



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:11 AM UTC

PDB ID : 8ZEE / pdb_00008zee
EMDB ID : EMD-60026
Title : Cryo-EM structure of an intermediate-state PSII-PRF2' complex during the process of photosystem II repair
Authors : Li, A.; Liu, Z.
Deposited on : 2024-05-06
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

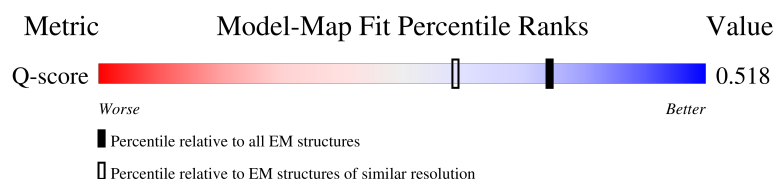
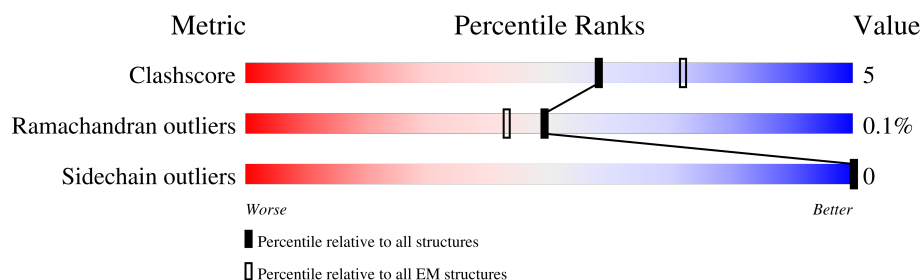
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.90 Å.

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



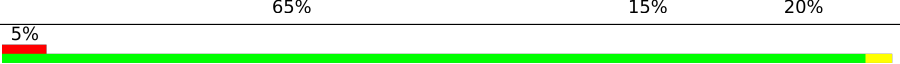
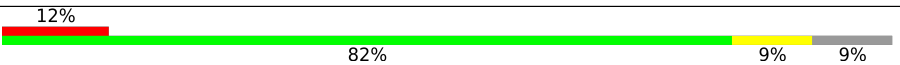
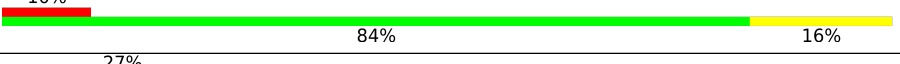
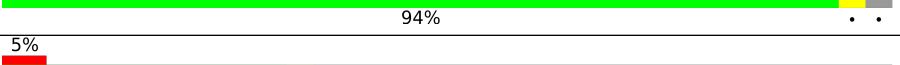
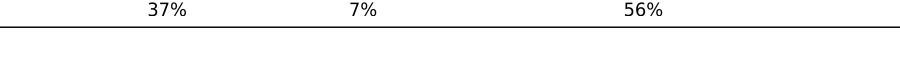
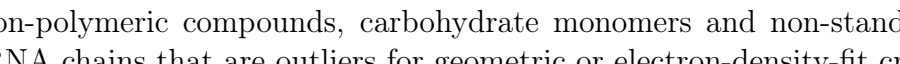
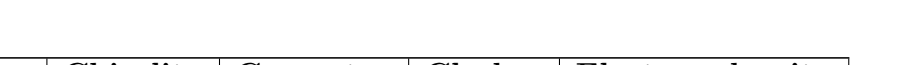
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	B	508	
2	D	352	
3	E	82	
4	F	44	

Continued on next page...

Continued from previous page...

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	C	461	
15	A	329	
16	1	99	

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
17	CLA	A	402	X	-	-	-
17	CLA	A	403	X	-	-	-
17	CLA	A	404	X	-	-	-
17	CLA	B	601	X	-	-	-
17	CLA	B	602	X	-	-	-
17	CLA	B	603	X	-	-	-
17	CLA	B	604	X	-	-	-
17	CLA	B	605	X	-	-	-
17	CLA	B	606	X	-	-	-
17	CLA	B	607	X	-	-	-
17	CLA	B	608	X	-	-	-
17	CLA	B	609	X	-	-	-
17	CLA	B	610	X	-	-	-
17	CLA	B	611	X	-	-	-
17	CLA	B	612	X	-	-	-
17	CLA	B	613	X	-	-	-
17	CLA	B	614	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	B	615	X	-	-	-
17	CLA	B	616	X	-	-	-
17	CLA	C	602	X	-	-	-
17	CLA	C	603	X	-	-	-
17	CLA	C	604	X	-	-	-
17	CLA	C	605	X	-	-	-
17	CLA	C	606	X	-	-	-
17	CLA	C	607	X	-	-	-
17	CLA	C	608	X	-	-	-
17	CLA	C	609	X	-	-	-
17	CLA	C	610	X	-	-	-
17	CLA	C	611	X	-	-	-
17	CLA	C	612	X	-	-	-
17	CLA	C	613	X	-	-	-
17	CLA	C	614	X	-	-	-
17	CLA	D	402	X	-	-	-
17	CLA	D	403	X	-	-	-
17	CLA	D	410	X	-	-	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 20218 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 Psb30.

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 4.1 kDa photosystem II subunit.

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 Photosystem II CP43 reaction center protein.

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

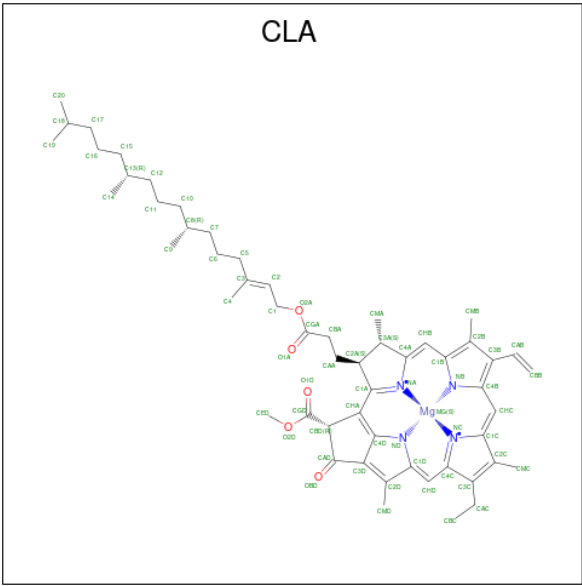
- Molecule 15 is a protein called Photosystem II protein D1.

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

- Molecule 16 is a protein called Chains: 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	1	44	Total	C	N	O	0	0
			313	204	51	58		

- Molecule 17 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

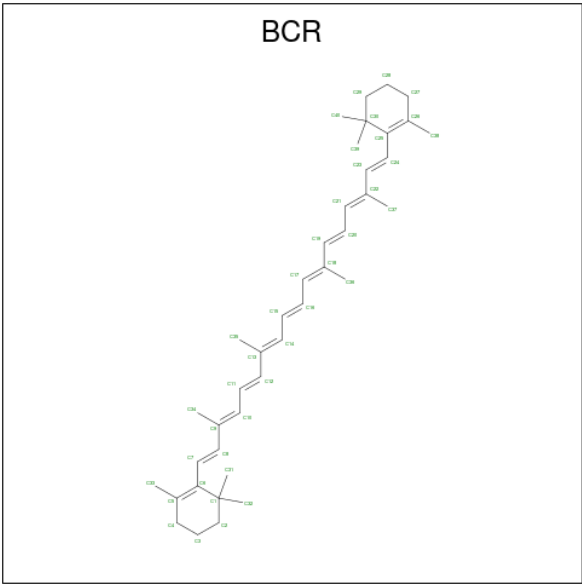
Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total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

Continued on next page...

Continued from previous page...

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

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



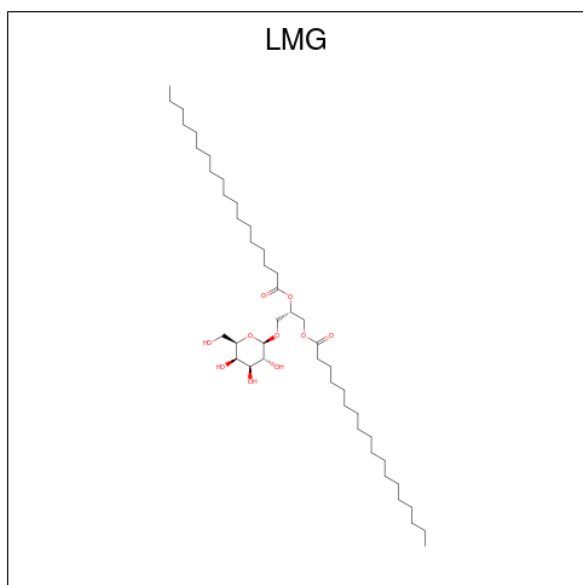
Mol	Chain	Residues	Atoms		AltConf
18	B	1	Total	C	0
			40	40	

Continued on next page...

Continued from previous page...

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

- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



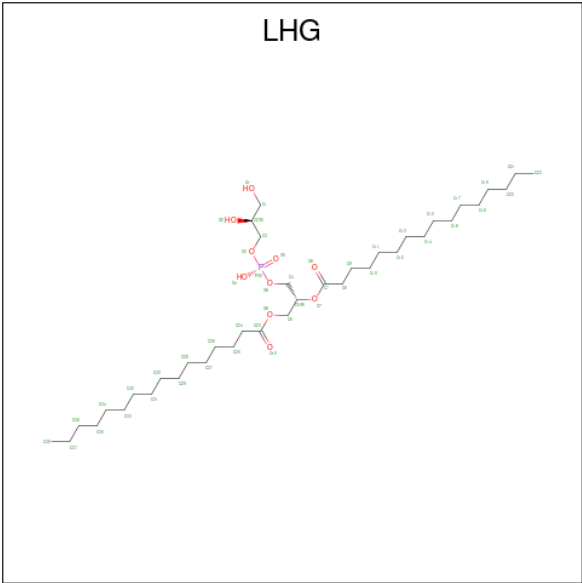
Mol	Chain	Residues	Atoms	AltConf
19	B	1	Total C O 46 36 10	0
19	D	1	Total C O 46 36 10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
19	H	1	Total	C	O	0
			48	38	10	
19	K	1	Total	C	O	0
			51	41	10	
19	C	1	Total	C	O	0
			49	39	10	
19	C	1	Total	C	O	0
			48	38	10	

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



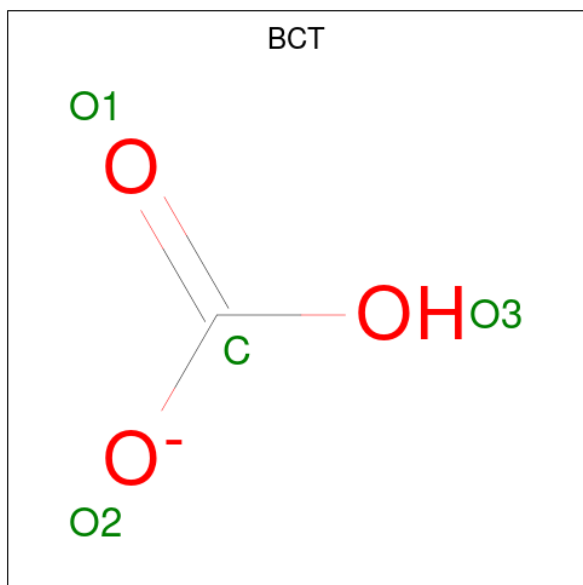
Mol	Chain	Residues	Atoms				AltConf
20	B	1	Total	C	O	P	0
			44	33	10	1	
20	B	1	Total	C	O	P	0
			47	36	10	1	
20	B	1	Total	C	O	P	0
			49	38	10	1	
20	D	1	Total	C	O	P	0
			49	38	10	1	
20	D	1	Total	C	O	P	0
			43	32	10	1	
20	D	1	Total	C	O	P	0
			49	38	10	1	
20	K	1	Total	C	O	P	0
			41	30	10	1	

Continued on next page...

Continued from previous page...

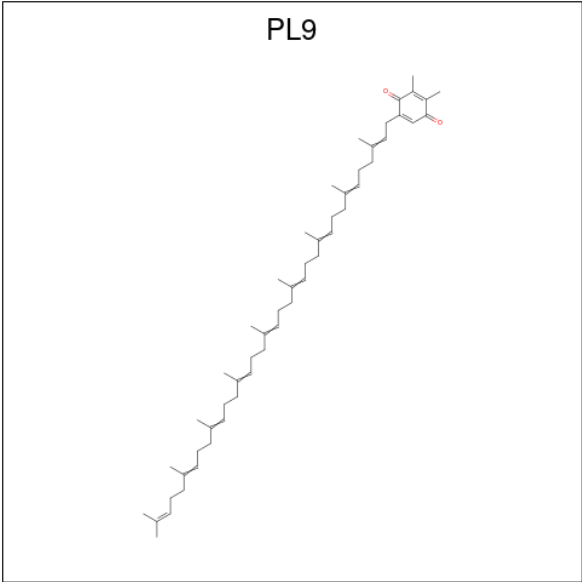
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
20	L	1	49	38	10	1	0

- Molecule 21 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



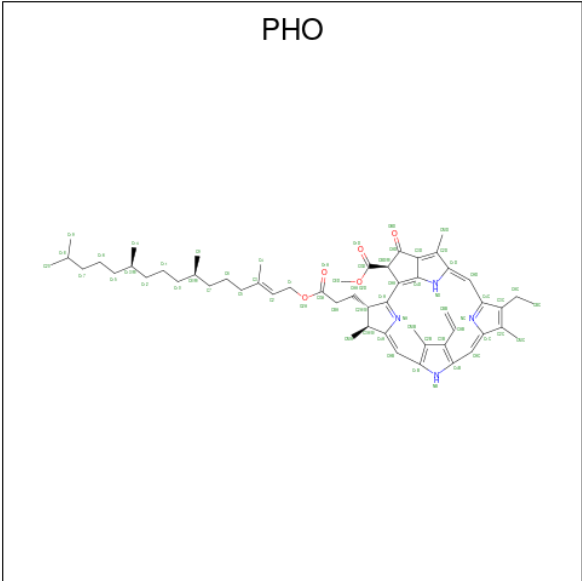
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
21	D	1	4	1	3	0

- Molecule 22 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: $\text{C}_{53}\text{H}_{80}\text{O}_2$) (labeled as "Ligand of Interest" by depositor).



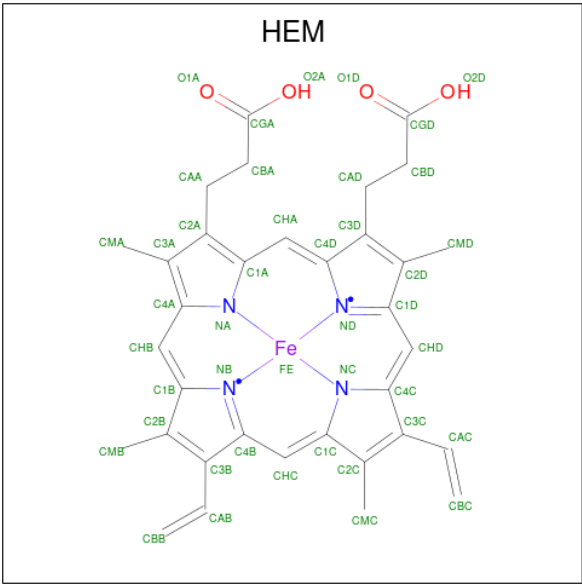
Mol	Chain	Residues	Atoms			AltConf
22	D	1	Total	C	O	0
			55	53	2	

- Molecule 23 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅) (labeled as "Ligand of Interest" by depositor).



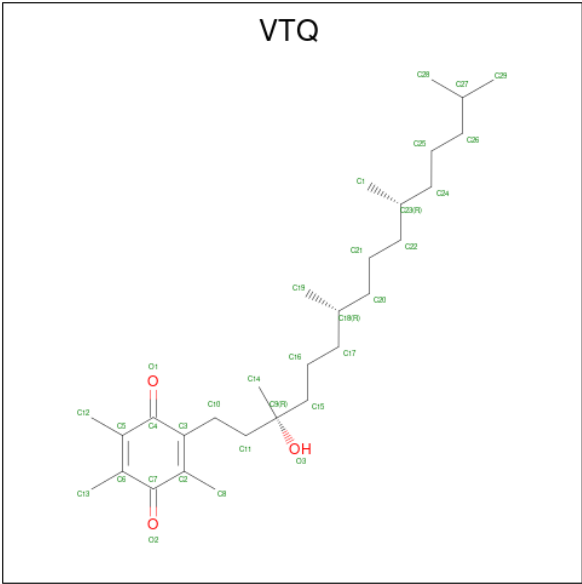
Mol	Chain	Residues	Atoms				AltConf
23	D	1	Total	C	N	O	0
			64	55	4	5	
23	D	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 24 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



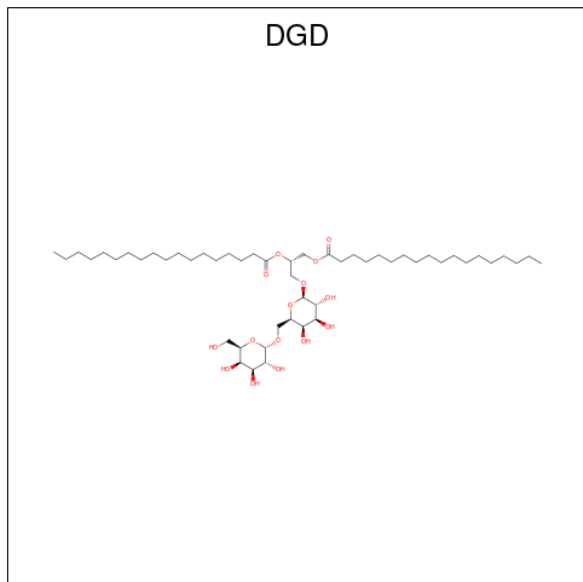
Mol	Chain	Residues	Atoms					AltConf
24	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 25 is RRR-ALPHA-TOCOPHERYLQUINONE (CCD ID: VTQ) (formula: $C_{29}H_{50}O_3$) (labeled as "Ligand of Interest" by depositor).



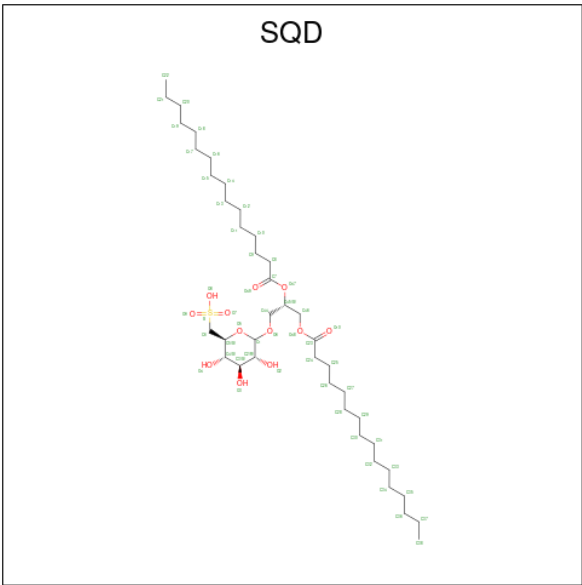
Mol	Chain	Residues	Atoms			AltConf
25	X	1	Total	C	O	0
			32	29	3	

- Molecule 26 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
26	C	1	Total	C	O	0
			55	40	15	
26	C	1	Total	C	O	0
			57	42	15	
26	C	1	Total	C	O	0
			59	44	15	

- Molecule 27 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
27	C	1	Total	C	O	S	0
			51	38	12	1	

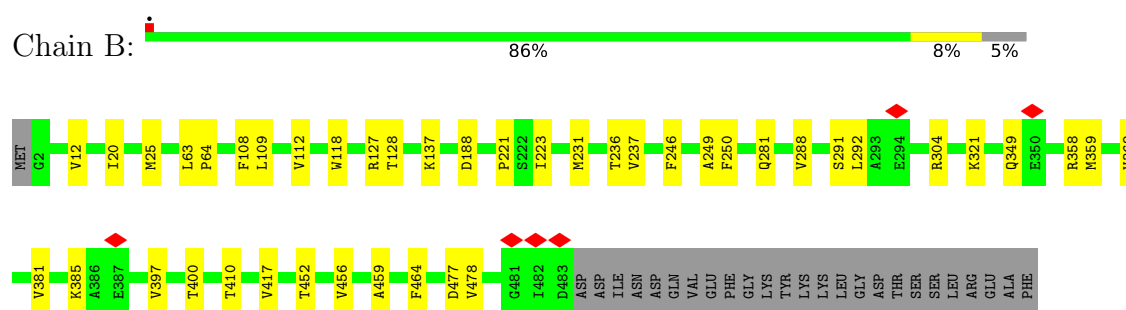
- Molecule 28 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

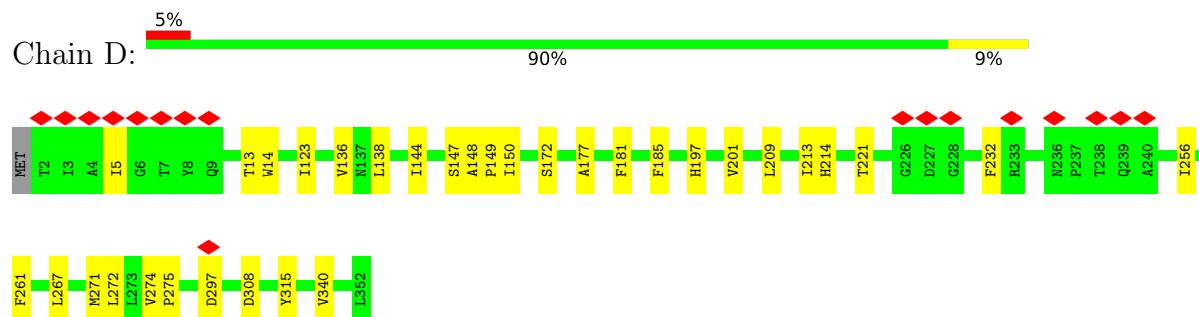
3 Residue-property plots [i](#)

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

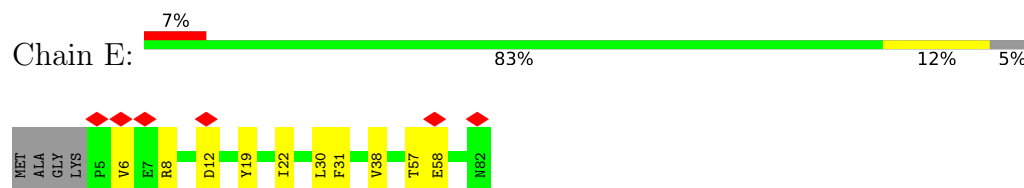
- Molecule 1: Photosystem II CP47 reaction center protein



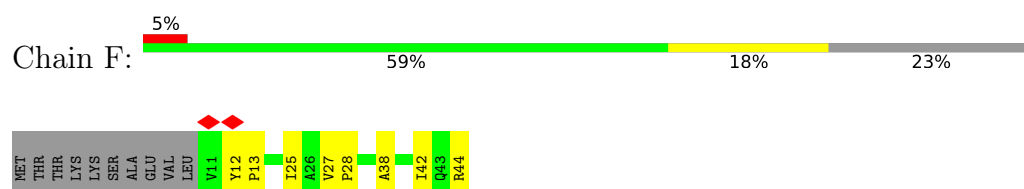
- Molecule 2: Photosystem II D2 protein



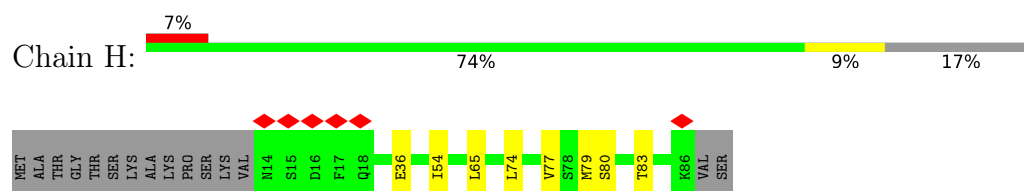
- Molecule 3: Cytochrome b559 subunit alpha



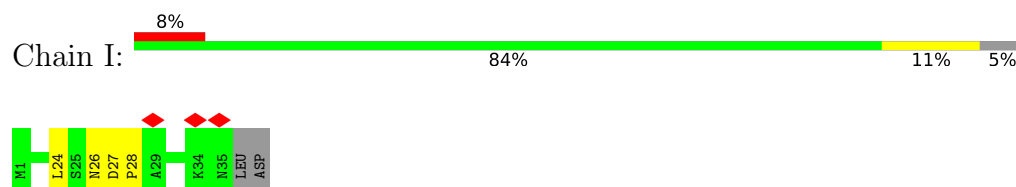
- Molecule 4: Cytochrome b559 subunit beta



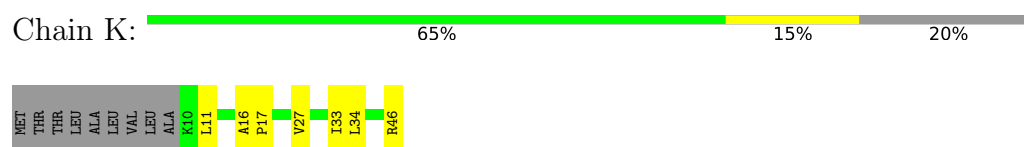
- Molecule 5: Photosystem II reaction center protein H



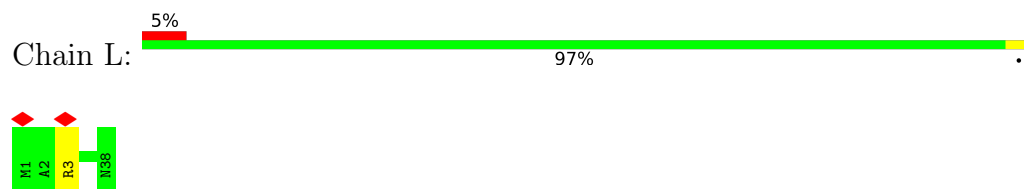
- Molecule 6: Photosystem II reaction center protein I



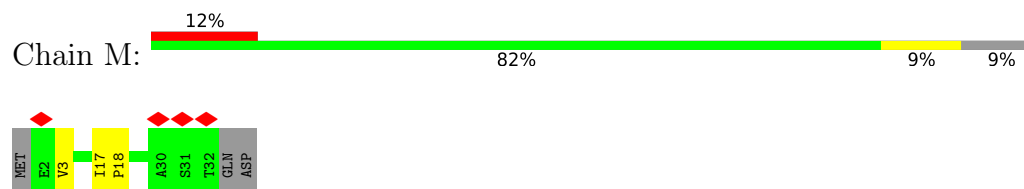
- Molecule 7: Photosystem II reaction center protein K



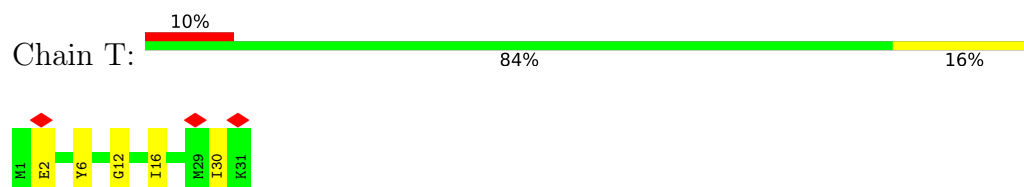
- Molecule 8: Photosystem II reaction center protein L



- Molecule 9: Photosystem II reaction center protein M

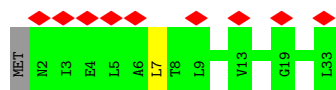


- Molecule 10: Photosystem II reaction center protein T

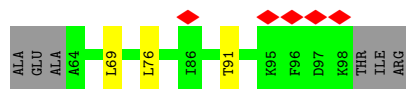
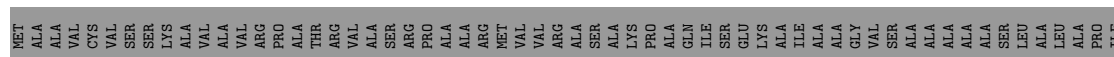


- Molecule 11: Photosystem II reaction center protein Psb30

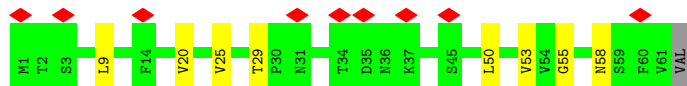
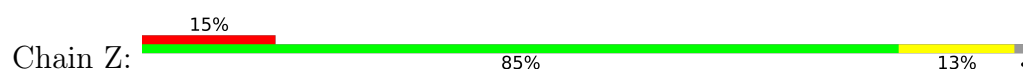




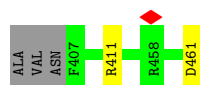
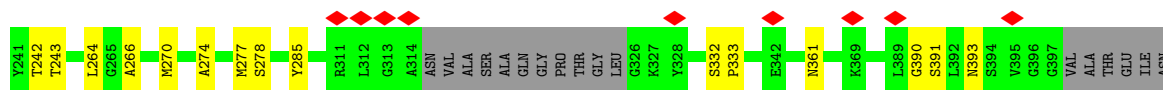
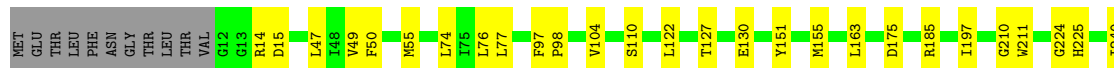
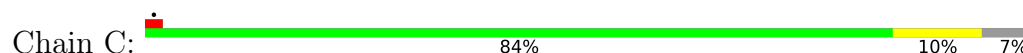
- Molecule 12: 4.1 kDa photosystem II subunit



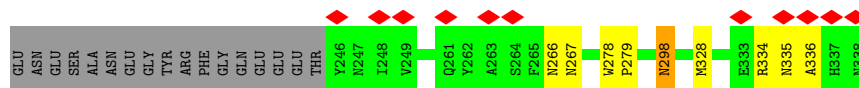
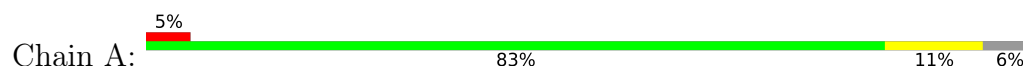
- Molecule 13: Photosystem II reaction center protein Z



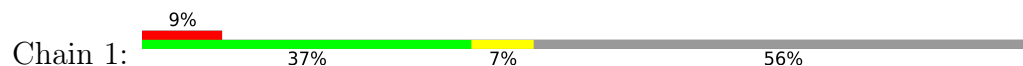
- Molecule 14: Photosystem II CP43 reaction center protein

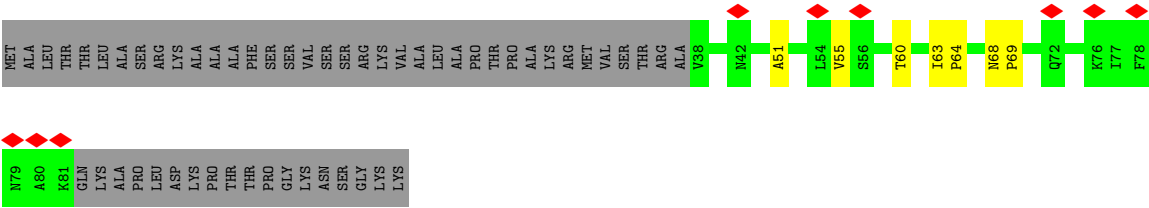


- Molecule 15: Photosystem II protein D1



- Molecule 16: Chains: 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	159928	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 K3 (6k x 4k)	Depositor
Maximum map value	0.215	Depositor
Minimum map value	-0.004	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	280.80002, 280.80002, 280.80002	wwPDB
Map dimensions	208, 208, 208	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3500001, 1.3500001, 1.3500001	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.13	0/3894	0.28	0/5302
2	D	0.13	0/2886	0.29	0/3937
3	E	0.12	0/652	0.31	0/890
4	F	0.13	0/286	0.26	0/389
5	H	0.10	0/573	0.26	0/783
6	I	0.16	0/291	0.31	0/394
7	K	0.10	0/309	0.29	0/425
8	L	0.14	0/322	0.23	0/437
9	M	0.07	0/243	0.20	0/333
10	T	0.14	0/263	0.21	0/354
11	V	0.07	0/224	0.18	0/307
12	X	0.10	0/244	0.20	0/330
13	Z	0.12	0/469	0.23	0/644
14	C	0.12	0/3486	0.28	0/4743
15	A	0.13	0/2495	0.32	0/3402
16	1	0.19	0/317	0.50	0/435
All	All	0.12	0/16954	0.29	0/23105

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

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	28	0
3	E	633	0	622	10	0
4	F	277	0	288	6	0
5	H	561	0	581	6	0
6	I	283	0	293	3	0
7	K	297	0	308	4	0
8	L	314	0	327	1	0
9	M	239	0	258	2	0
10	T	256	0	273	4	0
11	V	224	0	256	1	0
12	X	242	0	266	3	0
13	Z	458	0	490	7	0
14	C	3368	0	3240	37	0
15	A	2418	0	2349	25	0
16	1	313	0	331	8	0
17	A	174	0	170	0	0
17	B	1020	0	1113	8	0
17	C	845	0	936	16	0
17	D	195	0	216	4	0
18	A	40	0	56	2	0
18	B	120	0	168	3	0
18	C	80	0	112	11	0
18	D	40	0	56	0	0
18	H	40	0	56	5	0
18	K	40	0	56	1	0
18	Z	40	0	56	7	0
19	B	46	0	62	0	0
19	C	97	0	134	0	0
19	D	46	0	62	0	0
19	H	48	0	66	3	0
19	K	51	0	72	0	0
20	B	140	0	202	0	0
20	D	141	0	204	2	0
20	K	41	0	52	0	0
20	L	49	0	74	1	0
21	D	4	0	0	0	0
22	D	55	0	80	0	0
23	D	128	0	148	0	0
24	E	43	0	30	5	0
25	X	32	0	50	0	0
26	C	171	0	216	2	0
27	C	51	0	69	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	A	1	0	0	0	0
All	All	20218	0	20725	191	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (191) 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)
24:E:101:HEM:HHC	24:E:101:HEM:HBB2	1.67	0.77
14:C:390:GLY:O	15:A:298:ASN:ND2	2.19	0.76
14:C:74:LEU:HD13	14:C:77:LEU:HD12	1.70	0.74
20:D:407:LHG:O5	15:A:140:ARG:NH2	2.22	0.73
18:C:616:BCR:H383	18:C:616:BCR:H23C	1.72	0.72
18:Z:101:BCR:H333	14:C:104:VAL:HG11	1.73	0.71
15:A:184:ILE:HG23	15:A:328:MET:HE3	1.72	0.71
2:D:297:ASP:O	2:D:315:TYR:OH	2.08	0.69
7:K:46:ARG:NH1	14:C:14:ARG:O	2.27	0.67
15:A:32:TRP:O	15:A:35:VAL:HG22	1.95	0.66
18:B:618:BCR:H383	18:B:618:BCR:H23C	1.78	0.65
18:K:101:BCR:H343	13:Z:20:VAL:HG11	1.78	0.65
24:E:101:HEM:HBC2	24:E:101:HEM:HMC2	1.80	0.63
17:C:603:CLA:HED2	17:C:604:CLA:H43	1.81	0.62
1:B:477:ASP:OD1	1:B:478:VAL:N	2.34	0.60
17:B:602:CLA:H43	5:H:65:LEU:HA	1.83	0.60
3:E:19:TYR:OH	16:1:60:THR:O	2.18	0.60
14:C:285:TYR:OH	17:C:603:CLA:HED3	2.01	0.59
15:A:334:ARG:O	15:A:336:ALA:N	2.35	0.59
1:B:291:SER:OG	1:B:304:ARG:NH2	2.36	0.58
15:A:56:PRO:HG3	15:A:106:LEU:HD13	1.85	0.58
5:H:54:ILE:HG13	18:H:101:BCR:H333	1.85	0.58
10:T:6:TYR:HB3	15:A:77:ILE:HD11	1.86	0.56
14:C:224:GLY:HA3	18:C:615:BCR:H402	1.86	0.56
14:C:393:ASN:ND2	26:C:619:DGD:O1B	2.38	0.56
3:E:8:ARG:NH2	3:E:12:ASP:OD2	2.39	0.55
26:C:619:DGD:O5D	26:C:619:DGD:O4D	2.23	0.55
1:B:127:ARG:O	1:B:128:THR:OG1	2.22	0.55
1:B:368:VAL:HG22	1:B:381:VAL:HG22	1.88	0.55
17:B:602:CLA:H42	19:H:102:LMG:H112	1.88	0.55
18:Z:101:BCR:H382	18:Z:101:BCR:H23C	1.88	0.55
3:E:6:VAL:HG22	3:E:6:VAL:O	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:C:606:CLA:H11	18:C:615:BCR:H333	1.89	0.54
18:B:617:BCR:H382	18:B:617:BCR:H23C	1.88	0.53
2:D:221:THR:HG22	2:D:221:THR:O	2.09	0.53
14:C:49:VAL:HG23	14:C:110:SER:HB2	1.91	0.53
2:D:13:THR:HG22	2:D:14:TRP:N	2.24	0.53
2:D:136:VAL:HG13	2:D:138:LEU:HD13	1.91	0.53
15:A:85:THR:HG22	15:A:109:GLY:O	2.09	0.53
18:H:101:BCR:H23C	18:H:101:BCR:H383	1.91	0.52
17:D:403:CLA:H43	12:X:76:LEU:HD23	1.90	0.52
10:T:30:ILE:HG23	10:T:30:ILE:O	2.08	0.52
2:D:340:VAL:HG13	2:D:340:VAL:O	2.08	0.52
3:E:38:VAL:CG1	4:F:38:ALA:HB3	2.39	0.52
4:F:27:VAL:HB	4:F:28:PRO:HD3	1.91	0.52
2:D:232:PHE:O	15:A:267:ASN:ND2	2.42	0.52
1:B:221:PRO:CB	1:B:231:MET:HE1	2.41	0.51
2:D:201:VAL:HG22	17:D:402:CLA:C1B	2.41	0.51
7:K:27:VAL:O	7:K:27:VAL:HG12	2.11	0.51
13:Z:55:GLY:HA2	18:Z:101:BCR:H323	1.93	0.51
16:1:51:ALA:O	16:1:55:VAL:HG12	2.11	0.50
6:I:24:LEU:O	6:I:24:LEU:HD23	2.11	0.50
5:H:79:MET:HA	5:H:79:MET:HE2	1.92	0.50
18:Z:101:BCR:H23C	18:Z:101:BCR:C38	2.40	0.50
20:D:407:LHG:O3	20:D:407:LHG:O1	2.24	0.50
14:C:163:LEU:HD23	14:C:225:HIS:CD2	2.48	0.49
3:E:38:VAL:HG11	4:F:38:ALA:HB3	1.94	0.49
3:E:57:THR:HG22	3:E:58:GLU:N	2.28	0.49
1:B:12:VAL:HG12	1:B:12:VAL:O	2.12	0.49
24:E:101:HEM:HBC2	24:E:101:HEM:CMC	2.41	0.49
2:D:197:HIS:O	2:D:201:VAL:HG23	2.13	0.49
1:B:250:PHE:CE2	1:B:459:ALA:HB1	2.48	0.48
14:C:175:ASP:OD1	14:C:185:ARG:NH2	2.46	0.48
1:B:281:GLN:OE1	1:B:358:ARG:NH1	2.46	0.48
13:Z:50:LEU:HA	13:Z:53:VAL:HG12	1.96	0.48
14:C:391:SER:HA	15:A:298:ASN:HB2	1.94	0.48
2:D:148:ALA:HB3	2:D:149:PRO:CD	2.44	0.48
18:Z:101:BCR:C33	14:C:104:VAL:HG11	2.42	0.48
14:C:242:THR:HG22	14:C:243:THR:N	2.28	0.47
18:C:615:BCR:H311	18:C:615:BCR:HC8	1.95	0.47
3:E:30:LEU:HD11	24:E:101:HEM:HBB1	1.96	0.47
1:B:349:GLN:HA	1:B:349:GLN:OE1	2.14	0.47
11:V:7:LEU:HD23	11:V:7:LEU:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:264:LEU:HD21	17:C:609:CLA:HAB	1.96	0.47
2:D:261:PHE:CD2	2:D:267:LEU:HD13	2.49	0.47
14:C:197:ILE:HG23	18:C:615:BCR:H403	1.97	0.47
1:B:25:MET:HE1	1:B:108:PHE:HD1	1.80	0.47
18:H:101:BCR:H393	12:X:69:LEU:HD21	1.97	0.47
18:Z:101:BCR:H333	14:C:104:VAL:CG1	2.41	0.47
18:C:615:BCR:H382	18:C:615:BCR:H23C	1.97	0.47
17:C:606:CLA:C1	18:C:615:BCR:H333	2.46	0.46
18:A:405:BCR:H382	18:A:405:BCR:H23C	1.98	0.46
9:M:3:VAL:HG11	10:T:2:GLU:OE2	2.16	0.46
15:A:278:TRP:HB3	15:A:279:PRO:HD3	1.97	0.46
1:B:223:ILE:HD12	2:D:5:ILE:HG21	1.98	0.46
14:C:127:THR:OG1	14:C:130:GLU:OE2	2.28	0.46
16:1:63:ILE:N	16:1:64:PRO:CD	2.78	0.46
18:H:101:BCR:HC8	18:H:101:BCR:H331	1.98	0.46
15:A:111:PRO:O	15:A:115:ILE:HG12	2.15	0.46
17:B:602:CLA:H41	17:B:602:CLA:H71	1.97	0.46
2:D:272:LEU:C	2:D:272:LEU:HD23	2.40	0.46
13:Z:9:LEU:HD11	18:C:616:BCR:H312	1.97	0.45
2:D:214:HIS:CD2	2:D:271:MET:HE1	2.51	0.45
14:C:15:ASP:OD1	14:C:15:ASP:N	2.48	0.45
17:D:410:CLA:HMA1	17:D:410:CLA:H142	1.97	0.45
2:D:14:TRP:NE1	12:X:91:THR:OG1	2.40	0.45
2:D:209:LEU:HD21	2:D:213:ILE:HD12	1.97	0.45
14:C:266:ALA:O	14:C:270:MET:HG3	2.16	0.45
2:D:172:SER:HB2	2:D:177:ALA:HB1	1.98	0.45
15:A:110:GLY:N	15:A:111:PRO:HD2	2.32	0.45
17:B:602:CLA:H41	17:B:602:CLA:C7	2.46	0.45
14:C:55:MET:HG3	14:C:76:LEU:HD12	1.98	0.45
15:A:59:ASP:OD2	15:A:59:ASP:O	2.35	0.45
1:B:400:THR:HG23	1:B:410:THR:HG22	1.98	0.45
1:B:452:THR:O	1:B:456:VAL:HG23	2.17	0.44
15:A:30:ILE:O	15:A:34:GLY:HA3	2.17	0.44
15:A:127:MET:HE1	15:A:148:SER:HA	1.98	0.44
15:A:182:PHE:CE1	15:A:186:PHE:HE2	2.35	0.44
17:B:604:CLA:HAA2	17:B:612:CLA:H141	1.99	0.44
14:C:50:PHE:HB2	14:C:110:SER:OG	2.17	0.44
14:C:163:LEU:HD13	17:C:602:CLA:HMD1	2.00	0.44
1:B:321:LYS:HE2	1:B:359:MET:HE3	2.00	0.44
15:A:266:ASN:OD1	15:A:266:ASN:O	2.36	0.44
1:B:109:LEU:O	1:B:112:VAL:HG12	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:PHE:HE1	2:D:144:ILE:HG23	1.83	0.44
3:E:22:ILE:HD13	24:E:101:HEM:HMA3	1.99	0.43
15:A:214:MET:O	15:A:218:LEU:HD13	2.18	0.43
2:D:181:PHE:CZ	2:D:185:PHE:CZ	3.05	0.43
4:F:42:ILE:HG22	4:F:44:ARG:H	1.83	0.43
14:C:47:LEU:HD21	17:C:611:CLA:HMD2	1.99	0.43
15:A:109:GLY:C	15:A:111:PRO:HD2	2.43	0.43
13:Z:25:VAL:O	13:Z:29:THR:HG23	2.18	0.43
1:B:20:ILE:HG23	17:B:615:CLA:HED1	2.01	0.43
14:C:274:ALA:HB2	17:C:603:CLA:HMD2	1.99	0.43
18:C:616:BCR:H383	18:C:616:BCR:C23	2.47	0.43
1:B:25:MET:HE1	1:B:108:PHE:CD1	2.53	0.43
2:D:123:ILE:HD11	19:H:102:LMG:H401	1.99	0.43
2:D:308:ASP:O	2:D:308:ASP:OD1	2.37	0.43
4:F:25:ILE:O	4:F:25:ILE:HG22	2.18	0.43
19:H:102:LMG:O5	19:H:102:LMG:O4	2.28	0.43
17:C:606:CLA:C2	18:C:615:BCR:H333	2.48	0.43
14:C:14:ARG:HH11	14:C:14:ARG:HG3	1.84	0.43
14:C:122:LEU:HD11	17:C:612:CLA:H92	2.01	0.43
14:C:278:SER:O	14:C:411:ARG:NH1	2.52	0.43
15:A:188:ALA:HB2	15:A:328:MET:HB3	2.00	0.43
16:1:63:ILE:N	16:1:64:PRO:HD2	2.33	0.42
2:D:136:VAL:O	2:D:136:VAL:HG22	2.18	0.42
1:B:249:ALA:HB2	17:B:604:CLA:HBC3	2.02	0.42
17:B:615:CLA:H91	17:B:616:CLA:C11	2.49	0.42
2:D:147:SER:HA	2:D:150:ILE:HG22	2.01	0.42
2:D:209:LEU:CD2	2:D:213:ILE:HD12	2.49	0.42
1:B:477:ASP:OD1	1:B:478:VAL:HG23	2.19	0.42
14:C:97:PHE:N	14:C:98:PRO:CD	2.83	0.42
14:C:151:TYR:CE1	14:C:240:ILE:HD12	2.55	0.42
16:1:68:ASN:HB3	16:1:69:PRO:CD	2.49	0.42
2:D:274:VAL:HB	2:D:275:PRO:HD3	2.01	0.42
1:B:397:VAL:HG23	1:B:417:VAL:HG11	2.01	0.42
5:H:74:LEU:HB2	5:H:77:VAL:HG22	2.01	0.42
10:T:12:GLY:O	10:T:16:ILE:HG12	2.20	0.42
1:B:288:VAL:O	1:B:292:LEU:HD13	2.20	0.42
2:D:148:ALA:HB3	2:D:149:PRO:HD3	2.01	0.42
9:M:17:ILE:HB	9:M:18:PRO:HD3	2.02	0.42
3:E:38:VAL:HG22	3:E:38:VAL:O	2.19	0.42
1:B:246:PHE:HE1	1:B:250:PHE:CE2	2.38	0.41
18:H:101:BCR:HC7	18:H:101:BCR:H321	1.87	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ASP:OD1	1:B:188:ASP:N	2.53	0.41
4:F:12:TYR:N	4:F:13:PRO:HD2	2.35	0.41
6:I:26:ASN:O	6:I:26:ASN:OD1	2.38	0.41
14:C:270:MET:HE1	17:C:608:CLA:H42	2.02	0.41
14:C:361:ASN:OD1	14:C:361:ASN:N	2.54	0.41
1:B:137:LYS:NZ	5:H:36:GLU:OE2	2.41	0.41
13:Z:58:ASN:C	13:Z:58:ASN:HD22	2.27	0.41
14:C:277:MET:HE1	17:C:602:CLA:HMA3	2.02	0.41
6:I:27:ASP:N	6:I:28:PRO:HD2	2.36	0.41
1:B:118:TRP:NE1	8:L:3:ARG:O	2.46	0.41
5:H:80:SER:O	5:H:83:THR:HG22	2.19	0.41
7:K:33:ILE:HG23	7:K:34:LEU:N	2.35	0.41
13:Z:55:GLY:CA	18:Z:101:BCR:H323	2.51	0.41
14:C:155:MET:HE1	17:C:614:CLA:H172	2.01	0.41
15:A:29:TYR:O	15:A:129:ARG:NH1	2.54	0.41
15:A:42:LEU:HB3	18:A:405:BCR:H353	2.02	0.41
2:D:256:ILE:HG12	15:A:133:LEU:HD23	2.03	0.41
15:A:22:THR:HG22	15:A:22:THR:O	2.21	0.41
16:1:63:ILE:CG2	16:1:64:PRO:HD3	2.51	0.41
1:B:246:PHE:CE1	1:B:250:PHE:HE2	2.39	0.41
1:B:385:LYS:HG2	1:B:385:LYS:O	2.21	0.41
2:D:144:ILE:HD12	2:D:144:ILE:H	1.86	0.41
14:C:210:GLY:O	14:C:211:TRP:C	2.63	0.41
1:B:236:THR:HG23	1:B:237:VAL:N	2.36	0.41
17:C:602:CLA:H141	17:C:602:CLA:H162	1.91	0.41
17:C:607:CLA:H43	18:C:615:BCR:H313	2.02	0.41
16:1:55:VAL:HG22	16:1:55:VAL:O	2.20	0.40
18:B:619:BCR:H23C	18:B:619:BCR:H383	2.02	0.40
17:D:410:CLA:H92	20:L:101:LHG:H222	2.03	0.40
3:E:31:PHE:CE2	16:1:55:VAL:HG11	2.57	0.40
14:C:163:LEU:HD22	17:C:602:CLA:C2D	2.51	0.40
14:C:461:ASP:N	14:C:461:ASP:OD1	2.53	0.40
7:K:16:ALA:N	7:K:17:PRO:HD2	2.37	0.40
14:C:332:SER:OG	14:C:333:PRO:HD2	2.21	0.40
1:B:63:LEU:N	1:B:64:PRO:HD2	2.36	0.40
2:D:214:HIS:CG	2:D:271:MET:HE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	480/508 (94%)	470 (98%)	10 (2%)	0	100	100
2	D	349/352 (99%)	337 (97%)	12 (3%)	0	100	100
3	E	76/82 (93%)	72 (95%)	4 (5%)	0	100	100
4	F	32/44 (73%)	31 (97%)	1 (3%)	0	100	100
5	H	71/88 (81%)	68 (96%)	3 (4%)	0	100	100
6	I	33/37 (89%)	32 (97%)	1 (3%)	0	100	100
7	K	35/46 (76%)	34 (97%)	0	1 (3%)	3	15
8	L	36/38 (95%)	36 (100%)	0	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%)	30 (100%)	0	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
14	C	424/461 (92%)	415 (98%)	9 (2%)	0	100	100
15	A	305/329 (93%)	290 (95%)	13 (4%)	2 (1%)	18	48
16	1	42/99 (42%)	42 (100%)	0	0	100	100
All	All	2063/2345 (88%)	2005 (97%)	55 (3%)	3 (0%)	49	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	A	298	ASN
15	A	335	ASN
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
12	X	25/67 (37%)	25 (100%)	0	100	100
13	Z	51/52 (98%)	51 (100%)	0	100	100
14	C	338/362 (93%)	338 (100%)	0	100	100
15	A	251/268 (94%)	251 (100%)	0	100	100
16	1	32/75 (43%)	32 (100%)	0	100	100
All	All	1700/1887 (90%)	1700 (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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	201	HIS
2	D	142	ASN
5	H	18	GLN
8	L	9	GLN
15	A	108	ASN
15	A	322	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	1	71	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 70 ligands modelled in this entry, 1 is monoatomic - leaving 69 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$
17	CLA	B	607	-	69,73,73	1.17	7 (10%)	82,113,113	1.09	5 (6%)
19	LMG	H	102	-	48,48,55	0.97	2 (4%)	56,56,63	0.96	2 (3%)
18	BCR	D	404	-	41,41,41	0.77	1 (2%)	56,56,56	2.09	21 (37%)
20	LHG	D	406	-	48,48,48	0.93	2 (4%)	51,54,54	1.02	2 (3%)
18	BCR	B	617	-	41,41,41	0.80	1 (2%)	56,56,56	1.97	21 (37%)
17	CLA	B	604	-	69,73,73	1.17	7 (10%)	82,113,113	1.06	4 (4%)
17	CLA	A	402	-	69,73,73	1.17	7 (10%)	82,113,113	1.09	6 (7%)
17	CLA	B	609	-	69,73,73	1.16	5 (7%)	82,113,113	1.05	4 (4%)
17	CLA	C	611	-	69,73,73	1.18	6 (8%)	82,113,113	1.11	4 (4%)
20	LHG	B	621	-	43,43,48	1.00	2 (4%)	46,49,54	1.01	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	404	-	64,68,73	1.21	5 (7%)	76,107,113	1.09	4 (5%)
17	CLA	B	606	-	69,73,73	1.16	6 (8%)	82,113,113	1.07	5 (6%)
17	CLA	C	605	-	69,73,73	1.17	7 (10%)	82,113,113	1.06	4 (4%)
21	BCT	D	401	28	3,3,3	1.11	0	2,3,3	4.17	2 (100%)
17	CLA	C	610	-	69,73,73	1.16	5 (7%)	82,113,113	1.07	3 (3%)
17	CLA	B	602	-	69,73,73	1.18	6 (8%)	82,113,113	1.09	5 (6%)
17	CLA	B	610	-	69,73,73	1.15	6 (8%)	82,113,113	1.11	5 (6%)
17	CLA	B	608	-	69,73,73	1.15	6 (8%)	82,113,113	1.04	4 (4%)
17	CLA	B	612	-	69,73,73	1.17	7 (10%)	82,113,113	1.11	4 (4%)
18	BCR	C	616	-	41,41,41	0.76	1 (2%)	56,56,56	1.96	15 (26%)
27	SQD	C	620	-	49,51,54	1.15	3 (6%)	59,62,65	1.04	3 (5%)
19	LMG	D	408	-	46,46,55	0.99	2 (4%)	54,54,63	0.87	2 (3%)
17	CLA	B	613	-	69,73,73	1.17	6 (8%)	82,113,113	1.11	5 (6%)
17	CLA	B	614	-	49,53,73	1.37	6 (12%)	58,89,113	1.18	3 (5%)
17	CLA	B	615	-	69,73,73	1.17	6 (8%)	82,113,113	1.07	4 (4%)
17	CLA	B	605	-	69,73,73	1.15	5 (7%)	82,113,113	1.05	5 (6%)
17	CLA	B	616	-	69,73,73	1.17	6 (8%)	82,113,113	1.10	5 (6%)
17	CLA	C	609	-	69,73,73	1.17	7 (10%)	82,113,113	1.03	4 (4%)
17	CLA	A	403	-	53,57,73	1.31	7 (13%)	61,93,113	1.19	4 (6%)
26	DGD	C	618	-	58,58,67	0.92	2 (3%)	72,72,81	0.87	2 (2%)
20	LHG	B	623	-	48,48,48	0.94	2 (4%)	51,54,54	0.94	2 (3%)
18	BCR	C	615	-	41,41,41	0.81	1 (2%)	56,56,56	2.30	24 (42%)
18	BCR	Z	101	-	41,41,41	0.85	1 (2%)	56,56,56	1.92	19 (33%)
17	CLA	B	603	-	69,73,73	1.16	7 (10%)	82,113,113	1.07	5 (6%)
17	CLA	C	607	-	69,73,73	1.17	6 (8%)	82,113,113	1.09	5 (6%)
20	LHG	L	101	-	48,48,48	0.94	2 (4%)	51,54,54	0.92	2 (3%)
20	LHG	B	622	-	46,46,48	0.97	2 (4%)	49,52,54	0.96	2 (4%)
18	BCR	H	101	-	41,41,41	0.69	0	56,56,56	2.13	20 (35%)
24	HEM	E	101	3,4	50,50,50	1.44	9 (18%)	67,82,82	1.12	4 (5%)
19	LMG	K	102	-	51,51,55	0.95	2 (3%)	59,59,63	0.89	2 (3%)
17	CLA	C	602	-	69,73,73	1.17	7 (10%)	82,113,113	1.09	5 (6%)
20	LHG	D	407	-	42,42,48	1.02	2 (4%)	45,48,54	1.12	3 (6%)
17	CLA	C	604	-	69,73,73	1.16	5 (7%)	82,113,113	1.10	5 (6%)
17	CLA	C	612	14	69,73,73	1.17	8 (11%)	82,113,113	1.09	6 (7%)
25	VTQ	X	201	-	30,32,32	1.51	6 (20%)	39,44,44	1.06	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	DGD	C	619	-	60,60,67	0.90	2 (3%)	74,74,81	0.81	2 (2%)
17	CLA	B	611	-	69,73,73	1.16	5 (7%)	82,113,113	1.07	4 (4%)
26	DGD	C	617	-	56,56,67	0.93	2 (3%)	70,70,81	0.93	3 (4%)
22	PL9	D	405	-	55,55,55	1.03	4 (7%)	68,69,69	1.51	12 (17%)
17	CLA	C	613	-	69,73,73	1.17	5 (7%)	82,113,113	1.10	3 (3%)
18	BCR	B	618	-	41,41,41	0.77	0	56,56,56	1.92	20 (35%)
19	LMG	B	620	-	46,46,55	0.99	2 (4%)	54,54,63	0.88	2 (3%)
17	CLA	C	608	-	69,73,73	1.17	6 (8%)	82,113,113	1.11	4 (4%)
17	CLA	D	402	-	69,73,73	1.18	6 (8%)	82,113,113	1.22	4 (4%)
23	PHO	D	411	-	58,69,69	2.16	9 (15%)	55,99,99	1.49	7 (12%)
17	CLA	C	614	-	69,73,73	1.16	6 (8%)	82,113,113	1.11	6 (7%)
17	CLA	D	410	-	69,73,73	1.16	7 (10%)	82,113,113	1.09	7 (8%)
20	LHG	K	103	-	40,40,48	1.03	2 (5%)	43,46,54	1.02	3 (6%)
17	CLA	B	601	-	69,73,73	1.17	7 (10%)	82,113,113	1.05	5 (6%)
18	BCR	K	101	-	41,41,41	0.76	0	56,56,56	2.17	20 (35%)
18	BCR	B	619	-	41,41,41	0.79	1 (2%)	56,56,56	2.03	20 (35%)
17	CLA	C	603	-	69,73,73	1.17	6 (8%)	82,113,113	1.16	5 (6%)
18	BCR	A	405	-	41,41,41	0.78	1 (2%)	56,56,56	2.02	19 (33%)
20	LHG	D	409	-	48,48,48	0.94	2 (4%)	51,54,54	1.03	3 (5%)
19	LMG	C	621	-	48,48,55	0.99	3 (6%)	56,56,63	1.06	3 (5%)
23	PHO	D	412	-	58,69,69	2.16	9 (15%)	55,99,99	1.39	5 (9%)
17	CLA	C	606	-	69,73,73	1.16	6 (8%)	82,113,113	1.03	5 (6%)
19	LMG	C	601	-	49,49,55	0.96	2 (4%)	57,57,63	0.91	2 (3%)
17	CLA	D	403	-	69,73,73	1.16	6 (8%)	82,113,113	1.09	4 (4%)

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
17	CLA	B	607	-	1/1/15/20	18/39/115/115	-
19	LMG	H	102	-	-	10/43/63/70	0/1/1/1
18	BCR	D	404	-	-	4/29/63/63	0/2/2/2
20	LHG	D	406	-	-	8/53/53/53	-
18	BCR	B	617	-	-	4/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	604	-	1/1/15/20	17/39/115/115	-
17	CLA	A	402	-	1/1/15/20	10/39/115/115	-
17	CLA	B	609	-	1/1/15/20	13/39/115/115	-
17	CLA	C	611	-	1/1/15/20	8/39/115/115	-
20	LHG	B	621	-	-	9/48/48/53	-
17	CLA	A	404	-	1/1/14/20	6/33/109/115	-
17	CLA	B	606	-	1/1/15/20	12/39/115/115	-
17	CLA	C	605	-	1/1/15/20	8/39/115/115	-
17	CLA	C	610	-	1/1/15/20	16/39/115/115	-
17	CLA	B	602	-	1/1/15/20	8/39/115/115	-
17	CLA	B	610	-	1/1/15/20	13/39/115/115	-
17	CLA	B	608	-	1/1/15/20	8/39/115/115	-
17	CLA	B	612	-	1/1/15/20	10/39/115/115	-
18	BCR	C	616	-	-	4/29/63/63	0/2/2/2
27	SQD	C	620	-	-	13/46/66/69	0/1/1/1
19	LMG	D	408	-	-	6/41/61/70	0/1/1/1
17	CLA	B	613	-	1/1/15/20	13/39/115/115	-
17	CLA	B	614	-	1/1/11/20	3/15/91/115	-
17	CLA	B	615	-	1/1/15/20	6/39/115/115	-
17	CLA	B	605	-	1/1/15/20	15/39/115/115	-
17	CLA	B	616	-	1/1/15/20	12/39/115/115	-
17	CLA	C	609	-	1/1/15/20	17/39/115/115	-
17	CLA	A	403	-	1/1/11/20	6/20/96/115	-
26	DGD	C	618	-	-	7/46/86/95	0/2/2/2
20	LHG	B	623	-	-	10/53/53/53	-
18	BCR	C	615	-	-	2/29/63/63	0/2/2/2
18	BCR	Z	101	-	-	4/29/63/63	0/2/2/2
17	CLA	B	603	-	1/1/15/20	11/39/115/115	-
17	CLA	C	607	-	1/1/15/20	21/39/115/115	-
20	LHG	L	101	-	-	11/53/53/53	-
20	LHG	B	622	-	-	7/51/51/53	-
18	BCR	H	101	-	-	4/29/63/63	0/2/2/2
24	HEM	E	101	3,4	-	3/14/54/54	-
19	LMG	K	102	-	-	9/46/66/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	C	602	-	1/1/15/20	16/39/115/115	-
20	LHG	D	407	-	-	13/47/47/53	-
17	CLA	C	604	-	1/1/15/20	16/39/115/115	-
17	CLA	C	612	14	1/1/15/20	11/39/115/115	-
25	VTQ	X	201	-	-	6/25/49/49	0/1/1/1
26	DGD	C	619	-	-	5/48/88/95	0/2/2/2
17	CLA	B	611	-	1/1/15/20	14/39/115/115	-
26	DGD	C	617	-	-	6/44/84/95	0/2/2/2
22	PL9	D	405	-	-	8/53/73/73	0/1/1/1
17	CLA	C	613	-	1/1/15/20	14/39/115/115	-
18	BCR	B	618	-	-	4/29/63/63	0/2/2/2
19	LMG	B	620	-	-	3/41/61/70	0/1/1/1
17	CLA	C	608	-	1/1/15/20	6/39/115/115	-
17	CLA	D	402	-	1/1/15/20	17/39/115/115	-
23	PHO	D	411	-	-	11/37/103/103	0/5/6/6
17	CLA	C	614	-	1/1/15/20	15/39/115/115	-
17	CLA	D	410	-	1/1/15/20	5/39/115/115	-
20	LHG	K	103	-	-	8/45/45/53	-
17	CLA	B	601	-	1/1/15/20	13/39/115/115	-
18	BCR	K	101	-	-	4/29/63/63	0/2/2/2
18	BCR	B	619	-	-	4/29/63/63	0/2/2/2
17	CLA	C	603	-	1/1/15/20	12/39/115/115	-
18	BCR	A	405	-	-	4/29/63/63	0/2/2/2
20	LHG	D	409	-	-	10/53/53/53	-
19	LMG	C	621	-	-	8/43/63/70	0/1/1/1
23	PHO	D	412	-	-	10/37/103/103	0/5/6/6
17	CLA	C	606	-	1/1/15/20	15/39/115/115	-
19	LMG	C	601	-	-	5/44/64/70	0/1/1/1
17	CLA	D	403	-	1/1/15/20	17/39/115/115	-

All (298) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	412	PHO	C1B-C2B	9.74	1.50	1.39
23	D	411	PHO	C1B-C2B	9.66	1.50	1.39
23	D	412	PHO	C3B-C4B	8.51	1.50	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	411	PHO	C3B-C4B	8.46	1.50	1.41
27	C	620	SQD	O8-S	4.45	1.63	1.47
20	D	407	LHG	O8-C23	4.30	1.45	1.33
19	C	621	LMG	O8-C28	4.30	1.45	1.33
19	C	601	LMG	O8-C28	4.30	1.45	1.33
26	C	618	DGD	O1G-C1A	4.28	1.45	1.33
20	B	622	LHG	O8-C23	4.27	1.45	1.33
19	K	102	LMG	O7-C10	4.27	1.46	1.34
19	K	102	LMG	O8-C28	4.26	1.45	1.33
27	C	620	SQD	O48-C23	4.25	1.45	1.33
19	D	408	LMG	O7-C10	4.25	1.46	1.34
20	B	623	LHG	O8-C23	4.25	1.45	1.33
20	D	409	LHG	O8-C23	4.24	1.45	1.33
19	D	408	LMG	O8-C28	4.24	1.45	1.33
26	C	617	DGD	O1G-C1A	4.24	1.45	1.33
20	L	101	LHG	O8-C23	4.24	1.45	1.33
19	H	102	LMG	O8-C28	4.24	1.45	1.33
20	K	103	LHG	O8-C23	4.23	1.45	1.33
26	C	619	DGD	O1G-C1A	4.23	1.45	1.33
20	B	621	LHG	O8-C23	4.22	1.45	1.33
26	C	618	DGD	O2G-C1B	4.22	1.46	1.34
19	B	620	LMG	O8-C28	4.22	1.45	1.33
20	B	622	LHG	O7-C7	4.20	1.46	1.34
19	B	620	LMG	O7-C10	4.19	1.46	1.34
20	B	621	LHG	O7-C7	4.18	1.46	1.34
23	D	411	PHO	C1D-C2D	4.18	1.44	1.39
20	D	407	LHG	O7-C7	4.18	1.46	1.34
26	C	619	DGD	O2G-C1B	4.18	1.46	1.34
20	K	103	LHG	O7-C7	4.16	1.46	1.34
20	D	406	LHG	O8-C23	4.16	1.45	1.33
19	H	102	LMG	O7-C10	4.15	1.46	1.34
26	C	617	DGD	O2G-C1B	4.14	1.46	1.34
20	D	409	LHG	O7-C7	4.14	1.46	1.34
20	D	406	LHG	O7-C7	4.14	1.46	1.34
20	B	623	LHG	O7-C7	4.13	1.46	1.34
19	C	621	LMG	O7-C10	4.13	1.45	1.34
19	C	601	LMG	O7-C10	4.10	1.45	1.34
27	C	620	SQD	O47-C7	4.08	1.45	1.34
20	L	101	LHG	O7-C7	4.07	1.45	1.34
23	D	412	PHO	C1D-C2D	3.94	1.43	1.39
23	D	411	PHO	C4D-CHA	3.79	1.45	1.39
24	E	101	HEM	FE-NB	3.77	2.06	1.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	412	PHO	C4D-CHA	3.66	1.45	1.39
17	D	402	CLA	C1D-ND	3.63	1.42	1.37
17	C	611	CLA	C1D-ND	3.61	1.42	1.37
17	C	610	CLA	C1D-ND	3.59	1.42	1.37
17	B	614	CLA	C1D-ND	3.58	1.42	1.37
17	C	606	CLA	C1D-ND	3.58	1.42	1.37
17	B	616	CLA	C1D-ND	3.57	1.42	1.37
17	D	403	CLA	C1D-ND	3.56	1.42	1.37
17	D	410	CLA	C1D-ND	3.55	1.42	1.37
17	C	613	CLA	C1D-ND	3.55	1.42	1.37
17	B	612	CLA	C1D-ND	3.55	1.42	1.37
17	A	402	CLA	C1D-ND	3.55	1.42	1.37
17	B	601	CLA	C1D-ND	3.55	1.42	1.37
17	B	615	CLA	C1D-ND	3.55	1.42	1.37
17	B	607	CLA	C1D-ND	3.54	1.42	1.37
17	C	612	CLA	C1D-ND	3.54	1.42	1.37
17	B	609	CLA	C1D-ND	3.53	1.42	1.37
17	C	604	CLA	C1D-ND	3.53	1.42	1.37
17	A	404	CLA	C1D-ND	3.53	1.42	1.37
17	B	608	CLA	C1D-ND	3.53	1.42	1.37
17	B	613	CLA	C1D-ND	3.52	1.42	1.37
17	C	603	CLA	C1D-ND	3.52	1.42	1.37
17	C	614	CLA	C1D-ND	3.51	1.42	1.37
17	B	610	CLA	C1D-ND	3.51	1.42	1.37
17	B	602	CLA	C1D-ND	3.51	1.42	1.37
17	C	605	CLA	C1D-ND	3.51	1.42	1.37
17	B	611	CLA	C1D-ND	3.50	1.42	1.37
17	C	609	CLA	C1D-ND	3.50	1.42	1.37
17	B	606	CLA	C1D-ND	3.50	1.42	1.37
17	B	605	CLA	C1D-ND	3.49	1.42	1.37
17	C	607	CLA	C1D-ND	3.48	1.42	1.37
17	C	608	CLA	C1D-ND	3.48	1.42	1.37
17	B	604	CLA	C1D-ND	3.48	1.42	1.37
17	A	403	CLA	C1D-ND	3.47	1.42	1.37
17	C	602	CLA	C1D-ND	3.44	1.42	1.37
17	B	603	CLA	C1D-ND	3.40	1.42	1.37
24	E	101	HEM	FE-NA	3.35	2.06	1.95
17	C	613	CLA	C4B-NB	3.33	1.42	1.37
17	C	606	CLA	C4B-NB	3.30	1.42	1.37
17	C	609	CLA	C4B-NB	3.30	1.42	1.37
17	C	605	CLA	C4B-NB	3.29	1.42	1.37
17	C	611	CLA	C4B-NB	3.28	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	602	CLA	C4B-NB	3.27	1.42	1.37
17	B	604	CLA	C4B-NB	3.27	1.42	1.37
17	B	615	CLA	C4B-NB	3.27	1.42	1.37
17	D	402	CLA	C4B-NB	3.25	1.42	1.37
17	A	403	CLA	C4B-NB	3.25	1.42	1.37
17	C	610	CLA	C4B-NB	3.24	1.42	1.37
17	B	603	CLA	C4B-NB	3.24	1.42	1.37
17	B	609	CLA	C4B-NB	3.24	1.42	1.37
17	C	612	CLA	C4B-NB	3.24	1.42	1.37
22	D	405	PL9	C3-C4	-3.23	1.44	1.49
17	C	604	CLA	C4B-NB	3.23	1.42	1.37
17	B	606	CLA	C4B-NB	3.23	1.42	1.37
17	D	403	CLA	C4B-NB	3.22	1.42	1.37
17	D	410	CLA	C4B-NB	3.22	1.42	1.37
17	C	614	CLA	C4B-NB	3.20	1.42	1.37
17	C	602	CLA	C4B-NB	3.20	1.42	1.37
17	B	607	CLA	C4B-NB	3.20	1.42	1.37
17	B	613	CLA	C4B-NB	3.18	1.42	1.37
24	E	101	HEM	FE-ND	3.18	2.04	1.94
25	X	201	VTQ	O3-C9	-3.18	1.40	1.44
17	B	608	CLA	C4B-NB	3.17	1.42	1.37
17	B	612	CLA	C4B-NB	3.17	1.42	1.37
17	B	611	CLA	C4B-NB	3.16	1.42	1.37
17	C	607	CLA	C4B-NB	3.16	1.42	1.37
17	B	601	CLA	C4B-NB	3.16	1.42	1.37
17	A	404	CLA	C4B-NB	3.16	1.42	1.37
17	B	616	CLA	C4B-NB	3.15	1.42	1.37
17	A	402	CLA	C4B-NB	3.14	1.42	1.37
17	C	603	CLA	C4B-NB	3.12	1.42	1.37
17	B	614	CLA	C4B-NB	3.09	1.41	1.37
17	C	608	CLA	C4B-NB	3.08	1.41	1.37
17	B	605	CLA	C4B-NB	3.06	1.41	1.37
17	B	610	CLA	C4B-NB	3.03	1.41	1.37
24	E	101	HEM	CAC-C3C	2.97	1.55	1.47
17	C	613	CLA	C1B-C2B	2.96	1.50	1.43
17	B	605	CLA	C1B-C2B	2.93	1.50	1.43
24	E	101	HEM	CAB-C3B	2.91	1.55	1.47
17	A	404	CLA	C1B-C2B	2.88	1.49	1.43
17	B	607	CLA	C1B-C2B	2.84	1.49	1.43
17	B	615	CLA	C1B-C2B	2.82	1.49	1.43
24	E	101	HEM	FE-NC	2.81	2.04	1.95
17	B	611	CLA	C1B-C2B	2.81	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	608	CLA	C1B-C2B	2.80	1.49	1.43
17	B	614	CLA	C1B-C2B	2.78	1.49	1.43
17	B	613	CLA	C1B-C2B	2.78	1.49	1.43
17	C	610	CLA	C1B-C2B	2.78	1.49	1.43
17	C	603	CLA	C1B-C2B	2.77	1.49	1.43
17	C	604	CLA	C1B-C2B	2.77	1.49	1.43
17	B	602	CLA	C1B-C2B	2.77	1.49	1.43
17	B	609	CLA	C1B-C2B	2.77	1.49	1.43
17	C	611	CLA	C1B-C2B	2.76	1.49	1.43
17	C	612	CLA	C1B-C2B	2.76	1.49	1.43
17	B	608	CLA	C1B-C2B	2.75	1.49	1.43
17	D	403	CLA	C1B-C2B	2.74	1.49	1.43
17	C	609	CLA	C1B-C2B	2.74	1.49	1.43
17	C	602	CLA	C1B-C2B	2.74	1.49	1.43
17	C	606	CLA	C1B-C2B	2.74	1.49	1.43
17	B	612	CLA	C1B-C2B	2.73	1.49	1.43
17	C	605	CLA	C1B-C2B	2.72	1.49	1.43
17	B	604	CLA	C1B-C2B	2.71	1.49	1.43
17	B	616	CLA	C1B-C2B	2.71	1.49	1.43
17	A	402	CLA	C1B-C2B	2.71	1.49	1.43
17	B	601	CLA	C1B-C2B	2.69	1.49	1.43
17	C	607	CLA	C1B-C2B	2.66	1.49	1.43
17	B	610	CLA	C1B-C2B	2.66	1.49	1.43
17	B	603	CLA	C1B-C2B	2.64	1.49	1.43
22	D	405	PL9	C7-C3	-2.64	1.47	1.51
17	C	614	CLA	C1B-C2B	2.63	1.49	1.43
23	D	412	PHO	CMD-C2D	-2.62	1.46	1.51
17	D	402	CLA	C1B-C2B	2.62	1.49	1.43
17	A	403	CLA	C1B-C2B	2.61	1.49	1.43
17	B	606	CLA	C1B-C2B	2.60	1.49	1.43
17	D	410	CLA	C1B-C2B	2.58	1.49	1.43
23	D	412	PHO	CMC-C2C	-2.56	1.46	1.50
25	X	201	VTQ	C3-C4	2.55	1.53	1.46
25	X	201	VTQ	C10-C3	2.54	1.57	1.51
23	D	411	PHO	CMC-C2C	-2.52	1.46	1.50
23	D	411	PHO	CMB-C2B	-2.50	1.46	1.51
23	D	411	PHO	CMD-C2D	-2.49	1.46	1.51
22	D	405	PL9	C6-C1	-2.45	1.44	1.48
23	D	411	PHO	CAC-C3C	-2.43	1.47	1.51
23	D	412	PHO	CMB-C2B	-2.40	1.46	1.51
23	D	412	PHO	CAC-C3C	-2.39	1.47	1.51
17	C	614	CLA	C3B-C4B	2.36	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	411	PHO	C3D-C4D	2.35	1.44	1.41
17	D	410	CLA	C3B-C4B	2.35	1.49	1.42
17	B	612	CLA	C3B-C4B	2.34	1.49	1.42
17	C	613	CLA	C3B-C4B	2.33	1.49	1.42
17	B	613	CLA	C3B-C4B	2.32	1.49	1.42
23	D	412	PHO	C3D-C4D	2.31	1.44	1.41
22	D	405	PL9	C53-C6	-2.31	1.46	1.50
17	C	610	CLA	C3B-C4B	2.31	1.49	1.42
17	A	402	CLA	C3B-C4B	2.30	1.49	1.42
17	B	616	CLA	C3B-C4B	2.30	1.49	1.42
17	C	609	CLA	C3B-C4B	2.30	1.49	1.42
17	C	605	CLA	C3B-C4B	2.29	1.49	1.42
17	B	602	CLA	C3B-C4B	2.29	1.49	1.42
17	C	606	CLA	C3B-C4B	2.29	1.49	1.42
17	C	602	CLA	C3B-C4B	2.28	1.49	1.42
17	C	611	CLA	C3B-C4B	2.28	1.49	1.42
17	B	614	CLA	C3B-C4B	2.28	1.49	1.42
17	C	608	CLA	C3B-C4B	2.28	1.49	1.42
18	Z	101	BCR	C1-C6	-2.27	1.50	1.53
17	C	612	CLA	C3B-C4B	2.27	1.49	1.42
19	C	621	LMG	O1-C1	2.26	1.44	1.40
17	B	606	CLA	C3B-C4B	2.26	1.49	1.42
17	B	607	CLA	C3B-C4B	2.26	1.49	1.42
18	C	615	BCR	C30-C25	-2.26	1.50	1.53
17	A	403	CLA	C3B-C4B	2.25	1.49	1.42
17	B	609	CLA	C3B-C4B	2.25	1.49	1.42
17	C	604	CLA	C3B-C4B	2.24	1.49	1.42
17	B	608	CLA	C3B-C4B	2.24	1.49	1.42
18	A	405	BCR	C30-C25	-2.24	1.50	1.53
17	B	603	CLA	C3B-C4B	2.24	1.49	1.42
17	C	607	CLA	C3B-C4B	2.23	1.49	1.42
17	B	604	CLA	C3B-C4B	2.23	1.49	1.42
18	C	616	BCR	C1-C6	-2.22	1.50	1.53
17	B	615	CLA	C3B-C4B	2.22	1.49	1.42
17	B	611	CLA	C3B-C4B	2.21	1.49	1.42
17	D	402	CLA	C3B-C4B	2.21	1.49	1.42
17	D	403	CLA	C3B-C4B	2.21	1.49	1.42
17	B	610	CLA	C3B-C4B	2.20	1.49	1.42
18	B	617	BCR	C30-C25	-2.20	1.51	1.53
17	C	607	CLA	CMB-C2B	-2.19	1.46	1.50
17	B	601	CLA	C3B-C4B	2.19	1.49	1.42
25	X	201	VTQ	C5-C4	2.18	1.54	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	603	CLA	CMB-C2B	-2.17	1.46	1.50
17	C	603	CLA	C3B-C4B	2.17	1.49	1.42
17	C	608	CLA	CHC-C1C	2.17	1.42	1.38
17	B	613	CLA	CHC-C1C	2.16	1.42	1.38
17	D	402	CLA	CHC-C1C	2.15	1.42	1.38
17	B	605	CLA	C3B-C4B	2.15	1.49	1.42
17	C	602	CLA	CHC-C1C	2.14	1.42	1.38
17	A	404	CLA	C3B-C4B	2.14	1.49	1.42
17	B	612	CLA	CMD-C2D	-2.14	1.46	1.50
17	B	602	CLA	CHC-C1C	2.13	1.42	1.38
17	C	611	CLA	CHC-C1C	2.12	1.42	1.38
17	A	402	CLA	CMD-C2D	-2.12	1.46	1.50
17	C	605	CLA	CHC-C1C	2.11	1.42	1.38
17	C	603	CLA	CMB-C2B	-2.11	1.46	1.50
17	B	606	CLA	CMD-C2D	-2.10	1.46	1.50
17	C	602	CLA	CMD-C2D	-2.10	1.46	1.50
17	D	402	CLA	CMD-C2D	-2.10	1.46	1.50
17	B	601	CLA	CMD-C2D	-2.10	1.46	1.50
17	B	602	CLA	CMD-C2D	-2.10	1.46	1.50
17	C	612	CLA	CMB-C2B	-2.10	1.46	1.50
17	B	612	CLA	CMB-C2B	-2.09	1.46	1.50
17	C	611	CLA	CMD-C2D	-2.09	1.46	1.50
17	A	404	CLA	CMD-C2D	-2.09	1.46	1.50
17	B	603	CLA	CMD-C2D	-2.09	1.46	1.50
17	D	410	CLA	CMB-C2B	-2.09	1.46	1.50
17	B	608	CLA	CMD-C2D	-2.09	1.46	1.50
17	A	402	CLA	CHC-C1C	2.09	1.42	1.38
17	C	609	CLA	CHC-C1C	2.08	1.42	1.38
17	A	403	CLA	CMD-C2D	-2.08	1.46	1.50
17	B	616	CLA	CHC-C1C	2.07	1.42	1.38
17	C	608	CLA	CMD-C2D	-2.07	1.46	1.50
17	C	614	CLA	CMD-C2D	-2.07	1.46	1.50
17	B	605	CLA	CMD-C2D	-2.07	1.46	1.50
17	C	610	CLA	CMD-C2D	-2.07	1.46	1.50
17	B	609	CLA	CMD-C2D	-2.07	1.46	1.50
17	C	606	CLA	CHC-C1C	2.07	1.42	1.38
17	A	403	CLA	CMB-C2B	-2.07	1.46	1.50
17	B	614	CLA	CMD-C2D	-2.06	1.46	1.50
17	C	603	CLA	CMD-C2D	-2.06	1.46	1.50
17	B	607	CLA	CHC-C1C	2.06	1.42	1.38
17	B	601	CLA	CHC-C1C	2.06	1.42	1.38
17	B	613	CLA	CMD-C2D	-2.06	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	605	CLA	CMD-C2D	-2.06	1.46	1.50
17	C	612	CLA	CHC-C1C	2.06	1.42	1.38
17	B	601	CLA	CMB-C2B	-2.06	1.46	1.50
17	B	604	CLA	CMD-C2D	-2.06	1.46	1.50
25	X	201	VTQ	O1-C4	-2.05	1.18	1.23
17	D	403	CLA	CMD-C2D	-2.05	1.46	1.50
17	B	611	CLA	CMD-C2D	-2.05	1.46	1.50
17	C	607	CLA	CMD-C2D	-2.05	1.46	1.50
17	D	410	CLA	CHC-C1C	2.05	1.42	1.38
17	A	403	CLA	CHC-C1C	2.05	1.42	1.38
17	C	606	CLA	CMD-C2D	-2.05	1.46	1.50
17	B	610	CLA	CMD-C2D	-2.04	1.46	1.50
18	D	404	BCR	C30-C25	-2.04	1.51	1.53
17	B	612	CLA	CHC-C1C	2.04	1.42	1.38
17	B	606	CLA	CMB-C2B	-2.04	1.46	1.50
17	C	609	CLA	CMD-C2D	-2.04	1.46	1.50
17	B	616	CLA	CMD-C2D	-2.04	1.46	1.50
17	C	602	CLA	CMB-C2B	-2.04	1.46	1.50
17	C	614	CLA	CHC-C1C	2.04	1.42	1.38
17	B	615	CLA	CMB-C2B	-2.04	1.46	1.50
24	E	101	HEM	CMB-C2B	2.04	1.54	1.50
17	B	607	CLA	CMD-C2D	-2.03	1.46	1.50
17	B	614	CLA	CHC-C1C	2.03	1.42	1.38
17	B	604	CLA	CMB-C2B	-2.03	1.46	1.50
17	C	613	CLA	CHC-C1C	2.03	1.42	1.38
25	X	201	VTQ	C6-C7	2.03	1.54	1.47
17	C	604	CLA	CMD-C2D	-2.03	1.46	1.50
17	A	402	CLA	CMB-C2B	-2.02	1.46	1.50
17	B	603	CLA	CHC-C1C	2.02	1.42	1.38
17	B	615	CLA	CMD-C2D	-2.02	1.46	1.50
17	C	609	CLA	CMB-C2B	-2.02	1.46	1.50
24	E	101	HEM	CMC-C2C	2.01	1.54	1.50
18	B	619	BCR	C1-C6	-2.01	1.51	1.53
17	C	605	CLA	CMB-C2B	-2.01	1.46	1.50
17	B	607	CLA	CMB-C2B	-2.01	1.46	1.50
17	D	403	CLA	CMB-C2B	-2.01	1.46	1.50
17	D	410	CLA	CMD-C2D	-2.00	1.46	1.50
17	B	608	CLA	CHC-C1C	2.00	1.42	1.38
17	B	604	CLA	CHC-C1C	2.00	1.42	1.38
17	C	612	CLA	CMD-C2D	-2.00	1.46	1.50
24	E	101	HEM	CMA-C3A	2.00	1.54	1.50
17	C	612	CLA	CMC-C2C	-2.00	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	610	CLA	CHC-C1C	2.00	1.42	1.38

All (434) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	411	PHO	C4D-CHA-CBD	-6.13	105.52	108.45
18	C	615	BCR	C3-C4-C5	-5.92	103.49	114.06
23	D	412	PHO	C4D-CHA-CBD	-5.79	105.68	108.45
18	C	615	BCR	C30-C25-C26	-5.71	114.84	122.64
17	D	402	CLA	C4A-NA-C1A	5.50	109.19	106.68
21	D	401	BCT	O2-C-O1	5.50	133.74	119.68
17	C	603	CLA	C4A-NA-C1A	5.44	109.16	106.68
17	C	608	CLA	C4A-NA-C1A	5.21	109.06	106.68
17	B	612	CLA	C4A-NA-C1A	5.20	109.05	106.68
22	D	405	PL9	C7-C3-C4	5.20	121.19	116.91
18	K	101	BCR	C30-C25-C26	-5.14	115.62	122.64
18	B	619	BCR	C30-C25-C26	-5.13	115.62	122.64
18	Z	101	BCR	C33-C5-C6	-5.04	118.98	124.48
18	A	405	BCR	C30-C25-C26	-4.95	115.87	122.64
18	H	101	BCR	C7-C8-C9	-4.92	118.95	126.23
17	B	610	CLA	C4A-NA-C1A	4.91	108.92	106.68
17	B	613	CLA	C4A-NA-C1A	4.91	108.92	106.68
17	C	611	CLA	C4A-NA-C1A	4.77	108.86	106.68
18	H	101	BCR	C28-C27-C26	-4.75	105.59	114.06
18	Z	101	BCR	C1-C6-C5	-4.66	116.27	122.64
18	H	101	BCR	C3-C4-C5	-4.66	105.75	114.06
17	C	610	CLA	C4A-NA-C1A	4.62	108.79	106.68
17	C	602	CLA	C4A-NA-C1A	4.58	108.77	106.68
17	C	614	CLA	C4A-NA-C1A	4.56	108.76	106.68
17	B	602	CLA	C4A-NA-C1A	4.55	108.75	106.68
17	B	607	CLA	C4A-NA-C1A	4.54	108.75	106.68
18	D	404	BCR	C30-C25-C26	-4.54	116.43	122.64
17	C	605	CLA	C4A-NA-C1A	4.52	108.74	106.68
17	C	613	CLA	C4A-NA-C1A	4.52	108.74	106.68
18	D	404	BCR	C1-C6-C5	-4.50	116.48	122.64
17	D	403	CLA	C4A-NA-C1A	4.46	108.72	106.68
17	B	616	CLA	C4A-NA-C1A	4.43	108.70	106.68
18	C	616	BCR	C28-C27-C26	-4.41	106.19	114.06
18	K	101	BCR	C1-C6-C5	-4.39	116.63	122.64
17	C	612	CLA	C4A-NA-C1A	4.39	108.68	106.68
17	B	611	CLA	C4A-NA-C1A	4.39	108.68	106.68
17	B	606	CLA	C4A-NA-C1A	4.34	108.66	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	615	CLA	C4A-NA-C1A	4.33	108.65	106.68
18	K	101	BCR	C3-C4-C5	-4.30	106.39	114.06
17	B	605	CLA	C4A-NA-C1A	4.26	108.62	106.68
17	A	403	CLA	C4A-NA-C1A	4.25	108.62	106.68
17	C	609	CLA	C4A-NA-C1A	4.25	108.62	106.68
17	B	601	CLA	C4A-NA-C1A	4.24	108.61	106.68
17	A	404	CLA	C4A-NA-C1A	4.23	108.61	106.68
18	B	617	BCR	C1-C6-C5	-4.20	116.89	122.64
17	C	607	CLA	C4A-NA-C1A	4.20	108.59	106.68
20	D	407	LHG	O7-C7-C8	4.20	120.56	111.48
17	D	410	CLA	C4A-NA-C1A	4.13	108.56	106.68
18	C	615	BCR	C33-C5-C6	-4.11	120.00	124.48
18	B	618	BCR	C28-C27-C26	-4.07	106.80	114.06
20	K	103	LHG	O7-C7-C8	4.04	120.22	111.48
18	A	405	BCR	C3-C4-C5	-4.02	106.90	114.06
18	D	404	BCR	C3-C4-C5	-4.01	106.91	114.06
20	D	406	LHG	O7-C7-C8	4.01	120.15	111.48
22	D	405	PL9	C7-C3-C2	-4.00	118.67	123.39
20	D	409	LHG	O7-C7-C8	4.00	120.12	111.48
17	B	614	CLA	C4A-NA-C1A	3.97	108.49	106.68
19	C	621	LMG	O7-C10-C11	3.95	120.03	111.48
18	K	101	BCR	C37-C22-C23	3.92	124.08	118.09
18	C	616	BCR	C20-C21-C22	-3.92	121.78	127.28
23	D	412	PHO	C2B-C1B-NB	-3.91	106.60	109.43
26	C	618	DGD	O2G-C1B-C2B	3.88	119.87	111.48
18	C	615	BCR	C1-C6-C7	3.88	126.16	115.65
18	H	101	BCR	C20-C21-C22	-3.85	121.88	127.28
17	A	402	CLA	C4A-NA-C1A	3.84	108.43	106.68
20	B	621	LHG	O7-C7-C8	3.83	119.78	111.48
18	C	616	BCR	C16-C17-C18	-3.83	121.91	127.28
18	C	615	BCR	C33-C5-C4	3.81	121.72	113.60
18	B	619	BCR	C1-C6-C5	-3.81	117.43	122.64
26	C	617	DGD	O2G-C1B-C2B	3.81	119.72	111.48
18	K	101	BCR	C28-C27-C26	-3.80	107.28	114.06
19	H	102	LMG	O7-C10-C11	3.79	119.69	111.48
18	H	101	BCR	C16-C17-C18	-3.78	121.97	127.28
18	C	616	BCR	C1-C6-C5	-3.75	117.52	122.64
23	D	411	PHO	C2B-C1B-NB	-3.74	106.72	109.43
18	C	615	BCR	C28-C27-C26	-3.73	107.40	114.06
19	K	102	LMG	O7-C10-C11	3.72	119.53	111.48
18	D	404	BCR	C16-C17-C18	-3.72	122.06	127.28
18	B	619	BCR	C28-C27-C26	-3.71	107.43	114.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	617	BCR	C30-C25-C26	-3.69	117.59	122.64
18	B	618	BCR	C37-C22-C23	3.67	123.69	118.09
18	K	101	BCR	C16-C17-C18	-3.66	122.14	127.28
18	B	617	BCR	C36-C18-C19	3.66	123.68	118.09
17	B	603	CLA	C4A-NA-C1A	3.66	108.35	106.68
27	C	620	SQD	O47-C7-C8	3.65	119.37	111.48
26	C	619	DGD	O2G-C1B-C2B	3.64	119.36	111.48
18	B	618	BCR	C20-C21-C22	-3.64	122.17	127.28
17	B	604	CLA	C4A-NA-C1A	3.64	108.34	106.68
18	B	617	BCR	C20-C21-C22	-3.63	122.19	127.28
19	B	620	LMG	O7-C10-C11	3.61	119.29	111.48
18	K	101	BCR	C27-C26-C25	-3.61	117.83	122.70
20	B	622	LHG	O7-C7-C8	3.60	119.27	111.48
18	Z	101	BCR	C33-C5-C4	3.60	121.27	113.60
17	B	608	CLA	C4A-NA-C1A	3.59	108.32	106.68
18	B	619	BCR	C37-C22-C23	3.59	123.57	118.09
18	A	405	BCR	C20-C21-C22	-3.58	122.25	127.28
18	B	619	BCR	C16-C17-C18	-3.58	122.26	127.28
18	B	617	BCR	C37-C22-C23	3.58	123.55	118.09
19	C	601	LMG	O7-C10-C11	3.56	119.19	111.48
18	B	619	BCR	C20-C21-C22	-3.56	122.29	127.28
18	A	405	BCR	C7-C8-C9	-3.55	120.98	126.23
25	X	201	VTQ	C10-C11-C9	-3.55	109.23	118.08
17	C	604	CLA	C4A-NA-C1A	3.52	108.29	106.68
17	D	402	CLA	O2D-CGD-O1D	-3.51	117.01	123.85
18	D	404	BCR	C37-C22-C23	3.51	123.45	118.09
19	D	408	LMG	O7-C10-C11	3.49	119.04	111.48
18	H	101	BCR	C36-C18-C19	3.49	123.42	118.09
18	D	404	BCR	C20-C21-C22	-3.49	122.39	127.28
18	H	101	BCR	C4-C5-C6	-3.48	118.00	122.70
20	B	623	LHG	O7-C7-C8	3.48	119.02	111.48
18	K	101	BCR	C36-C18-C19	3.48	123.41	118.09
18	C	615	BCR	C1-C6-C5	-3.47	117.90	122.64
18	B	619	BCR	C36-C18-C19	3.46	123.37	118.09
18	B	618	BCR	C36-C18-C19	3.45	123.36	118.09
18	D	404	BCR	C27-C26-C25	-3.44	118.06	122.70
18	C	616	BCR	C7-C8-C9	-3.42	121.17	126.23
18	B	618	BCR	C7-C8-C9	-3.41	121.19	126.23
18	Z	101	BCR	C37-C22-C23	3.40	123.29	118.09
18	A	405	BCR	C16-C17-C18	-3.40	122.51	127.28
18	B	618	BCR	C1-C6-C5	-3.38	118.01	122.64
20	L	101	LHG	O7-C7-C8	3.35	118.74	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	618	BCR	C33-C5-C6	-3.35	120.83	124.48
18	C	615	BCR	C4-C5-C6	-3.35	118.18	122.70
18	H	101	BCR	C30-C25-C26	-3.31	118.11	122.64
18	A	405	BCR	C36-C18-C19	3.31	123.15	118.09
18	D	404	BCR	C4-C5-C6	-3.30	118.24	122.70
18	D	404	BCR	C36-C18-C19	3.28	123.10	118.09
18	K	101	BCR	C20-C21-C22	-3.28	122.67	127.28
18	A	405	BCR	C27-C26-C25	-3.27	118.28	122.70
18	H	101	BCR	C37-C22-C23	3.26	123.08	118.09
17	B	609	CLA	C4A-NA-C1A	3.25	108.16	106.68
18	B	618	BCR	C30-C25-C26	-3.23	118.22	122.64
18	B	617	BCR	C3-C4-C5	-3.23	108.30	114.06
18	D	404	BCR	C28-C27-C26	-3.23	108.30	114.06
17	B	606	CLA	O2D-CGD-O1D	-3.18	117.65	123.85
18	Z	101	BCR	C3-C4-C5	-3.18	108.38	114.06
18	C	615	BCR	C37-C22-C23	3.18	122.94	118.09
18	A	405	BCR	C38-C26-C27	3.18	120.37	113.60
18	B	619	BCR	C33-C5-C6	-3.16	121.04	124.48
18	C	615	BCR	C7-C8-C9	-3.13	121.60	126.23
18	H	101	BCR	C11-C10-C9	-3.13	122.88	127.28
18	C	615	BCR	C36-C18-C19	3.11	122.84	118.09
23	D	411	PHO	O1D-CGD-CBD	3.11	129.44	124.72
18	B	618	BCR	C16-C17-C18	-3.11	122.92	127.28
18	A	405	BCR	C1-C6-C5	-3.09	118.41	122.64
18	C	616	BCR	C29-C30-C25	3.09	114.92	110.44
18	A	405	BCR	C38-C26-C25	-3.08	121.12	124.48
18	B	619	BCR	C27-C26-C25	-3.07	118.55	122.70
18	Z	101	BCR	C16-C17-C18	-3.06	122.98	127.28
17	C	606	CLA	C4A-NA-C1A	3.06	108.07	106.68
18	C	616	BCR	C33-C5-C6	-3.05	121.16	124.48
18	Z	101	BCR	C36-C18-C19	3.05	122.74	118.09
18	A	405	BCR	C37-C22-C23	3.04	122.74	118.09
17	B	615	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
18	C	615	BCR	C38-C26-C25	-3.04	121.17	124.48
23	D	412	PHO	O1D-CGD-CBD	3.03	129.31	124.72
17	B	608	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
18	B	617	BCR	C33-C5-C6	-3.02	121.19	124.48
18	B	619	BCR	C7-C8-C9	-3.01	121.78	126.23
18	B	617	BCR	C38-C26-C25	-3.01	121.20	124.48
18	D	404	BCR	C38-C26-C27	3.01	120.00	113.60
17	B	614	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
17	C	613	CLA	O2D-CGD-O1D	-3.00	118.00	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	H	101	BCR	C2-C1-C6	3.00	114.80	110.44
17	C	603	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
18	C	616	BCR	C24-C23-C22	-3.00	121.80	126.23
17	B	611	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
17	A	404	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
18	B	617	BCR	C16-C17-C18	-2.99	123.09	127.28
18	C	616	BCR	C37-C22-C23	2.99	122.65	118.09
17	A	403	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
27	C	620	SQD	O48-C23-C24	2.98	120.92	111.83
17	D	403	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
18	K	101	BCR	C38-C26-C27	2.97	119.92	113.60
17	B	604	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
17	C	606	CLA	O2D-CGD-O1D	-2.96	118.10	123.85
17	D	410	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
18	B	617	BCR	C33-C5-C4	2.94	119.87	113.60
18	Z	101	BCR	C20-C21-C22	-2.94	123.16	127.28
17	B	612	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
17	C	612	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
22	D	405	PL9	C22-C23-C24	-2.90	120.99	127.62
18	C	615	BCR	C27-C26-C25	-2.89	118.80	122.70
18	B	617	BCR	C7-C8-C9	-2.89	121.96	126.23
18	A	405	BCR	C11-C10-C9	-2.88	123.23	127.28
18	K	101	BCR	C33-C5-C6	-2.88	121.34	124.48
18	C	616	BCR	C36-C18-C19	2.88	122.48	118.09
18	B	619	BCR	C38-C26-C27	2.86	119.69	113.60
17	C	605	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
17	C	610	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
18	H	101	BCR	C27-C26-C25	-2.85	118.85	122.70
23	D	411	PHO	O2D-CGD-O1D	-2.85	118.30	123.85
19	C	621	LMG	O8-C28-C29	2.84	120.51	111.83
20	D	407	LHG	O8-C23-C24	2.84	120.50	111.83
17	B	603	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
18	B	619	BCR	C33-C5-C4	2.84	119.64	113.60
17	D	402	CLA	O2D-CGD-CBD	2.84	116.19	111.23
19	C	601	LMG	O8-C28-C29	2.83	120.48	111.83
18	C	615	BCR	C38-C26-C27	2.83	119.64	113.60
17	B	616	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
17	B	602	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
17	B	610	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
17	C	609	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
18	B	617	BCR	C4-C5-C6	-2.82	118.90	122.70
18	H	101	BCR	C1-C6-C5	-2.82	118.79	122.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	C	608	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
17	B	607	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
18	C	615	BCR	C20-C21-C22	-2.81	123.33	127.28
17	C	604	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
20	B	622	LHG	O8-C23-C24	2.79	120.36	111.83
17	C	611	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
18	A	405	BCR	C28-C27-C26	-2.79	109.08	114.06
23	D	411	PHO	C1-C2-C3	-2.79	121.63	126.20
22	D	405	PL9	C40-C39-C41	2.78	120.06	115.23
18	B	618	BCR	C33-C5-C4	2.78	119.53	113.60
18	D	404	BCR	C33-C5-C4	2.78	119.52	113.60
17	B	609	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
23	D	412	PHO	O2D-CGD-O1D	-2.77	118.45	123.85
20	D	409	LHG	C5-O7-C7	-2.77	111.17	117.80
17	C	607	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
17	C	614	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
18	B	617	BCR	C15-C16-C17	-2.75	117.89	123.52
17	B	601	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
17	A	402	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
18	D	404	BCR	C16-C15-C14	-2.72	117.95	123.52
18	C	615	BCR	C16-C17-C18	-2.72	123.46	127.28
17	C	602	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
26	C	617	DGD	O1G-C1A-C2A	2.71	120.11	111.83
17	B	605	CLA	O2D-CGD-O1D	-2.71	118.56	123.85
26	C	618	DGD	O1G-C1A-C2A	2.71	120.10	111.83
18	C	615	BCR	C15-C16-C17	-2.70	118.00	123.52
20	B	623	LHG	O8-C23-C24	2.69	120.04	111.83
18	A	405	BCR	C24-C23-C22	-2.68	122.28	126.23
18	B	618	BCR	C3-C4-C5	-2.67	109.30	114.06
18	C	616	BCR	C16-C15-C14	-2.66	118.07	123.52
20	B	621	LHG	O8-C23-C24	2.66	119.94	111.83
20	L	101	LHG	O8-C23-C24	2.64	119.88	111.83
18	B	619	BCR	C38-C26-C25	-2.63	121.61	124.48
18	C	616	BCR	C11-C10-C9	-2.63	123.59	127.28
18	C	616	BCR	C33-C5-C4	2.62	119.19	113.60
18	H	101	BCR	C38-C26-C27	2.60	119.15	113.60
17	D	403	CLA	C1-C2-C3	-2.60	121.93	126.20
17	B	616	CLA	CHB-C4A-NA	2.59	128.14	124.40
18	B	618	BCR	C37-C22-C21	-2.59	118.62	122.82
18	Z	101	BCR	C29-C30-C25	2.58	114.19	110.44
24	E	101	HEM	C3B-C2B-C1B	2.58	108.35	106.41
18	B	618	BCR	C11-C10-C9	-2.56	123.68	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	101	BCR	C33-C5-C4	2.56	119.05	113.60
17	C	611	CLA	C1-C2-C3	-2.56	122.01	126.20
18	B	617	BCR	C37-C22-C21	-2.55	118.68	122.82
17	B	615	CLA	CHB-C4A-NA	2.55	128.07	124.40
18	B	619	BCR	C4-C5-C6	-2.55	119.26	122.70
18	B	617	BCR	C38-C26-C27	2.54	119.02	113.60
17	C	610	CLA	CHB-C4A-NA	2.54	128.07	124.40
19	B	620	LMG	O8-C28-C29	2.54	119.58	111.83
17	C	613	CLA	CHB-C4A-NA	2.52	128.03	124.40
18	A	405	BCR	C33-C5-C6	-2.51	121.74	124.48
17	B	613	CLA	O2D-CGD-O1D	-2.50	118.97	123.85
18	K	101	BCR	C16-C15-C14	-2.49	118.43	123.52
18	K	101	BCR	C30-C25-C24	2.49	122.40	115.65
18	C	615	BCR	C7-C6-C5	-2.48	115.85	121.56
26	C	617	DGD	O6D-C5D-C6D	2.48	111.60	106.69
24	E	101	HEM	C3B-C4B-NB	-2.48	107.69	109.47
17	C	614	CLA	CMB-C2B-C1B	-2.47	121.65	125.42
17	C	604	CLA	CHB-C4A-NA	2.47	127.97	124.40
18	A	405	BCR	C4-C5-C6	-2.47	119.36	122.70
20	D	406	LHG	O8-C23-C24	2.47	119.36	111.83
18	Z	101	BCR	C7-C8-C9	-2.47	122.58	126.23
18	D	404	BCR	C7-C8-C9	-2.45	122.61	126.23
18	H	101	BCR	C38-C26-C25	-2.45	121.81	124.48
17	B	606	CLA	CHB-C4A-NA	2.45	127.93	124.40
18	Z	101	BCR	C8-C7-C6	-2.45	120.46	127.00
22	D	405	PL9	O2-C1-C6	2.44	124.37	120.48
19	D	408	LMG	O8-C28-C29	2.44	119.28	111.83
18	D	404	BCR	C38-C26-C25	-2.44	121.82	124.48
24	E	101	HEM	C1B-NB-C4B	2.44	108.09	105.21
18	A	405	BCR	C33-C5-C4	2.43	118.79	113.60
20	D	409	LHG	O8-C23-C24	2.43	119.25	111.83
18	B	618	BCR	C15-C16-C17	-2.43	118.55	123.52
22	D	405	PL9	C7-C8-C9	-2.43	122.64	126.83
19	K	102	LMG	O8-C28-C29	2.43	119.24	111.83
18	B	619	BCR	C3-C4-C5	-2.42	109.74	114.06
18	K	101	BCR	C34-C9-C8	2.41	121.77	118.09
17	C	611	CLA	CHB-C4A-NA	2.40	127.87	124.40
18	K	101	BCR	C7-C8-C9	-2.40	122.68	126.23
23	D	411	PHO	CMB-C2B-C3B	2.39	129.47	124.68
18	K	101	BCR	C4-C5-C6	-2.39	119.47	122.70
18	B	619	BCR	C30-C25-C24	2.39	122.13	115.65
17	C	602	CLA	C3B-C4B-NB	-2.38	108.41	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	C	608	CLA	C3B-C4B-NB	-2.37	108.41	110.53
18	B	618	BCR	C15-C14-C13	-2.37	123.95	127.28
18	B	617	BCR	C15-C14-C13	-2.36	123.96	127.28
17	B	612	CLA	CHB-C4A-NA	2.36	127.81	124.40
18	H	101	BCR	C24-C23-C22	-2.36	122.74	126.23
18	H	101	BCR	C16-C15-C14	-2.36	118.69	123.52
24	E	101	HEM	C4D-ND-C1D	2.36	108.00	105.21
18	Z	101	BCR	C1-C6-C7	2.35	122.03	115.65
17	B	613	CLA	CHB-C4A-NA	2.35	127.79	124.40
17	B	602	CLA	C3B-C4B-NB	-2.35	108.43	110.53
18	A	405	BCR	C15-C16-C17	-2.35	118.71	123.52
17	B	604	CLA	CHB-C4A-NA	2.34	127.78	124.40
17	B	609	CLA	CHB-C4A-NA	2.34	127.78	124.40
17	B	607	CLA	CHB-C4A-NA	2.33	127.76	124.40
17	C	606	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
17	B	610	CLA	CHB-C4A-NA	2.33	127.76	124.40
18	Z	101	BCR	C15-C14-C13	-2.33	124.01	127.28
18	C	616	BCR	C4-C5-C6	-2.32	119.57	122.70
22	D	405	PL9	C20-C19-C21	2.32	119.25	115.23
18	H	101	BCR	C31-C1-C6	-2.32	106.61	110.24
18	C	616	BCR	C27-C26-C25	-2.31	119.58	122.70
18	A	405	BCR	C15-C14-C13	-2.31	124.04	127.28
17	B	605	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
18	C	615	BCR	C15-C14-C13	-2.30	124.05	127.28
18	B	618	BCR	C4-C5-C6	-2.30	119.59	122.70
17	A	402	CLA	CHB-C4A-NA	2.30	127.72	124.40
17	C	608	CLA	CHB-C4A-NA	2.30	127.72	124.40
18	B	619	BCR	C37-C22-C21	-2.30	119.09	122.82
20	K	103	LHG	O8-C23-C24	2.29	118.82	111.83
17	D	403	CLA	CHB-C4A-NA	2.29	127.71	124.40
26	C	619	DGD	O1G-C1A-C2A	2.29	118.80	111.83
17	B	616	CLA	C3B-C4B-NB	-2.28	108.49	110.53
17	B	603	CLA	CHB-C4A-NA	2.28	127.69	124.40
17	B	614	CLA	CHB-C4A-NA	2.28	127.69	124.40
17	C	612	CLA	CHB-C4A-NA	2.28	127.69	124.40
18	Z	101	BCR	C4-C5-C6	-2.28	119.62	122.70
22	D	405	PL9	O1-C4-C3	-2.28	118.33	120.73
18	B	617	BCR	C27-C26-C25	-2.27	119.64	122.70
18	B	619	BCR	C36-C18-C17	-2.27	119.14	122.82
18	H	101	BCR	C36-C18-C17	-2.27	119.14	122.82
17	C	603	CLA	CHB-C4A-NA	2.26	127.67	124.40
20	D	407	LHG	C5-O7-C7	-2.26	112.39	117.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	H	102	LMG	O8-C28-C29	2.25	118.70	111.83
17	C	602	CLA	CHB-C4A-NA	2.25	127.65	124.40
17	C	612	CLA	C3B-C4B-NB	-2.25	108.52	110.53
17	C	609	CLA	CHB-C4A-NA	2.25	127.64	124.40
17	A	404	CLA	C1-C2-C3	-2.24	122.52	126.20
17	B	613	CLA	C1-C2-C3	-2.23	122.54	126.20
22	D	405	PL9	C32-C33-C34	-2.23	122.51	127.62
17	B	605	CLA	CHB-C4A-NA	2.23	127.62	124.40
17	C	609	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
17	B	611	CLA	CHB-C4A-NA	2.23	127.61	124.40
17	B	615	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
17	B	603	CLA	C3B-C4B-NB	-2.21	108.56	110.53
22	D	405	PL9	C12-C13-C14	-2.21	122.57	127.62
17	B	611	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
17	C	607	CLA	CHB-C4A-NA	2.20	127.57	124.40
17	A	404	CLA	CHB-C4A-NA	2.20	127.57	124.40
17	C	607	CLA	C3B-C4B-NB	-2.19	108.57	110.53
18	B	618	BCR	C36-C18-C17	-2.19	119.27	122.82
17	C	604	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
18	D	404	BCR	C10-C11-C12	-2.19	116.86	123.20
17	B	608	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
18	B	618	BCR	C27-C26-C25	-2.19	119.75	122.70
23	D	411	PHO	O2A-CGA-O1A	-2.19	118.16	123.63
17	B	607	CLA	C3B-C4B-NB	-2.19	108.58	110.53
17	B	612	CLA	C3B-C4B-NB	-2.18	108.58	110.53
17	C	612	CLA	C1-C2-C3	-2.18	122.63	126.20
18	Z	101	BCR	C24-C25-C26	2.18	126.58	121.56
17	C	603	CLA	C1-C2-C3	-2.18	122.63	126.20
27	C	620	SQD	C45-O47-C7	-2.18	112.58	117.80
17	B	601	CLA	CHB-C4A-NA	2.18	127.54	124.40
18	B	617	BCR	C28-C27-C26	-2.17	110.18	114.06
17	C	606	CLA	C3B-C4B-NB	-2.17	108.59	110.53
18	C	615	BCR	C2-C1-C6	2.17	113.59	110.44
17	C	614	CLA	CHB-C4A-NA	2.17	127.53	124.40
18	D	404	BCR	C1-C6-C7	2.17	121.53	115.65
18	C	615	BCR	C23-C24-C25	-2.17	121.21	127.00
22	D	405	PL9	O2-C1-C2	-2.16	116.91	121.83
17	B	610	CLA	C3B-C4B-NB	-2.16	108.60	110.53
17	B	602	CLA	CHB-C4A-NA	2.16	127.52	124.40
17	C	606	CLA	CHB-C4A-NA	2.16	127.52	124.40
17	C	605	CLA	CHB-C4A-NA	2.16	127.51	124.40
17	B	613	CLA	C3B-C4B-NB	-2.15	108.61	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	617	BCR	C24-C23-C22	-2.15	123.05	126.23
17	B	608	CLA	CHB-C4A-NA	2.15	127.50	124.40
17	D	410	CLA	CHB-C4A-NA	2.15	127.50	124.40
18	B	619	BCR	C11-C10-C9	-2.15	124.27	127.28
17	C	612	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
17	A	403	CLA	CHB-C4A-NA	2.14	127.49	124.40
18	D	404	BCR	C33-C5-C6	-2.14	122.15	124.48
19	C	621	LMG	C8-O7-C10	-2.14	112.68	117.80
21	D	401	BCT	O3-C-O1	-2.13	114.22	119.68
18	D	404	BCR	C12-C13-C14	-2.13	115.66	119.01
17	A	402	CLA	C3B-C4B-NB	-2.13	108.63	110.53
17	C	604	CLA	C4-C3-C5	2.13	118.92	115.23
17	C	614	CLA	CMB-C2B-C3B	2.13	131.55	126.55
18	D	404	BCR	C8-C9-C10	-2.13	115.67	119.01
17	C	614	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
17	C	607	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
18	Z	101	BCR	C15-C16-C17	-2.12	119.19	123.52
22	D	405	PL9	C27-C28-C29	-2.11	122.79	127.62
18	K	101	BCR	C38-C26-C25	-2.11	122.18	124.48
17	A	402	CLA	C1-C2-C3	-2.11	122.74	126.20
17	B	601	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
17	D	410	CLA	O2D-CGD-CBD	2.10	114.90	111.23
17	B	616	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
17	D	410	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
17	B	604	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
18	B	618	BCR	C24-C23-C22	-2.09	123.14	126.23
25	X	201	VTQ	C8-C2-C3	-2.09	121.02	124.45
18	Z	101	BCR	C11-C10-C9	-2.09	124.35	127.28
18	K	101	BCR	C10-C11-C12	-2.08	117.16	123.20
17	C	605	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
18	H	101	BCR	C37-C22-C21	-2.08	119.44	122.82
18	Z	101	BCR	C24-C23-C22	-2.08	123.16	126.23
17	D	410	CLA	C1-C2-C3	-2.07	122.80	126.20
17	B	603	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
18	B	618	BCR	C29-C30-C25	2.07	113.44	110.44
17	D	410	CLA	C3B-C4B-NB	-2.07	108.68	110.53
25	X	201	VTQ	C16-C15-C9	-2.07	109.84	116.10
18	B	619	BCR	C15-C14-C13	-2.06	124.38	127.28
18	C	615	BCR	C11-C10-C9	-2.06	124.39	127.28
17	B	601	CLA	C3B-C4B-NB	-2.06	108.69	110.53
17	D	402	CLA	C3B-C4B-NB	-2.06	108.69	110.53
17	B	602	CLA	O2A-CGA-O1A	-2.05	118.50	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	K	103	LHG	C5-O7-C7	-2.05	112.89	117.80
17	B	606	CLA	O1D-CGD-CBD	2.04	128.55	124.52
17	B	609	CLA	O2A-CGA-O1A	-2.04	118.51	123.63
17	A	403	CLA	O2A-CGA-O1A	-2.04	118.51	123.63
17	B	610	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
18	C	615	BCR	C24-C23-C22	-2.04	123.22	126.23
17	C	602	CLA	C1-C2-C3	-2.04	122.86	126.20
18	B	617	BCR	C1-C6-C7	2.03	121.17	115.65
23	D	412	PHO	CMB-C2B-C3B	2.03	128.75	124.68
18	C	615	BCR	C30-C25-C24	2.03	121.16	115.65
18	Z	101	BCR	C29-C28-C27	-2.03	106.81	111.28
17	B	607	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
18	B	617	BCR	C11-C10-C9	-2.02	124.45	127.28
18	D	404	BCR	C36-C18-C17	-2.02	119.55	122.82
18	K	101	BCR	C37-C22-C21	-2.01	119.55	122.82
17	B	605	CLA	C3B-C4B-NB	-2.01	108.73	110.53
17	C	603	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
17	A	402	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
17	B	606	CLA	C3B-C4B-NB	-2.01	108.73	110.53

All (35) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	B	601	CLA	ND
17	B	602	CLA	ND
17	B	603	CLA	ND
17	B	604	CLA	ND
17	B	605	CLA	ND
17	B	606	CLA	ND
17	B	607	CLA	ND
17	B	608	CLA	ND
17	B	609	CLA	ND
17	B	610	CLA	ND
17	B	611	CLA	ND
17	B	612	CLA	ND
17	B	613	CLA	ND
17	B	614	CLA	ND
17	B	615	CLA	ND
17	B	616	CLA	ND
17	D	402	CLA	ND
17	D	403	CLA	ND
17	D	410	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
17	C	602	CLA	ND
17	C	603	CLA	ND
17	C	604	CLA	ND
17	C	605	CLA	ND
17	C	606	CLA	ND
17	C	607	CLA	ND
17	C	608	CLA	ND
17	C	609	CLA	ND
17	C	610	CLA	ND
17	C	611	CLA	ND
17	C	612	CLA	ND
17	C	613	CLA	ND
17	C	614	CLA	ND
17	A	402	CLA	ND
17	A	403	CLA	ND
17	A	404	CLA	ND

All (646) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	B	601	CLA	CAD-CBD-CGD-O2D
17	B	603	CLA	C1A-C2A-CAA-CBA
17	B	603	CLA	C3A-C2A-CAA-CBA
17	B	603	CLA	CAD-CBD-CGD-O1D
17	B	603	CLA	CAD-CBD-CGD-O2D
17	B	604	CLA	C1A-C2A-CAA-CBA
17	B	605	CLA	C1A-C2A-CAA-CBA
17	B	606	CLA	CAD-CBD-CGD-O1D
17	B	606	CLA	CAD-CBD-CGD-O2D
17	B	606	CLA	CBD-CGD-O2D-CED
17	B	607	CLA	C1A-C2A-CAA-CBA
17	B	607	CLA	C3A-C2A-CAA-CBA
17	B	608	CLA	C1A-C2A-CAA-CBA
17	B	608	CLA	CAD-CBD-CGD-O1D
17	B	608	CLA	CAD-CBD-CGD-O2D
17	B	609	CLA	CAD-CBD-CGD-O1D
17	B	609	CLA	CAD-CBD-CGD-O2D
17	B	610	CLA	CHA-CBD-CGD-O1D
17	B	610	CLA	CHA-CBD-CGD-O2D
17	B	611	CLA	CBD-CGD-O2D-CED
17	B	613	CLA	CHA-CBD-CGD-O1D
17	B	613	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	614	CLA	CAD-CBD-CGD-O1D
17	B	614	CLA	CAD-CBD-CGD-O2D
17	B	616	CLA	CHA-CBD-CGD-O1D
17	B	616	CLA	CHA-CBD-CGD-O2D
17	D	402	CLA	CAD-CBD-CGD-O1D
17	D	402	CLA	CAD-CBD-CGD-O2D
17	D	403	CLA	C1A-C2A-CAA-CBA
17	D	403	CLA	C3A-C2A-CAA-CBA
17	D	403	CLA	CAD-CBD-CGD-O1D
17	D	403	CLA	CAD-CBD-CGD-O2D
17	C	602	CLA	CAD-CBD-CGD-O1D
17	C	602	CLA	CAD-CBD-CGD-O2D
17	C	603	CLA	CBD-CGD-O2D-CED
17	C	604	CLA	C1A-C2A-CAA-CBA
17	C	604	CLA	CAD-CBD-CGD-O1D
17	C	604	CLA	CAD-CBD-CGD-O2D
17	C	606	CLA	C1A-C2A-CAA-CBA
17	C	607	CLA	CAD-CBD-CGD-O1D
17	C	607	CLA	CAD-CBD-CGD-O2D
17	C	607	CLA	CBD-CGD-O2D-CED
17	C	608	CLA	C1A-C2A-CAA-CBA
17	C	608	CLA	C3A-C2A-CAA-CBA
17	C	610	CLA	CHA-CBD-CGD-O1D
17	C	610	CLA	CHA-CBD-CGD-O2D
17	C	612	CLA	CAD-CBD-CGD-O1D
17	C	612	CLA	CAD-CBD-CGD-O2D
17	C	613	CLA	CHA-CBD-CGD-O1D
17	C	613	CLA	CHA-CBD-CGD-O2D
17	C	614	CLA	CBD-CGD-O2D-CED
17	A	404	CLA	CHA-CBD-CGD-O1D
17	A	404	CLA	CHA-CBD-CGD-O2D
18	B	617	BCR	C1-C6-C7-C8
18	B	617	BCR	C5-C6-C7-C8
18	B	617	BCR	C23-C24-C25-C26
18	B	617	BCR	C23-C24-C25-C30
18	B	618	BCR	C1-C6-C7-C8
18	B	618	BCR	C5-C6-C7-C8
18	B	618	BCR	C23-C24-C25-C26
18	B	619	BCR	C1-C6-C7-C8
18	B	619	BCR	C5-C6-C7-C8
18	B	619	BCR	C23-C24-C25-C26
18	D	404	BCR	C1-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	D	404	BCR	C5-C6-C7-C8
18	D	404	BCR	C23-C24-C25-C26
18	D	404	BCR	C23-C24-C25-C30
18	H	101	BCR	C1-C6-C7-C8
18	H	101	BCR	C5-C6-C7-C8
18	H	101	BCR	C23-C24-C25-C26
18	K	101	BCR	C5-C6-C7-C8
18	K	101	BCR	C23-C24-C25-C26
18	Z	101	BCR	C5-C6-C7-C8
18	Z	101	BCR	C23-C24-C25-C26
18	C	616	BCR	C5-C6-C7-C8
18	A	405	BCR	C5-C6-C7-C8
18	A	405	BCR	C23-C24-C25-C26
18	A	405	BCR	C23-C24-C25-C30
19	C	621	LMG	O6-C1-O1-C7
20	B	621	LHG	C3-O3-P-O4
20	B	621	LHG	C3-O3-P-O6
20	B	621	LHG	C4-O6-P-O3
20	B	621	LHG	C4-O6-P-O4
20	B	622	LHG	C4-O6-P-O4
20	B	623	LHG	C4-O6-P-O3
20	B	623	LHG	C4-O6-P-O4
20	D	406	LHG	C3-O3-P-O4
20	D	406	LHG	C3-O3-P-O6
20	D	406	LHG	C4-O6-P-O3
20	D	406	LHG	C4-O6-P-O4
20	D	409	LHG	C4-O6-P-O3
20	K	103	LHG	C3-O3-P-O5
20	K	103	LHG	C3-O3-P-O6
20	L	101	LHG	C3-O3-P-O5
25	X	201	VTQ	C16-C15-C9-C11
26	C	618	DGD	C4D-C5D-C6D-O5D
17	C	603	CLA	O1D-CGD-O2D-CED
17	B	609	CLA	O1D-CGD-O2D-CED
17	B	604	CLA	CBD-CGD-O2D-CED
17	B	609	CLA	CBD-CGD-O2D-CED
17	C	604	CLA	CBD-CGD-O2D-CED
17	C	605	CLA	CBD-CGD-O2D-CED
17	A	402	CLA	CBD-CGD-O2D-CED
17	B	607	CLA	O1A-CGA-O2A-C1
17	B	616	CLA	O1A-CGA-O2A-C1
17	C	607	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	C	604	CLA	O1D-CGD-O2D-CED
17	B	616	CLA	CBA-CGA-O2A-C1
23	D	411	PHO	CBA-CGA-O2A-C1
17	D	410	CLA	O1A-CGA-O2A-C1
17	C	607	CLA	O1A-CGA-O2A-C1
23	D	411	PHO	O1A-CGA-O2A-C1
17	B	606	CLA	O1D-CGD-O2D-CED
17	B	611	CLA	O1D-CGD-O2D-CED
17	C	614	CLA	O1D-CGD-O2D-CED
17	B	601	CLA	CBD-CGD-O2D-CED
17	A	404	CLA	C3-C5-C6-C7
17	B	605	CLA	CBA-CGA-O2A-C1
17	B	607	CLA	CBA-CGA-O2A-C1
17	D	410	CLA	CBA-CGA-O2A-C1
17	C	606	CLA	CBA-CGA-O2A-C1
17	C	607	CLA	CBA-CGA-O2A-C1
17	C	611	CLA	CBD-CGD-O2D-CED
17	B	606	CLA	O1A-CGA-O2A-C1
17	C	604	CLA	C4-C3-C5-C6
17	C	604	CLA	C2-C3-C5-C6
17	D	402	CLA	C3-C5-C6-C7
17	C	605	CLA	C3-C5-C6-C7
17	B	606	CLA	CBA-CGA-O2A-C1
17	C	609	CLA	CBA-CGA-O2A-C1
17	B	605	CLA	O1A-CGA-O2A-C1
17	B	611	CLA	O1A-CGA-O2A-C1
17	C	609	CLA	O1A-CGA-O2A-C1
17	C	612	CLA	O1A-CGA-O2A-C1
17	A	402	CLA	O1D-CGD-O2D-CED
17	B	603	CLA	C3-C5-C6-C7
23	D	412	PHO	C3-C5-C6-C7
17	B	603	CLA	CBD-CGD-O2D-CED
17	C	605	CLA	O1D-CGD-O2D-CED
17	B	601	CLA	CBA-CGA-O2A-C1
17	B	602	CLA	CBA-CGA-O2A-C1
17	C	614	CLA	CBA-CGA-O2A-C1
17	C	606	CLA	O1A-CGA-O2A-C1
20	D	409	LHG	C8-C7-O7-C5
17	C	614	CLA	O1A-CGA-O2A-C1
22	D	405	PL9	C47-C48-C49-C51
17	B	604	CLA	O1D-CGD-O2D-CED
17	C	612	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	611	CLA	CBA-CGA-O2A-C1
17	C	612	CLA	CBA-CGA-O2A-C1
17	B	615	CLA	C4-C3-C5-C6
17	B	602	CLA	O1A-CGA-O2A-C1
17	B	601	CLA	O1A-CGA-O2A-C1
17	B	615	CLA	CBD-CGD-O2D-CED
17	D	403	CLA	CBD-CGD-O2D-CED
17	B	601	CLA	O1D-CGD-O2D-CED
20	D	409	LHG	O9-C7-O7-C5
20	L	101	LHG	C1-C2-C3-O3
17	C	613	CLA	CBA-CGA-O2A-C1
19	C	621	LMG	C2-C1-O1-C7
20	L	101	LHG	O2-C2-C3-O3
17	C	603	CLA	C2A-CAA-CBA-CGA
17	C	612	CLA	C2A-CAA-CBA-CGA
17	C	613	CLA	O1A-CGA-O2A-C1
26	C	618	DGD	O6D-C5D-C6D-O5D
17	C	605	CLA	CBA-CGA-O2A-C1
17	C	613	CLA	C2-C1-O2A-CGA
17	C	612	CLA	C15-C16-C17-C18
22	D	405	PL9	C42-C43-C44-C46
23	D	412	PHO	CBA-CGA-O2A-C1
17	C	614	CLA	C10-C11-C12-C13
17	C	611	CLA	O1D-CGD-O2D-CED
17	B	605	CLA	C13-C15-C16-C17
17	D	402	CLA	C13-C15-C16-C17
17	C	602	CLA	C13-C15-C16-C17
25	X	201	VTQ	C16-C15-C9-C14
17	B	611	CLA	C2A-CAA-CBA-CGA
17	B	616	CLA	C2A-CAA-CBA-CGA
17	D	410	CLA	C2A-CAA-CBA-CGA
17	C	609	CLA	C2A-CAA-CBA-CGA
17	B	602	CLA	C10-C11-C12-C13
17	C	611	CLA	C10-C11-C12-C13
17	D	403	CLA	C3-C5-C6-C7
17	B	611	CLA	C5-C6-C7-C8
17	B	612	CLA	C13-C15-C16-C17
17	C	606	CLA	C8-C10-C11-C12
17	B	601	CLA	C10-C11-C12-C13
22	D	405	PL9	C47-C48-C49-C50
25	X	201	VTQ	C15-C16-C17-C18
17	C	605	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	603	CLA	O1D-CGD-O2D-CED
17	A	403	CLA	CBA-CGA-O2A-C1
23	D	412	PHO	O1A-CGA-O2A-C1
17	B	605	CLA	C2A-CAA-CBA-CGA
17	B	613	CLA	CBA-CGA-O2A-C1
17	C	602	CLA	CBA-CGA-O2A-C1
17	C	610	CLA	CBA-CGA-O2A-C1
17	A	402	CLA	CBA-CGA-O2A-C1
17	B	601	CLA	C5-C6-C7-C8
17	B	604	CLA	C15-C16-C17-C18
17	B	616	CLA	C10-C11-C12-C13
17	C	602	CLA	C10-C11-C12-C13
17	C	609	CLA	C8-C10-C11-C12
17	D	403	CLA	C15-C16-C17-C18
17	B	615	CLA	C2-C3-C5-C6
17	C	612	CLA	O1D-CGD-O2D-CED
17	D	402	CLA	C10-C11-C12-C13
17	B	607	CLA	CBD-CGD-O2D-CED
17	C	602	CLA	O1A-CGA-O2A-C1
19	C	601	LMG	C11-C12-C13-C14
17	C	609	CLA	C16-C17-C18-C19
17	C	607	CLA	C2A-CAA-CBA-CGA
27	C	620	SQD	C8-C7-O47-C45
17	A	402	CLA	C12-C13-C15-C16
26	C	619	DGD	C3B-C4B-C5B-C6B
20	B	621	LHG	C30-C31-C32-C33
26	C	619	DGD	C6B-C7B-C8B-C9B
17	B	613	CLA	O1A-CGA-O2A-C1
17	C	610	CLA	O1A-CGA-O2A-C1
17	A	403	CLA	O1A-CGA-O2A-C1
17	B	604	CLA	C3A-C2A-CAA-CBA
17	B	608	CLA	C3A-C2A-CAA-CBA
17	B	609	CLA	C3A-C2A-CAA-CBA
17	D	402	CLA	C3A-C2A-CAA-CBA
17	C	606	CLA	C3A-C2A-CAA-CBA
17	B	607	CLA	C5-C6-C7-C8
17	D	403	CLA	O1D-CGD-O2D-CED
17	C	609	CLA	C16-C17-C18-C20
17	A	402	CLA	O1A-CGA-O2A-C1
17	D	403	CLA	CBA-CGA-O2A-C1
18	B	618	BCR	C23-C24-C25-C30
18	B	619	BCR	C23-C24-C25-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	H	101	BCR	C23-C24-C25-C30
18	K	101	BCR	C1-C6-C7-C8
18	K	101	BCR	C23-C24-C25-C30
18	Z	101	BCR	C1-C6-C7-C8
18	Z	101	BCR	C23-C24-C25-C30
18	C	615	BCR	C23-C24-C25-C26
18	C	615	BCR	C23-C24-C25-C30
18	C	616	BCR	C1-C6-C7-C8
18	C	616	BCR	C23-C24-C25-C26
18	C	616	BCR	C23-C24-C25-C30
18	A	405	BCR	C1-C6-C7-C8
20	L	101	LHG	C8-C7-O7-C5
17	B	615	CLA	O1D-CGD-O2D-CED
26	C	618	DGD	C6B-C7B-C8B-C9B
17	C	608	CLA	C14-C13-C15-C16
17	D	403	CLA	O1A-CGA-O2A-C1
17	B	604	CLA	CBA-CGA-O2A-C1
17	B	616	CLA	C13-C15-C16-C17
17	B	608	CLA	C3-C5-C6-C7
17	C	614	CLA	C16-C17-C18-C19
17	C	614	CLA	C16-C17-C18-C20
27	C	620	SQD	C27-C28-C29-C30
17	B	602	CLA	C3-C5-C6-C7
27	C	620	SQD	O49-C7-O47-C45
20	D	407	LHG	O6-C4-C5-O7
19	B	620	LMG	O6-C5-C6-O5
19	C	621	LMG	C11-C10-O7-C8
20	B	623	LHG	C8-C7-O7-C5
17	B	610	CLA	C15-C16-C17-C18
17	D	403	CLA	C10-C11-C12-C13
27	C	620	SQD	O6-C44-C45-O47
17	C	612	CLA	C2-C1-O2A-CGA
17	B	609	CLA	C16-C17-C18-C20
19	K	102	LMG	C15-C16-C17-C18
17	C	611	CLA	C2-C3-C5-C6
17	D	402	CLA	CBD-CGD-O2D-CED
17	C	606	CLA	CBD-CGD-O2D-CED
19	K	102	LMG	O6-C5-C6-O5
17	C	614	CLA	C3-C5-C6-C7
17	B	609	CLA	C1A-C2A-CAA-CBA
17	B	614	CLA	C1A-C2A-CAA-CBA
17	C	602	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	C	607	CLA	C1A-C2A-CAA-CBA
20	D	407	LHG	O6-C4-C5-C6
17	B	601	CLA	C11-C10-C8-C7
17	B	605	CLA	C11-C12-C13-C15
17	B	608	CLA	C11-C12-C13-C15
17	B	610	CLA	C12-C13-C15-C16
17	B	612	CLA	C11-C10-C8-C7
17	C	603	CLA	C12-C13-C15-C16
17	B	604	CLA	C8-C10-C11-C12
17	C	604	CLA	C8-C10-C11-C12
23	D	411	PHO	C4-C3-C5-C6
17	C	607	CLA	C2-C3-C5-C6
17	C	610	CLA	C5-C6-C7-C8
19	H	102	LMG	C11-C10-O7-C8
17	B	601	CLA	C11-C10-C8-C9
20	B	621	LHG	C11-C12-C13-C14
26	C	617	DGD	C4B-C5B-C6B-C7B
20	L	101	LHG	O9-C7-O7-C5
17	B	602	CLA	C5-C6-C7-C8
19	D	408	LMG	O6-C5-C6-O5
20	B	623	LHG	C11-C12-C13-C14
23	D	412	PHO	CHA-CBD-CGD-O1D
23	D	412	PHO	CHA-CBD-CGD-O2D
23	D	411	PHO	C3-C5-C6-C7
17	C	607	CLA	C4-C3-C5-C6
17	C	611	CLA	C4-C3-C5-C6
22	D	405	PL9	C28-C29-C31-C32
22	D	405	PL9	C43-C44-C46-C47
17	C	608	CLA	C8-C10-C11-C12
17	B	604	CLA	O1A-CGA-O2A-C1
17	B	609	CLA	C8-C10-C11-C12
26	C	617	DGD	O6E-C5E-C6E-O5E
17	B	612	CLA	O2A-C1-C2-C3
17	B	615	CLA	O2A-C1-C2-C3
20	D	409	LHG	C26-C27-C28-C29
23	D	411	PHO	C2-C3-C5-C6
19	H	102	LMG	C38-C39-C40-C41
26	C	618	DGD	C2A-C1A-O1G-C1G
17	B	606	CLA	C5-C6-C7-C8
20	B	621	LHG	C11-C10-C9-C8
17	C	606	CLA	C4-C3-C5-C6
22	D	405	PL9	C45-C44-C46-C47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	D	408	LMG	C14-C15-C16-C17
19	C	621	LMG	O9-C10-O7-C8
17	B	605	CLA	C11-C12-C13-C14
17	B	608	CLA	C11-C12-C13-C14
17	B	610	CLA	C14-C13-C15-C16
17	B	612	CLA	C11-C10-C8-C9
17	B	616	CLA	C11-C10-C8-C9
17	C	603	CLA	C14-C13-C15-C16
17	A	402	CLA	C14-C13-C15-C16
25	X	201	VTQ	C21-C22-C23-C1
17	B	616	CLA	C11-C10-C8-C7
17	D	402	CLA	C6-C7-C8-C10
17	C	602	CLA	C11-C12-C13-C15
17	C	605	CLA	C11-C10-C8-C7
17	C	614	CLA	C11-C10-C8-C7
25	X	201	VTQ	C16-C17-C18-C20
17	B	605	CLA	C3A-C2A-CAA-CBA
17	B	610	CLA	C3A-C2A-CAA-CBA
17	C	610	CLA	C3A-C2A-CAA-CBA
17	C	607	CLA	C5-C6-C7-C8
19	H	102	LMG	C35-C36-C37-C38
17	C	604	CLA	CBA-CGA-O2A-C1
20	D	406	LHG	C9-C10-C11-C12
20	B	623	LHG	O9-C7-O7-C5
17	B	604	CLA	C2A-CAA-CBA-CGA
27	C	620	SQD	O6-C44-C45-C46
20	L	101	LHG	C14-C15-C16-C17
17	B	607	CLA	O1D-CGD-O2D-CED
20	D	409	LHG	C23-C24-C25-C26
17	C	602	CLA	C2B-C3B-CAB-CBB
17	B	613	CLA	C10-C11-C12-C13
17	C	611	CLA	C8-C10-C11-C12
17	B	609	CLA	C16-C17-C18-C19
19	H	102	LMG	O7-C8-C9-O8
17	C	606	CLA	C2-C3-C5-C6
20	B	623	LHG	C25-C26-C27-C28
17	C	605	CLA	C11-C10-C8-C9
23	D	412	PHO	C11-C10-C8-C9
20	D	409	LHG	C11-C12-C13-C14
19	C	621	LMG	C34-C35-C36-C37
19	D	408	LMG	C10-C11-C12-C13
17	B	610	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	C	603	CLA	CBA-CGA-O2A-C1
17	C	609	CLA	C5-C6-C7-C8
23	D	411	PHO	C15-C16-C17-C18
17	B	613	CLA	C16-C17-C18-C20
17	D	403	CLA	C12-C13-C15-C16
17	C	608	CLA	C11-C12-C13-C15
17	C	609	CLA	C12-C13-C15-C16
17	C	614	CLA	C12-C13-C15-C16
23	D	411	PHO	C11-C12-C13-C15
23	D	412	PHO	C11-C10-C8-C7
20	D	406	LHG	C11-C10-C9-C8
17	C	607	CLA	C15-C16-C17-C18
17	C	614	CLA	C5-C6-C7-C8
26	C	618	DGD	O1A-C1A-O1G-C1G
19	H	102	LMG	O9-C10-O7-C8
17	C	612	CLA	C3-C5-C6-C7
17	C	607	CLA	O2A-C1-C2-C3
17	C	604	CLA	O1A-CGA-O2A-C1
20	B	622	LHG	C31-C32-C33-C34
20	B	623	LHG	O6-C4-C5-O7
24	E	101	HEM	C4B-C3B-CAB-CBB
17	B	613	CLA	C3-C5-C6-C7
17	C	605	CLA	C15-C16-C17-C18
17	D	403	CLA	C11-C10-C8-C9
17	C	609	CLA	C14-C13-C15-C16
17	C	610	CLA	C14-C13-C15-C16
23	D	411	PHO	C11-C12-C13-C14
25	X	201	VTQ	C16-C17-C18-C19
19	B	620	LMG	C11-C12-C13-C14
17	B	610	CLA	O1A-CGA-O2A-C1
17	C	603	CLA	O1A-CGA-O2A-C1
17	C	609	CLA	C2-C1-O2A-CGA
17	B	610	CLA	C1A-C2A-CAA-CBA
17	D	402	CLA	C1A-C2A-CAA-CBA
17	C	602	CLA	C4B-C3B-CAB-CBB
17	C	606	CLA	O1D-CGD-O2D-CED
17	C	613	CLA	C4-C3-C5-C6
20	B	622	LHG	O6-C4-C5-C6
20	B	623	LHG	O6-C4-C5-C6
20	D	406	LHG	C30-C31-C32-C33
17	B	607	CLA	C11-C12-C13-C15
17	B	611	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	612	CLA	C6-C7-C8-C10
17	B	616	CLA	C11-C12-C13-C15
17	D	402	CLA	C11-C12-C13-C15
17	C	604	CLA	C11-C10-C8-C7
17	C	606	CLA	C12-C13-C15-C16
17	C	609	CLA	C6-C7-C8-C10
17	C	610	CLA	C6-C7-C8-C10
17	C	611	CLA	C6-C7-C8-C10
17	A	404	CLA	C11-C10-C8-C7
17	B	609	CLA	O1A-CGA-O2A-C1
17	B	609	CLA	CBA-CGA-O2A-C1
17	B	605	CLA	CBD-CGD-O2D-CED
17	B	606	CLA	C3A-C2A-CAA-CBA
17	C	604	CLA	C3A-C2A-CAA-CBA
17	C	607	CLA	C3A-C2A-CAA-CBA
17	B	613	CLA	C16-C17-C18-C19
17	C	602	CLA	CBD-CGD-O2D-CED
20	B	622	LHG	O6-C4-C5-O7
27	C	620	SQD	C33-C34-C35-C36
17	D	402	CLA	C6-C7-C8-C9
17	C	614	CLA	C14-C13-C15-C16
23	D	412	PHO	C14-C13-C15-C16
20	B	623	LHG	C31-C32-C33-C34
20	L	101	LHG	C11-C12-C13-C14
19	D	408	LMG	C33-C34-C35-C36
19	K	102	LMG	C17-C18-C19-C20
19	C	601	LMG	O7-C8-C9-O8
26	C	618	DGD	O1G-C1G-C2G-O2G
19	H	102	LMG	C7-C8-C9-O8
17	B	604	CLA	CAD-CBD-CGD-O2D
17	B	605	CLA	CAD-CBD-CGD-O2D
17	B	607	CLA	CAD-CBD-CGD-O2D
17	B	611	CLA	CAD-CBD-CGD-O2D
17	D	402	CLA	O1D-CGD-O2D-CED
17	B	601	CLA	CAD-CBD-CGD-O1D
17	B	604	CLA	CAD-CBD-CGD-O1D
17	B	605	CLA	CAD-CBD-CGD-O1D
17	B	607	CLA	CAD-CBD-CGD-O1D
17	B	611	CLA	CAD-CBD-CGD-O1D
17	C	609	CLA	CHA-CBD-CGD-O1D
17	C	609	CLA	CHA-CBD-CGD-O2D
17	A	403	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	403	CLA	CHA-CBD-CGD-O2D
20	B	622	LHG	C4-O6-P-O3
20	D	407	LHG	C4-O6-P-O4
20	D	409	LHG	C4-O6-P-O5
20	L	101	LHG	C4-O6-P-O5
27	C	620	SQD	C25-C26-C27-C28
17	C	603	CLA	C3-C5-C6-C7
17	A	404	CLA	C11-C12-C13-C15
17	C	607	CLA	C13-C15-C16-C17
22	D	405	PL9	C34-C36-C37-C38
17	B	611	CLA	C16-C17-C18-C19
20	D	409	LHG	C10-C11-C12-C13
17	B	611	CLA	C6-C7-C8-C9
17	C	602	CLA	C14-C13-C15-C16
17	C	604	CLA	C11-C10-C8-C9
17	C	611	CLA	C6-C7-C8-C9
17	C	614	CLA	C11-C10-C8-C9
17	C	610	CLA	C12-C13-C15-C16
23	D	412	PHO	C11-C12-C13-C15
19	C	601	LMG	C28-C29-C30-C31
17	D	402	CLA	C16-C17-C18-C19
17	C	606	CLA	C16-C17-C18-C20
20	D	407	LHG	C33-C34-C35-C36
17	A	403	CLA	O2A-C1-C2-C3
20	B	622	LHG	C30-C31-C32-C33
27	C	620	SQD	C9-C10-C11-C12
17	C	602	CLA	O1D-CGD-O2D-CED
17	D	410	CLA	C13-C15-C16-C17
17	B	605	CLA	O1D-CGD-O2D-CED
20	D	407	LHG	O9-C7-O7-C5
17	C	613	CLA	C16-C17-C18-C19
17	B	607	CLA	C11-C12-C13-C14
17	C	602	CLA	C11-C12-C13-C14
17	C	606	CLA	C14-C13-C15-C16
17	C	609	CLA	C6-C7-C8-C9
17	C	610	CLA	C6-C7-C8-C9
17	A	404	CLA	C11-C10-C8-C9
17	C	613	CLA	C2-C3-C5-C6
26	C	619	DGD	O6D-C5D-C6D-O5D
19	C	601	LMG	C12-C13-C14-C15
17	B	611	CLA	C16-C17-C18-C20
17	B	613	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	C	614	CLA	C6-C7-C8-C10
17	D	402	CLA	C16-C17-C18-C20
17	C	606	CLA	C16-C17-C18-C19
20	D	407	LHG	C24-C25-C26-C27
20	B	621	LHG	C23-C24-C25-C26
19	C	621	LMG	C33-C34-C35-C36
17	A	402	CLA	C4C-C3C-CAC-CBC
23	D	411	PHO	C5-C6-C7-C8
17	B	607	CLA	C3-C5-C6-C7
17	C	603	CLA	C13-C15-C16-C17
17	B	603	CLA	C11-C12-C13-C14
17	B	605	CLA	C6-C7-C8-C9
17	B	610	CLA	C11-C10-C8-C9
17	C	603	CLA	C11-C10-C8-C9
17	C	614	CLA	C6-C7-C8-C9
17	B	613	CLA	CBD-CGD-O2D-CED
19	C	621	LMG	C16-C17-C18-C19
20	D	409	LHG	C30-C31-C32-C33
17	B	613	CLA	O1D-CGD-O2D-CED
17	B	606	CLA	C1A-C2A-CAA-CBA
17	C	610	CLA	C1A-C2A-CAA-CBA
17	C	607	CLA	C16-C17-C18-C20
20	D	407	LHG	C8-C7-O7-C5
17	D	403	CLA	C4-C3-C5-C6
17	B	603	CLA	C11-C12-C13-C15
19	H	102	LMG	C33-C34-C35-C36
20	D	407	LHG	C11-C10-C9-C8
20	K	103	LHG	C24-C25-C26-C27
17	D	403	CLA	C5-C6-C7-C8
17	B	613	CLA	C2-C1-O2A-CGA
17	C	607	CLA	C8-C10-C11-C12
17	C	604	CLA	C6-C7-C8-C9
17	C	603	CLA	C4-C3-C5-C6
17	B	603	CLA	C13-C15-C16-C17
17	C	607	CLA	C3-C5-C6-C7
19	C	601	LMG	C7-C8-C9-O8
20	D	407	LHG	C32-C33-C34-C35
17	C	613	CLA	C16-C17-C18-C20
17	B	601	CLA	C2C-C3C-CAC-CBC
22	D	405	PL9	C30-C29-C31-C32
17	B	607	CLA	C16-C17-C18-C19
17	B	616	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	C	617	DGD	O6D-C5D-C6D-O5D
20	L	101	LHG	O7-C5-C6-O8
27	C	620	SQD	O47-C45-C46-O48
23	D	411	PHO	C6-C7-C8-C10
19	C	621	LMG	C15-C16-C17-C18
19	B	620	LMG	C10-C11-C12-C13
17	B	604	CLA	C11-C12-C13-C14
17	B	607	CLA	C6-C7-C8-C9
17	B	608	CLA	C14-C13-C15-C16
17	B	612	CLA	C6-C7-C8-C9
17	D	402	CLA	C11-C12-C13-C14
17	C	606	CLA	C6-C7-C8-C9
19	K	102	LMG	C14-C15-C16-C17
17	B	602	CLA	C2A-CAA-CBA-CGA
17	B	612	CLA	C3A-C2A-CAA-CBA
17	C	613	CLA	C3A-C2A-CAA-CBA
17	A	402	CLA	O2A-C1-C2-C3
19	D	408	LMG	C29-C30-C31-C32
20	K	103	LHG	C10-C11-C12-C13
19	K	102	LMG	O9-C10-O7-C8
26	C	618	DGD	O1G-C1G-C2G-C3G
17	C	609	CLA	C10-C11-C12-C13
19	D	408	LMG	C19-C20-C21-C22
23	D	411	PHO	C10-C11-C12-C13
19	K	102	LMG	C32-C33-C34-C35
26	C	617	DGD	C4A-C5A-C6A-C7A
17	B	616	CLA	C11-C12-C13-C14
17	C	607	CLA	C16-C17-C18-C19
17	B	611	CLA	CAA-CBA-CGA-O2A
20	D	407	LHG	O8-C23-C24-C25
20	D	407	LHG	C25-C26-C27-C28
17	D	410	CLA	C16-C17-C18-C19
17	B	604	CLA	C11-C12-C13-C15
17	B	607	CLA	C6-C7-C8-C10
17	B	610	CLA	C11-C10-C8-C7
17	C	602	CLA	C6-C7-C8-C10
17	C	604	CLA	C6-C7-C8-C10
17	B	610	CLA	CAA-CBA-CGA-O2A
17	B	601	CLA	C13-C15-C16-C17
17	C	604	CLA	C15-C16-C17-C18
17	B	612	CLA	CAA-CBA-CGA-O2A
17	B	607	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	C	610	CLA	CAA-CBA-CGA-O2A
26	C	619	DGD	C2B-C1B-O2G-C2G
17	B	604	CLA	C10-C11-C12-C13
17	C	610	CLA	C8-C10-C11-C12
17	D	402	CLA	CAA-CBA-CGA-O2A
17	C	613	CLA	CAA-CBA-CGA-O2A
17	B	606	CLA	CAA-CBA-CGA-O2A
17	C	609	CLA	CAA-CBA-CGA-O2A
17	B	604	CLA	C13-C15-C16-C17
19	K	102	LMG	C28-C29-C30-C31
19	H	102	LMG	C15-C16-C17-C18
19	H	102	LMG	C12-C13-C14-C15
26	C	617	DGD	C3A-C4A-C5A-C6A
17	D	403	CLA	C14-C13-C15-C16
20	K	103	LHG	O7-C7-C8-C9
17	B	602	CLA	C1A-C2A-CAA-CBA
17	C	613	CLA	C1A-C2A-CAA-CBA
17	C	613	CLA	C4B-C3B-CAB-CBB
26	C	619	DGD	O1B-C1B-O2G-C2G
20	K	103	LHG	C24-C23-O8-C6
24	E	101	HEM	CAA-CBA-CGA-O2A
17	B	607	CLA	CAA-CBA-CGA-O2A
17	B	609	CLA	CAA-CBA-CGA-O2A
17	A	402	CLA	C5-C6-C7-C8
17	C	607	CLA	CAA-CBA-CGA-O2A
20	B	622	LHG	O8-C23-C24-C25
17	B	605	CLA	CAA-CBA-CGA-O2A
17	C	606	CLA	C6-C7-C8-C10
17	C	612	CLA	C12-C13-C15-C16
17	B	606	CLA	C8-C10-C11-C12
20	D	409	LHG	C12-C13-C14-C15
17	B	613	CLA	C2A-CAA-CBA-CGA
17	C	610	CLA	C16-C17-C18-C20
27	C	620	SQD	C32-C33-C34-C35
17	C	610	CLA	C13-C15-C16-C17
17	C	603	CLA	CAA-CBA-CGA-O2A
17	D	403	CLA	C2-C3-C5-C6
17	B	610	CLA	CAA-CBA-CGA-O1A
19	H	102	LMG	C11-C12-C13-C14
20	L	101	LHG	C12-C13-C14-C15
17	C	608	CLA	C11-C12-C13-C14
17	B	612	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	C	610	CLA	CAA-CBA-CGA-O1A
17	C	613	CLA	CAA-CBA-CGA-O1A
17	D	402	CLA	CAA-CBA-CGA-O1A
17	B	604	CLA	CAA-CBA-CGA-O2A
20	L	101	LHG	O8-C23-C24-C25
17	B	611	CLA	CAA-CBA-CGA-O1A
20	K	103	LHG	O9-C7-C8-C9
26	C	617	DGD	C5D-C6D-O5D-C1E
24	E	101	HEM	CAA-CBA-CGA-O1A
17	B	612	CLA	C3-C5-C6-C7
23	D	412	PHO	CAA-CBA-CGA-O2A
27	C	620	SQD	O47-C7-C8-C9
17	C	602	CLA	C15-C16-C17-C18
20	B	621	LHG	C35-C36-C37-C38
20	D	407	LHG	O10-C23-C24-C25
17	B	601	CLA	CAA-CBA-CGA-O2A
17	C	609	CLA	CAA-CBA-CGA-O1A
17	B	615	CLA	CAD-CBD-CGD-O2D
17	A	403	CLA	CAA-CBA-CGA-O2A
20	D	406	LHG	C25-C26-C27-C28
17	B	606	CLA	CAA-CBA-CGA-O1A
17	C	607	CLA	CAA-CBA-CGA-O1A
20	B	623	LHG	O8-C23-C24-C25
20	D	407	LHG	C29-C30-C31-C32
17	B	609	CLA	CAA-CBA-CGA-O1A
17	B	602	CLA	CAA-CBA-CGA-O2A
19	K	102	LMG	C11-C10-O7-C8
17	B	603	CLA	C16-C17-C18-C20
27	C	620	SQD	O49-C7-C8-C9
19	K	102	LMG	C33-C34-C35-C36
17	A	402	CLA	CAA-CBA-CGA-O2A
27	C	620	SQD	C10-C11-C12-C13
20	K	103	LHG	O10-C23-O8-C6
17	B	604	CLA	CAA-CBA-CGA-O1A
17	B	605	CLA	CAA-CBA-CGA-O1A
17	B	607	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

32 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	H	102	LMG	3	0

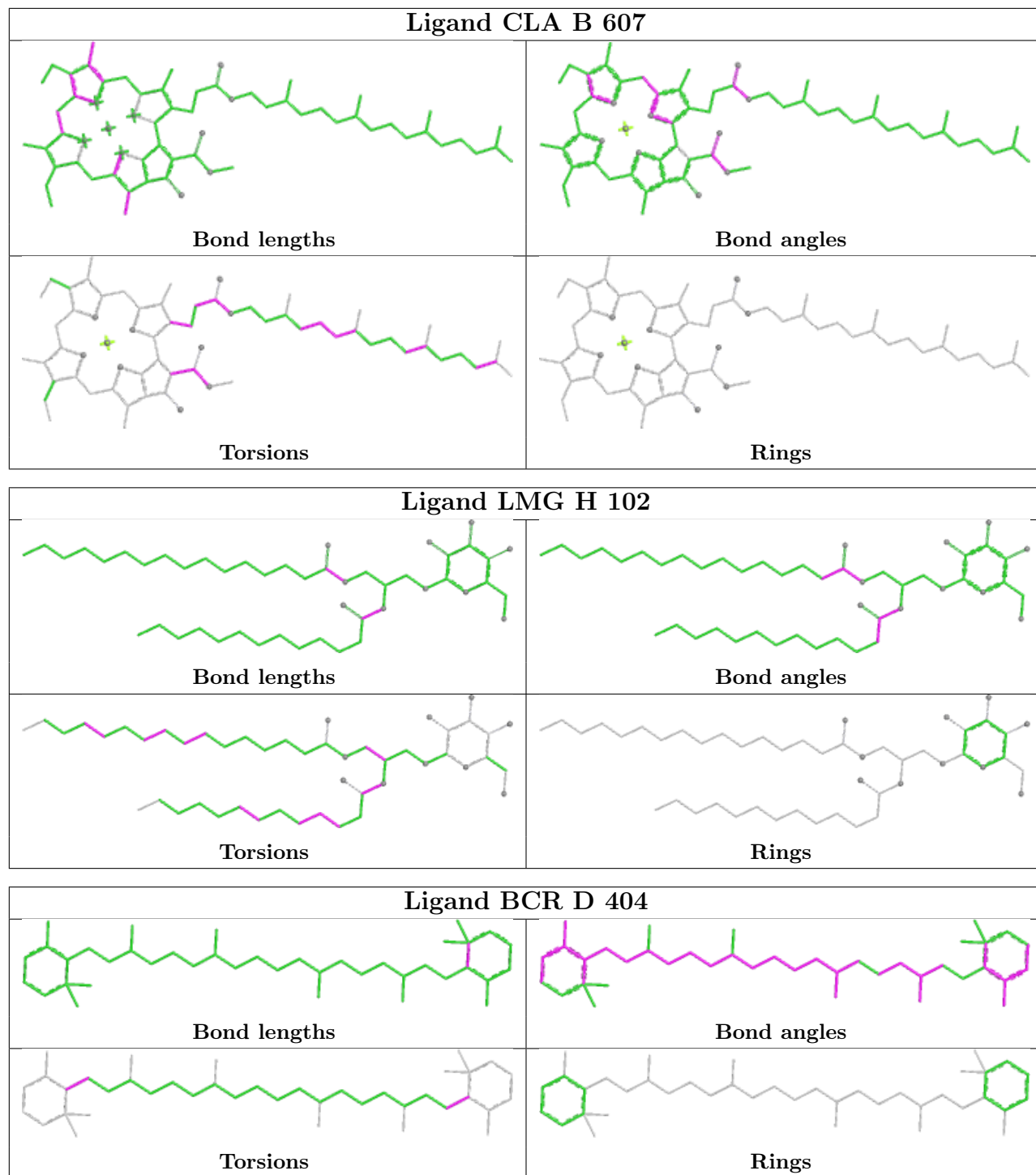
Continued on next page...

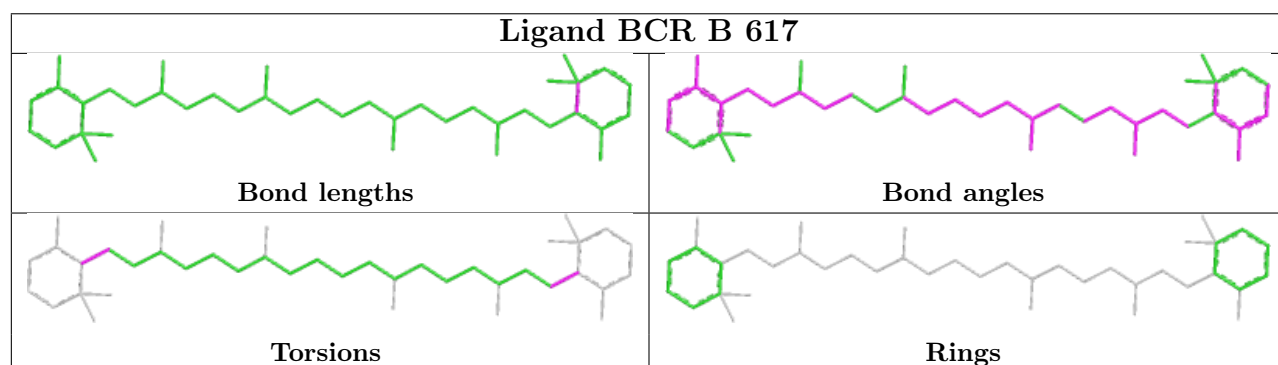
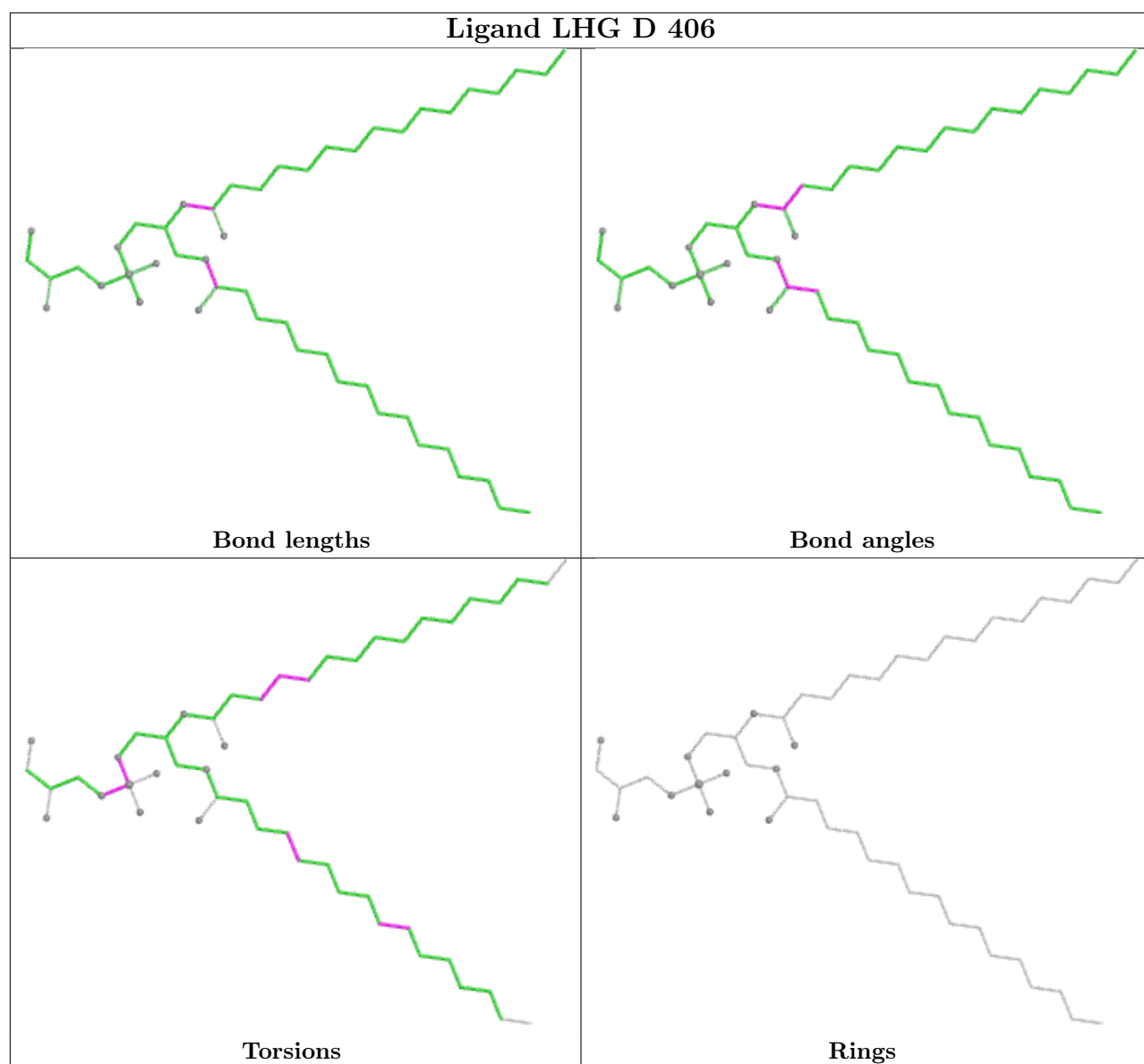
Continued from previous page...

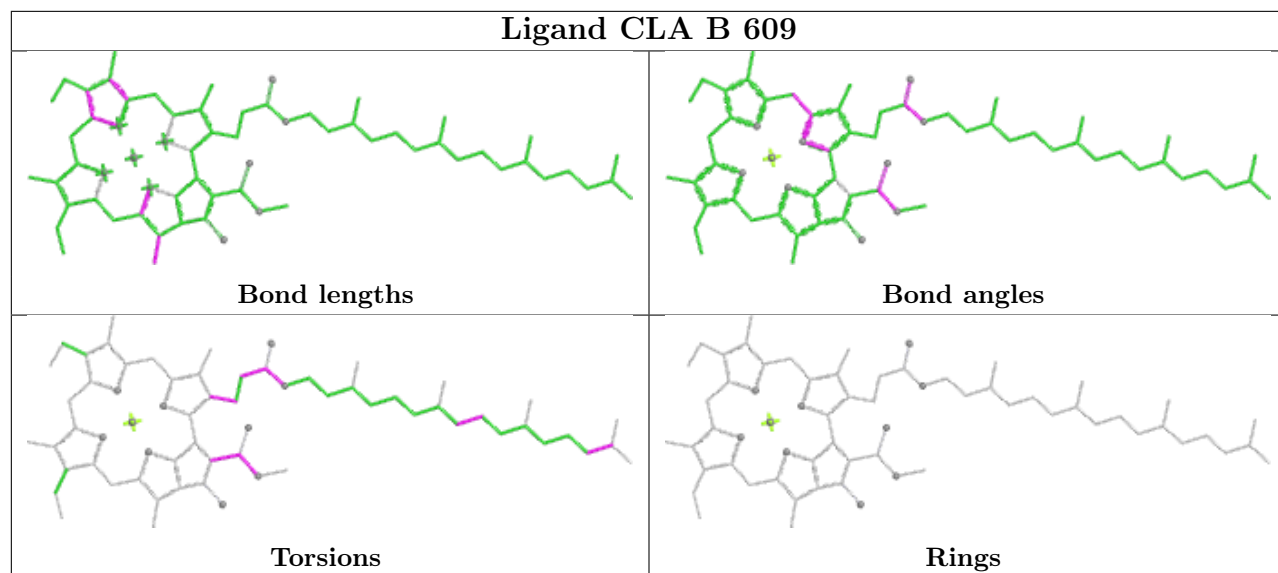
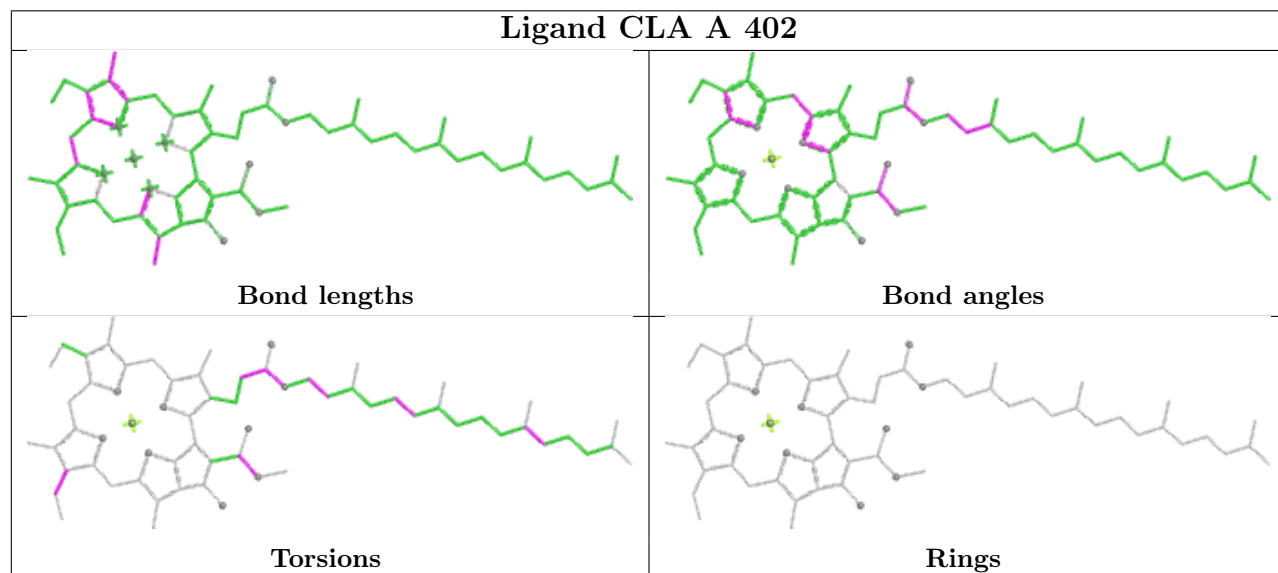
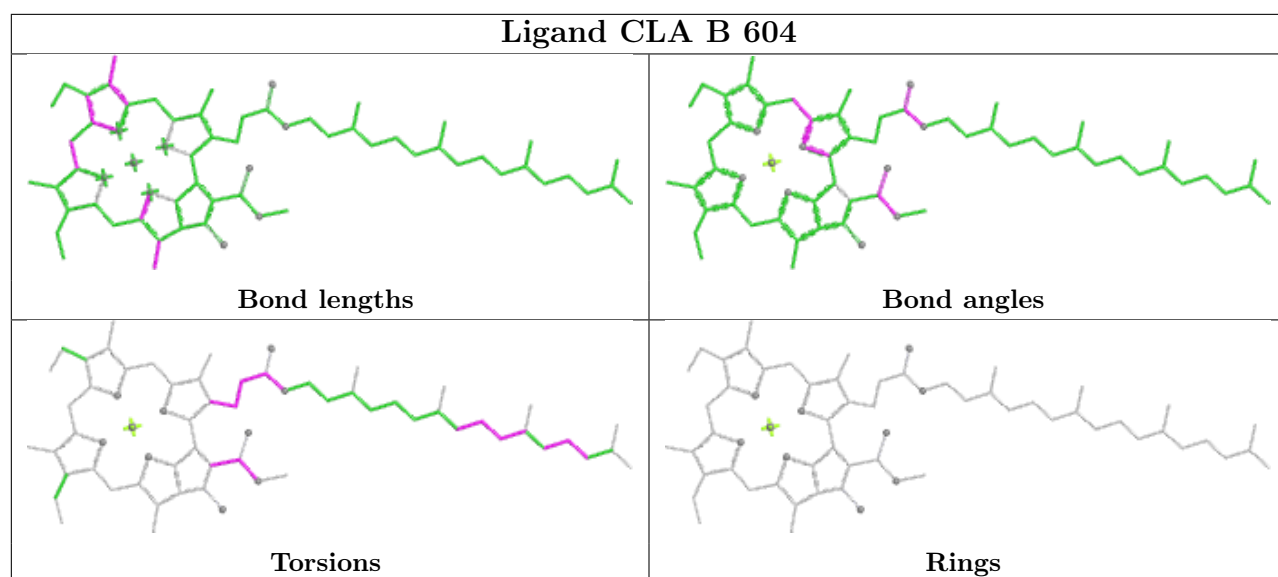
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	617	BCR	1	0
17	B	604	CLA	2	0
17	C	611	CLA	1	0
17	B	602	CLA	4	0
17	B	612	CLA	1	0
18	C	616	BCR	3	0
17	B	615	CLA	2	0
17	B	616	CLA	1	0
17	C	609	CLA	1	0
18	C	615	BCR	8	0
18	Z	101	BCR	7	0
17	C	607	CLA	1	0
20	L	101	LHG	1	0
18	H	101	BCR	5	0
24	E	101	HEM	5	0
17	C	602	CLA	4	0
20	D	407	LHG	2	0
17	C	604	CLA	1	0
17	C	612	CLA	1	0
26	C	619	DGD	2	0
18	B	618	BCR	1	0
17	C	608	CLA	1	0
17	D	402	CLA	1	0
17	C	614	CLA	1	0
17	D	410	CLA	2	0
18	K	101	BCR	1	0
18	B	619	BCR	1	0
17	C	603	CLA	3	0
18	A	405	BCR	2	0
17	C	606	CLA	3	0
17	D	403	CLA	1	0

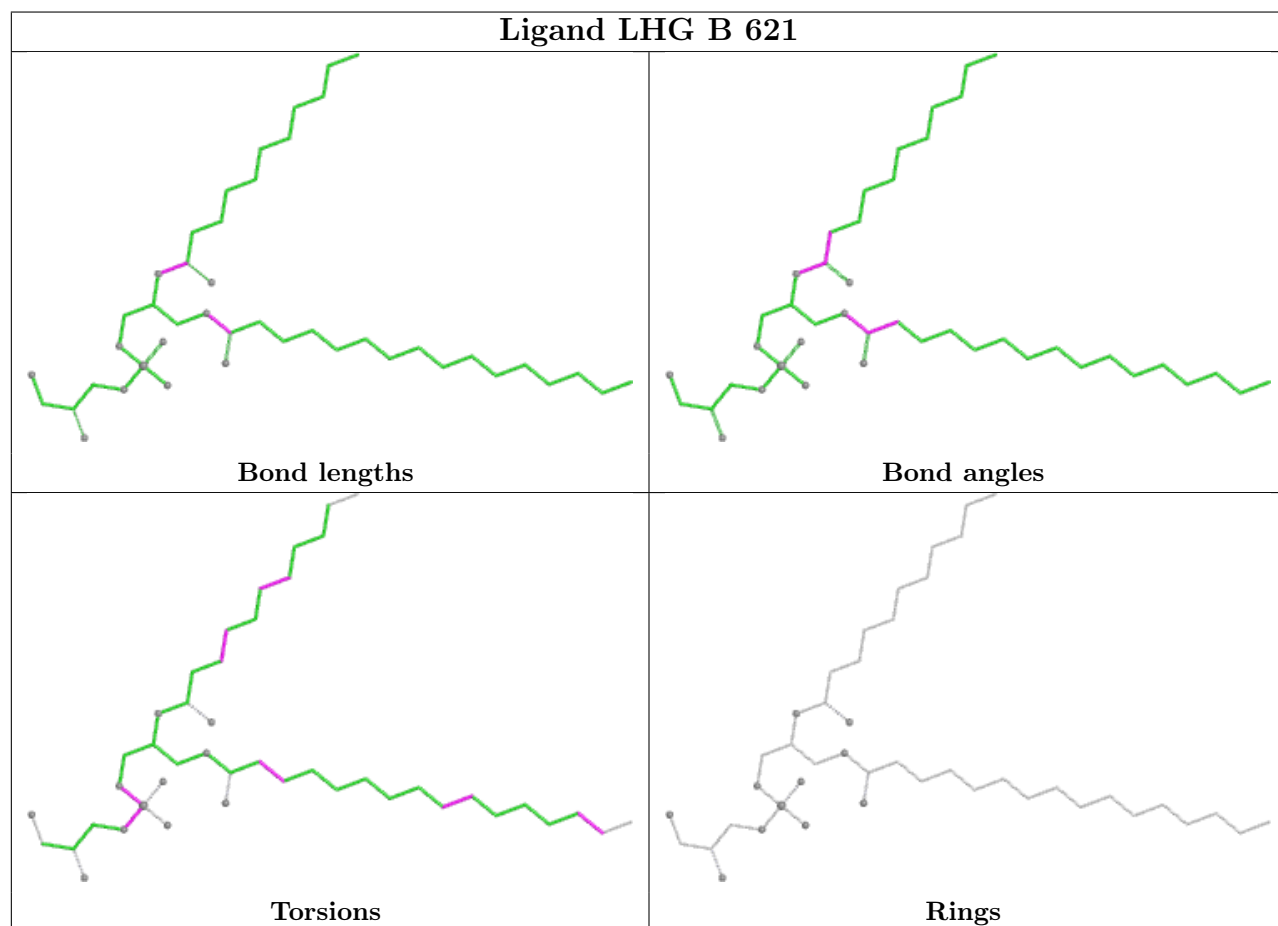
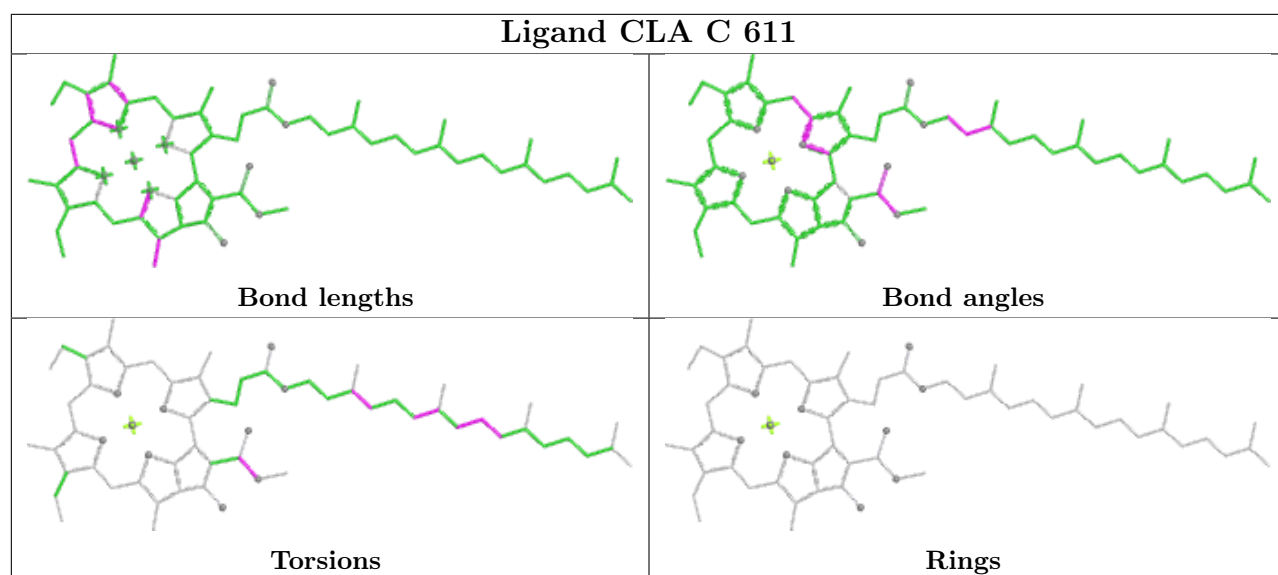
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

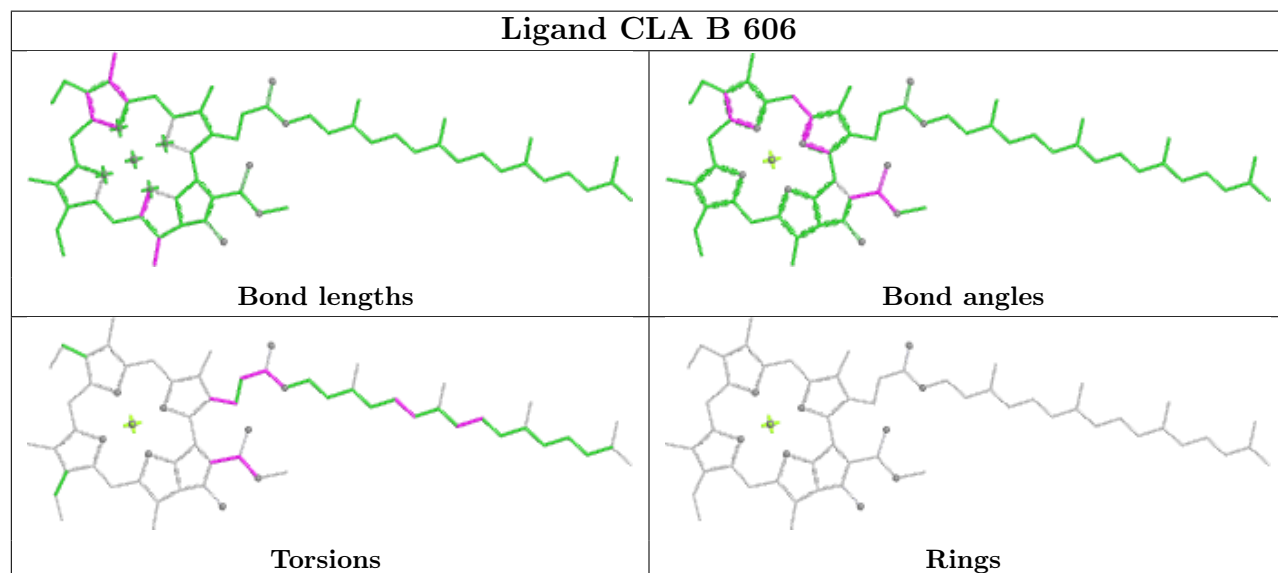
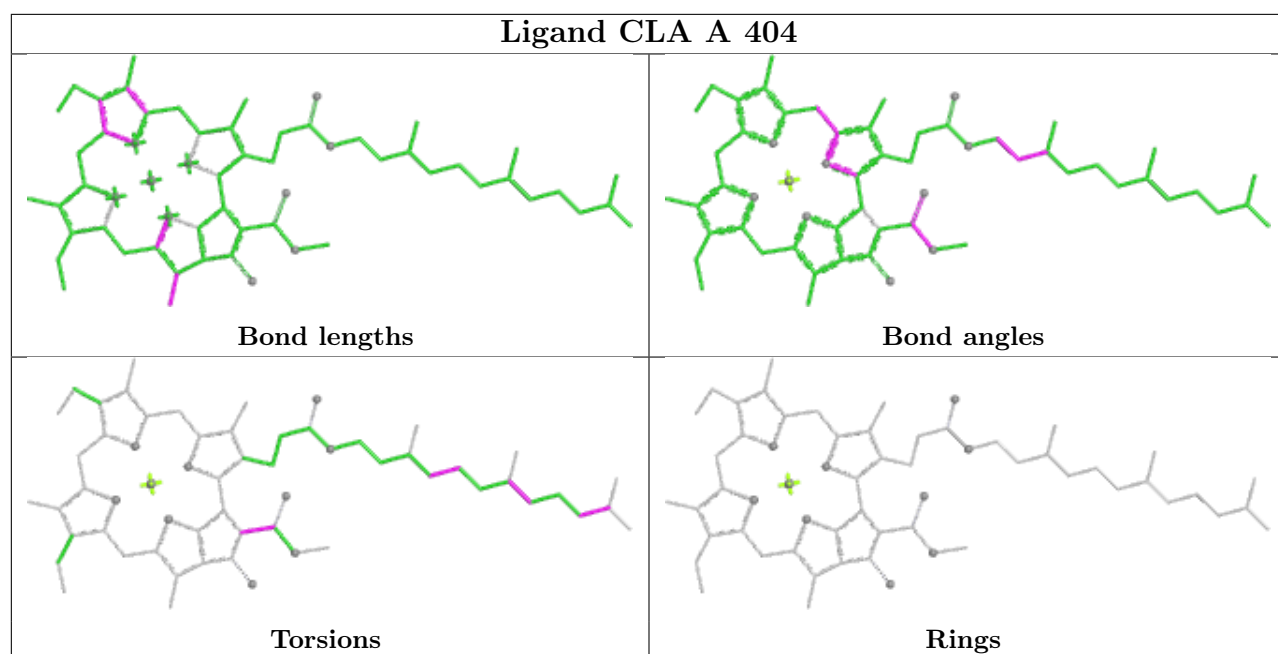
equivalents in the CSD to analyse the geometry.

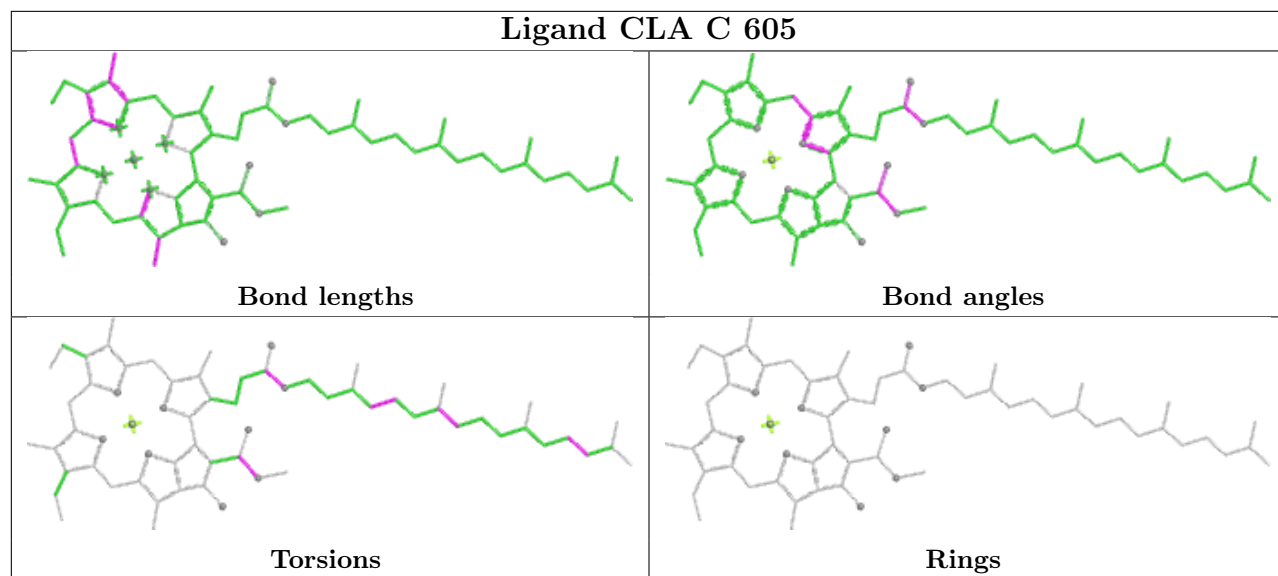


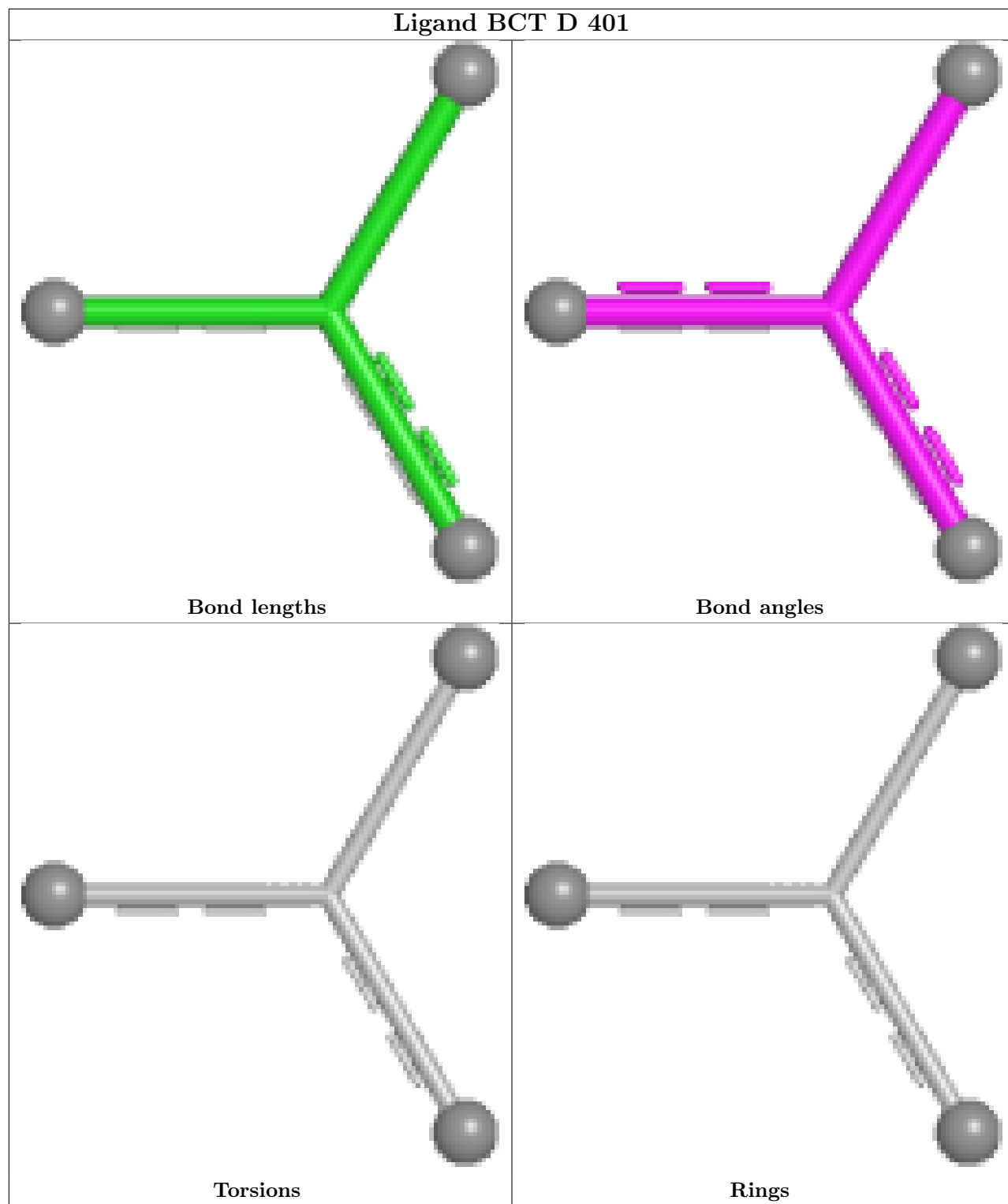


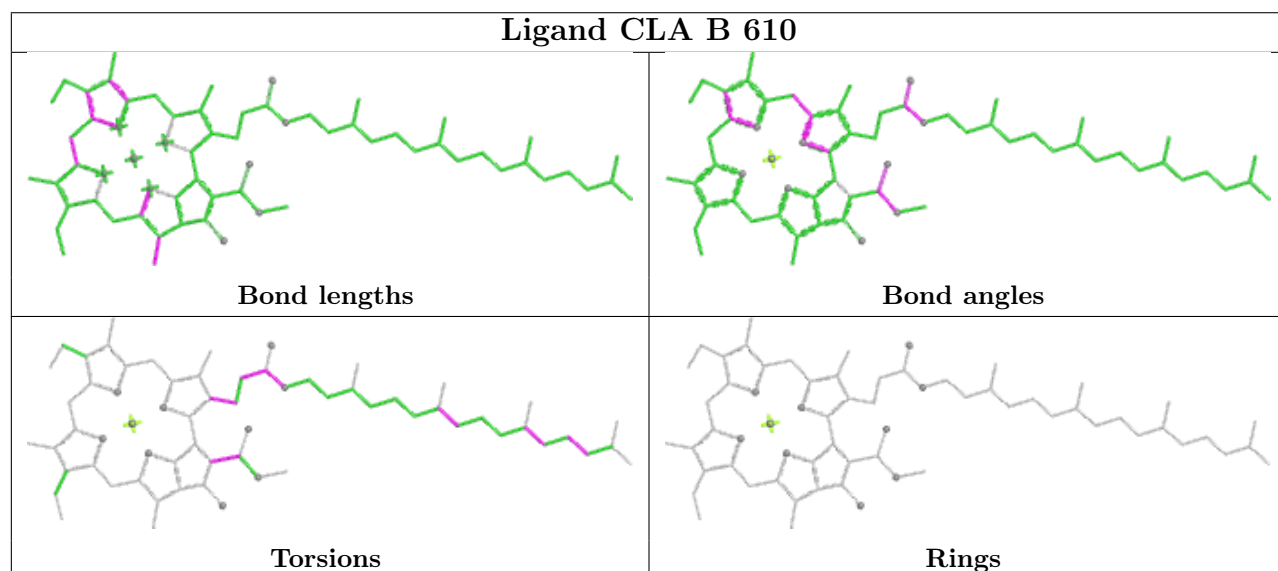
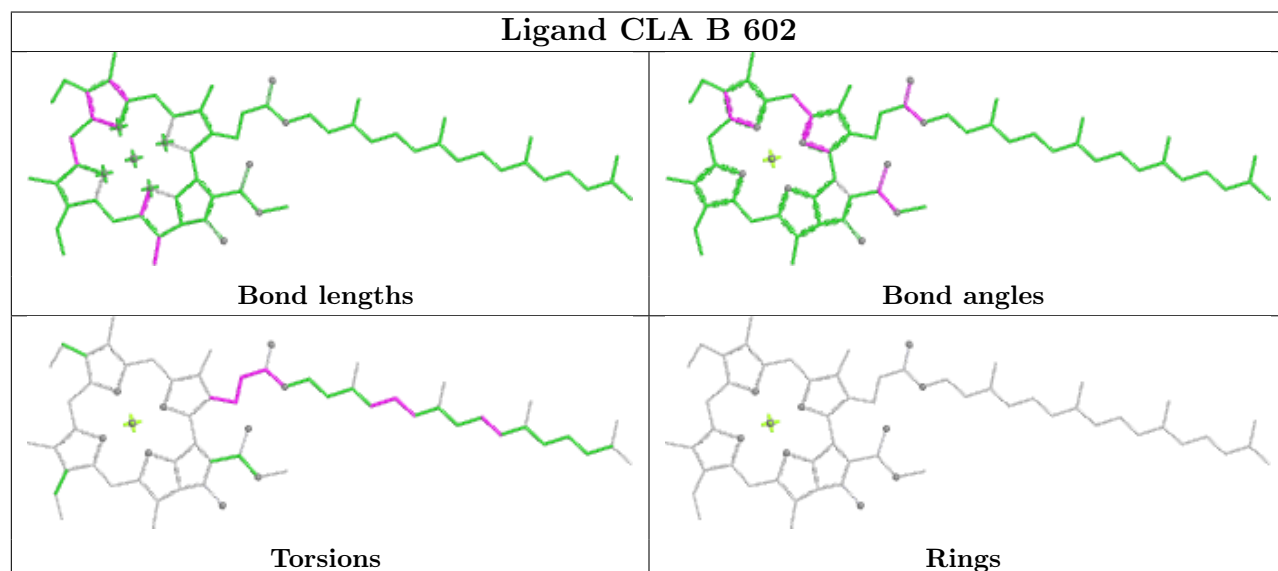
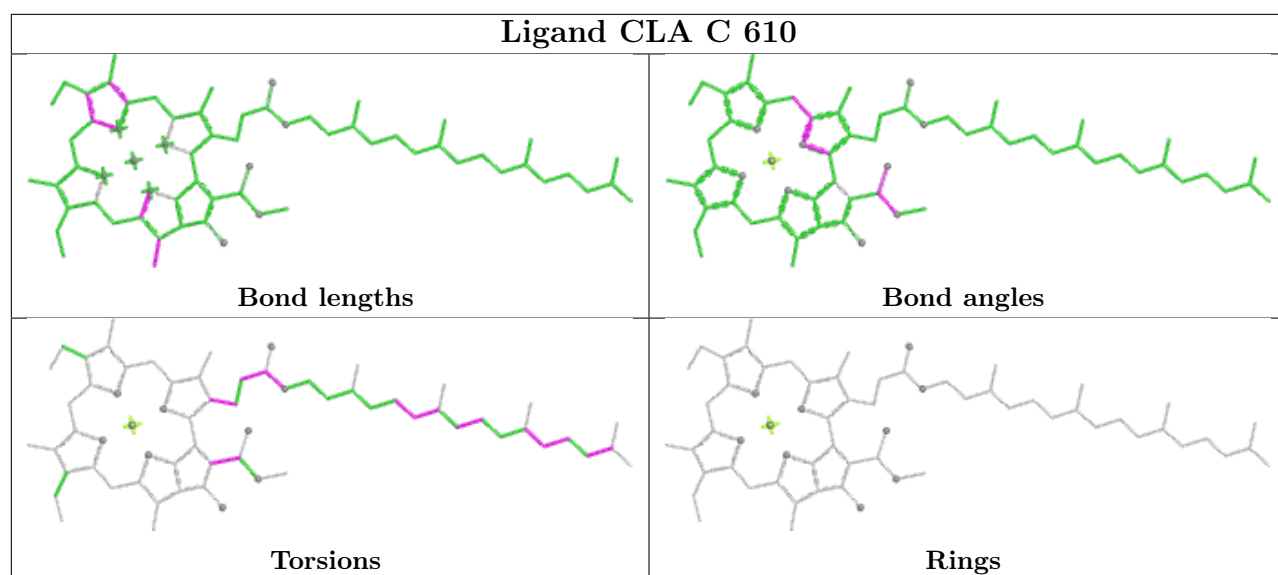


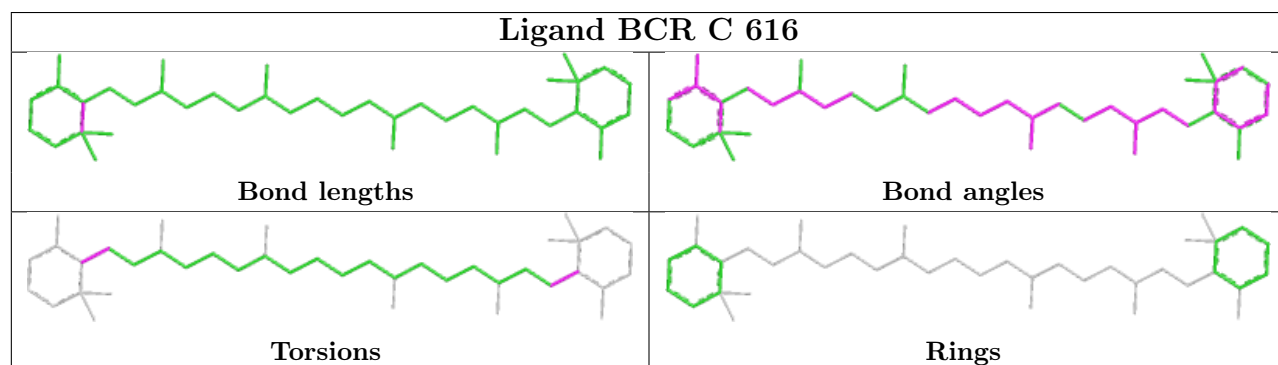
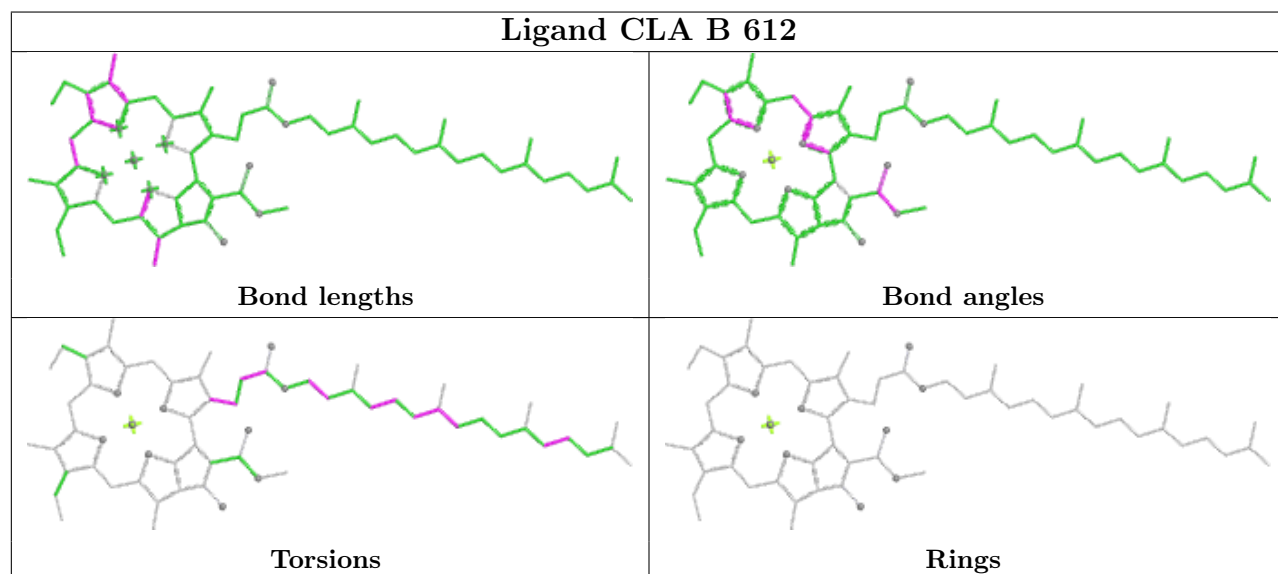
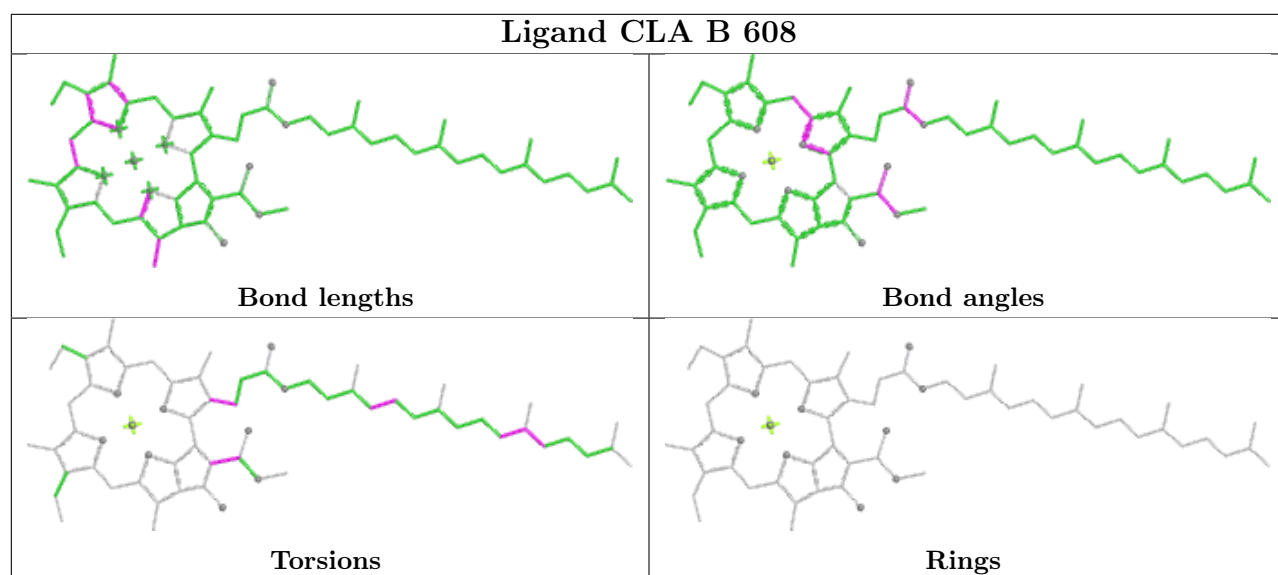


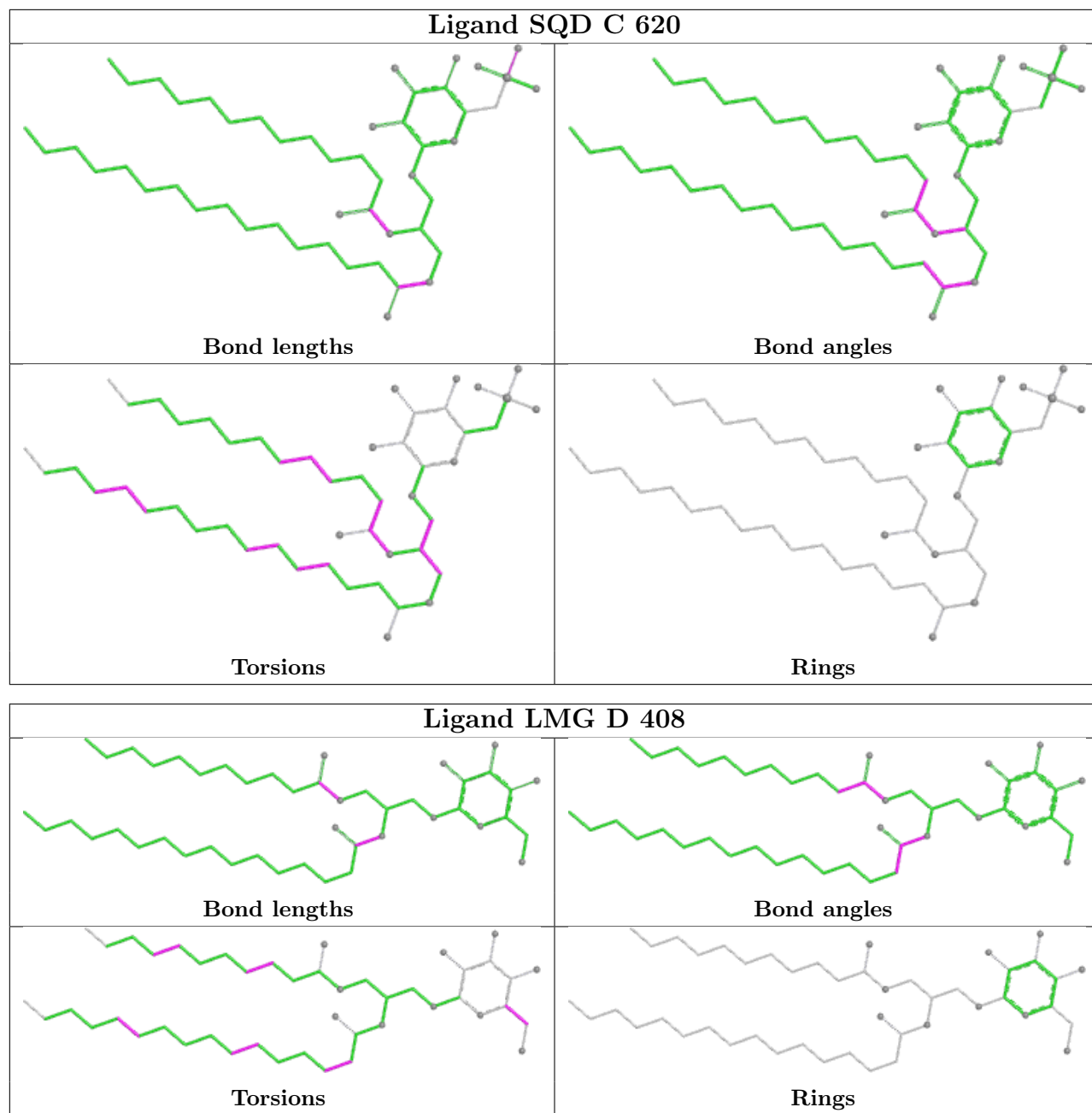


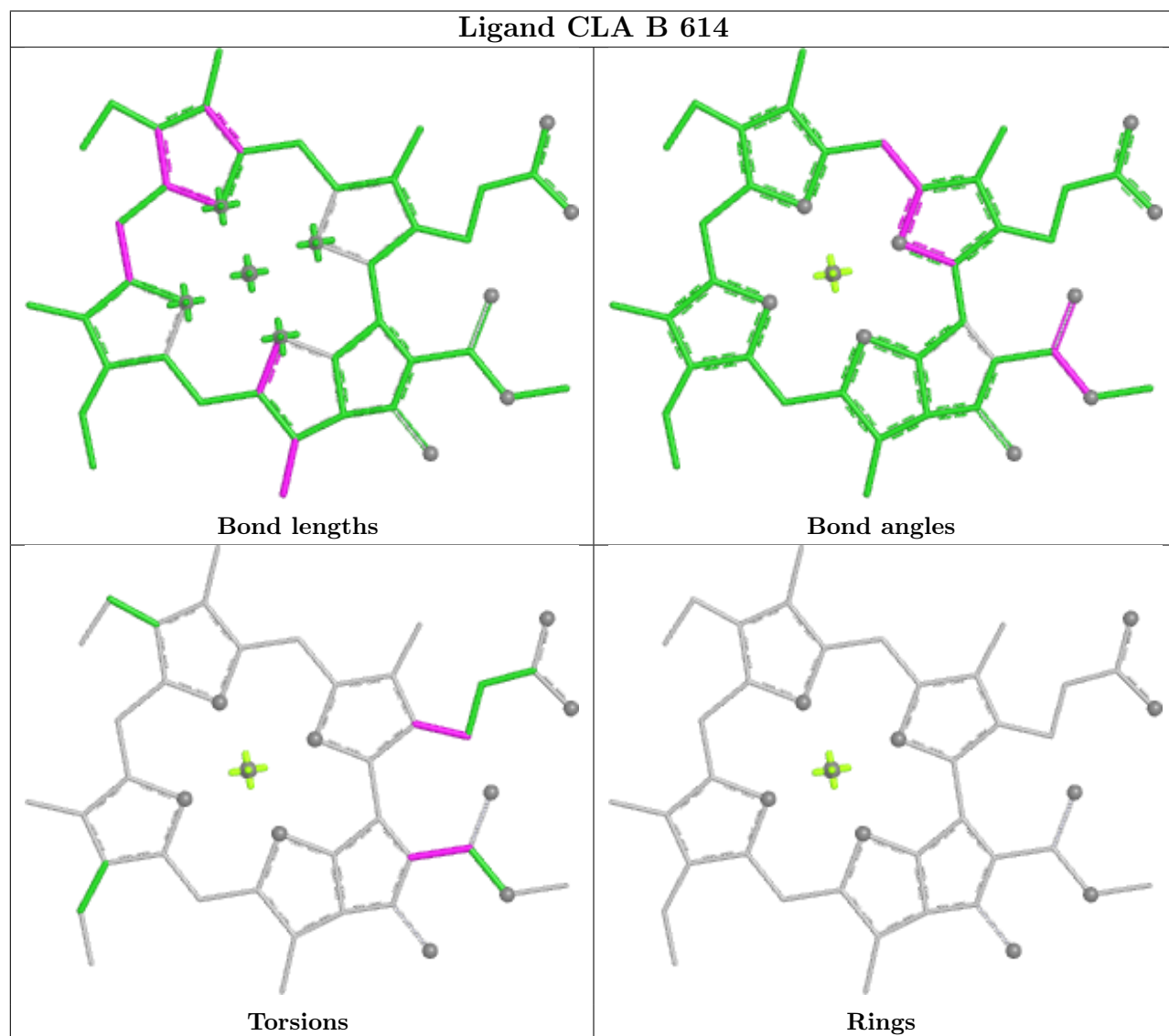
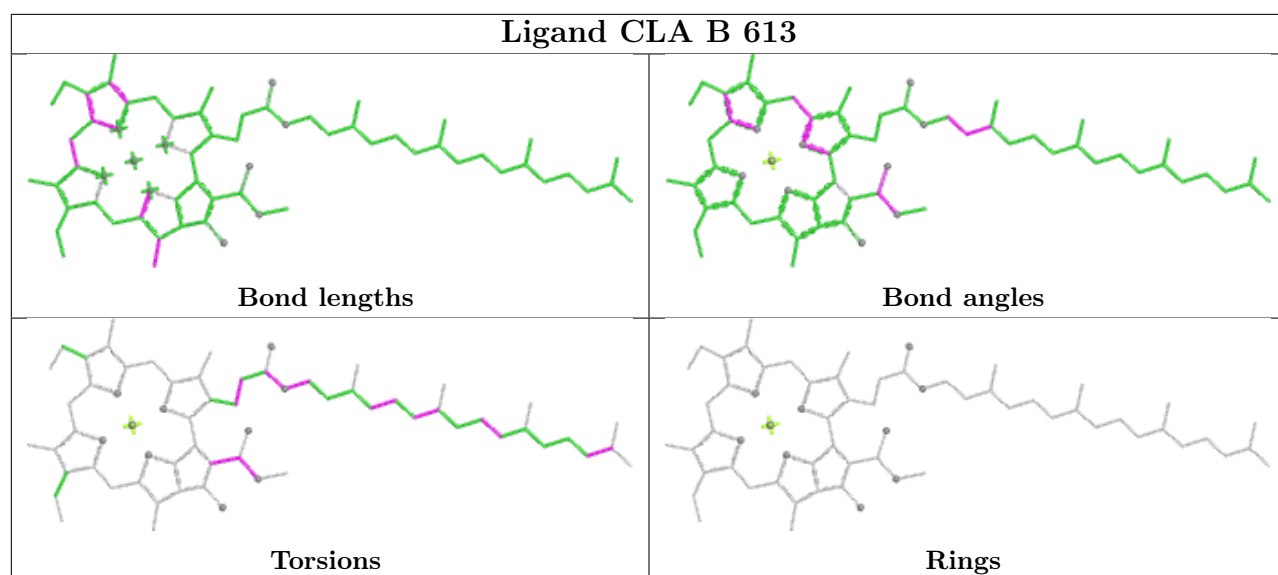


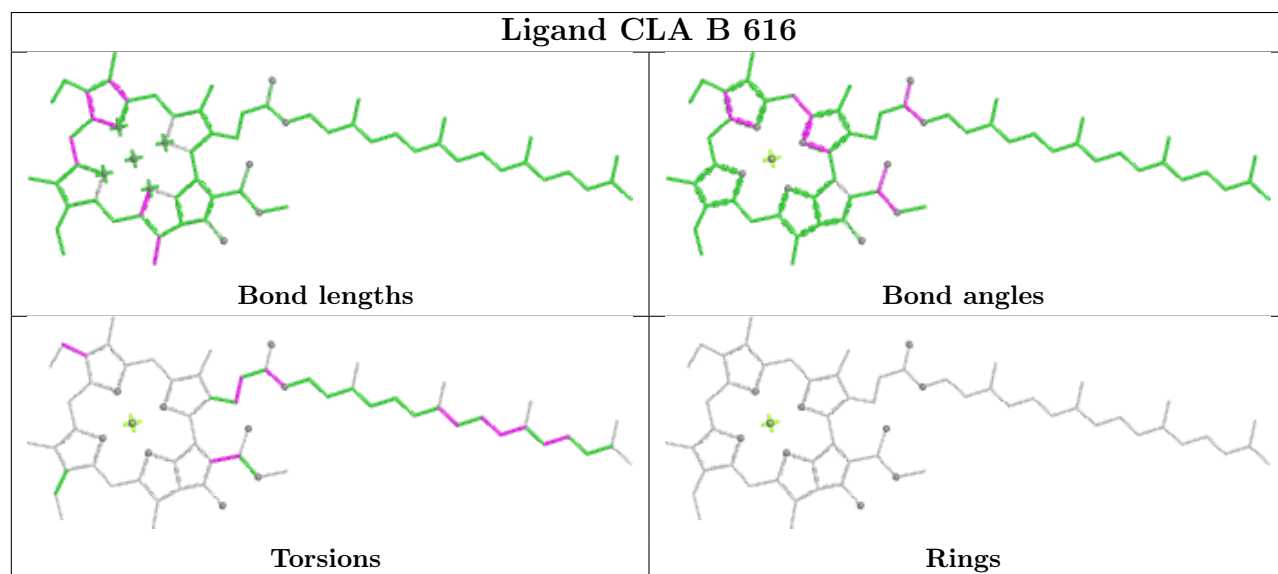
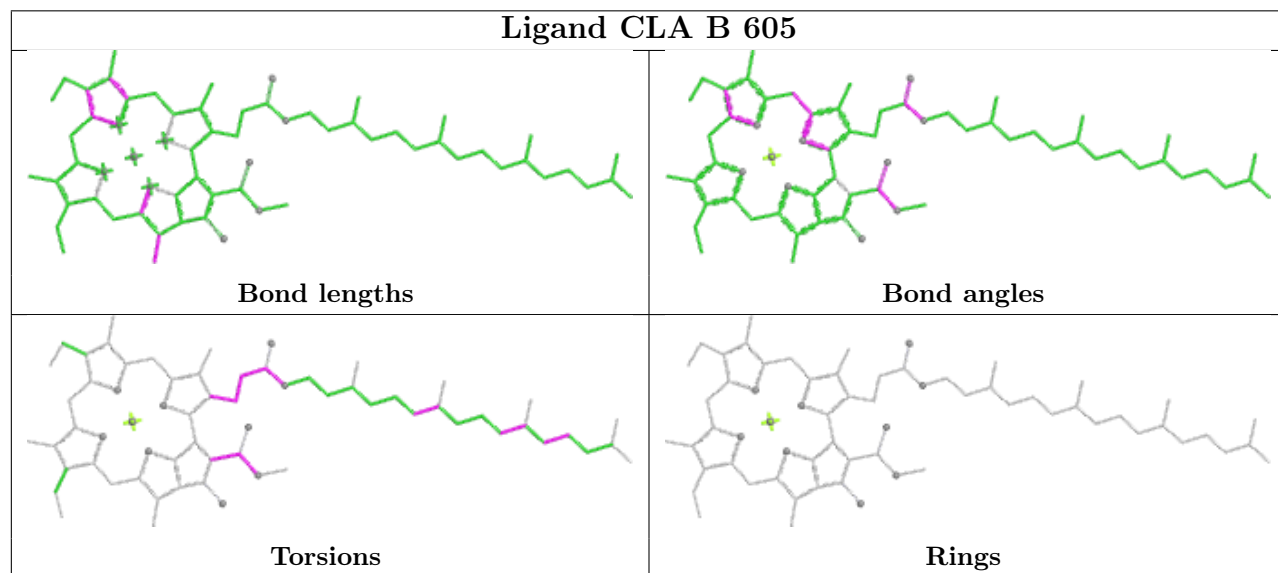
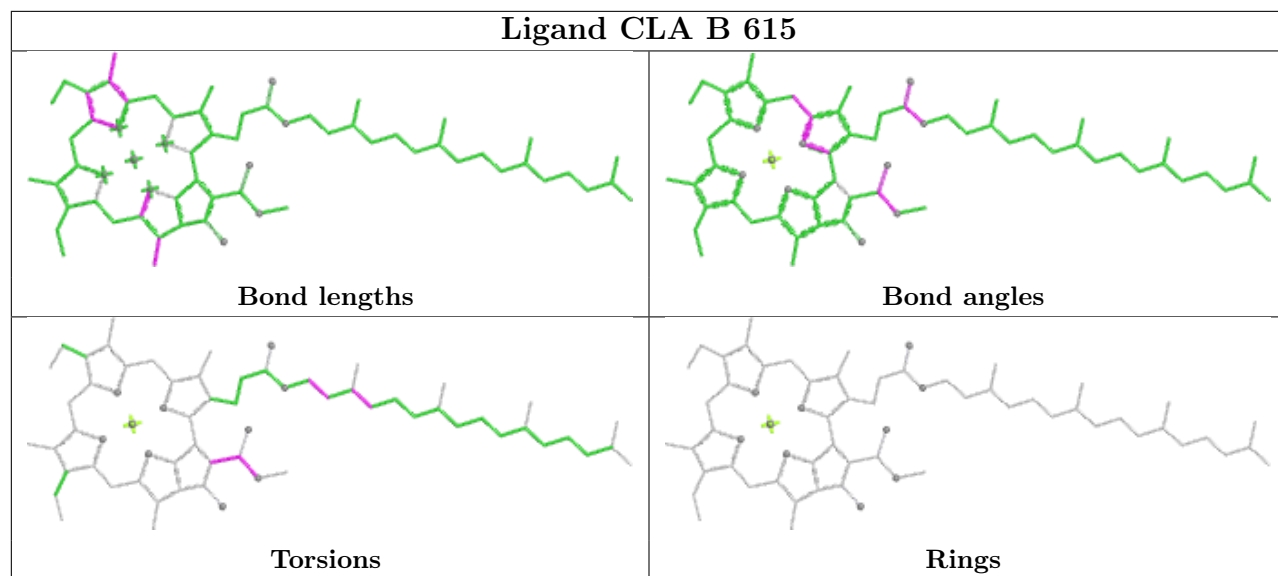




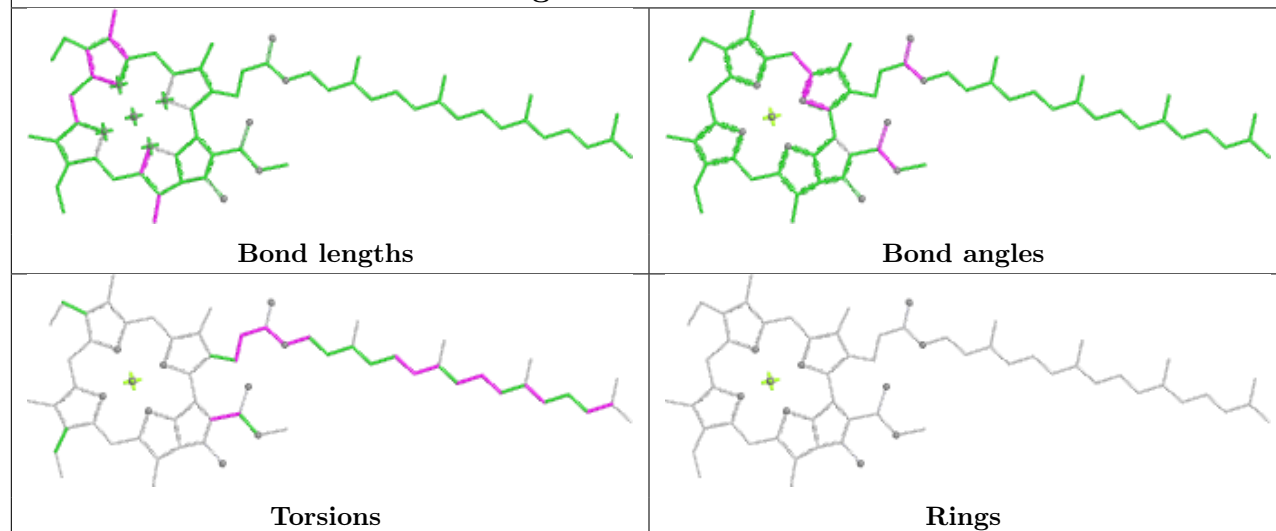




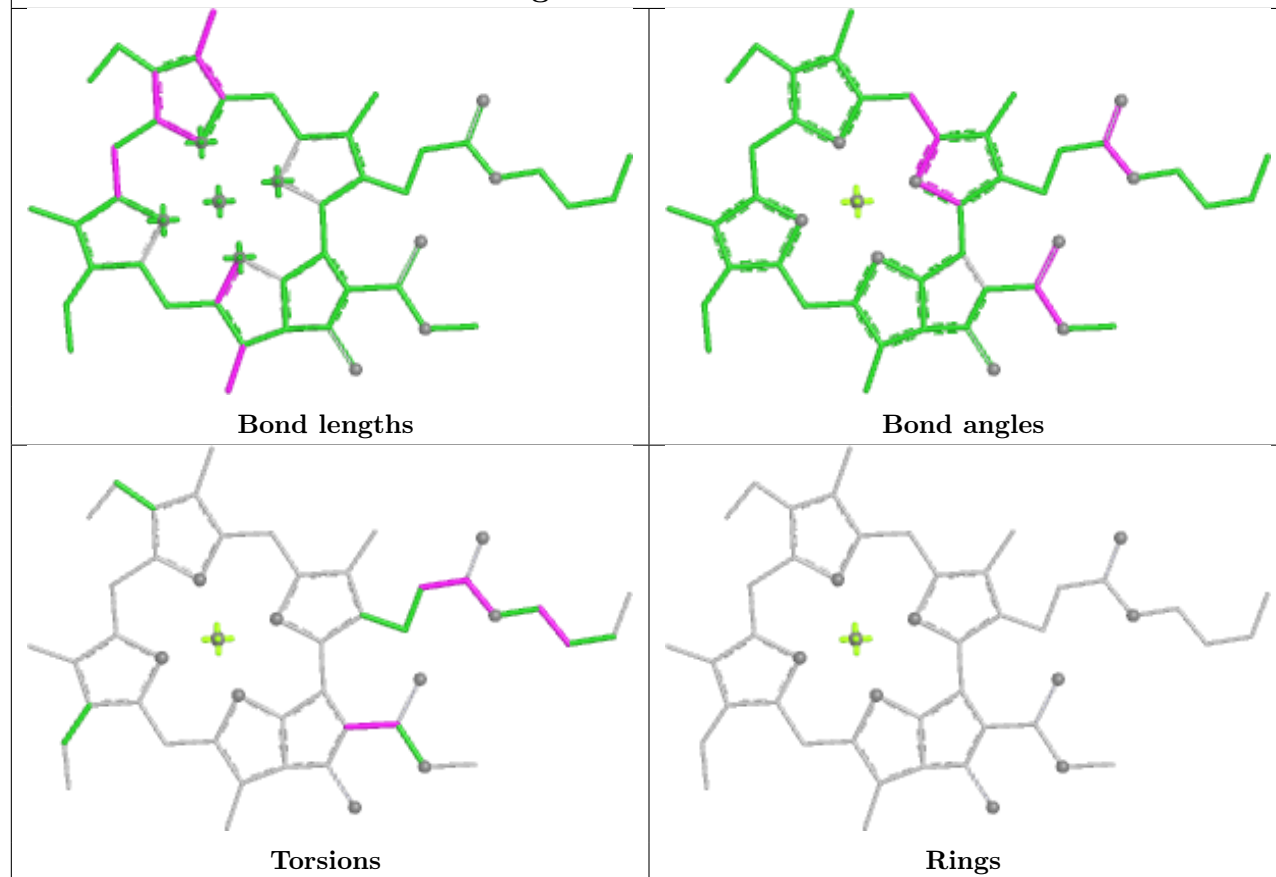


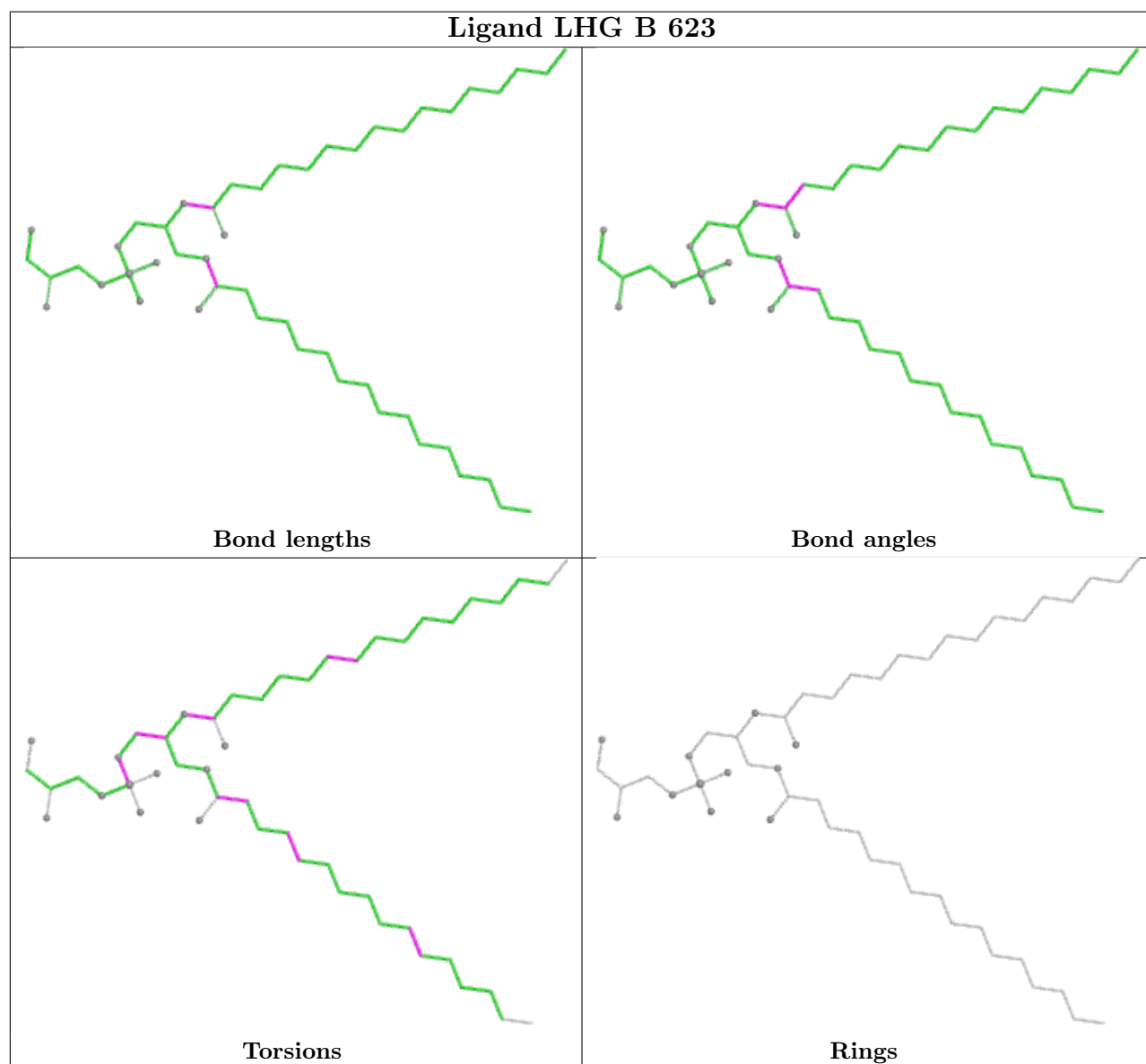
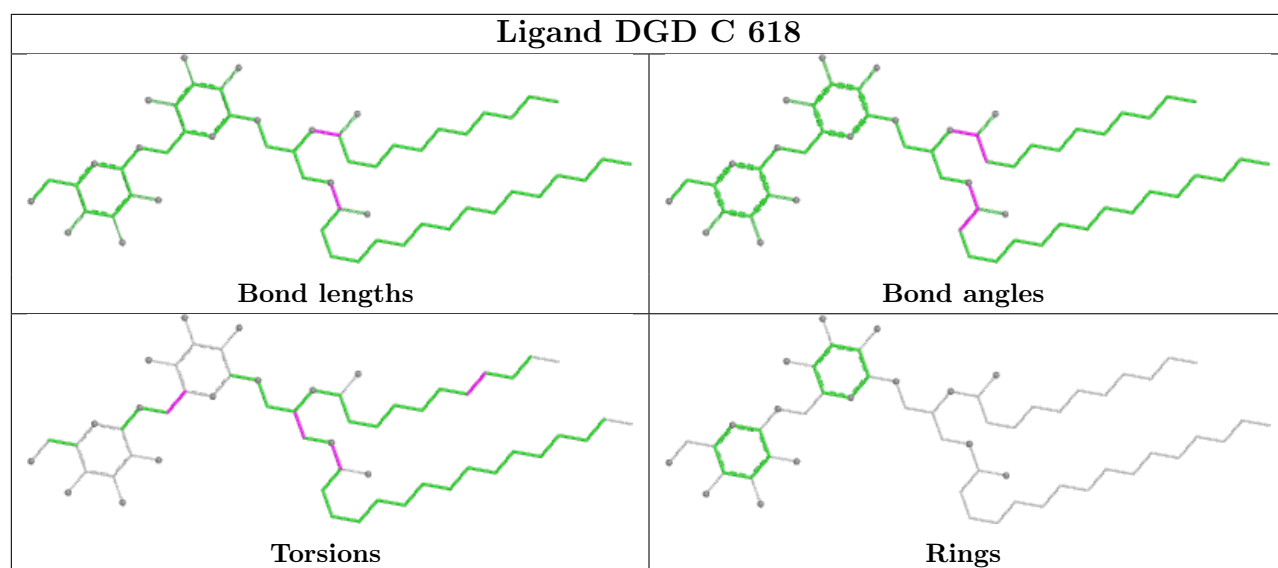


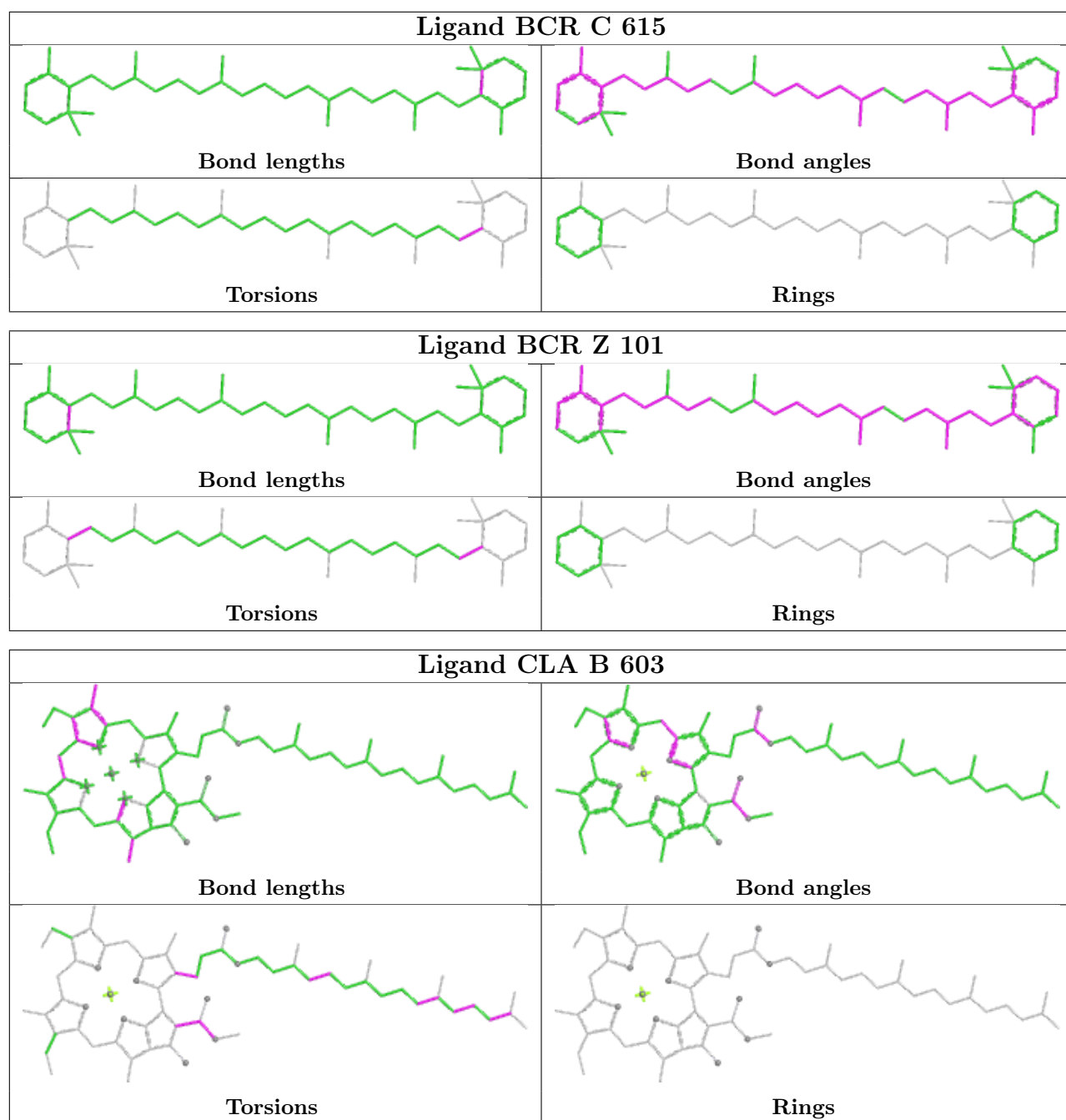
Ligand CLA C 609

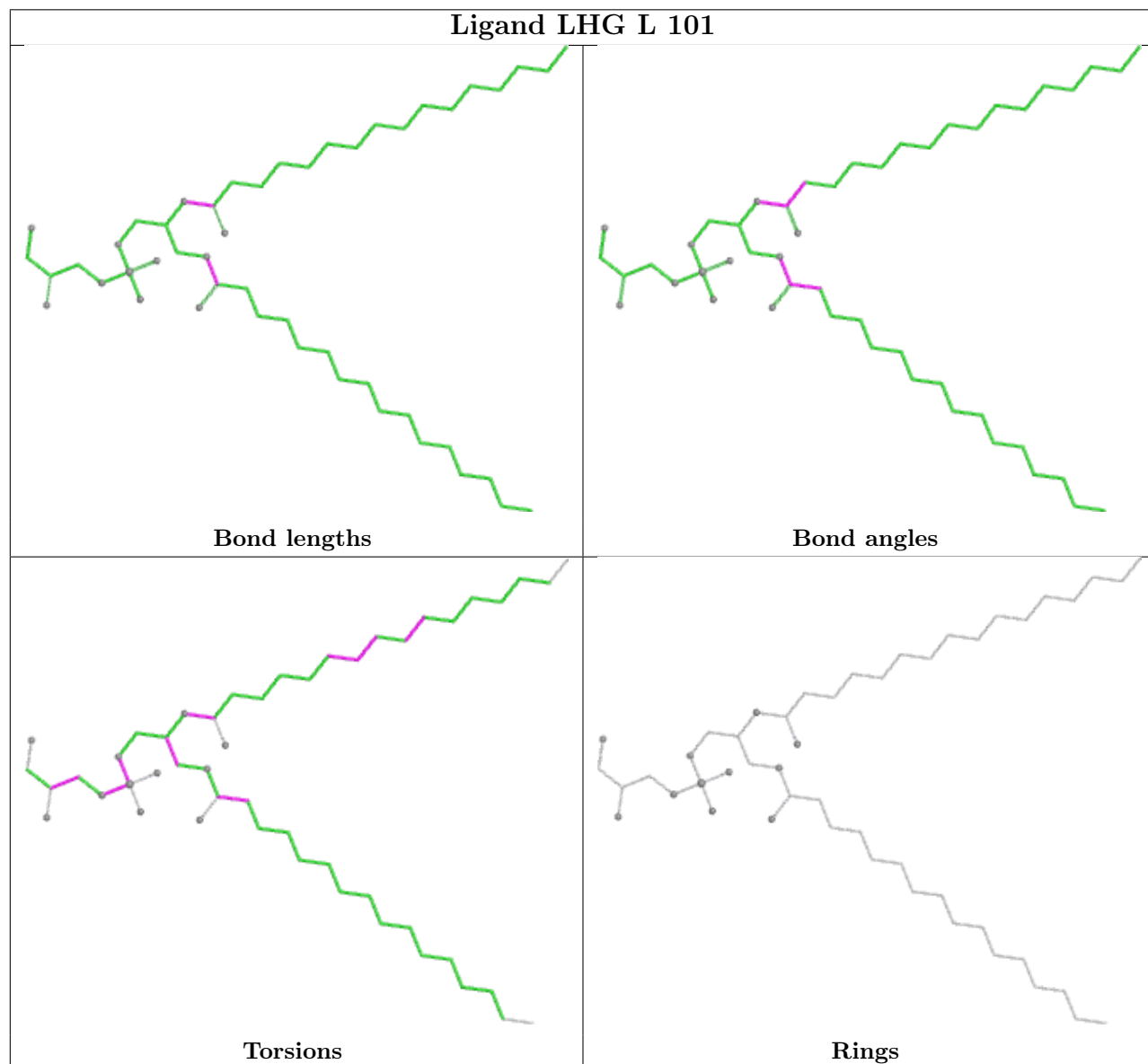
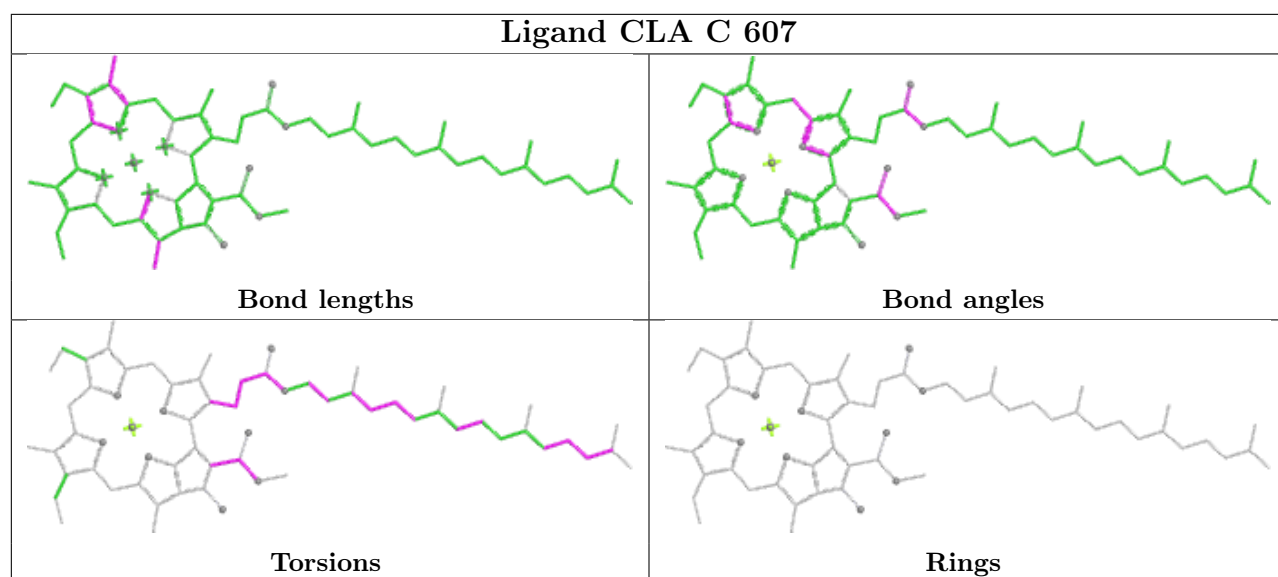


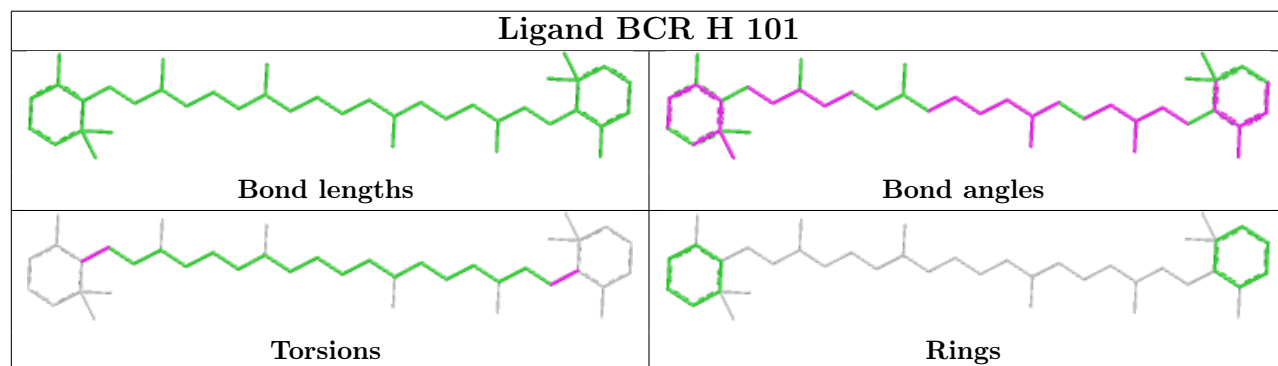
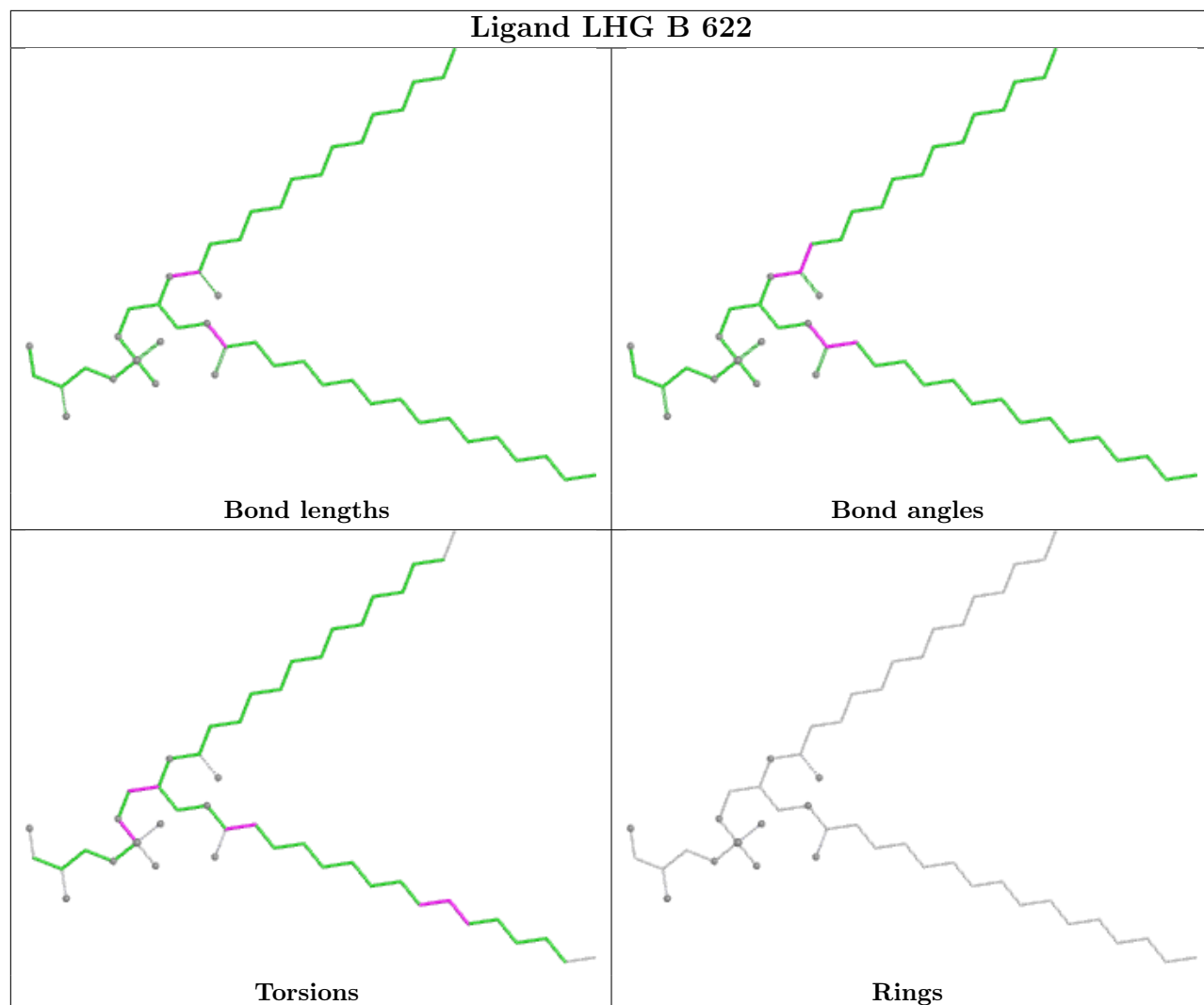
Ligand CLA A 403

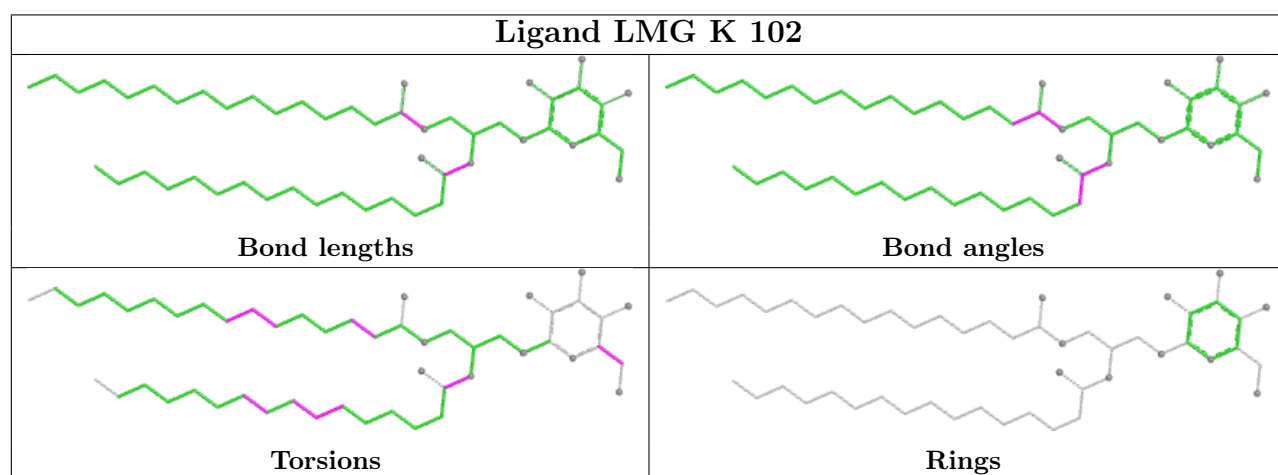
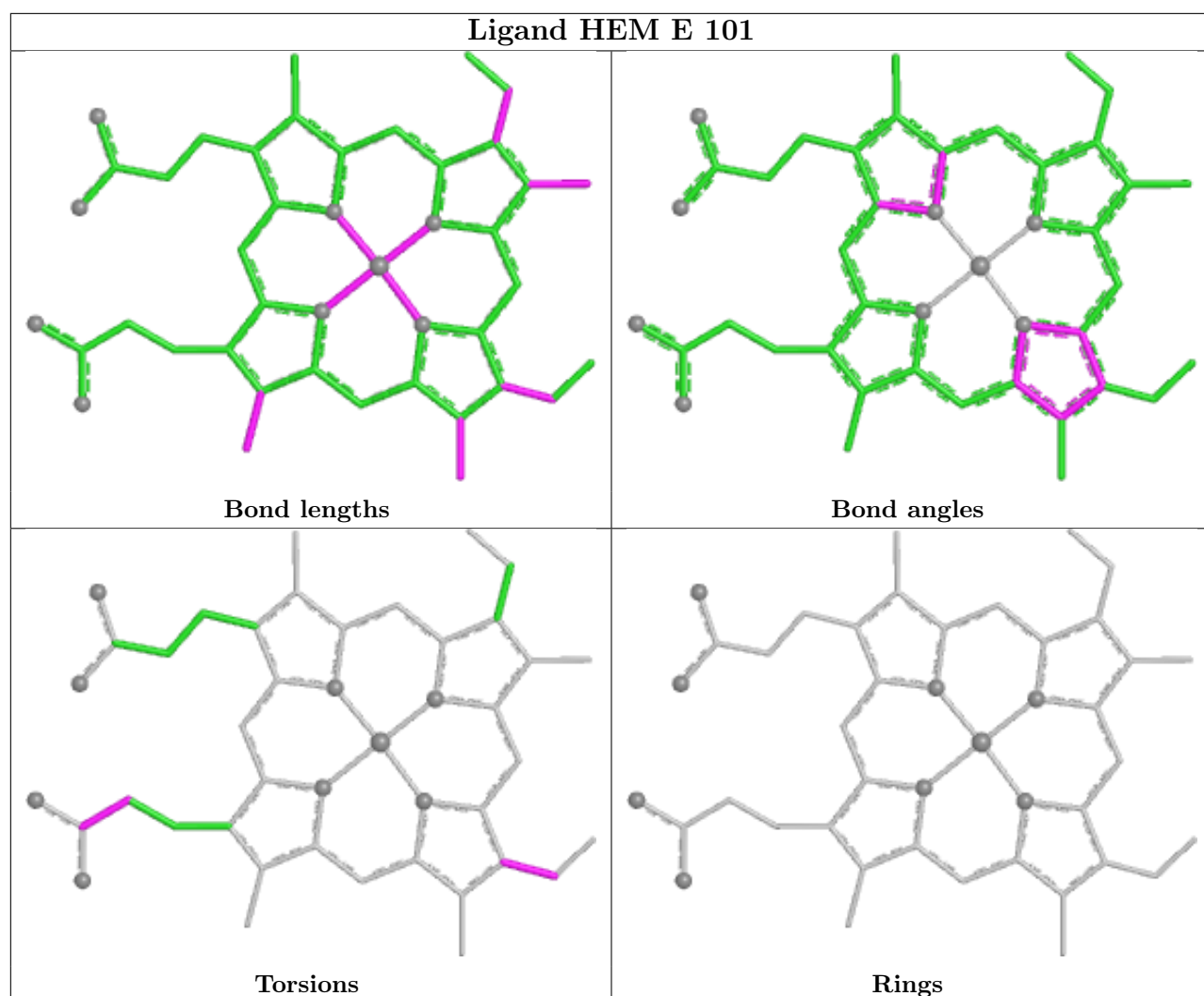


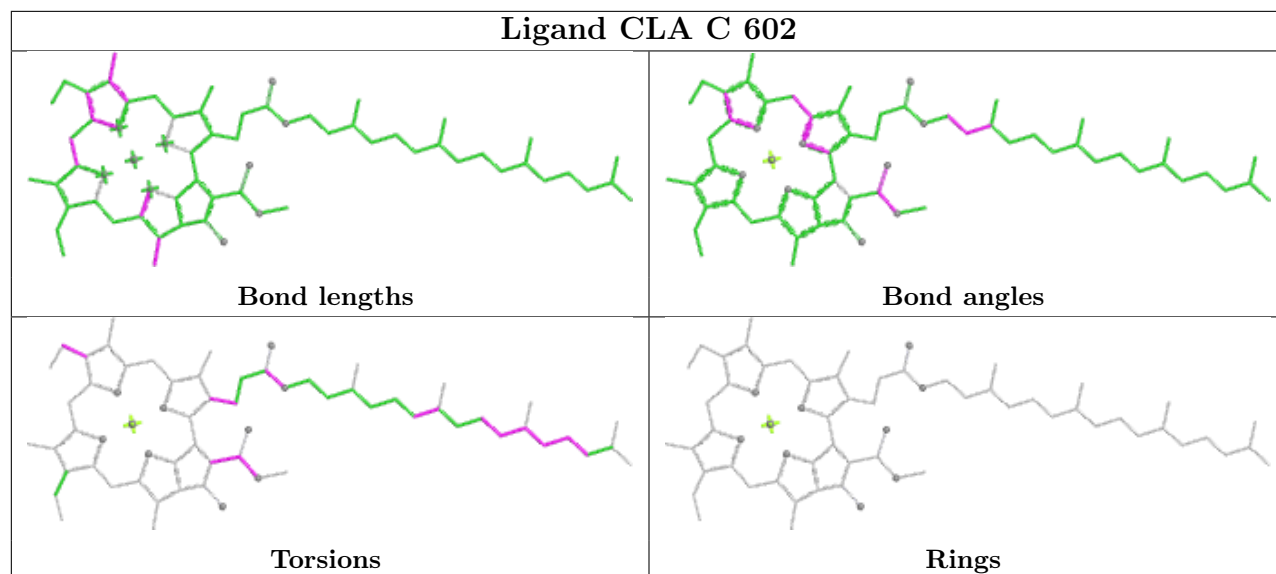
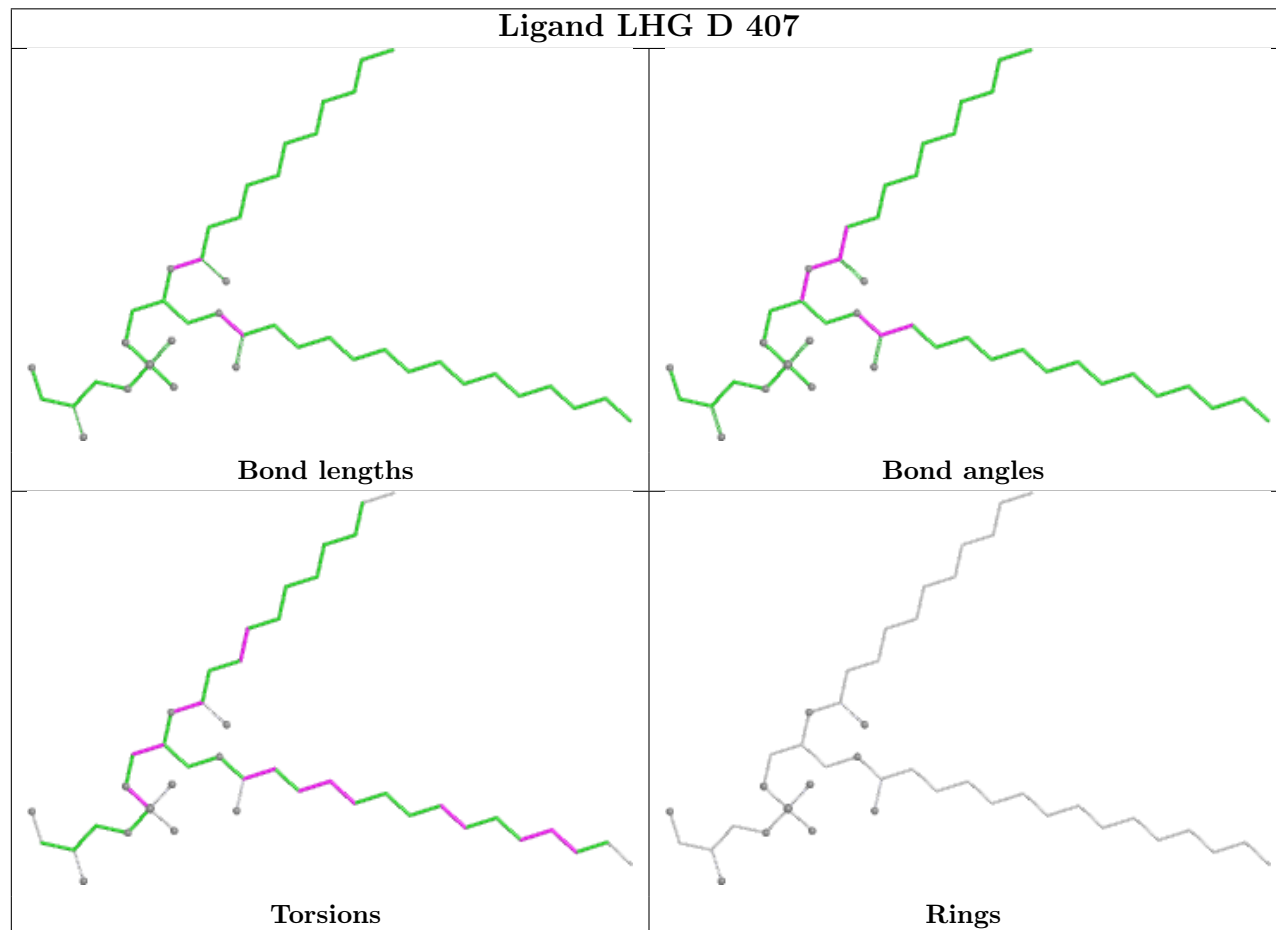


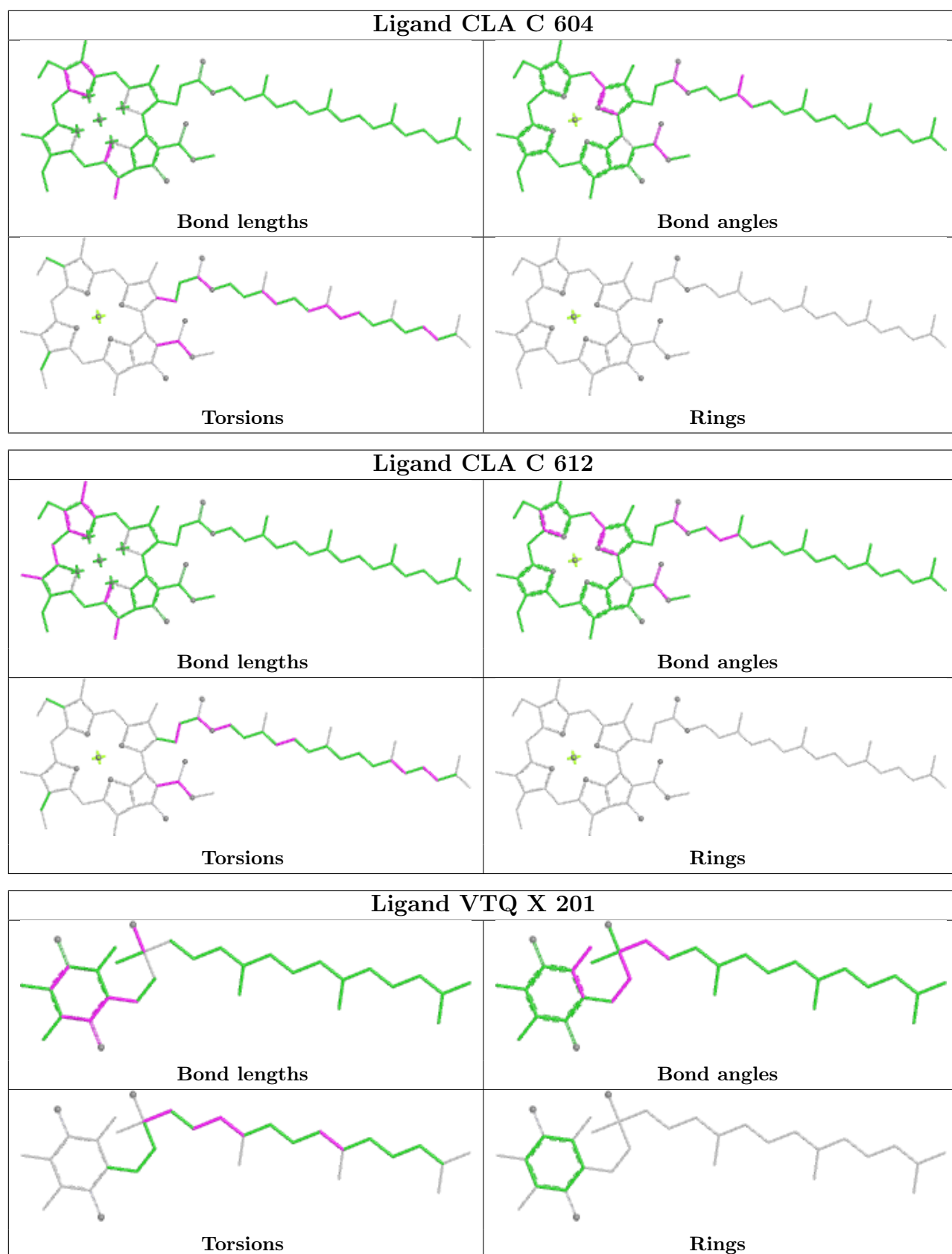


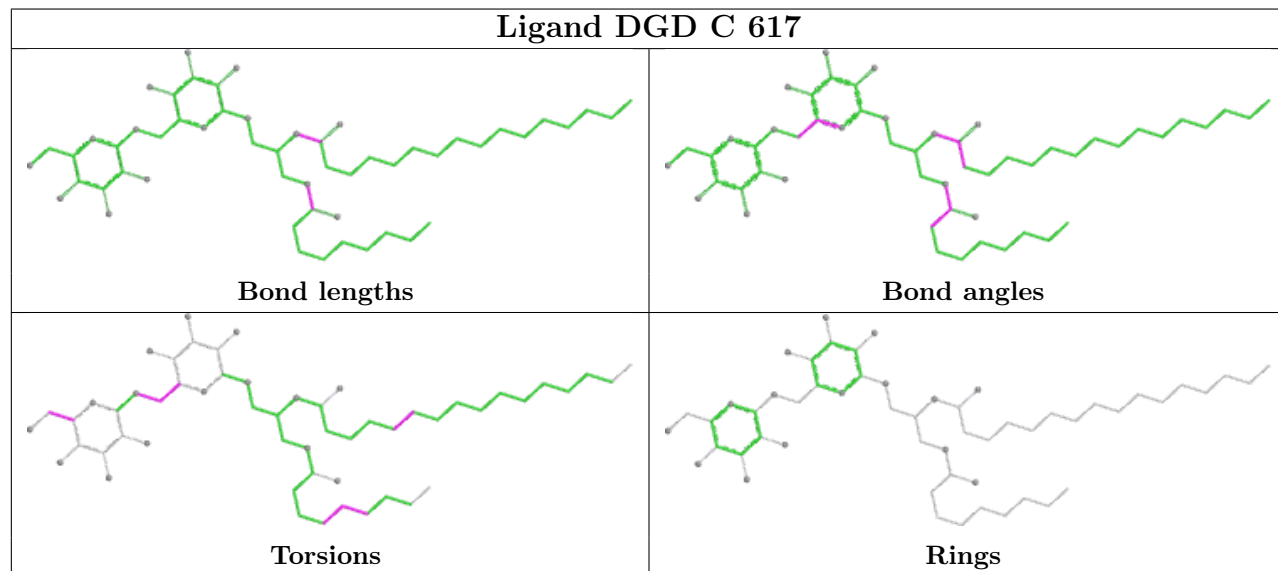
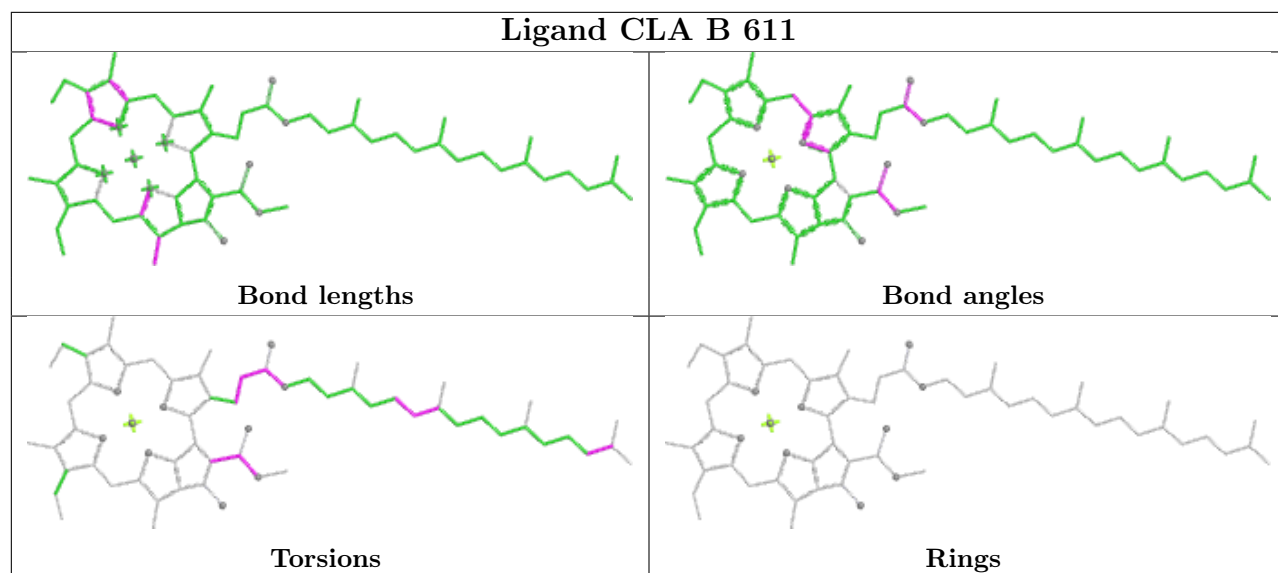
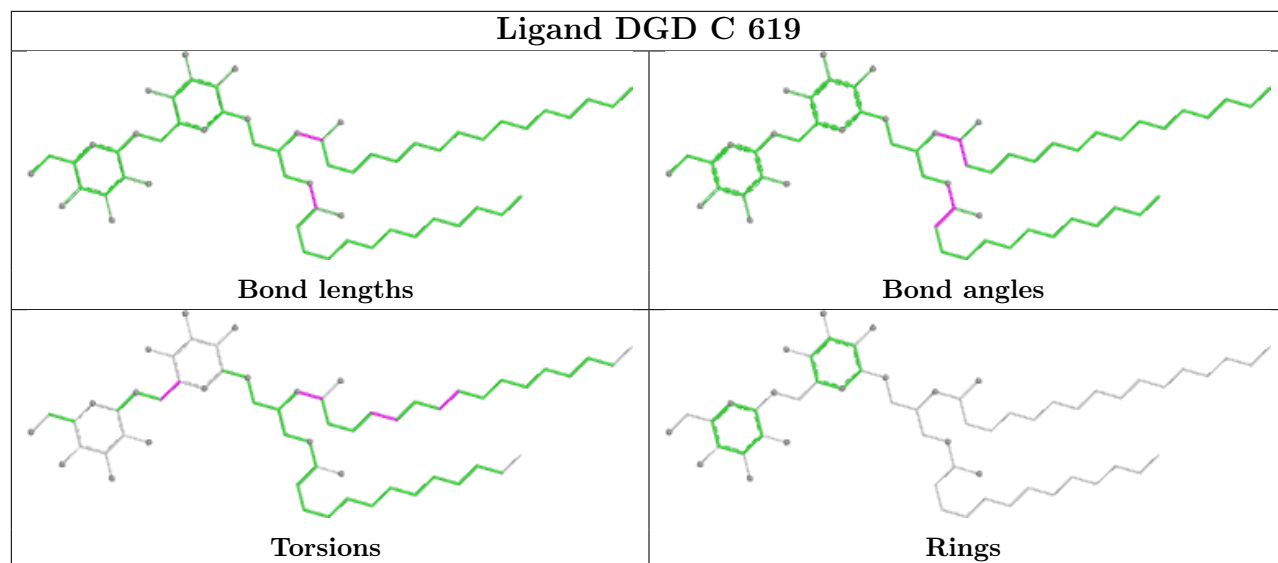


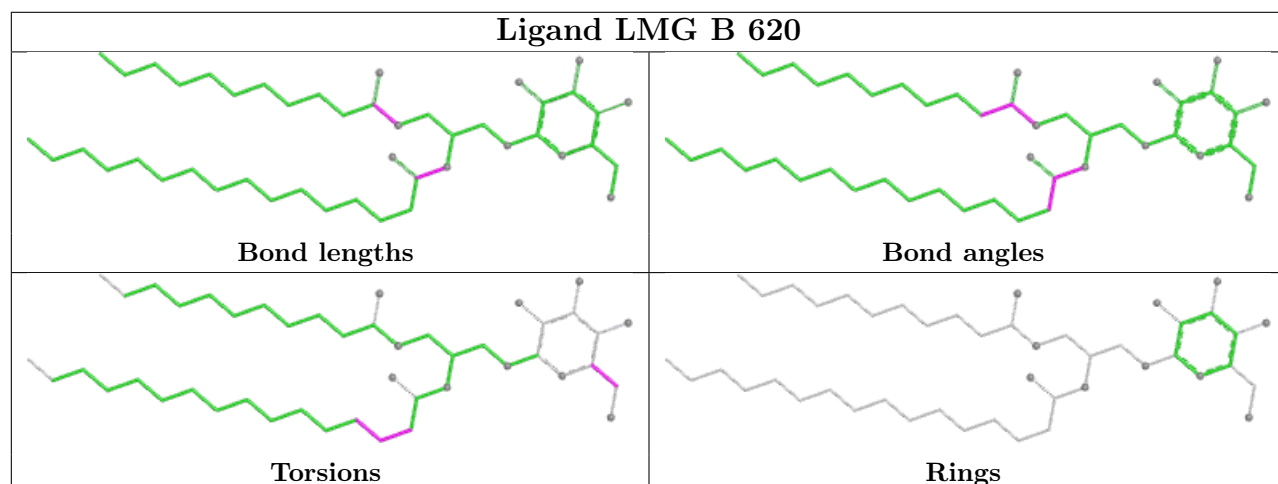
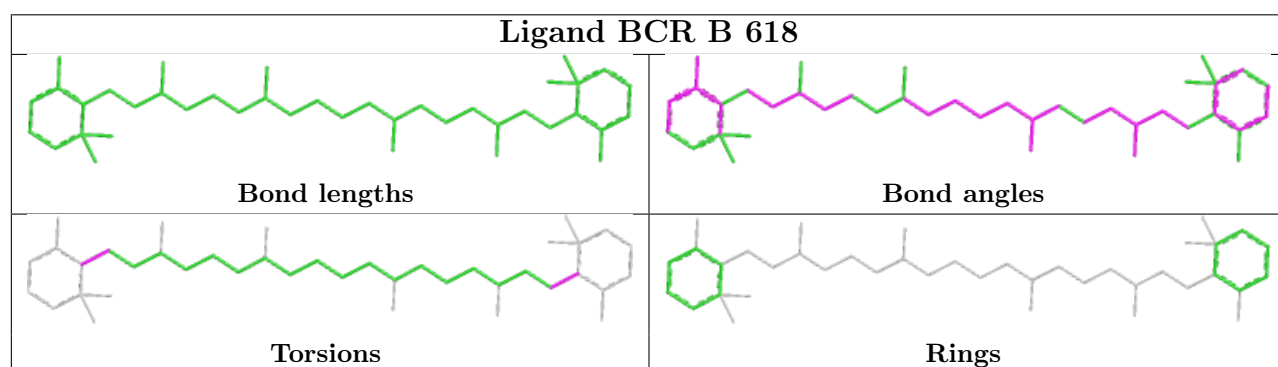
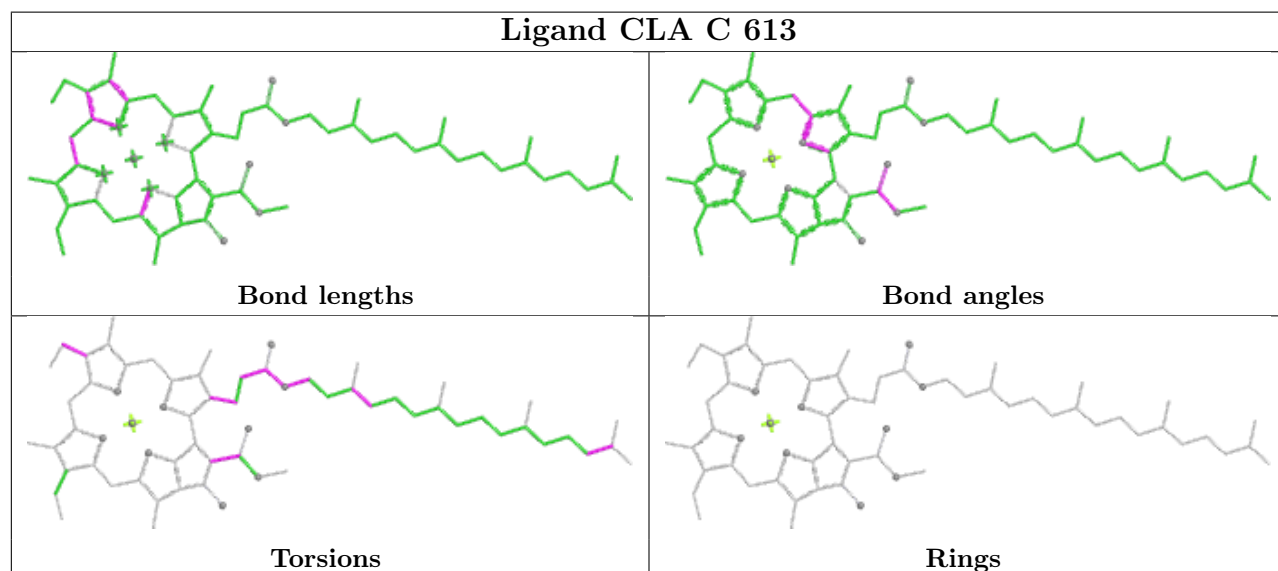
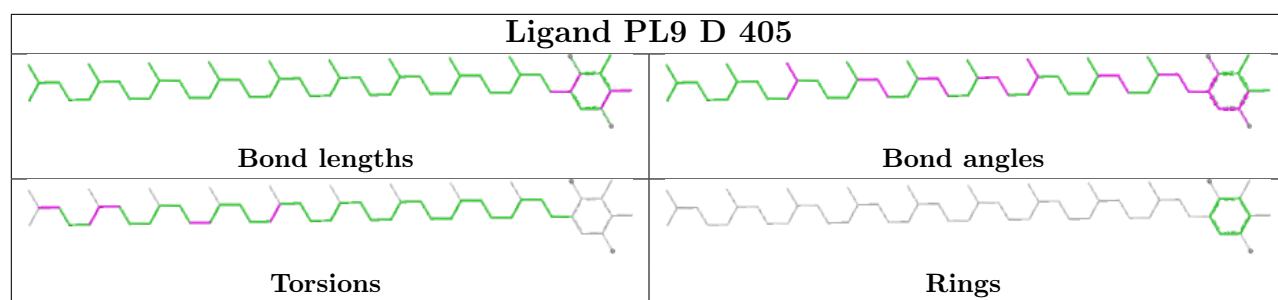


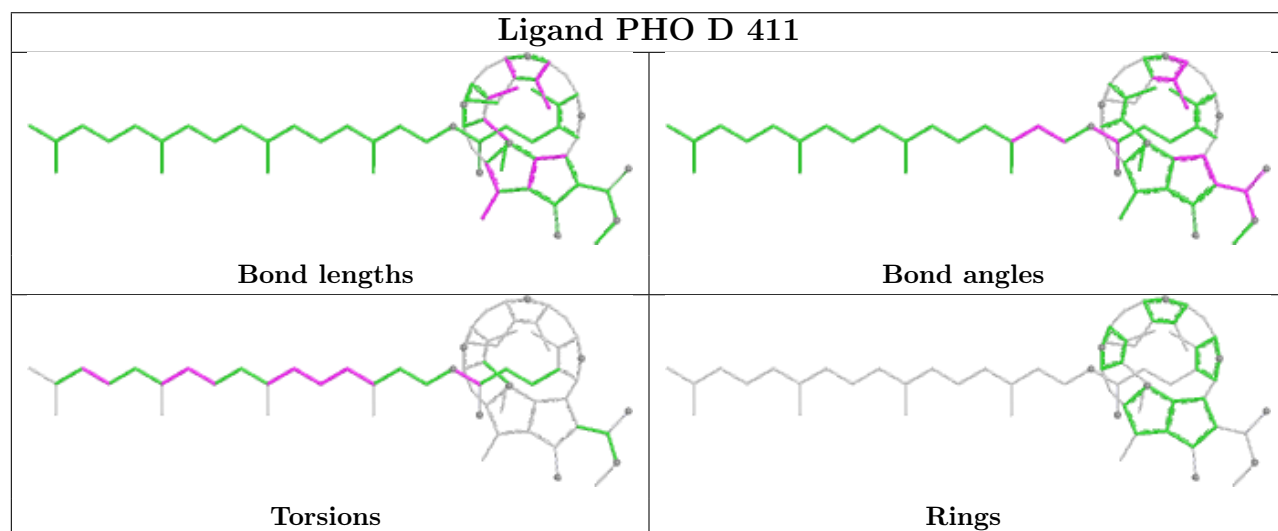
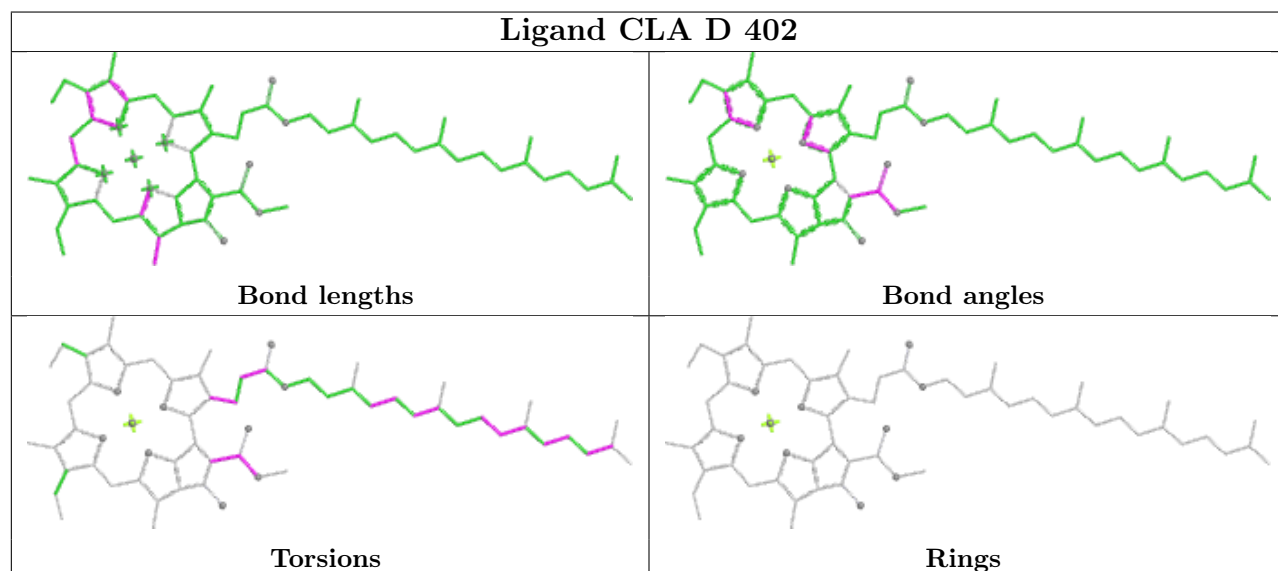
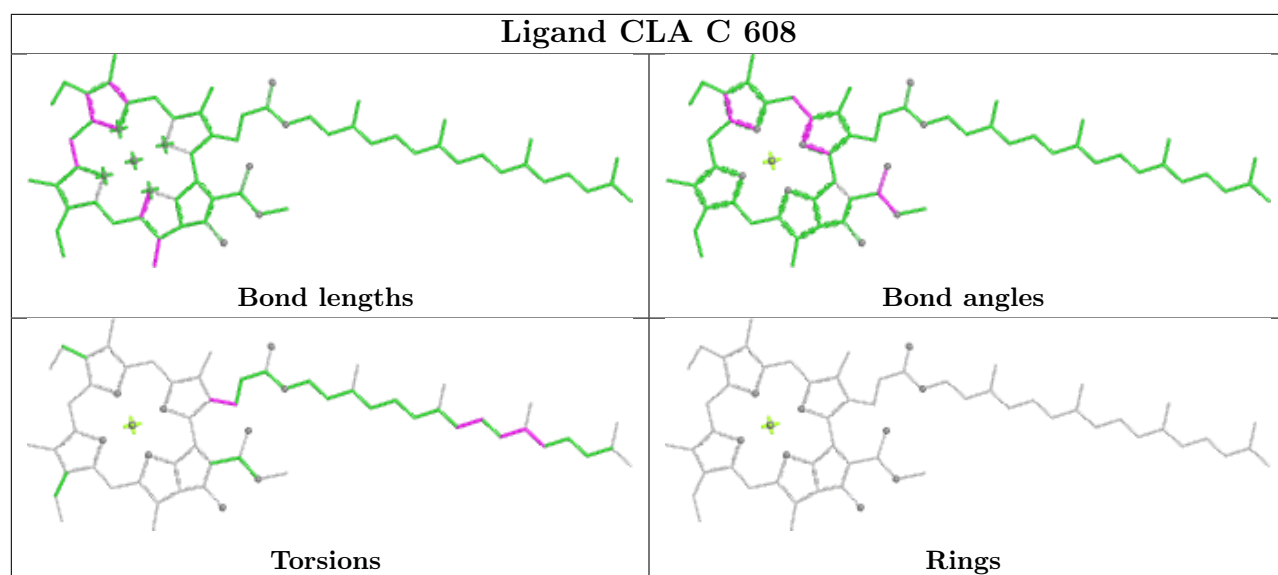


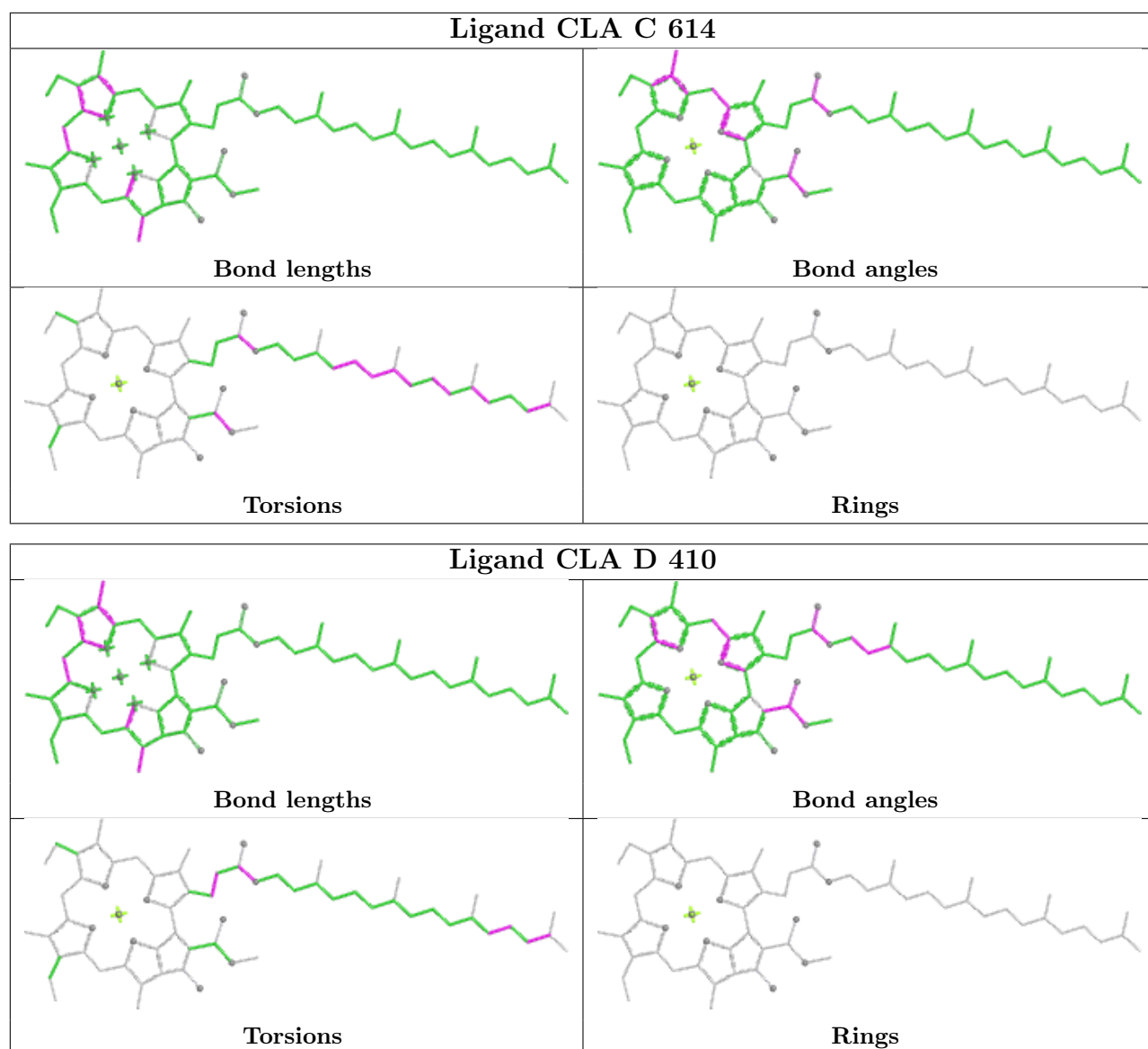
Ligand CLA C 602**Ligand LHG D 407**

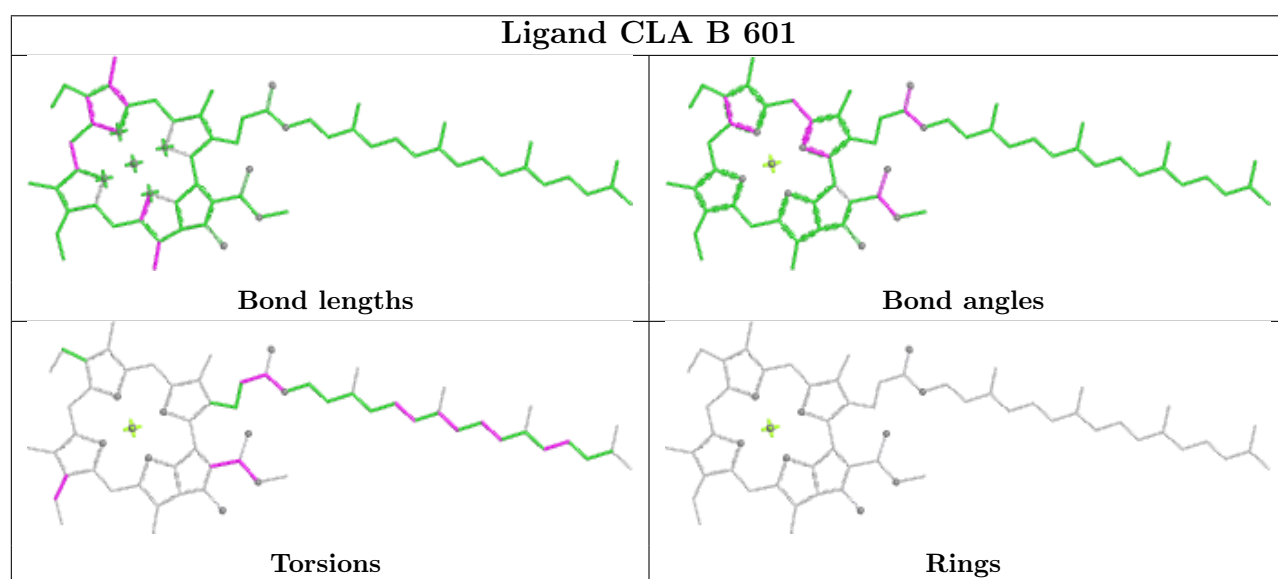
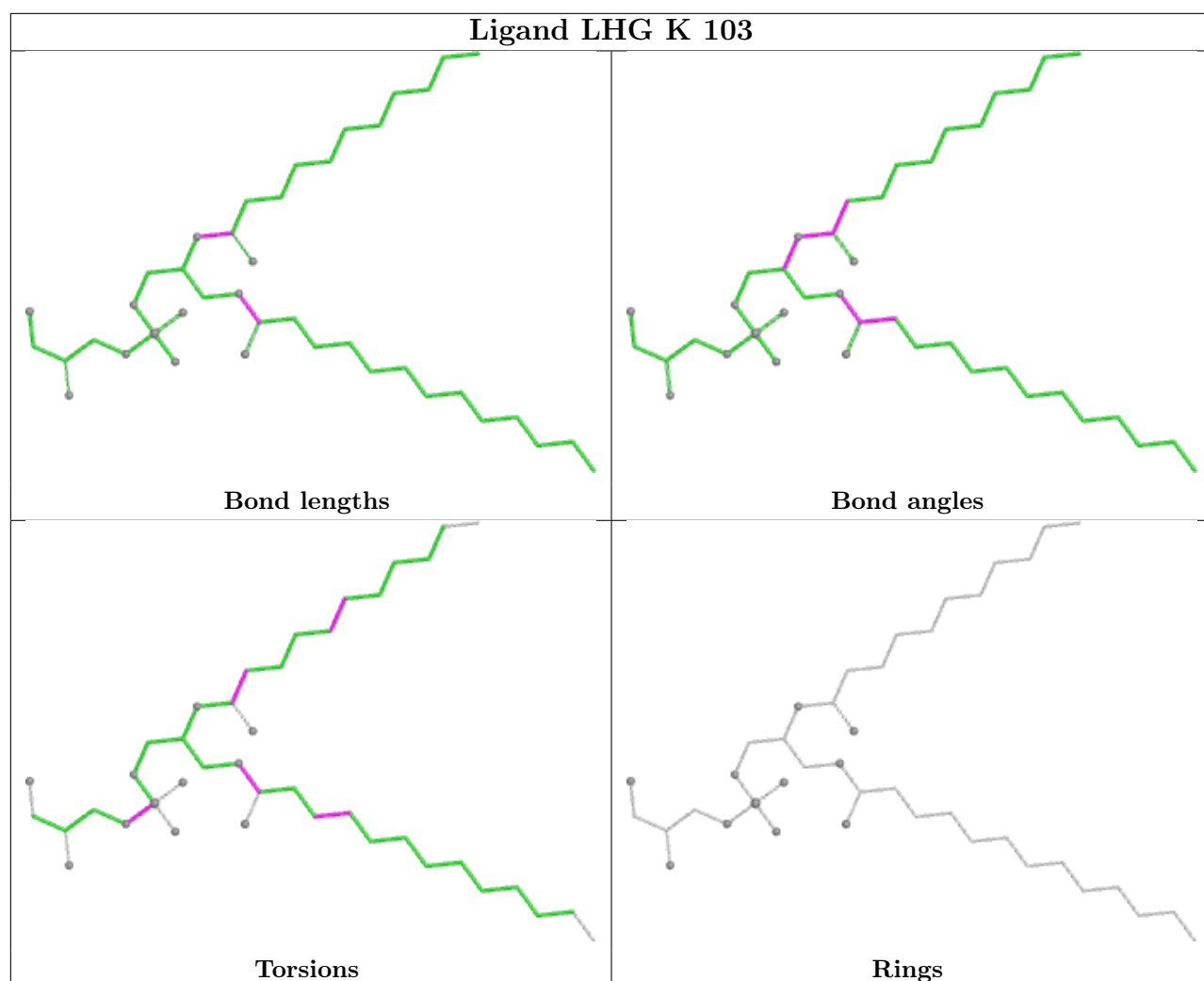


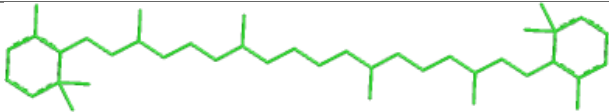
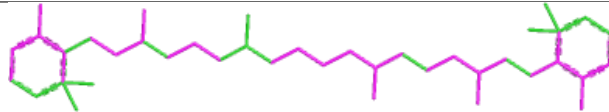
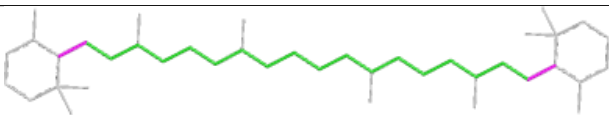
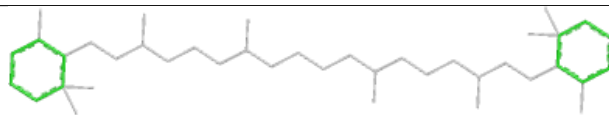


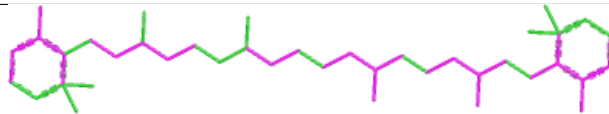
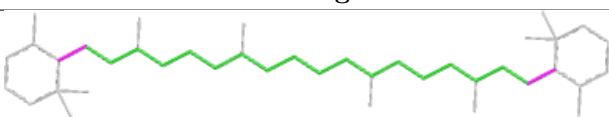
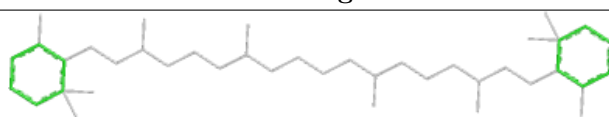


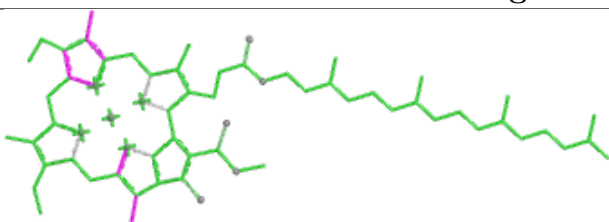
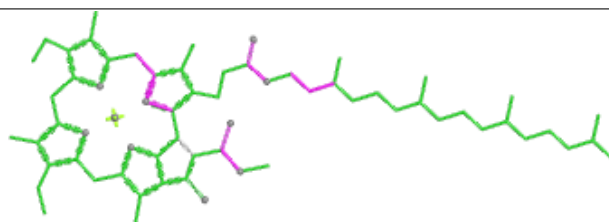
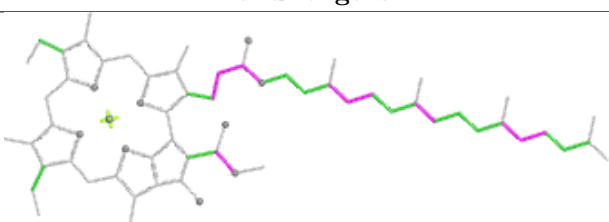
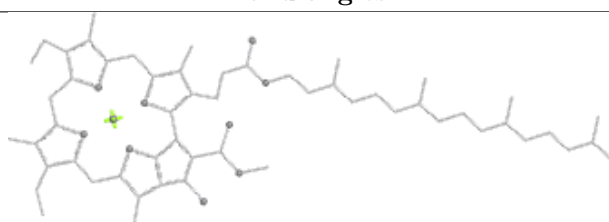


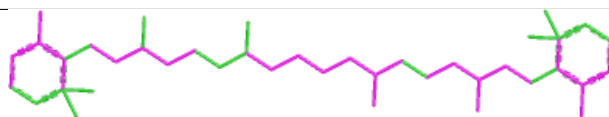
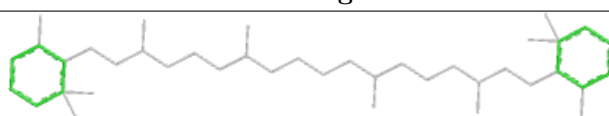


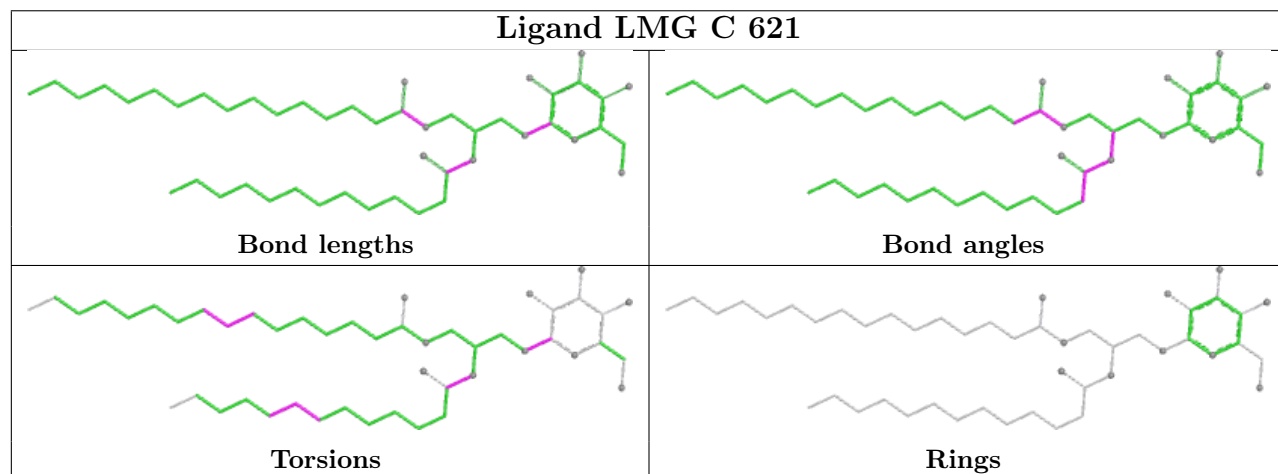
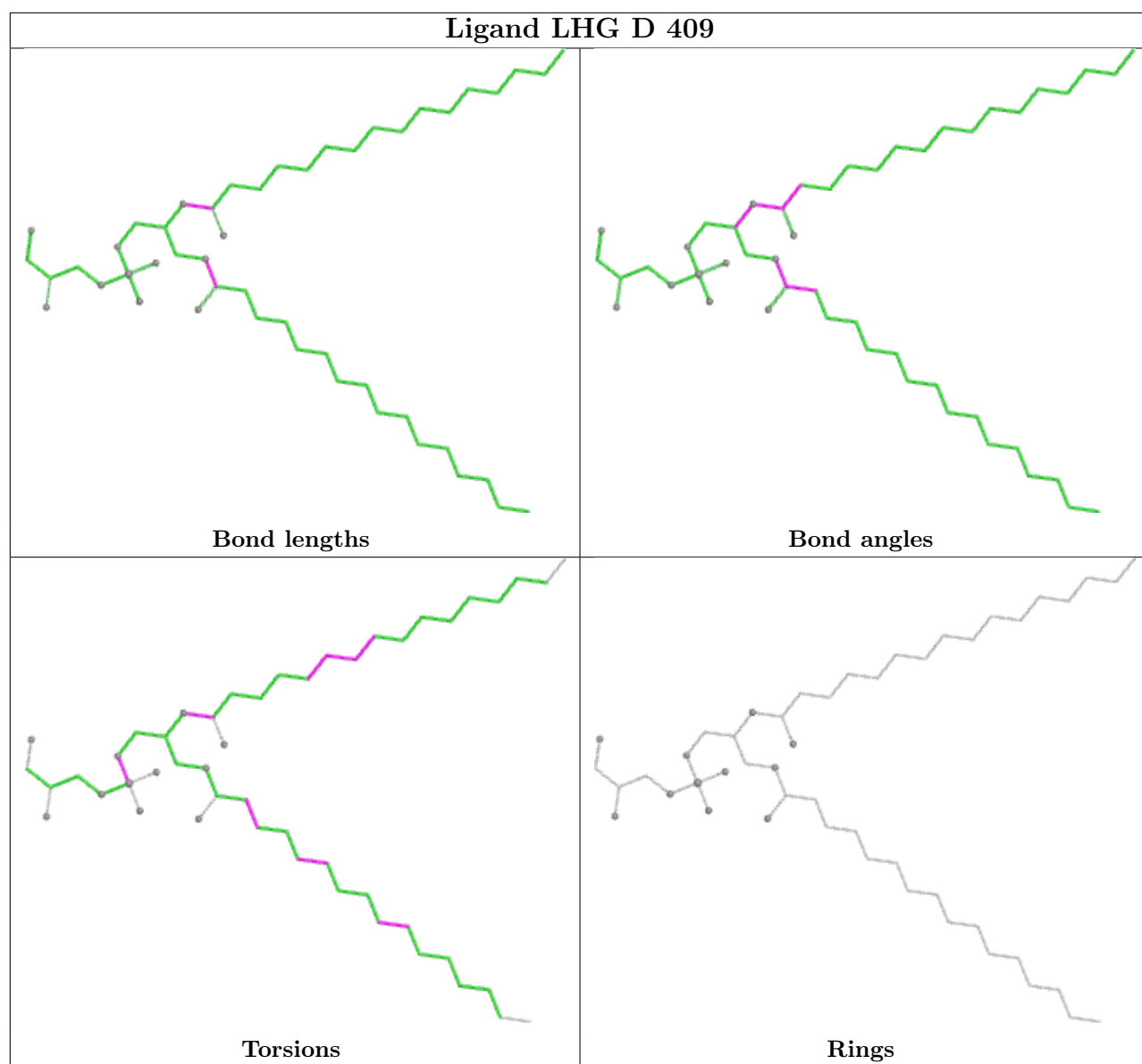


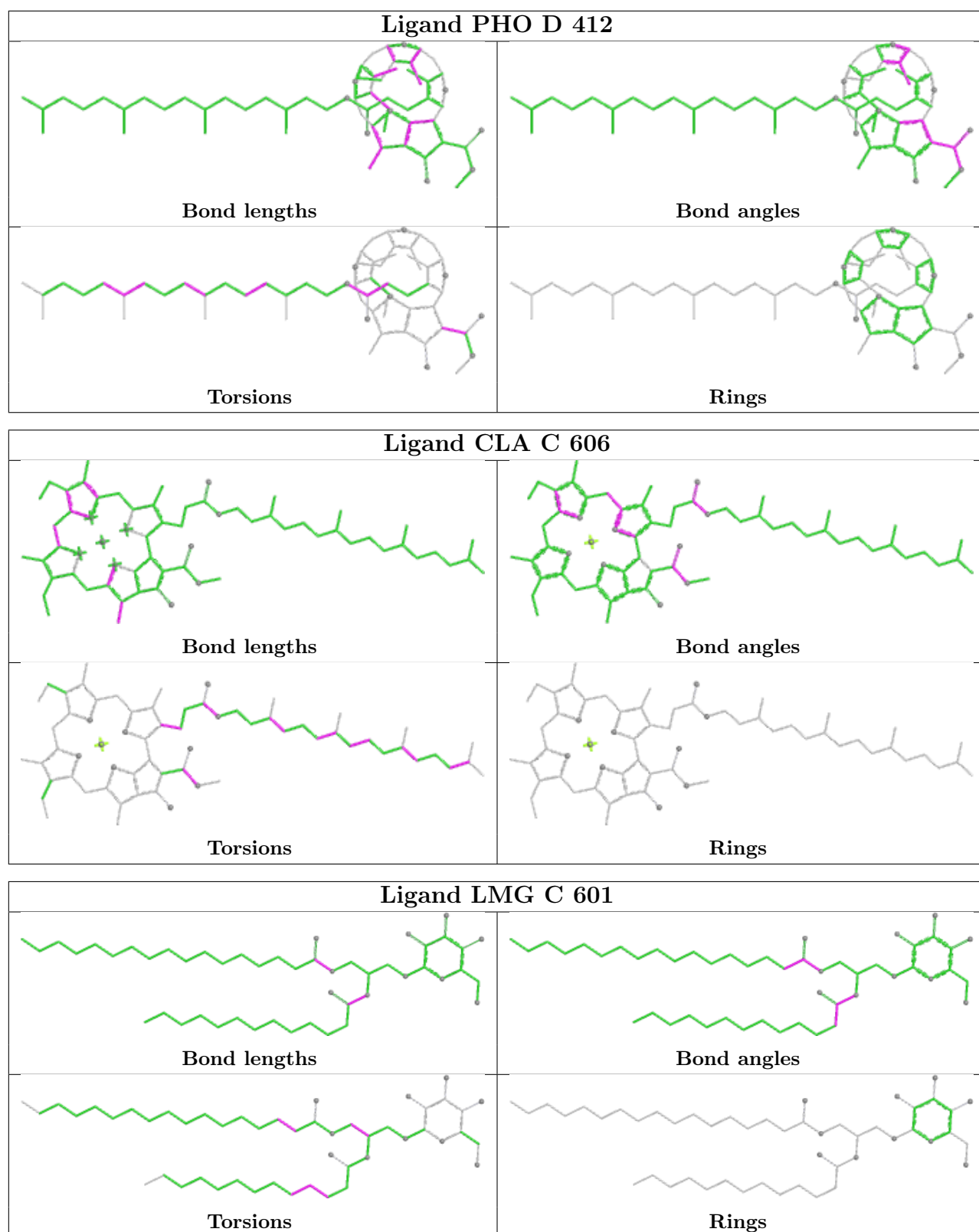
Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

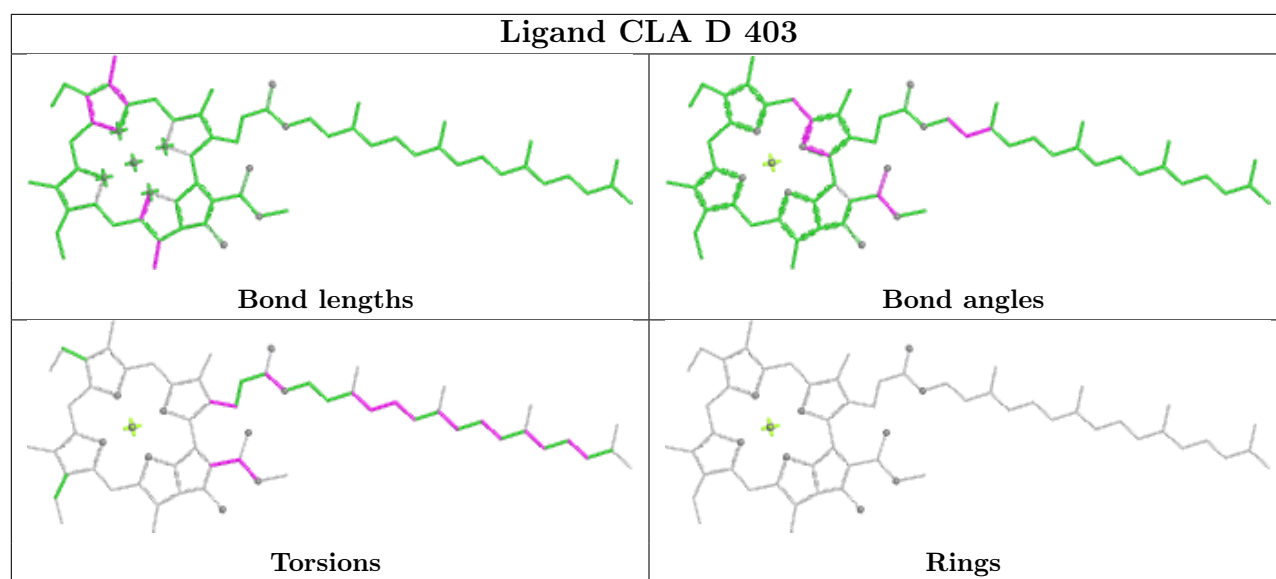
Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 405	
	
Bond lengths	Bond angles
	
Torsions	Rings







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.

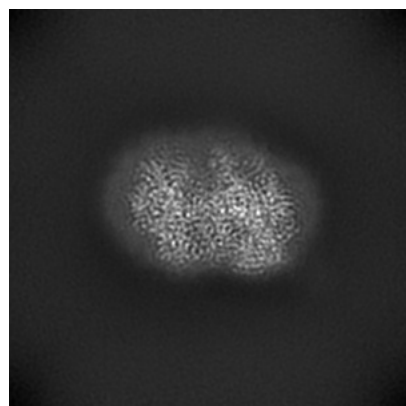
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60026. These allow visual inspection of the internal detail of the map and identification of artifacts.

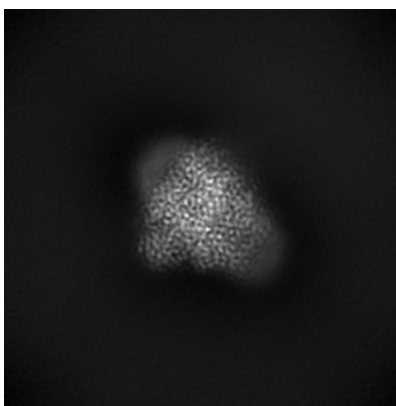
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

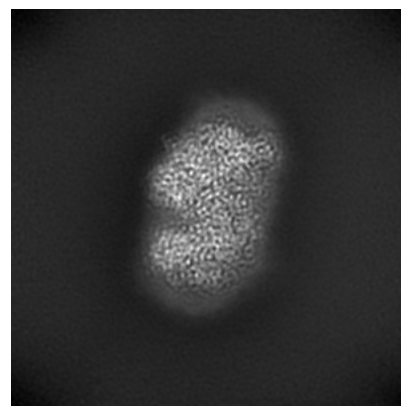
6.1.1 Primary map



X

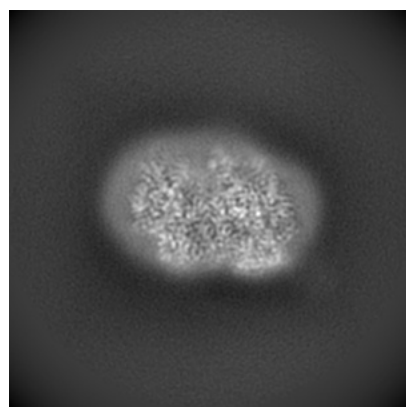


Y

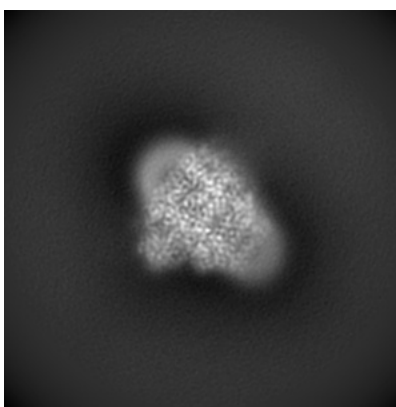


Z

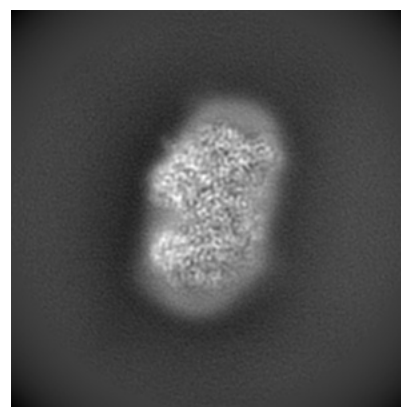
6.1.2 Raw map



X



Y

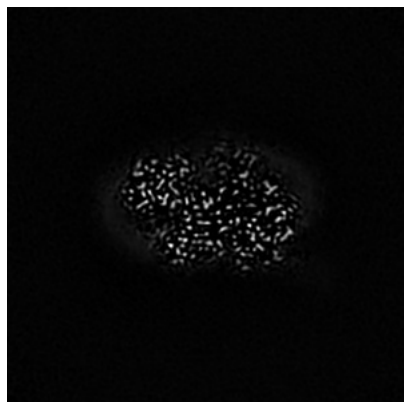


Z

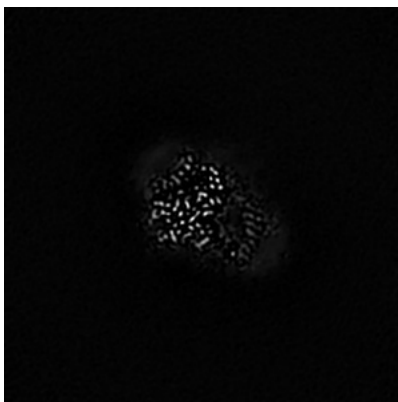
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

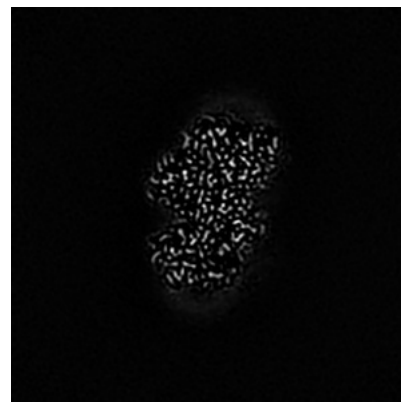
6.2.1 Primary map



X Index: 104

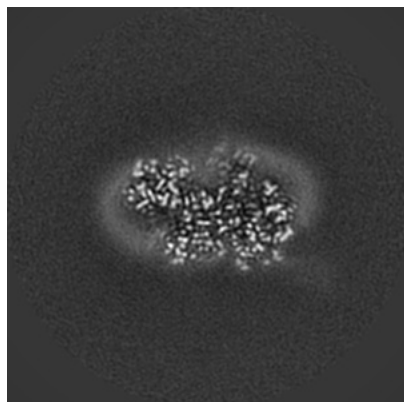


Y Index: 104

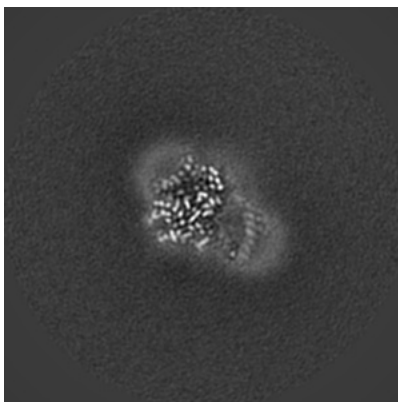


Z Index: 104

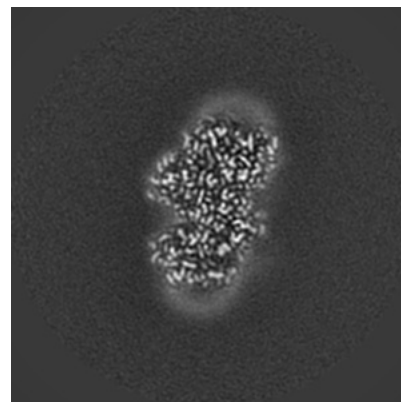
6.2.2 Raw map



X Index: 104



Y Index: 104

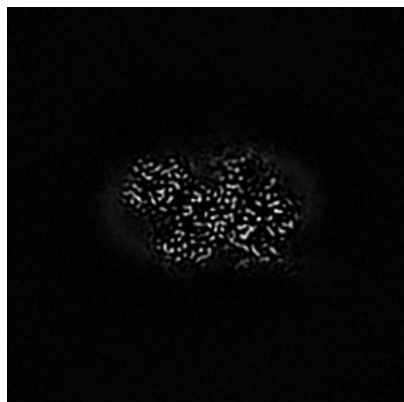


Z Index: 104

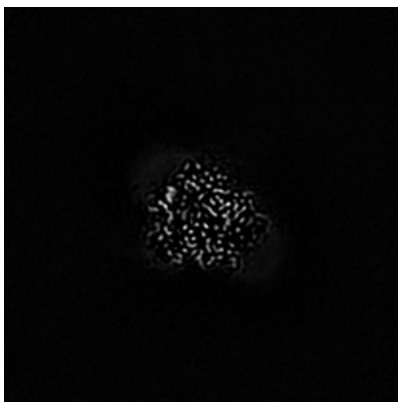
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

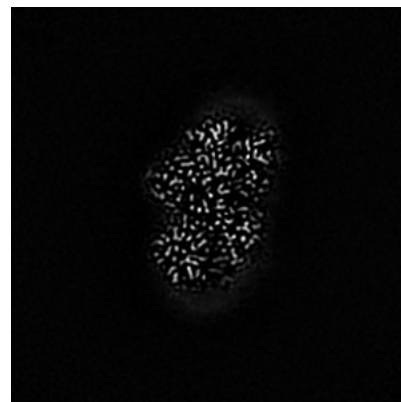
6.3.1 Primary map



X Index: 106

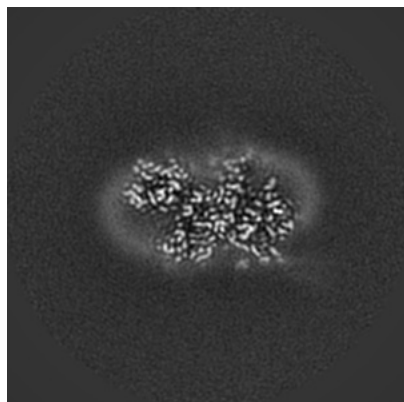


Y Index: 85

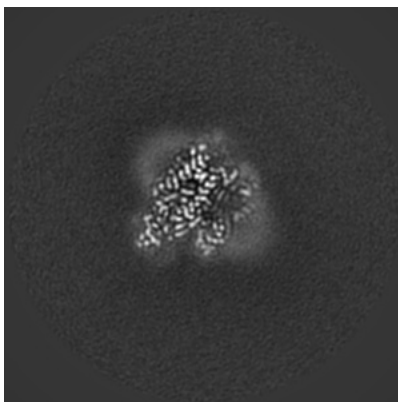


Z Index: 101

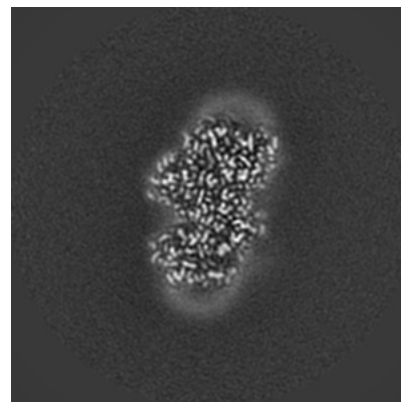
6.3.2 Raw map



X Index: 106



Y Index: 129

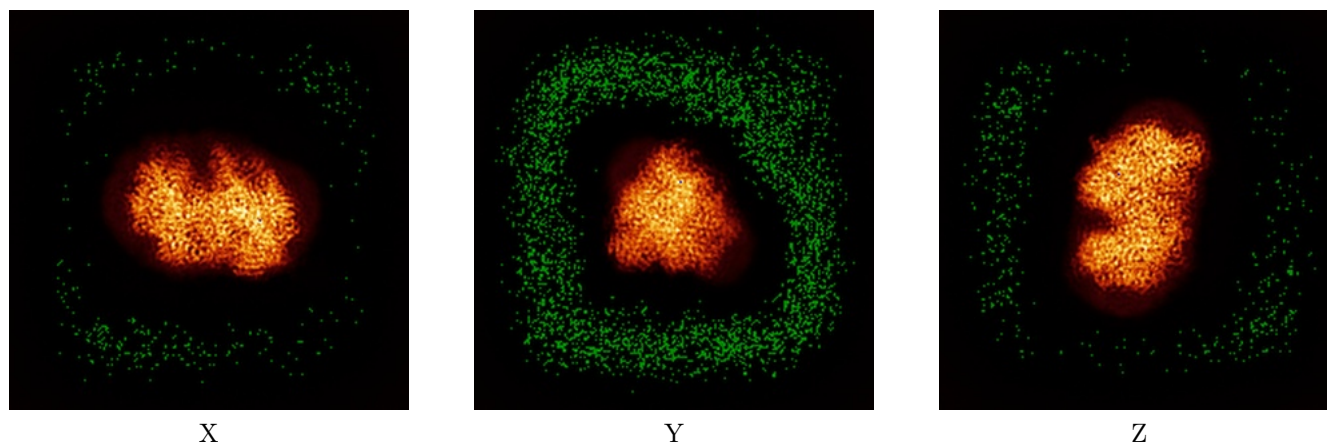


Z Index: 104

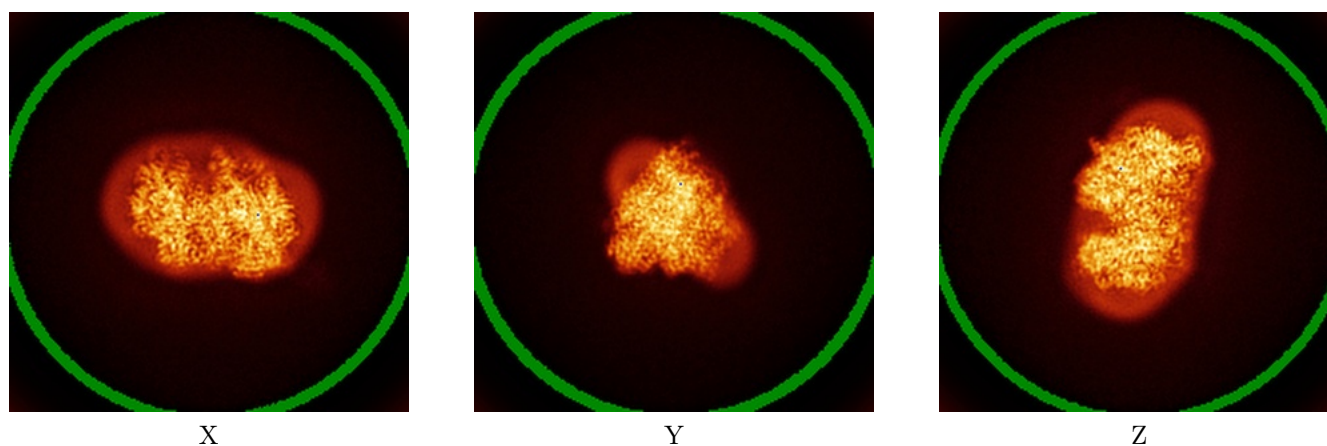
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

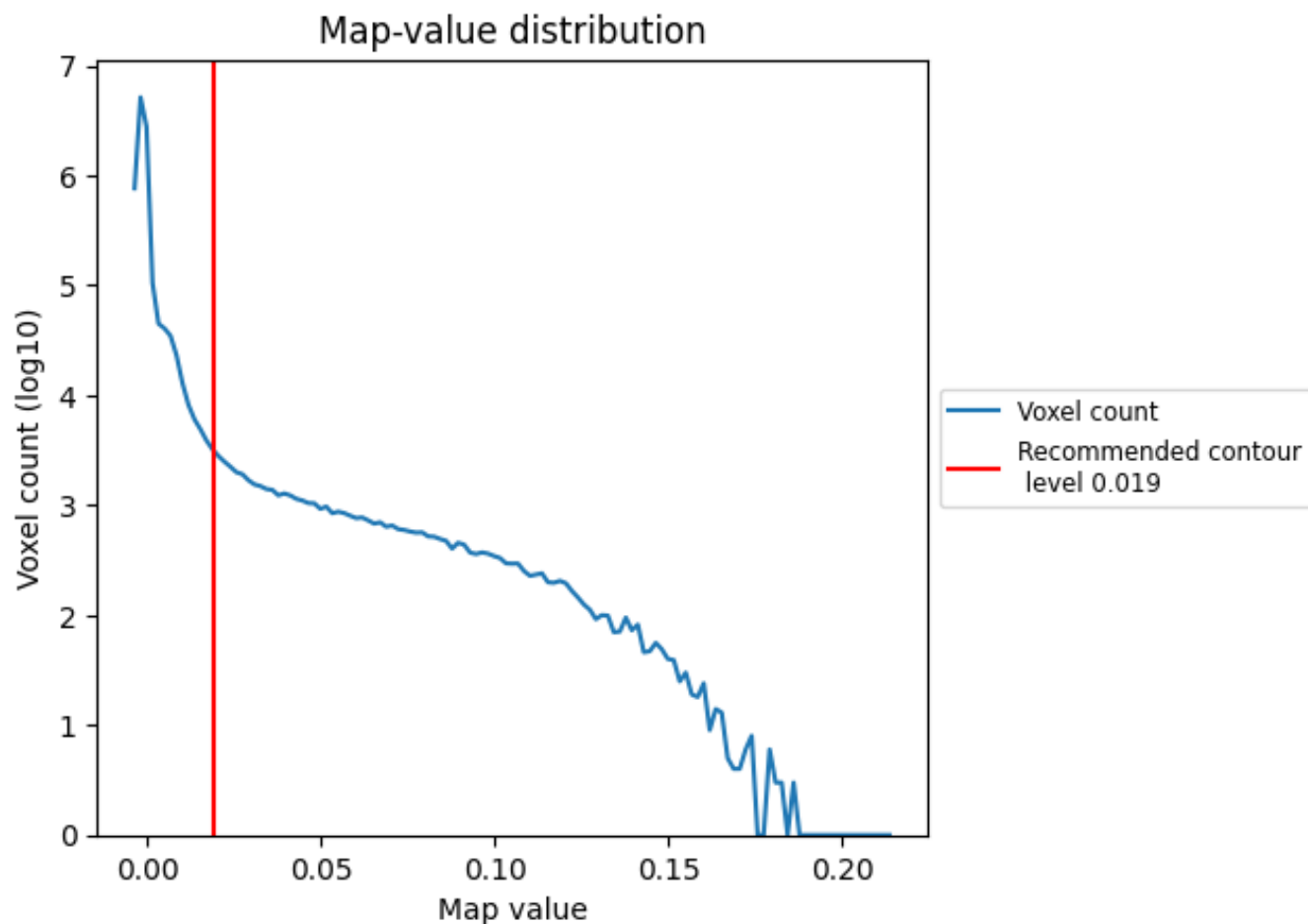
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

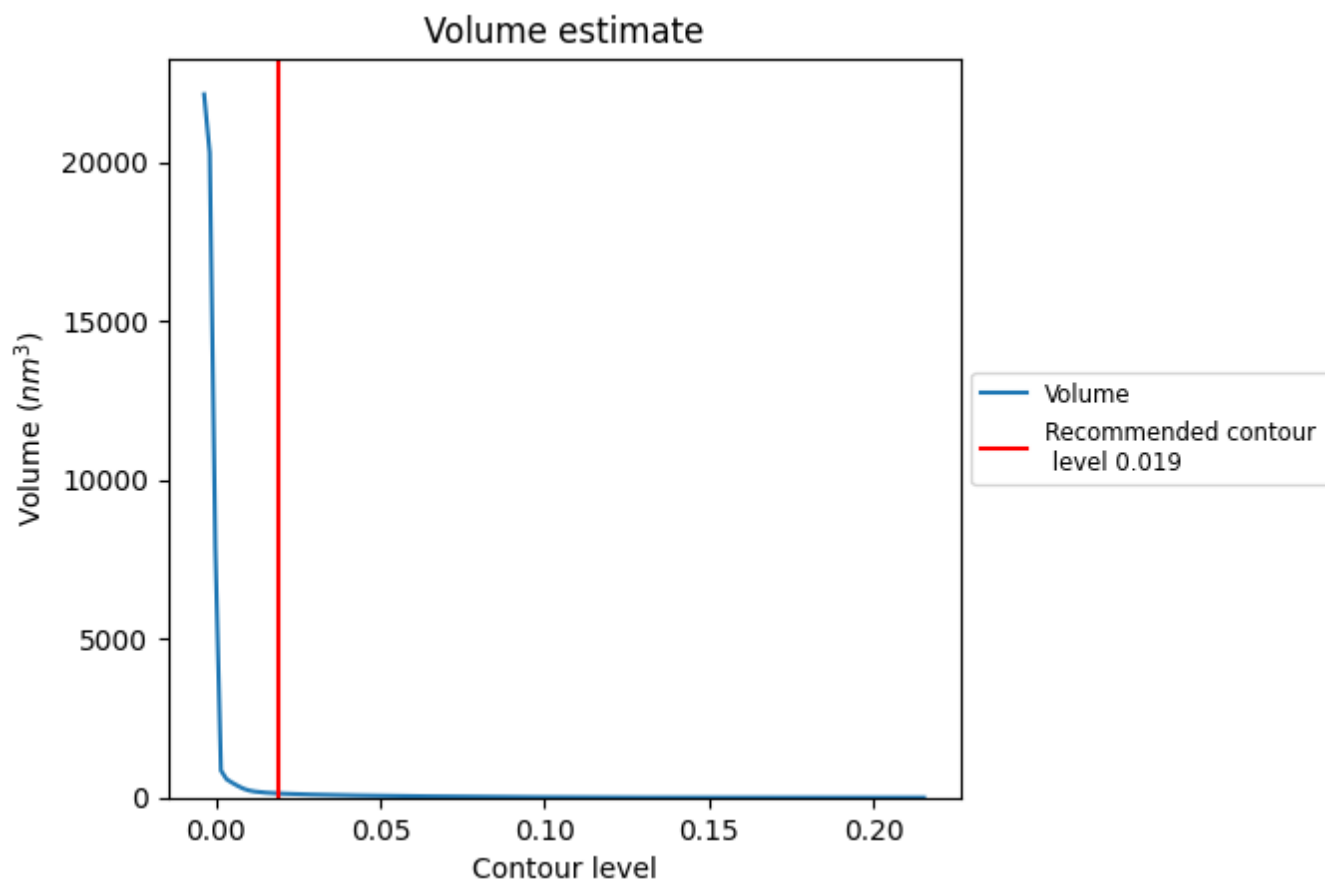
This section contains the results of statistical analysis of the map.

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.

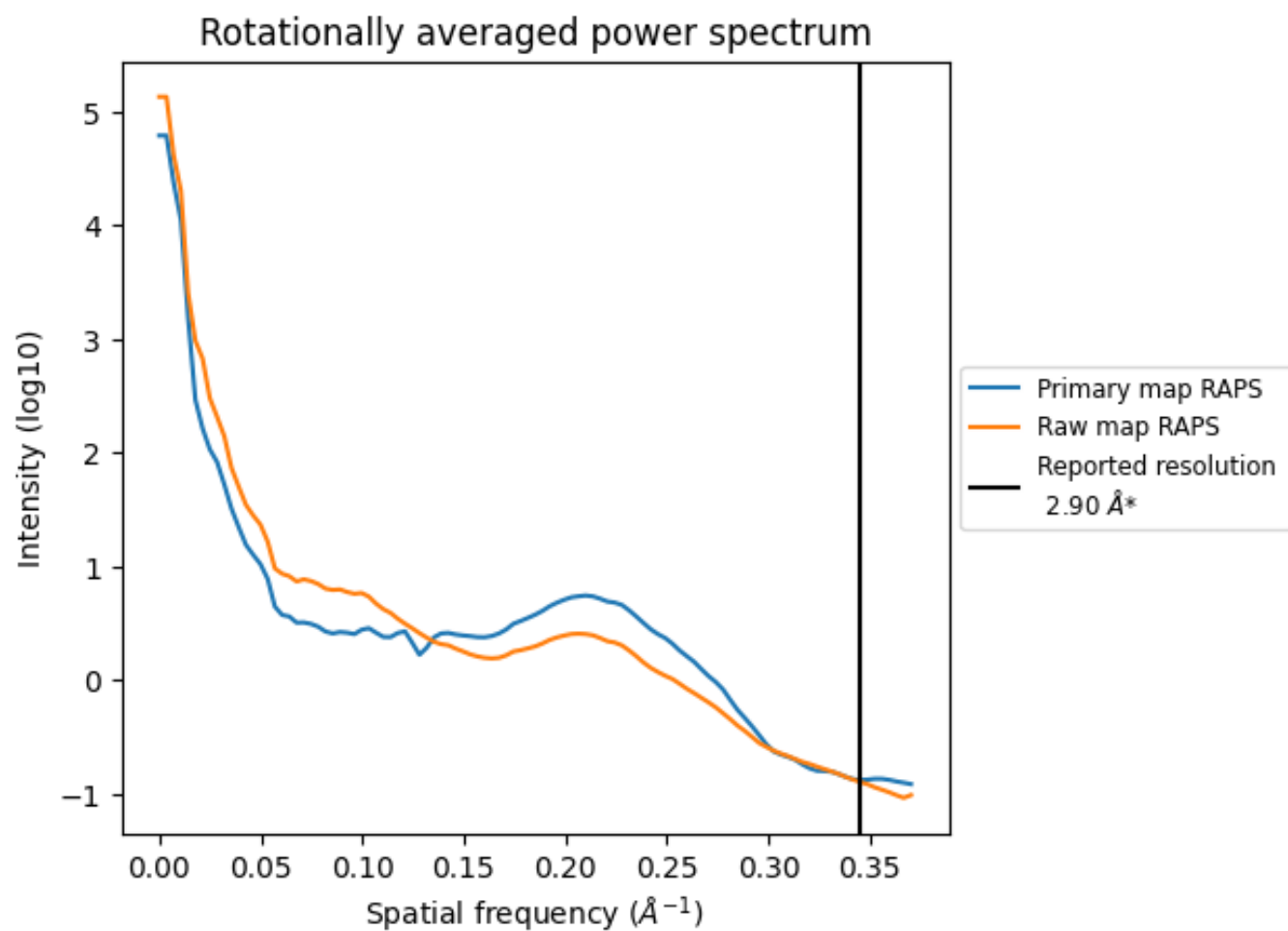
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 130 nm³; this corresponds to an approximate mass of 117 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

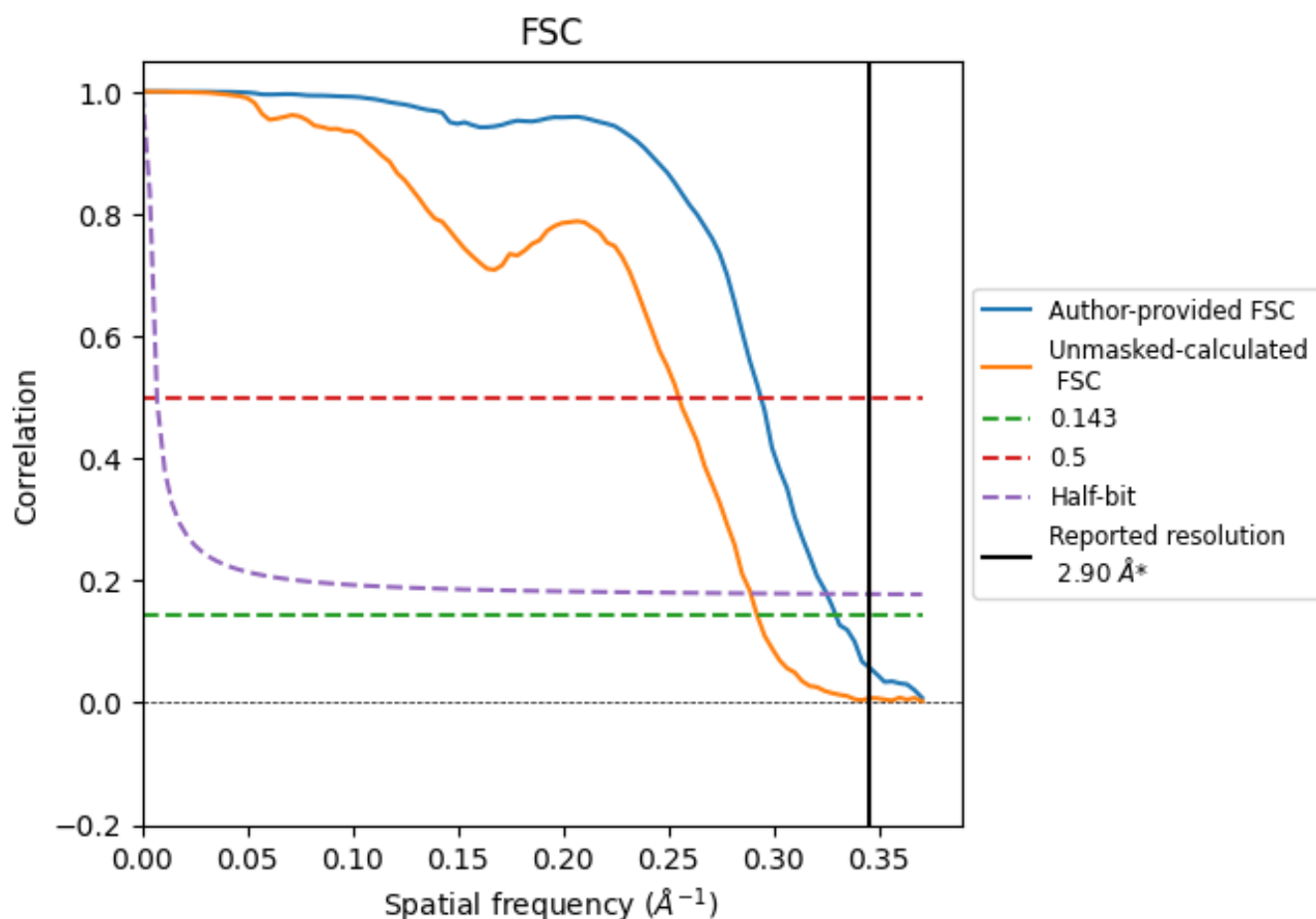


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

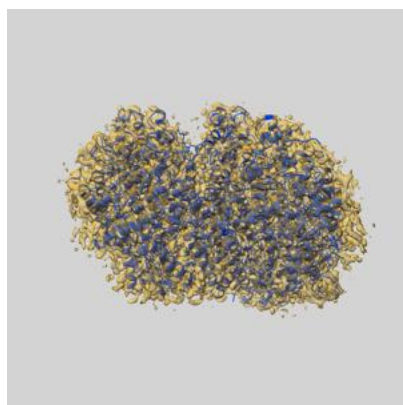
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	3.04	3.40	3.08
Unmasked-calculated*	3.42	3.92	3.46

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.42 differs from the reported value 2.9 by more than 10 %

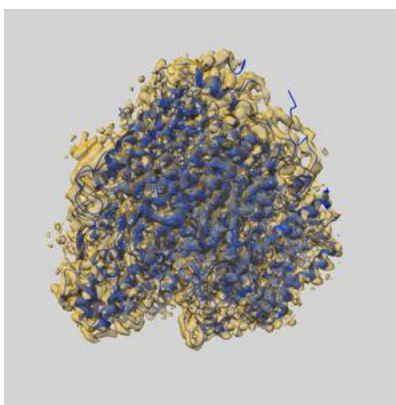
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60026 and PDB model 8ZEE. Per-residue inclusion information can be found in section 3 on page 17.

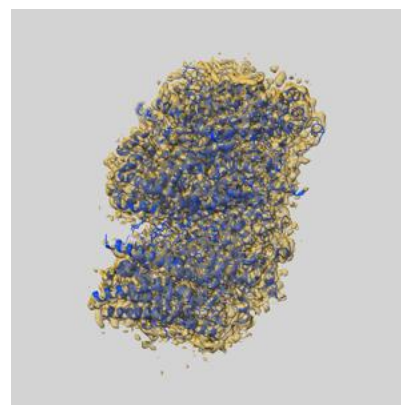
9.1 Map-model overlay [i](#)



X



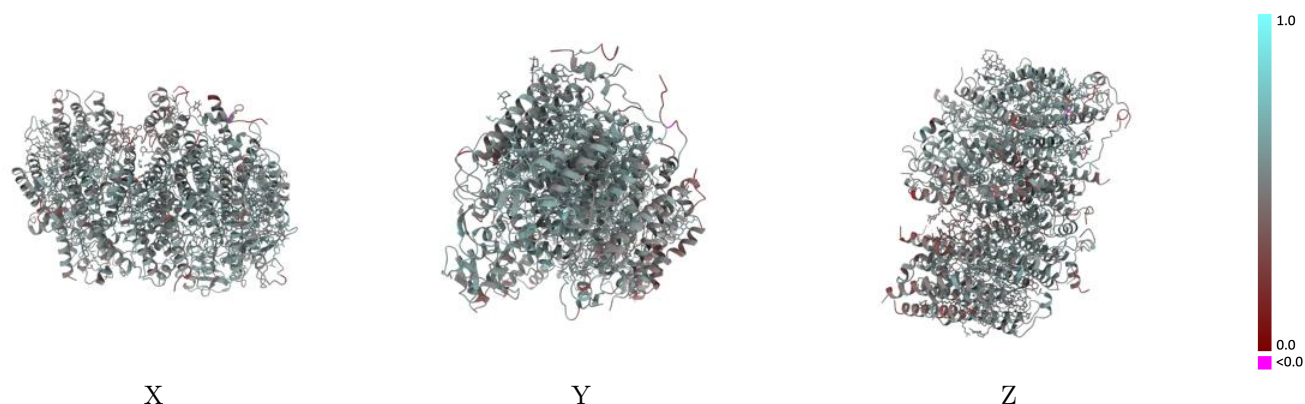
Y



Z

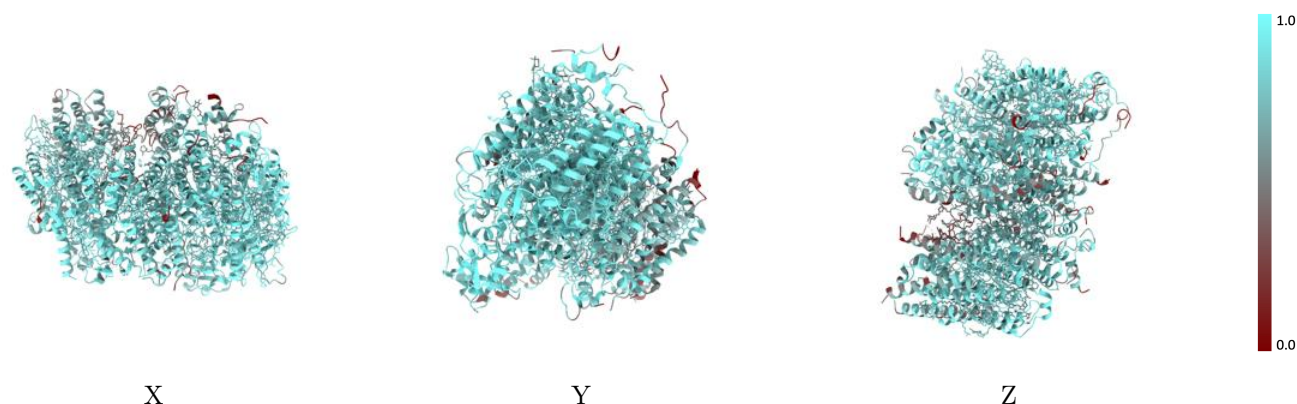
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



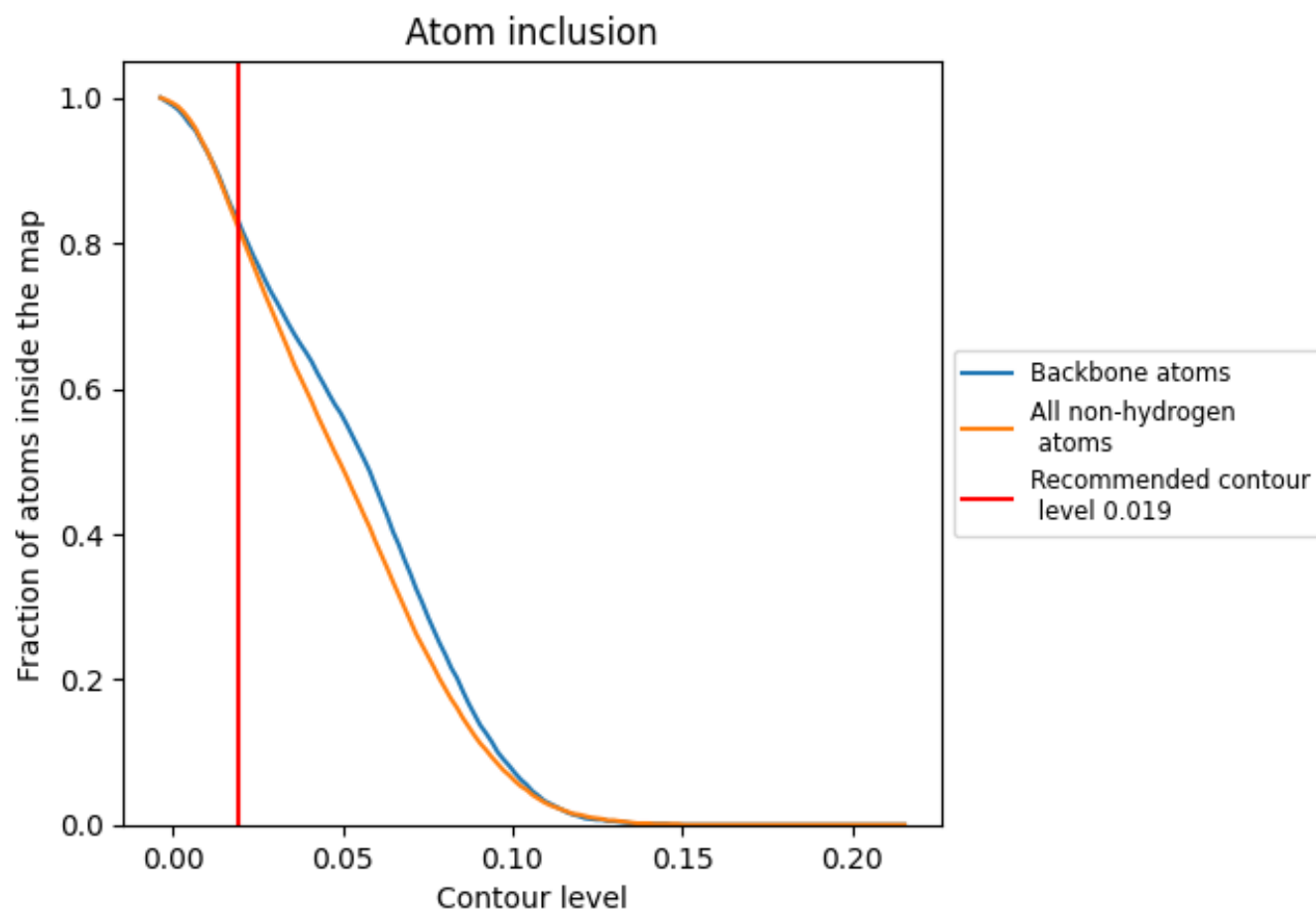
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.019).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8240	 0.5180
1	 0.5220	 0.4240
A	 0.8550	 0.5230
B	 0.8810	 0.5440
C	 0.8350	 0.5190
D	 0.8550	 0.5380
E	 0.7870	 0.4950
F	 0.7600	 0.4810
H	 0.8090	 0.5080
I	 0.7750	 0.4920
K	 0.6780	 0.4490
L	 0.7920	 0.5040
M	 0.6670	 0.4450
T	 0.7370	 0.4750
V	 0.5270	 0.4180
X	 0.6020	 0.4440
Z	 0.6390	 0.4300

