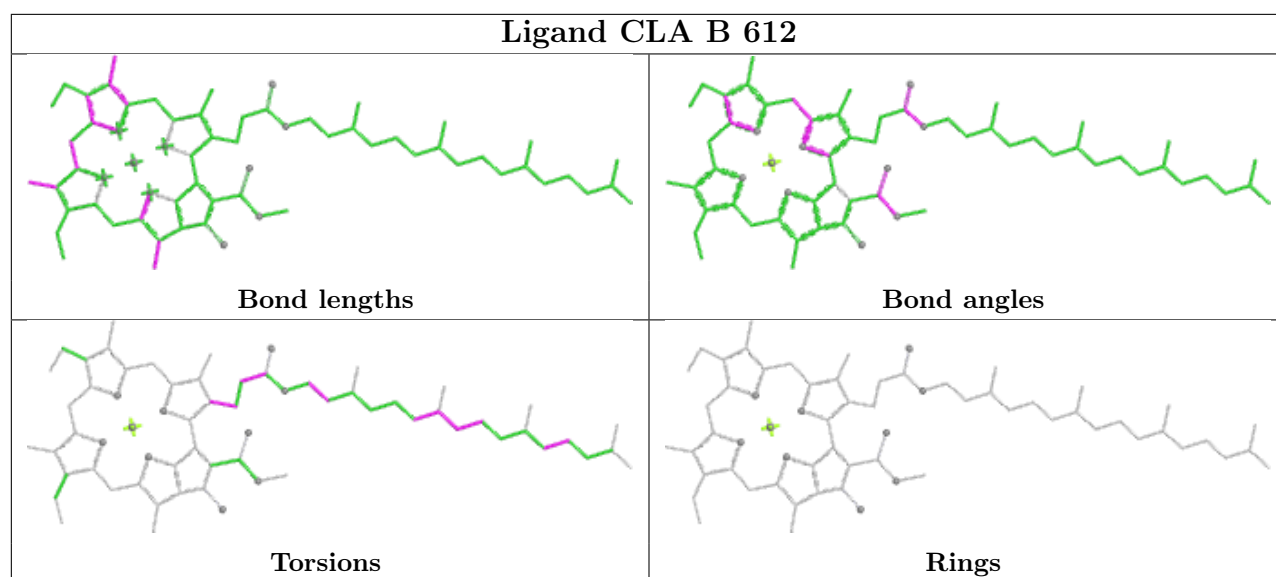


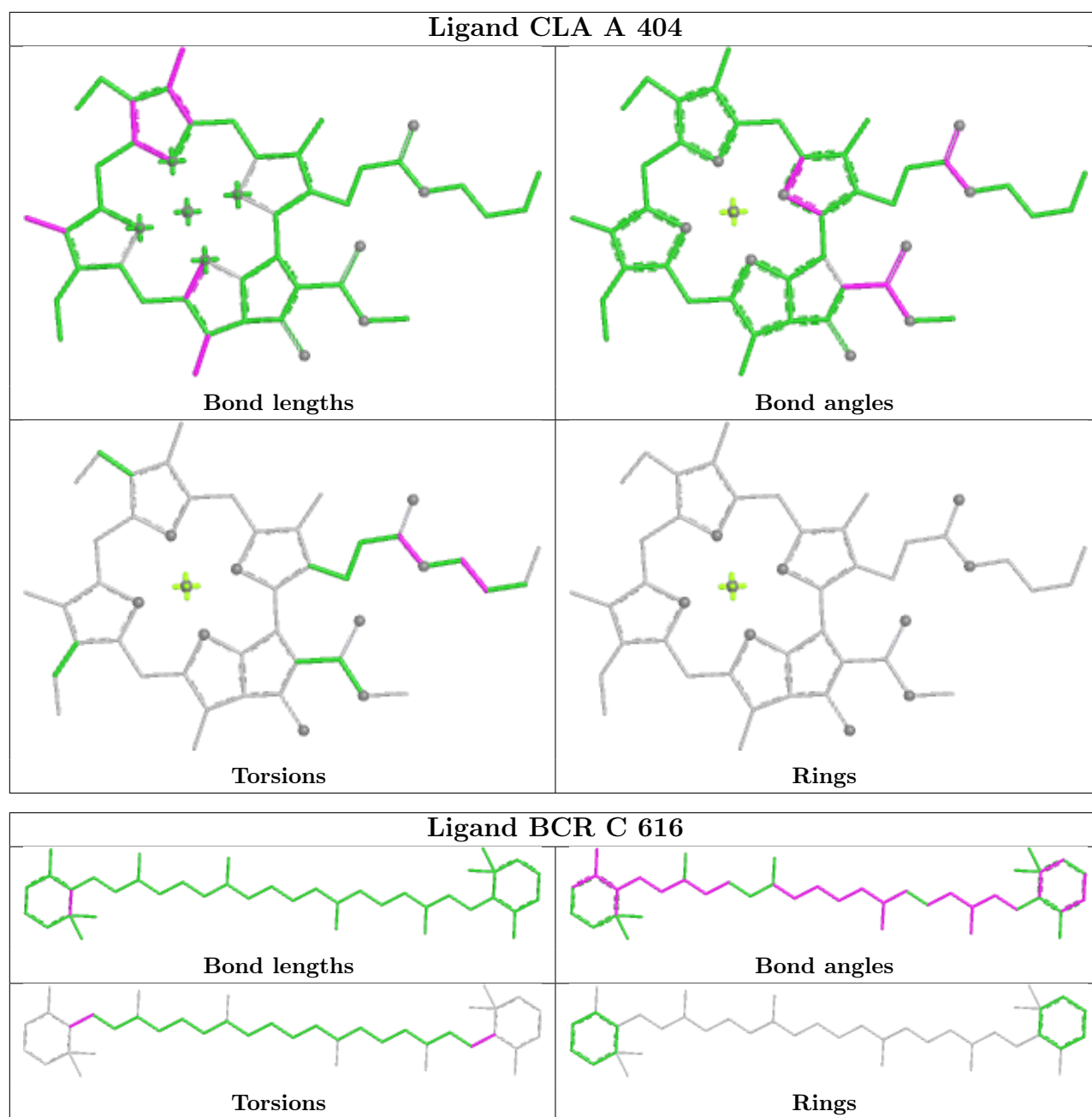


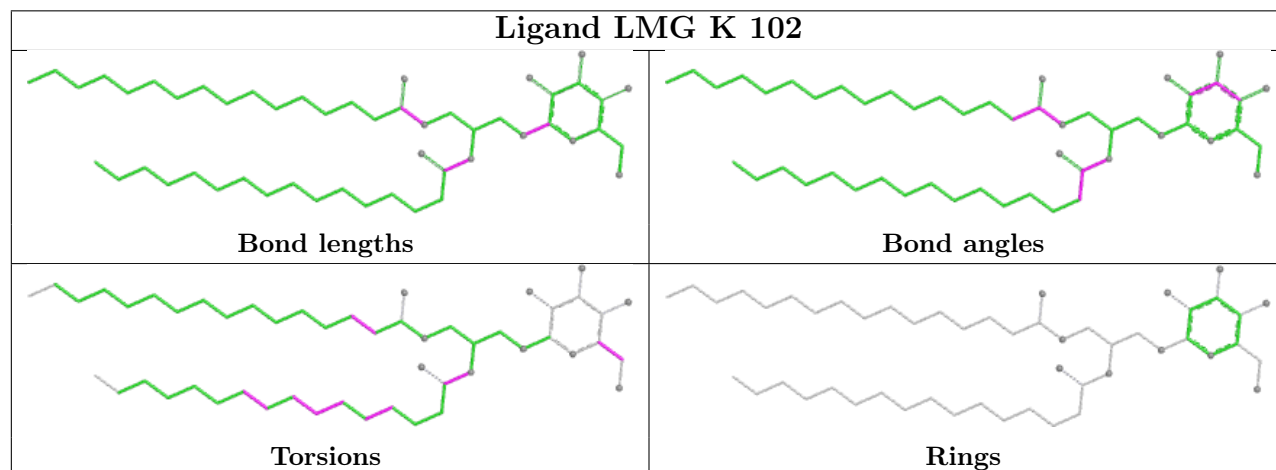
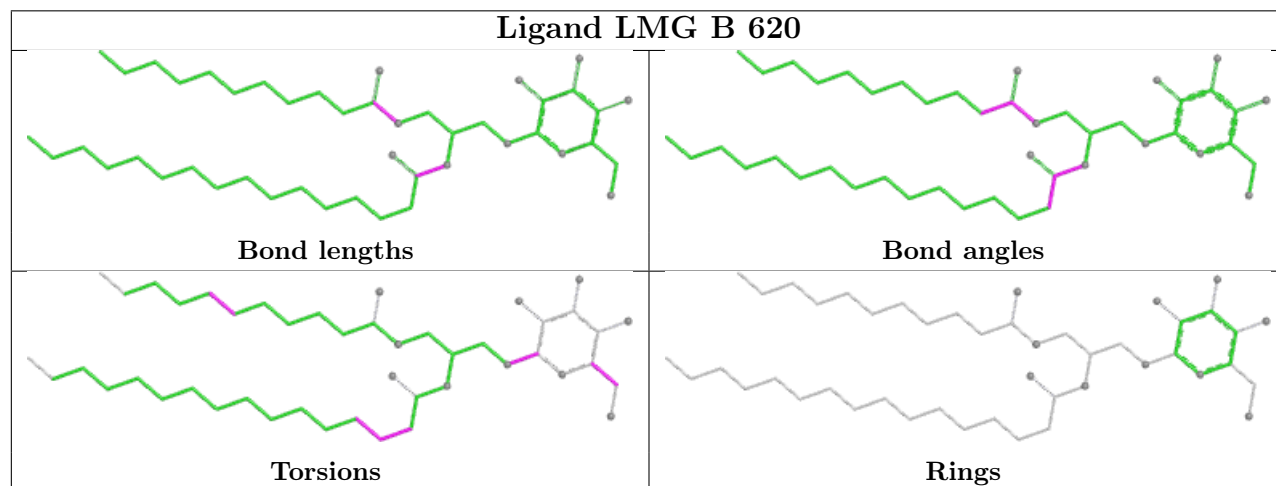
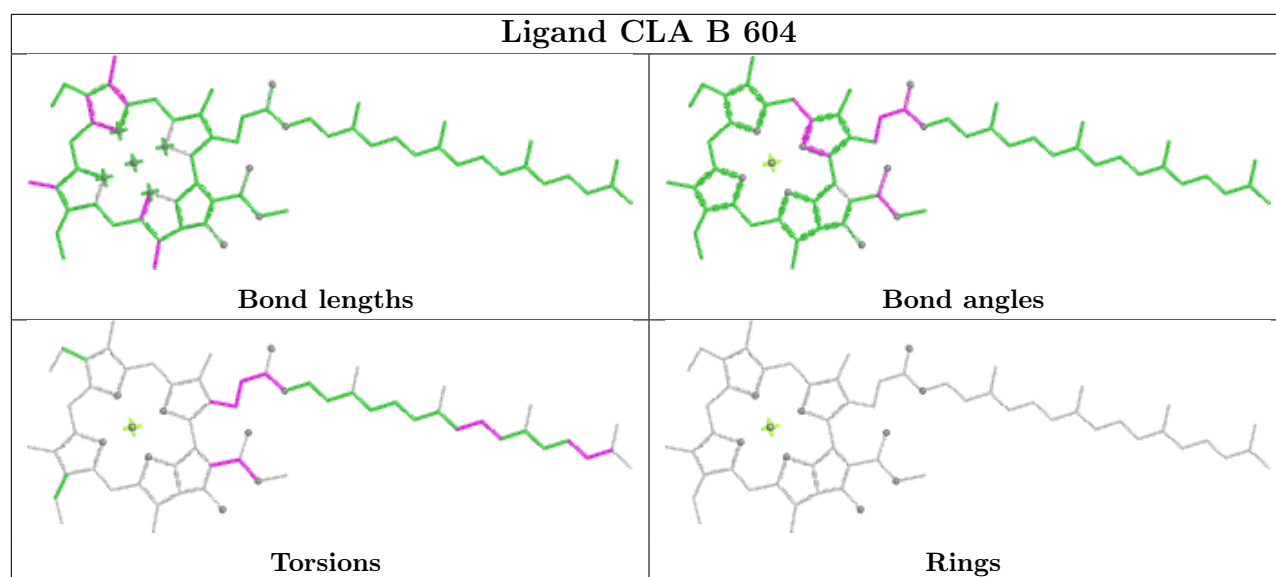


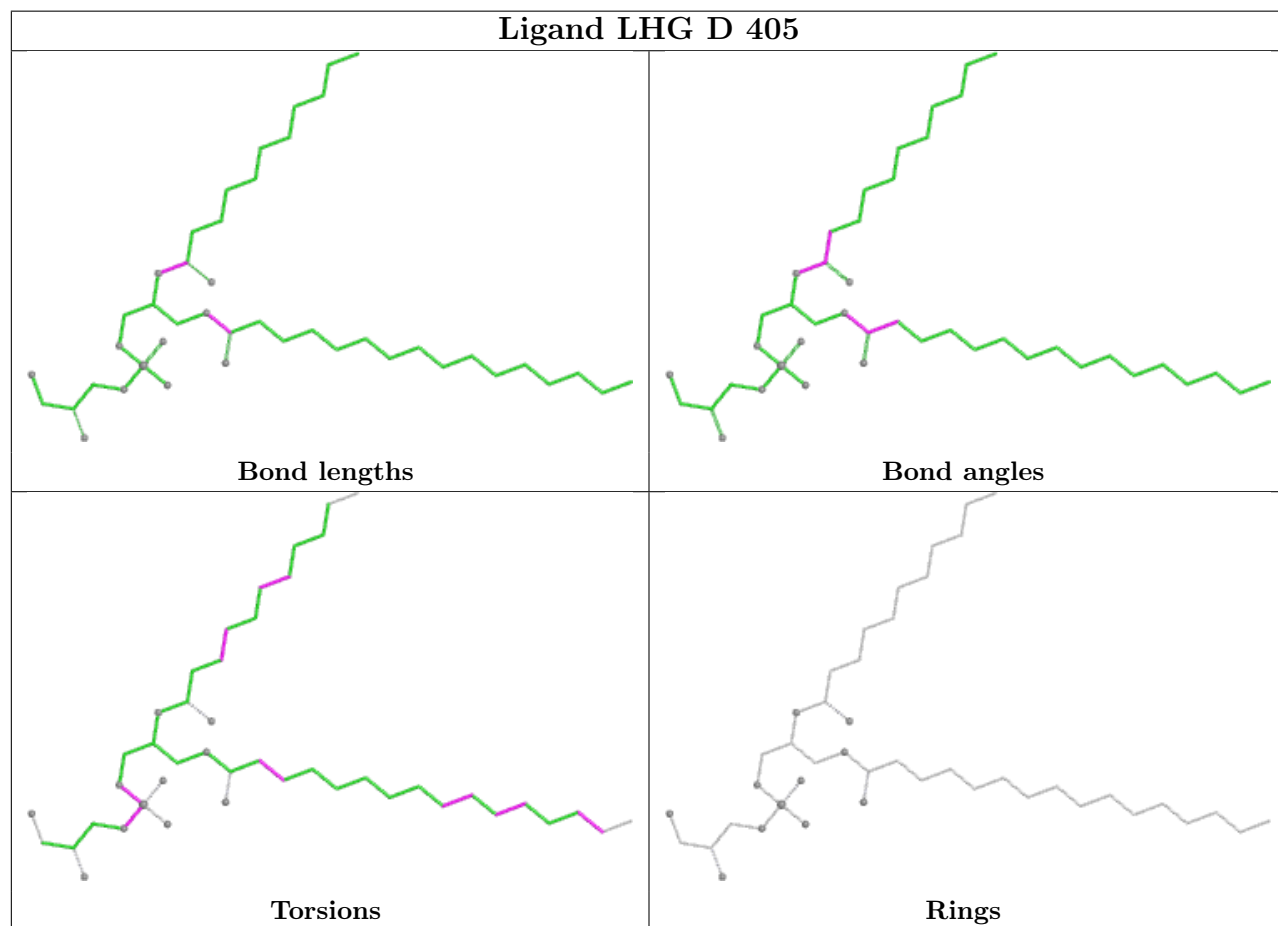
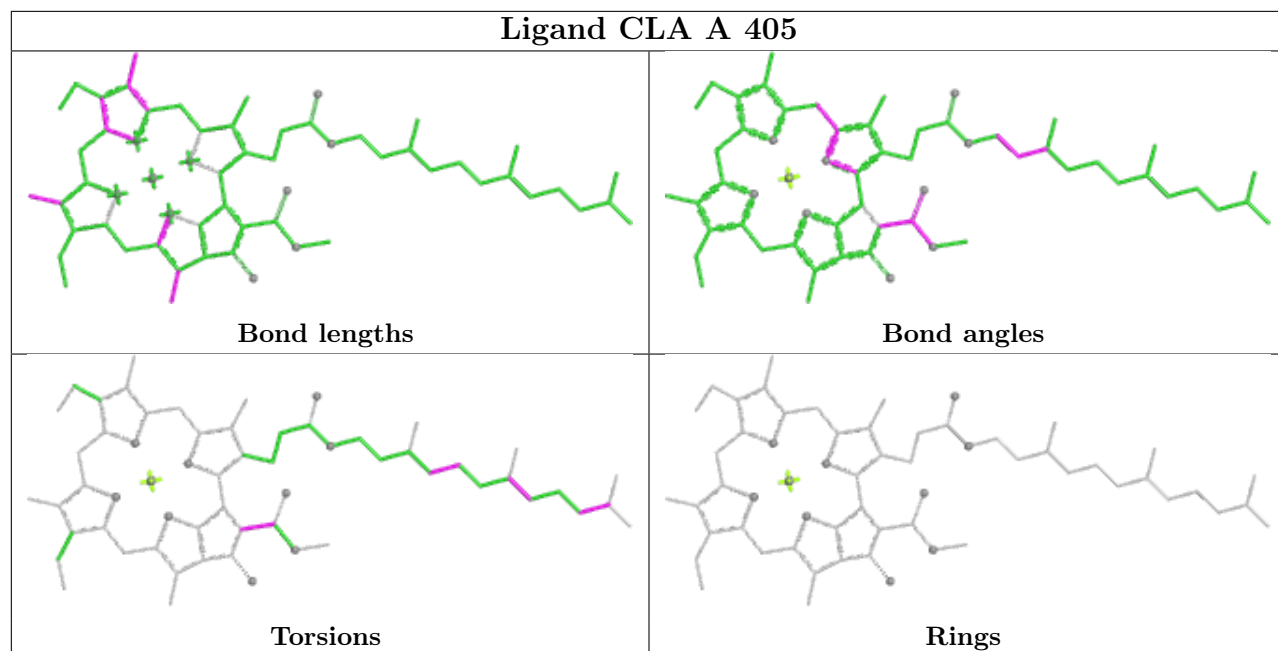


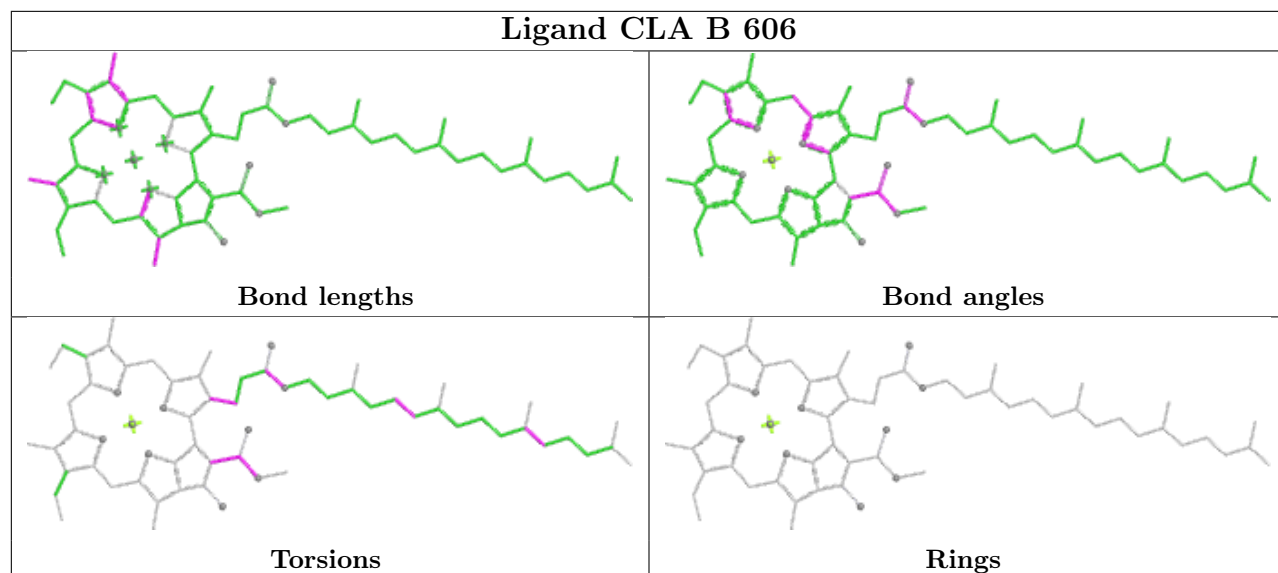
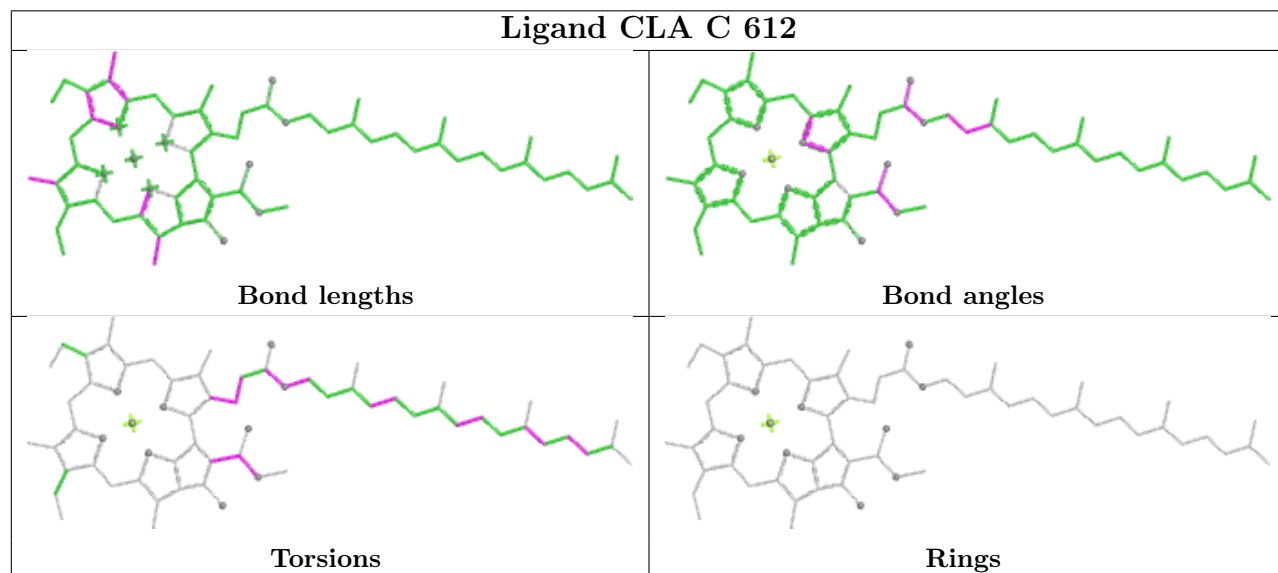
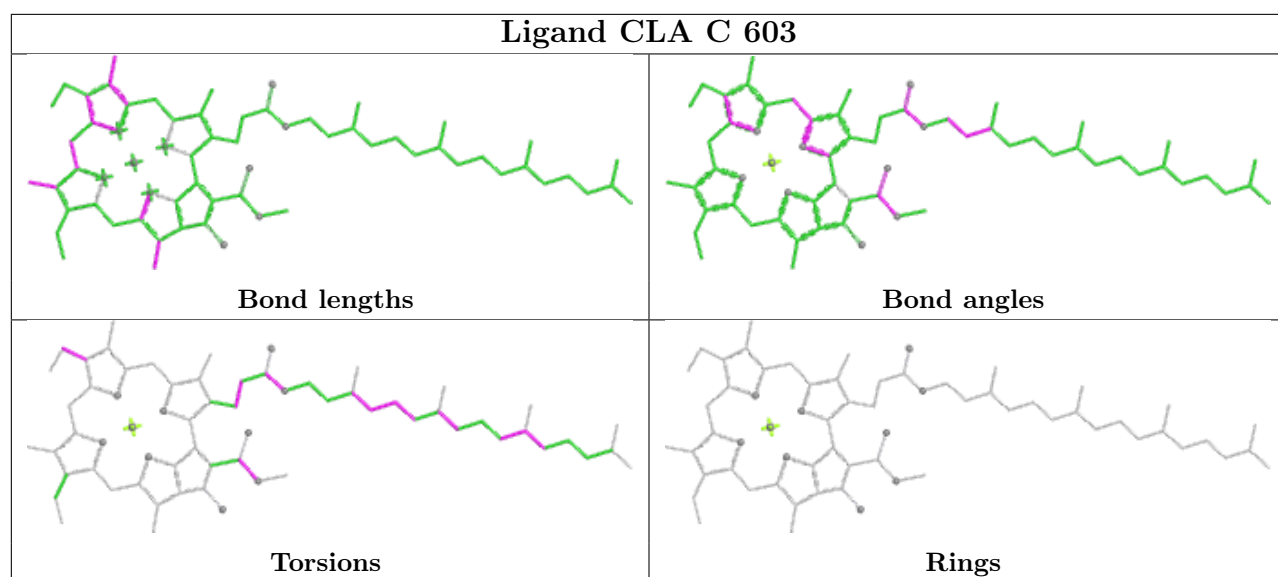


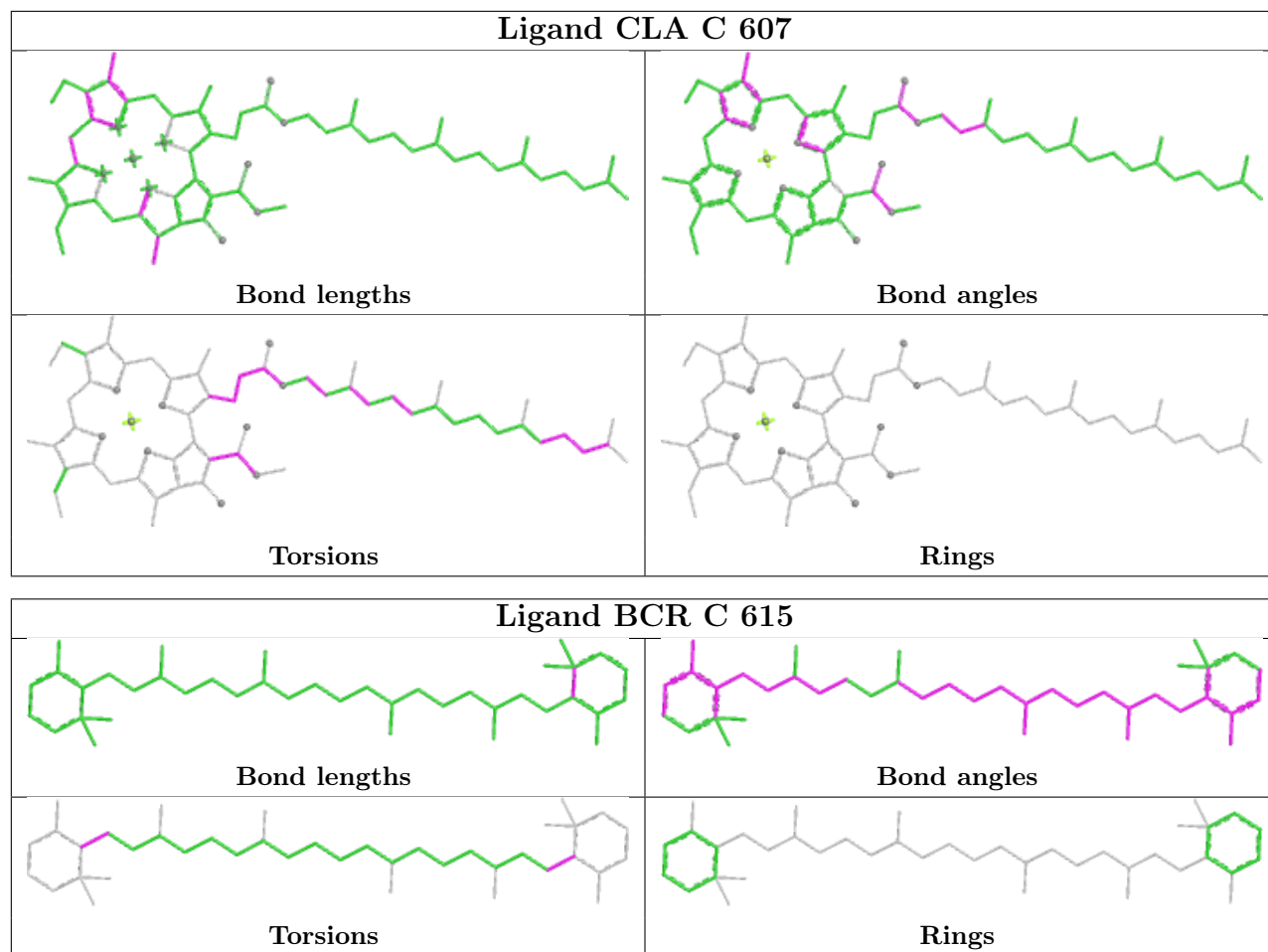


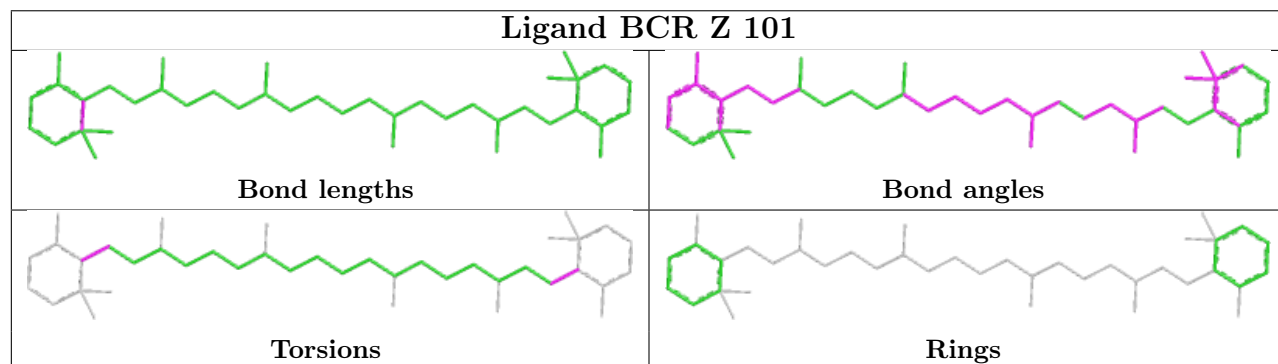
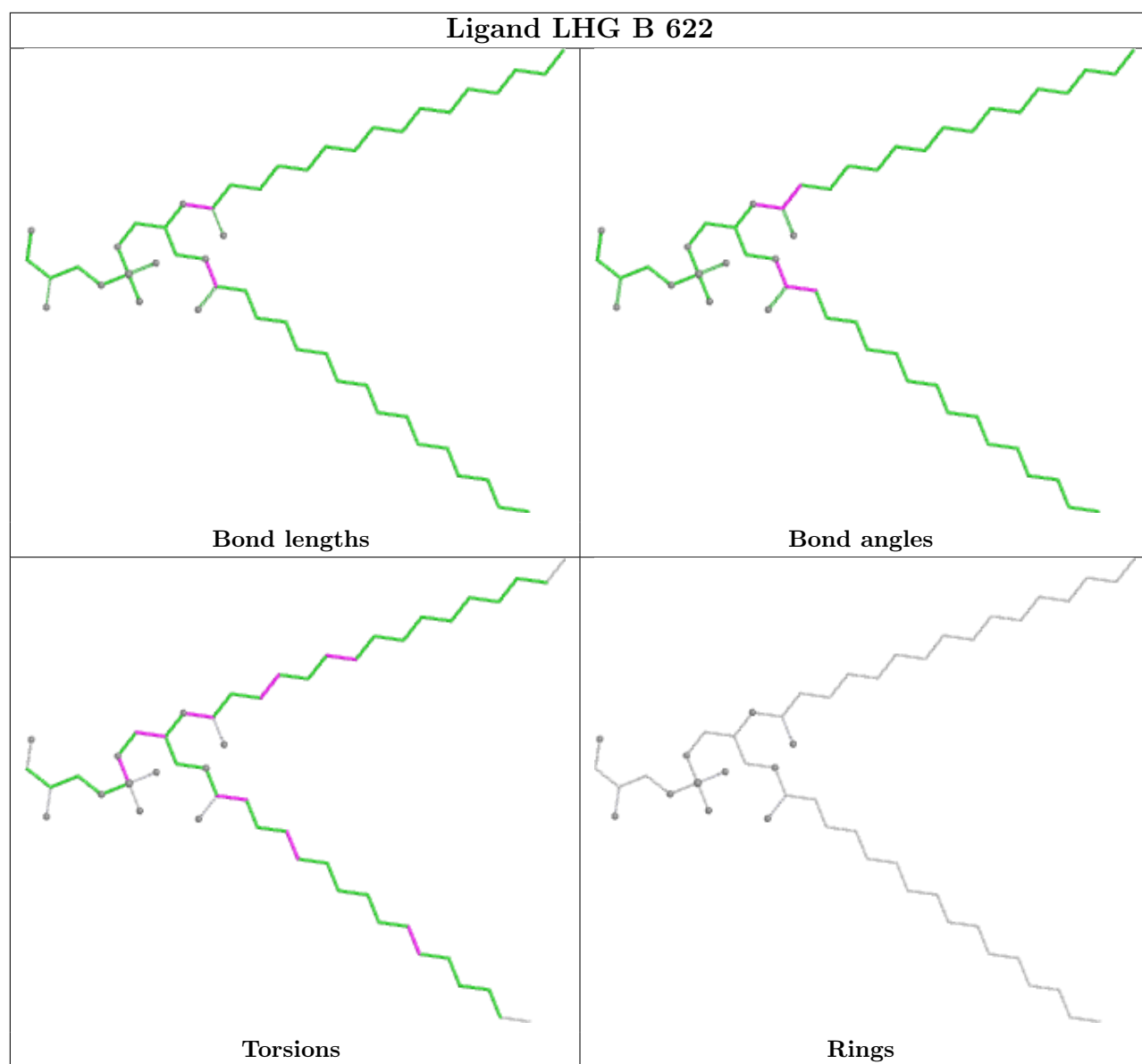


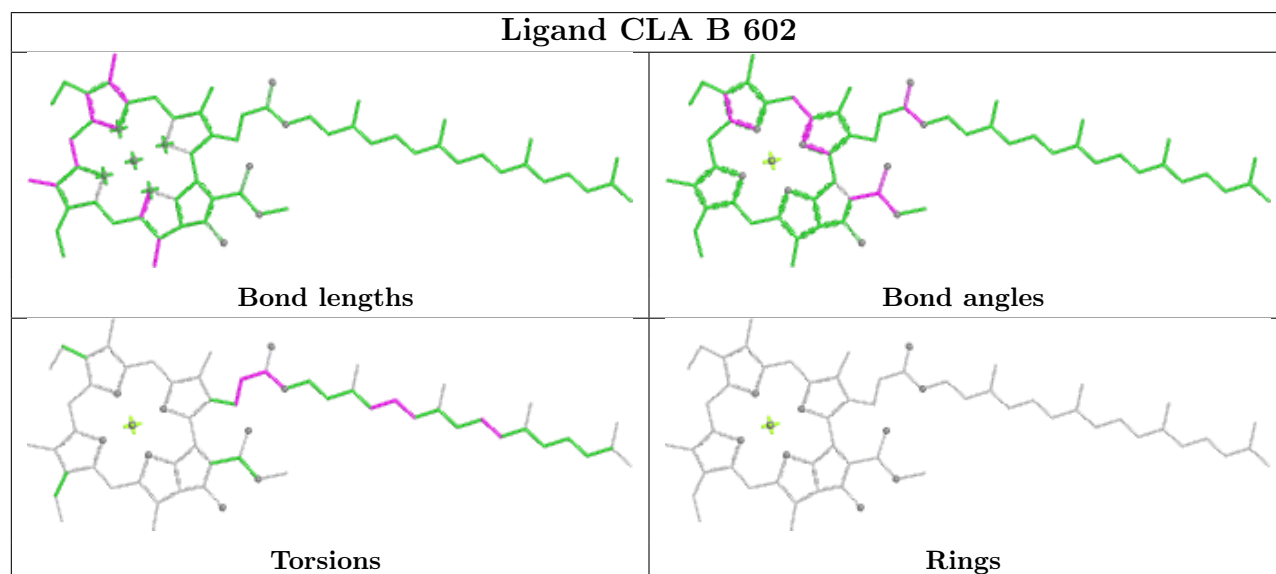
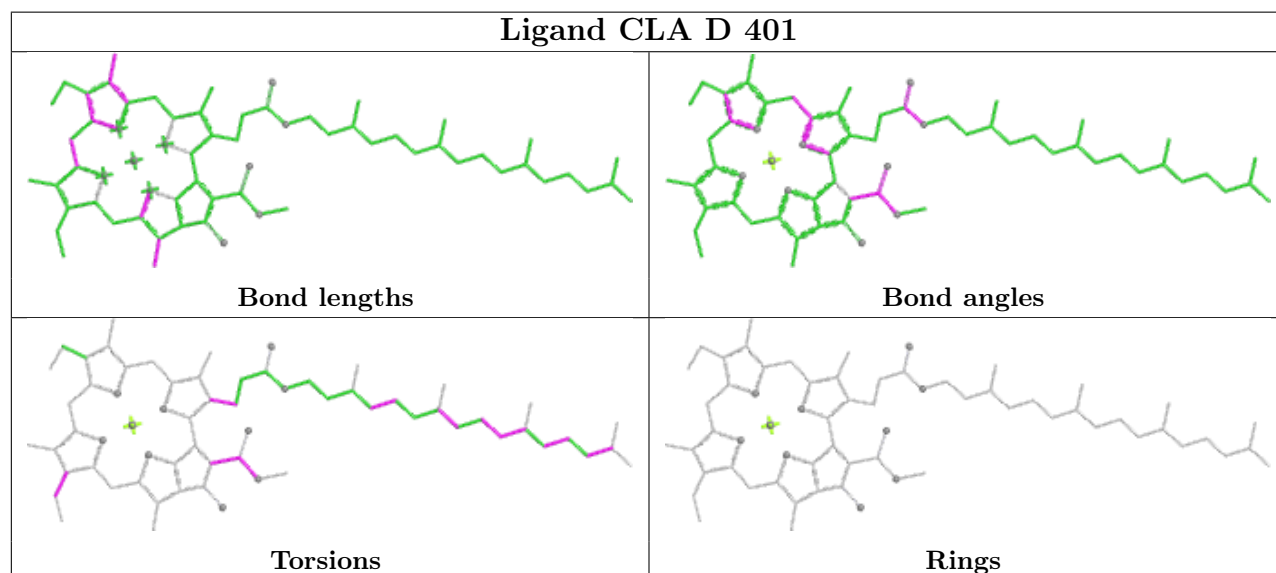
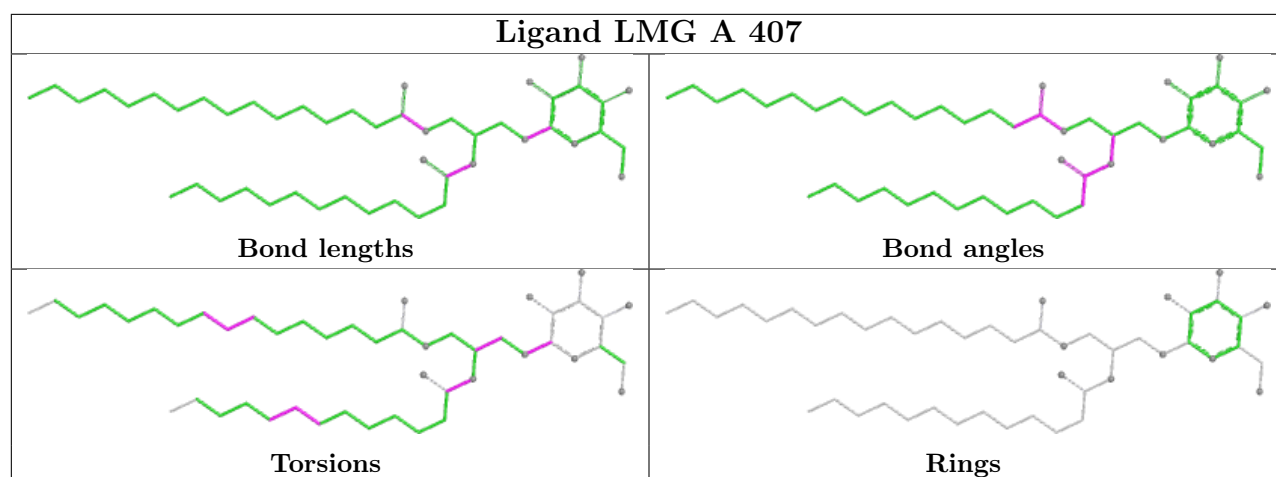


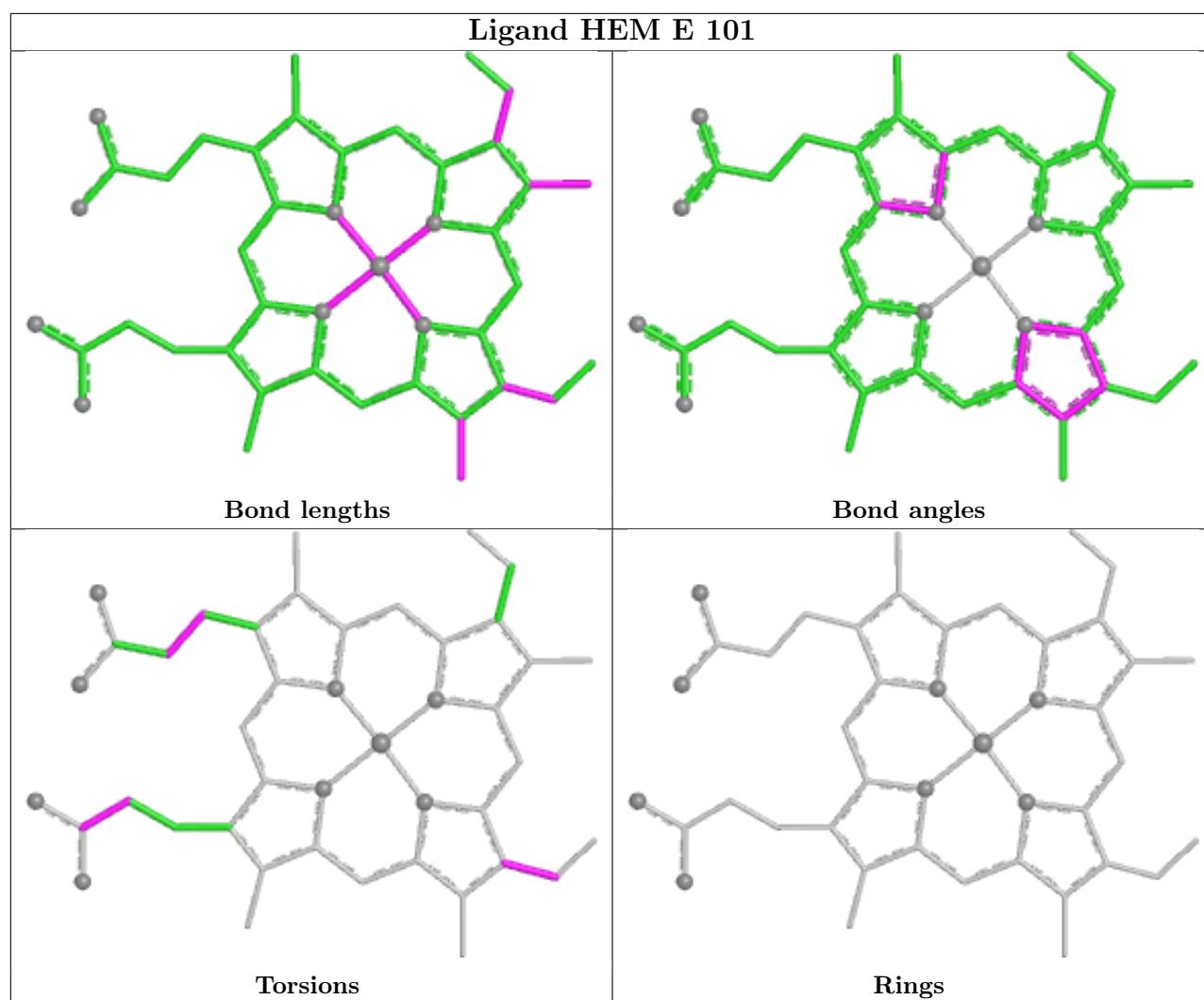












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

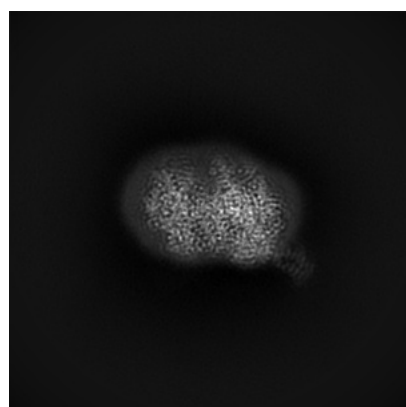
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37133. These allow visual inspection of the internal detail of the map and identification of artifacts.

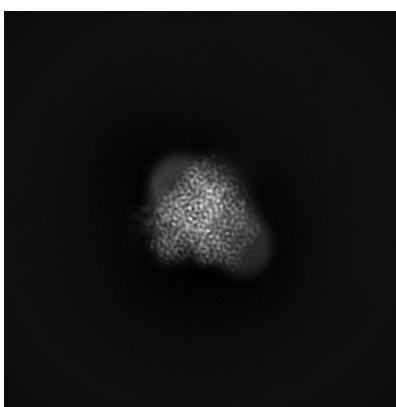
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

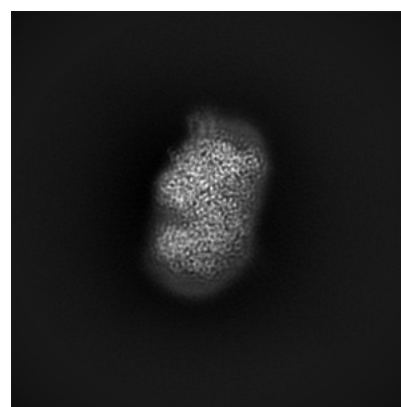
6.1.1 Primary map



X



Y

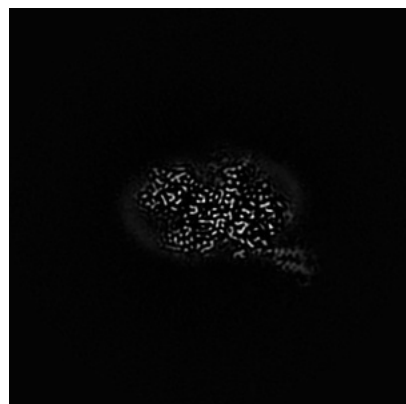


Z

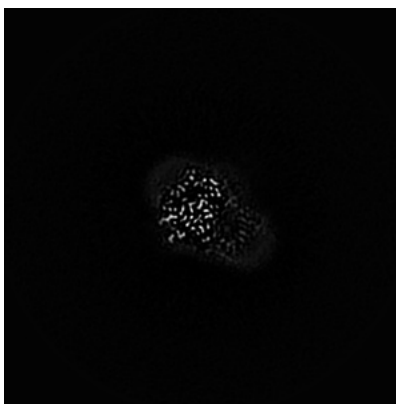
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

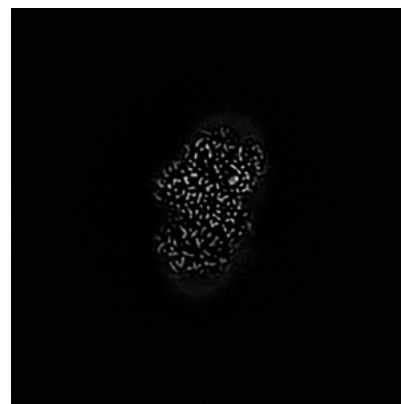
6.2.1 Primary map



X Index: 160



Y Index: 160

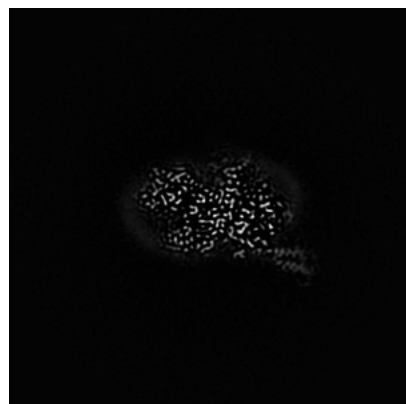


Z Index: 160

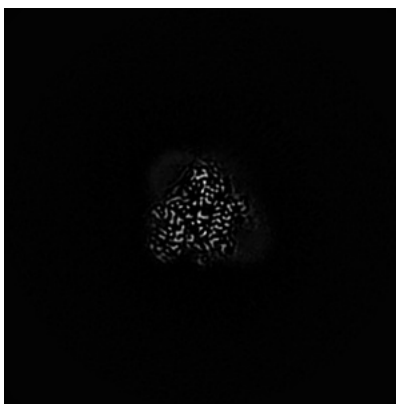
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 160



Y Index: 183

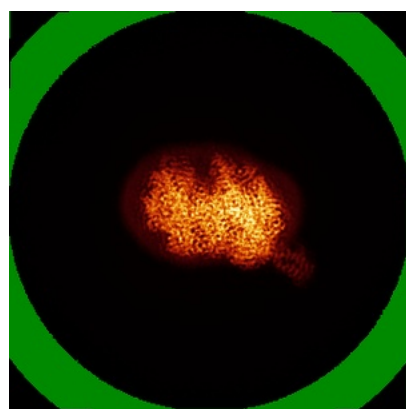


Z Index: 162

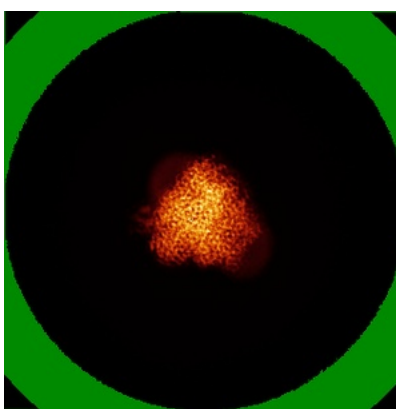
The images above show the largest variance slices of the map in three orthogonal directions.

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

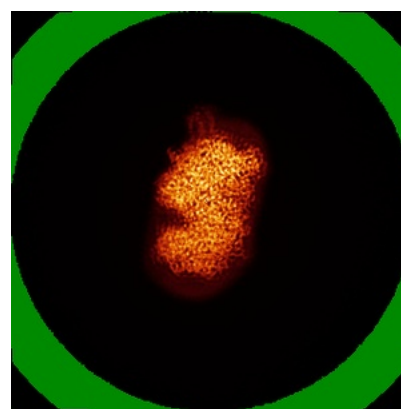
6.4.1 Primary map



X



Y

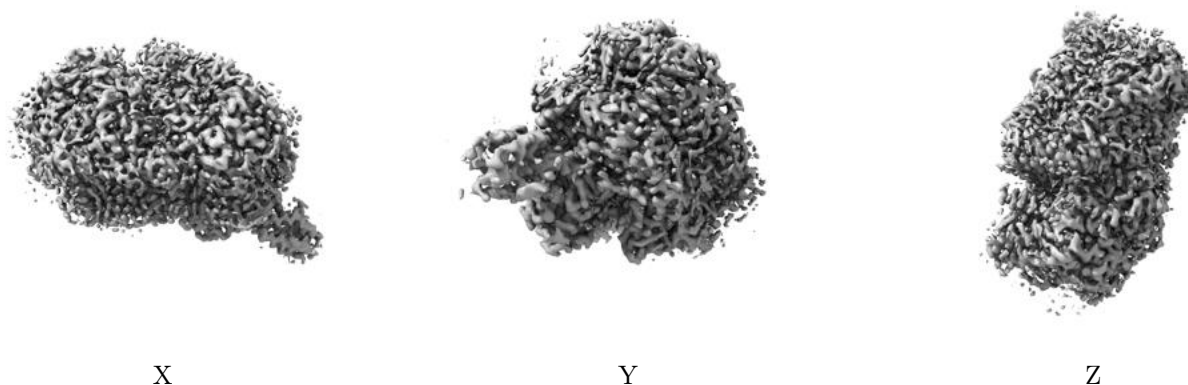


Z

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 3.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

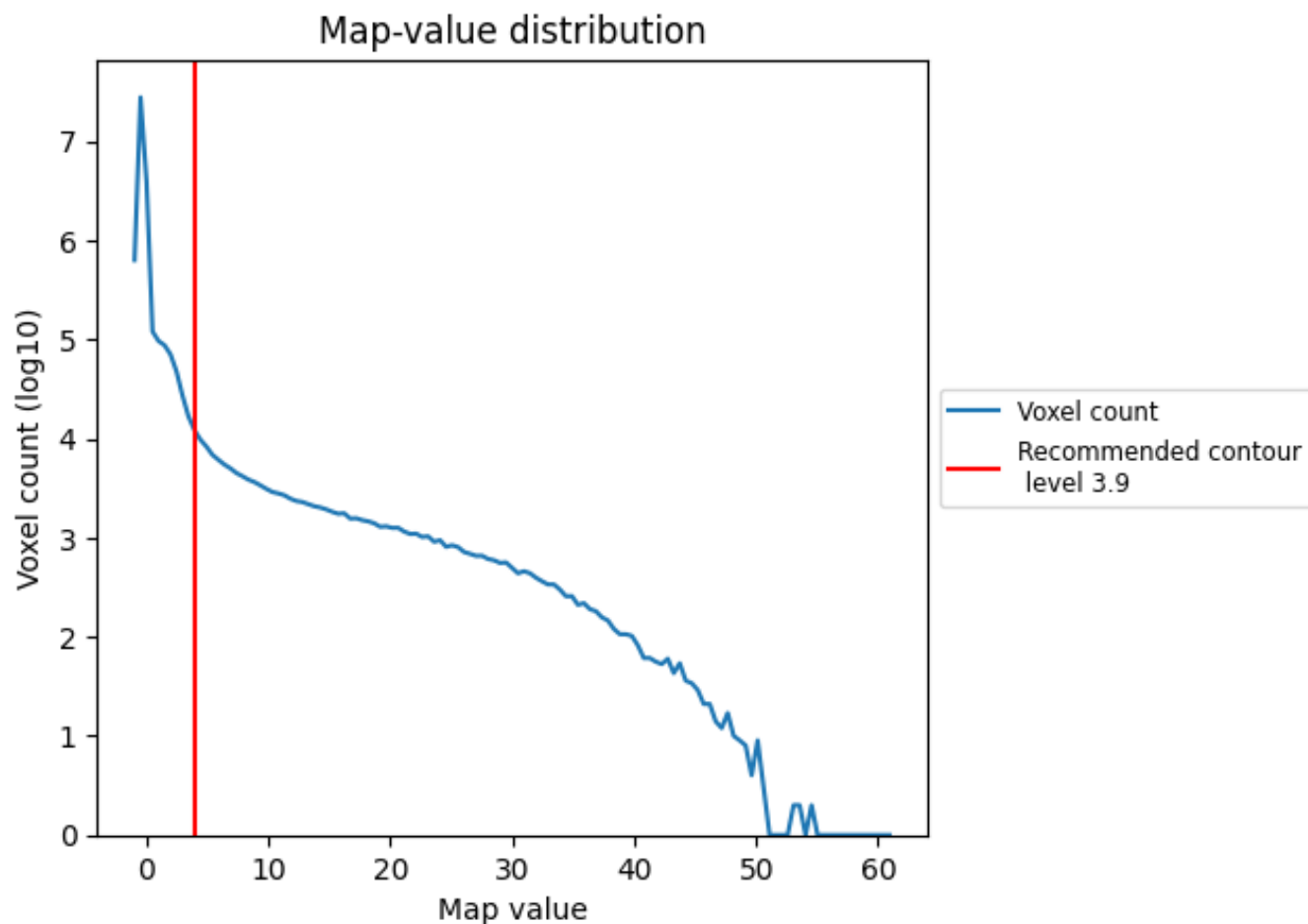
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

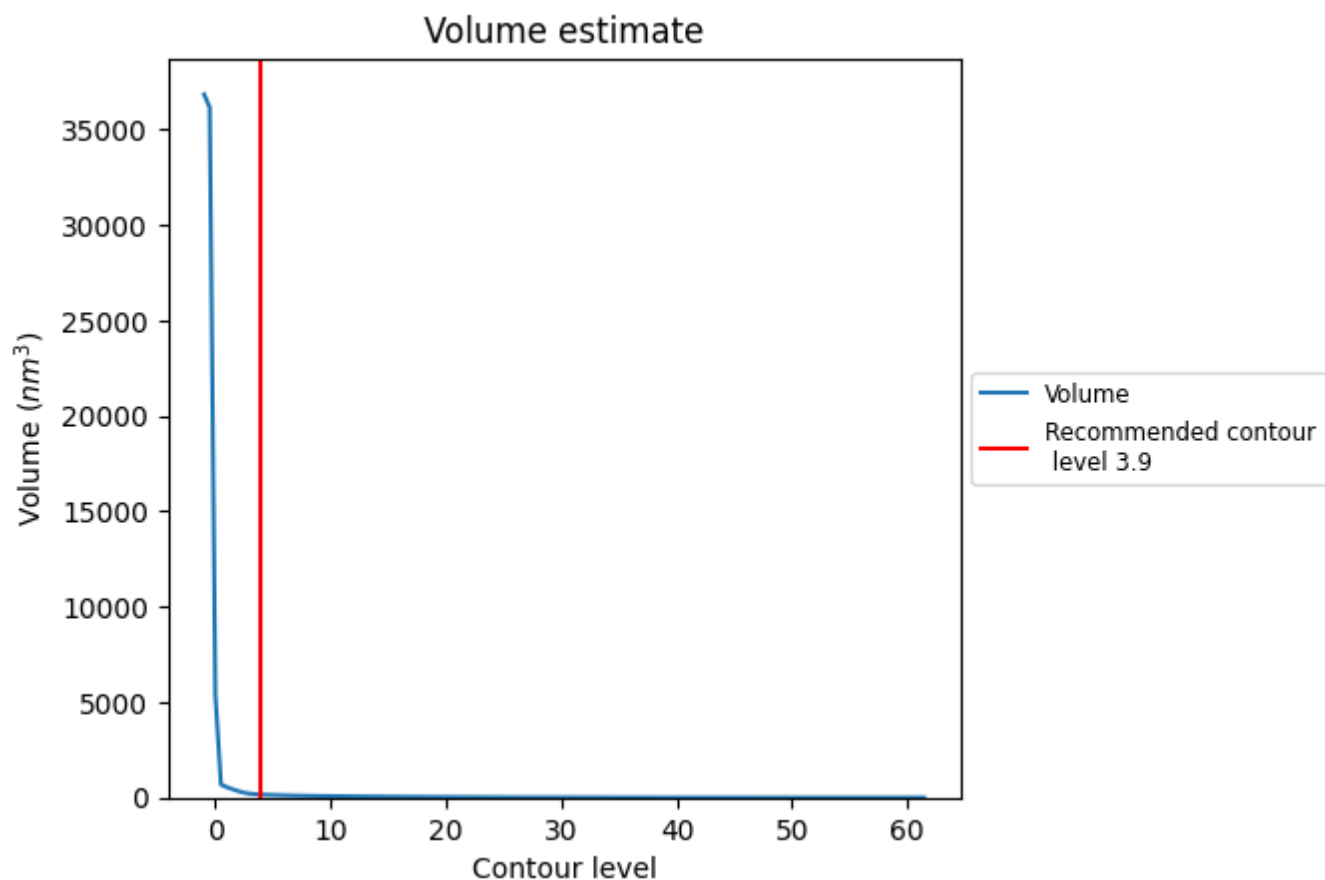
This section contains the results of statistical analysis of the map.

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.

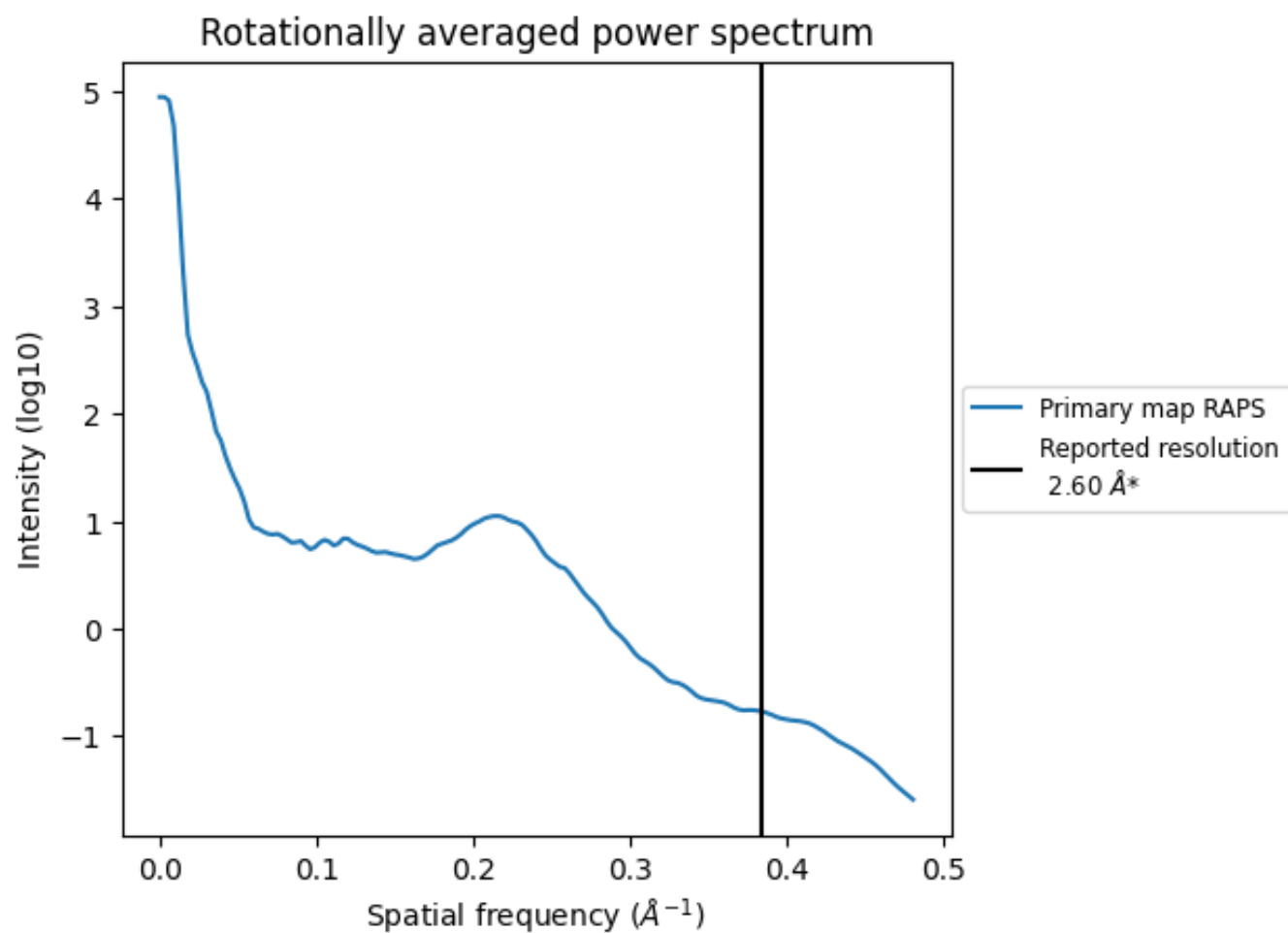
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 158 nm^3 ; this corresponds to an approximate mass of 142 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 ⓘ

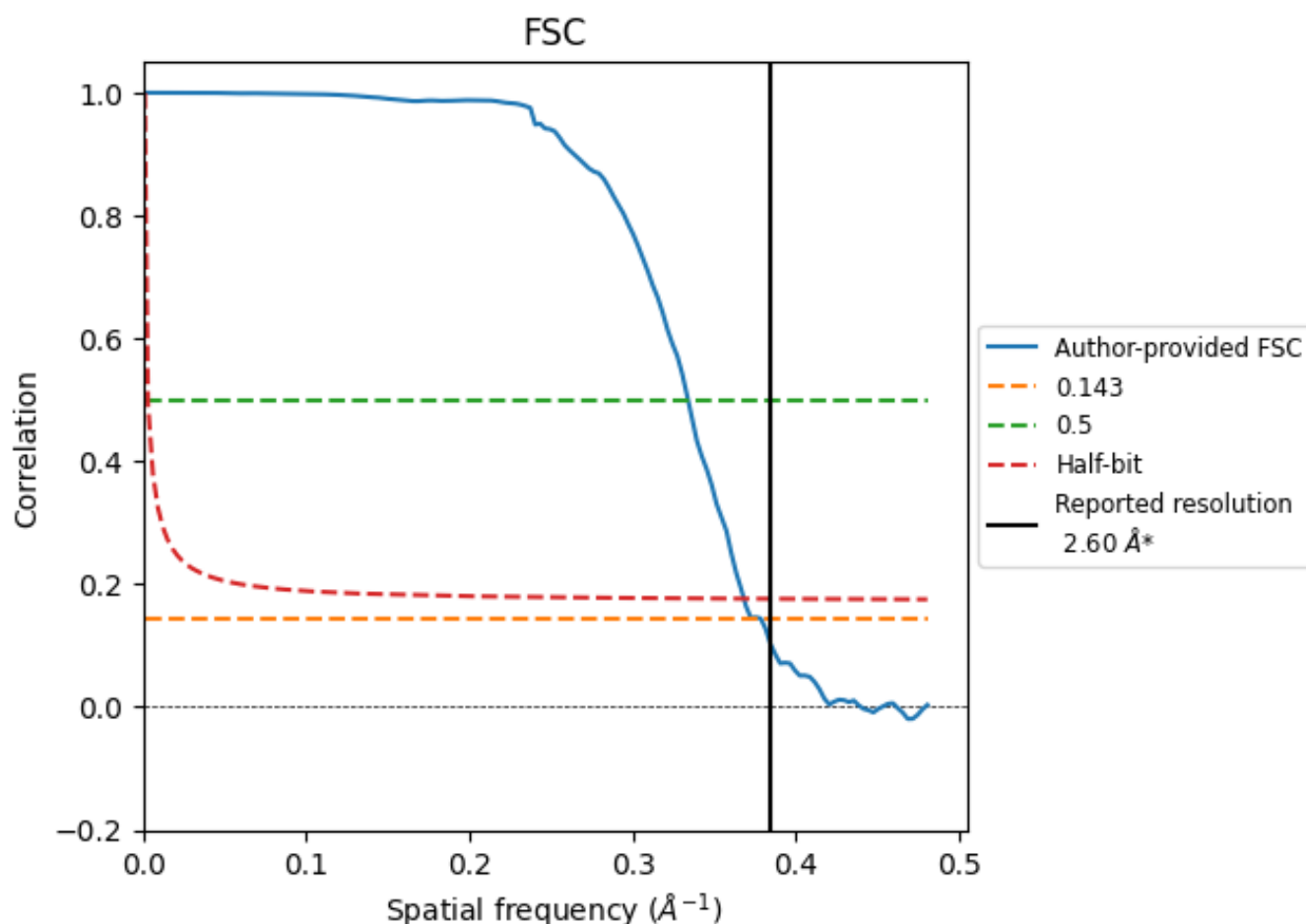


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 Å⁻¹

8.2 Resolution estimates [i](#)

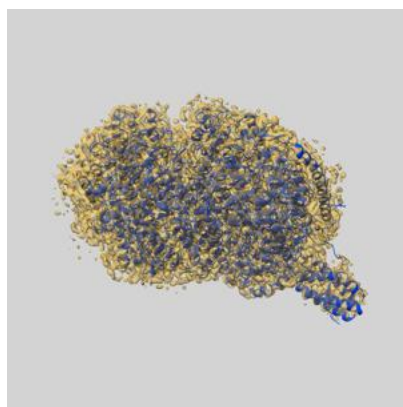
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.64	2.99	2.72
Unmasked-calculated*	-	-	-

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

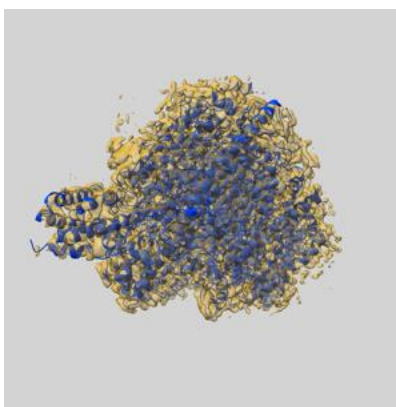
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37133 and PDB model 8KDE. Per-residue inclusion information can be found in section [3](#) on page [18](#).

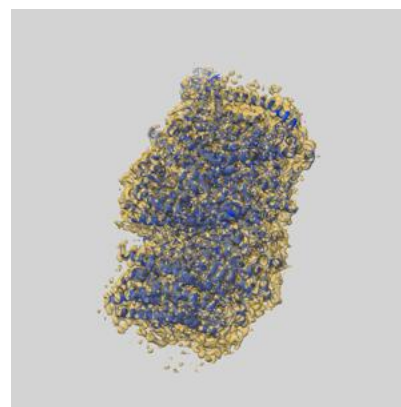
9.1 Map-model overlay [i](#)



X



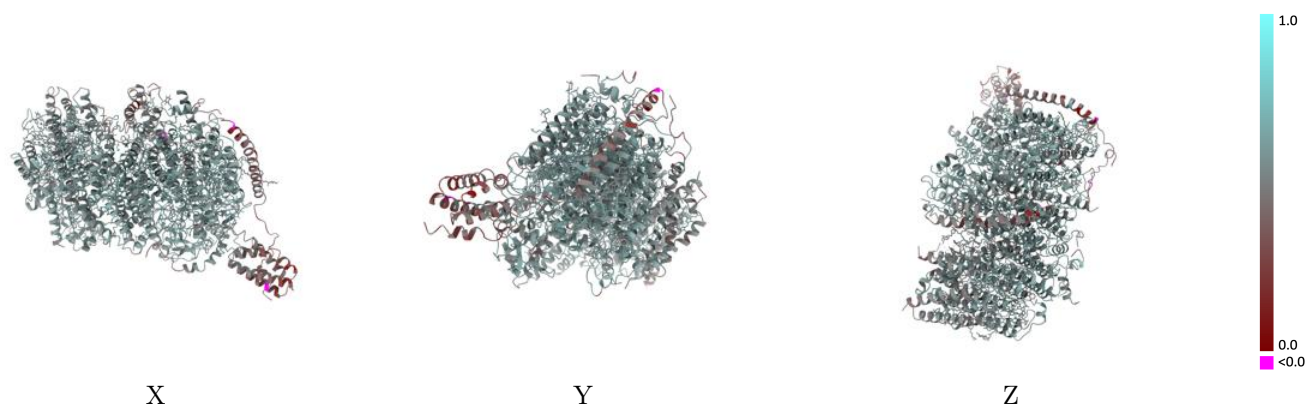
Y



Z

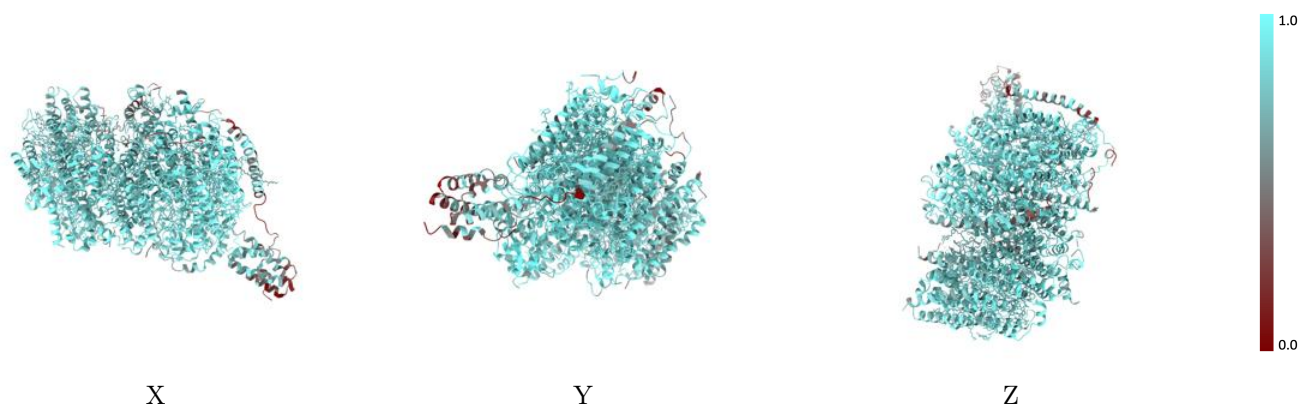
The images above show the 3D surface view of the map at the recommended contour level 3.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



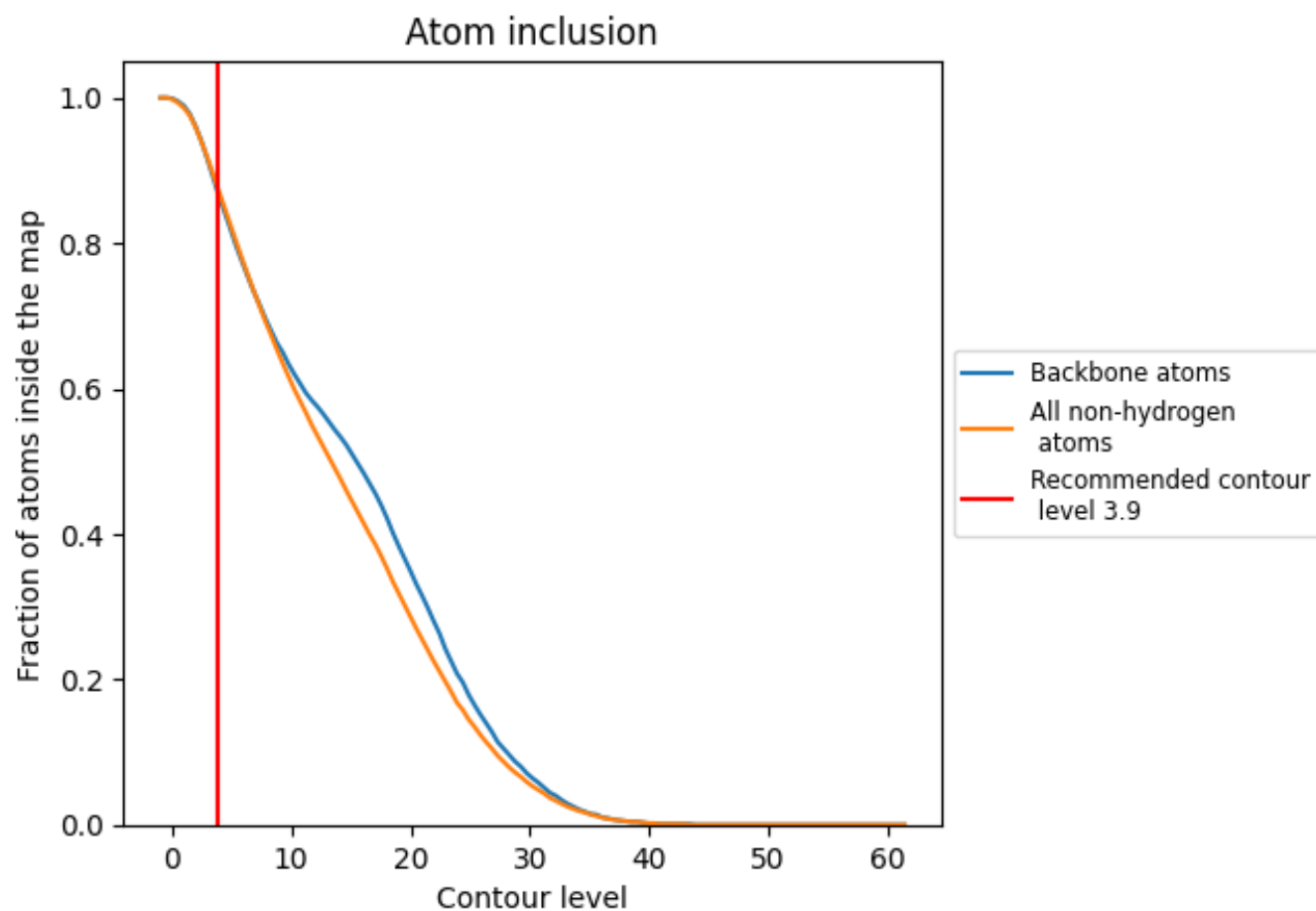
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.9).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (3.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8730	 0.5480
1	 0.6020	 0.3960
3	 0.5530	 0.3920
A	 0.9080	 0.5660
B	 0.9380	 0.5830
C	 0.8950	 0.5590
D	 0.9260	 0.5830
E	 0.8750	 0.5390
F	 0.8670	 0.5110
G	 0.6420	 0.4010
H	 0.8730	 0.5470
I	 0.8820	 0.5470
K	 0.7930	 0.5090
L	 0.8960	 0.5600
M	 0.7760	 0.5220
T	 0.8370	 0.5440
V	 0.7160	 0.4850
X	 0.8510	 0.5440
Z	 0.7860	 0.4900

