



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:25 AM UTC

PDB ID : 7UEA / pdb_00007uea
EMDB ID : EMD-26469
Title : Photosynthetic assembly of Chlorobaculum tepidum (RC-FMO1)
Authors : Puskar, R.; Truong, C.D.; Swain, K.; Li, S.; Cheng, K.-W.; Wang, T.Y.; Poh, Y.-P.; Liu, H.; Chou, T.-F.; Nannenga, B.; Chiu, P.-L.
Deposited on : 2022-03-21
Resolution : 3.49 Å(reported)
Based on initial model : 6M32

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:

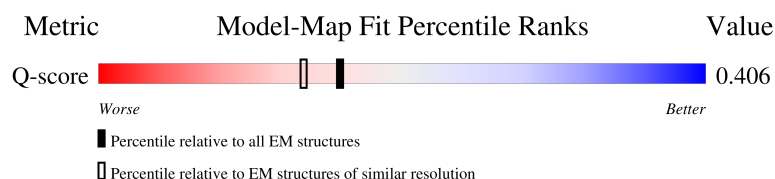
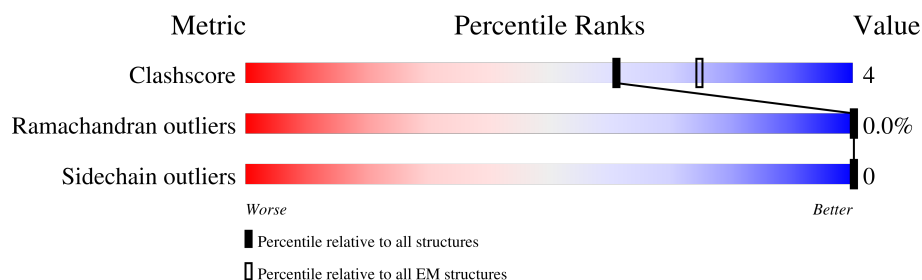
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.49 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	13600 (2.99 - 3.99)

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

Mol	Chain	Length	Quality of chain
1	A	731	8% 80% 8% 12%
1	a	731	8% 77% 10% 13%
2	B	231	14% 44% 52%
3	C	206	35% 50% 6% 43%

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Mol	Chain	Length	Quality of chain
3	c	206	
4	D	143	
5	U	366	
5	V	366	
5	W	366	

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
13	G2O	A	824	X	-	-	-
13	G2O	a	801	X	-	-	-
13	G2O	a	802	X	-	-	-
13	G2O	a	805	X	-	-	-
6	GS0	A	801	X	-	-	-
6	GS0	a	804	X	-	-	-
9	F26	a	820	-	X	-	-

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 26313 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 P840 reaction center, large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	645	Total	C	N	O	S	0	0
			5167	3449	821	871	26		
1	a	633	Total	C	N	O	S	0	0
			5079	3398	804	852	25		

- Molecule 2 is a protein called Photosystem P840 reaction center iron-sulfur protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	110	Total	C	N	O	S	0	0
			855	545	143	158	9		

- Molecule 3 is a protein called Cytochrome c.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	117	Total	C	N	O	S	0	0
			916	617	142	150	7		
3	c	105	Total	C	N	O	S	0	0
			839	565	130	138	6		

- Molecule 4 is a protein called P840 reaction center 17 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	100	Total	C	N	O	S	0	0
			817	520	144	149	4		

- Molecule 5 is a protein called Bacteriochlorophyll a protein.

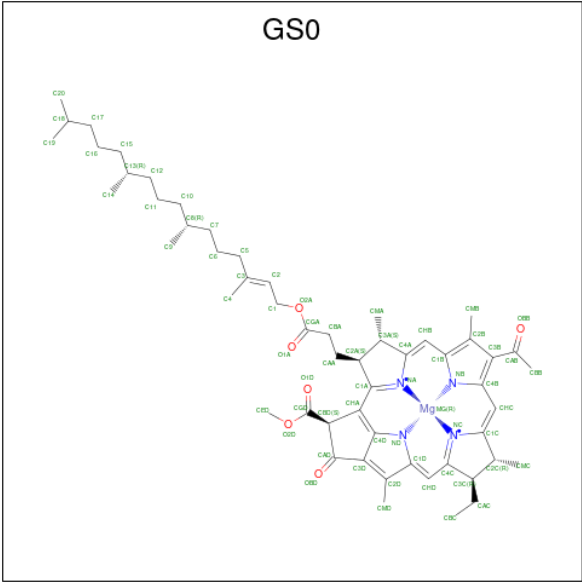
Mol	Chain	Residues	Atoms					AltConf	Trace
5	U	364	Total	C	N	O	S	0	0
			2834	1798	503	526	7		
5	V	360	Total	C	N	O	S	0	0
			2805	1778	499	521	7		

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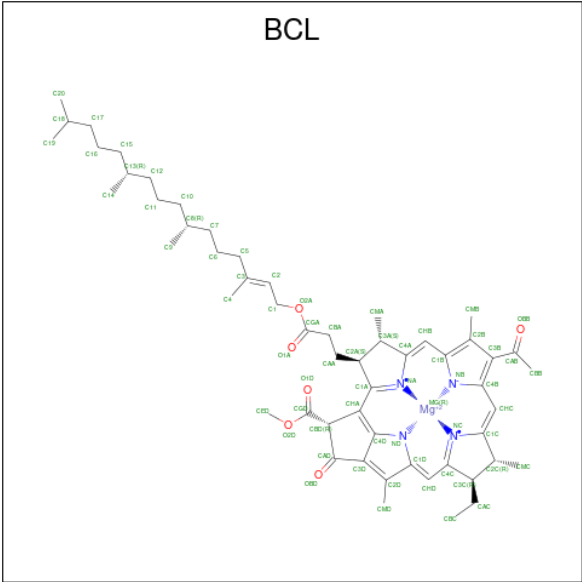
Mol	Chain	Residues	Atoms					AltConf	Trace
5	W	359	Total	C	N	O	S	0	0
			2797	1774	497	519	7		

- Molecule 6 is Bacteriochlorophyll A isomer (CCD ID: GS0) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 7 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	A	1	Total 65	C 54	Mg 1	N 4	O 6	0
7	a	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	a	1	Total 66	C 55	Mg 1	N 4	O 6	0

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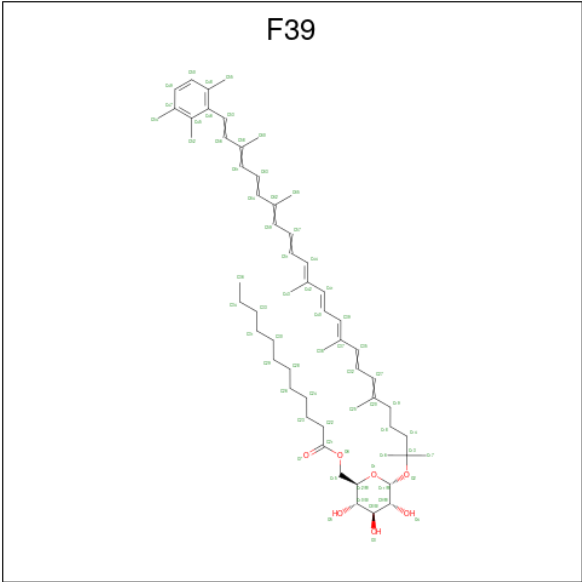
Mol	Chain	Residues	Atoms					AltConf
7	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
7	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	U	1	Total	C	Mg	N	O	1
			46	35	1	4	6	
7	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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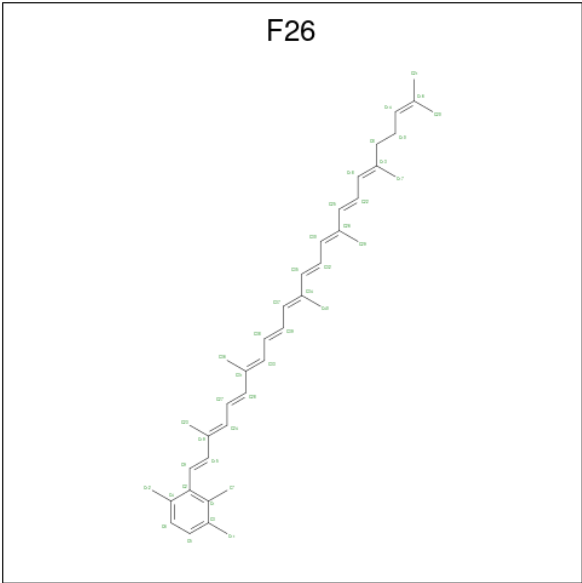
Mol	Chain	Residues	Atoms					AltConf
7	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	V	1	Total	C	Mg	N	O	1
			46	35	1	4	6	
7	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	W	1	Total	C	Mg	N	O	1
			46	35	1	4	6	

- Molecule 8 is [(2R,3S,4S,5R,6R)-6-[(10E,12E,14E)-2,6,10,14,19,23-hexamethyl-25-(2,3,6-trimethylphenyl)pentacos-6,8,10,12,14,16,18,20,22,24-decaen-2-yl]oxy-3,4,5-tris(oxidanyl)oxan-2-yl]methyl dodecanoate (CCD ID: F39) (formula: C₅₈H₈₆O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			65	58	7	
8	a	1	Total	C	O	0
			65	58	7	

- Molecule 9 is 2-[(1E,3E,5E,7E,9E,11E,13E,15E,17E,19E)-3,7,12,16,20,24-hexamethylpentaco sa-1,3,5,7,9,11,13,15,17,19,23-undecaenyl]-1,3,4-trimethyl-benzene (CCD ID: F26) (formula: C₄₀H₅₂) (labeled as "Ligand of Interest" by depositor).



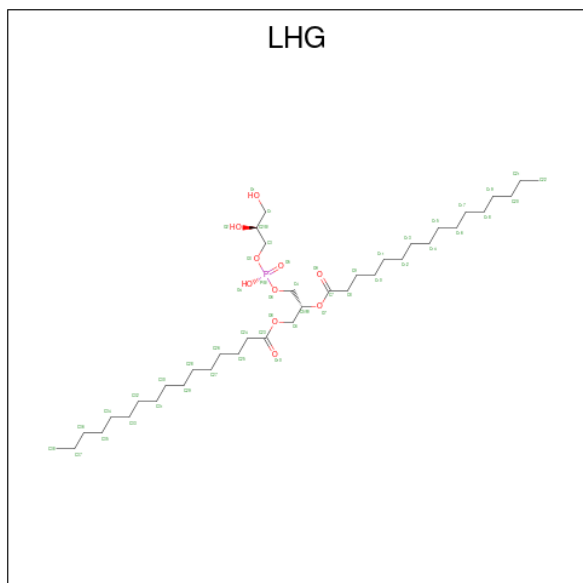
Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	C	0
			40	40	

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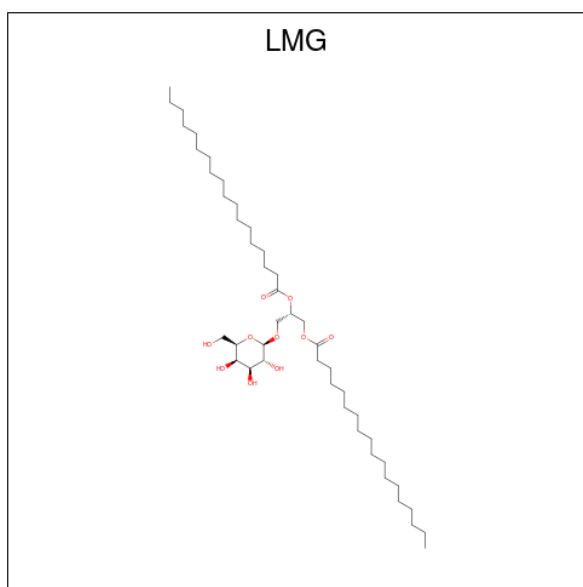
Mol	Chain	Residues	Atoms	AltConf
9	a	1	Total C 40 40	0
9	a	1	Total C 40 40	0

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



Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C O P 26 15 10 1	0
10	A	1	Total C O P 41 30 10 1	0
10	a	1	Total C O P 33 22 10 1	0
10	a	1	Total C O P 26 15 10 1	0
10	a	1	Total C O P 40 29 10 1	0
10	C	1	Total C O P 34 23 10 1	0

- Molecule 11 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).

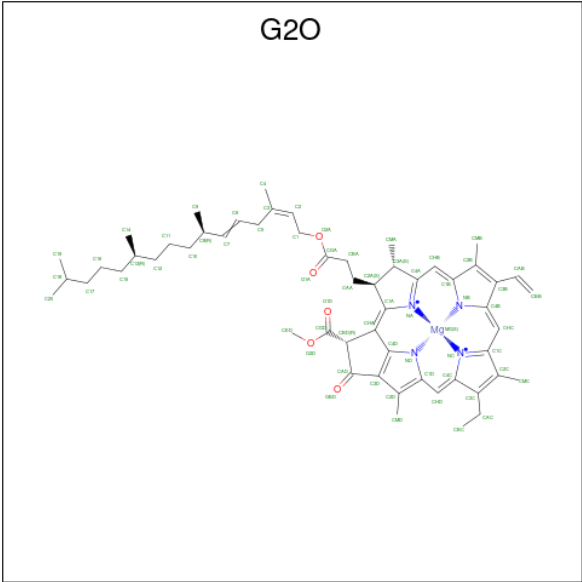


Mol	Chain	Residues	Atoms			AltConf
11	A	1	Total	C	O	0
			42	32	10	
11	A	1	Total	C	O	0
			39	29	10	
11	A	1	Total	C	O	0
			36	26	10	
11	A	1	Total	C	O	0
			27	17	10	
11	A	1	Total	C	O	0
			30	20	10	
11	a	1	Total	C	O	0
			40	30	10	
11	C	1	Total	C	O	0
			35	25	10	

- Molecule 12 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

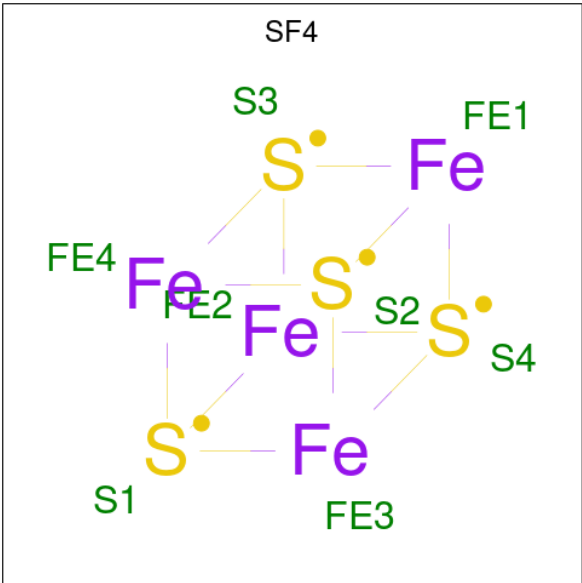
Mol	Chain	Residues	Atoms		AltConf
12	A	1	Total	Ca	0
			1	1	
12	a	1	Total	Ca	0
			1	1	

- Molecule 13 is Chlorophyll A ester (CCD ID: G2O) (formula: C₅₅H₇₀MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 14 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

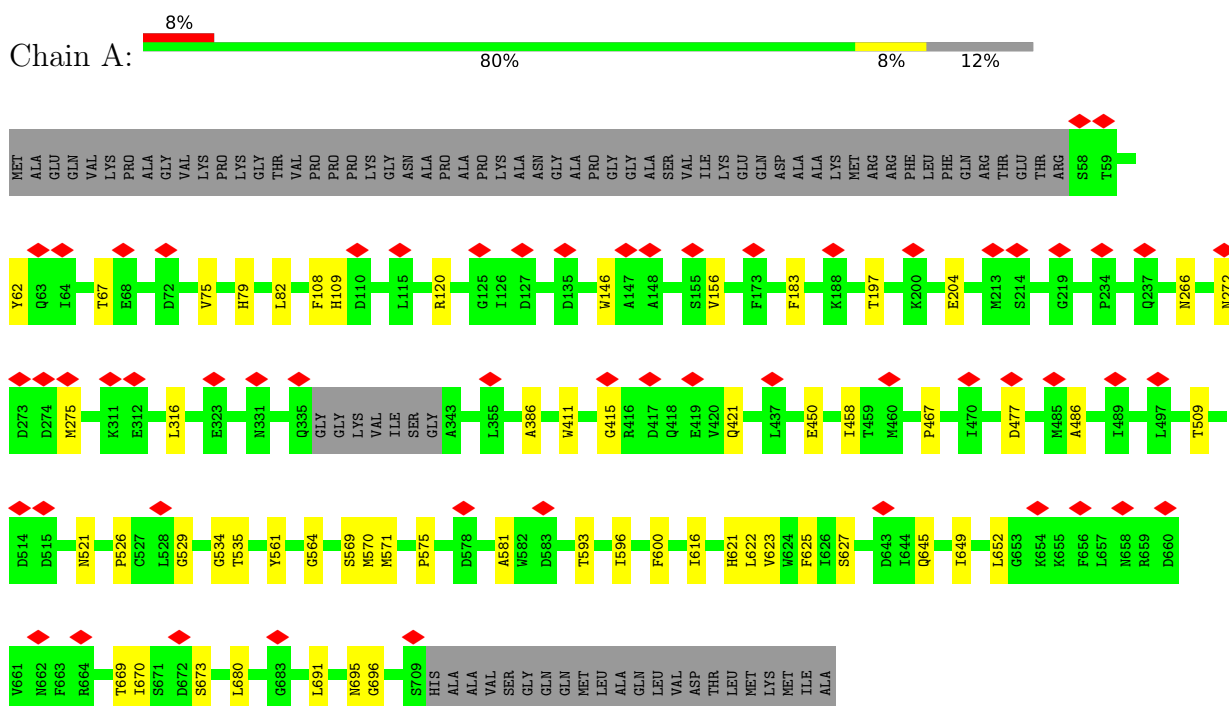


Mol	Chain	Residues	Atoms			AltConf
14	a	1	Total 8	Fe 4	S 4	0
14	B	1	Total 8	Fe 4	S 4	0
14	B	1	Total 8	Fe 4	S 4	0

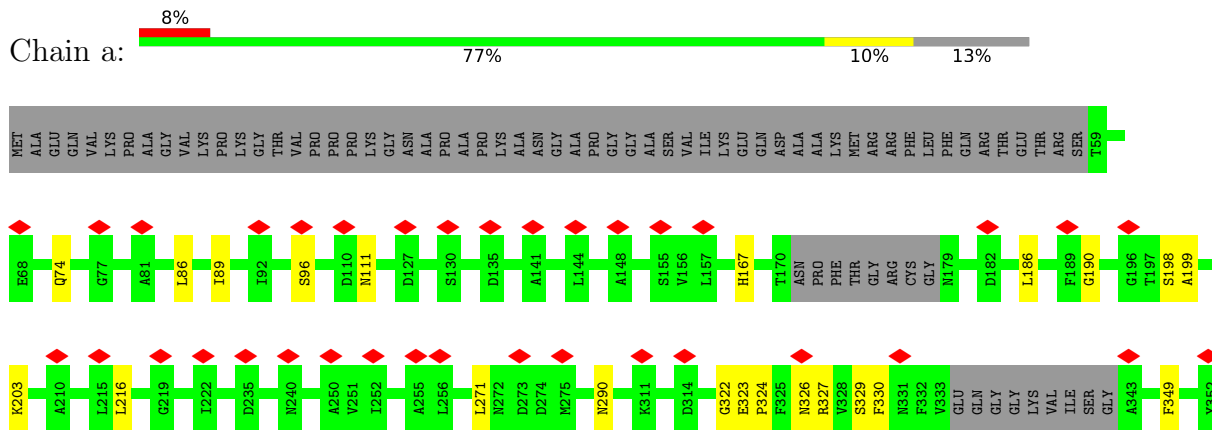
3 Residue-property plots

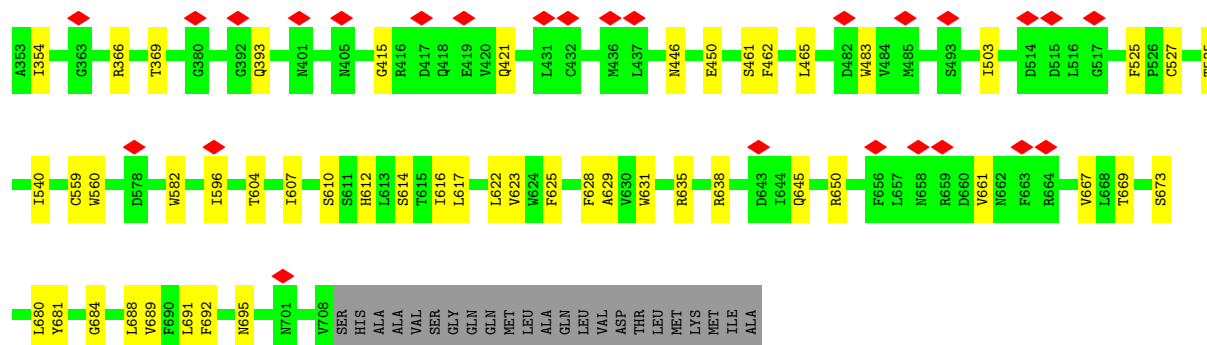
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem P840 reaction center, large subunit

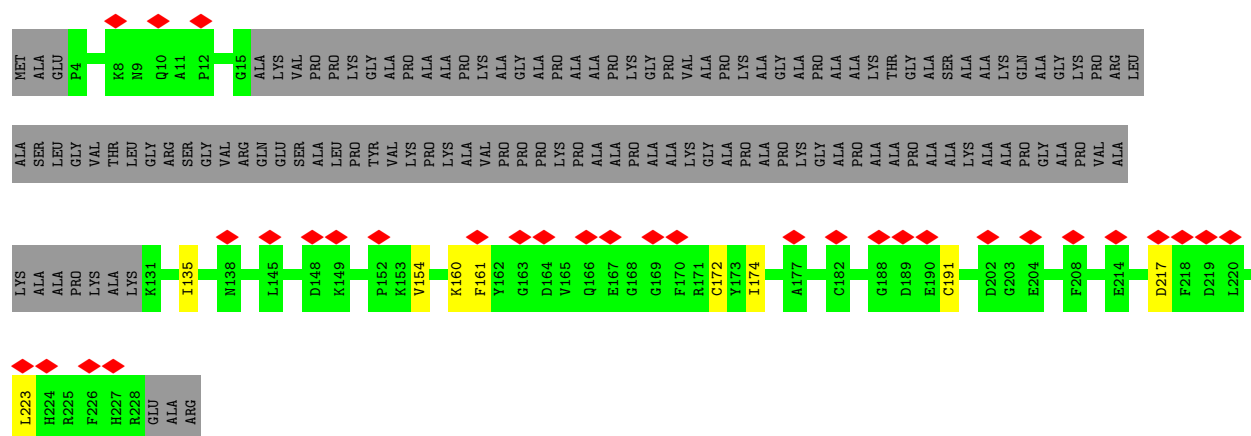


- Molecule 1: Photosystem P840 reaction center, large subunit

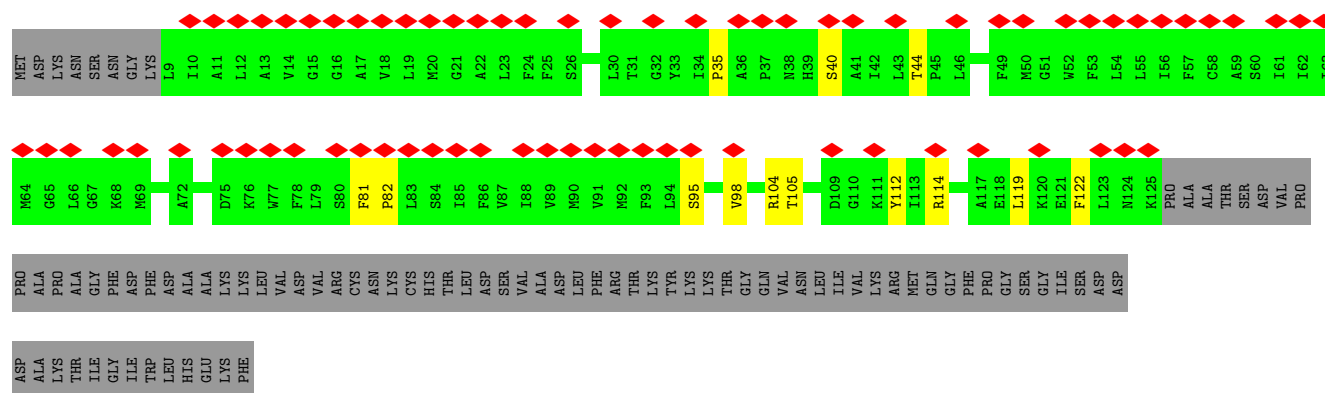




• Molecule 2: Photosystem P840 reaction center iron-sulfur protein

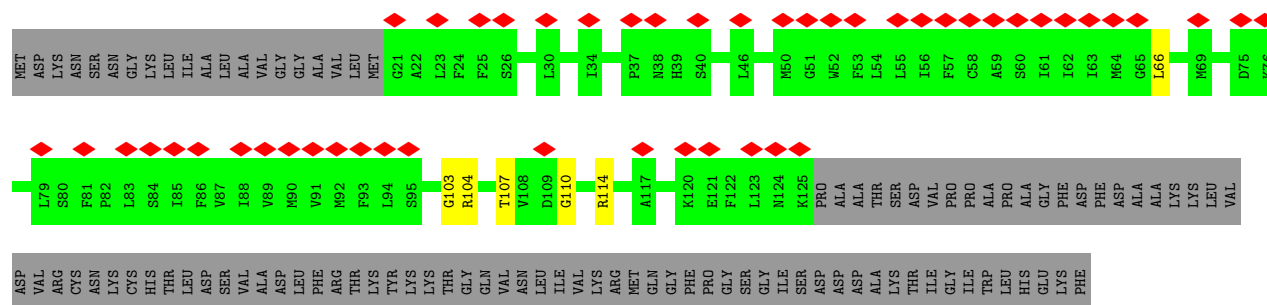


• Molecule 3: Cytochrome c

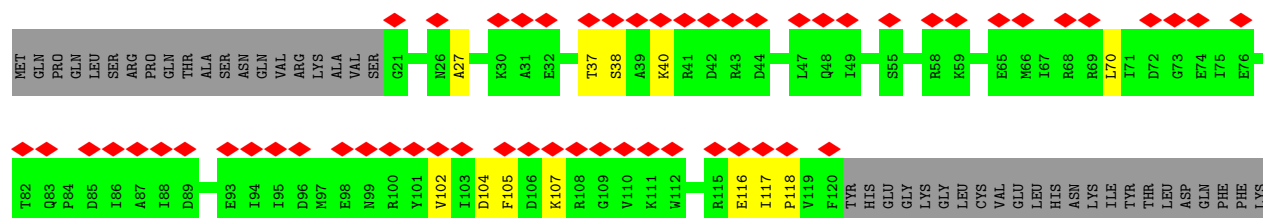
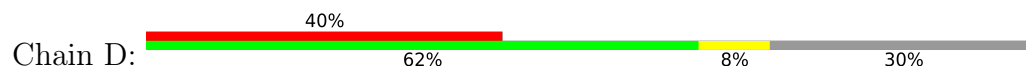


• Molecule 3: Cytochrome c

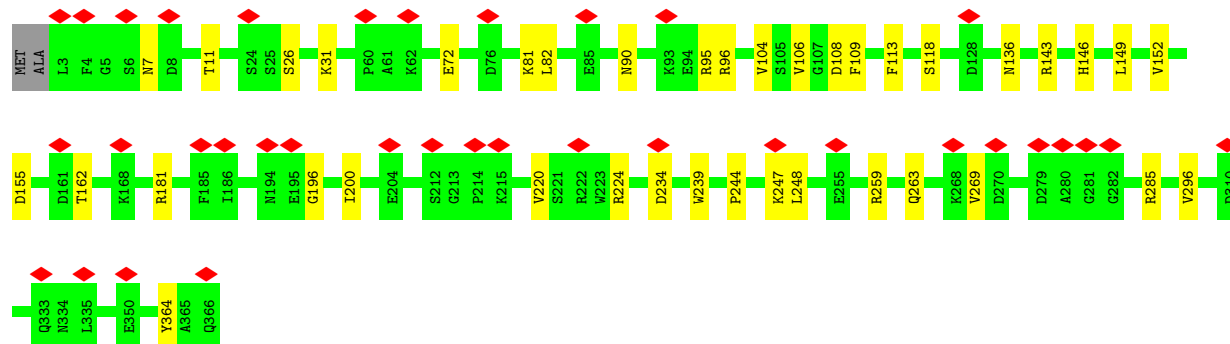
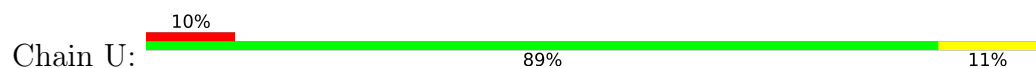




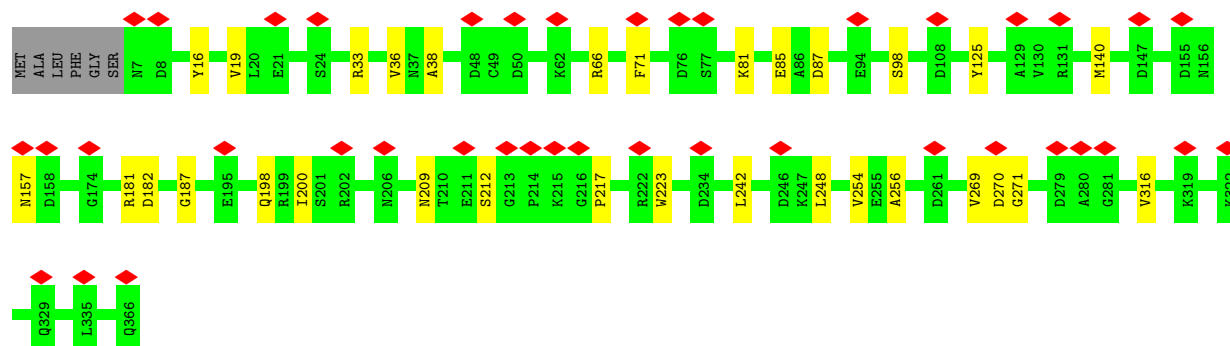
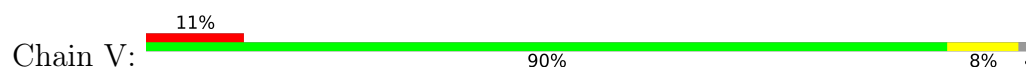
• Molecule 4: P840 reaction center 17 kDa protein



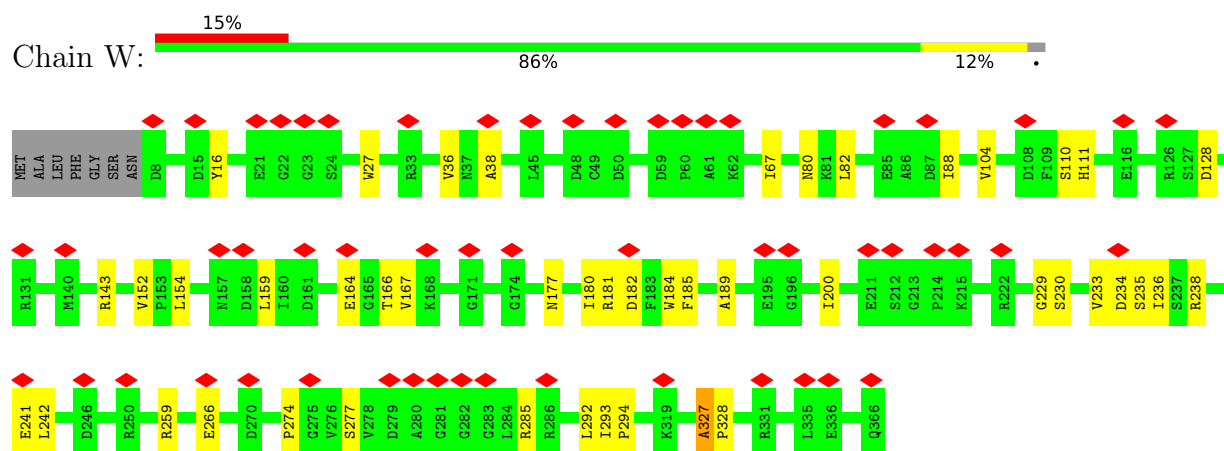
• Molecule 5: Bacteriochlorophyll a protein



• Molecule 5: Bacteriochlorophyll a protein



● Molecule 5: Bacteriochlorophyll a protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	142020	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 ($e^-/\text{\AA}^2$)	45.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	47259	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	8.114	Depositor
Minimum map value	-3.718	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.090	Depositor
Recommended contour level	0.352	Depositor
Map size (Å)	374.4, 374.4, 374.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, G2O, LHG, F26, BCL, SF4, LMG, GS0, F39

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.18	0/5348	0.31	0/7288
1	a	0.18	0/5257	0.32	0/7164
2	B	0.18	0/878	0.33	0/1187
3	C	0.15	0/940	0.35	0/1272
3	c	0.16	0/863	0.34	0/1167
4	D	0.14	0/833	0.36	0/1122
5	U	0.18	0/2905	0.34	0/3937
5	V	0.17	0/2875	0.32	0/3897
5	W	0.17	0/2867	0.35	0/3886
All	All	0.17	0/22766	0.33	0/30920

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
5	W	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	40	LYS	Peptide
5	W	327	ALA	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5167	0	5051	45	0
1	a	5079	0	4974	48	0
2	B	855	0	805	8	0
3	C	916	0	962	8	0
3	c	839	0	870	5	0
4	D	817	0	834	7	0
5	U	2834	0	2770	27	0
5	V	2805	0	2742	23	0
5	W	2797	0	2736	31	0
6	A	66	0	0	0	0
6	a	66	0	0	2	0
7	A	791	0	884	19	0
7	U	574	0	627	6	0
7	V	508	0	553	17	0
7	W	442	0	479	11	0
7	a	772	0	849	18	0
8	A	65	0	0	0	0
8	a	65	0	0	0	0
9	A	40	0	0	0	0
9	a	80	0	0	0	0
10	A	67	0	77	3	0
10	C	34	0	38	2	0
10	a	99	0	111	5	0
11	A	174	0	198	8	0
11	C	35	0	40	1	0
11	a	40	0	50	0	0
12	A	1	0	0	0	0
12	a	1	0	0	0	0
13	A	65	0	0	0	0
13	a	195	0	0	2	0
14	B	16	0	0	1	0
14	a	8	0	0	1	0
All	All	26313	0	25650	230	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (230) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:PHE:O	3:c:104:ARG:NH2	2.09	0.84
1:a:617:LEU:HD12	1:a:688:LEU:HD23	1.61	0.81
5:V:242:LEU:HD21	7:V:406:BCL:HMD1	1.65	0.79
1:a:692:PHE:O	1:a:695:ASN:ND2	2.16	0.79
1:A:529:GLY:O	1:A:535:THR:OG1	2.02	0.77
1:a:415:GLY:O	1:a:421:GLN:NE2	2.24	0.70
1:A:669:THR:O	1:A:673:SER:N	2.24	0.69
1:a:326:ASN:ND2	1:a:349:PHE:O	2.27	0.68
5:U:269:VAL:HG11	7:U:405:BCL:H41	1.77	0.67
1:A:575:PRO:O	1:a:327:ARG:NH2	2.28	0.66
1:a:684:GLY:O	1:a:688:LEU:HD12	1.95	0.66
5:W:16:TYR:OH	7:W:402:BCL:OBB	2.11	0.66
5:V:182:ASP:OD2	5:W:143:ARG:NH2	2.29	0.66
7:a:816:BCL:HHC	7:a:816:BCL:HBB3	1.76	0.65
5:V:33:ARG:NH1	5:V:270:ASP:OD1	2.31	0.64
5:U:90:ASN:OD1	5:U:96:ARG:NE	2.30	0.63
5:U:95:ARG:NH1	5:U:118:SER:OG	2.32	0.62
1:a:74:GLN:OE1	1:a:167:HIS:NE2	2.33	0.62
7:W:402:BCL:HBB	7:W:403:BCL:H93	1.82	0.61
7:A:802:BCL:H191	7:A:809:BCL:HHD	1.82	0.60
7:a:812:BCL:HBB3	7:a:812:BCL:HHC	1.83	0.60
7:A:802:BCL:C19	7:A:809:BCL:HHD	2.32	0.59
5:V:16:TYR:OH	7:V:403:BCL:OBB	2.19	0.59
1:a:198:SER:OG	1:a:199:ALA:N	2.36	0.59
1:A:183:PHE:O	1:A:197:THR:OG1	2.19	0.58
1:a:669:THR:O	1:a:673:SER:N	2.32	0.58
1:A:645:GLN:NE2	13:a:802:G2O:O1D	2.37	0.58
4:D:70:LEU:HD21	4:D:107:LYS:HD2	1.86	0.57
5:W:184:TRP:HE1	7:W:405:BCL:HBB1	1.69	0.57
1:A:272:ASN:ND2	5:U:263:GLN:OE1	2.36	0.57
1:A:521:ASN:ND2	2:B:191:CYS:O	2.38	0.57
1:a:446:ASN:ND2	1:a:461:SER:OG	2.37	0.57
1:A:266:ASN:OD1	5:U:11:THR:OG1	2.22	0.57
1:A:120:ARG:HB3	7:A:804:BCL:HED1	1.86	0.56
5:U:181:ARG:NH1	5:U:200:ILE:O	2.40	0.55
5:W:185:PHE:HB3	5:W:189:ALA:HB3	1.88	0.55
1:a:186:LEU:O	1:a:190:GLY:N	2.39	0.55
3:C:112:TYR:O	3:C:114:ARG:NE	2.40	0.55
11:A:820:LMG:H151	3:c:66:LEU:HD13	1.89	0.54
1:A:109:HIS:NE2	3:c:103:GLY:O	2.41	0.53
1:a:393:GLN:NE2	7:a:815:BCL:O1D	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:203:LYS:HD2	1:a:271:LEU:HD13	1.89	0.53
5:W:234:ASP:OD2	5:W:292:LEU:N	2.39	0.53
1:A:564:GLY:O	1:A:593:THR:OG1	2.21	0.53
1:a:635:ARG:NH1	1:a:667:VAL:O	2.40	0.53
7:a:810:BCL:HED1	7:a:810:BCL:H42	1.90	0.53
5:U:26:SER:OG	5:U:285:ARG:NH2	2.42	0.52
11:A:821:LMG:HO3	11:A:821:LMG:HO5	1.57	0.52
7:W:402:BCL:HHC	7:W:402:BCL:HBB2	1.91	0.52
7:A:807:BCL:HHC	7:A:807:BCL:HBB3	1.91	0.52
5:V:187:GLY:N	5:W:230:SER:O	2.38	0.51
3:c:107:THR:O	3:c:110:GLY:N	2.42	0.51
10:a:823:LHG:H241	10:C:301:LHG:H152	1.91	0.51
1:A:467:PRO:HB3	7:A:812:BCL:HED1	1.93	0.51
3:C:104:ARG:O	3:C:105:THR:OG1	2.25	0.51
1:A:450:GLU:OE2	1:A:569:SER:OG	2.29	0.51
1:A:616:ILE:HB	1:A:691:LEU:HD21	1.93	0.51
1:a:354:ILE:HB	3:C:105:THR:HG21	1.93	0.51
7:V:401:BCL:H43	7:V:402:BCL:H43	1.92	0.50
2:B:154:VAL:HG11	14:B:302:SF4:S3	2.51	0.50
5:V:242:LEU:HD21	7:V:406:BCL:CMD	2.39	0.50
5:U:82:LEU:HD13	5:U:104:VAL:HG12	1.94	0.50
1:A:477:ASP:OD1	1:A:477:ASP:N	2.44	0.50
7:a:806:BCL:HBB3	7:a:806:BCL:HHC	1.93	0.50
5:V:198:GLN:NE2	7:V:407:BCL:OBB	2.45	0.50
10:A:816:LHG:O9	10:A:816:LHG:HC41	2.08	0.49
7:a:813:BCL:H201	7:a:815:BCL:H202	1.94	0.49
1:A:627:SER:HB2	1:A:680:LEU:HB2	1.94	0.49
1:A:204:GLU:OE2	5:U:7:ASN:ND2	2.45	0.49
7:a:810:BCL:H101	7:a:810:BCL:H143	1.95	0.49
5:W:181:ARG:NH1	5:W:200:ILE:O	2.45	0.49
5:V:66:ARG:NH1	5:V:85:GLU:OE2	2.44	0.49
7:a:810:BCL:H42	7:a:810:BCL:CED	2.42	0.49
7:A:802:BCL:H202	7:A:810:BCL:HBB1	1.93	0.49
1:A:561:TYR:CE2	11:A:818:LMG:HC72	2.48	0.49
5:W:238:ARG:HB3	5:W:241:GLU:HB3	1.95	0.49
5:W:327:ALA:HB1	5:W:328:PRO:HD2	1.95	0.49
1:A:415:GLY:O	1:A:421:GLN:NE2	2.44	0.48
4:D:37:THR:HG22	4:D:38:SER:H	1.78	0.48
5:U:285:ARG:O	5:U:364:TYR:N	2.43	0.48
1:A:411:TRP:HA	7:A:803:BCL:H42	1.95	0.48
5:W:259:ARG:NH2	5:W:266:GLU:OE1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:GLY:O	1:A:535:THR:OG1	2.30	0.48
1:a:216:LEU:HD22	7:a:810:BCL:H92	1.95	0.48
5:W:80:ASN:OD1	5:W:80:ASN:N	2.47	0.48
5:V:248:LEU:HD13	7:V:405:BCL:HBB2	1.96	0.47
5:W:128:ASP:OD1	5:W:128:ASP:N	2.47	0.47
1:a:323:GLU:HB3	1:a:354:ILE:HG23	1.96	0.47
7:V:401:BCL:H41	7:V:401:BCL:H203	1.96	0.47
5:W:229:GLY:HA2	5:W:236:ILE:HD13	1.95	0.47
1:a:604:THR:HA	1:a:607:ILE:HB	1.97	0.47
7:A:802:BCL:HHC	7:A:802:BCL:HBB2	1.95	0.47
1:a:638:ARG:NE	10:a:823:LHG:O4	2.43	0.47
7:V:404:BCL:HBC3	7:V:404:BCL:HHD	1.97	0.47
1:a:650:ARG:HD2	1:a:661:VAL:HG23	1.96	0.47
5:U:248:LEU:HD11	7:U:405:BCL:HBB2	1.96	0.47
1:A:156:VAL:HG12	7:A:805:BCL:HBC1	1.96	0.47
7:A:810:BCL:H72	7:A:810:BCL:HBB2	1.97	0.46
1:a:461:SER:OG	1:a:462:PHE:N	2.48	0.46
2:B:135:ILE:HD13	2:B:172:CYS:SG	2.55	0.46
1:A:571:MET:SD	1:a:614:SER:OG	2.72	0.46
5:U:143:ARG:NH2	5:W:182:ASP:OD2	2.48	0.46
1:a:324:PRO:HD3	1:a:610:SER:HA	1.97	0.46
5:W:233:VAL:HG12	5:W:293:ILE:HD12	1.98	0.46
7:a:809:BCL:O2A	7:a:809:BCL:H43	2.16	0.46
1:A:649:ILE:O	1:A:652:LEU:HB2	2.16	0.45
1:A:486:ALA:HA	11:A:818:LMG:H322	1.98	0.45
5:W:327:ALA:O	5:W:328:PRO:C	2.59	0.45
2:B:135:ILE:HD12	2:B:174:ILE:HD11	1.98	0.45
7:A:803:BCL:HHD	7:A:808:BCL:OBB	2.17	0.45
5:V:125:TYR:OH	5:V:140:MET:SD	2.64	0.45
10:A:816:LHG:H241	11:A:818:LMG:H292	1.97	0.45
1:A:386:ALA:HB2	7:A:811:BCL:HMC3	1.99	0.45
5:U:106:VAL:O	5:U:108:ASP:N	2.49	0.45
7:a:816:BCL:HHC	7:a:816:BCL:CBB	2.45	0.45
2:B:174:ILE:N	4:D:116:GLU:OE2	2.42	0.45
3:C:95:SER:HA	3:C:98:VAL:HG22	1.99	0.45
1:A:623:VAL:HG13	1:A:680:LEU:HD22	1.98	0.44
1:a:329:SER:OG	1:a:330:PHE:N	2.49	0.44
5:U:108:ASP:OD1	5:U:109:PHE:N	2.50	0.44
5:W:277:SER:OG	5:W:285:ARG:NH2	2.40	0.44
7:V:404:BCL:H122	7:V:405:BCL:H143	1.99	0.44
5:W:82:LEU:HD13	7:W:406:BCL:H191	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:527:CYS:HB3	14:a:803:SF4:S1	2.57	0.44
10:a:823:LHG:HC91	10:C:301:LHG:H132	1.99	0.44
7:W:402:BCL:HBC3	7:W:402:BCL:HHD	1.98	0.44
1:a:560:TRP:HZ3	1:a:596:ILE:HA	1.82	0.44
7:V:403:BCL:H42	7:V:405:BCL:H171	2.00	0.44
5:W:104:VAL:HG22	5:W:111:HIS:ND1	2.33	0.44
1:A:680:LEU:HD11	10:A:817:LHG:H252	1.99	0.44
1:a:290:ASN:HD21	7:a:814:BCL:HMC3	1.81	0.44
7:U:404:BCL:H203	7:U:405:BCL:H192	2.00	0.44
5:V:256:ALA:HB1	7:V:404:BCL:H143	1.99	0.44
1:a:525:PHE:CG	1:a:525:PHE:O	2.70	0.44
5:V:256:ALA:HB3	7:V:405:BCL:H92	1.99	0.44
5:U:113:PHE:HB3	5:U:152:VAL:HG22	2.00	0.43
1:a:625:PHE:CD2	1:a:625:PHE:C	2.96	0.43
5:W:152:VAL:HG21	7:W:401:BCL:HHC	2.01	0.43
7:a:817:BCL:HHB	11:C:302:LMG:HC72	2.00	0.43
7:W:402:BCL:H121	7:W:406:BCL:HBB3	2.00	0.43
5:V:269:VAL:HG21	7:V:404:BCL:H62	1.99	0.43
7:A:802:BCL:HED1	11:A:819:LMG:C41	2.49	0.43
1:a:604:THR:HG21	6:a:804:GS0:CAC	2.49	0.43
3:C:40:SER:O	3:C:44:THR:OG1	2.37	0.43
3:C:122:PHE:C	3:C:122:PHE:CD2	2.97	0.43
7:U:404:BCL:OBB	7:U:404:BCL:HHC	2.19	0.43
1:A:621:HIS:HB3	13:a:801:G2O:CED	2.49	0.43
5:W:104:VAL:O	5:W:110:SER:HA	2.19	0.43
1:a:616:ILE:HB	1:a:691:LEU:HD21	1.99	0.43
7:a:813:BCL:HBC3	7:a:813:BCL:HHD	2.00	0.43
5:W:235:SER:HA	5:W:242:LEU:HD11	2.01	0.43
7:W:405:BCL:H92	7:W:406:BCL:HMC1	2.00	0.43
5:W:67:ILE:HD12	5:W:88:ILE:HD12	2.01	0.43
1:a:645:GLN:NE2	10:a:823:LHG:O1	2.49	0.43
1:A:570:MET:HA	1:A:596:ILE:HB	2.01	0.42
7:A:807:BCL:HHC	7:A:807:BCL:CBB	2.49	0.42
1:a:465:LEU:HD21	1:a:483:TRP:CD2	2.53	0.42
2:B:160:LYS:NZ	2:B:161:PHE:O	2.51	0.42
5:V:212:SER:HA	5:V:217:PRO:HA	2.00	0.42
7:V:401:BCL:HMC1	7:V:402:BCL:H192	2.00	0.42
4:D:104:ASP:O	4:D:105:PHE:CG	2.72	0.42
5:W:27:TRP:HA	5:W:274:PRO:HA	2.01	0.42
1:A:79:HIS:ND1	7:A:806:BCL:OBD	2.53	0.42
7:a:808:BCL:HMD2	7:a:814:BCL:H141	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:808:BCL:HBC2	7:a:812:BCL:H143	2.02	0.42
7:V:404:BCL:HBB1	7:V:405:BCL:H142	2.02	0.42
1:A:600:PHE:HB2	6:a:804:GS0:CMC	2.49	0.42
5:U:196:GLY:HA2	5:U:296:VAL:HG11	2.02	0.42
5:W:36:VAL:HG22	5:W:38:ALA:H	1.83	0.42
1:A:67:THR:HB	1:A:275:MET:HB3	2.00	0.42
5:U:162:THR:HG23	7:V:408[B]:BCL:HHC	2.02	0.42
5:V:209:ASN:OD1	5:V:209:ASN:N	2.51	0.42
1:A:62:TYR:HB3	11:A:819:LMG:H351	2.00	0.42
1:A:526:PRO:HB3	1:A:670:ILE:HB	2.01	0.42
1:a:623:VAL:HG13	1:a:680:LEU:HD22	2.02	0.42
5:W:166:THR:HG21	7:W:401:BCL:H91	2.02	0.42
1:a:450:GLU:CG	1:a:582:TRP:HE1	2.32	0.42
3:C:81:PHE:HB3	3:C:82:PRO:HD3	2.02	0.42
5:V:254:VAL:HA	5:V:271:GLY:HA3	2.01	0.42
7:W:401:BCL:H2	7:W:401:BCL:H71	2.01	0.42
5:U:234:ASP:N	5:U:234:ASP:OD1	2.52	0.42
1:A:82:LEU:HD11	7:A:802:BCL:HBD	2.02	0.41
1:a:86:LEU:HA	1:a:89:ILE:HG12	2.02	0.41
1:a:622:LEU:HA	1:a:625:PHE:CE1	2.55	0.41
5:U:146:HIS:O	5:U:224:ARG:HA	2.20	0.41
5:U:239:TRP:HZ3	7:U:406:BCL:HMD2	1.85	0.41
5:U:244:PRO:HB3	5:U:247:LYS:HB2	2.02	0.41
1:a:86:LEU:HD11	7:a:814:BCL:H42	2.02	0.41
1:a:527:CYS:O	1:a:535:THR:OG1	2.32	0.41
1:a:322:GLY:HA3	1:a:612:HIS:HB2	2.02	0.41
5:U:72:GLU:OE2	5:U:81:LYS:NZ	2.52	0.41
5:V:36:VAL:HG22	5:V:38:ALA:H	1.86	0.41
5:W:293:ILE:HG22	5:W:294:PRO:HD3	2.02	0.41
4:D:117:ILE:N	4:D:118:PRO:CD	2.84	0.41
1:A:146:TRP:CZ3	7:A:804:BCL:HHB	2.55	0.41
1:A:534:GLY:HA2	1:a:635:ARG:HD2	2.02	0.41
5:W:177:ASN:O	5:W:180:ILE:HG22	2.20	0.41
1:A:509:THR:HG21	4:D:27:ALA:HB1	2.03	0.41
1:a:366:ARG:HA	1:a:369:THR:HG22	2.03	0.41
4:D:102:VAL:HG23	4:D:105:PHE:HA	2.03	0.41
5:V:223:TRP:HH2	7:V:406:BCL:HBB3	1.85	0.41
5:W:154:LEU:HA	5:W:159:LEU:HD22	2.02	0.41
11:A:820:LMG:H291	11:A:820:LMG:H121	2.02	0.41
7:a:812:BCL:O2A	7:a:812:BCL:H43	2.20	0.41
1:A:75:VAL:HG23	7:A:806:BCL:HMD1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ILE:HD11	1:A:581:ALA:HB3	2.03	0.41
1:a:503:ILE:HG23	1:a:540:ILE:HG23	2.02	0.41
5:V:19:VAL:HA	5:V:316:VAL:HB	2.02	0.41
5:V:181:ARG:NH1	5:V:200:ILE:O	2.52	0.41
1:a:629:ALA:HB3	10:a:823:LHG:HC5	2.03	0.40
2:B:217:ASP:OD1	5:U:259:ARG:NH2	2.47	0.40
2:B:223:LEU:HD11	5:U:31:LYS:HB2	2.02	0.40
5:U:136:ASN:OD1	5:U:136:ASN:N	2.53	0.40
5:V:71:PHE:O	5:V:81:LYS:HA	2.20	0.40
1:A:316:LEU:HD13	3:c:114:ARG:HE	1.86	0.40
1:A:695:ASN:OD1	1:A:696:GLY:O	2.39	0.40
7:A:805:BCL:HBC3	7:A:805:BCL:HHD	2.03	0.40
1:a:559:CYS:SG	1:a:689:VAL:HG13	2.61	0.40
1:a:628:PHE:HA	1:a:631:TRP:HB2	2.03	0.40
3:C:119:LEU:HA	3:C:122:PHE:CE1	2.56	0.40
5:U:149:LEU:HD11	5:U:220:VAL:CG1	2.51	0.40
5:V:87:ASP:O	5:V:98:SER:HA	2.22	0.40
1:a:96:SER:OG	1:a:111:ASN:OD1	2.39	0.40
5:W:293:ILE:N	5:W:294:PRO:CD	2.85	0.40
1:a:631:TRP:HE1	1:a:681:TYR:HB2	1.87	0.40
7:U:405:BCL:HMB2	7:U:406:BCL:H202	2.04	0.40
5:V:157:ASN:OD1	5:V:157:ASN:N	2.55	0.40
1:A:622:LEU:HA	1:A:625:PHE:CE1	2.56	0.40
5:U:155:ASP:OD1	5:U:155:ASP:N	2.50	0.40
5:W:164:GLU:HA	5:W:167:VAL:HG22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	641/731 (88%)	620 (97%)	21 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	627/731 (86%)	600 (96%)	27 (4%)	0	100	100
2	B	106/231 (46%)	99 (93%)	7 (7%)	0	100	100
3	C	115/206 (56%)	110 (96%)	4 (4%)	1 (1%)	14	47
3	c	103/206 (50%)	102 (99%)	1 (1%)	0	100	100
4	D	98/143 (68%)	84 (86%)	14 (14%)	0	100	100
5	U	362/366 (99%)	348 (96%)	14 (4%)	0	100	100
5	V	358/366 (98%)	351 (98%)	7 (2%)	0	100	100
5	W	357/366 (98%)	344 (96%)	13 (4%)	0	100	100
All	All	2767/3346 (83%)	2658 (96%)	108 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	35	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	536/599 (90%)	536 (100%)	0	100	100
1	a	526/599 (88%)	526 (100%)	0	100	100
2	B	93/162 (57%)	93 (100%)	0	100	100
3	C	99/173 (57%)	99 (100%)	0	100	100
3	c	92/173 (53%)	92 (100%)	0	100	100
4	D	89/128 (70%)	89 (100%)	0	100	100
5	U	301/302 (100%)	301 (100%)	0	100	100
5	V	298/302 (99%)	298 (100%)	0	100	100
5	W	297/302 (98%)	297 (100%)	0	100	100
All	All	2331/2740 (85%)	2331 (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 (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	167	HIS
1	A	303	GLN
1	A	405	ASN
1	A	590	HIS
1	A	591	HIS
1	a	446	ASN
1	a	645	GLN
2	B	9	ASN
2	B	155	ASN
2	B	166	GLN
2	B	176	GLN
2	B	227	HIS
3	C	38	ASN
5	U	144	GLN
5	U	146	HIS
5	V	146	HIS
5	V	263	GLN
5	V	297	HIS
5	V	306	ASN
5	V	333	GLN
5	V	359	GLN
5	W	306	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 77 ligands modelled in this entry, 2 are monoatomic - leaving 75 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
7	BCL	A	808	-	69,74,74	1.09	5 (7%)	79,115,115	1.38	10 (12%)
6	GS0	A	801	-	69,74,74	2.36	14 (20%)	79,115,115	2.80	32 (40%)
10	LHG	A	817	-	40,40,48	0.70	1 (2%)	43,46,54	1.01	2 (4%)
10	LHG	a	822	-	25,25,48	0.83	1 (4%)	28,31,54	0.98	1 (3%)
7	BCL	a	815	-	69,74,74	1.13	6 (8%)	79,115,115	1.37	10 (12%)
10	LHG	A	816	-	25,25,48	0.84	1 (4%)	28,31,54	0.97	1 (3%)
7	BCL	V	407	-	69,74,74	1.06	5 (7%)	79,115,115	1.39	10 (12%)
10	LHG	a	821	-	32,32,48	0.76	2 (6%)	35,38,54	1.01	2 (5%)
13	G2O	A	824	-	68,73,73	4.47	40 (58%)	81,113,113	2.79	20 (24%)
7	BCL	W	406	-	69,74,74	1.05	4 (5%)	79,115,115	1.37	11 (13%)
7	BCL	A	805	-	69,74,74	1.18	4 (5%)	79,115,115	1.58	12 (15%)
13	G2O	a	801	-	68,73,73	4.05	41 (60%)	81,113,113	2.97	17 (20%)
7	BCL	a	809	-	69,74,74	1.14	3 (4%)	79,115,115	1.65	15 (18%)
7	BCL	a	813	-	69,74,74	1.14	5 (7%)	79,115,115	1.42	10 (12%)
7	BCL	V	405	-	69,74,74	1.07	5 (7%)	79,115,115	1.40	8 (10%)
7	BCL	W	404	5	69,74,74	1.12	4 (5%)	79,115,115	1.41	10 (12%)
11	LMG	A	819	-	39,39,55	0.82	0	47,47,63	1.13	5 (10%)
7	BCL	a	806	-	69,74,74	1.10	4 (5%)	79,115,115	1.44	10 (12%)
8	F39	a	818	-	66,66,66	2.85	20 (30%)	83,85,85	2.15	22 (26%)
6	GS0	a	804	-	69,74,74	2.33	15 (21%)	79,115,115	2.77	28 (35%)
11	LMG	A	818	-	42,42,55	0.80	0	50,50,63	1.17	5 (10%)
7	BCL	U	401	-	69,74,74	1.12	4 (5%)	79,115,115	1.43	11 (13%)
7	BCL	V	401	-	69,74,74	1.13	4 (5%)	79,115,115	1.41	11 (13%)
7	BCL	W	405	-	69,74,74	1.10	5 (7%)	79,115,115	1.51	11 (13%)
7	BCL	U	402	-	69,74,74	1.11	6 (8%)	79,115,115	1.34	8 (10%)
7	BCL	A	813	-	68,73,74	1.12	5 (7%)	77,113,115	1.45	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BCL	U	407	-	69,74,74	1.09	5 (7%)	79,115,115	1.35	9 (11%)
14	SF4	B	302	2	0,12,12	-	-	-		
11	LMG	C	302	-	35,35,55	0.89	1 (2%)	43,43,63	1.17	4 (9%)
7	BCL	V	403	-	69,74,74	1.09	5 (7%)	79,115,115	1.46	8 (10%)
7	BCL	a	810	-	69,74,74	1.09	6 (8%)	79,115,115	1.36	10 (12%)
13	G2O	a	802	-	68,73,73	4.16	41 (60%)	81,113,113	2.88	17 (20%)
7	BCL	W	402	-	69,74,74	1.11	6 (8%)	79,115,115	1.44	9 (11%)
7	BCL	a	814	-	69,74,74	1.11	5 (7%)	79,115,115	1.47	9 (11%)
7	BCL	a	807	-	69,74,74	1.18	6 (8%)	79,115,115	1.28	5 (6%)
11	LMG	A	822	-	30,30,55	0.96	1 (3%)	38,38,63	1.28	4 (10%)
9	F26	A	815	-	40,40,40	1.80	10 (25%)	49,50,50	2.17	15 (30%)
9	F26	a	819	-	40,40,40	1.67	10 (25%)	49,50,50	2.35	14 (28%)
7	BCL	U	405	5	69,74,74	1.12	5 (7%)	79,115,115	1.43	9 (11%)
7	BCL	W	401	-	69,74,74	1.13	5 (7%)	79,115,115	1.55	9 (11%)
7	BCL	V	406	-	69,74,74	1.12	5 (7%)	79,115,115	1.46	13 (16%)
11	LMG	A	820	-	36,36,55	0.91	0	44,44,63	1.12	4 (9%)
7	BCL	A	802	-	69,74,74	1.11	5 (7%)	79,115,115	1.40	11 (13%)
11	LMG	A	821	-	27,27,55	1.02	1 (3%)	35,35,63	1.24	5 (14%)
7	BCL	A	810	-	69,74,74	1.13	4 (5%)	79,115,115	1.47	10 (12%)
7	BCL	U	406	-	69,74,74	1.13	3 (4%)	79,115,115	1.39	9 (11%)
14	SF4	a	803	1	0,12,12	-	-	-		
7	BCL	V	408[B]	5	49,54,74	1.25	4 (8%)	55,91,115	1.46	9 (16%)
7	BCL	W	403	-	69,74,74	1.08	4 (5%)	79,115,115	1.38	11 (13%)
14	SF4	B	301	2	0,12,12	-	-	-		
7	BCL	A	804	-	69,74,74	1.10	6 (8%)	79,115,115	1.39	9 (11%)
7	BCL	U	408[B]	5	49,54,74	1.24	5 (10%)	55,91,115	1.42	6 (10%)
7	BCL	A	809	-	69,74,74	1.09	6 (8%)	79,115,115	1.41	9 (11%)
10	LHG	a	823	-	39,39,48	0.67	0	42,45,54	0.99	2 (4%)
13	G2O	a	805	-	68,73,73	4.21	40 (58%)	81,113,113	2.78	18 (22%)
9	F26	a	820	-	40,40,40	1.75	10 (25%)	49,50,50	2.25	13 (26%)
8	F39	A	814	-	66,66,66	2.82	20 (30%)	83,85,85	2.20	23 (27%)
7	BCL	a	812	-	69,74,74	1.15	6 (8%)	79,115,115	1.35	8 (10%)
7	BCL	U	404	-	69,74,74	1.11	4 (5%)	79,115,115	1.46	13 (16%)
7	BCL	a	817	-	69,74,74	1.08	4 (5%)	79,115,115	1.37	9 (11%)
10	LHG	C	301	-	33,33,48	0.74	1 (3%)	36,39,54	1.01	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BCL	A	806	-	69,74,74	1.09	5 (7%)	79,115,115	1.32	9 (11%)
11	LMG	a	824	-	40,40,55	0.83	1 (2%)	48,48,63	1.18	4 (8%)
7	BCL	W	407[B]	5	49,54,74	1.24	4 (8%)	55,91,115	1.43	8 (14%)
7	BCL	U	403	-	69,74,74	1.09	4 (5%)	79,115,115	1.40	8 (10%)
7	BCL	A	812	-	69,74,74	1.14	5 (7%)	79,115,115	1.25	6 (7%)
7	BCL	A	811	-	69,74,74	1.09	4 (5%)	79,115,115	1.42	14 (17%)
7	BCL	a	811	1	49,54,74	1.24	5 (10%)	55,91,115	1.61	10 (18%)
7	BCL	a	816	-	69,74,74	1.10	5 (7%)	79,115,115	1.32	8 (10%)
7	BCL	A	803	-	69,74,74	1.14	4 (5%)	79,115,115	1.30	9 (11%)
7	BCL	V	402	-	69,74,74	1.08	5 (7%)	79,115,115	1.38	9 (11%)
7	BCL	a	808	-	69,74,74	1.14	5 (7%)	79,115,115	1.43	10 (12%)
7	BCL	V	404	-	69,74,74	1.11	5 (7%)	79,115,115	1.34	8 (10%)
7	BCL	A	807	-	69,74,74	1.12	5 (7%)	79,115,115	1.37	10 (12%)
7	BCL	U	409	-	69,74,74	1.08	4 (5%)	79,115,115	1.31	9 (11%)

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
7	BCL	A	808	-	-	11/41/137/137	-
6	GS0	A	801	-	2/2/21/25	21/41/137/137	-
10	LHG	A	817	-	-	19/45/45/53	-
10	LHG	a	822	-	-	17/30/30/53	-
7	BCL	a	815	-	-	10/41/137/137	-
10	LHG	A	816	-	-	11/30/30/53	-
7	BCL	V	407	-	-	5/41/137/137	-
10	LHG	a	821	-	-	12/37/37/53	-
13	G2O	A	824	-	3/3/15/22	20/39/115/115	-
7	BCL	W	406	-	-	9/41/137/137	-
7	BCL	A	805	-	-	19/41/137/137	-
13	G2O	a	801	-	4/4/15/22	21/39/115/115	-
7	BCL	a	809	-	-	12/41/137/137	-
7	BCL	a	813	-	-	11/41/137/137	-
7	BCL	V	405	-	-	6/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	U	409	-	-	6/41/137/137	-
7	BCL	W	404	5	-	8/41/137/137	-
7	BCL	a	806	-	-	19/41/137/137	-
8	F39	a	818	-	-	25/58/78/78	0/2/2/2
6	GS0	a	804	-	2/2/21/25	25/41/137/137	-
11	LMG	A	819	-	-	20/34/54/70	0/1/1/1
11	LMG	A	818	-	-	20/37/57/70	0/1/1/1
7	BCL	U	401	-	-	6/41/137/137	-
7	BCL	V	401	-	-	6/41/137/137	-
7	BCL	W	405	-	-	7/41/137/137	-
7	BCL	U	402	-	-	11/41/137/137	-
7	BCL	A	813	-	-	20/40/136/137	-
7	BCL	U	407	-	-	4/41/137/137	-
14	SF4	B	302	2	-	-	0/6/5/5
11	LMG	C	302	-	-	16/30/50/70	0/1/1/1
7	BCL	V	403	-	-	14/41/137/137	-
13	G2O	a	802	-	3/3/15/22	15/39/115/115	-
7	BCL	a	810	-	-	9/41/137/137	-
7	BCL	W	402	-	-	13/41/137/137	-
7	BCL	a	814	-	-	9/41/137/137	-
7	BCL	a	807	-	-	11/41/137/137	-
11	LMG	A	822	-	-	11/24/44/70	0/1/1/1
9	F26	A	815	-	-	15/36/36/36	0/1/1/1
9	F26	a	819	-	-	19/36/36/36	0/1/1/1
7	BCL	U	405	5	-	9/41/137/137	-
7	BCL	W	401	-	-	6/41/137/137	-
7	BCL	V	406	-	-	4/41/137/137	-
11	LMG	A	820	-	-	14/31/51/70	0/1/1/1
7	BCL	A	802	-	-	11/41/137/137	-
11	LMG	A	821	-	-	12/22/42/70	0/1/1/1
7	BCL	A	810	-	-	9/41/137/137	-
7	BCL	U	406	-	-	7/41/137/137	-
14	SF4	a	803	1	-	-	0/6/5/5
7	BCL	V	408[B]	5	-	6/17/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	W	403	-	-	7/41/137/137	-
14	SF4	B	301	2	-	-	0/6/5/5
7	BCL	A	804	-	-	8/41/137/137	-
7	BCL	U	408[B]	5	-	3/17/113/137	-
7	BCL	A	809	-	-	11/41/137/137	-
10	LHG	a	823	-	-	18/44/44/53	-
9	F26	a	820	-	-	28/36/36/36	0/1/1/1
8	F39	A	814	-	-	31/58/78/78	0/2/2/2
7	BCL	a	812	-	-	15/41/137/137	-
7	BCL	U	404	-	-	6/41/137/137	-
7	BCL	a	817	-	-	10/41/137/137	-
10	LHG	C	301	-	-	18/38/38/53	-
7	BCL	A	806	-	-	11/41/137/137	-
11	LMG	a	824	-	-	15/35/55/70	0/1/1/1
7	BCL	W	407[B]	5	-	5/17/113/137	-
7	BCL	U	403	-	-	12/41/137/137	-
7	BCL	A	812	-	-	16/41/137/137	-
7	BCL	A	811	-	-	7/41/137/137	-
7	BCL	a	811	1	-	7/17/113/137	-
7	BCL	a	816	-	-	12/41/137/137	-
7	BCL	A	803	-	-	10/41/137/137	-
7	BCL	V	402	-	-	3/41/137/137	-
7	BCL	a	808	-	-	9/41/137/137	-
7	BCL	V	404	-	-	7/41/137/137	-
7	BCL	A	807	-	-	5/41/137/137	-
13	G2O	a	805	-	3/3/15/22	20/39/115/115	-

All (499) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	824	G2O	MG-ND	18.24	2.41	2.05
13	a	805	G2O	MG-ND	15.56	2.36	2.05
13	A	824	G2O	MG-NA	14.77	2.41	2.06
13	a	802	G2O	MG-ND	14.64	2.34	2.05
13	a	801	G2O	MG-ND	12.77	2.31	2.05
13	a	805	G2O	MG-NA	12.75	2.36	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	801	G2O	MG-NC	12.01	2.34	2.06
13	a	802	G2O	MG-NC	11.41	2.33	2.06
6	a	804	GS0	MG-NC	10.63	2.31	2.06
13	a	802	G2O	MG-NA	10.52	2.31	2.06
6	A	801	GS0	MG-NC	10.30	2.30	2.06
13	A	824	G2O	MG-NC	9.97	2.29	2.06
13	a	801	G2O	MG-NA	9.69	2.29	2.06
13	a	805	G2O	MG-NC	9.52	2.28	2.06
13	a	802	G2O	C4B-NB	8.74	1.49	1.37
13	a	801	G2O	C4B-NB	8.74	1.49	1.37
13	a	805	G2O	C4B-NB	8.59	1.49	1.37
13	A	824	G2O	C4B-NB	7.91	1.48	1.37
8	a	818	F39	C35-C37	7.50	1.62	1.46
8	A	814	F39	C35-C37	7.48	1.62	1.46
13	a	801	G2O	C1A-CHA	7.30	1.51	1.37
8	a	818	F39	C56-C58	7.20	1.61	1.46
8	A	814	F39	C56-C58	7.15	1.61	1.46
13	a	802	G2O	C1A-CHA	7.12	1.51	1.37
6	a	804	GS0	MG-NA	7.10	2.23	2.06
13	a	801	G2O	CAA-C2A	-7.03	1.41	1.54
13	a	805	G2O	C1A-CHA	6.99	1.51	1.37
6	A	801	GS0	MG-ND	-6.97	1.92	2.05
8	a	818	F39	C64-C62	6.96	1.60	1.46
13	a	802	G2O	CAA-C2A	-6.79	1.41	1.54
13	A	824	G2O	C1A-CHA	6.78	1.50	1.37
8	A	814	F39	C64-C62	6.77	1.60	1.46
13	a	805	G2O	CAA-C2A	-6.72	1.41	1.54
13	A	824	G2O	CAA-C2A	-6.71	1.41	1.54
6	a	804	GS0	MG-ND	-6.56	1.92	2.05
13	a	805	G2O	C3B-C4B	6.53	1.57	1.46
6	A	801	GS0	MG-NA	6.50	2.21	2.06
13	a	802	G2O	C3B-C4B	6.45	1.57	1.46
13	A	824	G2O	C3B-C4B	6.34	1.57	1.46
8	A	814	F39	C41-C42	6.33	1.59	1.46
13	a	802	G2O	C1B-C2B	6.32	1.57	1.45
13	a	801	G2O	C1B-C2B	6.29	1.57	1.45
8	a	818	F39	C41-C42	6.28	1.59	1.46
13	A	824	G2O	C1B-C2B	6.28	1.57	1.45
6	A	801	GS0	MG-NB	-6.22	1.93	2.05
13	a	801	G2O	C3B-C4B	6.16	1.56	1.46
8	a	818	F39	C46-C53	6.15	1.60	1.47
8	A	814	F39	C46-C53	5.92	1.60	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	805	G2O	C1B-C2B	5.89	1.57	1.45
13	A	824	G2O	C1D-ND	5.79	1.45	1.37
13	a	802	G2O	C1D-ND	5.69	1.45	1.37
13	a	801	G2O	C1D-ND	5.57	1.45	1.37
13	a	805	G2O	C1D-ND	5.51	1.45	1.37
8	a	818	F39	C51-C44	5.51	1.60	1.43
13	a	802	G2O	C4C-NC	5.50	1.46	1.37
13	a	801	G2O	C4C-NC	5.49	1.46	1.37
13	a	805	G2O	C4C-NC	5.49	1.46	1.37
8	A	814	F39	C51-C44	5.38	1.59	1.43
8	A	814	F39	C32-C27	5.35	1.59	1.43
8	a	818	F39	C57-C59	5.34	1.59	1.43
8	a	818	F39	C32-C27	5.34	1.59	1.43
8	a	818	F39	C63-C61	5.27	1.59	1.43
8	A	814	F39	C40-C39	5.23	1.59	1.43
8	A	814	F39	C63-C61	5.21	1.59	1.43
8	a	818	F39	C40-C39	5.19	1.59	1.43
13	A	824	G2O	CMA-C3A	-5.10	1.42	1.53
13	A	824	G2O	C4C-NC	5.09	1.46	1.37
8	A	814	F39	C57-C59	5.08	1.58	1.43
13	A	824	G2O	C3C-C2C	5.01	1.47	1.36
13	A	824	G2O	CHB-C1B	4.96	1.48	1.38
13	a	801	G2O	CMA-C3A	-4.93	1.42	1.53
13	a	802	G2O	CMA-C3A	-4.93	1.42	1.53
13	a	805	G2O	CMA-C3A	-4.92	1.42	1.53
8	a	818	F39	C14-C13	4.92	1.60	1.53
13	a	802	G2O	CHB-C1B	4.86	1.47	1.38
6	a	804	GS0	MG-NB	-4.85	1.96	2.05
8	A	814	F39	C14-C13	4.80	1.60	1.53
13	a	805	G2O	CHB-C1B	4.78	1.47	1.38
13	a	801	G2O	CHB-C1B	4.72	1.47	1.38
13	a	802	G2O	C3C-C2C	4.69	1.46	1.36
13	A	824	G2O	CHC-C1C	4.68	1.49	1.39
13	A	824	G2O	CHD-C4C	4.68	1.47	1.38
8	A	814	F39	C19-C20	4.67	1.60	1.51
13	a	805	G2O	C3C-C2C	4.66	1.46	1.36
13	a	801	G2O	C3C-C2C	4.65	1.46	1.36
13	a	802	G2O	CHD-C4C	4.65	1.47	1.38
13	a	805	G2O	CHD-C4C	4.61	1.47	1.38
7	U	401	BCL	MG-NA	4.57	2.17	2.06
13	a	802	G2O	C1C-C2C	4.52	1.53	1.44
13	a	801	G2O	CBD-CGD	-4.51	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	805	G2O	C1C-C2C	4.50	1.53	1.44
13	A	824	G2O	C1C-C2C	4.50	1.53	1.44
13	a	801	G2O	CHD-C4C	4.50	1.47	1.38
13	a	802	G2O	CBD-CGD	-4.49	1.38	1.52
7	W	401	BCL	MG-NA	4.48	2.16	2.06
13	a	805	G2O	CBD-CGD	-4.48	1.38	1.52
13	a	805	G2O	CHC-C1C	4.47	1.49	1.39
7	V	408[B]	BCL	MG-NA	4.43	2.16	2.06
7	a	812	BCL	MG-NA	4.41	2.16	2.06
7	A	804	BCL	MG-NA	4.41	2.16	2.06
7	U	406	BCL	MG-NA	4.39	2.16	2.06
13	A	824	G2O	CBD-CGD	-4.39	1.39	1.52
7	a	815	BCL	MG-NA	4.38	2.16	2.06
13	a	801	G2O	C1C-C2C	4.38	1.53	1.44
13	a	802	G2O	CHC-C1C	4.34	1.49	1.39
7	V	403	BCL	MG-NA	4.34	2.16	2.06
8	a	818	F39	C19-C20	4.33	1.60	1.51
7	V	401	BCL	MG-NA	4.32	2.16	2.06
7	A	807	BCL	MG-NA	4.32	2.16	2.06
7	W	402	BCL	MG-NA	4.31	2.16	2.06
6	a	804	GS0	OBD-CAD	4.31	1.29	1.22
6	a	804	GS0	O1D-CGD	-4.30	1.10	1.21
7	V	406	BCL	MG-NA	4.29	2.16	2.06
7	U	408[B]	BCL	MG-NA	4.28	2.16	2.06
7	W	404	BCL	MG-NA	4.27	2.16	2.06
7	V	402	BCL	MG-NA	4.24	2.16	2.06
6	A	801	GS0	OBD-CAD	4.24	1.29	1.22
7	U	407	BCL	MG-NA	4.23	2.16	2.06
7	a	808	BCL	MG-NA	4.22	2.16	2.06
7	A	805	BCL	MG-NA	4.20	2.16	2.06
7	V	407	BCL	MG-NA	4.18	2.16	2.06
6	A	801	GS0	O1D-CGD	-4.17	1.10	1.21
7	A	808	BCL	MG-NA	4.16	2.16	2.06
7	a	816	BCL	MG-NA	4.16	2.16	2.06
7	A	803	BCL	MG-NA	4.15	2.16	2.06
7	a	807	BCL	MG-NA	4.13	2.16	2.06
13	a	801	G2O	CHC-C1C	4.13	1.48	1.39
7	U	403	BCL	MG-NA	4.12	2.16	2.06
7	a	806	BCL	MG-NA	4.09	2.16	2.06
7	V	404	BCL	MG-NA	4.09	2.16	2.06
7	W	405	BCL	MG-NA	4.09	2.16	2.06
7	a	811	BCL	MG-NA	4.08	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	U	402	BCL	MG-NA	4.07	2.15	2.06
13	a	801	G2O	C4C-C3C	4.07	1.51	1.45
13	A	824	G2O	C3B-C2B	4.07	1.45	1.37
7	W	403	BCL	MG-NA	4.06	2.15	2.06
7	A	811	BCL	MG-NA	4.04	2.15	2.06
13	A	824	G2O	O2D-CGD	4.04	1.43	1.33
7	a	813	BCL	MG-NA	4.02	2.15	2.06
13	a	801	G2O	O2D-CGD	4.02	1.43	1.33
7	U	404	BCL	MG-NA	4.00	2.15	2.06
13	a	805	G2O	O2D-CGD	4.00	1.43	1.33
7	A	813	BCL	MG-NA	3.99	2.15	2.06
7	A	812	BCL	MG-NA	3.99	2.15	2.06
7	V	405	BCL	MG-NA	3.99	2.15	2.06
13	A	824	G2O	CHB-C4A	3.98	1.50	1.39
7	W	406	BCL	MG-NA	3.98	2.15	2.06
7	U	405	BCL	MG-NA	3.97	2.15	2.06
13	a	802	G2O	C4C-C3C	3.96	1.51	1.45
7	A	806	BCL	MG-NA	3.95	2.15	2.06
7	A	810	BCL	MG-NA	3.94	2.15	2.06
13	a	802	G2O	O2D-CGD	3.94	1.42	1.33
7	W	407[B]	BCL	MG-NA	3.92	2.15	2.06
13	A	824	G2O	C4C-C3C	3.92	1.51	1.45
7	A	809	BCL	MG-NA	3.90	2.15	2.06
13	a	805	G2O	C4C-C3C	3.89	1.51	1.45
13	A	824	G2O	O2A-CGA	3.88	1.44	1.33
13	a	802	G2O	O2A-CGA	3.86	1.44	1.33
7	a	810	BCL	MG-NA	3.86	2.15	2.06
7	U	409	BCL	MG-NA	3.85	2.15	2.06
7	A	802	BCL	MG-NA	3.84	2.15	2.06
13	a	801	G2O	O2A-CGA	3.84	1.44	1.33
13	a	801	G2O	C3B-C2B	3.82	1.44	1.37
7	a	809	BCL	MG-NA	3.82	2.15	2.06
13	a	805	G2O	O2A-CGA	3.81	1.44	1.33
13	a	802	G2O	CHB-C4A	3.80	1.49	1.39
9	A	815	F26	C35-C34	3.79	1.54	1.46
13	a	802	G2O	C3B-C2B	3.76	1.44	1.37
13	a	805	G2O	C3B-C2B	3.75	1.44	1.37
7	A	805	BCL	CHD-C1D	3.73	1.45	1.38
7	a	817	BCL	MG-NA	3.72	2.15	2.06
13	a	805	G2O	CHB-C4A	3.69	1.49	1.39
7	A	805	BCL	MG-ND	-3.67	1.98	2.05
13	a	801	G2O	CHB-C4A	3.65	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	810	BCL	CHD-C1D	3.65	1.45	1.38
7	a	814	BCL	MG-NA	3.60	2.14	2.06
9	A	815	F26	C28-C31	3.59	1.53	1.46
7	V	401	BCL	CHD-C1D	3.58	1.45	1.38
9	a	819	F26	C28-C31	3.54	1.53	1.46
9	a	819	F26	C15-C19	3.54	1.53	1.46
13	A	824	G2O	C2-C3	3.53	1.41	1.33
9	a	820	F26	C35-C34	3.52	1.53	1.46
13	a	802	G2O	C2-C3	3.51	1.41	1.33
7	a	809	BCL	MG-ND	-3.51	1.98	2.05
7	a	809	BCL	CHD-C1D	3.51	1.45	1.38
6	A	801	GS0	O2D-CED	3.51	1.53	1.45
9	a	820	F26	C28-C31	3.49	1.53	1.46
7	U	405	BCL	CHD-C1D	3.48	1.45	1.38
7	W	404	BCL	CHD-C1D	3.47	1.45	1.38
13	a	801	G2O	C2-C3	3.46	1.41	1.33
6	a	804	GS0	O2D-CED	3.46	1.53	1.45
9	A	815	F26	C25-C26	3.42	1.53	1.46
13	A	824	G2O	OBD-CAD	3.42	1.28	1.22
13	a	801	G2O	O1D-CGD	3.42	1.29	1.21
13	a	805	G2O	OBD-CAD	3.41	1.28	1.22
13	A	824	G2O	O1D-CGD	3.41	1.29	1.21
13	a	802	G2O	OBD-CAD	3.40	1.28	1.22
13	a	805	G2O	C2-C3	3.40	1.40	1.33
13	a	805	G2O	O1D-CGD	3.40	1.29	1.21
13	a	802	G2O	O1D-CGD	3.38	1.29	1.21
7	U	401	BCL	CHD-C1D	3.37	1.45	1.38
9	a	820	F26	C15-C19	3.36	1.53	1.46
7	V	405	BCL	CHD-C1D	3.35	1.44	1.38
7	A	812	BCL	CHD-C1D	3.35	1.44	1.38
7	W	403	BCL	CHD-C1D	3.34	1.44	1.38
9	a	820	F26	C25-C26	3.33	1.53	1.46
6	A	801	GS0	O2D-CGD	-3.33	1.25	1.33
7	a	812	BCL	CHD-C1D	3.33	1.44	1.38
7	a	811	BCL	CHD-C1D	3.32	1.44	1.38
7	V	404	BCL	CHD-C1D	3.30	1.44	1.38
9	A	815	F26	C15-C19	3.30	1.53	1.46
7	A	812	BCL	MG-ND	-3.30	1.99	2.05
7	W	406	BCL	CHD-C1D	3.29	1.44	1.38
9	A	815	F26	C39-C37	3.26	1.53	1.43
7	W	401	BCL	CHD-C1D	3.26	1.44	1.38
7	a	814	BCL	CHD-C1D	3.25	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	a	807	BCL	CHD-C1D	3.24	1.44	1.38
7	A	811	BCL	CHD-C1D	3.23	1.44	1.38
7	A	807	BCL	CHD-C1D	3.20	1.44	1.38
7	V	407	BCL	CHD-C1D	3.19	1.44	1.38
9	A	815	F26	C32-C30	3.19	1.53	1.43
7	a	812	BCL	MG-ND	-3.19	1.99	2.05
9	a	820	F26	C38-C33	3.18	1.53	1.43
7	A	803	BCL	CHD-C1D	3.18	1.44	1.38
7	W	405	BCL	MG-ND	-3.17	1.99	2.05
7	W	405	BCL	CHD-C1D	3.17	1.44	1.38
7	a	813	BCL	CHD-C1D	3.16	1.44	1.38
7	U	407	BCL	CHD-C1D	3.15	1.44	1.38
9	A	815	F26	C27-C24	3.15	1.53	1.43
7	A	810	BCL	MG-ND	-3.13	1.99	2.05
7	U	404	BCL	CHD-C1D	3.13	1.44	1.38
6	a	804	GS0	O2A-CGA	-3.13	1.24	1.33
13	a	801	G2O	OBD-CAD	3.13	1.27	1.22
7	a	815	BCL	CHD-C1D	3.12	1.44	1.38
7	a	817	BCL	CHD-C1D	3.12	1.44	1.38
7	a	814	BCL	MG-ND	-3.12	1.99	2.05
6	a	804	GS0	O2D-CGD	-3.11	1.25	1.33
7	a	816	BCL	CHD-C1D	3.10	1.44	1.38
7	A	806	BCL	CHD-C1D	3.10	1.44	1.38
7	A	802	BCL	CHD-C1D	3.10	1.44	1.38
7	A	808	BCL	CHD-C1D	3.10	1.44	1.38
9	A	815	F26	C38-C33	3.10	1.52	1.43
13	a	801	G2O	C3D-C4D	3.09	1.48	1.40
7	U	406	BCL	CHD-C1D	3.09	1.44	1.38
9	a	820	F26	C39-C37	3.08	1.52	1.43
7	V	408[B]	BCL	CHD-C1D	3.07	1.44	1.38
7	U	402	BCL	CHD-C1D	3.07	1.44	1.38
7	W	402	BCL	CHD-C1D	3.07	1.44	1.38
7	a	810	BCL	CHD-C1D	3.05	1.44	1.38
7	A	813	BCL	CHD-C1D	3.05	1.44	1.38
13	a	802	G2O	C3D-C4D	3.05	1.48	1.40
9	a	819	F26	C39-C37	3.04	1.52	1.43
7	U	403	BCL	CHD-C1D	3.04	1.44	1.38
9	a	820	F26	C32-C30	3.04	1.52	1.43
13	a	805	G2O	C3D-C4D	3.03	1.48	1.40
7	U	409	BCL	CHD-C1D	3.03	1.44	1.38
7	a	806	BCL	CHD-C1D	3.03	1.44	1.38
9	a	820	F26	C27-C24	3.02	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	819	F26	C38-C33	3.02	1.52	1.43
7	U	408[B]	BCL	CHD-C1D	3.01	1.44	1.38
9	A	815	F26	C22-C18	3.01	1.52	1.43
9	a	819	F26	C27-C24	3.00	1.52	1.43
6	A	801	GS0	O2A-CGA	-2.99	1.24	1.33
6	A	801	GS0	C1D-C2D	-2.98	1.39	1.45
7	A	804	BCL	CHD-C1D	2.98	1.44	1.38
13	A	824	G2O	C3D-C4D	2.97	1.47	1.40
7	a	810	BCL	MG-ND	-2.97	1.99	2.05
7	W	402	BCL	MG-ND	-2.96	1.99	2.05
7	a	811	BCL	MG-ND	-2.95	1.99	2.05
7	U	405	BCL	MG-ND	-2.95	1.99	2.05
9	a	819	F26	C25-C26	2.95	1.52	1.46
9	a	819	F26	C35-C34	2.95	1.52	1.46
7	V	406	BCL	CHD-C1D	2.94	1.44	1.38
7	V	403	BCL	MG-ND	-2.92	2.00	2.05
7	A	813	BCL	MG-ND	-2.92	2.00	2.05
13	A	824	G2O	C1D-C2D	2.92	1.50	1.43
9	a	820	F26	C22-C18	2.92	1.52	1.43
7	V	406	BCL	MG-ND	-2.92	2.00	2.05
7	a	808	BCL	CHD-C1D	2.92	1.44	1.38
7	V	403	BCL	CHD-C1D	2.91	1.44	1.38
13	a	805	G2O	C1D-C2D	2.91	1.50	1.43
7	V	404	BCL	MG-ND	-2.90	2.00	2.05
7	W	404	BCL	MG-ND	-2.89	2.00	2.05
7	A	807	BCL	MG-ND	-2.89	2.00	2.05
6	A	801	GS0	O1A-CGA	-2.88	1.13	1.22
7	W	407[B]	BCL	CHD-C1D	2.88	1.44	1.38
7	A	803	BCL	MG-ND	-2.87	2.00	2.05
7	V	405	BCL	MG-ND	-2.86	2.00	2.05
13	a	802	G2O	C5-C6	2.86	1.59	1.50
7	A	806	BCL	MG-ND	-2.86	2.00	2.05
13	A	824	G2O	C5-C6	2.85	1.59	1.50
7	a	813	BCL	MG-ND	-2.85	2.00	2.05
7	U	404	BCL	MG-ND	-2.84	2.00	2.05
13	a	805	G2O	C5-C6	2.83	1.59	1.50
6	a	804	GS0	O1A-CGA	-2.83	1.14	1.22
7	V	402	BCL	CHD-C1D	2.82	1.43	1.38
7	a	807	BCL	MG-ND	-2.82	2.00	2.05
13	A	824	G2O	C3A-C2A	-2.82	1.46	1.54
13	a	802	G2O	C1D-C2D	2.82	1.49	1.43
7	V	401	BCL	MG-ND	-2.81	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	W	401	BCL	MG-ND	-2.81	2.00	2.05
7	A	808	BCL	MG-ND	-2.81	2.00	2.05
9	a	820	F26	C8-C13	2.81	1.57	1.51
9	a	819	F26	C32-C30	2.80	1.51	1.43
7	V	402	BCL	MG-ND	-2.80	2.00	2.05
7	W	403	BCL	MG-ND	-2.80	2.00	2.05
7	U	401	BCL	MG-ND	-2.79	2.00	2.05
13	a	801	G2O	C5-C6	2.79	1.58	1.50
7	U	403	BCL	MG-ND	-2.79	2.00	2.05
13	a	801	G2O	C1D-C2D	2.73	1.49	1.43
7	A	804	BCL	MG-ND	-2.71	2.00	2.05
7	A	809	BCL	CHD-C1D	2.71	1.43	1.38
7	A	802	BCL	MG-ND	-2.70	2.00	2.05
7	a	815	BCL	MG-ND	-2.70	2.00	2.05
9	A	815	F26	C8-C13	2.70	1.56	1.51
7	U	408[B]	BCL	MG-ND	-2.70	2.00	2.05
9	a	819	F26	C22-C18	2.67	1.51	1.43
7	U	409	BCL	MG-ND	-2.67	2.00	2.05
7	a	808	BCL	MG-ND	-2.67	2.00	2.05
7	A	809	BCL	MG-ND	-2.66	2.00	2.05
7	U	407	BCL	MG-ND	-2.66	2.00	2.05
7	U	402	BCL	MG-ND	-2.65	2.00	2.05
7	A	811	BCL	MG-ND	-2.65	2.00	2.05
7	U	406	BCL	MG-ND	-2.65	2.00	2.05
13	a	801	G2O	C5-C3	2.64	1.58	1.51
7	W	406	BCL	MG-ND	-2.63	2.00	2.05
7	V	408[B]	BCL	MG-ND	-2.63	2.00	2.05
13	a	805	G2O	C5-C3	2.63	1.58	1.51
13	a	805	G2O	O1A-CGA	2.63	1.30	1.22
8	a	818	F39	C50-C49	2.62	1.43	1.38
7	a	806	BCL	MG-ND	-2.59	2.00	2.05
13	A	824	G2O	C1-C2	2.59	1.56	1.49
13	a	801	G2O	C3A-C2A	-2.59	1.47	1.54
13	A	824	G2O	C5-C3	2.59	1.58	1.51
13	a	805	G2O	C3A-C2A	-2.58	1.47	1.54
6	A	801	GS0	OBB-CAB	-2.57	1.17	1.23
8	A	814	F39	C50-C49	2.57	1.43	1.38
13	a	802	G2O	C1-C2	2.57	1.56	1.49
7	W	407[B]	BCL	MG-ND	-2.57	2.00	2.05
7	a	817	BCL	MG-ND	-2.56	2.00	2.05
13	a	802	G2O	O1A-CGA	2.56	1.30	1.22
13	a	801	G2O	C1-C2	2.55	1.56	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	V	407	BCL	MG-ND	-2.54	2.00	2.05
7	a	816	BCL	MG-ND	-2.54	2.00	2.05
13	a	801	G2O	O1A-CGA	2.53	1.30	1.22
13	A	824	G2O	O1A-CGA	2.53	1.30	1.22
13	a	802	G2O	C3A-C2A	-2.53	1.47	1.54
13	a	802	G2O	CBA-CGA	2.53	1.58	1.50
13	a	801	G2O	C1B-NB	2.52	1.41	1.37
13	a	802	G2O	C5-C3	2.51	1.58	1.51
13	a	805	G2O	C1-C2	2.50	1.56	1.49
8	a	818	F39	C47-C45	2.49	1.44	1.40
13	A	824	G2O	CBA-CGA	2.49	1.57	1.50
13	a	805	G2O	CBA-CGA	2.48	1.57	1.50
7	A	802	BCL	C3B-C4B	2.48	1.46	1.41
8	a	818	F39	C11-C9	2.48	1.59	1.52
9	a	819	F26	C8-C13	2.48	1.56	1.51
8	a	818	F39	C46-C48	2.46	1.44	1.41
13	a	801	G2O	CBA-CGA	2.46	1.57	1.50
13	a	801	G2O	C4-C3	2.46	1.56	1.50
6	a	804	GS0	OBB-CAB	-2.46	1.17	1.23
6	a	804	GS0	C1B-C2B	-2.44	1.37	1.43
6	A	801	GS0	C1B-C2B	-2.43	1.37	1.43
13	A	824	G2O	C4-C3	2.43	1.56	1.50
8	A	814	F39	C23-C22	2.43	1.61	1.52
8	a	818	F39	O6-C21	2.42	1.40	1.33
6	a	804	GS0	C1D-C2D	-2.41	1.40	1.45
13	a	805	G2O	C4-C3	2.40	1.56	1.50
10	A	817	LHG	O7-C5	-2.39	1.41	1.46
7	a	807	BCL	CAC-C3C	2.39	1.58	1.54
8	A	814	F39	C47-C45	2.39	1.44	1.40
8	A	814	F39	O6-C21	2.38	1.40	1.33
13	a	801	G2O	O2D-CED	2.38	1.50	1.45
8	A	814	F39	C46-C48	2.36	1.44	1.41
13	a	802	G2O	C4-C3	2.33	1.56	1.50
8	a	818	F39	C23-C22	2.32	1.60	1.52
7	a	812	BCL	C3B-C4B	2.32	1.45	1.41
8	a	818	F39	C38-C37	2.30	1.55	1.50
7	A	810	BCL	C3D-C4D	-2.29	1.39	1.44
7	A	812	BCL	C3B-C4B	2.29	1.45	1.41
11	a	824	LMG	O7-C8	-2.28	1.41	1.46
7	A	805	BCL	C3D-C4D	-2.28	1.39	1.44
7	a	807	BCL	C3D-C4D	-2.28	1.39	1.44
7	A	813	BCL	C3D-C4D	-2.28	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	a	814	BCL	C3D-C4D	-2.27	1.39	1.44
7	V	406	BCL	C3D-C4D	-2.26	1.39	1.44
13	a	802	G2O	C1B-NB	2.25	1.40	1.37
13	a	802	G2O	C7-C6	2.25	1.40	1.31
6	A	801	GS0	C3B-CAB	2.25	1.53	1.46
13	a	805	G2O	CAA-CBA	2.24	1.59	1.52
13	A	824	G2O	MG-NB	-2.24	2.01	2.05
7	a	811	BCL	C3D-C4D	-2.24	1.39	1.44
13	a	805	G2O	CHD-C1D	2.24	1.44	1.39
6	a	804	GS0	C3B-CAB	2.24	1.53	1.46
7	a	816	BCL	C3B-C4B	2.24	1.45	1.41
7	a	812	BCL	C3D-C4D	-2.23	1.39	1.44
7	V	406	BCL	C1D-C2D	-2.23	1.40	1.45
7	U	409	BCL	C3D-C4D	-2.22	1.39	1.44
7	W	407[B]	BCL	C3D-C4D	-2.22	1.39	1.44
7	W	406	BCL	C3D-C4D	-2.21	1.39	1.44
13	A	824	G2O	CHD-C1D	2.21	1.44	1.39
7	V	404	BCL	C3D-C4D	-2.21	1.39	1.44
10	C	301	LHG	O7-C5	-2.20	1.41	1.46
7	a	813	BCL	C3D-C4D	-2.20	1.39	1.44
7	U	404	BCL	C3D-C4D	-2.20	1.39	1.44
7	V	401	BCL	C3D-C4D	-2.20	1.39	1.44
8	A	814	F39	C18-C19	2.20	1.60	1.52
13	a	805	G2O	C7-C6	2.19	1.40	1.31
7	V	404	BCL	C3B-C4B	2.19	1.45	1.41
13	A	824	G2O	C7-C6	2.19	1.40	1.31
7	A	806	BCL	C3B-C4B	2.19	1.45	1.41
7	a	814	BCL	C3B-C4B	2.19	1.45	1.41
7	a	808	BCL	C3B-C4B	2.18	1.45	1.41
10	a	821	LHG	O7-C5	-2.18	1.41	1.46
13	a	802	G2O	CHD-C1D	2.18	1.44	1.39
7	V	403	BCL	C3D-C4D	-2.18	1.39	1.44
10	A	816	LHG	P-O6	2.18	1.67	1.59
7	W	402	BCL	C3B-C4B	2.17	1.45	1.41
13	A	824	G2O	CAA-CBA	2.17	1.59	1.52
13	A	824	G2O	O2D-CED	2.17	1.50	1.45
7	W	401	BCL	MG-NC	2.17	2.11	2.06
13	a	801	G2O	C7-C6	2.17	1.40	1.31
7	U	408[B]	BCL	C3D-C4D	-2.17	1.39	1.44
7	U	402	BCL	C3D-C4D	-2.16	1.39	1.44
7	A	807	BCL	C3D-C4D	-2.16	1.39	1.44
13	a	802	G2O	CAA-CBA	2.16	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	812	BCL	C3D-C4D	-2.16	1.39	1.44
7	W	403	BCL	C3D-C4D	-2.16	1.39	1.44
13	a	802	G2O	O2D-CED	2.16	1.50	1.45
8	a	818	F39	C18-C19	2.15	1.60	1.52
13	a	805	G2O	C1B-NB	2.15	1.40	1.37
8	A	814	F39	C11-C9	2.15	1.58	1.52
7	U	407	BCL	C3D-C4D	-2.15	1.39	1.44
7	a	812	BCL	C5-C3	2.15	1.55	1.51
13	a	801	G2O	CAA-CBA	2.15	1.59	1.52
7	a	815	BCL	C3D-C4D	-2.14	1.39	1.44
7	U	402	BCL	C3B-C4B	2.14	1.45	1.41
13	a	805	G2O	O2D-CED	2.14	1.50	1.45
7	a	808	BCL	C3D-C4D	-2.14	1.39	1.44
7	W	401	BCL	C3D-C4D	-2.14	1.39	1.44
7	U	403	BCL	C3D-C4D	-2.14	1.39	1.44
11	C	302	LMG	C4-C5	2.13	1.57	1.53
8	A	814	F39	C38-C37	2.13	1.55	1.50
7	A	811	BCL	C3D-C4D	-2.13	1.39	1.44
7	A	808	BCL	C3D-C4D	-2.13	1.39	1.44
7	A	803	BCL	C3D-C4D	-2.12	1.39	1.44
7	a	817	BCL	C3D-C4D	-2.12	1.39	1.44
7	V	407	BCL	C3D-C4D	-2.12	1.39	1.44
7	W	405	BCL	C3D-C4D	-2.12	1.39	1.44
7	U	408[B]	BCL	MG-NC	2.11	2.11	2.06
7	a	810	BCL	C3D-C4D	-2.11	1.39	1.44
11	A	822	LMG	O7-C8	-2.11	1.41	1.46
7	a	815	BCL	C3B-C4B	2.10	1.45	1.41
7	W	402	BCL	C3D-C4D	-2.10	1.39	1.44
7	A	809	BCL	C3D-C4D	-2.10	1.39	1.44
7	A	804	BCL	MG-NC	2.09	2.11	2.06
7	a	810	BCL	C3B-C4B	2.09	1.45	1.41
7	A	804	BCL	C3D-C4D	-2.09	1.39	1.44
7	V	402	BCL	C3D-C4D	-2.09	1.39	1.44
7	V	408[B]	BCL	C3D-C4D	-2.09	1.39	1.44
7	U	401	BCL	C3D-C4D	-2.09	1.39	1.44
7	V	405	BCL	CBD-CGD	-2.08	1.46	1.52
7	U	407	BCL	MG-NC	2.08	2.11	2.06
7	W	404	BCL	C3D-C4D	-2.08	1.39	1.44
7	a	807	BCL	C3B-C4B	2.08	1.45	1.41
7	a	815	BCL	MG-NC	2.08	2.11	2.06
13	a	801	G2O	CBB-CAB	2.08	1.40	1.30
7	A	804	BCL	CBD-CGD	-2.08	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	a	806	BCL	C3D-C4D	-2.08	1.39	1.44
7	V	405	BCL	C3D-C4D	-2.08	1.39	1.44
10	a	822	LHG	P-O6	2.08	1.67	1.59
6	a	804	GS0	C3B-C2B	-2.08	1.35	1.42
7	A	807	BCL	C3B-C4B	2.07	1.45	1.41
7	U	405	BCL	C3D-C4D	-2.07	1.39	1.44
7	A	806	BCL	C3D-C4D	-2.07	1.39	1.44
7	V	407	BCL	MG-NC	2.07	2.11	2.06
7	V	402	BCL	C1D-C2D	-2.06	1.41	1.45
11	A	821	LMG	O7-C8	-2.06	1.41	1.46
7	W	402	BCL	C1D-C2D	-2.06	1.41	1.45
7	U	402	BCL	CBD-CGD	-2.06	1.46	1.52
7	A	802	BCL	C3D-C4D	-2.06	1.39	1.44
7	A	813	BCL	C3B-C4B	2.05	1.45	1.41
13	a	801	G2O	CHD-C1D	2.05	1.44	1.39
13	A	824	G2O	CBB-CAB	2.05	1.40	1.30
13	a	802	G2O	CBB-CAB	2.05	1.40	1.30
7	A	808	BCL	MG-NC	2.04	2.11	2.06
10	a	821	LHG	P-O6	2.04	1.67	1.59
13	a	801	G2O	O2A-C1	2.04	1.51	1.46
7	U	405	BCL	CBD-CGD	-2.04	1.46	1.52
7	W	405	BCL	CBD-CGD	-2.04	1.46	1.52
7	V	403	BCL	C1D-C2D	-2.03	1.41	1.45
7	a	816	BCL	C3D-C4D	-2.03	1.39	1.44
13	a	805	G2O	CBB-CAB	2.02	1.40	1.30
7	a	813	BCL	CBD-CGD	-2.02	1.46	1.52
7	a	811	BCL	MG-NC	2.01	2.11	2.06
7	A	809	BCL	CBD-CGD	-2.01	1.46	1.52
7	A	809	BCL	C3B-C4B	2.01	1.45	1.41
7	a	810	BCL	CBD-CGD	-2.00	1.46	1.52
13	a	802	G2O	O2A-C1	2.00	1.51	1.46

All (719) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	801	G2O	C1A-NA-C4A	20.15	115.87	106.68
13	a	802	G2O	C1A-NA-C4A	19.47	115.56	106.68
13	a	805	G2O	C1A-NA-C4A	17.54	114.68	106.68
13	A	824	G2O	C1A-NA-C4A	17.37	114.60	106.68
6	A	801	GS0	C4A-NA-C1A	12.50	112.38	106.68
6	a	804	GS0	C4A-NA-C1A	12.40	112.33	106.68
6	a	804	GS0	C4D-CHA-C1A	7.70	130.43	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	a	804	GS0	C1C-NC-C4C	7.57	110.13	106.68
13	a	801	G2O	C5-C6-C7	-7.17	108.76	125.05
13	a	805	G2O	C5-C6-C7	-7.16	108.81	125.05
6	A	801	GS0	C4D-CHA-C1A	7.14	129.76	121.24
13	A	824	G2O	C5-C6-C7	-7.11	108.92	125.05
13	a	801	G2O	C1D-ND-C4D	6.53	110.90	106.31
13	a	802	G2O	C5-C6-C7	-6.52	110.25	125.05
6	A	801	GS0	C1C-NC-C4C	6.51	109.65	106.68
9	a	819	F26	C22-C18-C13	-6.32	118.80	127.69
8	a	818	F39	C11-O1-C12	6.17	125.78	113.72
13	a	802	G2O	C1D-ND-C4D	6.07	110.57	106.31
9	A	815	F26	C38-C33-C31	-6.05	118.79	127.28
7	W	401	BCL	C1-C2-C3	-6.00	116.37	126.20
9	a	820	F26	C22-C18-C13	-5.94	119.34	127.69
9	a	819	F26	C32-C30-C26	-5.85	119.07	127.28
9	a	819	F26	C38-C33-C31	-5.85	119.08	127.28
8	A	814	F39	C11-O1-C12	5.81	125.07	113.72
9	a	820	F26	C23-C19-C15	-5.79	109.24	118.09
13	A	824	G2O	CMA-C3A-C4A	5.77	127.27	111.77
13	a	805	G2O	C1D-ND-C4D	5.75	110.35	106.31
7	U	406	BCL	C4D-CHA-C1A	5.68	128.02	121.24
7	a	813	BCL	C4D-CHA-C1A	5.63	127.96	121.24
7	U	405	BCL	C4D-CHA-C1A	5.61	127.94	121.24
7	A	807	BCL	C4D-CHA-C1A	5.61	127.93	121.24
13	a	805	G2O	CAA-C2A-C3A	5.59	128.12	113.00
7	V	403	BCL	C4D-CHA-C1A	5.56	127.88	121.24
7	U	407	BCL	C4D-CHA-C1A	5.55	127.86	121.24
7	V	405	BCL	C4D-CHA-C1A	5.54	127.85	121.24
7	A	805	BCL	C4D-CHA-C1A	5.52	127.83	121.24
7	V	407	BCL	C4D-CHA-C1A	5.50	127.80	121.24
8	a	818	F39	C32-C27-C20	-5.48	119.98	127.69
7	W	405	BCL	C4D-CHA-C1A	5.47	127.76	121.24
7	a	815	BCL	C4D-CHA-C1A	5.46	127.76	121.24
7	a	807	BCL	C4D-CHA-C1A	5.46	127.75	121.24
7	a	808	BCL	C4D-CHA-C1A	5.43	127.72	121.24
7	A	813	BCL	C4D-CHA-C1A	5.42	127.70	121.24
9	a	819	F26	C23-C19-C15	-5.41	109.82	118.09
9	A	815	F26	C22-C18-C13	-5.39	120.10	127.69
7	A	803	BCL	C4D-CHA-C1A	5.37	127.65	121.24
7	V	404	BCL	C4D-CHA-C1A	5.37	127.65	121.24
7	A	812	BCL	C4D-CHA-C1A	5.36	127.64	121.24
13	a	801	G2O	CMA-C3A-C4A	5.36	126.18	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	814	F39	C57-C59-C62	-5.35	119.77	127.28
7	U	401	BCL	C4D-CHA-C1A	5.35	127.62	121.24
9	A	815	F26	C23-C19-C15	-5.35	109.92	118.09
7	V	406	BCL	C4D-CHA-C1A	5.35	127.62	121.24
7	W	401	BCL	C4D-CHA-C1A	5.34	127.62	121.24
7	a	812	BCL	C4D-CHA-C1A	5.34	127.61	121.24
7	A	809	BCL	C4D-CHA-C1A	5.31	127.58	121.24
8	A	814	F39	C51-C44-C42	-5.31	119.83	127.28
13	a	805	G2O	CMA-C3A-C4A	5.30	126.03	111.77
7	W	406	BCL	C4D-CHA-C1A	5.30	127.56	121.24
13	a	802	G2O	CMA-C3A-C4A	5.29	125.99	111.77
7	a	810	BCL	C4D-CHA-C1A	5.28	127.54	121.24
8	A	814	F39	C32-C27-C20	-5.27	120.28	127.69
7	A	808	BCL	C4D-CHA-C1A	5.27	127.52	121.24
7	W	402	BCL	C4D-CHA-C1A	5.25	127.50	121.24
7	U	403	BCL	C4D-CHA-C1A	5.24	127.50	121.24
7	a	814	BCL	C4D-CHA-C1A	5.23	127.48	121.24
7	W	404	BCL	C4D-CHA-C1A	5.23	127.48	121.24
6	a	804	GS0	O2D-CGD-CBD	5.21	120.34	111.23
7	W	403	BCL	C4D-CHA-C1A	5.20	127.45	121.24
13	a	802	G2O	CAA-C2A-C3A	5.19	127.04	113.00
7	V	408[B]	BCL	C4D-CHA-C1A	5.19	127.43	121.24
7	U	402	BCL	C4D-CHA-C1A	5.19	127.43	121.24
7	a	806	BCL	C4D-CHA-C1A	5.18	127.43	121.24
7	A	810	BCL	C4D-CHA-C1A	5.18	127.42	121.24
7	V	401	BCL	C4D-CHA-C1A	5.18	127.42	121.24
8	A	814	F39	C40-C39-C37	-5.17	120.02	127.28
7	A	811	BCL	C4D-CHA-C1A	5.15	127.38	121.24
13	A	824	G2O	CAA-C2A-C3A	5.12	126.85	113.00
7	U	404	BCL	C4D-CHA-C1A	5.07	127.29	121.24
8	a	818	F39	C40-C39-C37	-5.04	120.21	127.28
6	a	804	GS0	C2A-C1A-CHA	5.03	132.60	123.87
8	a	818	F39	C63-C61-C58	-5.03	120.23	127.28
7	A	806	BCL	C4D-CHA-C1A	5.02	127.23	121.24
7	a	817	BCL	C4D-CHA-C1A	5.00	127.21	121.24
13	a	801	G2O	CAA-C2A-C3A	4.97	126.44	113.00
8	A	814	F39	C63-C61-C58	-4.97	120.31	127.28
13	A	824	G2O	CAA-C2A-C1A	4.97	128.25	111.97
7	U	409	BCL	C4D-CHA-C1A	4.96	127.16	121.24
8	a	818	F39	C51-C44-C42	-4.96	120.33	127.28
7	a	816	BCL	C4D-CHA-C1A	4.95	127.15	121.24
6	A	801	GS0	C2A-C1A-CHA	4.95	132.46	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	820	F26	C38-C33-C31	-4.94	120.34	127.28
7	U	402	BCL	C1-C2-C3	-4.92	118.13	126.20
7	A	805	BCL	C1C-NC-C4C	4.92	108.92	106.68
6	A	801	GS0	CMB-C2B-C1B	-4.91	117.94	125.42
7	a	811	BCL	C4D-CHA-C1A	4.88	127.07	121.24
7	V	402	BCL	C4D-CHA-C1A	4.87	127.05	121.24
7	a	809	BCL	C4A-NA-C1A	4.87	108.90	106.68
7	a	809	BCL	CHD-C1D-ND	-4.86	117.96	124.80
8	A	814	F39	O6-C21-C22	4.82	126.52	111.83
13	a	801	G2O	CAA-C2A-C1A	4.80	127.70	111.97
6	a	804	GS0	O2D-CGD-O1D	-4.77	114.56	123.85
7	W	402	BCL	C4A-NA-C1A	4.77	108.86	106.68
13	a	802	G2O	CAA-C2A-C1A	4.75	127.53	111.97
6	A	801	GS0	O2D-CGD-CBD	4.74	119.52	111.23
7	A	802	BCL	C4D-CHA-C1A	4.72	126.88	121.24
13	A	824	G2O	C1D-ND-C4D	4.72	109.62	106.31
9	a	819	F26	C27-C24-C19	-4.71	120.67	127.28
7	A	804	BCL	C4D-CHA-C1A	4.71	126.86	121.24
9	a	820	F26	C27-C24-C19	-4.71	120.67	127.28
7	W	407[B]	BCL	C4D-CHA-C1A	4.68	126.83	121.24
8	a	818	F39	C57-C59-C62	-4.66	120.75	127.28
9	A	815	F26	C32-C30-C26	-4.61	120.82	127.28
7	V	403	BCL	C4A-NA-C1A	4.59	108.78	106.68
7	W	405	BCL	C4A-NA-C1A	4.56	108.76	106.68
9	a	820	F26	C32-C30-C26	-4.52	120.94	127.28
7	A	805	BCL	CHD-C1D-ND	-4.49	118.49	124.80
13	a	805	G2O	CAA-C2A-C1A	4.48	126.66	111.97
7	V	405	BCL	C4A-NA-C1A	4.45	108.71	106.68
6	A	801	GS0	O2D-CGD-O1D	-4.42	115.25	123.85
9	A	815	F26	C27-C24-C19	-4.40	121.11	127.28
7	A	809	BCL	CHD-C1D-ND	-4.36	118.67	124.80
7	W	407[B]	BCL	CHD-C1D-ND	-4.35	118.68	124.80
7	a	814	BCL	CHD-C1D-ND	-4.32	118.72	124.80
8	a	818	F39	O6-C21-C22	4.32	124.99	111.83
6	a	804	GS0	CMB-C2B-C1B	-4.31	118.85	125.42
7	A	805	BCL	C4A-NA-C1A	4.31	108.65	106.68
7	a	806	BCL	C1-C2-C3	-4.31	119.13	126.20
6	A	801	GS0	CGD-CBD-CAD	4.27	124.66	110.85
7	a	815	BCL	C4A-NA-C1A	4.26	108.62	106.68
6	a	804	GS0	CHB-C1B-NB	4.26	130.44	124.05
6	A	801	GS0	C3B-C4B-NB	-4.26	104.14	109.76
7	V	406	BCL	CHD-C1D-ND	-4.26	118.81	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	815	F26	C39-C37-C34	-4.26	121.31	127.28
6	A	801	GS0	OBB-CAB-CBB	-4.25	110.26	119.77
7	a	808	BCL	CHD-C1D-ND	-4.23	118.86	124.80
6	A	801	GS0	CHA-C1A-NA	-4.22	116.82	126.39
7	a	806	BCL	CHD-C1D-ND	-4.22	118.86	124.80
7	a	817	BCL	CHD-C1D-ND	-4.20	118.89	124.80
7	W	405	BCL	C1C-NC-C4C	4.15	108.57	106.68
7	A	804	BCL	CHD-C1D-ND	-4.15	118.97	124.80
7	a	807	BCL	C1C-NC-C4C	4.14	108.57	106.68
7	V	407	BCL	CHD-C1D-ND	-4.11	119.02	124.80
7	U	405	BCL	C1C-NC-C4C	4.10	108.55	106.68
9	a	820	F26	C39-C37-C34	-4.08	121.55	127.28
7	A	813	BCL	CHD-C1D-ND	-4.08	119.06	124.80
9	a	819	F26	C2-C9-C15	-4.07	119.29	128.50
7	U	408[B]	BCL	C4D-CHA-C1A	4.06	126.09	121.24
7	A	811	BCL	CHD-C1D-ND	-4.03	119.13	124.80
7	A	810	BCL	CHD-C1D-ND	-4.02	119.14	124.80
7	W	405	BCL	CHD-C1D-ND	-4.01	119.15	124.80
7	U	404	BCL	C4A-NA-C1A	4.01	108.51	106.68
6	a	804	GS0	OBB-CAB-CBB	-4.00	110.82	119.77
8	A	814	F39	O6-C21-O7	-3.99	113.65	123.63
7	a	813	BCL	C4A-NA-C1A	3.99	108.50	106.68
7	a	811	BCL	CHD-C1D-ND	-3.98	119.20	124.80
7	W	403	BCL	C4A-NA-C1A	3.98	108.49	106.68
7	U	405	BCL	CHD-C1D-ND	-3.97	119.21	124.80
9	a	820	F26	C2-C9-C15	-3.97	119.51	128.50
7	a	809	BCL	C4D-CHA-C1A	3.96	125.97	121.24
7	V	405	BCL	C1C-NC-C4C	3.96	108.49	106.68
7	a	811	BCL	C1C-NC-C4C	3.95	108.48	106.68
7	V	405	BCL	CHD-C1D-ND	-3.95	119.24	124.80
7	a	816	BCL	C4A-NA-C1A	3.94	108.48	106.68
7	a	808	BCL	C4A-NA-C1A	3.93	108.47	106.68
7	V	402	BCL	C4A-NA-C1A	3.92	108.47	106.68
13	A	824	G2O	C3C-C4C-NC	-3.92	105.71	109.90
7	U	409	BCL	CHD-C1D-ND	-3.91	119.30	124.80
13	A	824	G2O	C2C-C1C-NC	-3.90	105.62	110.45
7	A	807	BCL	CHD-C1D-ND	-3.90	119.32	124.80
7	U	406	BCL	CHD-C1D-ND	-3.89	119.32	124.80
7	V	402	BCL	C1-C2-C3	-3.89	119.82	126.20
7	V	403	BCL	CHD-C1D-ND	-3.89	119.33	124.80
8	a	818	F39	C35-C37-C39	-3.89	112.89	119.01
7	A	805	BCL	CHA-C1A-NA	-3.87	117.63	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	W	406	BCL	CHD-C1D-ND	-3.87	119.36	124.80
6	A	801	GS0	C2B-C1B-NB	-3.85	106.33	110.33
13	A	824	G2O	C2B-C1B-NB	-3.85	106.32	110.13
7	A	807	BCL	C4A-NA-C1A	3.84	108.43	106.68
8	A	814	F39	C56-C58-C61	-3.83	112.98	119.01
7	U	407	BCL	CHD-C1D-ND	-3.83	119.41	124.80
7	W	403	BCL	CHD-C1D-ND	-3.83	119.42	124.80
7	W	401	BCL	C4A-NA-C1A	3.81	108.42	106.68
7	A	810	BCL	C1-C2-C3	-3.81	119.95	126.20
7	a	812	BCL	CHD-C1D-ND	-3.81	119.44	124.80
13	a	802	G2O	C2D-C1D-ND	-3.79	106.40	110.33
7	a	806	BCL	C4A-NA-C1A	3.79	108.41	106.68
13	a	805	G2O	CGD-CBD-CAD	3.78	123.09	110.85
7	a	815	BCL	CHD-C1D-ND	-3.78	119.48	124.80
7	U	403	BCL	CHD-C1D-ND	-3.78	119.48	124.80
7	U	406	BCL	C4A-NA-C1A	3.78	108.40	106.68
7	a	816	BCL	C1C-NC-C4C	3.77	108.40	106.68
7	a	817	BCL	C4A-NA-C1A	3.77	108.40	106.68
7	A	808	BCL	C1-C2-C3	-3.77	120.03	126.20
7	U	403	BCL	C4A-NA-C1A	3.77	108.40	106.68
7	a	809	BCL	C4D-C3D-CAD	-3.76	104.02	108.11
7	U	402	BCL	CHD-C1D-ND	-3.76	119.51	124.80
7	A	812	BCL	CHD-C1D-ND	-3.74	119.53	124.80
7	W	402	BCL	CHD-C1D-ND	-3.74	119.53	124.80
7	A	813	BCL	C1C-NC-C4C	3.74	108.39	106.68
7	V	404	BCL	C4A-NA-C1A	3.74	108.38	106.68
6	a	804	GS0	CGD-CBD-CAD	3.73	122.93	110.85
7	U	408[B]	BCL	CHD-C1D-ND	-3.73	119.55	124.80
7	U	404	BCL	CHD-C1D-ND	-3.72	119.57	124.80
8	a	818	F39	O6-C21-O7	-3.70	114.36	123.63
7	A	806	BCL	C1C-NC-C4C	3.70	108.37	106.68
7	W	404	BCL	CHD-C1D-ND	-3.70	119.59	124.80
7	A	810	BCL	C1C-NC-C4C	3.70	108.37	106.68
7	W	406	BCL	C4A-NA-C1A	3.68	108.36	106.68
7	A	802	BCL	CHD-C1D-ND	-3.67	119.63	124.80
7	a	812	BCL	C4A-NA-C1A	3.67	108.35	106.68
7	W	401	BCL	C1C-NC-C4C	3.65	108.35	106.68
7	a	809	BCL	CHA-C1A-NA	-3.65	118.12	126.39
7	U	401	BCL	CHD-C1D-ND	-3.65	119.66	124.80
7	a	816	BCL	CHD-C1D-ND	-3.65	119.67	124.80
13	a	805	G2O	C2D-C1D-ND	-3.65	106.54	110.33
7	U	401	BCL	C4A-NA-C1A	3.65	108.34	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	802	G2O	CGD-CBD-CAD	3.64	122.64	110.85
7	V	408[B]	BCL	CHD-C1D-ND	-3.63	119.69	124.80
8	A	814	F39	C41-C42-C44	-3.63	113.30	119.01
7	U	403	BCL	C1C-NC-C4C	3.63	108.34	106.68
7	a	813	BCL	CHD-C1D-ND	-3.62	119.70	124.80
7	a	809	BCL	C1C-NC-C4C	3.62	108.33	106.68
7	a	807	BCL	CHD-C1D-ND	-3.61	119.72	124.80
8	A	814	F39	C46-C53-C56	-3.61	120.33	128.50
7	V	404	BCL	CHD-C1D-ND	-3.60	119.74	124.80
7	A	803	BCL	CHD-C1D-ND	-3.58	119.76	124.80
6	A	801	GS0	CMA-C3A-C4A	-3.58	102.15	111.77
7	V	402	BCL	CHD-C1D-ND	-3.57	119.78	124.80
7	A	806	BCL	CHD-C1D-ND	-3.56	119.79	124.80
13	A	824	G2O	CGD-CBD-CAD	3.56	122.37	110.85
7	a	810	BCL	CHD-C1D-ND	-3.55	119.80	124.80
6	A	801	GS0	CMC-C2C-C3C	-3.55	100.25	113.98
8	a	818	F39	C46-C53-C56	-3.55	120.46	128.50
8	a	818	F39	C41-C42-C44	-3.53	113.45	119.01
7	U	405	BCL	C4A-NA-C1A	3.53	108.29	106.68
13	A	824	G2O	C2A-C3A-C4A	3.53	107.57	101.87
7	W	404	BCL	C1C-NC-C4C	3.52	108.28	106.68
7	W	404	BCL	C1-C2-C3	-3.51	120.44	126.20
7	V	401	BCL	CHD-C1D-ND	-3.51	119.86	124.80
7	A	813	BCL	CHA-C1A-NA	-3.50	118.46	126.39
7	a	814	BCL	C1C-NC-C4C	3.50	108.28	106.68
7	A	808	BCL	CHD-C1D-ND	-3.50	119.88	124.80
7	V	402	BCL	C1C-NC-C4C	3.50	108.27	106.68
13	A	824	G2O	O2D-CGD-O1D	-3.49	117.05	123.85
7	U	401	BCL	C1C-NC-C4C	3.49	108.27	106.68
7	W	401	BCL	CHD-C1D-ND	-3.47	119.92	124.80
13	a	801	G2O	CGD-CBD-CAD	3.47	122.08	110.85
13	a	805	G2O	CMA-C3A-C2A	3.46	127.36	113.98
7	A	805	BCL	C1-C2-C3	-3.46	120.53	126.20
13	a	801	G2O	C2D-C1D-ND	-3.46	106.74	110.33
7	a	814	BCL	CHA-C1A-NA	-3.45	118.57	126.39
7	U	408[B]	BCL	C2A-C1A-CHA	3.45	129.86	123.87
13	a	801	G2O	CMA-C3A-C2A	3.45	127.33	113.98
7	A	809	BCL	C4A-NA-C1A	3.45	108.25	106.68
7	V	403	BCL	C1C-NC-C4C	3.44	108.25	106.68
7	a	814	BCL	C2A-C1A-CHA	3.44	129.84	123.87
8	a	818	F39	C32-C35-C37	-3.44	116.94	126.36
6	a	804	GS0	CHA-C1A-NA	-3.44	118.61	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	403	BCL	C1-C2-C3	-3.43	120.57	126.20
8	a	818	F39	C56-C58-C61	-3.43	113.61	119.01
7	a	813	BCL	C1C-NC-C4C	3.43	108.24	106.68
13	a	802	G2O	CMA-C3A-C2A	3.43	127.23	113.98
7	A	810	BCL	CHA-C1A-NA	-3.42	118.65	126.39
7	a	810	BCL	C2A-C1A-CHA	3.41	129.79	123.87
9	a	819	F26	C39-C37-C34	-3.40	122.51	127.28
13	A	824	G2O	C2D-C1D-ND	-3.40	106.80	110.33
7	U	409	BCL	C2A-C1A-CHA	3.40	129.76	123.87
6	A	801	GS0	CHB-C1B-NB	3.39	129.14	124.05
7	a	811	BCL	CHA-C1A-NA	-3.38	118.73	126.39
7	W	405	BCL	C4-C3-C5	-3.38	109.37	115.23
7	V	403	BCL	CHA-C1A-NA	-3.37	118.75	126.39
7	A	802	BCL	C1C-NC-C4C	3.37	108.22	106.68
7	U	401	BCL	CHA-C1A-NA	-3.36	118.77	126.39
7	V	401	BCL	CHA-C1A-NA	-3.36	118.78	126.39
13	a	805	G2O	C3C-C4C-NC	-3.36	106.31	109.90
7	A	812	BCL	CHA-C1A-NA	-3.35	118.80	126.39
7	V	406	BCL	C4A-NA-C1A	3.32	108.19	106.68
7	V	407	BCL	C4A-NA-C1A	3.30	108.18	106.68
7	A	809	BCL	C1C-NC-C4C	3.30	108.18	106.68
7	A	807	BCL	CHA-C1A-NA	-3.29	118.94	126.39
7	A	811	BCL	C4A-NA-C1A	3.29	108.18	106.68
7	V	406	BCL	CHA-C1A-NA	-3.28	118.95	126.39
7	A	806	BCL	C4A-NA-C1A	3.27	108.17	106.68
7	A	812	BCL	C1-C2-C3	-3.27	120.83	126.20
7	V	404	BCL	C1C-NC-C4C	3.27	108.17	106.68
7	a	817	BCL	C1C-NC-C4C	3.26	108.17	106.68
7	A	805	BCL	C2A-C1A-CHA	3.26	129.52	123.87
7	A	802	BCL	C17-C16-C15	3.25	127.86	113.28
7	V	401	BCL	C4A-NA-C1A	3.24	108.16	106.68
7	a	811	BCL	C4A-NA-C1A	3.24	108.16	106.68
7	V	401	BCL	C2A-C1A-CHA	3.23	129.47	123.87
7	A	804	BCL	CHA-C1A-NA	-3.22	119.09	126.39
7	a	809	BCL	C2A-C1A-CHA	3.22	129.45	123.87
7	V	408[B]	BCL	CHA-C1A-NA	-3.21	119.12	126.39
7	V	406	BCL	C1D-ND-C4D	-3.21	104.06	106.31
6	A	801	GS0	C16-C15-C13	-3.21	105.31	115.97
7	A	804	BCL	CAB-C3B-C2B	3.20	134.40	127.74
8	A	814	F39	C32-C35-C37	-3.20	117.59	126.36
8	A	814	F39	C35-C37-C39	-3.19	113.98	119.01
7	a	812	BCL	CHA-C1A-NA	-3.19	119.17	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	a	804	GS0	CMA-C3A-C4A	-3.18	103.22	111.77
7	a	810	BCL	C1C-NC-C4C	3.18	108.13	106.68
7	V	401	BCL	CAB-C3B-C2B	3.17	134.33	127.74
7	U	403	BCL	CHA-C1A-NA	-3.17	119.22	126.39
6	A	801	GS0	C7-C6-C5	-3.16	104.83	113.26
6	a	804	GS0	C16-C15-C13	-3.16	105.47	115.97
7	a	807	BCL	CHA-C1A-NA	-3.15	119.25	126.39
7	W	405	BCL	CHA-C1A-NA	-3.15	119.26	126.39
7	W	407[B]	BCL	CHA-C1A-NA	-3.14	119.27	126.39
7	A	803	BCL	CHA-C1A-NA	-3.14	119.28	126.39
13	a	805	G2O	C2B-C1B-NB	-3.14	107.02	110.13
7	A	808	BCL	CHA-C1A-NA	-3.13	119.30	126.39
8	A	814	F39	C25-C20-C27	-3.13	108.98	122.50
7	W	401	BCL	CHA-C1A-NA	-3.12	119.32	126.39
7	U	405	BCL	CHA-C1A-NA	-3.12	119.33	126.39
6	a	804	GS0	C7-C6-C5	-3.10	105.00	113.26
8	a	818	F39	C25-C20-C27	-3.10	109.11	122.50
7	U	402	BCL	CHA-C1A-NA	-3.10	119.38	126.39
7	a	808	BCL	CHA-C1A-NA	-3.09	119.39	126.39
7	A	809	BCL	C1-C2-C3	-3.09	121.14	126.20
7	a	806	BCL	C1D-ND-C4D	-3.08	104.15	106.31
7	U	402	BCL	C2A-C1A-CHA	3.08	129.21	123.87
7	a	815	BCL	C11-C10-C8	3.07	126.18	115.97
7	U	406	BCL	CHA-C1A-NA	-3.07	119.44	126.39
7	A	808	BCL	C1C-NC-C4C	3.07	108.08	106.68
6	a	804	GS0	C11-C10-C8	-3.07	105.78	115.97
7	W	402	BCL	CHA-C1A-NA	-3.06	119.46	126.39
7	U	409	BCL	CHA-C1A-NA	-3.06	119.47	126.39
7	W	402	BCL	C1C-NC-C4C	3.06	108.07	106.68
7	a	810	BCL	CHA-C1A-NA	-3.05	119.49	126.39
13	a	802	G2O	C2A-C3A-C4A	3.03	106.77	101.87
7	A	811	BCL	CHA-C1A-NA	-3.02	119.54	126.39
7	U	408[B]	BCL	CHA-C1A-NA	-3.02	119.55	126.39
7	A	811	BCL	C2A-C1A-CHA	3.02	129.10	123.87
13	a	801	G2O	C3A-C2A-C1A	3.02	105.86	101.34
7	a	808	BCL	C2A-C1A-CHA	3.00	129.08	123.87
7	a	808	BCL	C4D-C3D-CAD	-3.00	104.84	108.11
7	W	403	BCL	C1C-NC-C4C	3.00	108.05	106.68
6	A	801	GS0	C3C-C2C-C1C	3.00	106.71	101.87
7	A	804	BCL	C1D-ND-C4D	-3.00	104.21	106.31
7	A	811	BCL	C1-C2-C3	-2.99	121.29	126.20
7	A	810	BCL	C2A-C1A-CHA	2.99	129.06	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	809	BCL	CHA-C1A-NA	-2.99	119.61	126.39
13	A	824	G2O	CHC-C4B-C3B	2.99	130.25	125.21
13	a	802	G2O	C3C-C4C-NC	-2.98	106.71	109.90
7	V	407	BCL	CHA-C1A-NA	-2.98	119.64	126.39
7	V	403	BCL	C2A-C1A-CHA	2.98	129.04	123.87
7	V	403	BCL	C1D-ND-C4D	-2.98	104.22	106.31
7	U	407	BCL	CHA-C1A-NA	-2.98	119.65	126.39
7	a	808	BCL	C1D-ND-C4D	-2.97	104.23	106.31
7	A	809	BCL	C2A-C1A-CHA	2.97	129.02	123.87
7	a	806	BCL	CHA-C1A-NA	-2.97	119.67	126.39
7	U	402	BCL	C1C-NC-C4C	2.96	108.03	106.68
7	W	405	BCL	C2A-C1A-CHA	2.96	129.00	123.87
13	a	802	G2O	O2D-CGD-O1D	-2.96	118.09	123.85
7	V	408[B]	BCL	C1C-NC-C4C	2.96	108.03	106.68
7	W	404	BCL	CHA-C1A-NA	-2.95	119.71	126.39
7	a	817	BCL	CHA-C1A-NA	-2.95	119.72	126.39
7	a	815	BCL	CHA-C1A-NA	-2.94	119.72	126.39
7	A	810	BCL	CAC-C3C-C4C	2.94	119.12	112.58
7	V	404	BCL	CHA-C1A-NA	-2.94	119.74	126.39
13	a	805	G2O	C2C-C1C-NC	-2.94	106.81	110.45
13	a	805	G2O	C2A-C3A-C4A	2.94	106.61	101.87
7	V	406	BCL	C2A-C1A-CHA	2.93	128.96	123.87
7	a	809	BCL	O2D-CGD-O1D	-2.93	118.14	123.85
6	a	804	GS0	C3B-C4B-NB	-2.91	105.92	109.76
7	A	813	BCL	O2A-CGA-O1A	-2.91	116.35	123.63
7	W	404	BCL	C4A-NA-C1A	2.91	108.01	106.68
7	U	405	BCL	C2A-C1A-CHA	2.91	128.91	123.87
7	a	813	BCL	CHA-C1A-NA	-2.91	119.81	126.39
7	a	809	BCL	C5-C3-C2	-2.90	114.66	121.17
7	A	803	BCL	C1C-NC-C4C	2.90	108.00	106.68
7	V	402	BCL	CHA-C1A-NA	-2.89	119.84	126.39
13	A	824	G2O	CMA-C3A-C2A	2.89	125.16	113.98
7	A	802	BCL	CHA-C1A-NA	-2.89	119.85	126.39
7	A	808	BCL	C4A-NA-C1A	2.89	108.00	106.68
8	A	814	F39	C53-C56-C58	-2.89	119.40	126.25
7	V	405	BCL	CHA-C1A-NA	-2.89	119.86	126.39
8	A	814	F39	C25-C20-C19	2.88	120.23	115.23
7	U	403	BCL	C2A-C1A-CHA	2.88	128.87	123.87
7	W	403	BCL	CHA-C1A-NA	-2.88	119.86	126.39
7	V	404	BCL	C2A-C1A-CHA	2.88	128.87	123.87
6	A	801	GS0	C11-C10-C8	-2.88	106.39	115.97
7	V	406	BCL	C1C-NC-C4C	2.88	107.99	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	W	401	BCL	C2A-C1A-CHA	2.88	128.86	123.87
7	A	802	BCL	C2A-C1A-CHA	2.86	128.84	123.87
7	A	804	BCL	C2A-C1A-CHA	2.86	128.83	123.87
13	a	801	G2O	C2A-C3A-C4A	2.86	106.49	101.87
7	U	407	BCL	C4A-NA-C1A	2.86	107.98	106.68
13	a	802	G2O	C2B-C1B-NB	-2.85	107.30	110.13
7	W	402	BCL	C2A-C1A-CHA	2.84	128.80	123.87
6	A	801	GS0	CMA-C3A-C2A	-2.83	103.03	113.98
7	a	813	BCL	C16-C15-C13	-2.83	106.55	115.97
7	A	809	BCL	C1D-ND-C4D	-2.83	104.33	106.31
6	A	801	GS0	CHB-C4A-NA	-2.83	120.32	124.40
7	W	406	BCL	CHA-C1A-NA	-2.82	120.00	126.39
13	a	805	G2O	O2D-CGD-O1D	-2.82	118.35	123.85
7	W	405	BCL	C1-C2-C3	-2.82	121.57	126.20
13	a	801	G2O	C2A-C1A-CHA	2.82	131.98	126.36
7	A	808	BCL	C2A-C1A-CHA	2.82	128.76	123.87
10	A	816	LHG	O8-C23-C24	2.81	120.42	111.83
6	A	801	GS0	CBB-CAB-C3B	2.81	126.33	120.40
7	A	813	BCL	C4-C3-C5	-2.80	110.36	115.23
7	A	811	BCL	C1D-ND-C4D	-2.80	104.35	106.31
6	A	801	GS0	O2A-CGA-O1A	-2.80	116.64	123.63
7	a	816	BCL	CHA-C1A-NA	-2.80	120.06	126.39
7	U	404	BCL	CHA-C1A-NA	-2.79	120.07	126.39
9	a	819	F26	C17-C13-C8	2.78	120.05	115.23
7	U	407	BCL	C1C-NC-C4C	2.77	107.94	106.68
10	a	821	LHG	O8-C23-C24	2.77	119.56	111.15
7	V	407	BCL	C2A-C1A-CHA	2.77	128.67	123.87
7	V	403	BCL	C1-C2-C3	-2.77	121.66	126.20
7	W	403	BCL	C2A-C1A-CHA	2.76	128.66	123.87
7	V	407	BCL	C1D-ND-C4D	-2.76	104.37	106.31
7	a	814	BCL	O2D-CGD-O1D	-2.76	118.47	123.85
9	a	819	F26	C32-C35-C34	-2.75	118.82	126.36
13	a	801	G2O	C2B-C1B-NB	-2.75	107.41	110.13
7	A	807	BCL	C2A-C1A-CHA	2.74	128.62	123.87
11	A	822	LMG	O6-C1-O1	-2.74	103.58	110.04
7	U	401	BCL	C4-C3-C5	-2.73	110.48	115.23
6	a	804	GS0	C11-C12-C13	-2.73	106.89	115.97
13	a	802	G2O	C3A-C2A-C1A	2.73	105.43	101.34
11	a	824	LMG	O6-C1-O1	-2.73	103.59	110.04
13	a	802	G2O	C2A-C1A-CHA	2.73	131.80	126.36
7	W	407[B]	BCL	C2A-C1A-CHA	2.71	128.57	123.87
6	a	804	GS0	O2A-CGA-O1A	-2.71	116.84	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	820	F26	C22-C25-C26	-2.71	118.93	126.36
10	a	822	LHG	O8-C23-C24	2.71	120.09	111.83
7	a	811	BCL	C4D-C3D-CAD	-2.70	105.17	108.11
7	a	806	BCL	O2D-CGD-O1D	-2.70	118.59	123.85
7	U	408[B]	BCL	C1D-ND-C4D	-2.70	104.42	106.31
11	A	821	LMG	O6-C1-O1	-2.70	103.67	110.04
7	W	407[B]	BCL	C1D-ND-C4D	-2.69	104.43	106.31
7	a	817	BCL	C2A-C1A-CHA	2.68	128.52	123.87
7	a	816	BCL	C2A-C1A-CHA	2.68	128.51	123.87
9	A	815	F26	C17-C13-C8	2.67	119.87	115.23
10	a	823	LHG	O8-C23-C24	2.66	119.96	111.83
7	U	404	BCL	C5-C3-C2	-2.66	115.19	121.17
13	a	801	G2O	C3C-C4C-NC	-2.66	107.05	109.90
7	A	806	BCL	CHA-C1A-NA	-2.66	120.36	126.39
7	a	811	BCL	C2A-C1A-CHA	2.66	128.48	123.87
7	W	404	BCL	C2A-C1A-CHA	2.66	128.48	123.87
7	A	805	BCL	CHD-C1D-C2D	2.65	130.99	125.49
7	V	401	BCL	C1C-NC-C4C	2.64	107.89	106.68
7	W	406	BCL	C2A-C1A-CHA	2.64	128.45	123.87
10	A	817	LHG	O8-C23-C24	2.64	119.89	111.83
6	a	804	GS0	C3C-C2C-C1C	2.64	106.13	101.87
13	a	801	G2O	O2D-CGD-O1D	-2.64	118.71	123.85
8	a	818	F39	C25-C20-C19	2.64	119.81	115.23
9	a	820	F26	C17-C13-C8	2.64	119.81	115.23
7	V	402	BCL	C1D-ND-C4D	-2.64	104.46	106.31
9	a	819	F26	C22-C25-C26	-2.63	119.14	126.36
7	U	406	BCL	C1C-NC-C4C	2.62	107.88	106.68
7	A	810	BCL	O2A-CGA-O1A	-2.62	117.07	123.63
7	U	404	BCL	C2A-C1A-CHA	2.62	128.42	123.87
9	a	819	F26	C38-C39-C37	-2.62	118.16	123.52
7	a	806	BCL	C2A-C1A-CHA	2.62	128.41	123.87
7	U	406	BCL	C2A-C1A-CHA	2.62	128.41	123.87
7	a	809	BCL	CHD-C1D-C2D	2.61	130.92	125.49
7	W	406	BCL	CAB-C3B-C2B	2.61	133.16	127.74
7	U	404	BCL	C6-C5-C3	2.60	119.80	113.47
6	a	804	GS0	C2B-C1B-NB	-2.60	107.63	110.33
9	A	815	F26	C27-C28-C31	-2.60	119.24	126.36
6	A	801	GS0	C11-C12-C13	-2.60	107.33	115.97
7	U	401	BCL	C2A-C1A-CHA	2.59	128.37	123.87
7	V	401	BCL	C4-C3-C5	-2.59	110.73	115.23
7	A	803	BCL	C2A-C1A-CHA	2.59	128.36	123.87
13	a	805	G2O	C3A-C2A-C1A	2.59	105.22	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	401	BCL	C1-C2-C3	-2.59	121.96	126.20
7	W	402	BCL	C1-C2-C3	-2.59	121.96	126.20
7	a	813	BCL	C2A-C1A-CHA	2.59	128.36	123.87
11	C	302	LMG	C1-C2-C3	-2.57	104.59	110.01
8	a	818	F39	C46-C45-C47	2.57	121.55	118.96
7	a	810	BCL	CBA-CAA-C2A	2.57	121.44	113.79
10	A	817	LHG	C11-C10-C9	-2.56	101.41	114.37
7	A	805	BCL	C1-O2A-CGA	2.56	122.85	116.65
6	A	801	GS0	CHC-C4B-NB	2.56	127.89	124.05
11	A	820	LMG	O6-C1-O1	-2.55	104.01	110.04
7	A	802	BCL	C16-C15-C13	-2.55	107.48	115.97
7	W	406	BCL	C1D-ND-C4D	-2.55	104.53	106.31
7	V	401	BCL	C1-C2-C3	-2.55	122.03	126.20
7	V	402	BCL	C2A-C1A-CHA	2.55	128.28	123.87
7	U	407	BCL	C2A-C1A-CHA	2.54	128.28	123.87
7	a	815	BCL	C2A-C1A-CHA	2.54	128.28	123.87
9	a	820	F26	C9-C15-C19	-2.54	120.22	126.25
7	A	806	BCL	C1-C2-C3	-2.54	122.04	126.20
13	a	802	G2O	C2C-C1C-NC	-2.54	107.31	110.45
7	A	806	BCL	C4D-C3D-CAD	-2.53	105.36	108.11
7	U	407	BCL	C4-C3-C5	-2.53	110.83	115.23
7	A	811	BCL	CAC-C3C-C4C	2.53	118.20	112.58
7	A	802	BCL	C4D-C3D-CAD	-2.53	105.36	108.11
8	A	814	F39	C46-C45-C47	2.53	121.50	118.96
7	U	401	BCL	C1D-ND-C4D	-2.52	104.55	106.31
7	U	402	BCL	C4-C3-C5	-2.52	110.86	115.23
7	A	813	BCL	C2A-C1A-CHA	2.52	128.23	123.87
7	a	817	BCL	C1D-ND-C4D	-2.51	104.55	106.31
10	C	301	LHG	O8-C23-C24	2.49	119.43	111.83
7	U	407	BCL	C1D-ND-C4D	-2.49	104.57	106.31
7	U	404	BCL	C1D-ND-C4D	-2.48	104.57	106.31
7	V	406	BCL	C4D-C3D-CAD	-2.47	105.42	108.11
7	V	405	BCL	C2A-C1A-CHA	2.47	128.16	123.87
11	A	818	LMG	O6-C1-O1	-2.47	104.20	110.04
7	a	810	BCL	C4-C3-C5	-2.47	110.94	115.23
7	a	815	BCL	C1-C2-C3	-2.47	122.15	126.20
7	A	803	BCL	C6-C5-C3	2.47	119.48	113.47
11	A	822	LMG	O1-C7-C8	-2.47	104.82	110.82
10	C	301	LHG	C11-C10-C9	-2.47	101.91	114.37
7	U	409	BCL	C1C-NC-C4C	2.46	107.80	106.68
11	A	820	LMG	O2-C2-C1	-2.46	104.21	110.08
13	a	805	G2O	CHC-C4B-C3B	2.46	129.35	125.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	GS0	C2D-C1D-ND	2.45	112.55	110.13
7	W	402	BCL	C1D-ND-C4D	-2.44	104.60	106.31
7	A	804	BCL	C4A-NA-C1A	2.44	107.79	106.68
7	A	810	BCL	C1D-ND-C4D	-2.44	104.60	106.31
8	a	818	F39	C53-C56-C58	-2.43	120.48	126.25
7	A	807	BCL	C1D-ND-C4D	-2.42	104.61	106.31
13	a	801	G2O	O2A-CGA-O1A	-2.42	117.56	123.63
7	a	814	BCL	CHD-C1D-C2D	2.42	130.53	125.49
10	a	823	LHG	C11-C10-C9	-2.42	102.14	114.37
7	V	404	BCL	C6-C5-C3	2.42	119.36	113.47
9	A	815	F26	C22-C25-C26	-2.42	119.74	126.36
7	A	805	BCL	C6-C5-C3	2.41	119.34	113.47
6	A	801	GS0	OBD-CAD-C3D	2.41	134.04	128.42
7	a	815	BCL	C1C-NC-C4C	2.41	107.78	106.68
7	A	802	BCL	C1D-ND-C4D	-2.40	104.63	106.31
7	U	402	BCL	C1D-ND-C4D	-2.40	104.63	106.31
7	A	806	BCL	C2A-C1A-CHA	2.39	128.01	123.87
7	W	403	BCL	C11-C10-C8	-2.39	108.03	115.97
11	A	819	LMG	O6-C1-O1	-2.39	104.40	110.04
6	a	804	GS0	CBB-CAB-C3B	2.39	125.43	120.40
7	U	403	BCL	C1D-ND-C4D	-2.38	104.64	106.31
7	a	806	BCL	O2A-CGA-O1A	-2.38	117.67	123.63
13	A	824	G2O	C3A-C2A-C1A	2.38	104.90	101.34
7	U	408[B]	BCL	O2D-CGD-O1D	-2.38	119.22	123.85
7	V	405	BCL	C1D-ND-C4D	-2.38	104.64	106.31
7	V	408[B]	BCL	C1D-ND-C4D	-2.38	104.64	106.31
10	a	821	LHG	C11-C10-C9	-2.37	102.41	114.37
7	A	803	BCL	C4D-C3D-CAD	-2.36	105.54	108.11
9	A	815	F26	C32-C35-C34	-2.36	119.89	126.36
13	a	805	G2O	C2A-C1A-CHA	2.36	131.06	126.36
8	A	814	F39	C63-C64-C62	-2.35	119.91	126.36
7	U	406	BCL	C1D-ND-C4D	-2.35	104.67	106.31
11	A	822	LMG	O3-C3-C2	-2.34	104.85	110.38
7	A	811	BCL	C1C-NC-C4C	2.34	107.75	106.68
13	a	805	G2O	C1-C2-C3	-2.34	122.36	126.20
7	W	404	BCL	O2D-CGD-O1D	-2.34	119.30	123.85
7	a	808	BCL	C1C-NC-C4C	2.33	107.74	106.68
7	V	406	BCL	C17-C16-C15	2.33	123.72	113.28
7	a	809	BCL	C1D-ND-C4D	-2.33	104.68	106.31
7	A	807	BCL	C4D-C3D-CAD	-2.32	105.58	108.11
8	a	818	F39	O5-C10-C12	-2.32	103.60	109.32
7	U	405	BCL	C1D-ND-C4D	-2.32	104.68	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	808	BCL	C1D-ND-C4D	-2.32	104.68	106.31
11	A	819	LMG	O3-C3-C2	-2.32	104.90	110.38
7	W	403	BCL	CAB-C3B-C2B	2.32	132.56	127.74
11	A	818	LMG	O2-C2-C1	-2.32	104.55	110.08
7	a	812	BCL	C2A-C1A-CHA	2.32	127.89	123.87
7	A	806	BCL	C1D-ND-C4D	-2.32	104.69	106.31
7	a	810	BCL	C4A-NA-C1A	2.32	107.74	106.68
7	a	813	BCL	C5-C3-C2	-2.31	115.97	121.17
8	a	818	F39	C40-C41-C42	-2.31	120.02	126.36
7	a	810	BCL	CAB-C3B-C2B	2.31	132.55	127.74
7	V	408[B]	BCL	C2A-C1A-CHA	2.31	127.88	123.87
8	A	814	F39	C9-C8-C10	-2.31	106.77	110.83
8	A	814	F39	C40-C41-C42	-2.31	120.03	126.36
11	A	819	LMG	C1-O6-C5	-2.30	109.22	113.72
11	C	302	LMG	O6-C1-O1	-2.30	104.61	110.04
7	a	811	BCL	CAB-C3B-C2B	2.30	132.52	127.74
7	a	815	BCL	C1D-ND-C4D	-2.30	104.70	106.31
6	A	801	GS0	CMB-C2B-C3B	2.29	132.89	125.67
7	U	404	BCL	CAB-C3B-C2B	2.29	132.49	127.74
7	W	401	BCL	C1D-ND-C4D	-2.28	104.71	106.31
7	W	401	BCL	CAB-C3B-C2B	2.27	132.46	127.74
7	W	405	BCL	C1D-ND-C4D	-2.27	104.72	106.31
7	U	405	BCL	C1-C2-C3	-2.27	122.48	126.20
13	A	824	G2O	CHD-C4C-C3C	2.27	129.41	125.23
9	A	815	F26	C10-C14-C16	-2.26	120.09	127.64
11	C	302	LMG	O3-C3-C2	-2.26	105.04	110.38
8	A	814	F39	O4-C9-C11	-2.26	104.69	110.08
7	a	811	BCL	CHD-C1D-C2D	2.26	130.19	125.49
7	a	810	BCL	C1D-ND-C4D	-2.26	104.73	106.31
7	U	404	BCL	CMB-C2B-C1B	-2.26	121.98	125.42
7	U	409	BCL	C1D-ND-C4D	-2.25	104.73	106.31
11	A	818	LMG	O1-C1-C2	-2.25	104.86	108.27
11	A	821	LMG	O2-C2-C1	-2.25	104.72	110.08
7	W	402	BCL	C5-C3-C2	-2.25	116.13	121.17
6	a	804	GS0	CMC-C2C-C3C	-2.24	105.32	113.98
7	a	813	BCL	C1-C2-C3	-2.24	122.53	126.20
11	A	819	LMG	O2-C2-C1	-2.24	104.74	110.08
7	A	813	BCL	CHD-C1D-C2D	2.24	130.14	125.49
9	A	815	F26	C38-C39-C37	-2.23	118.95	123.52
7	W	407[B]	BCL	CHD-C1D-C2D	2.23	130.13	125.49
8	a	818	F39	O4-C9-C11	-2.23	104.75	110.08
7	W	407[B]	BCL	C4A-NA-C1A	2.23	107.70	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	a	814	BCL	CBA-CAA-C2A	2.23	120.43	113.79
7	W	403	BCL	O2D-CGD-O1D	-2.23	119.52	123.85
9	a	819	F26	C10-C14-C16	-2.22	120.22	127.64
11	a	824	LMG	O3-C3-C2	-2.22	105.13	110.38
7	A	804	BCL	C1-C2-C3	-2.22	122.56	126.20
11	a	824	LMG	O1-C7-C8	-2.22	105.42	110.82
9	a	820	F26	C10-C14-C16	-2.22	120.24	127.64
7	W	403	BCL	C1D-ND-C4D	-2.22	104.75	106.31
6	a	804	GS0	CHB-C4A-NA	-2.21	121.20	124.40
7	a	812	BCL	C1D-ND-C4D	-2.21	104.76	106.31
7	V	401	BCL	CBA-CAA-C2A	2.21	120.37	113.79
7	a	808	BCL	O2A-CGA-CBA	-2.21	105.10	111.83
7	a	807	BCL	C1D-ND-C4D	-2.21	104.76	106.31
7	a	813	BCL	C1D-ND-C4D	-2.21	104.76	106.31
7	A	812	BCL	O2D-CGD-O1D	-2.21	119.56	123.85
11	A	821	LMG	O3-C3-C2	-2.21	105.18	110.38
11	A	822	LMG	O2-C2-C1	-2.20	104.82	110.08
9	A	815	F26	C20-C16-C21	2.20	119.65	114.59
7	a	816	BCL	C1D-ND-C4D	-2.20	104.77	106.31
7	a	809	BCL	O2D-CGD-CBD	2.20	115.07	111.23
7	a	817	BCL	CHD-C1D-C2D	2.20	130.05	125.49
6	a	804	GS0	C12-C11-C10	-2.19	103.44	113.28
7	a	806	BCL	C1C-NC-C4C	2.19	107.68	106.68
13	a	802	G2O	O2A-CGA-O1A	-2.19	118.15	123.63
6	a	804	GS0	C2D-C1D-ND	2.19	112.29	110.13
7	A	805	BCL	C4D-C3D-CAD	-2.19	105.73	108.11
7	A	812	BCL	C2A-C1A-CHA	2.19	127.66	123.87
7	V	404	BCL	C1D-ND-C4D	-2.18	104.78	106.31
7	a	809	BCL	C6-C7-C8	2.18	123.20	115.97
7	a	817	BCL	C1-C2-C3	-2.18	122.63	126.20
7	A	807	BCL	CAC-C3C-C4C	2.17	117.41	112.58
7	A	803	BCL	C1D-ND-C4D	-2.17	104.79	106.31
13	a	801	G2O	C2C-C1C-NC	-2.17	107.76	110.45
7	A	811	BCL	C4D-C3D-CAD	-2.17	105.75	108.11
6	A	801	GS0	CMD-C2D-C3D	2.17	132.67	127.69
7	V	406	BCL	CAB-C3B-C2B	2.17	132.25	127.74
7	U	409	BCL	C15-C13-C12	-2.17	101.09	112.07
9	a	819	F26	C27-C28-C31	-2.16	120.44	126.36
9	a	820	F26	C32-C35-C34	-2.15	120.47	126.36
6	a	804	GS0	OBD-CAD-C3D	2.15	133.44	128.42
13	A	824	G2O	CHC-C1C-C2C	2.15	128.42	125.03
7	A	802	BCL	C4-C3-C5	-2.15	111.50	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	810	BCL	CHD-C1D-C2D	2.15	129.95	125.49
7	A	811	BCL	C6-C5-C3	2.15	118.70	113.47
7	U	409	BCL	C1-C2-C3	-2.14	122.68	126.20
7	V	402	BCL	C4-C3-C5	-2.14	111.51	115.23
6	A	801	GS0	CED-O2D-CGD	-2.14	111.06	115.92
11	A	818	LMG	O3-C3-C2	-2.14	105.33	110.38
8	a	818	F39	C63-C64-C62	-2.14	120.50	126.36
9	a	819	F26	C9-C15-C19	-2.14	121.18	126.25
7	A	813	BCL	O2D-CGD-O1D	-2.14	119.69	123.85
7	V	406	BCL	C6-C5-C3	2.13	118.66	113.47
6	A	801	GS0	C12-C11-C10	-2.13	103.73	113.28
7	A	808	BCL	C4-C3-C5	-2.13	111.53	115.23
8	A	814	F39	O5-C10-C12	-2.13	104.08	109.32
7	W	407[B]	BCL	C1C-NC-C4C	2.13	107.65	106.68
7	U	401	BCL	CAB-C3B-C2B	2.13	132.16	127.74
7	a	809	BCL	C6-C5-C3	2.13	118.64	113.47
7	U	405	BCL	CHD-C1D-C2D	2.12	129.90	125.49
7	A	808	BCL	C4D-C3D-CAD	-2.12	105.81	108.11
7	a	808	BCL	CHD-C1D-C2D	2.12	129.89	125.49
7	a	812	BCL	C1-O2A-CGA	-2.12	111.53	116.65
7	U	406	BCL	C5-C3-C2	-2.11	116.42	121.17
7	W	406	BCL	C1-C2-C3	-2.11	122.74	126.20
6	a	804	GS0	C3D-C2D-C1D	-2.11	102.95	105.83
7	U	401	BCL	CBA-CAA-C2A	2.11	120.07	113.79
7	a	811	BCL	C1D-ND-C4D	-2.11	104.83	106.31
9	A	815	F26	C23-C19-C24	-2.11	119.40	122.82
7	V	401	BCL	C1D-ND-C4D	-2.11	104.83	106.31
11	A	821	LMG	O1-C1-C2	-2.11	105.07	108.27
7	W	404	BCL	C4-C3-C5	-2.10	111.59	115.23
11	a	824	LMG	O2-C2-C1	-2.09	105.09	110.08
7	W	405	BCL	CAB-C3B-C2B	2.09	132.08	127.74
7	V	406	BCL	C16-C17-C18	-2.09	106.61	115.94
7	U	407	BCL	C6-C5-C3	2.09	118.56	113.47
7	V	407	BCL	CHD-C1D-C2D	2.09	129.83	125.49
7	U	404	BCL	O2D-CGD-O1D	-2.09	119.79	123.85
8	a	818	F39	C38-C37-C39	-2.09	119.44	122.82
7	A	807	BCL	C6-C5-C3	2.09	118.55	113.47
7	V	408[B]	BCL	C4A-NA-C1A	2.08	107.63	106.68
7	a	814	BCL	C4D-C3D-CAD	-2.08	105.84	108.11
7	V	408[B]	BCL	C4D-C3D-CAD	-2.08	105.85	108.11
7	A	811	BCL	CHD-C1D-C2D	2.08	129.81	125.49
11	A	820	LMG	C1-O6-C5	-2.08	109.67	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	a	804	GS0	CMC-C2C-C1C	-2.08	106.20	111.77
7	V	405	BCL	CHD-C1D-C2D	2.07	129.80	125.49
7	W	404	BCL	C1D-ND-C4D	-2.07	104.86	106.31
11	A	820	LMG	O3-C3-C2	-2.07	105.49	110.38
7	U	406	BCL	C6-C5-C3	2.07	118.52	113.47
7	W	406	BCL	C1C-NC-C4C	2.07	107.62	106.68
7	V	406	BCL	CHD-C1D-C2D	2.07	129.79	125.49
7	W	403	BCL	CHD-C1D-C2D	2.07	129.79	125.49
7	A	802	BCL	CAA-CBA-CGA	2.07	119.08	113.21
7	V	407	BCL	CAB-C3B-C2B	2.07	132.03	127.74
7	A	811	BCL	C5-C3-C2	-2.06	116.55	121.17
11	A	821	LMG	O1-C7-C8	-2.06	105.81	110.82
9	a	820	F26	C20-C16-C21	2.06	119.32	114.59
7	A	807	BCL	CHD-C1D-C2D	2.05	129.76	125.49
7	A	803	BCL	C4A-NA-C1A	2.05	107.62	106.68
7	V	407	BCL	O2A-CGA-O1A	-2.05	118.49	123.63
13	A	824	G2O	C2A-C1A-CHA	2.05	130.45	126.36
7	W	406	BCL	O2D-CGD-O1D	-2.04	119.87	123.85
7	V	408[B]	BCL	O2D-CGD-O1D	-2.04	119.88	123.85
6	A	801	GS0	C1D-ND-C4D	-2.04	104.88	106.31
7	A	804	BCL	C4D-C3D-CAD	-2.04	105.89	108.11
9	A	815	F26	C36-C31-C33	-2.04	119.52	122.82
7	W	405	BCL	CHD-C1D-C2D	2.03	129.72	125.49
7	A	809	BCL	CHD-C1D-C2D	2.03	129.72	125.49
7	W	406	BCL	CHD-C1D-C2D	2.03	129.72	125.49
11	C	302	LMG	O2-C2-C1	-2.03	105.24	110.08
8	A	814	F39	C14-C18-C19	2.03	117.21	112.33
7	A	805	BCL	O2D-CGD-O1D	-2.03	119.90	123.85
11	A	818	LMG	O1-C7-C8	-2.03	105.89	110.82
7	a	812	BCL	CHD-C1D-C2D	2.02	129.69	125.49
11	A	819	LMG	O1-C7-C8	-2.02	105.91	110.82
7	a	816	BCL	C1-C2-C3	-2.01	122.90	126.20
7	U	404	BCL	C1-O2A-CGA	2.01	121.52	116.65
7	U	404	BCL	CAC-C3C-C4C	2.01	117.05	112.58
13	A	824	G2O	O2A-CGA-O1A	-2.01	118.60	123.63
7	a	809	BCL	CAA-CBA-CGA	2.01	118.92	113.21
7	U	409	BCL	CHD-C1D-C2D	2.01	129.66	125.49
7	a	815	BCL	CHD-C1D-C2D	2.01	129.66	125.49
7	V	407	BCL	C1C-NC-C4C	2.01	107.59	106.68
7	A	811	BCL	O2D-CGD-O1D	-2.00	119.95	123.85

All (17) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	801	GS0	C13
6	A	801	GS0	CBD
6	a	804	GS0	C3C
6	a	804	GS0	CBD
13	A	824	G2O	C3A
13	A	824	G2O	C2A
13	A	824	G2O	CBD
13	a	801	G2O	C3A
13	a	801	G2O	C2A
13	a	801	G2O	C8
13	a	801	G2O	CBD
13	a	802	G2O	C3A
13	a	802	G2O	C2A
13	a	802	G2O	CBD
13	a	805	G2O	C3A
13	a	805	G2O	C2A
13	a	805	G2O	CBD

All (885) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	801	GS0	C1A-C2A-CAA-CBA
6	A	801	GS0	C3A-C2A-CAA-CBA
6	A	801	GS0	C4-C3-C5-C6
6	A	801	GS0	C2C-C3C-CAC-CBC
6	A	801	GS0	C6-C7-C8-C9
6	A	801	GS0	CBA-CGA-O2A-C1
6	A	801	GS0	O1A-CGA-O2A-C1
6	A	801	GS0	CBD-CGD-O2D-CED
6	a	804	GS0	C1-C2-C3-C4
6	a	804	GS0	C1-C2-C3-C5
6	a	804	GS0	C3A-C2A-CAA-CBA
6	a	804	GS0	C2B-C3B-CAB-OBB
6	a	804	GS0	C4B-C3B-CAB-OBB
6	a	804	GS0	C2C-C3C-CAC-CBC
6	a	804	GS0	C4C-C3C-CAC-CBC
6	a	804	GS0	CBD-CGD-O2D-CED
7	A	802	BCL	C4C-C3C-CAC-CBC
7	A	805	BCL	C2B-C3B-CAB-OBB
7	A	805	BCL	C2B-C3B-CAB-CBB
7	A	806	BCL	C2B-C3B-CAB-OBB
7	A	806	BCL	C2B-C3B-CAB-CBB
7	A	806	BCL	C4B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
7	A	806	BCL	C4B-C3B-CAB-CBB
7	A	806	BCL	CHA-CBD-CGD-O1D
7	A	808	BCL	C2B-C3B-CAB-OB
7	A	808	BCL	C2B-C3B-CAB-CBB
7	A	808	BCL	C4B-C3B-CAB-OB
7	A	808	BCL	C4B-C3B-CAB-CBB
7	A	808	BCL	CAD-CBD-CGD-O2D
7	A	811	BCL	C2C-C3C-CAC-CBC
7	A	811	BCL	C4C-C3C-CAC-CBC
7	A	812	BCL	C2B-C3B-CAB-OB
7	A	812	BCL	C2B-C3B-CAB-CBB
7	A	812	BCL	C4B-C3B-CAB-OB
7	A	812	BCL	C4B-C3B-CAB-CBB
7	A	812	BCL	C4C-C3C-CAC-CBC
7	A	812	BCL	CAD-CBD-CGD-O1D
7	A	812	BCL	CAD-CBD-CGD-O2D
7	A	813	BCL	C2B-C3B-CAB-OB
7	A	813	BCL	C2B-C3B-CAB-CBB
7	A	813	BCL	C4B-C3B-CAB-OB
7	A	813	BCL	C4B-C3B-CAB-CBB
7	a	806	BCL	C2B-C3B-CAB-OB
7	a	806	BCL	C2B-C3B-CAB-CBB
7	a	806	BCL	C4B-C3B-CAB-OB
7	a	806	BCL	C4B-C3B-CAB-CBB
7	a	806	BCL	CHA-CBD-CGD-O1D
7	a	807	BCL	C2B-C3B-CAB-OB
7	a	807	BCL	C2B-C3B-CAB-CBB
7	a	807	BCL	C2C-C3C-CAC-CBC
7	a	807	BCL	C4C-C3C-CAC-CBC
7	a	808	BCL	C2C-C3C-CAC-CBC
7	a	808	BCL	C4C-C3C-CAC-CBC
7	a	808	BCL	C4-C3-C5-C6
7	a	809	BCL	O2A-C1-C2-C3
7	a	811	BCL	C2C-C3C-CAC-CBC
7	a	811	BCL	C4C-C3C-CAC-CBC
7	a	812	BCL	C4B-C3B-CAB-CBB
7	a	812	BCL	C2C-C3C-CAC-CBC
7	a	812	BCL	C4C-C3C-CAC-CBC
7	a	812	BCL	CAD-CBD-CGD-O2D
7	a	812	BCL	O2A-C1-C2-C3
7	a	813	BCL	C2C-C3C-CAC-CBC
7	a	813	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
7	a	814	BCL	C4C-C3C-CAC-CBC
7	a	814	BCL	CHA-CBD-CGD-O1D
7	a	815	BCL	C2B-C3B-CAB-OBB
7	a	815	BCL	C2B-C3B-CAB-CBB
7	a	816	BCL	CAD-CBD-CGD-O2D
7	a	817	BCL	C2B-C3B-CAB-OBB
7	a	817	BCL	C2B-C3B-CAB-CBB
7	U	402	BCL	C2B-C3B-CAB-OBB
7	U	402	BCL	C2B-C3B-CAB-CBB
7	U	402	BCL	C4B-C3B-CAB-OBB
7	U	402	BCL	C4B-C3B-CAB-CBB
7	U	403	BCL	C2B-C3B-CAB-OBB
7	U	403	BCL	C2B-C3B-CAB-CBB
7	U	403	BCL	C4B-C3B-CAB-OBB
7	U	403	BCL	C4B-C3B-CAB-CBB
7	U	403	BCL	C2C-C3C-CAC-CBC
7	U	403	BCL	C4C-C3C-CAC-CBC
7	U	403	BCL	CAD-CBD-CGD-O2D
7	U	406	BCL	C2B-C3B-CAB-OBB
7	U	406	BCL	C2B-C3B-CAB-CBB
7	U	406	BCL	C4B-C3B-CAB-OBB
7	U	406	BCL	C4B-C3B-CAB-CBB
7	V	403	BCL	C2B-C3B-CAB-OBB
7	V	403	BCL	C2B-C3B-CAB-CBB
7	V	403	BCL	C4B-C3B-CAB-OBB
7	V	403	BCL	C4B-C3B-CAB-CBB
7	V	403	BCL	C2C-C3C-CAC-CBC
7	V	403	BCL	C4C-C3C-CAC-CBC
7	W	402	BCL	C2C-C3C-CAC-CBC
7	W	402	BCL	C4C-C3C-CAC-CBC
7	W	403	BCL	C2C-C3C-CAC-CBC
7	W	403	BCL	C4C-C3C-CAC-CBC
8	A	814	F39	C25-C20-C27-C32
8	A	814	F39	C32-C35-C37-C39
8	A	814	F39	C39-C40-C41-C42
8	A	814	F39	C40-C41-C42-C43
8	A	814	F39	C41-C42-C44-C51
8	A	814	F39	C43-C42-C44-C51
8	A	814	F39	C44-C51-C57-C59
8	A	814	F39	C46-C53-C56-C58
8	A	814	F39	C56-C58-C61-C63
8	A	814	F39	C60-C58-C61-C63

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Mol	Chain	Res	Type	Atoms
8	A	814	F39	C57-C59-C62-C64
8	A	814	F39	C57-C59-C62-C65
8	A	814	F39	C58-C61-C63-C64
8	A	814	F39	C59-C62-C64-C63
8	A	814	F39	C65-C62-C64-C63
8	a	818	F39	C17-C13-C14-C18
8	a	818	F39	C19-C20-C27-C32
8	a	818	F39	C25-C20-C27-C32
8	a	818	F39	C22-C21-O6-C15
8	a	818	F39	O7-C21-O6-C15
8	a	818	F39	C38-C37-C39-C40
8	a	818	F39	C41-C42-C44-C51
8	a	818	F39	C42-C44-C51-C57
8	a	818	F39	C44-C51-C57-C59
8	a	818	F39	C53-C56-C58-C61
8	a	818	F39	C56-C58-C61-C63
8	a	818	F39	C61-C63-C64-C62
9	A	815	F26	C9-C15-C19-C23
9	A	815	F26	C23-C19-C24-C27
9	A	815	F26	C15-C19-C24-C27
9	A	815	F26	C19-C24-C27-C28
9	A	815	F26	C22-C25-C26-C29
9	A	815	F26	C22-C25-C26-C30
9	A	815	F26	C35-C34-C37-C39
9	A	815	F26	C40-C34-C37-C39
9	a	819	F26	C9-C15-C19-C24
9	a	819	F26	C23-C19-C24-C27
9	a	819	F26	C15-C19-C24-C27
9	a	819	F26	C10-C14-C16-C20
9	a	819	F26	C22-C25-C26-C29
9	a	819	F26	C22-C25-C26-C30
9	a	819	F26	C25-C26-C30-C32
9	a	819	F26	C29-C26-C30-C32
9	a	819	F26	C35-C34-C37-C39
9	a	819	F26	C40-C34-C37-C39
9	a	820	F26	C17-C13-C18-C22
9	a	820	F26	C8-C13-C18-C22
9	a	820	F26	C9-C15-C19-C24
9	a	820	F26	C15-C19-C24-C27
9	a	820	F26	C10-C14-C16-C21
9	a	820	F26	C10-C14-C16-C20
9	a	820	F26	C8-C10-C14-C16

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Mol	Chain	Res	Type	Atoms
9	a	820	F26	C22-C25-C26-C30
9	a	820	F26	C25-C26-C30-C32
9	a	820	F26	C29-C26-C30-C32
9	a	820	F26	C28-C31-C33-C38
9	a	820	F26	C36-C31-C33-C38
9	a	820	F26	C31-C33-C38-C39
9	a	820	F26	C35-C34-C37-C39
9	a	820	F26	C40-C34-C37-C39
9	a	820	F26	C34-C37-C39-C38
10	A	816	LHG	C3-O3-P-O4
10	A	816	LHG	C3-O3-P-O5
10	A	816	LHG	C3-O3-P-O6
10	A	816	LHG	C8-C7-O7-C5
10	A	817	LHG	C3-O3-P-O4
10	A	817	LHG	C3-O3-P-O5
10	A	817	LHG	C3-O3-P-O6
10	a	821	LHG	C8-C7-O7-C5
10	a	822	LHG	C3-O3-P-O4
10	a	822	LHG	C3-O3-P-O6
10	a	822	LHG	C4-O6-P-O3
10	a	823	LHG	C4-O6-P-O5
10	a	823	LHG	C6-C5-O7-C7
10	C	301	LHG	C1-C2-C3-O3
10	C	301	LHG	C3-O3-P-O4
10	C	301	LHG	C3-O3-P-O5
10	C	301	LHG	C3-O3-P-O6
10	C	301	LHG	C4-O6-P-O5
10	C	301	LHG	O9-C7-O7-C5
10	C	301	LHG	C8-C7-O7-C5
11	A	818	LMG	C2-C1-O1-C7
11	A	818	LMG	O6-C1-O1-C7
11	A	820	LMG	O9-C10-O7-C8
11	A	820	LMG	C11-C10-O7-C8
11	A	821	LMG	C2-C1-O1-C7
11	A	821	LMG	O6-C1-O1-C7
11	A	822	LMG	O9-C10-O7-C8
11	A	822	LMG	C11-C10-O7-C8
11	a	824	LMG	O7-C8-C9-O8
11	C	302	LMG	O9-C10-O7-C8
13	A	824	G2O	C1-C2-C3-C4
13	A	824	G2O	C1-C2-C3-C5
13	A	824	G2O	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
13	A	824	G2O	C2B-C3B-CAB-CBB
13	A	824	G2O	C4B-C3B-CAB-CBB
13	A	824	G2O	CBD-CGD-O2D-CED
13	a	801	G2O	C5-C6-C7-C8
13	a	801	G2O	C11-C10-C8-C7
13	a	801	G2O	C11-C10-C8-C9
13	a	801	G2O	C1A-C2A-CAA-CBA
13	a	801	G2O	C6-C7-C8-C10
13	a	801	G2O	C6-C7-C8-C9
13	a	801	G2O	CBD-CGD-O2D-CED
13	a	801	G2O	O1D-CGD-O2D-CED
13	a	802	G2O	C5-C6-C7-C8
13	a	802	G2O	C1A-C2A-CAA-CBA
13	a	802	G2O	CBD-CGD-O2D-CED
13	a	805	G2O	C3-C5-C6-C7
13	a	805	G2O	C5-C6-C7-C8
13	a	805	G2O	C11-C10-C8-C9
13	a	805	G2O	C1A-C2A-CAA-CBA
13	a	805	G2O	CBD-CGD-O2D-CED
13	A	824	G2O	O1D-CGD-O2D-CED
13	a	805	G2O	O1D-CGD-O2D-CED
13	a	801	G2O	C2C-C3C-CAC-CBC
6	a	804	GS0	O1D-CGD-O2D-CED
13	a	802	G2O	O1D-CGD-O2D-CED
8	A	814	F39	O7-C21-O6-C15
10	a	822	LHG	O10-C23-O8-C6
11	A	821	LMG	O10-C28-O8-C9
13	a	802	G2O	C13-C15-C16-C17
9	A	815	F26	C10-C14-C16-C21
9	A	815	F26	C10-C14-C16-C20
9	a	819	F26	C10-C14-C16-C21
13	a	801	G2O	C4C-C3C-CAC-CBC
6	A	801	GS0	O1D-CGD-O2D-CED
8	A	814	F39	C22-C21-O6-C15
10	a	823	LHG	O10-C23-O8-C6
6	a	804	GS0	C15-C16-C17-C18
13	A	824	G2O	C8-C10-C11-C12
8	A	814	F39	O1-C12-C15-O6
10	A	816	LHG	O9-C7-O7-C5
10	a	821	LHG	O9-C7-O7-C5
10	a	822	LHG	O9-C7-O7-C5
10	a	823	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
10	a	822	LHG	C24-C23-O8-C6
11	A	821	LMG	C29-C28-O8-C9
11	C	302	LMG	C11-C10-O7-C8
13	a	805	G2O	C2C-C3C-CAC-CBC
7	A	805	BCL	C4-C3-C5-C6
7	a	817	BCL	C4-C3-C5-C6
7	U	404	BCL	C4-C3-C5-C6
7	V	403	BCL	C4-C3-C5-C6
8	A	814	F39	C18-C19-C20-C25
7	A	811	BCL	C2-C3-C5-C6
7	a	808	BCL	C2-C3-C5-C6
7	a	809	BCL	C2-C3-C5-C6
7	a	813	BCL	C2-C3-C5-C6
7	a	817	BCL	C2-C3-C5-C6
7	U	406	BCL	C2-C3-C5-C6
7	V	406	BCL	C2-C3-C5-C6
7	a	812	BCL	C2A-CAA-CBA-CGA
7	V	408[B]	BCL	C2A-CAA-CBA-CGA
13	A	824	G2O	C2A-CAA-CBA-CGA
10	a	823	LHG	C24-C23-O8-C6
13	A	824	G2O	CBA-CGA-O2A-C1
8	a	818	F39	C37-C39-C40-C41
9	A	815	F26	C26-C30-C32-C35
11	a	824	LMG	O10-C28-O8-C9
10	a	821	LHG	O2-C2-C3-O3
11	a	824	LMG	C29-C28-O8-C9
13	A	824	G2O	O1A-CGA-O2A-C1
11	C	302	LMG	O6-C5-C6-O5
10	a	823	LHG	C8-C7-O7-C5
13	a	801	G2O	O1A-CGA-O2A-C1
11	A	818	LMG	O6-C5-C6-O5
13	a	802	G2O	C2-C3-C5-C6
13	A	824	G2O	C4-C3-C5-C6
7	A	803	BCL	C4-C3-C5-C6
7	a	813	BCL	C4-C3-C5-C6
9	a	820	F26	C17-C13-C8-C10
6	A	801	GS0	C2-C3-C5-C6
7	U	404	BCL	C2-C3-C5-C6
7	V	403	BCL	C2-C3-C5-C6
7	W	402	BCL	C2-C3-C5-C6
9	a	820	F26	C18-C13-C8-C10
11	A	819	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
9	a	819	F26	C14-C10-C8-C13
9	a	820	F26	C14-C10-C8-C13
13	a	805	G2O	C4C-C3C-CAC-CBC
11	a	824	LMG	O6-C1-O1-C7
11	C	302	LMG	O6-C1-O1-C7
13	a	801	G2O	CBA-CGA-O2A-C1
13	a	802	G2O	C2C-C3C-CAC-CBC
10	a	822	LHG	C8-C7-O7-C5
8	a	818	F39	C51-C57-C59-C62
8	A	814	F39	C10-C12-C15-O6
13	A	824	G2O	C2-C3-C5-C6
7	A	803	BCL	C2-C3-C5-C6
7	A	813	BCL	C11-C10-C8-C9
7	a	806	BCL	C6-C7-C8-C9
7	a	809	BCL	C6-C7-C8-C9
7	a	815	BCL	C6-C7-C8-C9
7	U	405	BCL	C11-C12-C13-C14
7	U	409	BCL	C6-C7-C8-C9
13	A	824	G2O	C14-C13-C15-C16
11	C	302	LMG	C2-C1-O1-C7
10	C	301	LHG	O2-C2-C3-O3
8	A	814	F39	C32-C35-C37-C38
8	A	814	F39	C53-C56-C58-C60
8	a	818	F39	C40-C41-C42-C43
9	a	820	F26	C9-C15-C19-C23
9	a	820	F26	C22-C25-C26-C29
8	a	818	F39	C32-C35-C37-C39
9	A	815	F26	C9-C15-C19-C24
10	A	817	LHG	C7-C8-C9-C10
11	A	820	LMG	C28-C29-C30-C31
6	a	804	GS0	C6-C7-C8-C10
7	A	810	BCL	C6-C7-C8-C10
13	a	802	G2O	C4-C3-C5-C6
11	A	818	LMG	C4-C5-C6-O5
11	A	818	LMG	C10-C11-C12-C13
7	A	809	BCL	C10-C11-C12-C13
13	a	802	G2O	C2A-CAA-CBA-CGA
13	a	805	G2O	C2A-CAA-CBA-CGA
7	A	804	BCL	C13-C15-C16-C17
7	a	817	BCL	C10-C11-C12-C13
10	a	821	LHG	C7-C8-C9-C10
11	A	819	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
11	C	302	LMG	C28-C29-C30-C31
7	a	814	BCL	O1D-CGD-O2D-CED
11	A	819	LMG	O6-C1-O1-C7
6	A	801	GS0	C13-C15-C16-C17
7	a	806	BCL	C8-C10-C11-C12
7	W	404	BCL	C8-C10-C11-C12
7	W	405	BCL	C13-C15-C16-C17
7	W	406	BCL	C15-C16-C17-C18
11	C	302	LMG	C29-C28-O8-C9
7	W	404	BCL	O1D-CGD-O2D-CED
11	C	302	LMG	C4-C5-C6-O5
7	A	806	BCL	C8-C10-C11-C12
7	a	806	BCL	C13-C15-C16-C17
13	A	824	G2O	C13-C15-C16-C17
13	a	805	G2O	C15-C16-C17-C18
6	a	804	GS0	CBA-CGA-O2A-C1
11	A	820	LMG	C29-C28-O8-C9
11	A	818	LMG	C28-C29-C30-C31
7	V	402	BCL	C8-C10-C11-C12
8	A	814	F39	C37-C39-C40-C41
9	a	820	F26	C19-C24-C27-C28
11	a	824	LMG	C28-C29-C30-C31
10	a	821	LHG	C1-C2-C3-O3
7	A	812	BCL	C10-C11-C12-C13
7	A	813	BCL	C10-C11-C12-C13
7	W	404	BCL	C5-C6-C7-C8
13	a	802	G2O	C8-C10-C11-C12
6	a	804	GS0	C5-C6-C7-C8
7	A	805	BCL	C4B-C3B-CAB-CBB
7	a	807	BCL	C4B-C3B-CAB-OB
7	a	807	BCL	C4B-C3B-CAB-CBB
7	a	812	BCL	C4B-C3B-CAB-OB
7	a	815	BCL	C4B-C3B-CAB-OB
7	a	815	BCL	C4B-C3B-CAB-CBB
7	a	817	BCL	C4B-C3B-CAB-CBB
11	A	819	LMG	C2-C1-O1-C7
11	a	824	LMG	C2-C1-O1-C7
6	a	804	GS0	C10-C11-C12-C13
8	A	814	F39	C38-C37-C39-C40
8	a	818	F39	C43-C42-C44-C51
8	a	818	F39	C60-C58-C61-C63
9	A	815	F26	C29-C26-C30-C32

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Mol	Chain	Res	Type	Atoms
9	a	819	F26	C40-C34-C35-C32
9	a	820	F26	C27-C28-C31-C36
8	A	814	F39	C40-C41-C42-C44
8	A	814	F39	C53-C56-C58-C61
9	a	819	F26	C37-C34-C35-C32
9	a	820	F26	C27-C28-C31-C33
7	a	817	BCL	C2A-CAA-CBA-CGA
13	a	801	G2O	C2A-CAA-CBA-CGA
10	A	817	LHG	O1-C1-C2-C3
10	a	822	LHG	O1-C1-C2-C3
7	A	804	BCL	O1D-CGD-O2D-CED
7	A	812	BCL	O2A-C1-C2-C3
7	a	812	BCL	C2B-C3B-CAB-CBB
9	A	815	F26	C25-C26-C30-C32
11	A	822	LMG	O6-C1-O1-C7
11	A	819	LMG	C11-C10-O7-C8
7	U	408[B]	BCL	O1D-CGD-O2D-CED
7	A	806	BCL	O1D-CGD-O2D-CED
7	A	809	BCL	C16-C17-C18-C20
7	V	403	BCL	O1D-CGD-O2D-CED
10	A	817	LHG	C25-C26-C27-C28
10	C	301	LHG	C13-C14-C15-C16
13	a	802	G2O	C4C-C3C-CAC-CBC
11	A	818	LMG	C15-C16-C17-C18
7	V	408[B]	BCL	O1D-CGD-O2D-CED
7	W	402	BCL	O1D-CGD-O2D-CED
7	a	806	BCL	C2A-CAA-CBA-CGA
7	a	809	BCL	C2A-CAA-CBA-CGA
11	a	824	LMG	C12-C13-C14-C15
10	a	823	LHG	C23-C24-C25-C26
7	A	803	BCL	C10-C11-C12-C13
7	A	813	BCL	O1D-CGD-O2D-CED
7	U	409	BCL	C15-C16-C17-C18
11	C	302	LMG	C32-C33-C34-C35
11	A	818	LMG	C11-C12-C13-C14
11	A	818	LMG	C31-C32-C33-C34
10	A	817	LHG	C26-C27-C28-C29
11	A	820	LMG	C32-C33-C34-C35
7	a	808	BCL	O1D-CGD-O2D-CED
10	a	823	LHG	C12-C13-C14-C15
10	a	823	LHG	C11-C12-C13-C14
6	a	804	GS0	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
7	W	405	BCL	C8-C10-C11-C12
13	a	801	G2O	C15-C16-C17-C18
7	W	407[B]	BCL	O1D-CGD-O2D-CED
10	A	817	LHG	C11-C12-C13-C14
10	A	817	LHG	C15-C16-C17-C18
8	A	814	F39	C27-C32-C35-C37
8	a	818	F39	C39-C40-C41-C42
11	A	820	LMG	C31-C32-C33-C34
7	U	402	BCL	C5-C6-C7-C8
11	A	820	LMG	C11-C12-C13-C14
10	A	817	LHG	C12-C13-C14-C15
7	U	404	BCL	O1D-CGD-O2D-CED
11	A	821	LMG	C11-C10-O7-C8
11	A	822	LMG	C28-C29-C30-C31
7	U	405	BCL	C8-C10-C11-C12
7	A	807	BCL	C2A-CAA-CBA-CGA
7	W	401	BCL	C4-C3-C5-C6
7	W	401	BCL	C2-C3-C5-C6
11	A	819	LMG	C29-C30-C31-C32
11	A	822	LMG	C31-C32-C33-C34
6	a	804	GS0	C13-C15-C16-C17
11	A	820	LMG	O10-C28-O8-C9
7	a	806	BCL	O1D-CGD-O2D-CED
7	a	809	BCL	O1D-CGD-O2D-CED
10	a	821	LHG	C12-C13-C14-C15
6	a	804	GS0	C3-C5-C6-C7
7	A	805	BCL	O1D-CGD-O2D-CED
7	a	816	BCL	C10-C11-C12-C13
7	a	816	BCL	C15-C16-C17-C18
10	A	816	LHG	C2-C3-O3-P
7	A	810	BCL	C2A-CAA-CBA-CGA
7	W	403	BCL	O1D-CGD-O2D-CED
11	A	818	LMG	C29-C30-C31-C32
11	A	820	LMG	C8-C9-O8-C28
7	A	809	BCL	O1D-CGD-O2D-CED
6	a	804	GS0	C1A-C2A-CAA-CBA
13	A	824	G2O	C1A-C2A-CAA-CBA
10	a	823	LHG	C17-C18-C19-C20
13	A	824	G2O	C6-C7-C8-C9
13	a	805	G2O	C6-C7-C8-C9
10	C	301	LHG	C11-C10-C9-C8
10	A	816	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
7	A	803	BCL	C6-C7-C8-C10
7	a	809	BCL	C6-C7-C8-C10
7	W	405	BCL	C10-C11-C12-C13
7	a	810	BCL	O1A-CGA-O2A-C1
7	A	802	BCL	C2C-C3C-CAC-CBC
7	a	814	BCL	C2C-C3C-CAC-CBC
7	a	817	BCL	O1D-CGD-O2D-CED
11	A	818	LMG	C32-C33-C34-C35
7	a	807	BCL	C2-C3-C5-C6
7	a	806	BCL	O1A-CGA-O2A-C1
6	A	801	GS0	C15-C16-C17-C18
7	a	817	BCL	C4B-C3B-CAB-OB
7	U	405	BCL	C4B-C3B-CAB-OB
7	V	408[B]	BCL	C4B-C3B-CAB-OB
7	A	804	BCL	C11-C10-C8-C9
7	A	804	BCL	C11-C12-C13-C14
10	A	817	LHG	C24-C23-O8-C6
7	A	812	BCL	O1D-CGD-O2D-CED
10	a	822	LHG	C4-C5-C6-O8
10	A	817	LHG	C18-C19-C20-C21
11	C	302	LMG	C29-C30-C31-C32
7	W	405	BCL	O1D-CGD-O2D-CED
11	a	824	LMG	O6-C5-C6-O5
9	a	820	F26	C23-C19-C24-C27
11	a	824	LMG	C16-C17-C18-C19
7	U	401	BCL	C2-C3-C5-C6
7	V	401	BCL	C2-C3-C5-C6
7	U	409	BCL	C10-C11-C12-C13
7	a	811	BCL	O1D-CGD-O2D-CED
7	V	404	BCL	C10-C11-C12-C13
10	A	817	LHG	C13-C14-C15-C16
10	a	821	LHG	C13-C14-C15-C16
7	A	809	BCL	C15-C16-C17-C18
11	A	819	LMG	C37-C38-C39-C40
7	A	802	BCL	O2A-C1-C2-C3
7	A	805	BCL	O2A-C1-C2-C3
7	a	812	BCL	C2B-C3B-CAB-OB
10	a	822	LHG	C6-C5-O7-C7
11	A	820	LMG	C7-C8-O7-C10
8	a	818	F39	C22-C23-C24-C26
7	A	812	BCL	C5-C6-C7-C8
7	A	803	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	A	818	LMG	C16-C17-C18-C19
7	U	402	BCL	O1D-CGD-O2D-CED
10	a	823	LHG	C19-C20-C21-C22
10	a	823	LHG	C14-C15-C16-C17
10	C	301	LHG	C11-C12-C13-C14
11	A	819	LMG	C12-C13-C14-C15
7	W	406	BCL	O1D-CGD-O2D-CED
7	A	806	BCL	C4-C3-C5-C6
11	A	821	LMG	O9-C10-O7-C8
10	a	822	LHG	O1-C1-C2-O2
7	A	805	BCL	C6-C7-C8-C9
7	A	810	BCL	C6-C7-C8-C9
7	W	402	BCL	C11-C10-C8-C9
7	W	405	BCL	C11-C12-C13-C14
10	a	822	LHG	C2-C3-O3-P
7	A	808	BCL	O1D-CGD-O2D-CED
7	V	405	BCL	CAA-CBA-CGA-O2A
7	A	811	BCL	O1D-CGD-O2D-CED
11	A	822	LMG	C2-C1-O1-C7
8	a	818	F39	C16-C13-C14-C18
11	A	822	LMG	C33-C34-C35-C36
6	A	801	GS0	C6-C7-C8-C10
7	A	804	BCL	C11-C10-C8-C7
7	A	804	BCL	C11-C12-C13-C15
7	A	805	BCL	C6-C7-C8-C10
7	a	815	BCL	C6-C7-C8-C10
7	W	402	BCL	C11-C10-C8-C7
7	W	405	BCL	C11-C12-C13-C15
7	A	810	BCL	C4-C3-C5-C6
7	A	813	BCL	C4-C3-C5-C6
7	W	406	BCL	C4-C3-C5-C6
13	a	805	G2O	C3A-C2A-CAA-CBA
7	a	813	BCL	O1D-CGD-O2D-CED
7	a	814	BCL	C2A-CAA-CBA-CGA
10	A	817	LHG	C24-C25-C26-C27
10	C	301	LHG	C4-C5-C6-O8
7	A	809	BCL	C16-C17-C18-C19
7	A	805	BCL	C1-C2-C3-C4
7	A	808	BCL	C1-C2-C3-C4
7	A	809	BCL	C1-C2-C3-C4
7	A	812	BCL	C1-C2-C3-C4
7	A	813	BCL	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
7	a	806	BCL	C1-C2-C3-C4
7	a	812	BCL	C1-C2-C3-C4
7	a	813	BCL	C1-C2-C3-C4
7	W	405	BCL	C1-C2-C3-C4
7	W	406	BCL	C1-C2-C3-C4
13	a	801	G2O	C1-C2-C3-C4
13	a	802	G2O	C1-C2-C3-C4
7	a	814	BCL	C15-C16-C17-C18
7	A	812	BCL	C4-C3-C5-C6
7	A	806	BCL	C2-C3-C5-C6
11	A	818	LMG	C30-C31-C32-C33
10	C	301	LHG	C2-C3-O3-P
6	A	801	GS0	C5-C6-C7-C8
7	a	806	BCL	C10-C11-C12-C13
10	a	822	LHG	O7-C5-C6-O8
13	a	805	G2O	C4-C3-C5-C6
10	a	823	LHG	C26-C27-C28-C29
7	U	407	BCL	C4-C3-C5-C6
7	a	810	BCL	C2-C3-C5-C6
7	a	812	BCL	C2-C3-C5-C6
13	a	801	G2O	C1-C2-C3-C5
7	A	805	BCL	C4B-C3B-CAB-OBB
7	A	809	BCL	C4B-C3B-CAB-OBB
7	a	816	BCL	C4B-C3B-CAB-OBB
7	a	816	BCL	C4B-C3B-CAB-CBB
7	a	813	BCL	C11-C10-C8-C9
7	V	404	BCL	O1D-CGD-O2D-CED
7	U	404	BCL	O1A-CGA-O2A-C1
10	a	821	LHG	C11-C12-C13-C14
7	A	805	BCL	C4C-C3C-CAC-CBC
7	A	808	BCL	C4C-C3C-CAC-CBC
7	U	408[B]	BCL	C4C-C3C-CAC-CBC
7	V	404	BCL	C4C-C3C-CAC-CBC
8	a	818	F39	O2-C13-C14-C18
7	V	405	BCL	O1D-CGD-O2D-CED
11	A	818	LMG	C33-C34-C35-C36
7	a	809	BCL	C8-C10-C11-C12
11	A	821	LMG	C4-C5-C6-O5
6	A	801	GS0	C3-C5-C6-C7
7	a	807	BCL	C15-C16-C17-C18
7	A	805	BCL	C12-C13-C15-C16
7	a	808	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
7	a	817	BCL	O1A-CGA-O2A-C1
7	U	401	BCL	O1A-CGA-O2A-C1
7	a	816	BCL	C2A-CAA-CBA-CGA
7	W	402	BCL	C2A-CAA-CBA-CGA
11	A	818	LMG	C11-C10-O7-C8
11	a	824	LMG	C30-C31-C32-C33
7	a	807	BCL	C4-C3-C5-C6
7	V	407	BCL	O1A-CGA-O2A-C1
13	a	805	G2O	C2B-C3B-CAB-CBB
7	a	816	BCL	C2B-C3B-CAB-OB
7	a	816	BCL	C2B-C3B-CAB-CBB
7	W	402	BCL	C2B-C3B-CAB-OB
7	W	402	BCL	C2B-C3B-CAB-CBB
7	W	403	BCL	C8-C10-C11-C12
7	V	407	BCL	O1D-CGD-O2D-CED
7	A	813	BCL	C16-C17-C18-C19
10	A	816	LHG	O6-C4-C5-O7
10	a	822	LHG	O6-C4-C5-O7
11	A	821	LMG	O1-C7-C8-C9
11	a	824	LMG	C7-C8-C9-O8
7	U	404	BCL	C10-C11-C12-C13
7	V	405	BCL	C2-C3-C5-C6
9	A	815	F26	C19-C15-C9-C2
11	A	821	LMG	O1-C7-C8-O7
11	C	302	LMG	O1-C7-C8-O7
11	C	302	LMG	O7-C8-C9-O8
10	C	301	LHG	C12-C13-C14-C15
7	A	805	BCL	O1A-CGA-O2A-C1
7	A	813	BCL	C8-C10-C11-C12
7	a	816	BCL	C13-C15-C16-C17
10	a	821	LHG	C2-C3-O3-P
11	A	821	LMG	O6-C5-C6-O5
6	A	801	GS0	C8-C10-C11-C12
7	a	808	BCL	O1A-CGA-O2A-C1
13	a	802	G2O	C11-C10-C8-C7
11	C	302	LMG	O10-C28-O8-C9
7	a	816	BCL	O1D-CGD-O2D-CED
10	A	817	LHG	O1-C1-C2-O2
7	A	809	BCL	C1A-C2A-CAA-CBA
7	A	802	BCL	O1D-CGD-O2D-CED
11	A	819	LMG	C29-C28-O8-C9
8	a	818	F39	C31-C33-C34-C36

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Mol	Chain	Res	Type	Atoms
10	a	822	LHG	O6-C4-C5-C6
7	a	806	BCL	C6-C7-C8-C10
7	a	814	BCL	C12-C13-C15-C16
7	U	402	BCL	C12-C13-C15-C16
7	V	403	BCL	C11-C10-C8-C7
10	C	301	LHG	C9-C10-C11-C12
11	a	824	LMG	C18-C19-C20-C21
7	A	802	BCL	O1A-CGA-O2A-C1
7	A	813	BCL	O1A-CGA-O2A-C1
11	A	819	LMG	C11-C12-C13-C14
7	A	805	BCL	C2C-C3C-CAC-CBC
7	V	404	BCL	C2C-C3C-CAC-CBC
7	A	808	BCL	O1A-CGA-O2A-C1
11	A	820	LMG	C12-C13-C14-C15
6	a	804	GS0	C4B-C3B-CAB-CBB
7	U	405	BCL	C4B-C3B-CAB-CBB
7	V	408[B]	BCL	C4B-C3B-CAB-CBB
7	W	402	BCL	C4B-C3B-CAB-OB
7	W	402	BCL	C4B-C3B-CAB-CBB
9	a	819	F26	C19-C24-C27-C28
11	A	818	LMG	C13-C14-C15-C16
10	C	301	LHG	O7-C5-C6-O8
11	A	820	LMG	O1-C7-C8-O7
7	a	807	BCL	C10-C11-C12-C13
11	A	818	LMG	C7-C8-C9-O8
11	A	820	LMG	O1-C7-C8-C9
11	C	302	LMG	C7-C8-C9-O8
7	a	815	BCL	C2-C3-C5-C6
11	a	824	LMG	C14-C15-C16-C17
7	A	802	BCL	CAD-CBD-CGD-O2D
7	A	811	BCL	CAD-CBD-CGD-O2D
7	A	813	BCL	CAD-CBD-CGD-O2D
7	a	809	BCL	CAD-CBD-CGD-O2D
7	U	408[B]	BCL	CAD-CBD-CGD-O2D
13	a	805	G2O	C13-C15-C16-C17
7	A	812	BCL	C2A-CAA-CBA-CGA
7	A	803	BCL	CHA-CBD-CGD-O1D
7	A	808	BCL	CAD-CBD-CGD-O1D
7	a	806	BCL	CHA-CBD-CGD-O2D
7	a	811	BCL	CHA-CBD-CGD-O2D
7	a	812	BCL	CAD-CBD-CGD-O1D
7	a	816	BCL	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
7	U	403	BCL	CAD-CBD-CGD-O1D
7	V	408[B]	BCL	CHA-CBD-CGD-O1D
7	W	403	BCL	CHA-CBD-CGD-O1D
7	W	406	BCL	CHA-CBD-CGD-O1D
8	A	814	F39	C20-C27-C32-C35
9	a	820	F26	C26-C30-C32-C35
10	a	822	LHG	C3-O3-P-O5
10	a	822	LHG	C4-O6-P-O5
10	a	823	LHG	C3-O3-P-O5
7	V	404	BCL	C4-C3-C5-C6
7	A	810	BCL	O1D-CGD-O2D-CED
11	C	302	LMG	C12-C13-C14-C15
7	U	405	BCL	C10-C11-C12-C13
10	A	816	LHG	C4-C5-O7-C7
11	A	819	LMG	C7-C8-O7-C10
7	A	803	BCL	C11-C10-C8-C9
7	A	805	BCL	C14-C13-C15-C16
10	C	301	LHG	C16-C17-C18-C19
7	U	401	BCL	C4-C3-C5-C6
7	A	805	BCL	C2-C3-C5-C6
11	A	820	LMG	C34-C35-C36-C37
10	A	816	LHG	O7-C5-C6-O8
13	a	801	G2O	C10-C11-C12-C13
7	V	406	BCL	O1D-CGD-O2D-CED
7	a	806	BCL	C4-C3-C5-C6
10	A	816	LHG	C4-C5-C6-O8
11	A	818	LMG	C14-C15-C16-C17
6	A	801	GS0	C16-C17-C18-C19
11	A	822	LMG	C8-C7-O1-C1
7	a	810	BCL	C4-C3-C5-C6
7	U	405	BCL	C4-C3-C5-C6
7	U	409	BCL	C4-C3-C5-C6
11	A	819	LMG	C38-C39-C40-C41
7	A	809	BCL	C4B-C3B-CAB-CBB
7	A	810	BCL	C4B-C3B-CAB-OB
7	a	808	BCL	C4B-C3B-CAB-OB
7	a	809	BCL	C4B-C3B-CAB-OB
7	V	402	BCL	C4B-C3B-CAB-OB
7	W	407[B]	BCL	C4B-C3B-CAB-OB
7	V	405	BCL	C11-C10-C8-C9
7	W	401	BCL	C6-C7-C8-C9
7	V	406	BCL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
7	W	406	BCL	O1A-CGA-O2A-C1
6	a	804	GS0	C16-C17-C18-C20
7	a	815	BCL	O1D-CGD-O2D-CED
7	A	802	BCL	C6-C7-C8-C10
7	A	803	BCL	C11-C10-C8-C7
7	W	401	BCL	C6-C7-C8-C10
11	A	818	LMG	O7-C8-C9-O8
7	a	815	BCL	C4-C3-C5-C6
11	A	819	LMG	C31-C32-C33-C34
7	a	809	BCL	C5-C6-C7-C8
7	A	804	BCL	C4-C3-C5-C6
9	a	819	F26	C17-C13-C8-C10
7	A	813	BCL	C2-C3-C5-C6
11	A	819	LMG	C7-C8-C9-O8
7	V	405	BCL	C8-C10-C11-C12
11	a	824	LMG	C13-C14-C15-C16
7	A	809	BCL	C11-C10-C8-C9
7	a	814	BCL	C11-C10-C8-C9
7	U	403	BCL	C11-C10-C8-C9
7	V	401	BCL	C14-C13-C15-C16
13	a	801	G2O	C14-C13-C15-C16
6	A	801	GS0	C16-C17-C18-C20
7	a	811	BCL	CAA-CBA-CGA-O2A
7	A	802	BCL	C2B-C3B-CAB-OB
7	a	810	BCL	O2A-C1-C2-C3
10	C	301	LHG	C6-C5-O7-C7
11	A	822	LMG	C9-C8-O7-C10
6	A	801	GS0	C1-C2-C3-C4
7	A	811	BCL	C1-C2-C3-C4
7	a	809	BCL	C1-C2-C3-C4
7	a	810	BCL	C1-C2-C3-C4
7	U	402	BCL	C1-C2-C3-C4
7	U	406	BCL	C1-C2-C3-C4
7	U	407	BCL	C1-C2-C3-C4
7	U	409	BCL	C1-C2-C3-C4
7	W	402	BCL	C1-C2-C3-C4
10	a	821	LHG	C11-C10-C9-C8
7	A	808	BCL	C1A-C2A-CAA-CBA
7	a	813	BCL	C1A-C2A-CAA-CBA
10	A	817	LHG	O6-C4-C5-O7
6	a	804	GS0	C4-C3-C5-C6
7	A	804	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
8	a	818	F39	C21-C22-C23-C24
7	a	813	BCL	C12-C13-C15-C16
7	U	403	BCL	C11-C10-C8-C7
7	V	405	BCL	C11-C10-C8-C7
11	A	819	LMG	O7-C8-C9-O8
10	a	823	LHG	C13-C14-C15-C16
7	A	812	BCL	C2C-C3C-CAC-CBC
11	A	819	LMG	C32-C33-C34-C35
7	a	812	BCL	C4-C3-C5-C6
7	W	406	BCL	C2-C3-C5-C6
9	a	819	F26	C18-C13-C8-C10
6	A	801	GS0	C1-C2-C3-C5
7	V	401	BCL	O1D-CGD-O2D-CED
10	A	817	LHG	C11-C10-C9-C8
7	A	803	BCL	C4B-C3B-CAB-OB
7	a	808	BCL	C4B-C3B-CAB-CB
13	a	805	G2O	C2-C3-C5-C6
7	V	407	BCL	C4-C3-C5-C6
7	V	406	BCL	C4C-C3C-CAC-CBC
7	W	407[B]	BCL	C4C-C3C-CAC-CBC
13	a	801	G2O	C4-C3-C5-C6
7	W	404	BCL	CAA-CBA-CGA-O2A
13	A	824	G2O	C6-C7-C8-C10
7	a	806	BCL	CAA-CBA-CGA-O2A
7	A	805	BCL	CAA-CBA-CGA-O1A
7	U	405	BCL	CAA-CBA-CGA-O1A
7	A	805	BCL	CAA-CBA-CGA-O2A
13	a	801	G2O	C8-C10-C11-C12
7	U	407	BCL	O1A-CGA-O2A-C1
10	A	817	LHG	O6-C4-C5-C6
7	W	404	BCL	C3-C5-C6-C7
7	W	407[B]	BCL	CAA-CBA-CGA-O2A
7	U	405	BCL	CAA-CBA-CGA-O2A
6	a	804	GS0	C6-C7-C8-C9
7	A	803	BCL	C14-C13-C15-C16
7	V	403	BCL	C11-C10-C8-C9
11	A	819	LMG	C8-C7-O1-C1
7	a	807	BCL	CAA-CBA-CGA-O2A
7	W	407[B]	BCL	CAA-CBA-CGA-O1A
7	A	811	BCL	C2-C1-O2A-CGA
13	a	802	G2O	C3A-C2A-CAA-CBA
7	W	404	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
11	A	819	LMG	C30-C31-C32-C33
7	A	810	BCL	CAA-CBA-CGA-O2A
11	A	822	LMG	O8-C28-C29-C30
7	A	807	BCL	C2B-C3B-CAB-OB
7	V	408[B]	BCL	C2B-C3B-CAB-OB
7	V	401	BCL	C10-C11-C12-C13
7	a	811	BCL	CAA-CBA-CGA-O1A
7	A	806	BCL	O1A-CGA-O2A-C1
11	A	819	LMG	O10-C28-O8-C9
13	a	805	G2O	C4B-C3B-CAB-CBB
10	a	823	LHG	C18-C19-C20-C21
7	A	813	BCL	C5-C6-C7-C8
7	A	807	BCL	C4B-C3B-CAB-CBB
10	a	823	LHG	O7-C5-C6-O8
6	a	804	GS0	C14-C13-C15-C16
7	A	802	BCL	C4-C3-C5-C6
7	A	813	BCL	CAA-CBA-CGA-O1A
6	a	804	GS0	C11-C12-C13-C15
6	a	804	GS0	C12-C13-C15-C16
7	A	813	BCL	C11-C10-C8-C7
7	V	407	BCL	C6-C7-C8-C10
7	W	404	BCL	C11-C12-C13-C15
13	A	824	G2O	C12-C13-C15-C16
8	A	814	F39	C45-C46-C53-C56
8	A	814	F39	C48-C46-C53-C56
9	a	820	F26	C4-C2-C9-C15
7	V	404	BCL	C2-C1-O2A-CGA
7	W	404	BCL	C2-C1-O2A-CGA
7	a	806	BCL	C5-C6-C7-C8
11	A	822	LMG	C30-C31-C32-C33
7	U	401	BCL	CAA-CBA-CGA-O2A
13	a	802	G2O	C11-C10-C8-C9
7	W	402	BCL	CAA-CBA-CGA-O2A
7	U	406	BCL	O1A-CGA-O2A-C1
7	a	809	BCL	CAA-CBA-CGA-O2A
11	A	821	LMG	O7-C10-C11-C12
10	a	823	LHG	O6-C4-C5-O7
13	A	824	G2O	C11-C10-C8-C7
7	V	404	BCL	C2-C3-C5-C6
10	a	821	LHG	C14-C15-C16-C17
7	W	401	BCL	CAA-CBA-CGA-O2A
9	a	819	F26	C1-C2-C9-C15

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Mol	Chain	Res	Type	Atoms
7	A	810	BCL	C11-C10-C8-C9
7	U	402	BCL	C14-C13-C15-C16
7	U	404	BCL	CAA-CBA-CGA-O2A
7	U	402	BCL	C13-C15-C16-C17
7	a	806	BCL	C1A-C2A-CAA-CBA
7	A	812	BCL	C2-C3-C5-C6
7	W	403	BCL	C2-C3-C5-C6
7	a	815	BCL	C13-C15-C16-C17
7	a	813	BCL	CAA-CBA-CGA-O2A
7	A	813	BCL	C2A-CAA-CBA-CGA
7	A	806	BCL	CAA-CBA-CGA-O2A
7	V	401	BCL	CAA-CBA-CGA-O2A
7	U	402	BCL	C8-C10-C11-C12
7	a	812	BCL	O1D-CGD-O2D-CED
7	A	802	BCL	C2B-C3B-CAB-CBB
7	A	807	BCL	C2B-C3B-CAB-CBB
7	A	809	BCL	C2B-C3B-CAB-OB
7	U	405	BCL	C2B-C3B-CAB-OB
7	V	407	BCL	CAA-CBA-CGA-O2A
6	A	801	GS0	C10-C11-C12-C13
7	W	406	BCL	C10-C11-C12-C13
13	a	801	G2O	C16-C17-C18-C19
9	a	820	F26	C1-C2-C9-C15
7	A	802	BCL	CAA-CBA-CGA-O2A
7	a	810	BCL	C10-C11-C12-C13
7	A	813	BCL	C3A-C2A-CAA-CBA
7	W	401	BCL	CAA-CBA-CGA-O1A
10	A	817	LHG	O10-C23-C24-C25
11	A	818	LMG	C19-C20-C21-C22
7	a	810	BCL	C8-C10-C11-C12
7	U	403	BCL	CAA-CBA-CGA-O1A
7	V	403	BCL	CAA-CBA-CGA-O1A
7	A	810	BCL	C16-C17-C18-C20
11	a	824	LMG	C29-C30-C31-C32
7	A	807	BCL	C4B-C3B-CAB-OB
7	a	813	BCL	C14-C13-C15-C16
7	a	814	BCL	C14-C13-C15-C16
11	A	821	LMG	O9-C10-C11-C12
7	W	403	BCL	C10-C11-C12-C13
7	U	407	BCL	CAA-CBA-CGA-O2A
7	a	812	BCL	C15-C16-C17-C18
8	a	818	F39	C40-C41-C42-C44

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Mol	Chain	Res	Type	Atoms
8	A	814	F39	C29-C30-C31-C33
7	V	403	BCL	CAA-CBA-CGA-O2A
7	a	811	BCL	C2A-CAA-CBA-CGA
11	C	302	LMG	O1-C7-C8-C9
7	a	810	BCL	CAA-CBA-CGA-O1A
10	a	821	LHG	C15-C16-C17-C18
7	W	406	BCL	C8-C10-C11-C12
7	U	403	BCL	C5-C6-C7-C8
9	a	819	F26	C13-C18-C22-C25
13	a	805	G2O	C6-C7-C8-C10
13	a	805	G2O	CAD-CBD-CGD-O2D
7	U	409	BCL	C13-C15-C16-C17
7	A	805	BCL	C2-C1-O2A-CGA
7	V	401	BCL	CAA-CBA-CGA-O1A
7	a	816	BCL	C1-C2-C3-C4
7	U	401	BCL	C1-C2-C3-C4
7	V	402	BCL	C1-C2-C3-C4
7	V	403	BCL	C1-C2-C3-C4
13	a	805	G2O	C1-C2-C3-C4
7	U	401	BCL	C15-C16-C17-C18
7	A	813	BCL	CAA-CBA-CGA-O2A
7	a	810	BCL	CAA-CBA-CGA-O2A
11	A	819	LMG	O8-C28-C29-C30

There are no ring outliers.

51 monomers are involved in 91 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	808	BCL	1	0
10	A	817	LHG	1	0
7	a	815	BCL	2	0
10	A	816	LHG	2	0
7	V	407	BCL	1	0
7	W	406	BCL	3	0
7	A	805	BCL	2	0
13	a	801	G2O	1	0
7	a	809	BCL	1	0
7	a	813	BCL	2	0
7	V	405	BCL	5	0
11	A	819	LMG	2	0
7	a	806	BCL	1	0
6	a	804	GS0	2	0

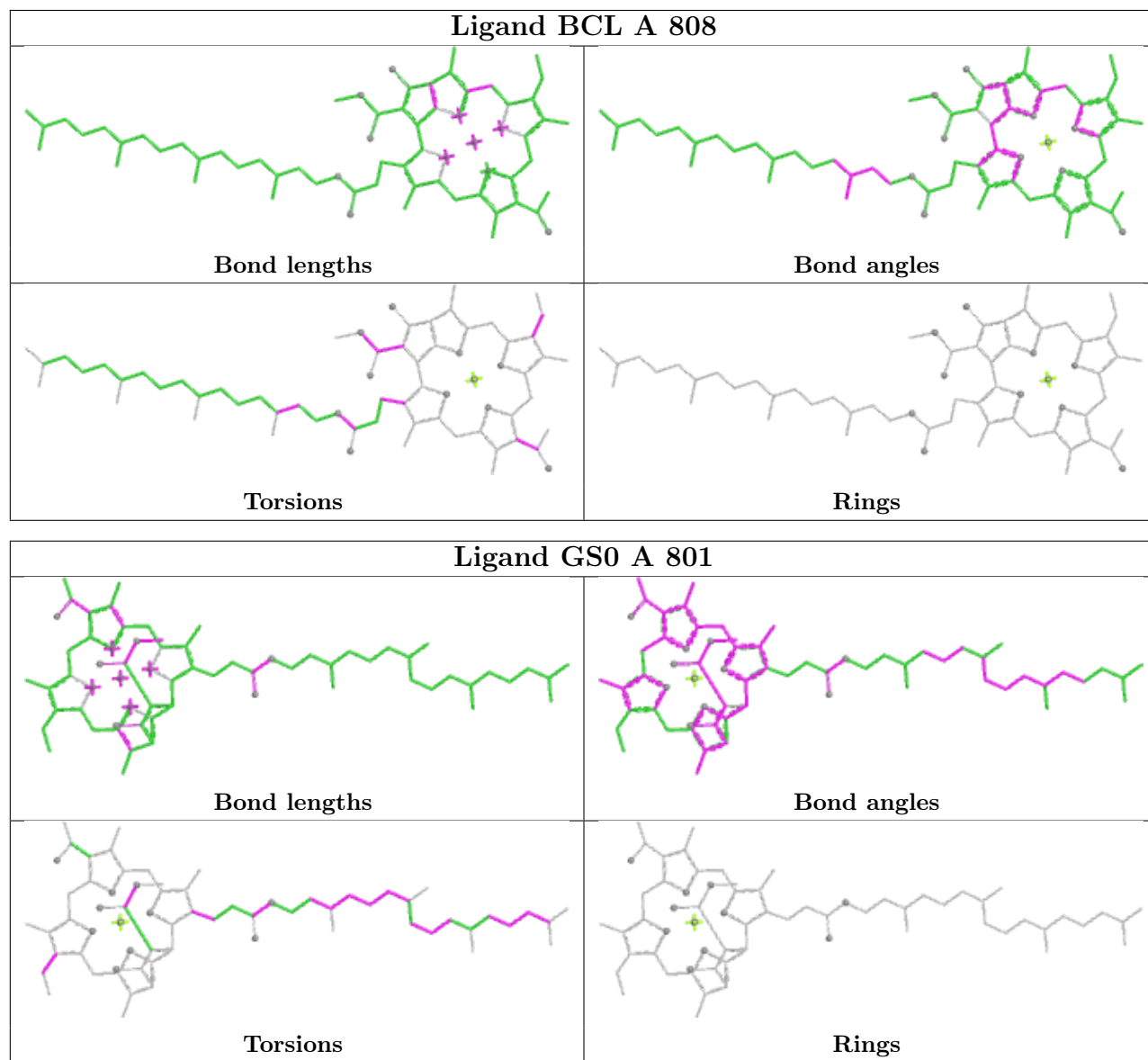
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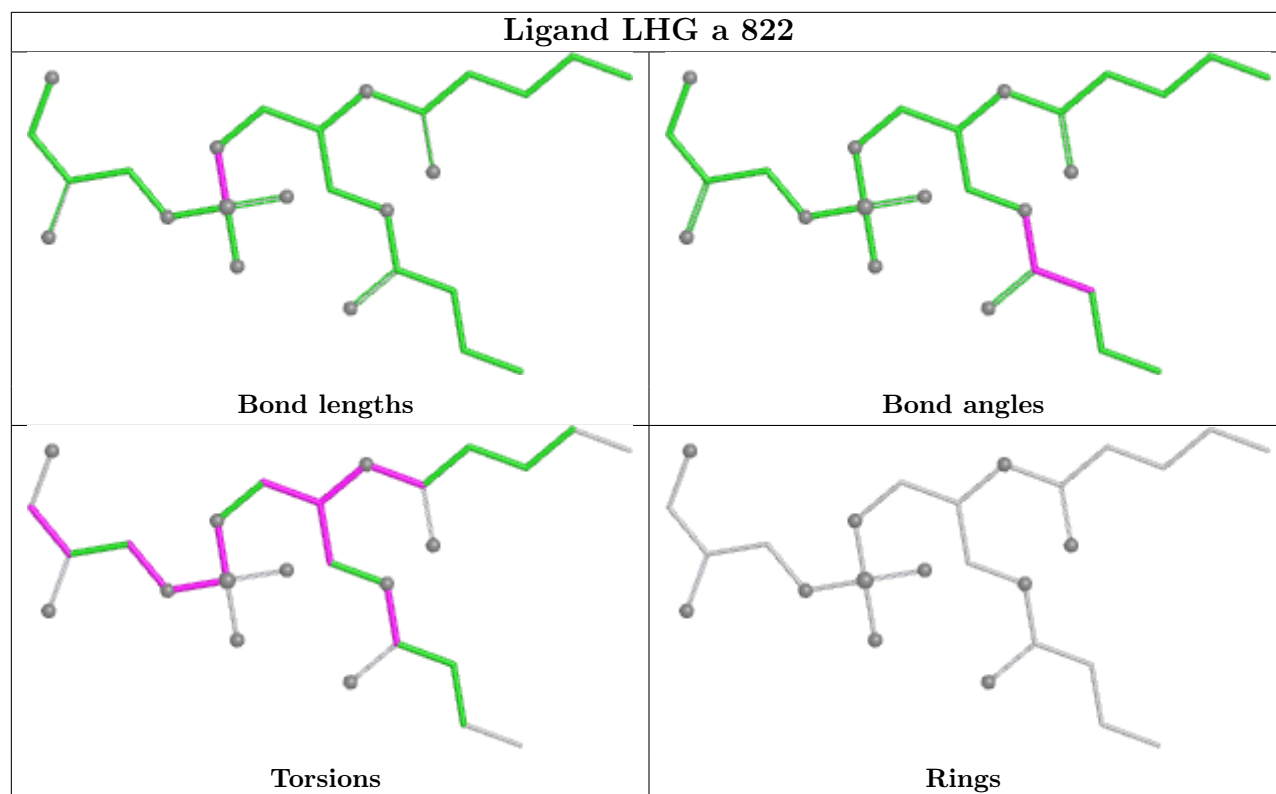
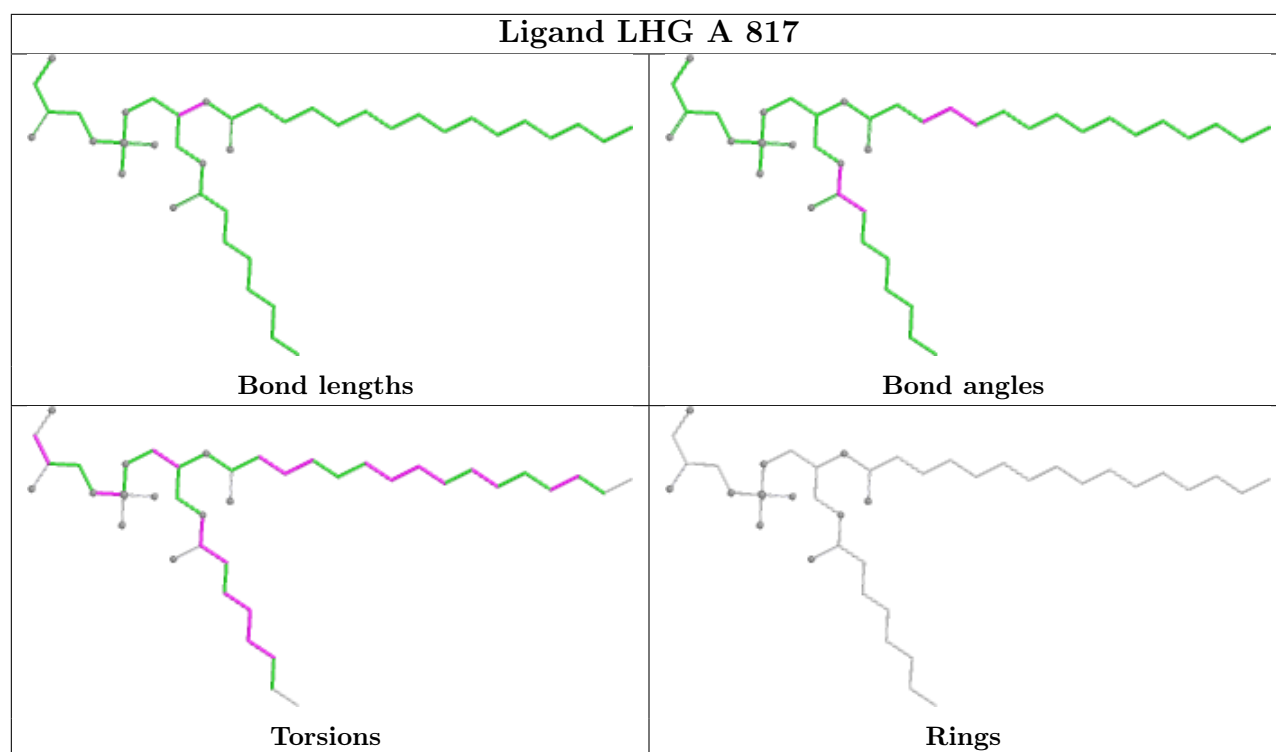
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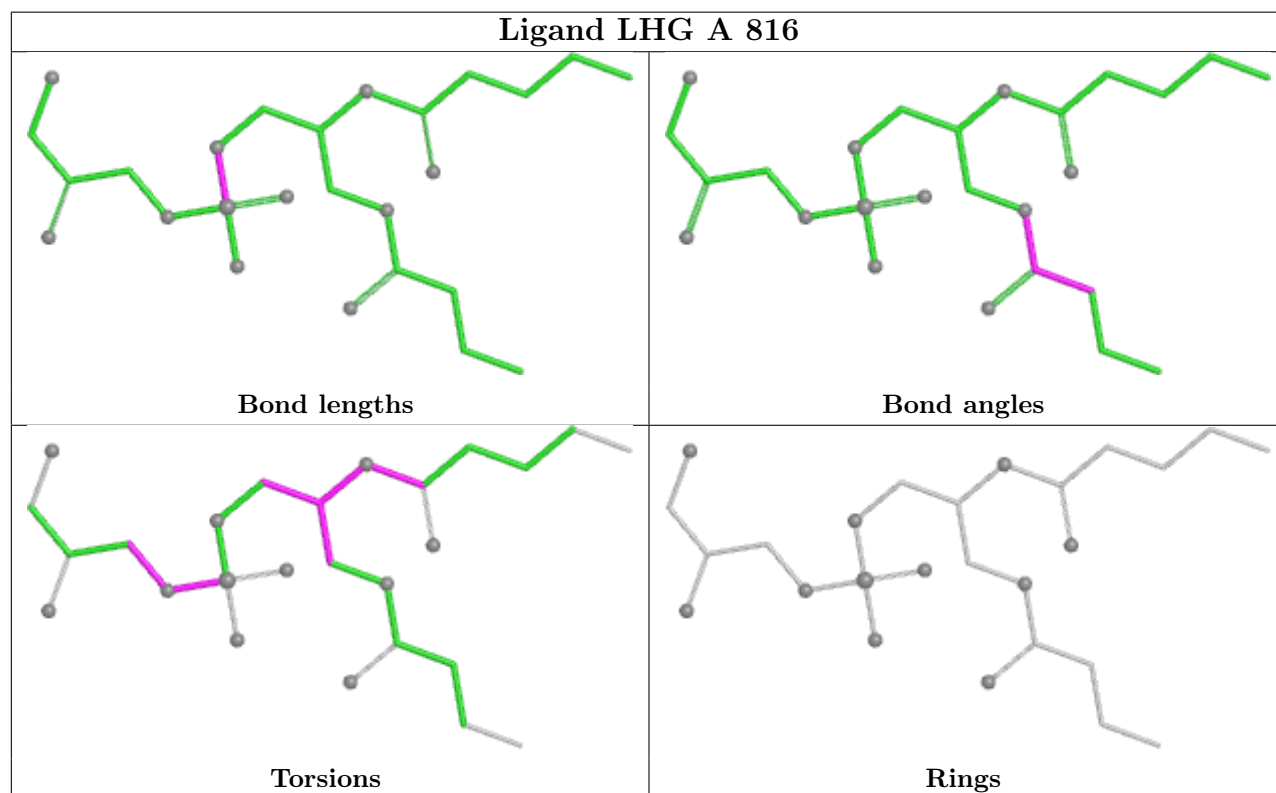
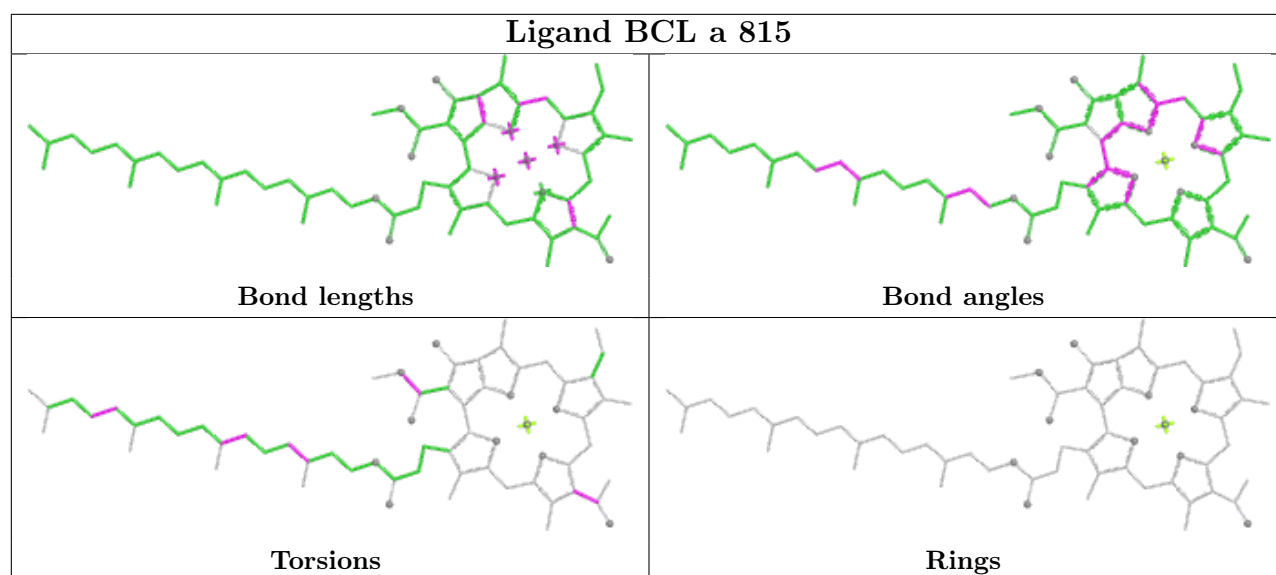
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	818	LMG	3	0
7	V	401	BCL	3	0
7	W	405	BCL	2	0
14	B	302	SF4	1	0
11	C	302	LMG	1	0
7	V	403	BCL	2	0
7	a	810	BCL	4	0
13	a	802	G2O	1	0
7	W	402	BCL	5	0
7	a	814	BCL	3	0
7	U	405	BCL	4	0
7	W	401	BCL	3	0
7	V	406	BCL	3	0
11	A	820	LMG	2	0
7	A	802	BCL	6	0
11	A	821	LMG	1	0
7	A	810	BCL	2	0
7	U	406	BCL	2	0
14	a	803	SF4	1	0
7	V	408[B]	BCL	1	0
7	W	403	BCL	1	0
7	A	804	BCL	2	0
7	A	809	BCL	2	0
10	a	823	LHG	5	0
7	a	812	BCL	3	0
7	U	404	BCL	2	0
7	a	817	BCL	1	0
10	C	301	LHG	2	0
7	A	806	BCL	2	0
7	A	812	BCL	1	0
7	A	811	BCL	1	0
7	a	816	BCL	2	0
7	A	803	BCL	2	0
7	V	402	BCL	2	0
7	a	808	BCL	2	0
7	V	404	BCL	5	0
7	A	807	BCL	2	0

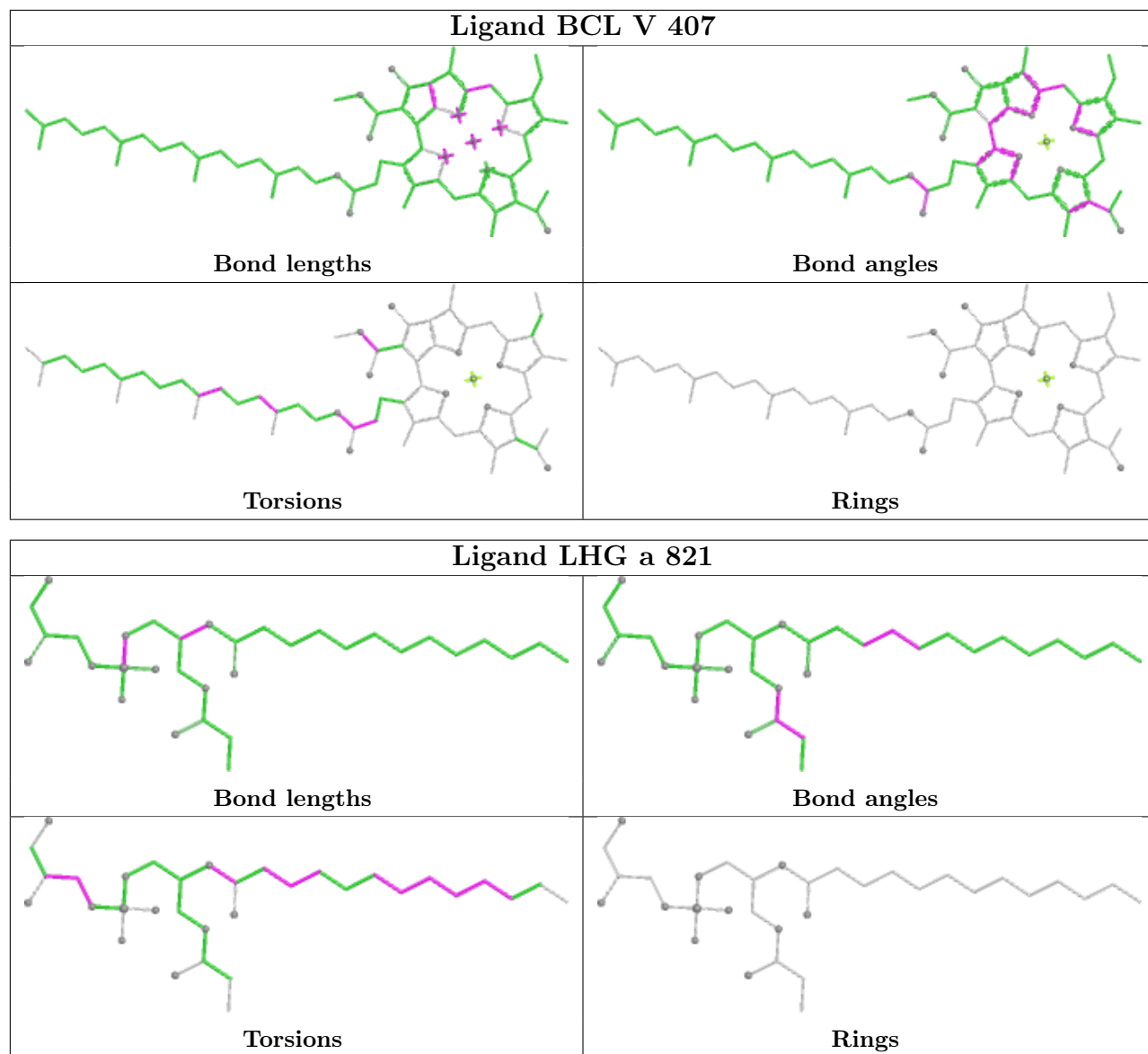
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

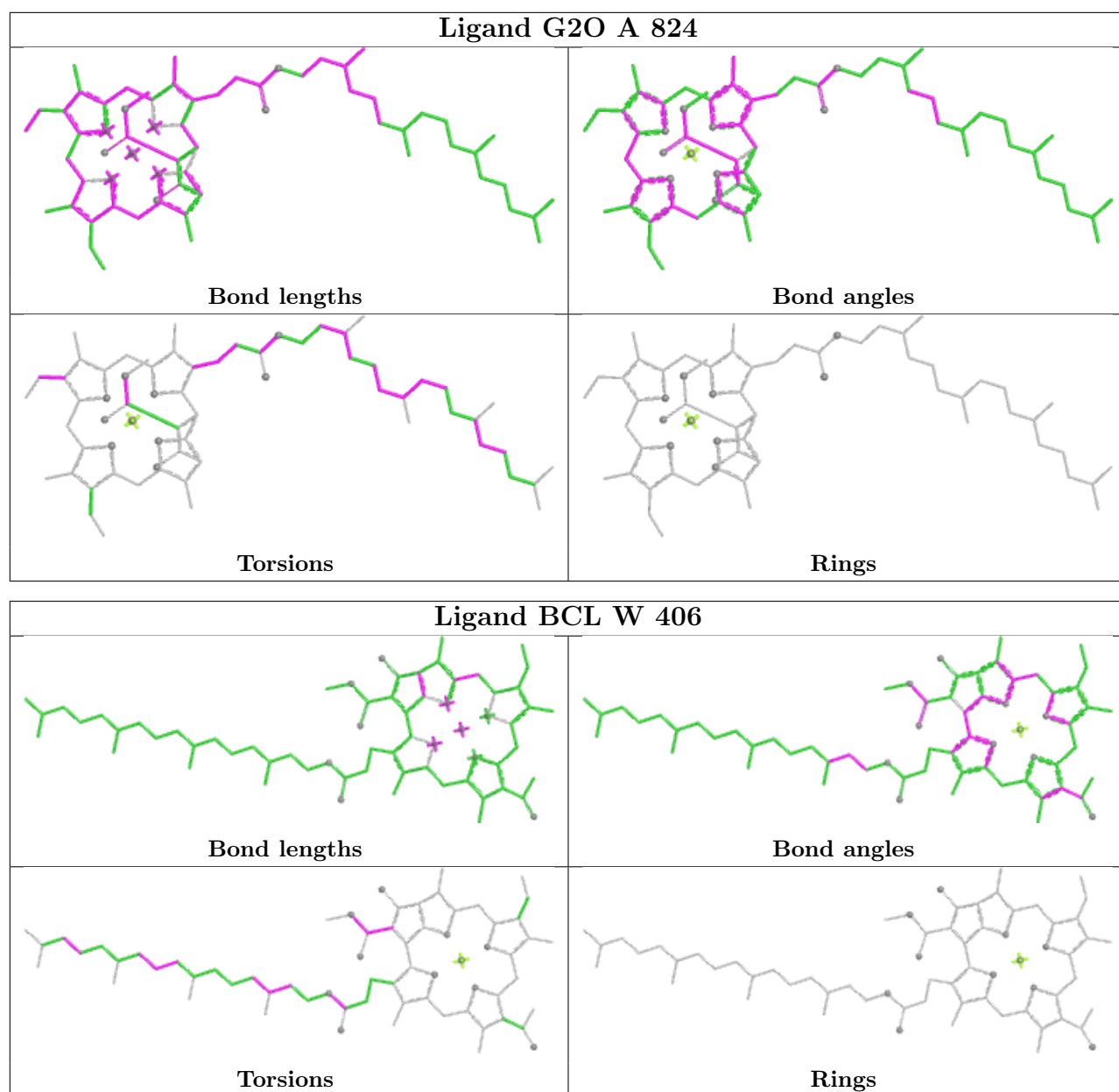
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

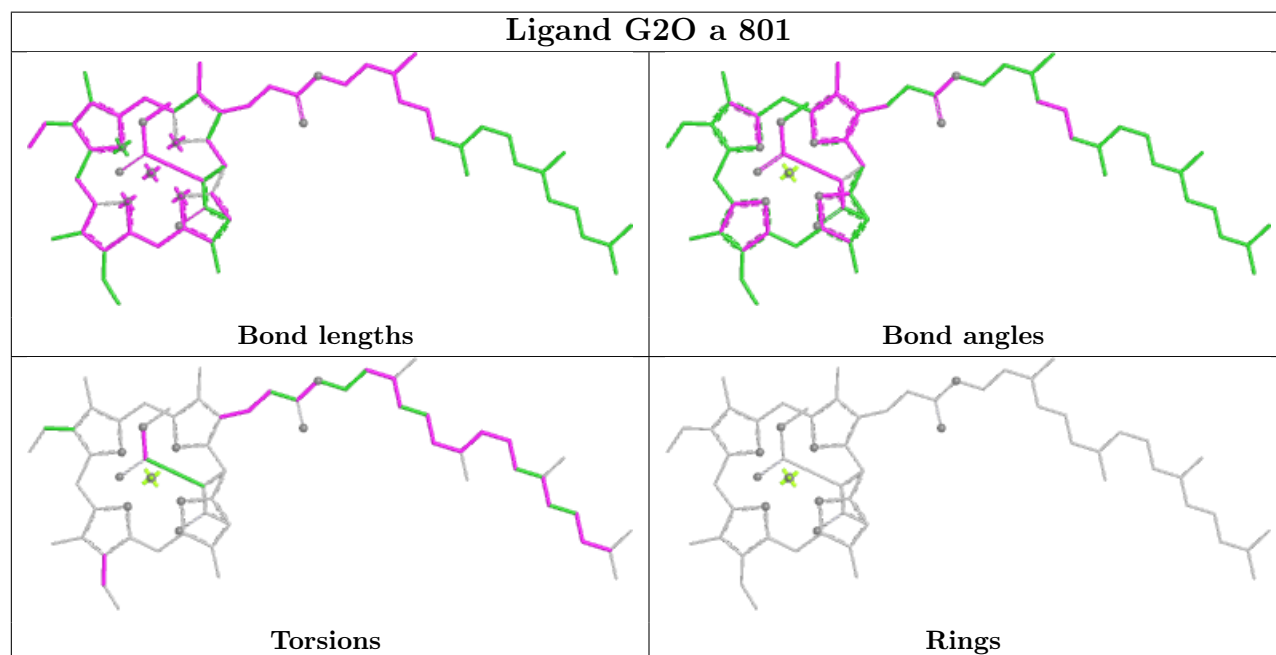
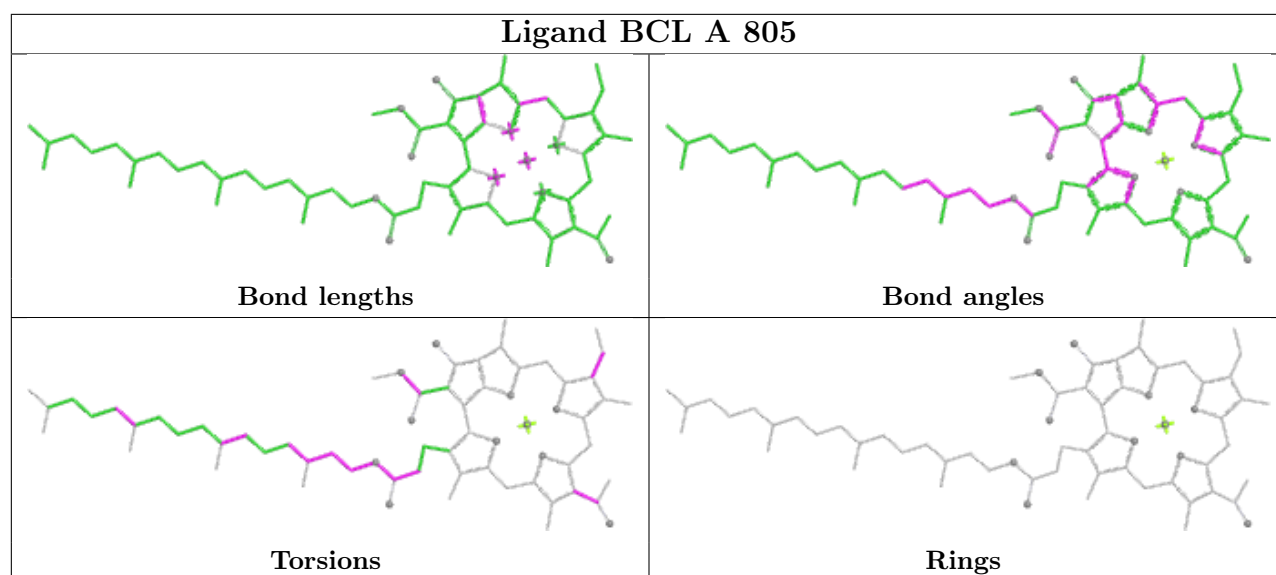


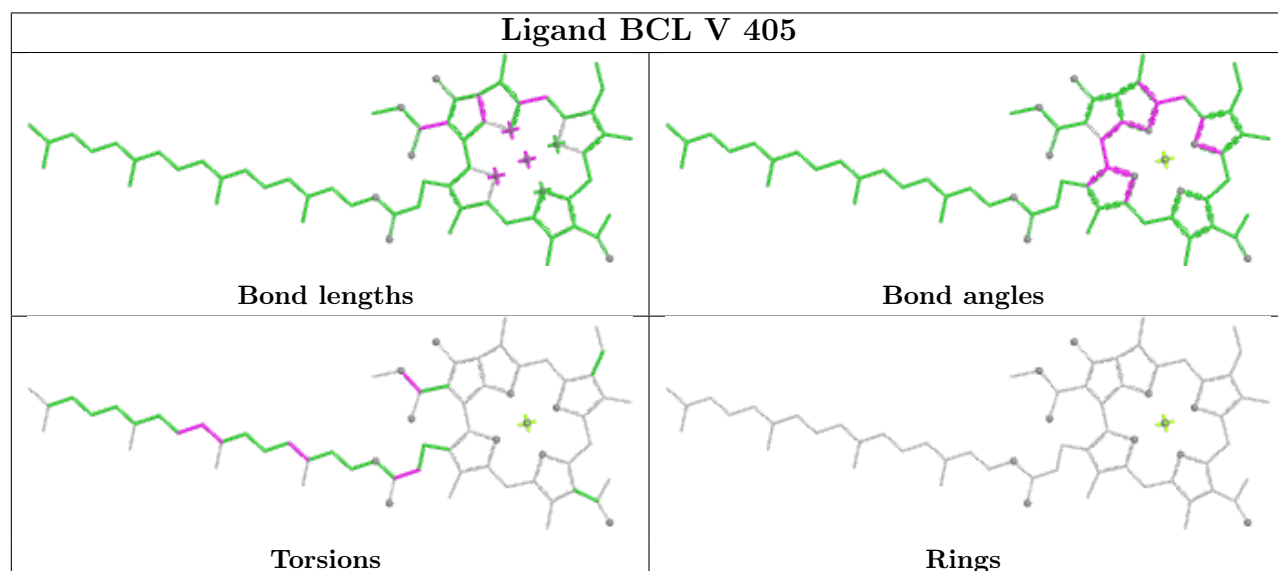
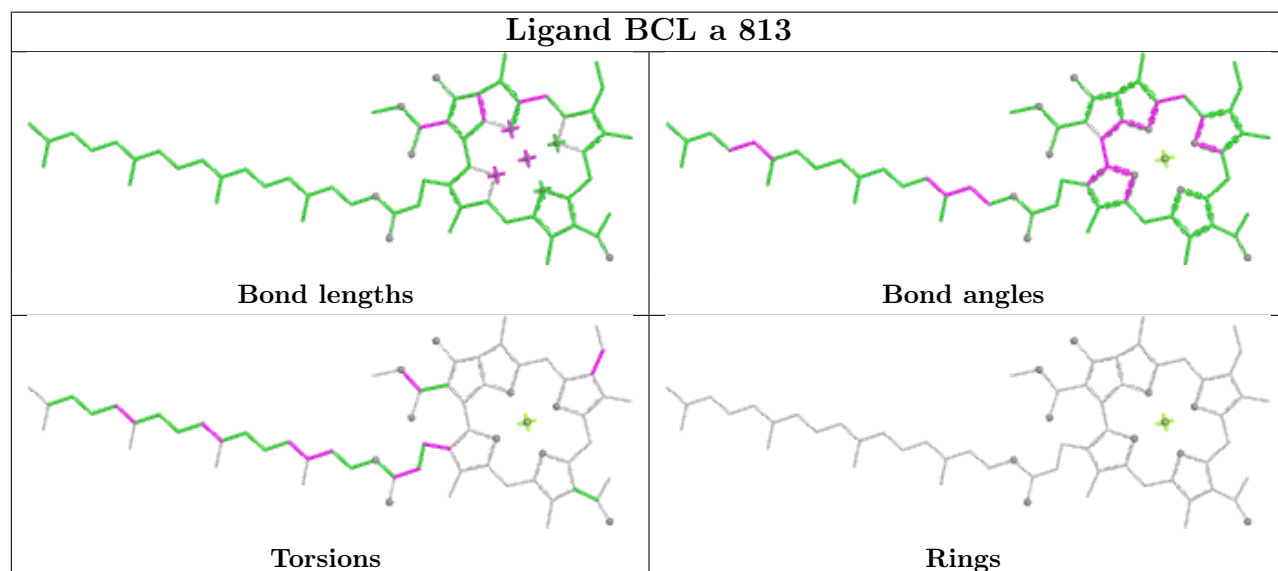
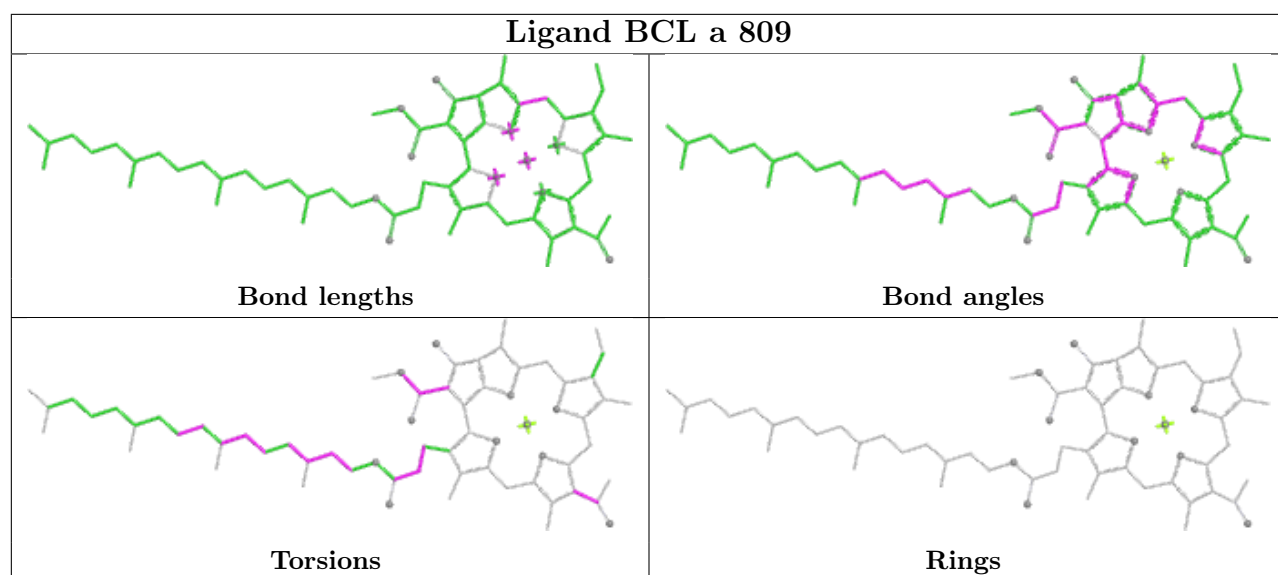


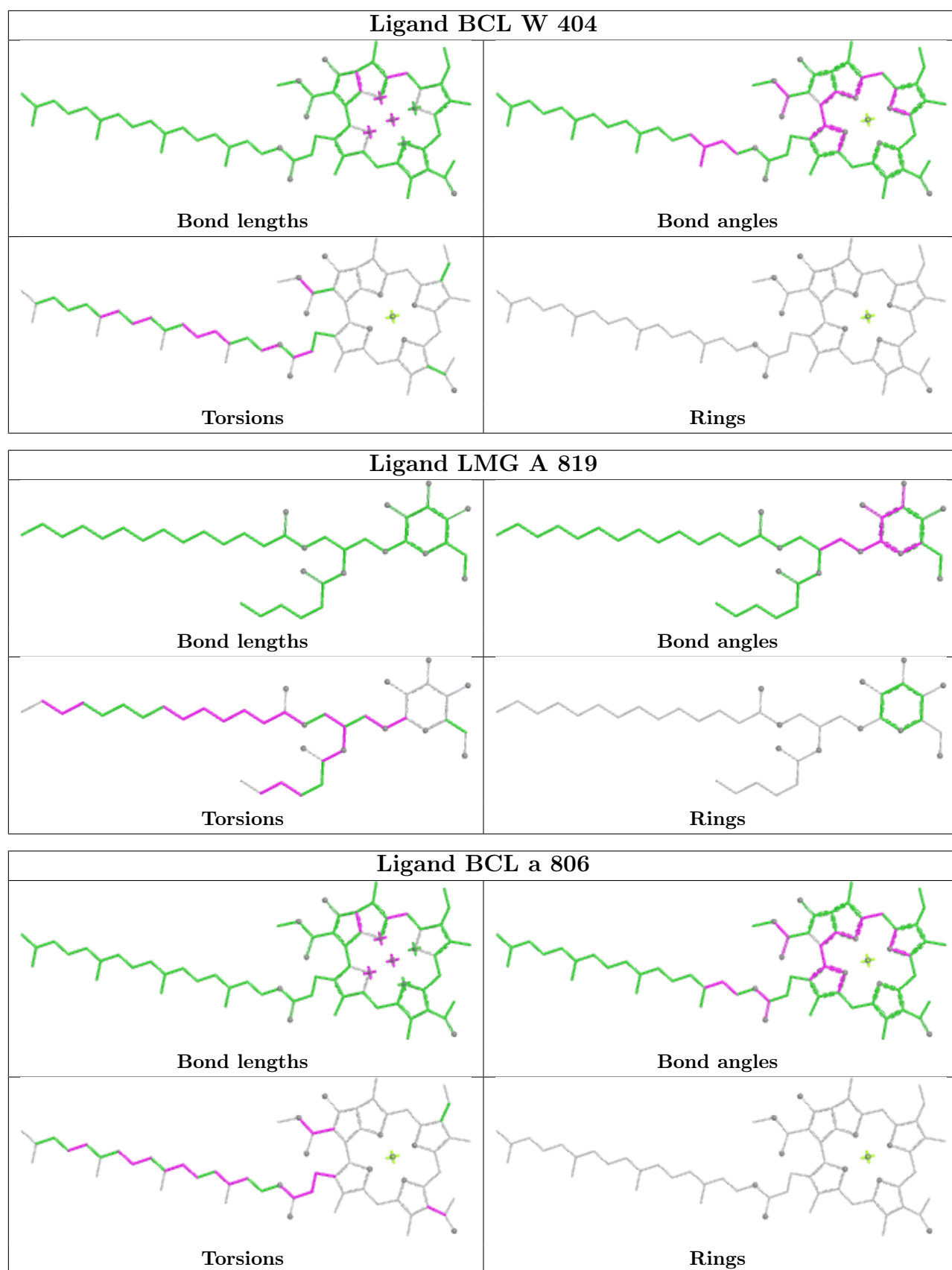


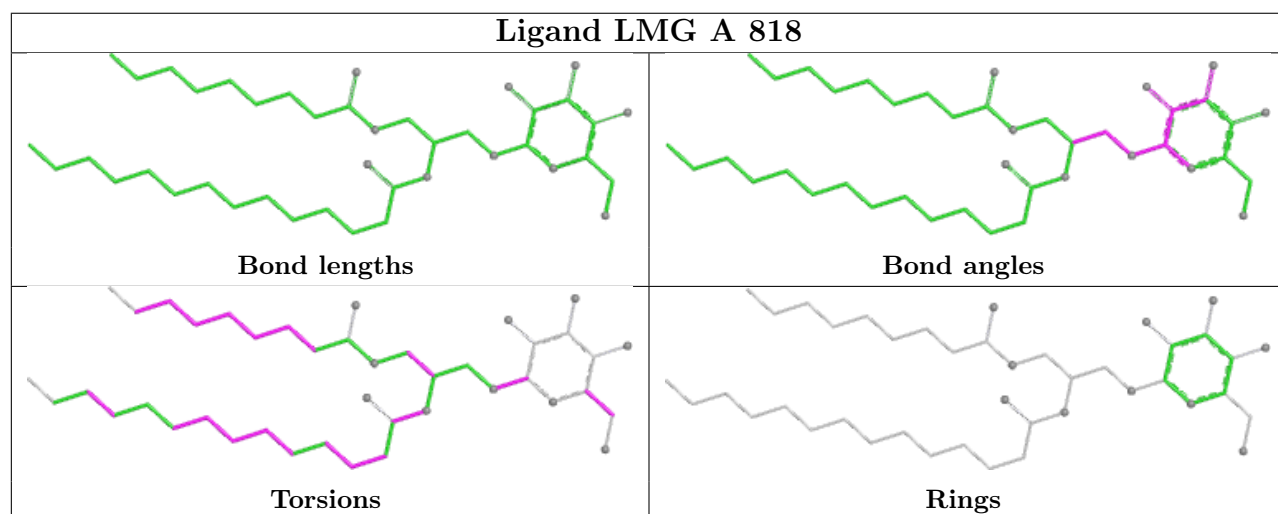
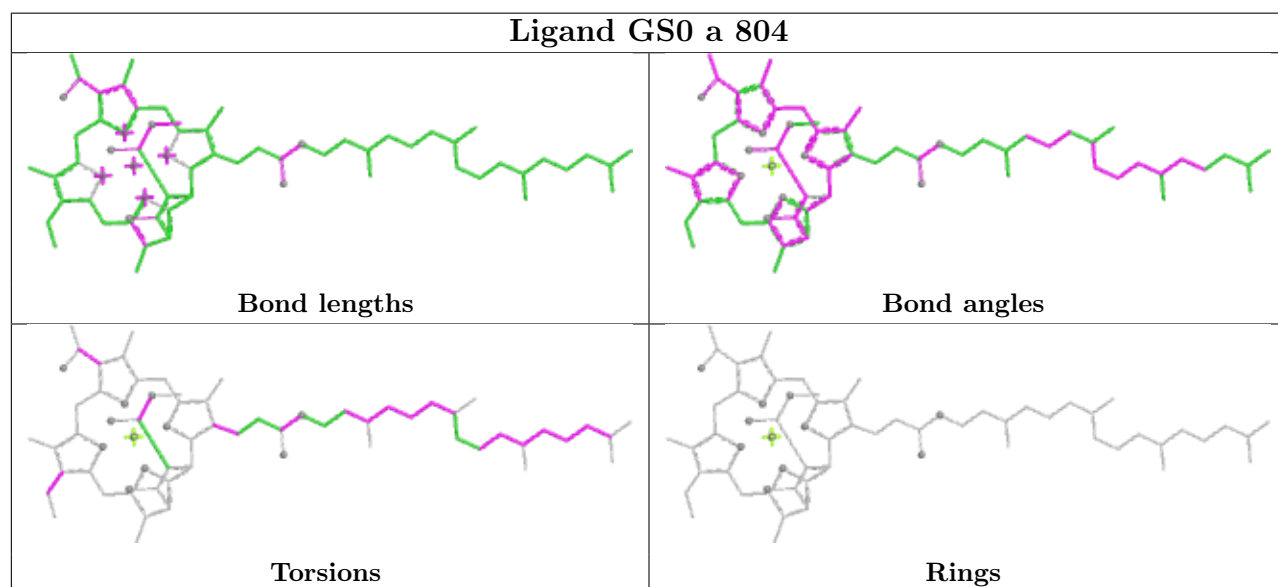
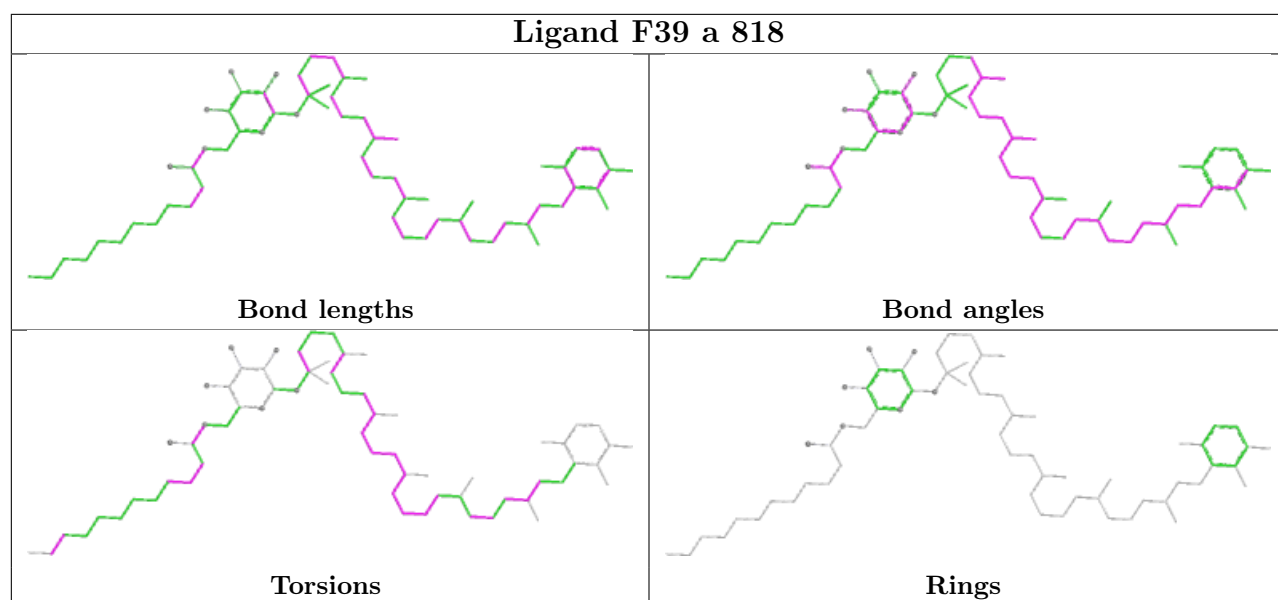


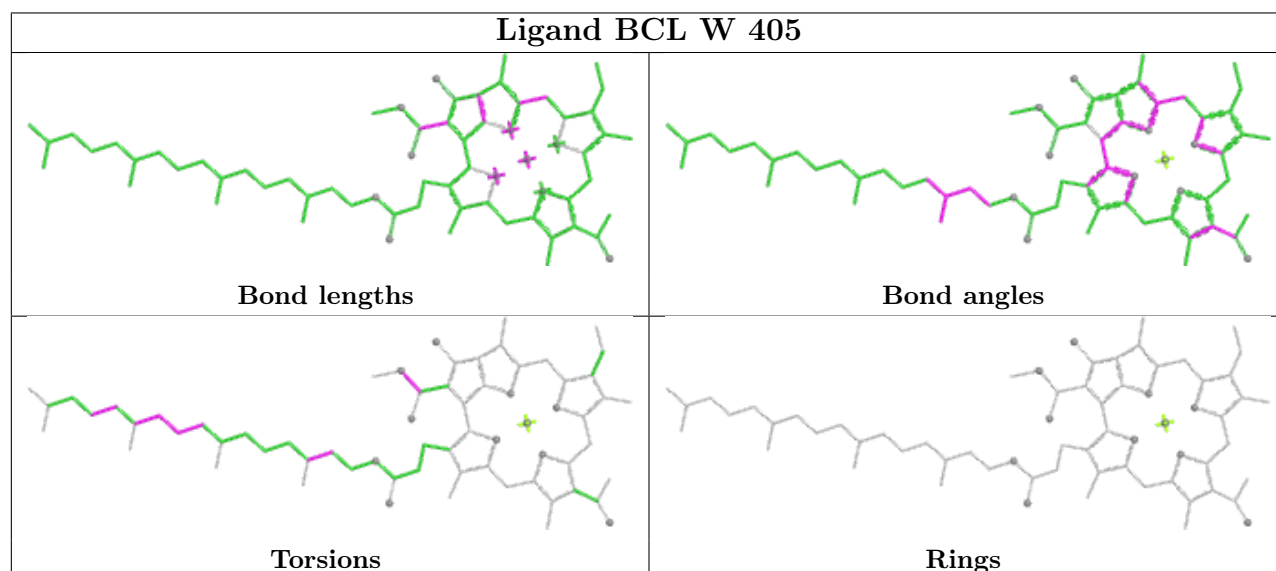
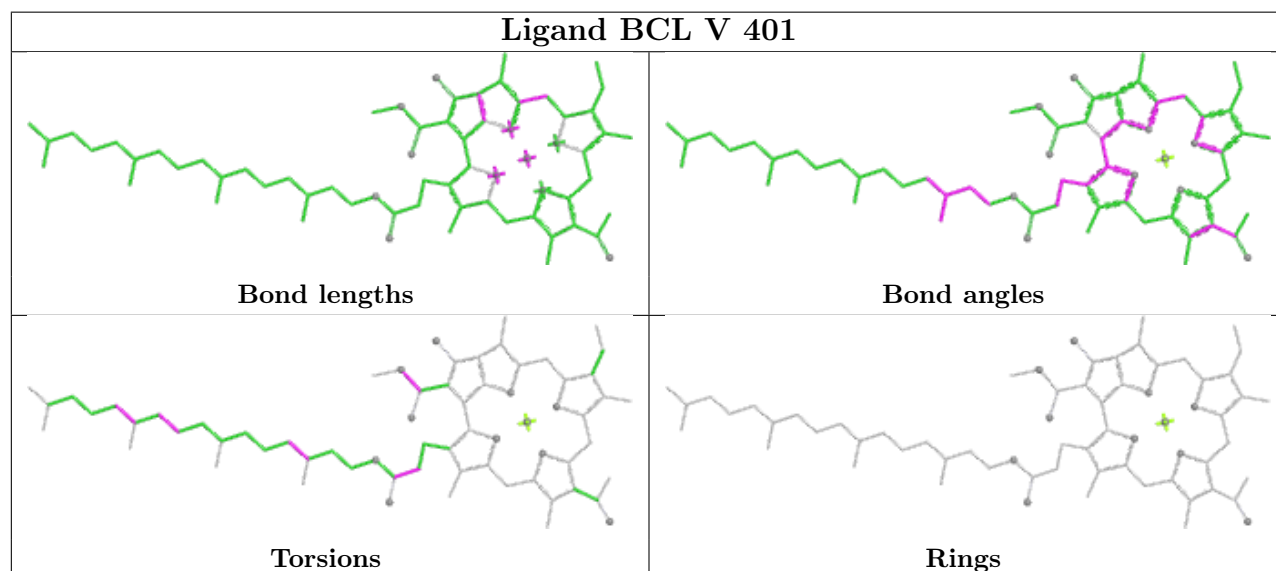
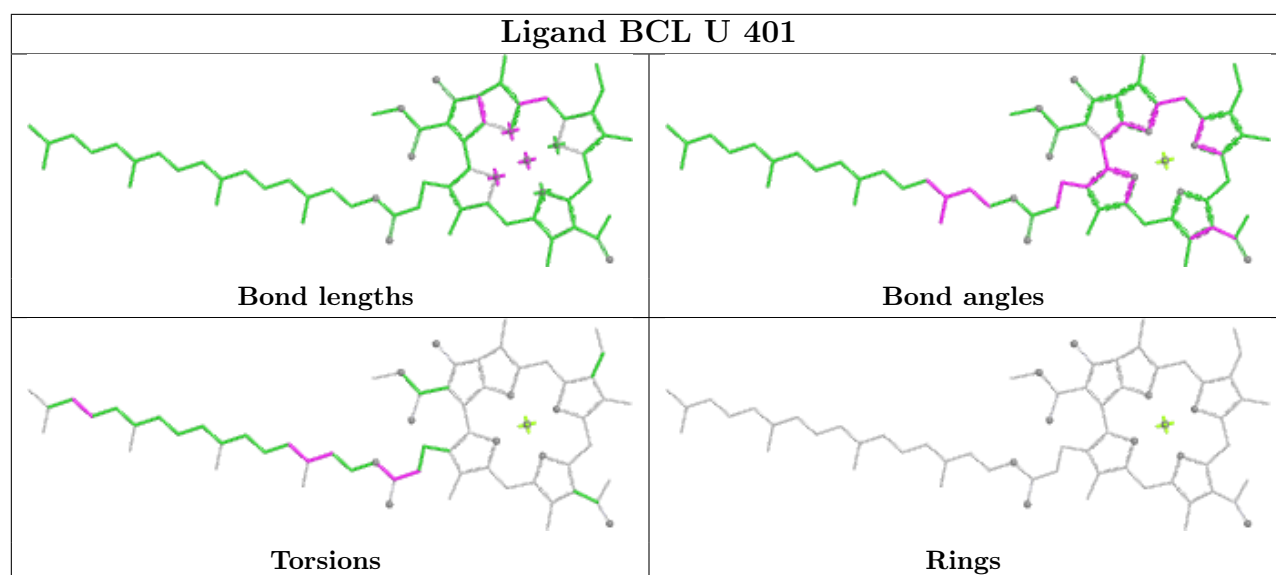


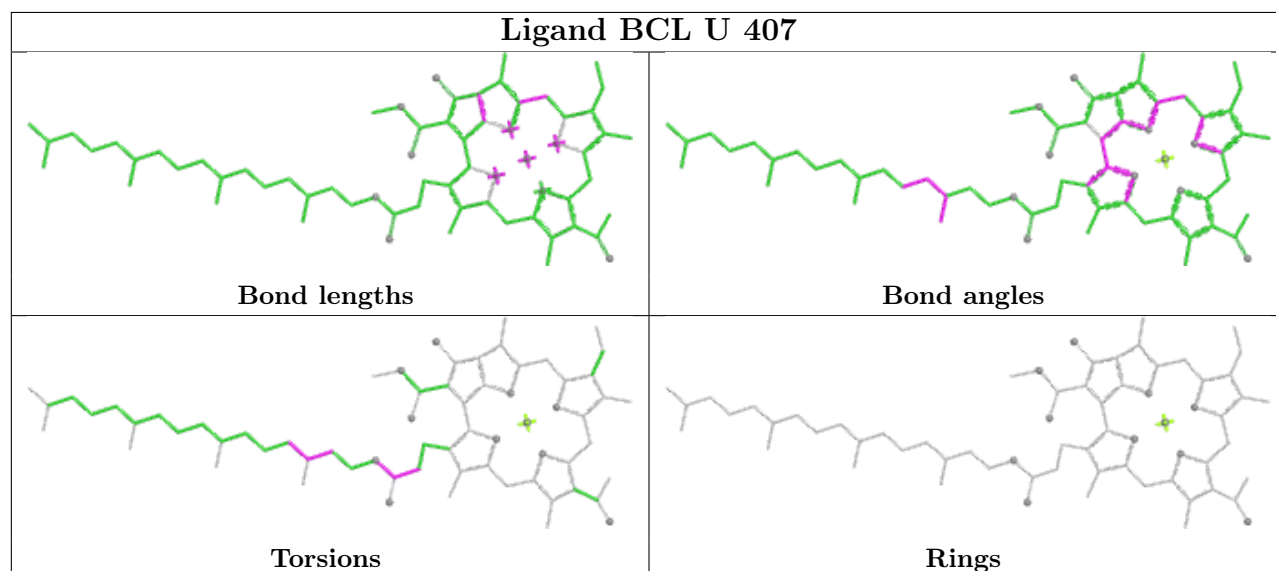
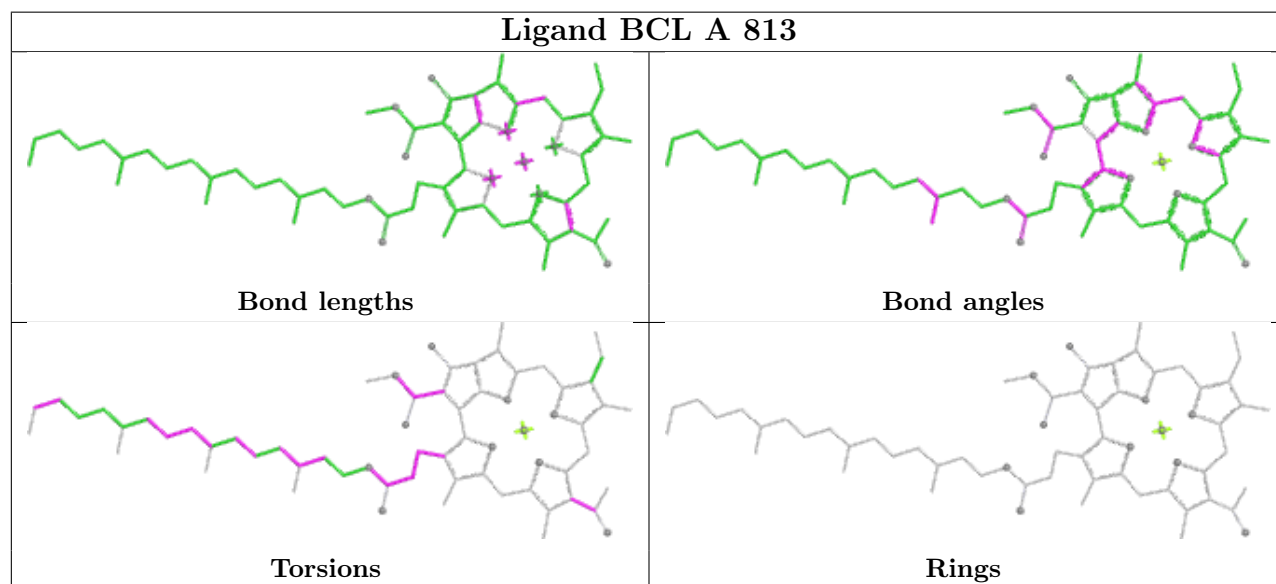
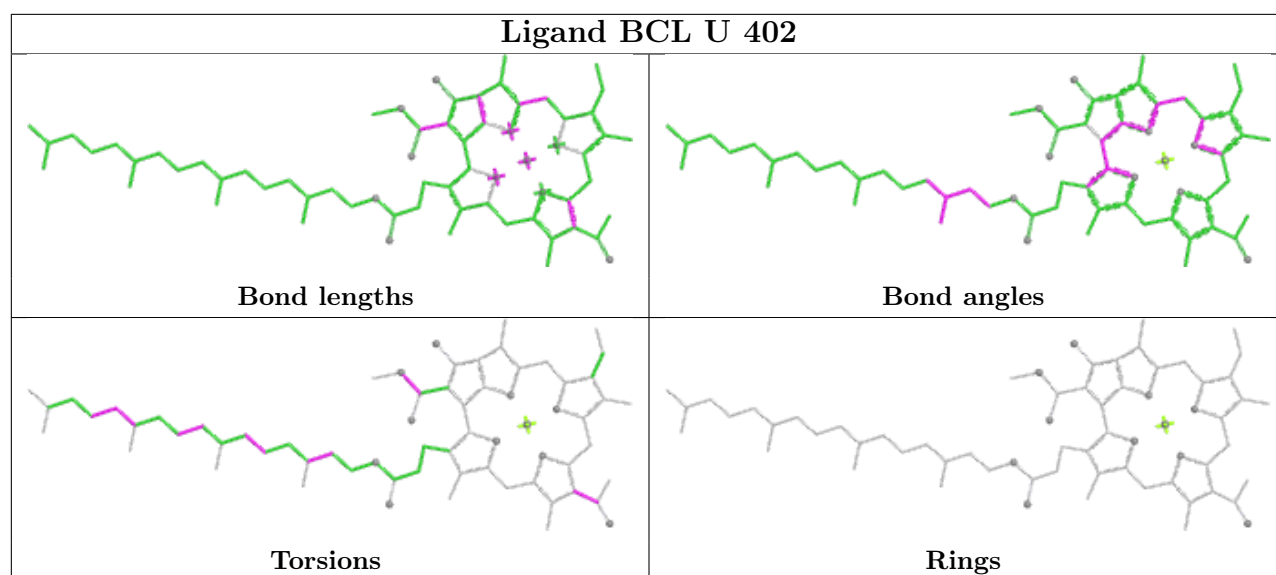


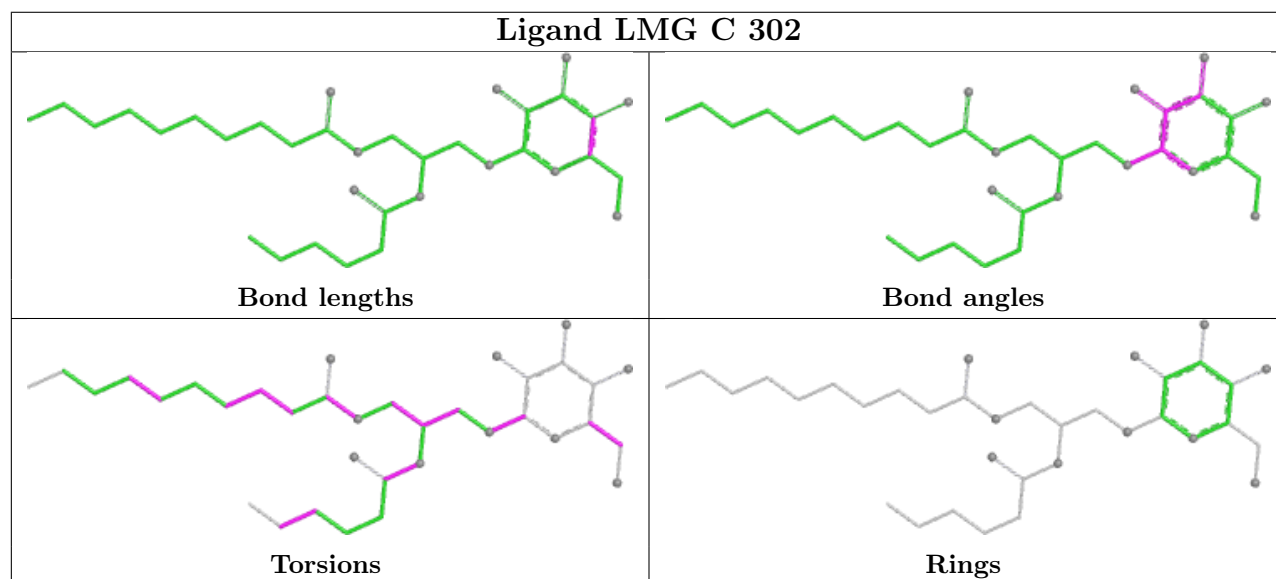
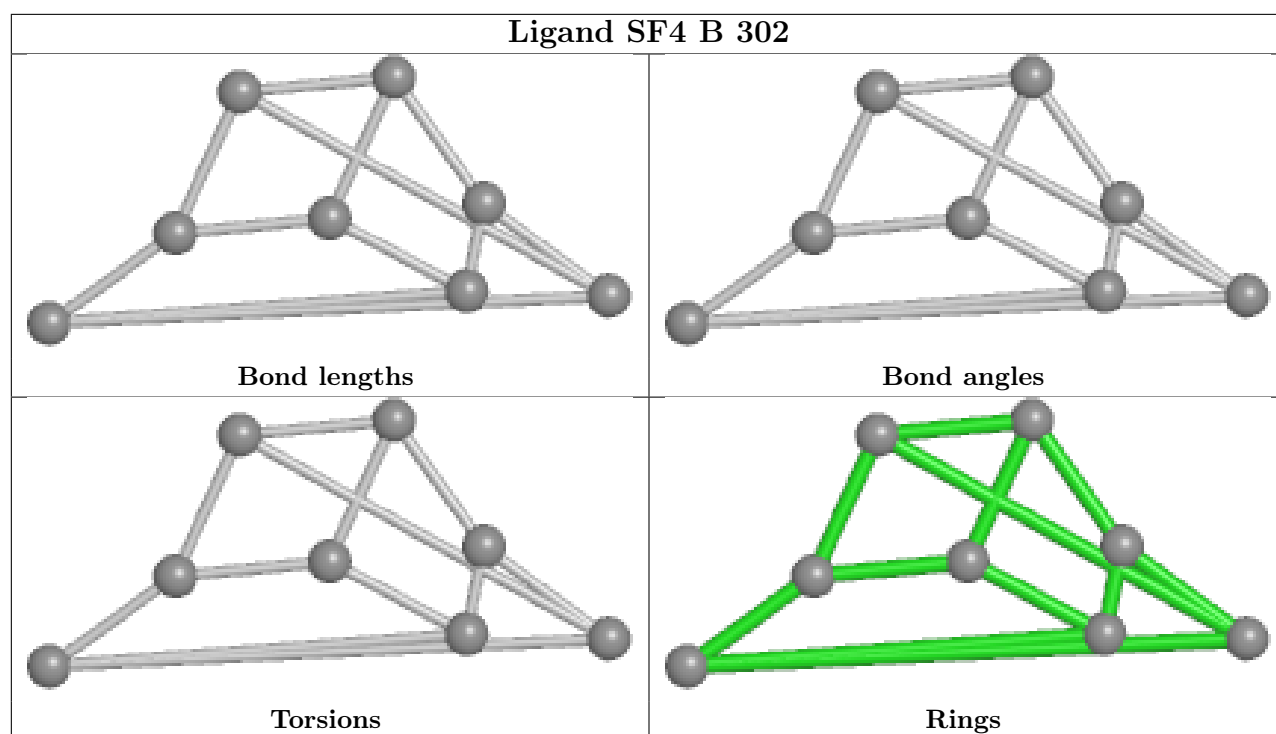


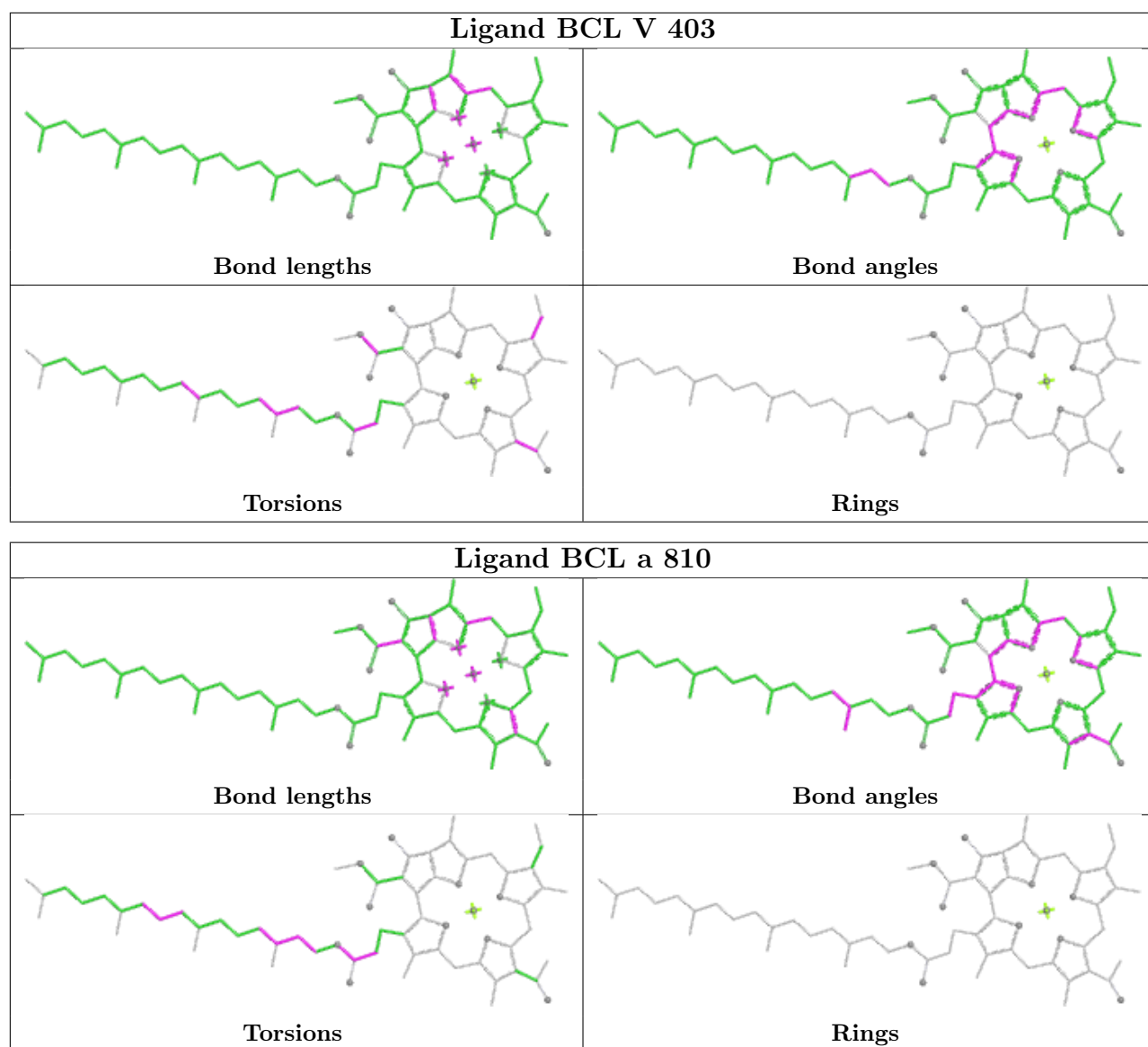


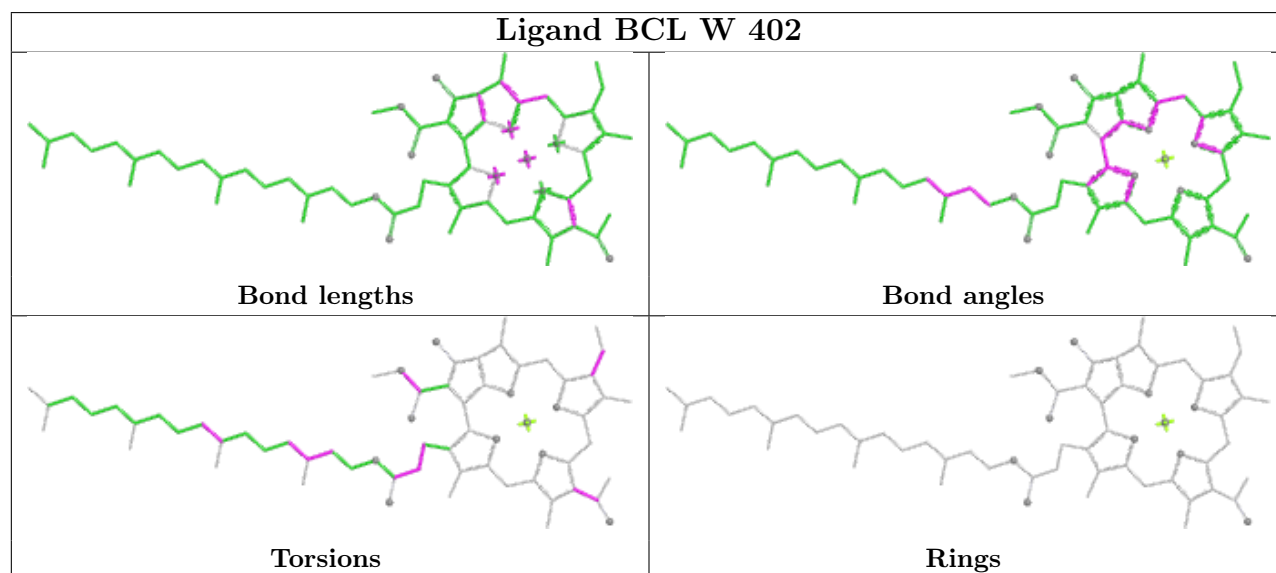
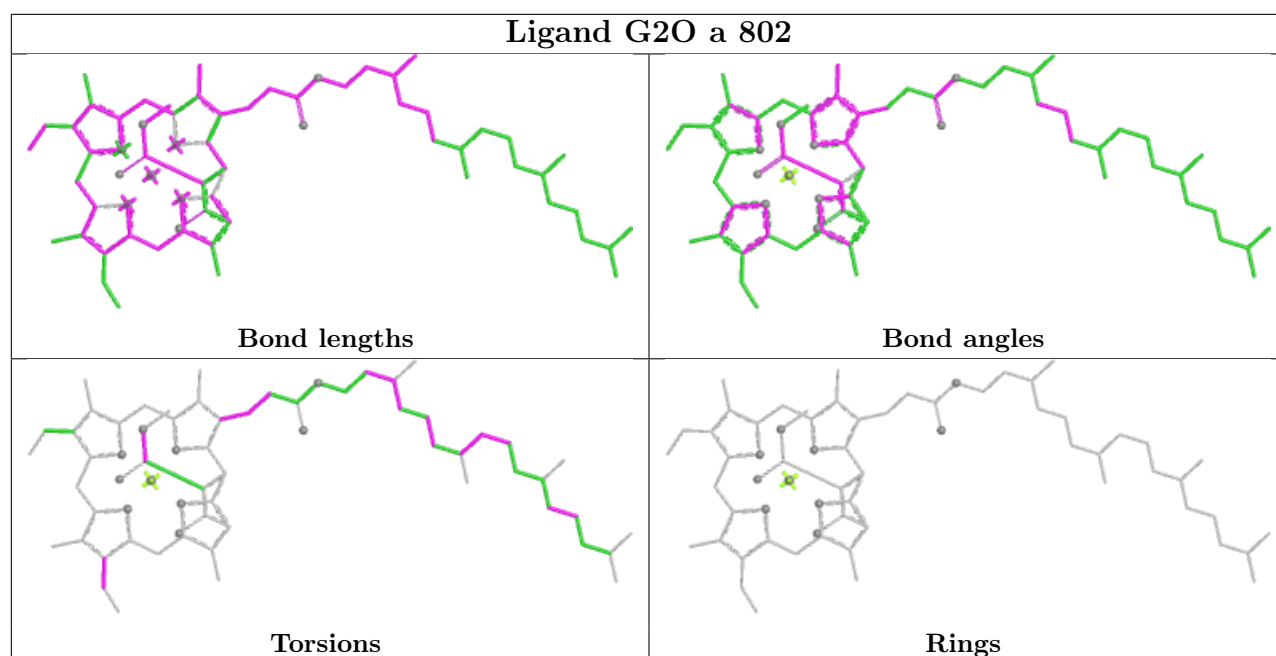


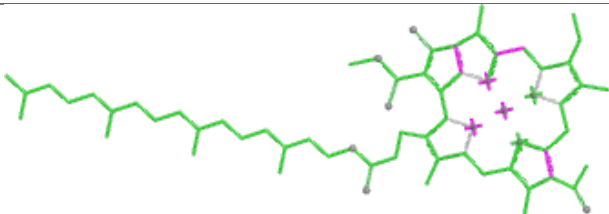
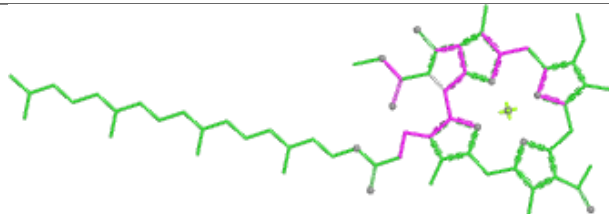
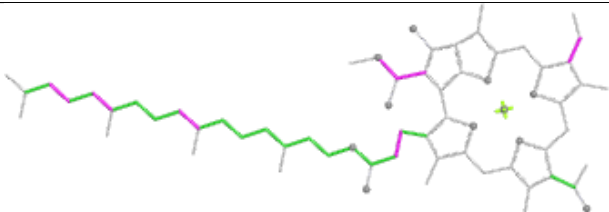
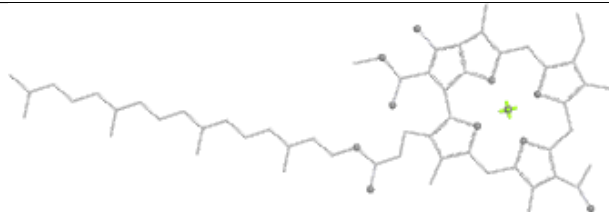


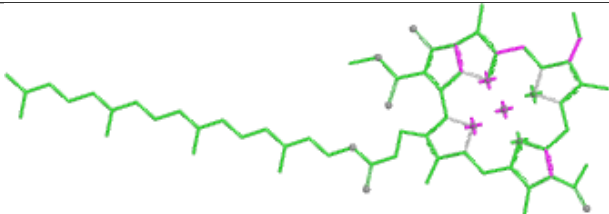
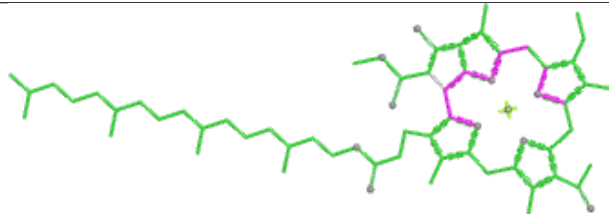
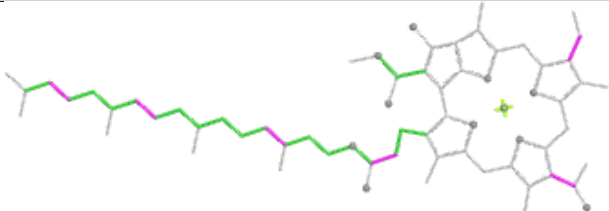
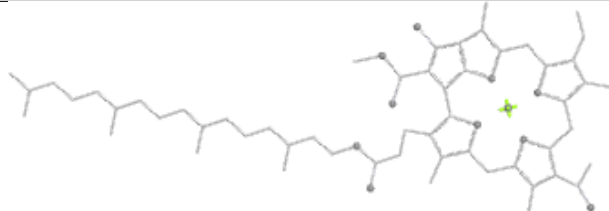


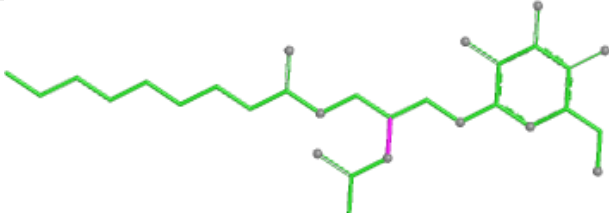
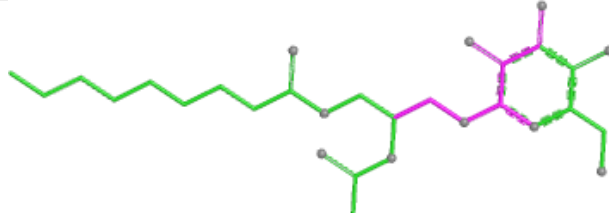
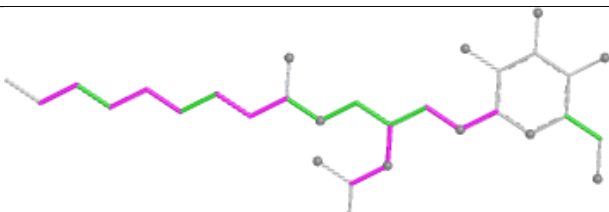
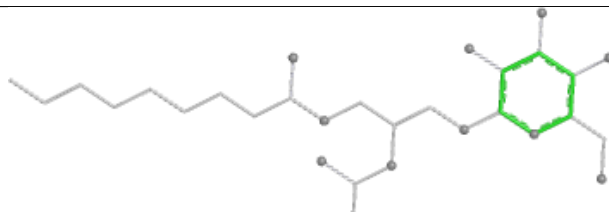


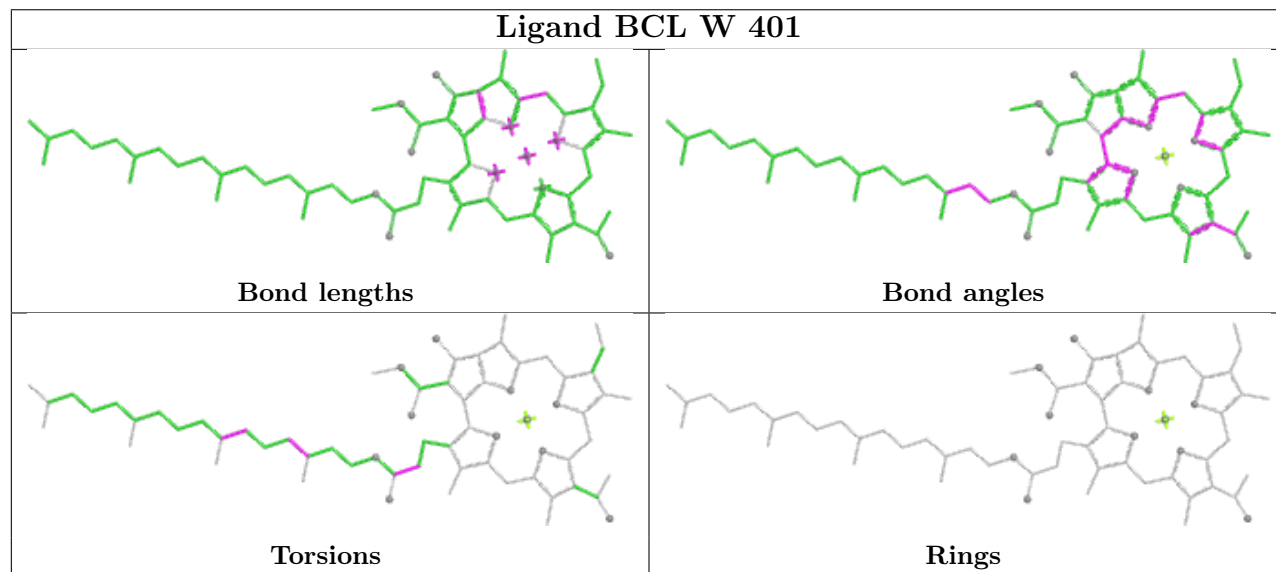
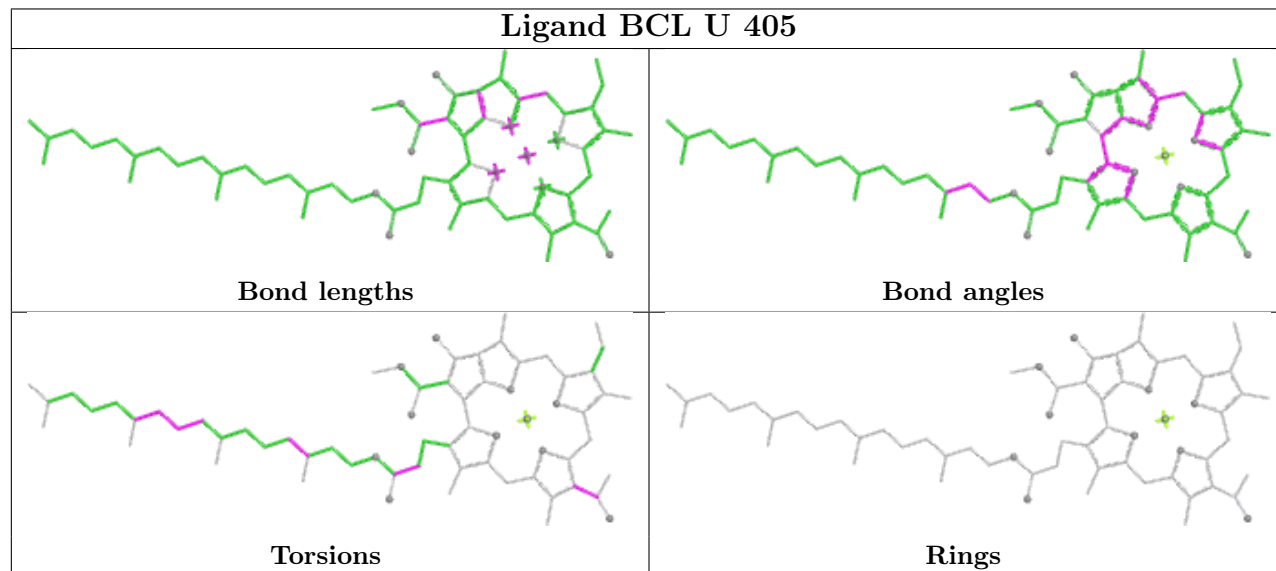
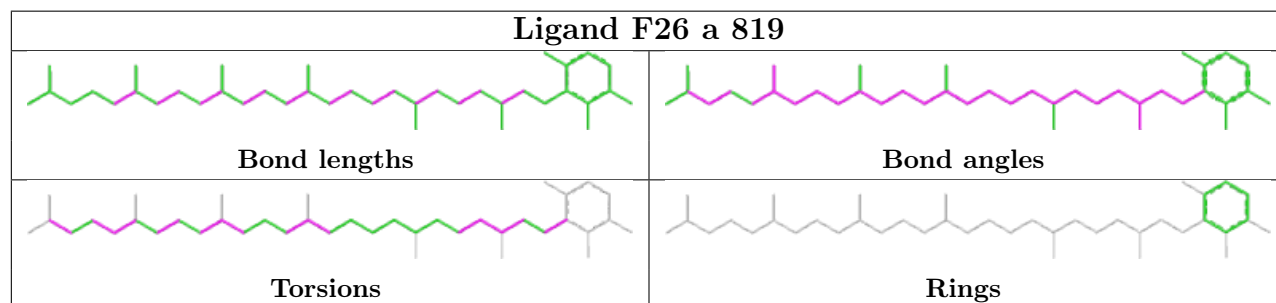
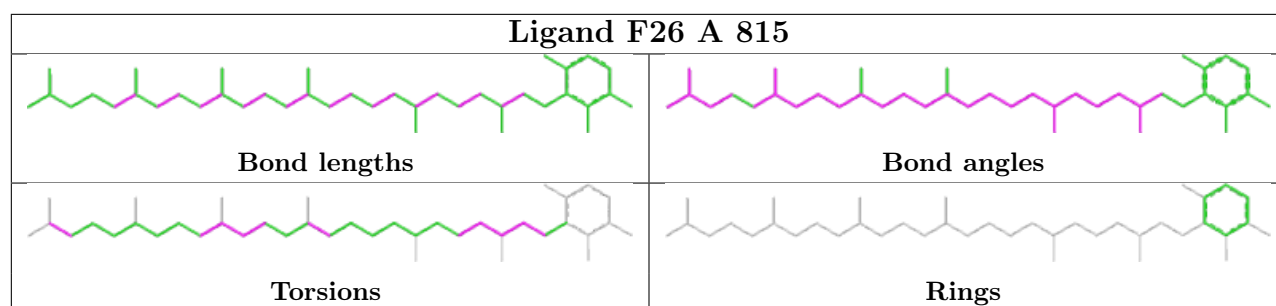


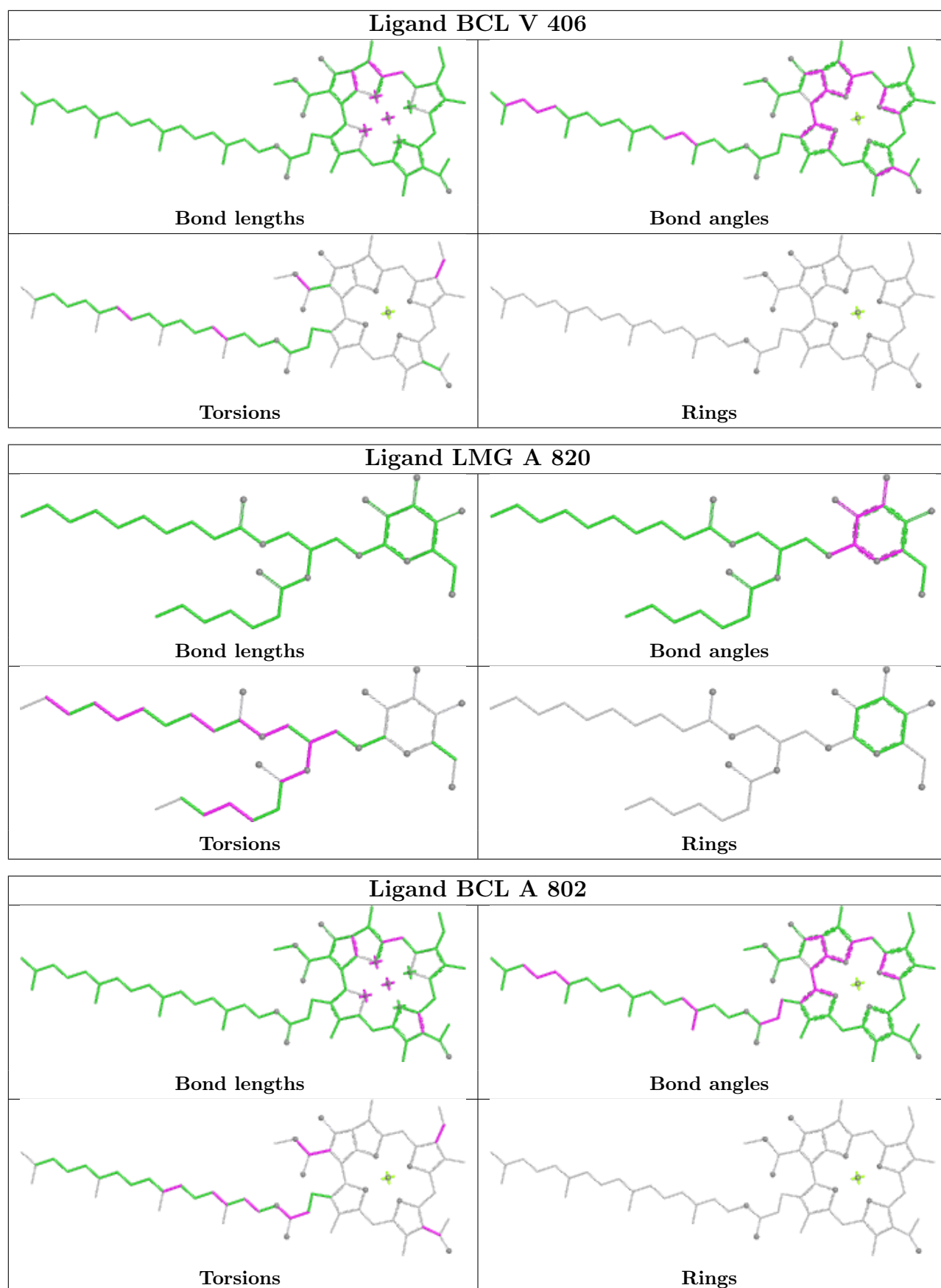


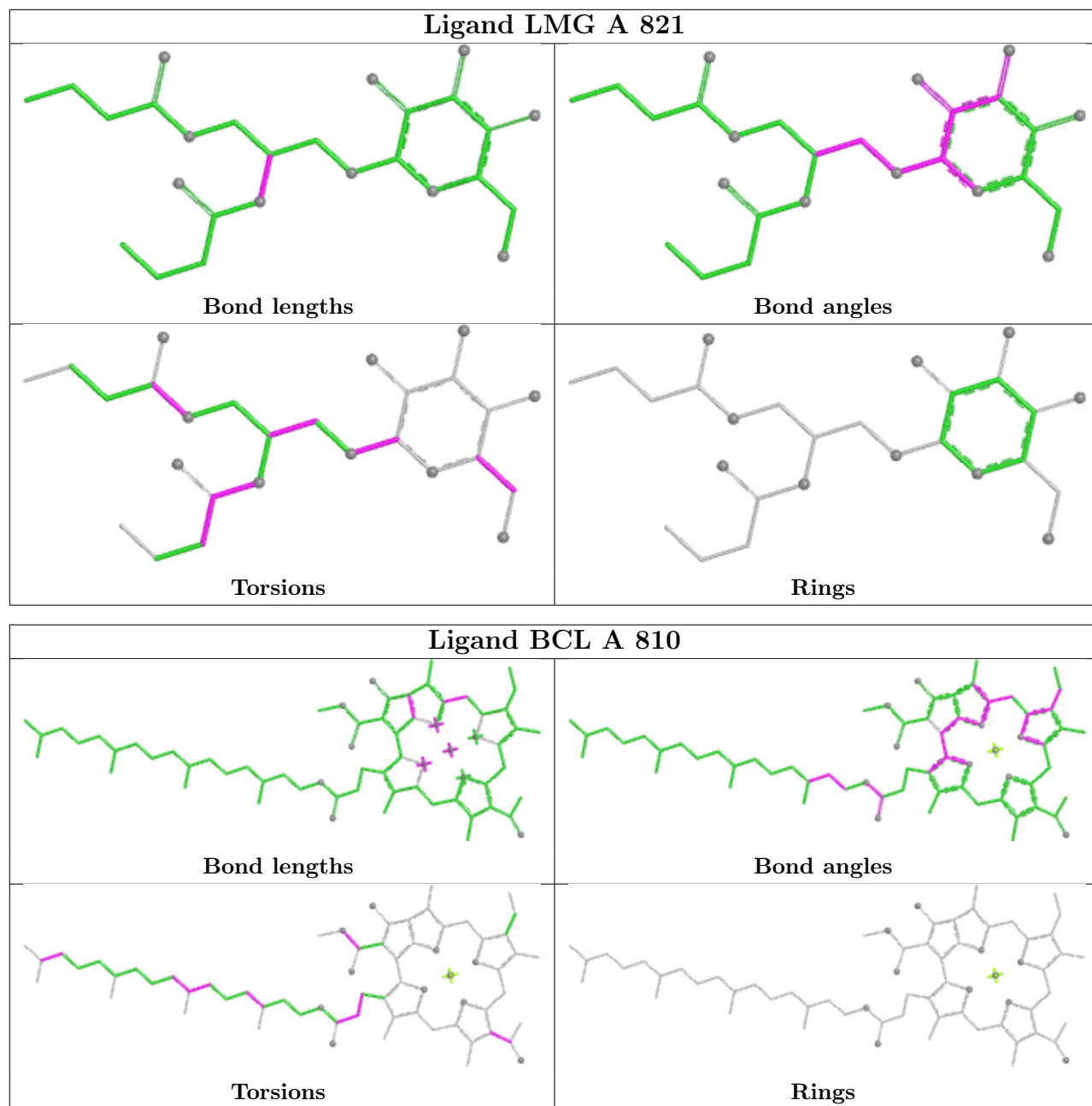
Ligand BCL a 814	
	
Bond lengths	Bond angles
	
Torsions	Rings

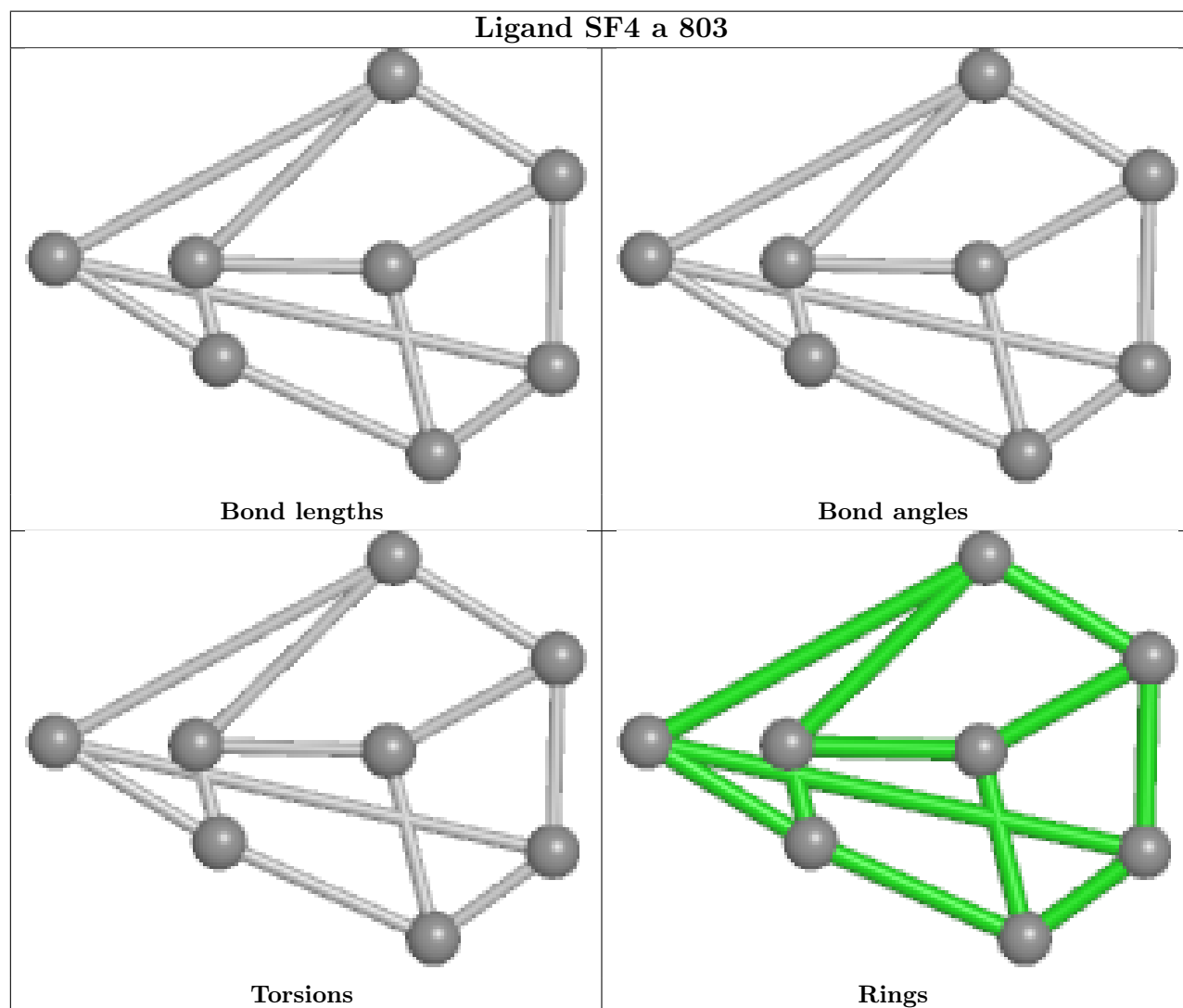
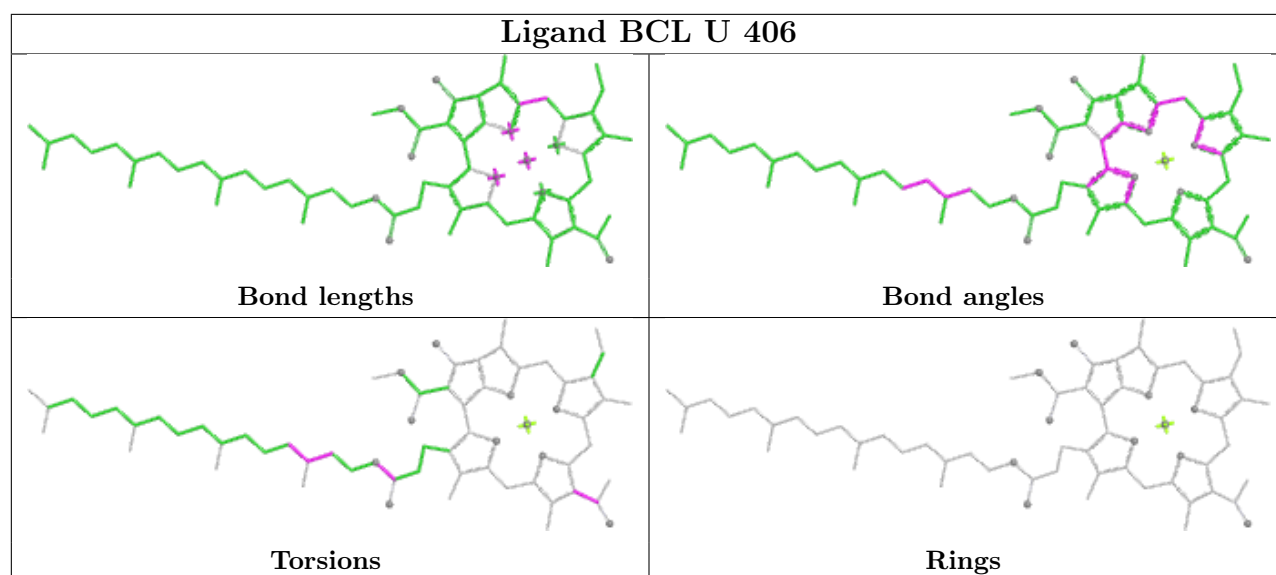
Ligand BCL a 807	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG A 822	
	
Bond lengths	Bond angles
	
Torsions	Rings

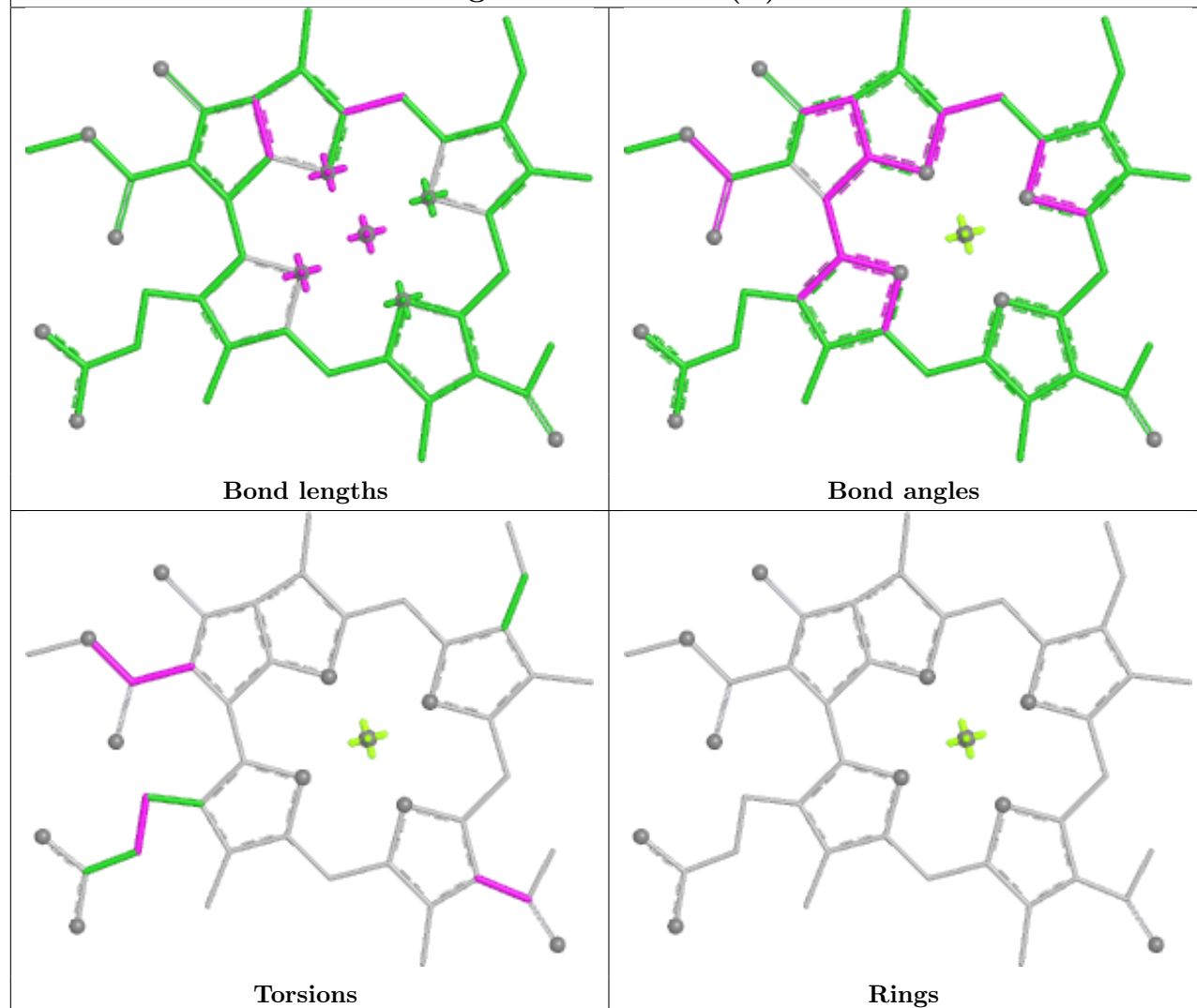




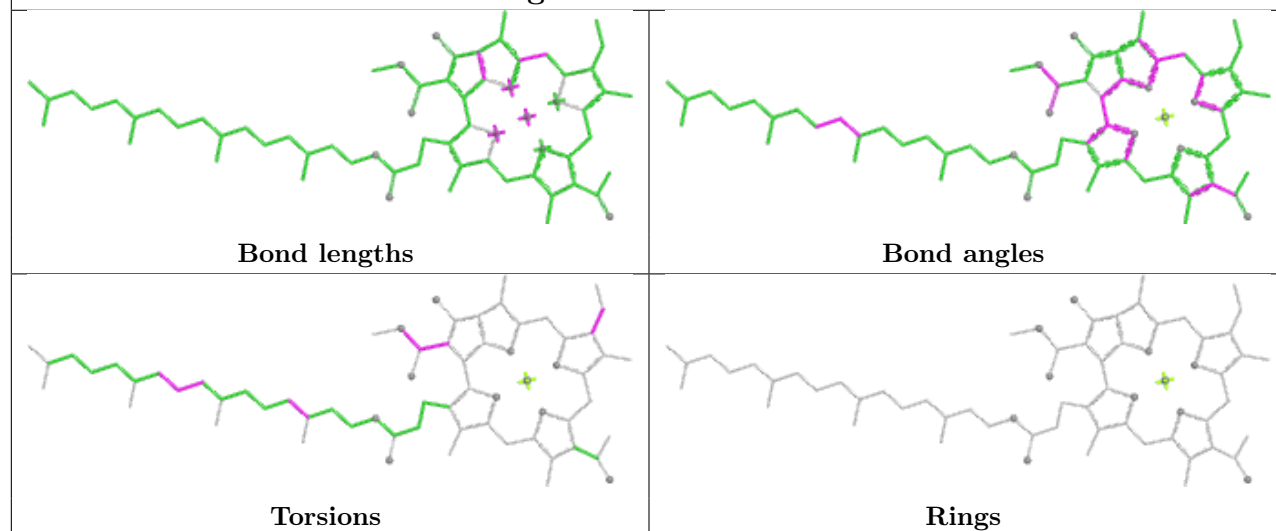


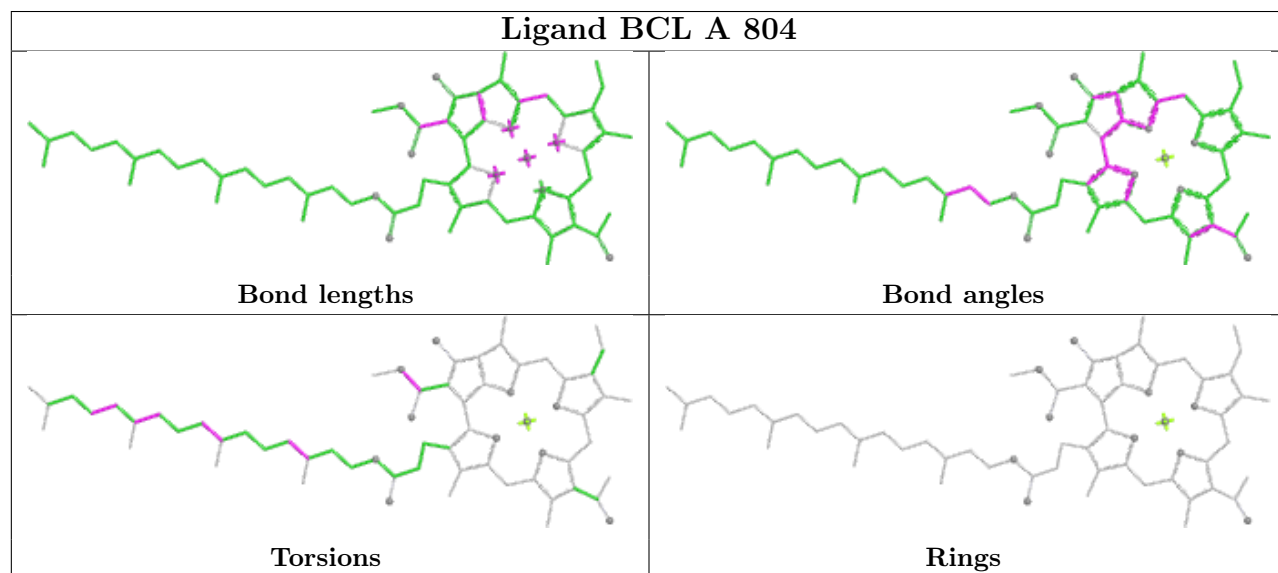
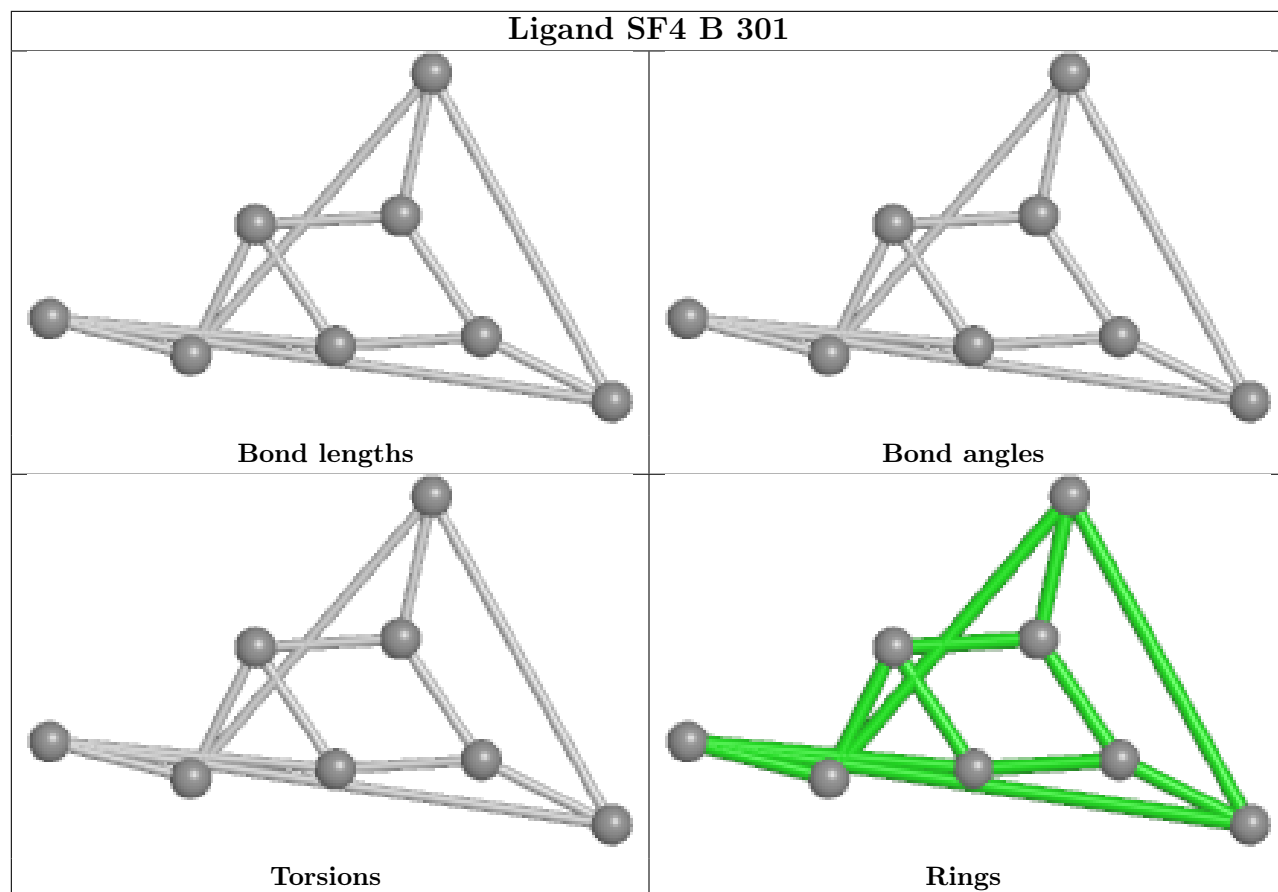


Ligand BCL V 408 (B)

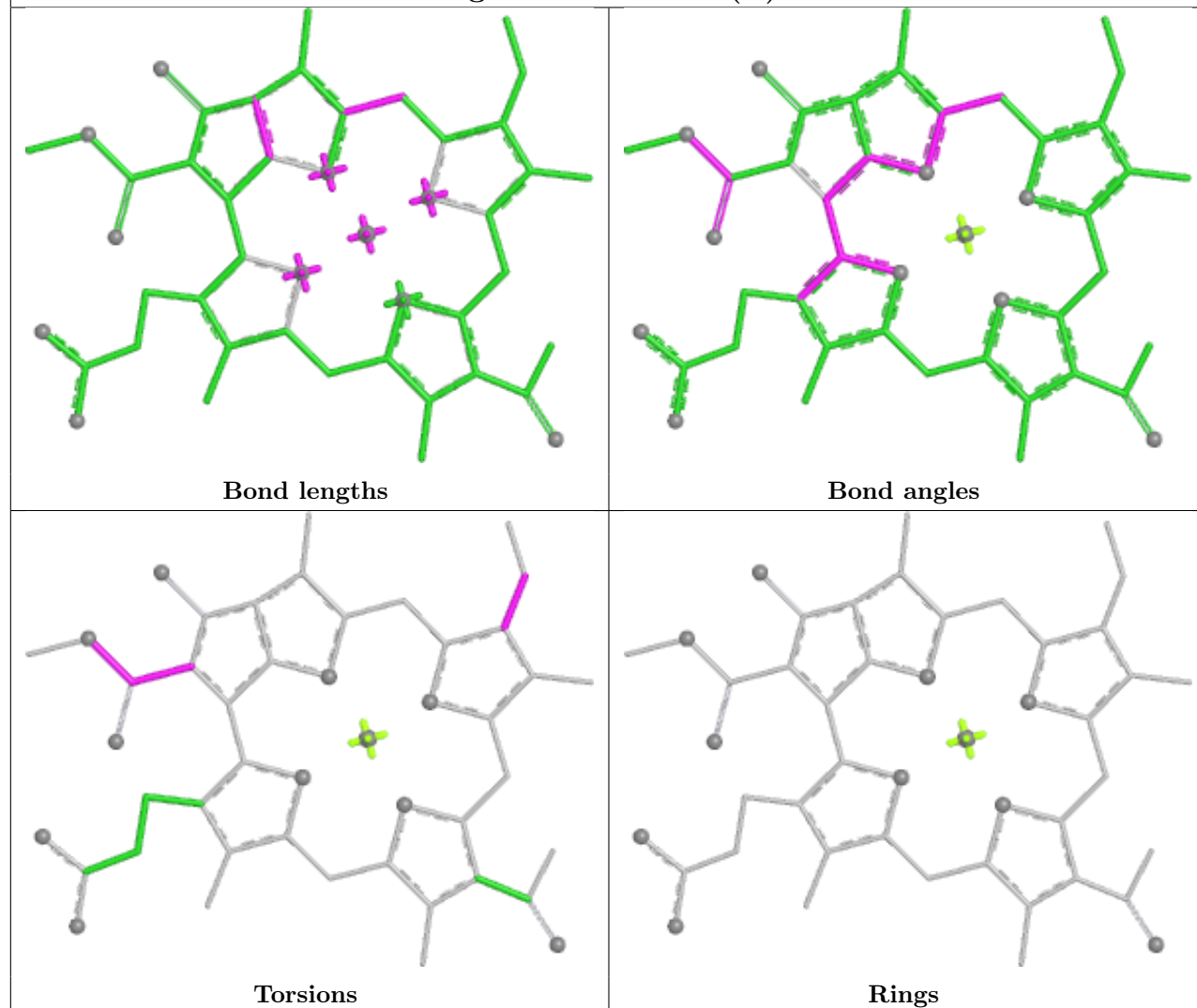


Ligand BCL W 403

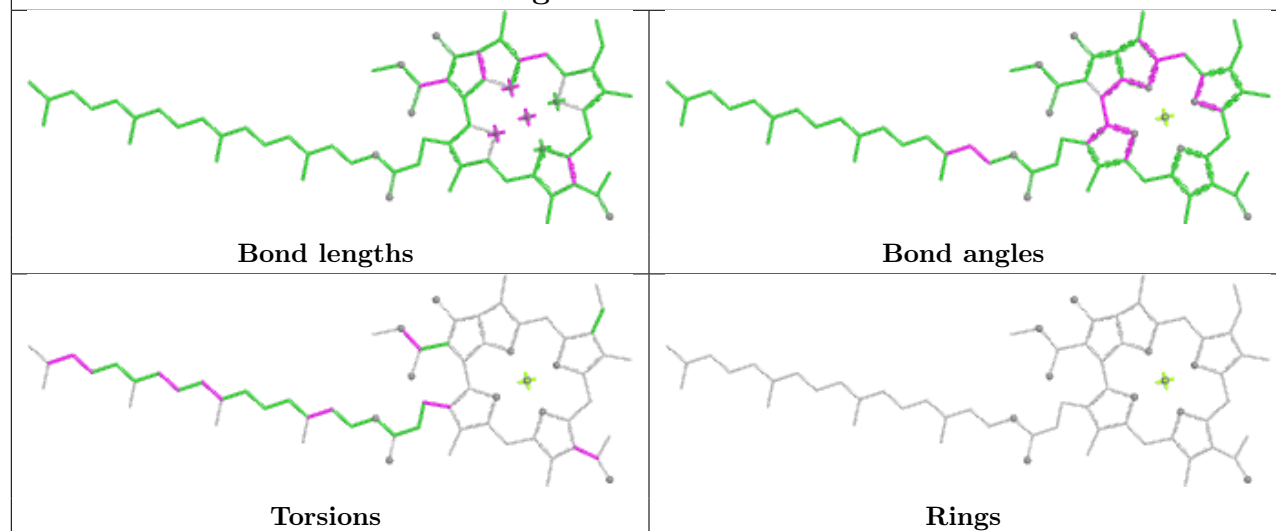


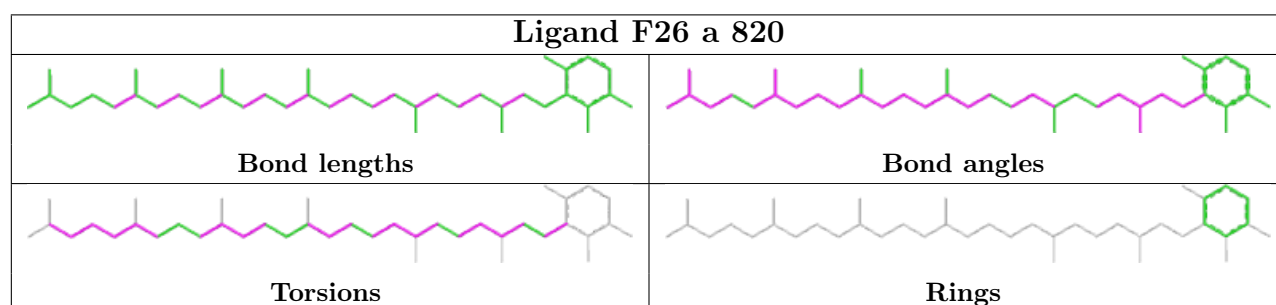
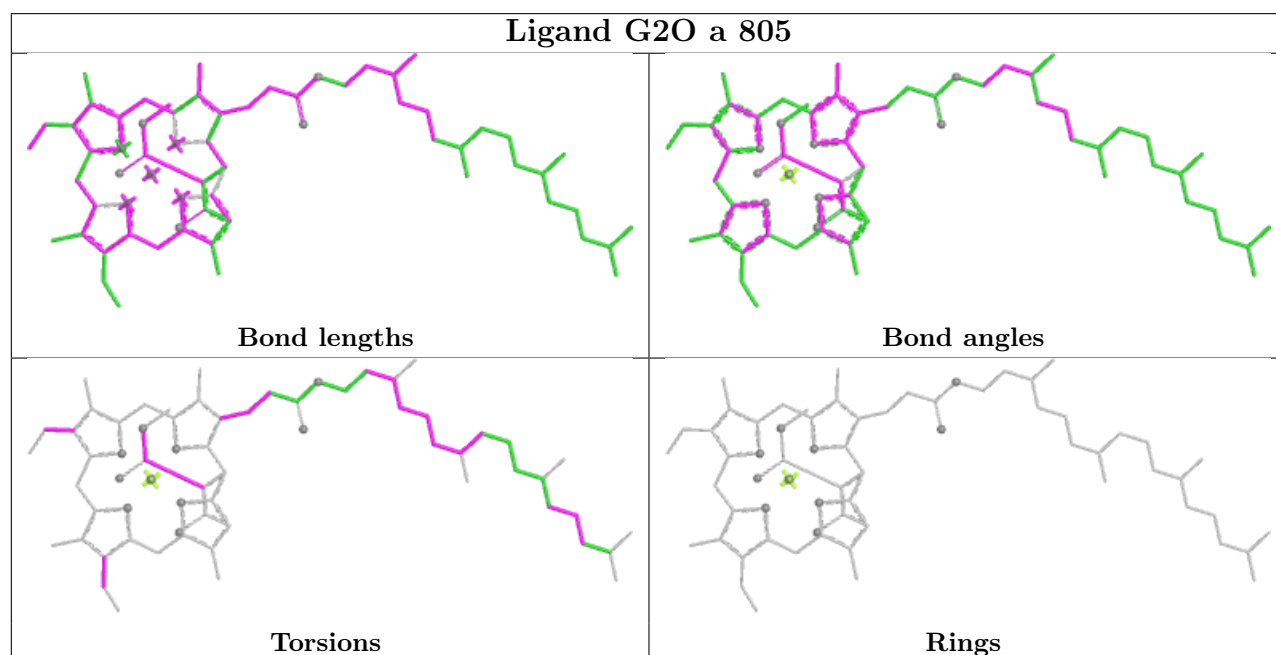
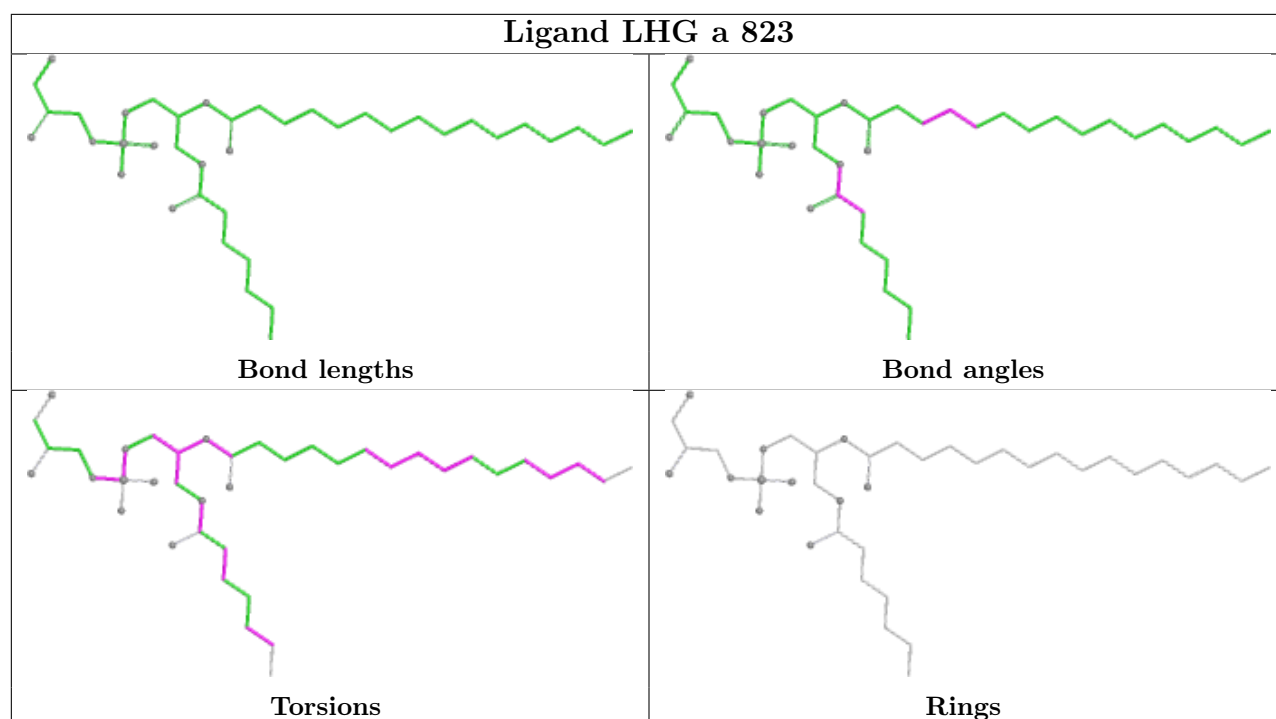


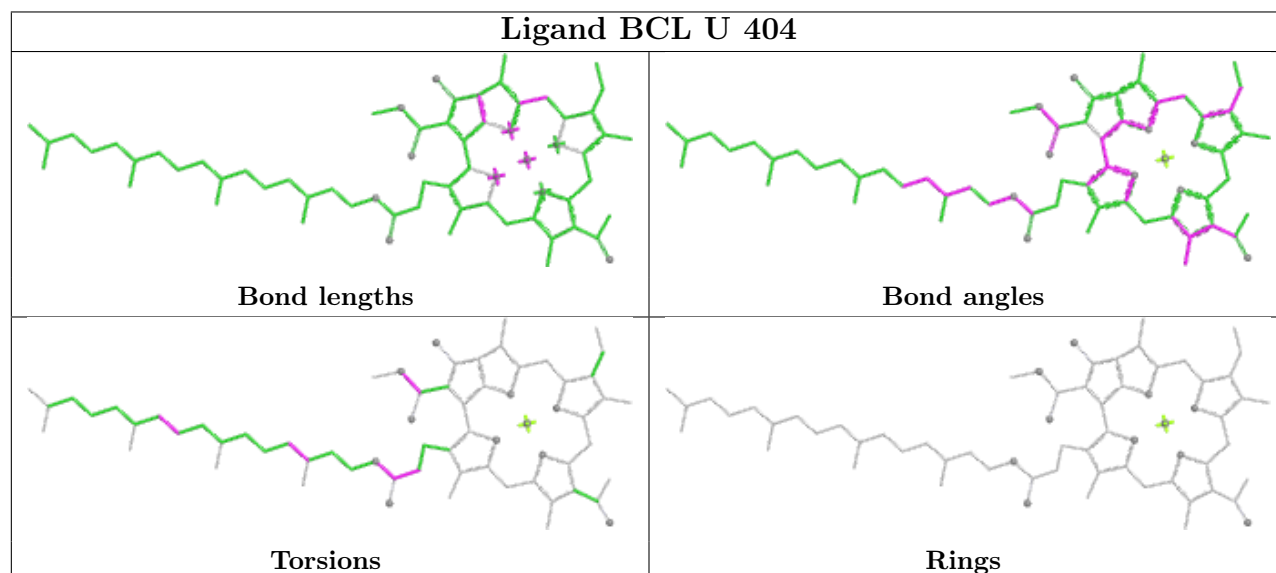
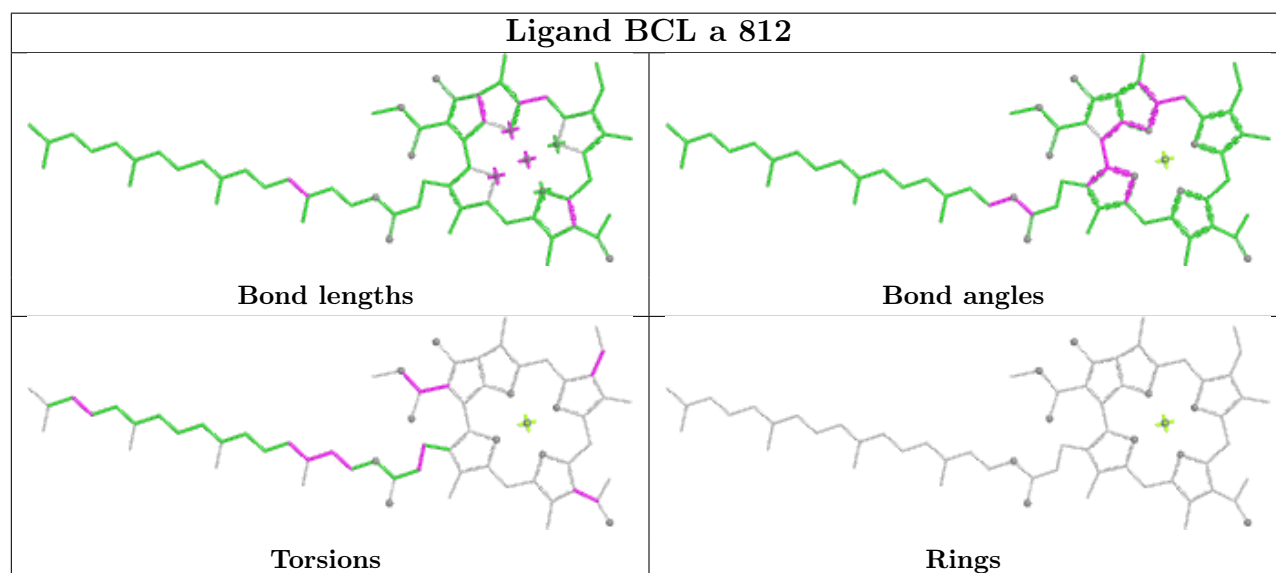
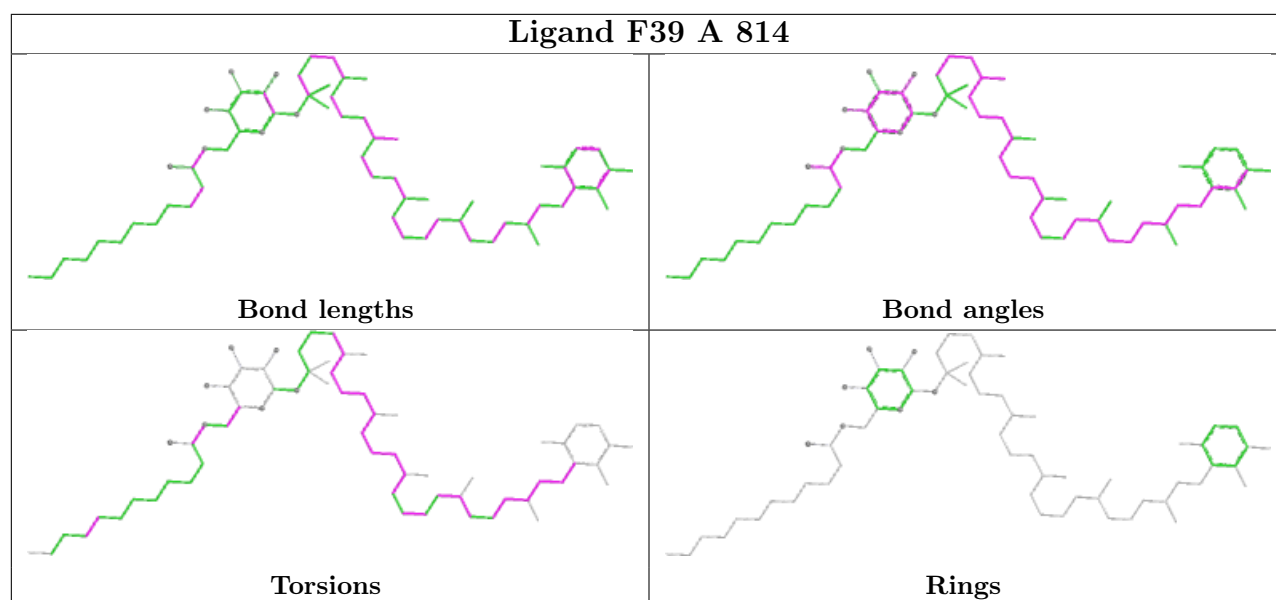
Ligand BCL U 408 (B)

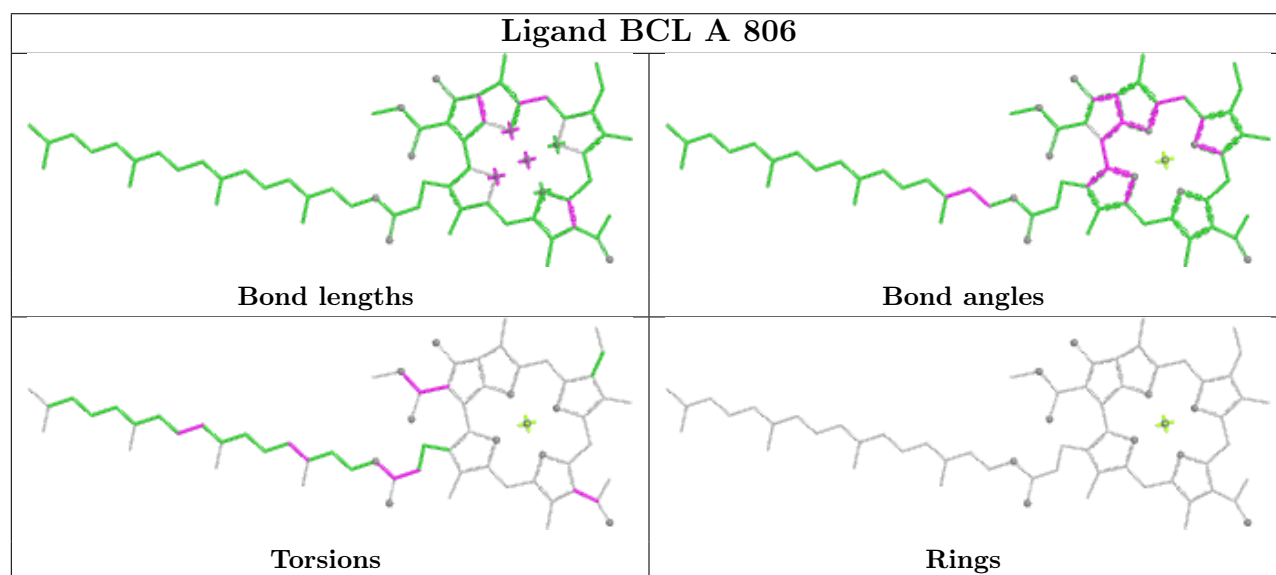
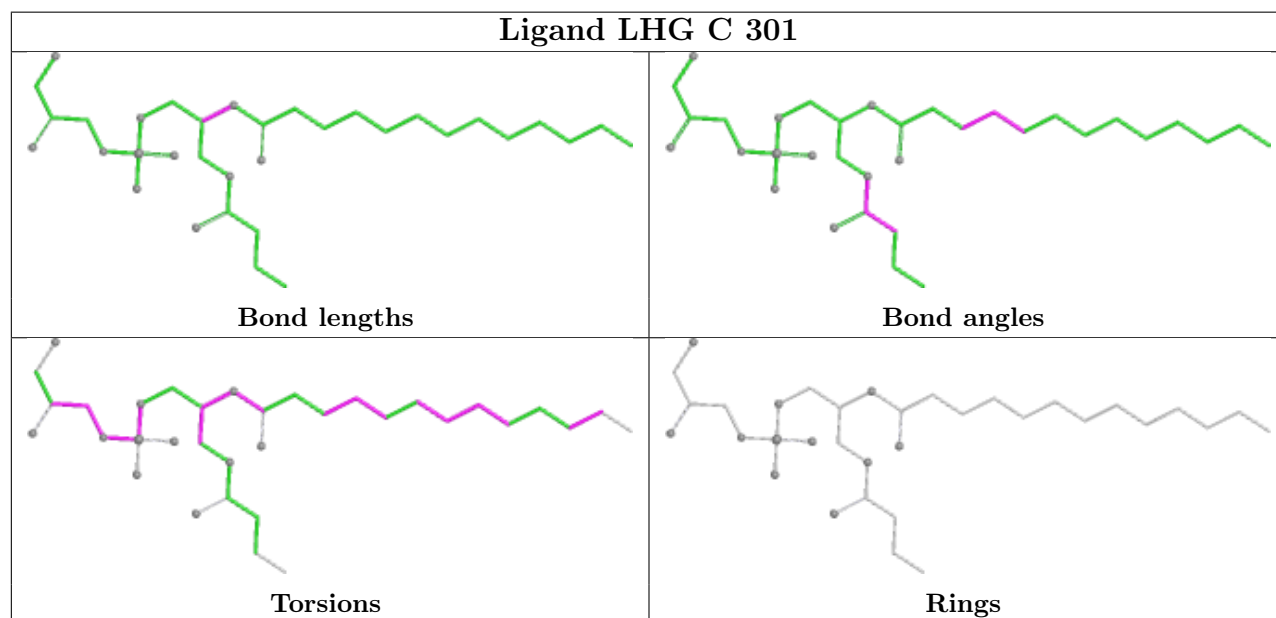
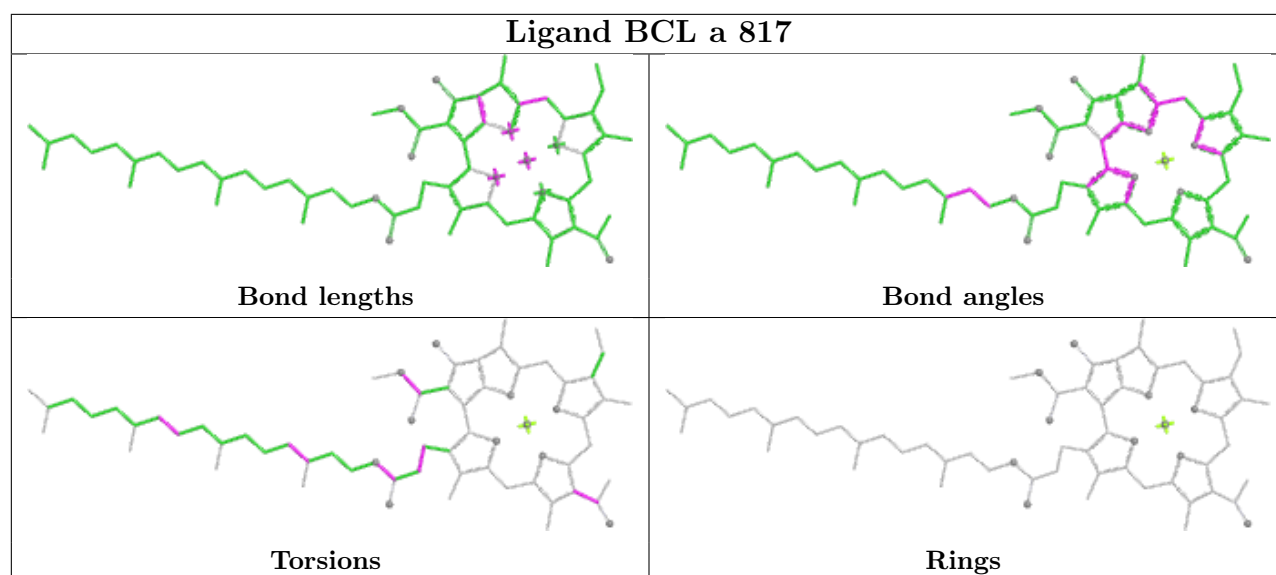


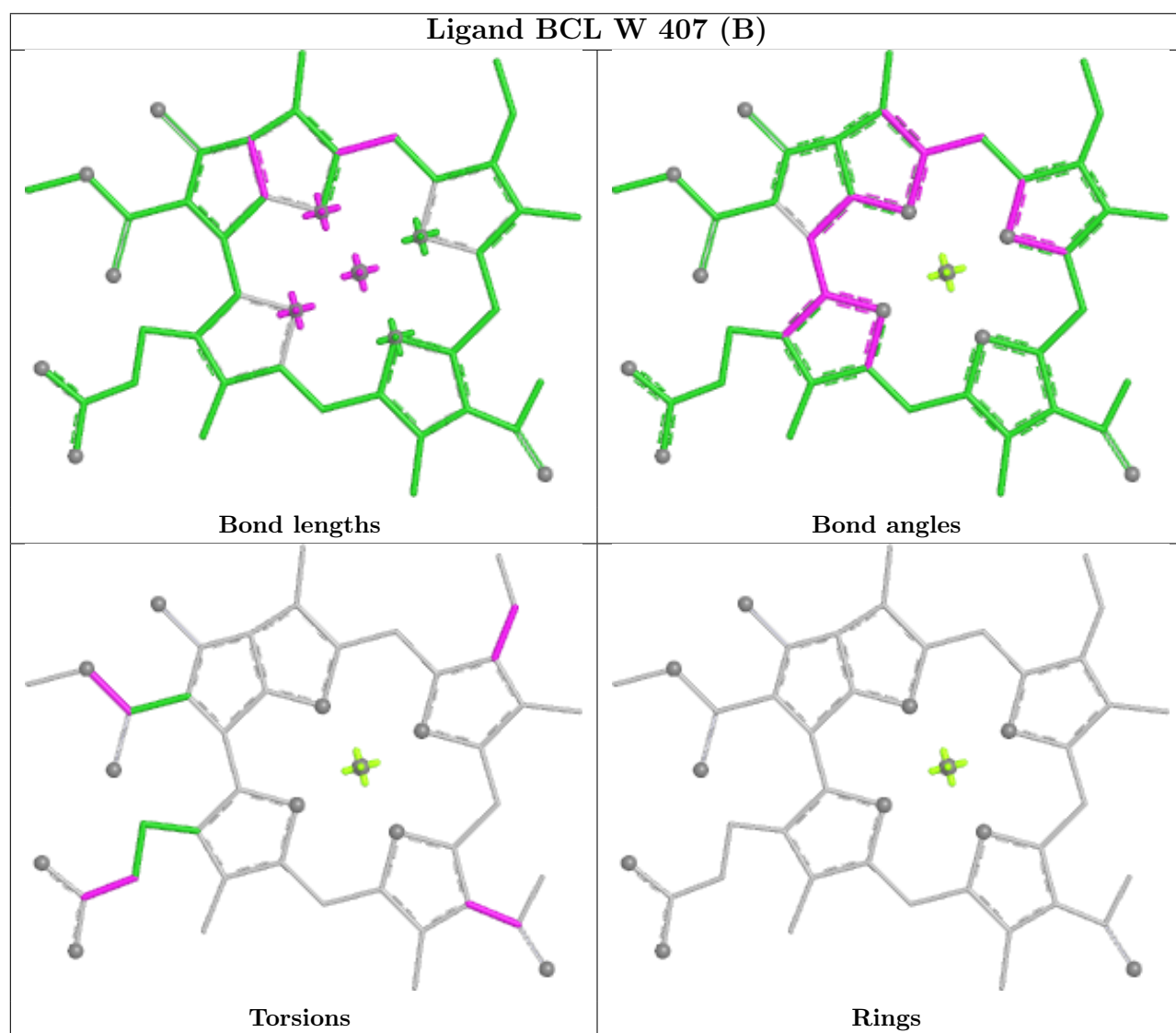
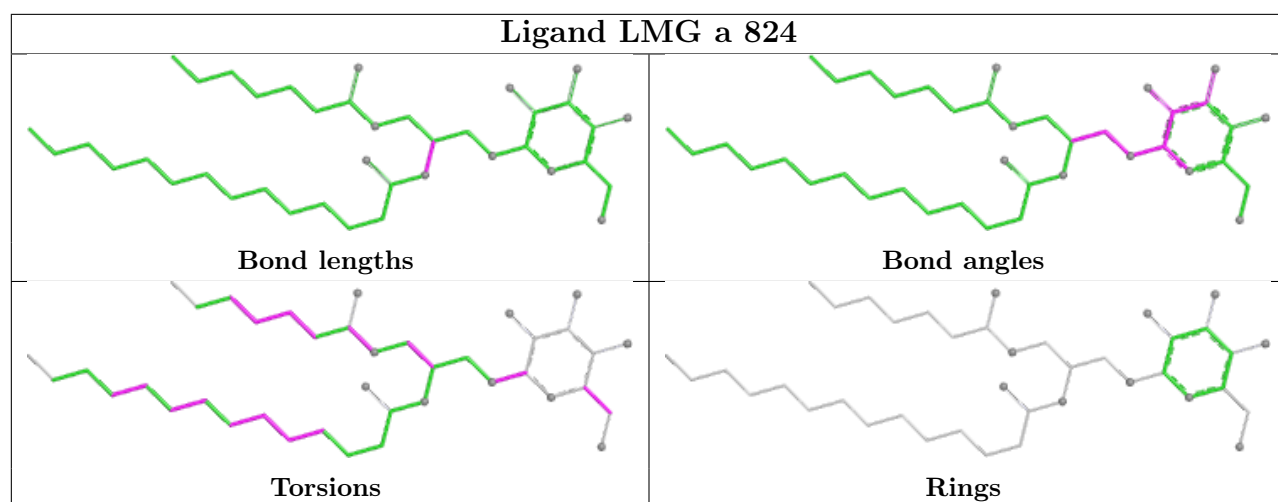
Ligand BCL A 809

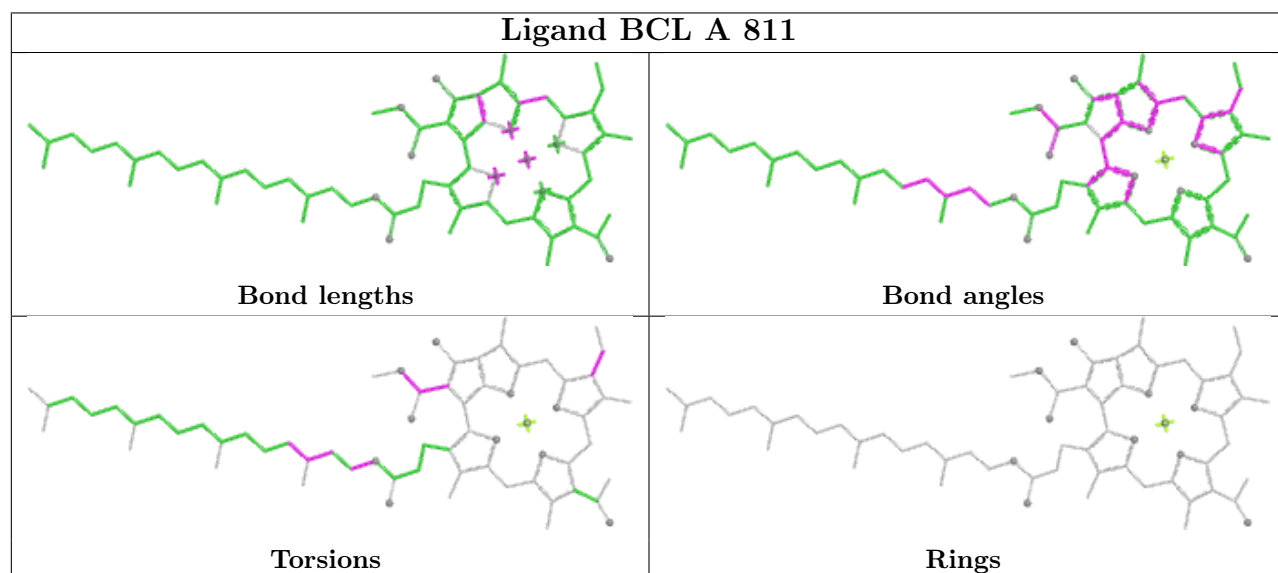
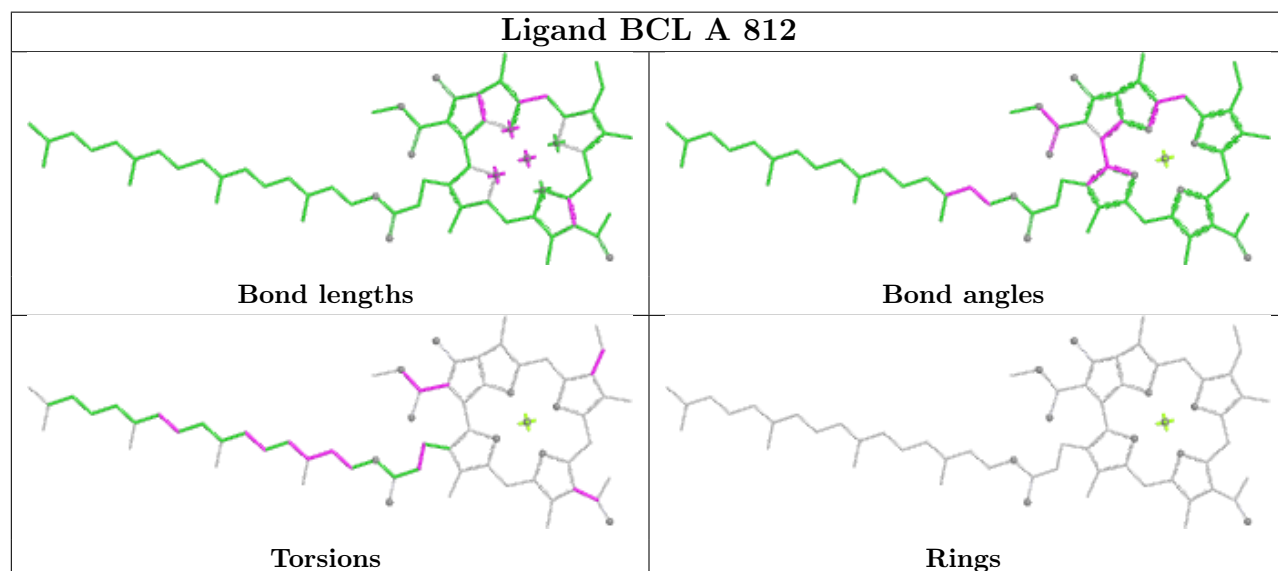
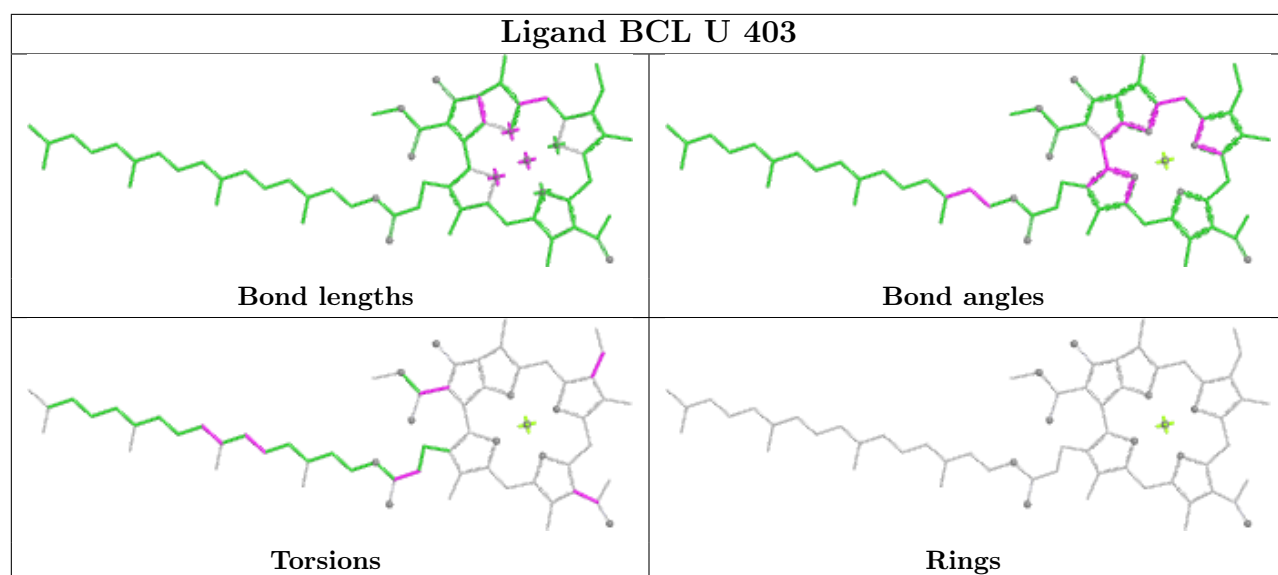




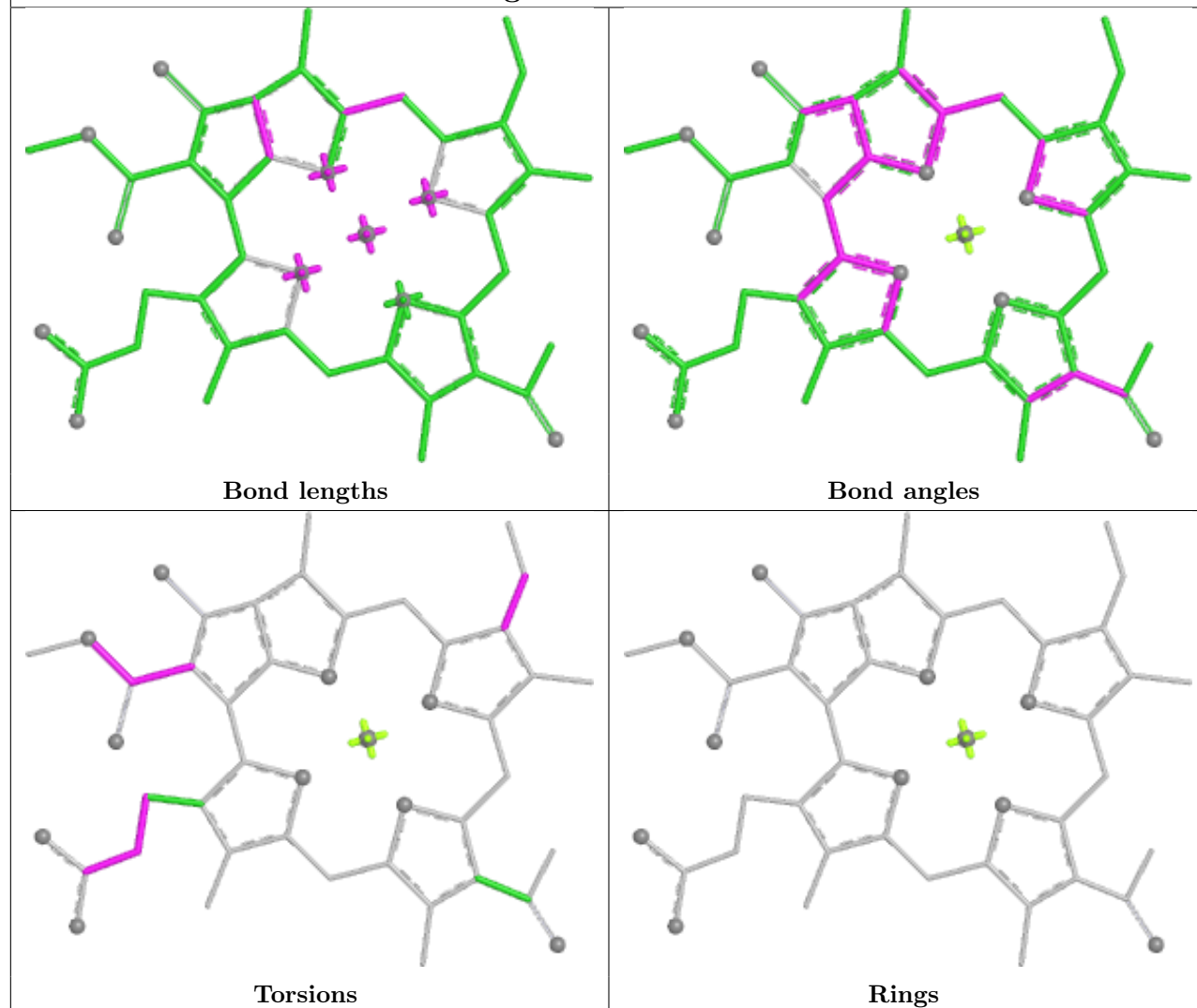




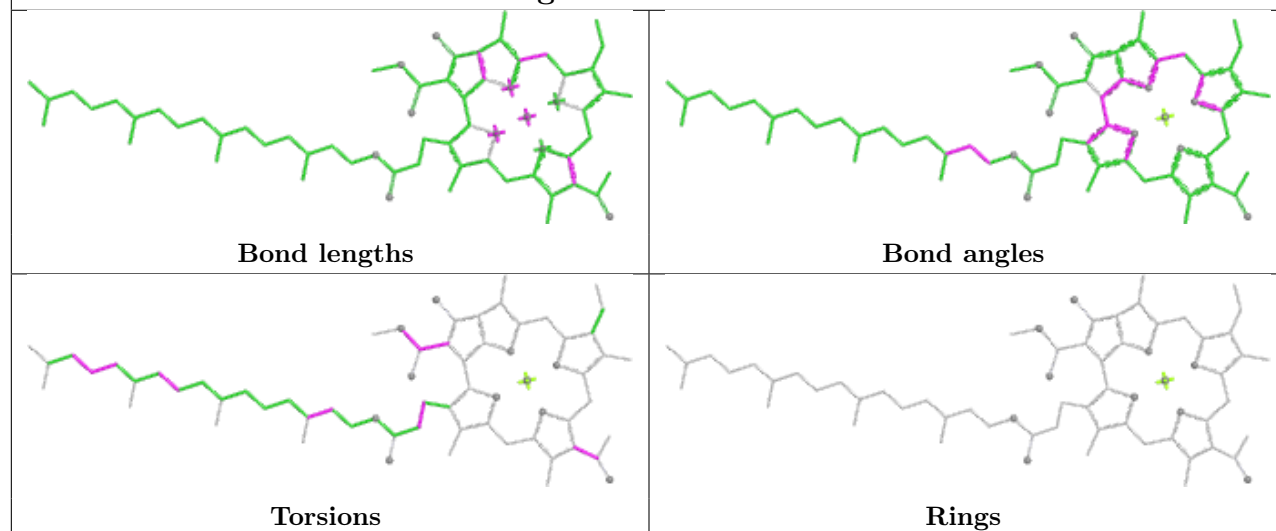


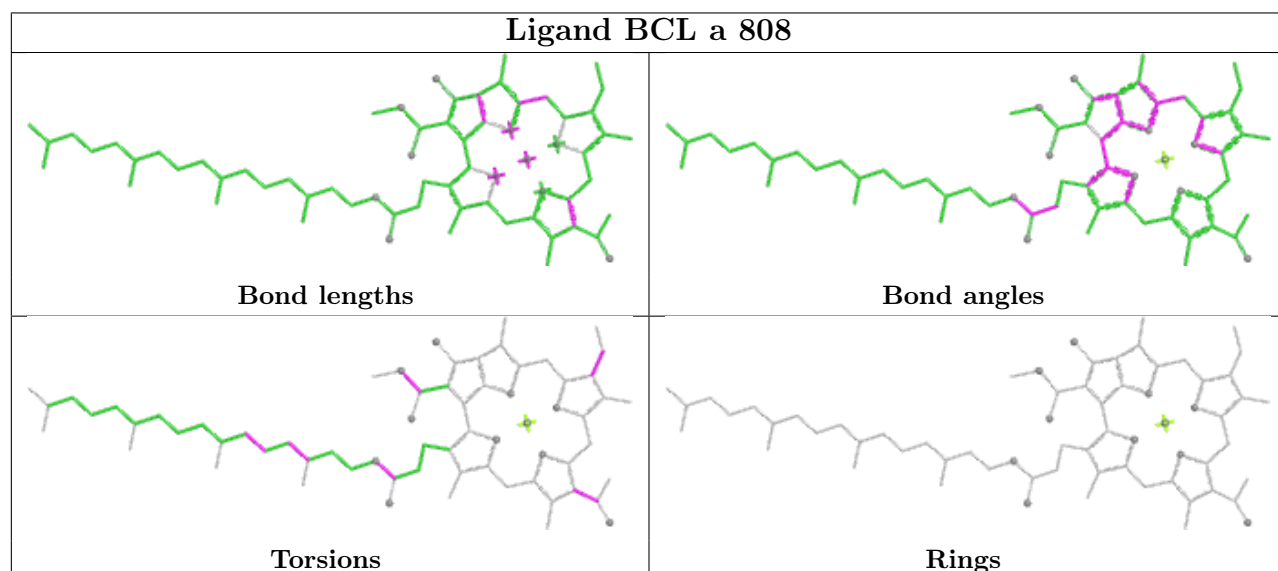
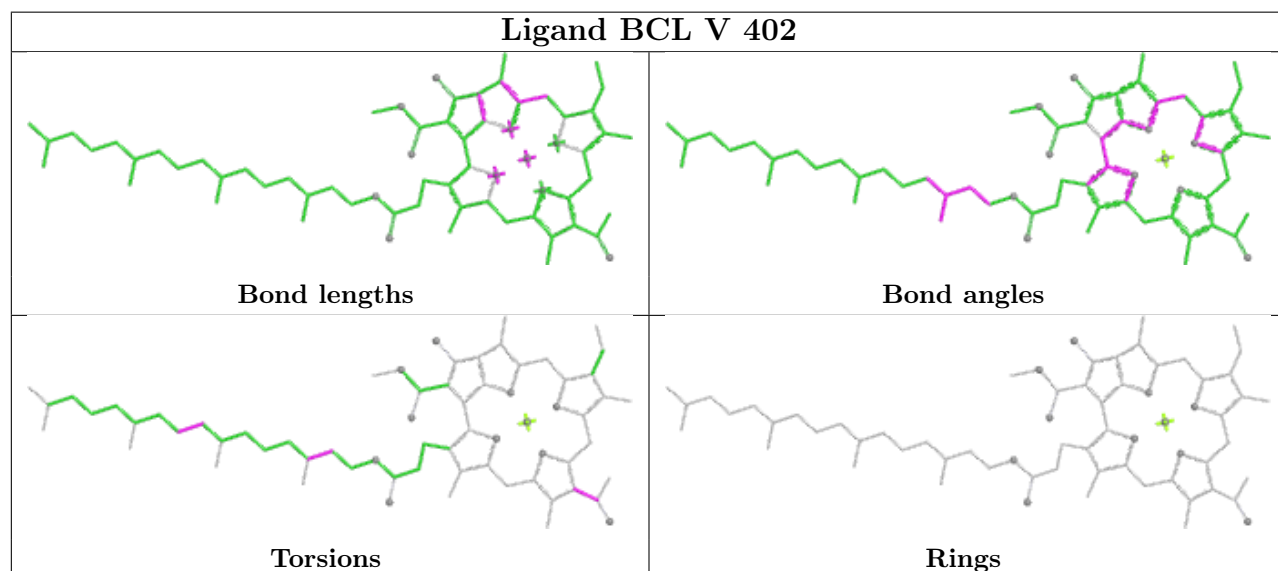
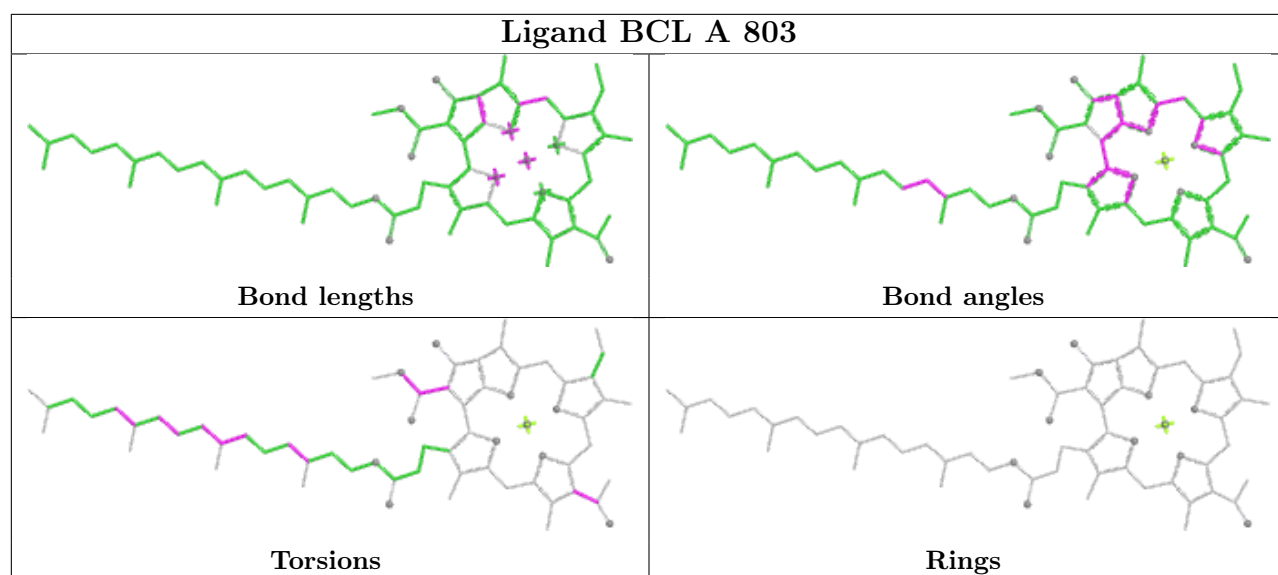


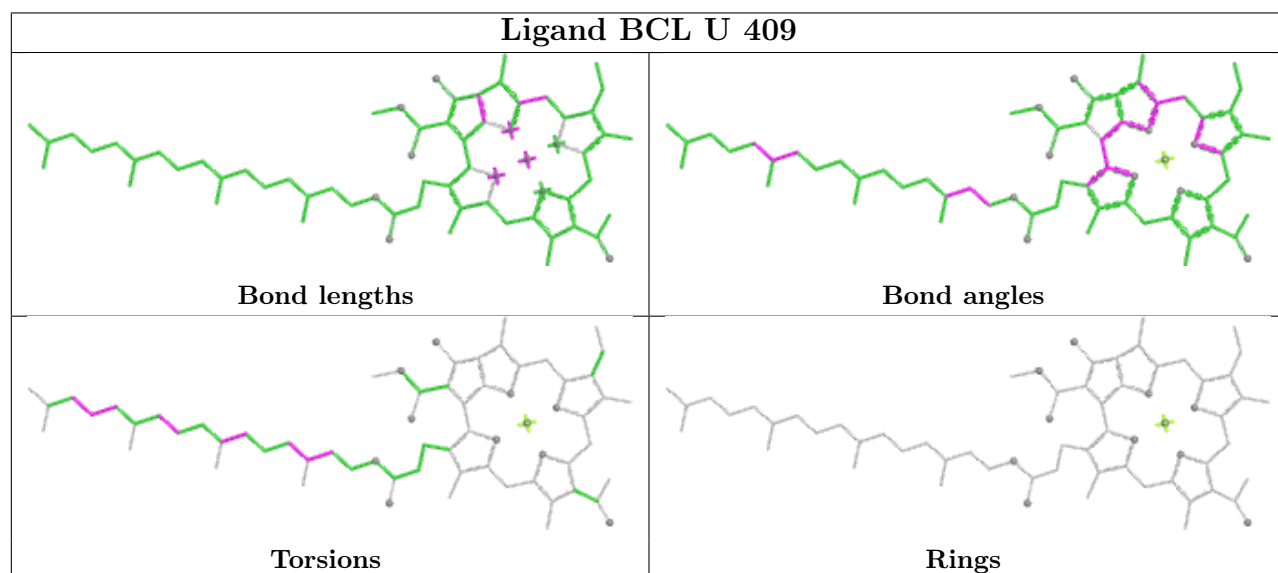
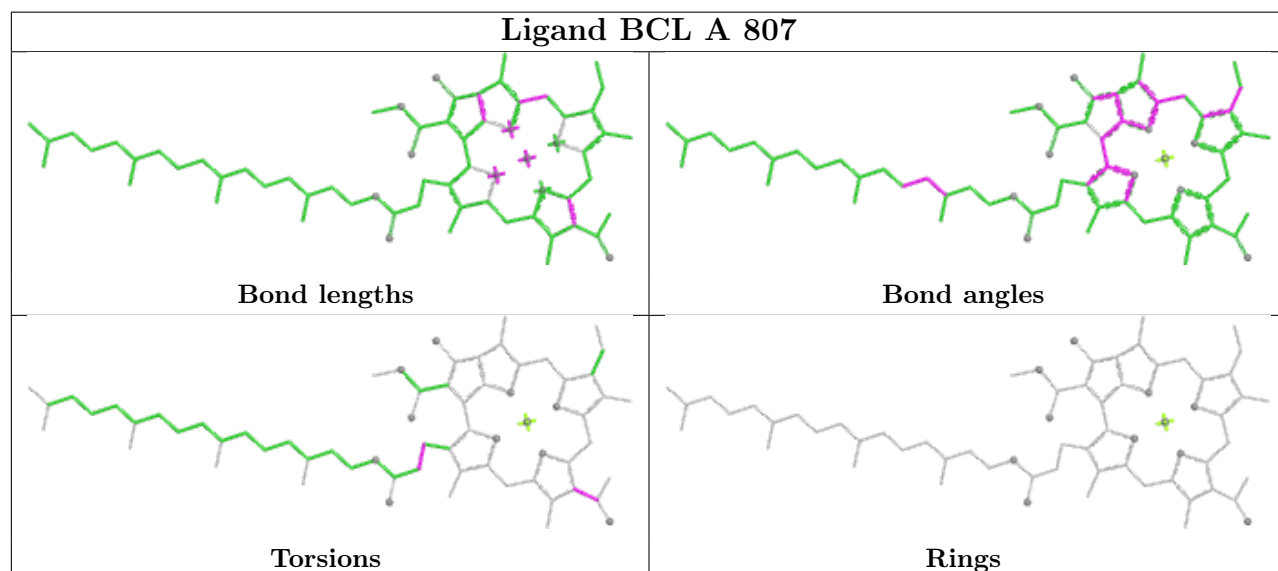
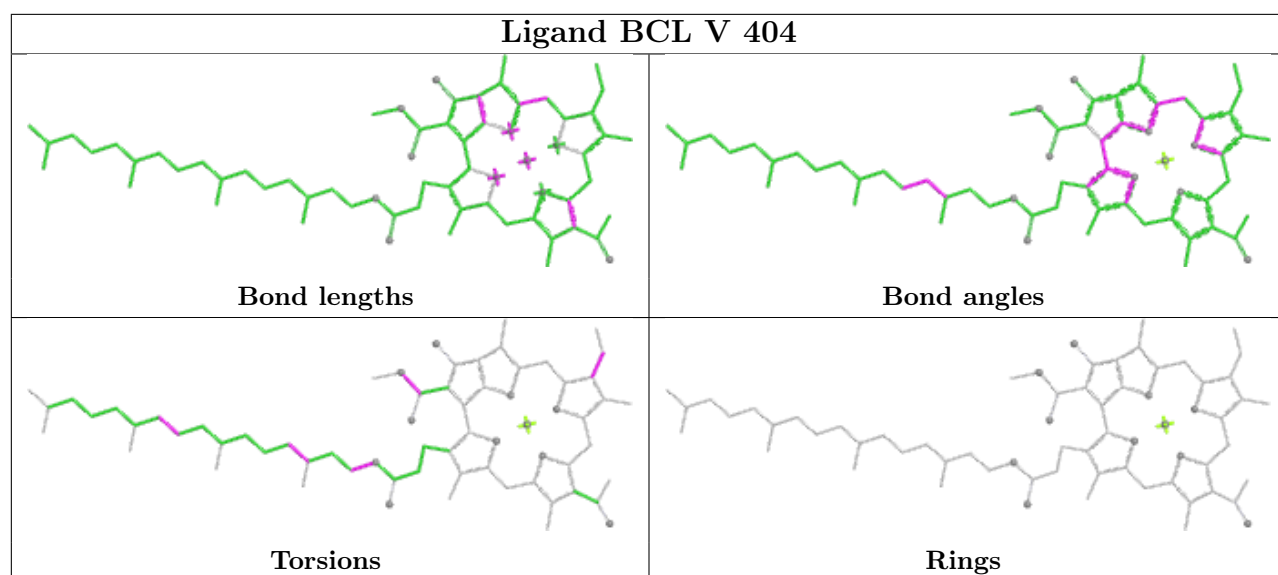
Ligand BCL a 811



Ligand BCL a 816







5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

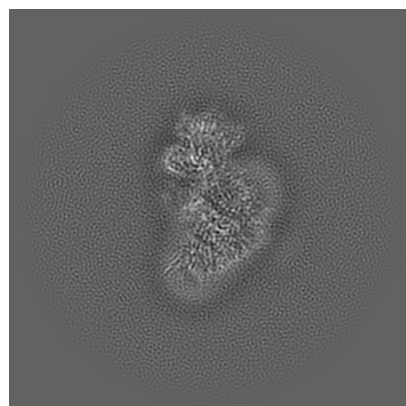
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26469. These allow visual inspection of the internal detail of the map and identification of artifacts.

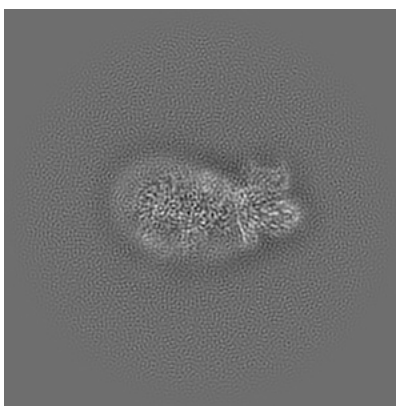
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

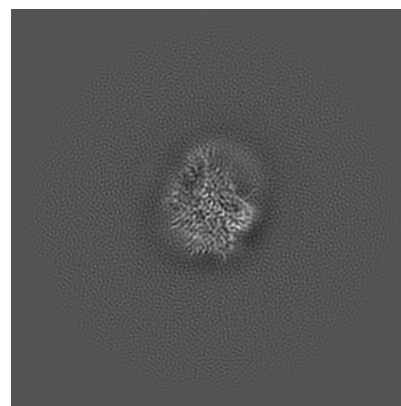
6.1.1 Primary map



X

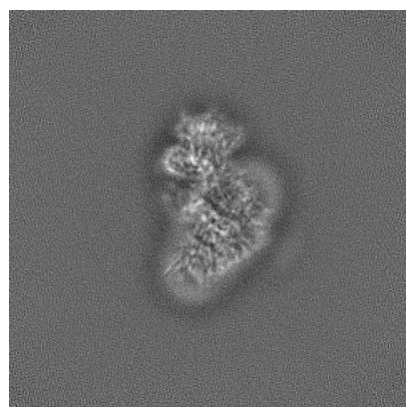


Y

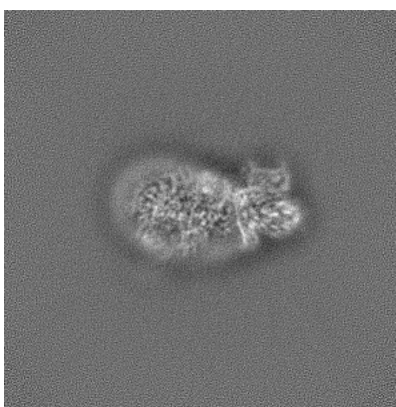


Z

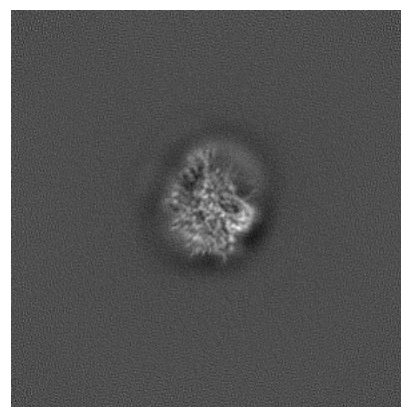
6.1.2 Raw map



X



Y

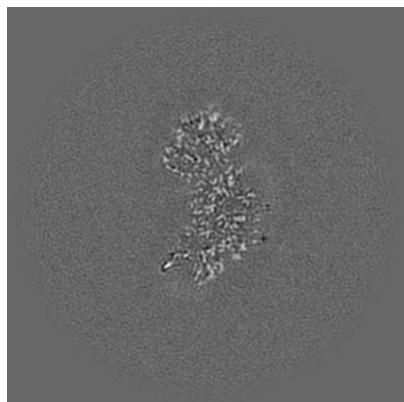


Z

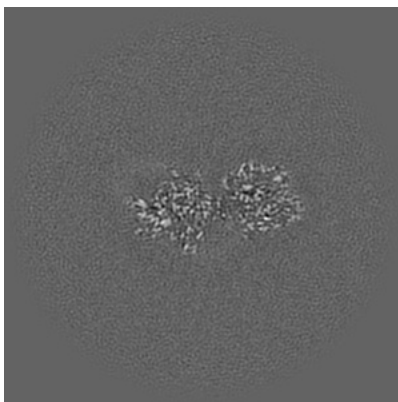
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

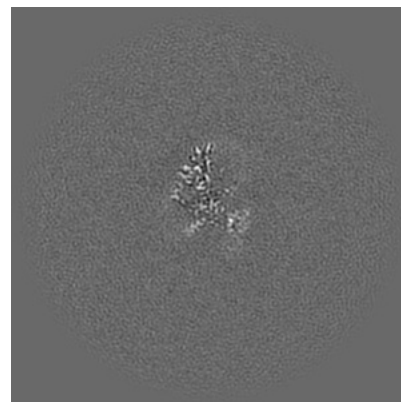
6.2.1 Primary map



X Index: 180

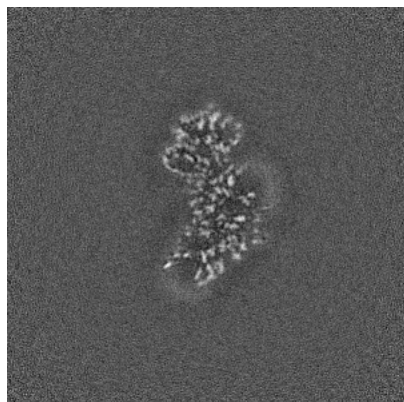


Y Index: 180

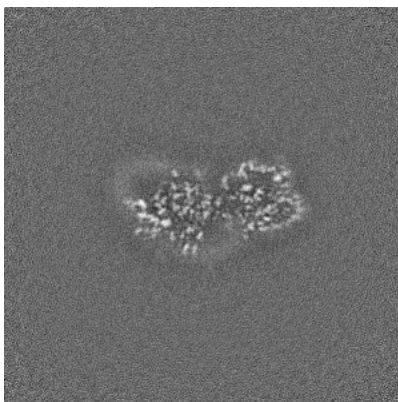


Z Index: 180

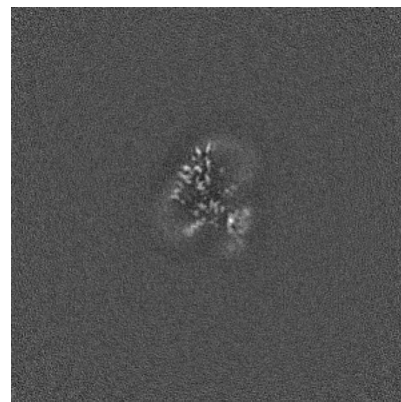
6.2.2 Raw map



X Index: 180



Y Index: 180

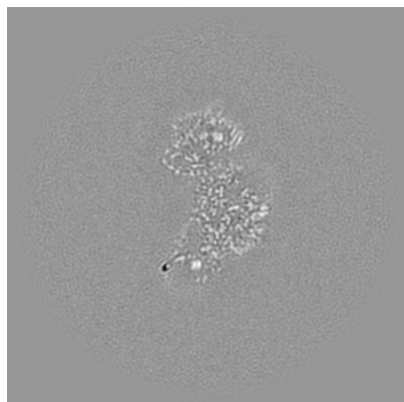


Z Index: 180

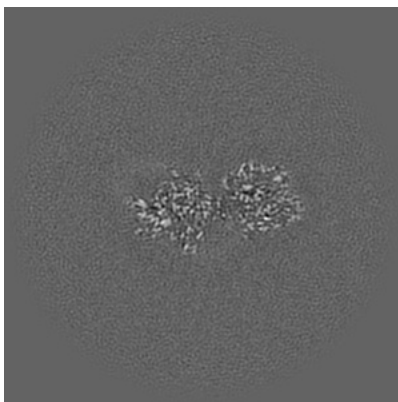
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

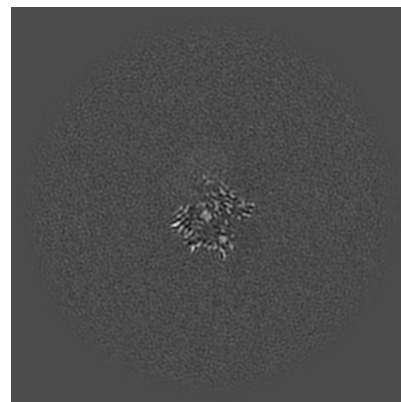
6.3.1 Primary map



X Index: 176

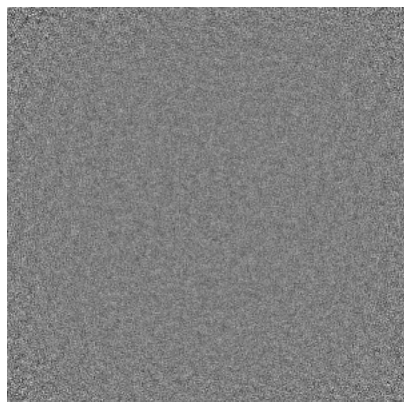


Y Index: 180

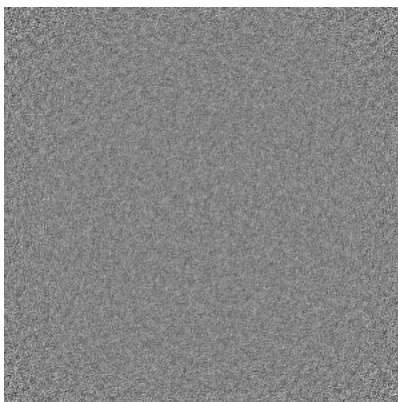


Z Index: 217

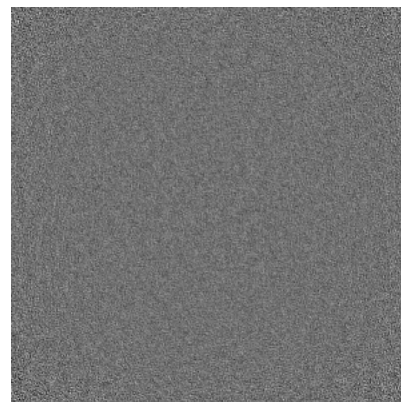
6.3.2 Raw map



X Index: 0



Y Index: 0

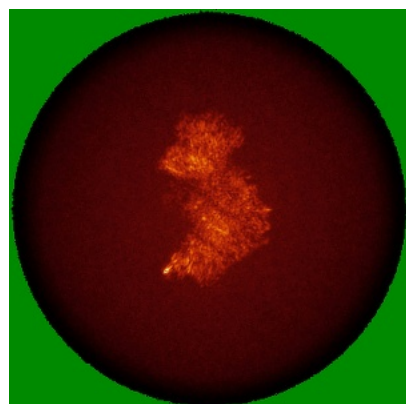


Z Index: 359

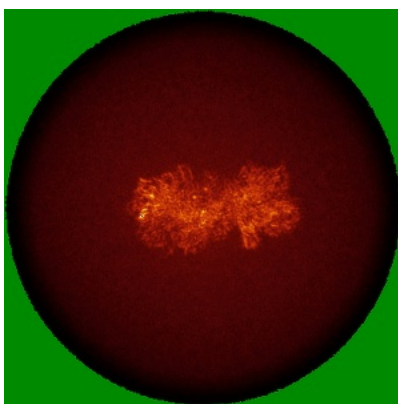
The images above show the largest variance slices of the map in three orthogonal directions.

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

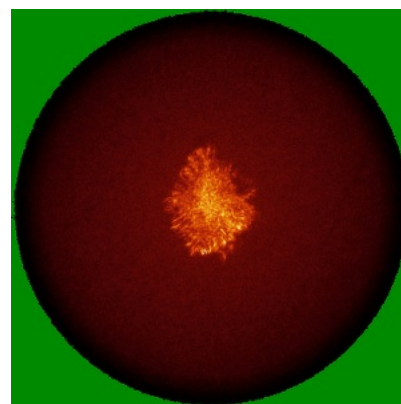
6.4.1 Primary map



X

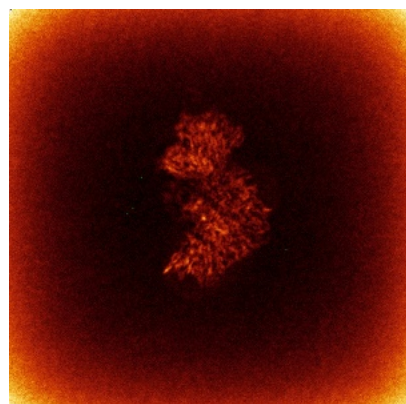


Y

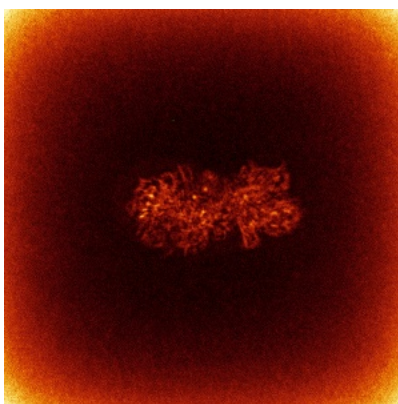


Z

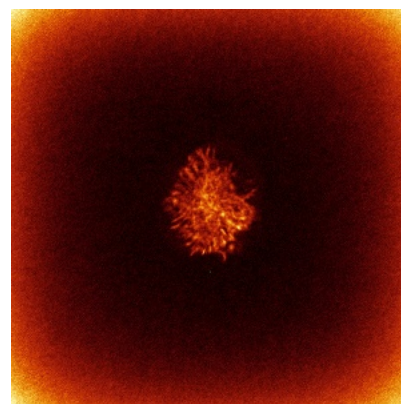
6.4.2 Raw map



X



Y

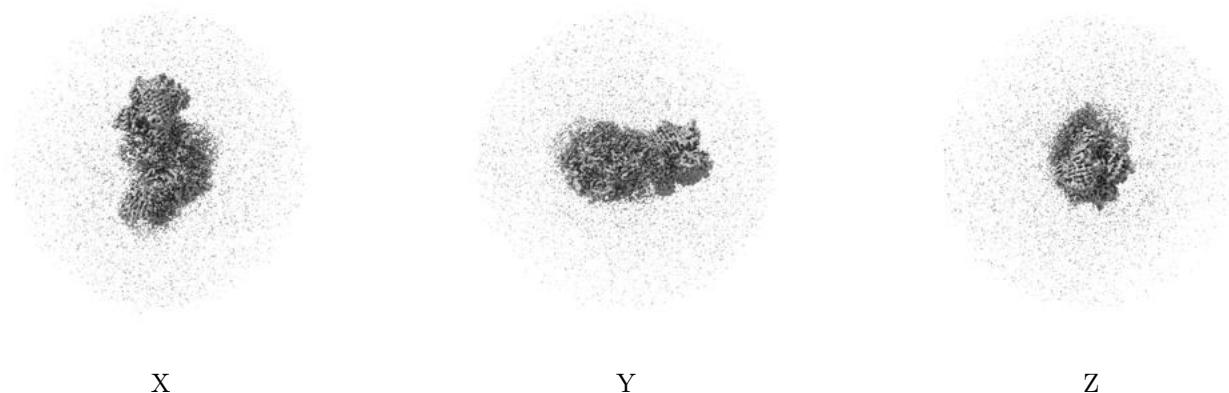


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.352. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

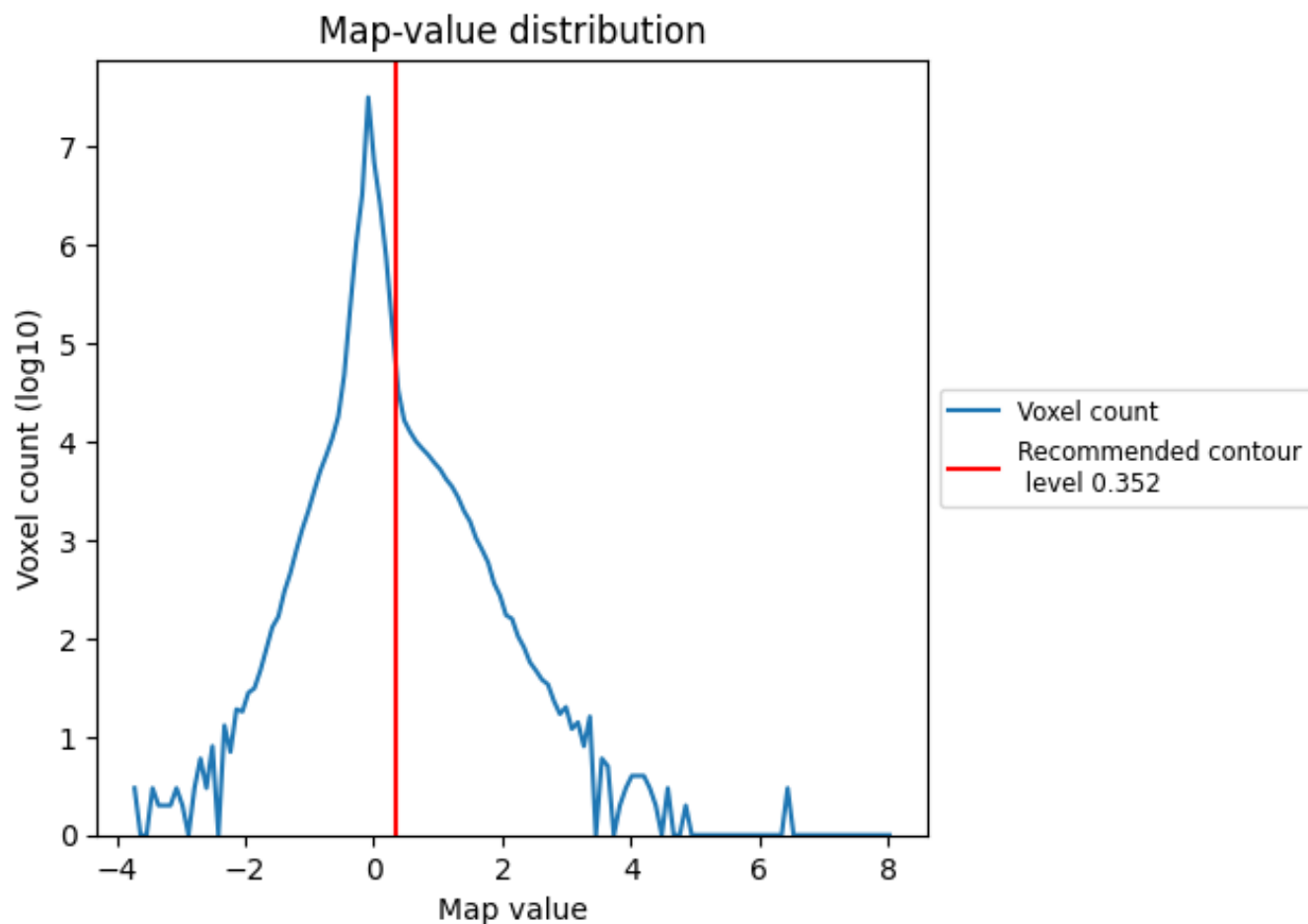
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

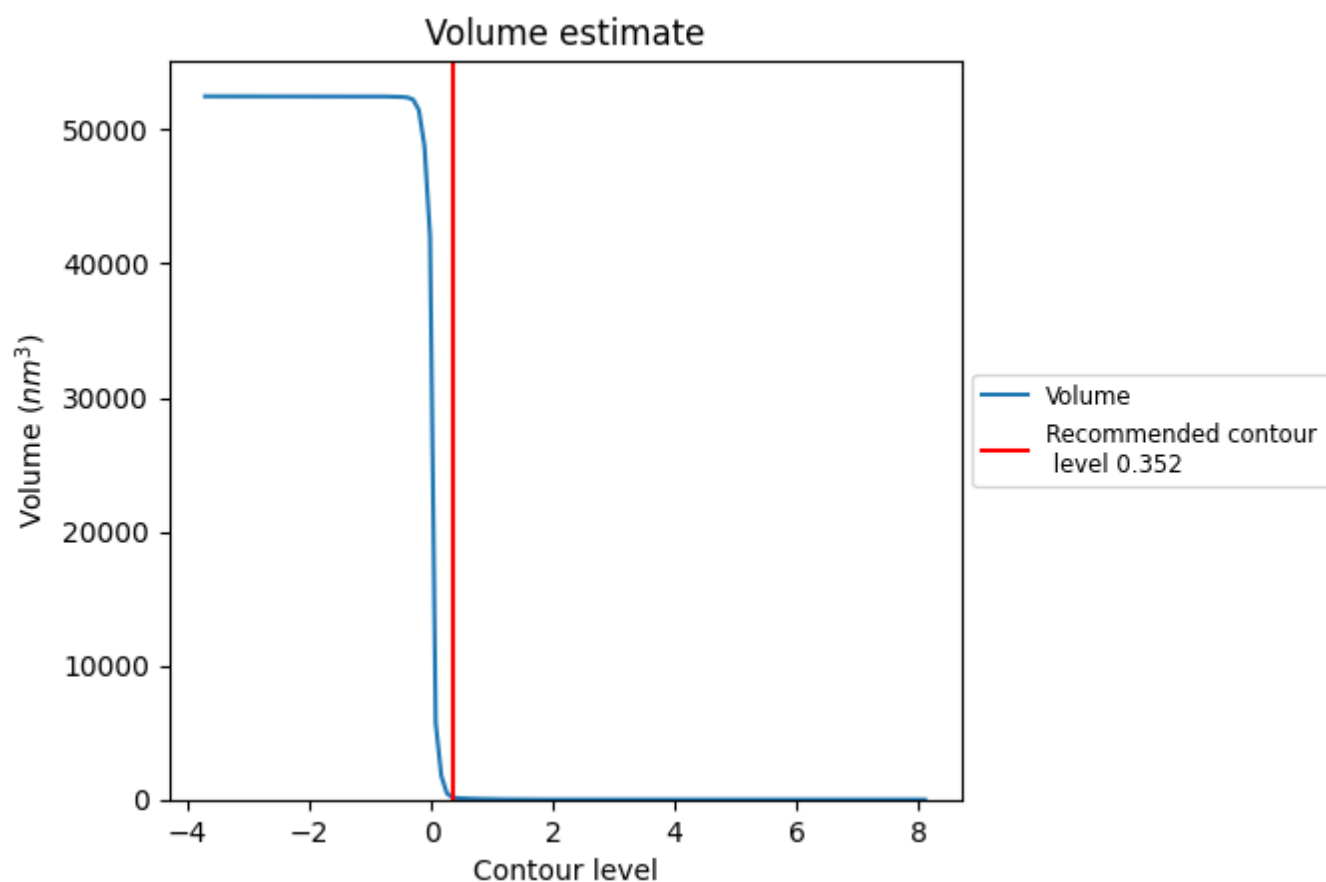
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

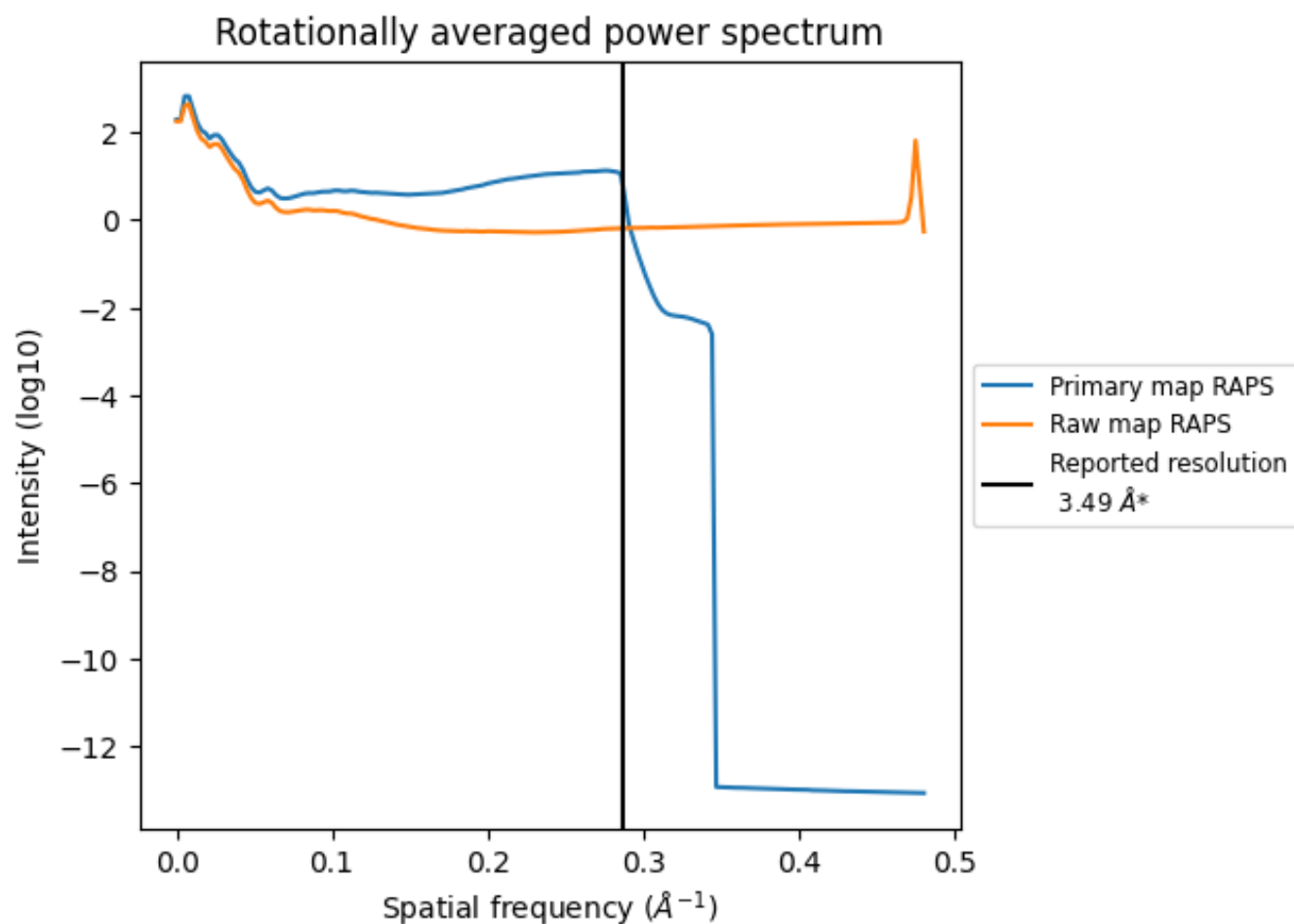
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 160 nm^3 ; this corresponds to an approximate mass of 145 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 ⓘ

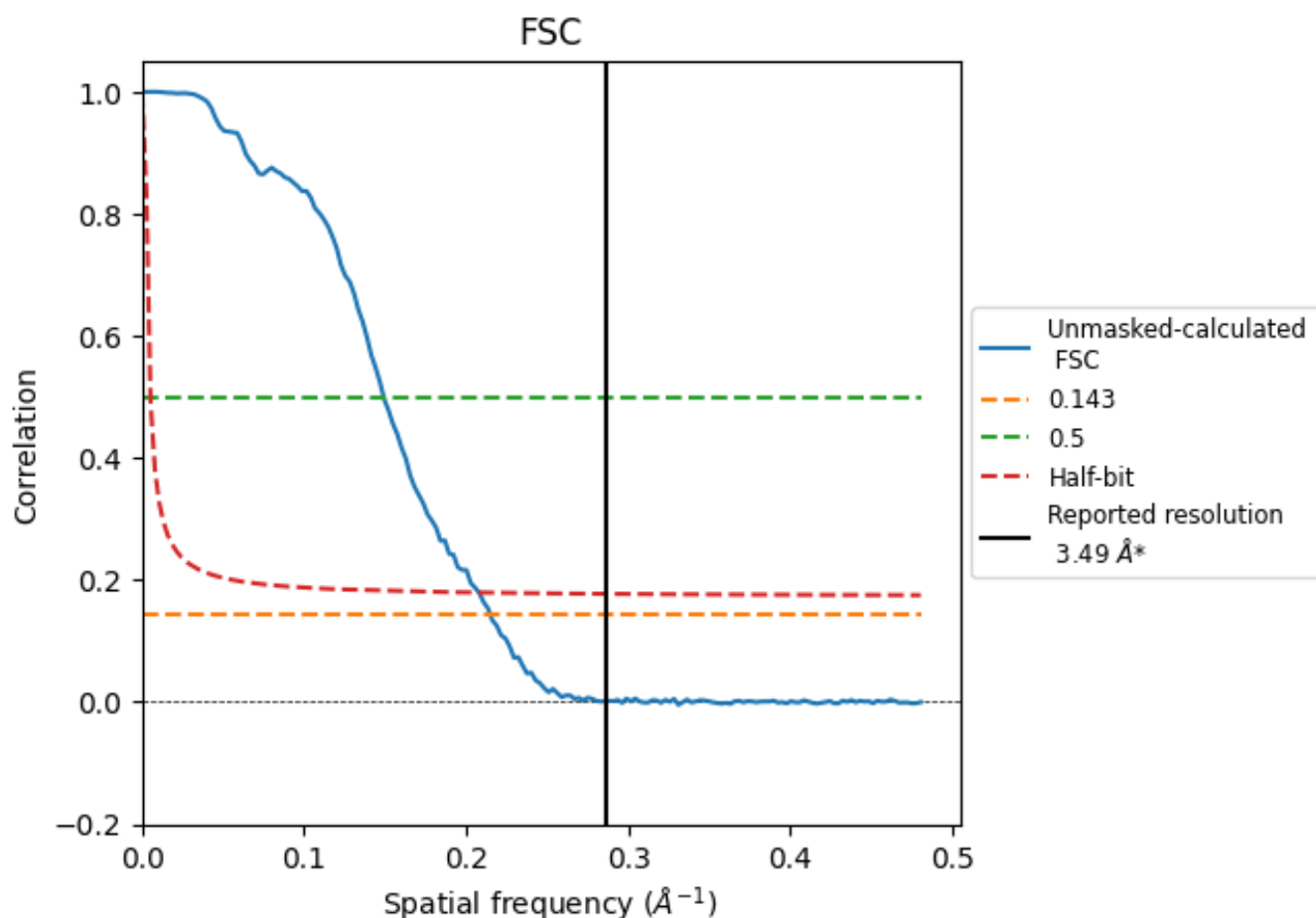


*Reported resolution corresponds to spatial frequency of 0.287 $\text{\AA}^{-1}$

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 0.287 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

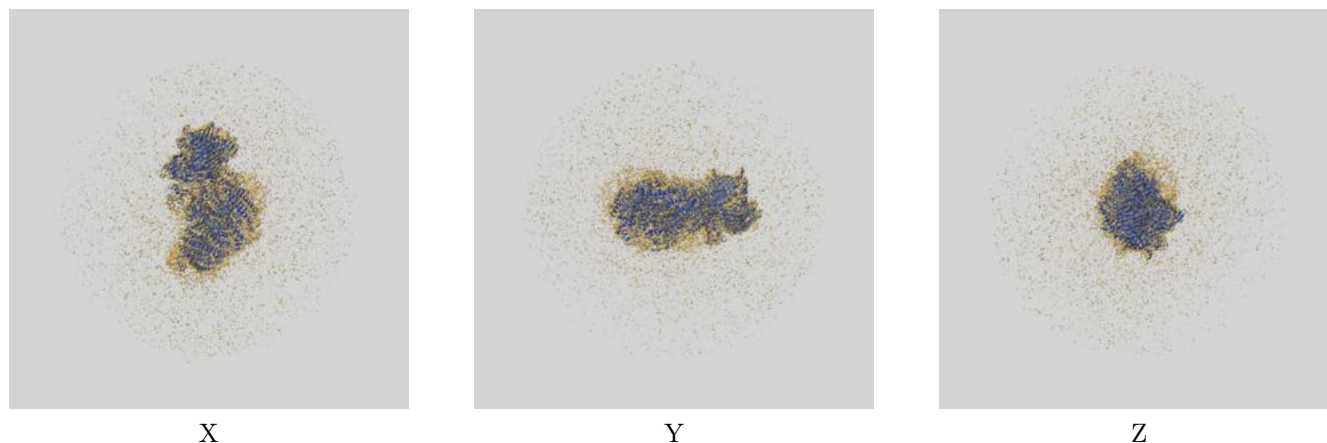
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.49	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.65	6.71	4.81

*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 4.65 differs from the reported value 3.49 by more than 10 %

9 Map-model fit [i](#)

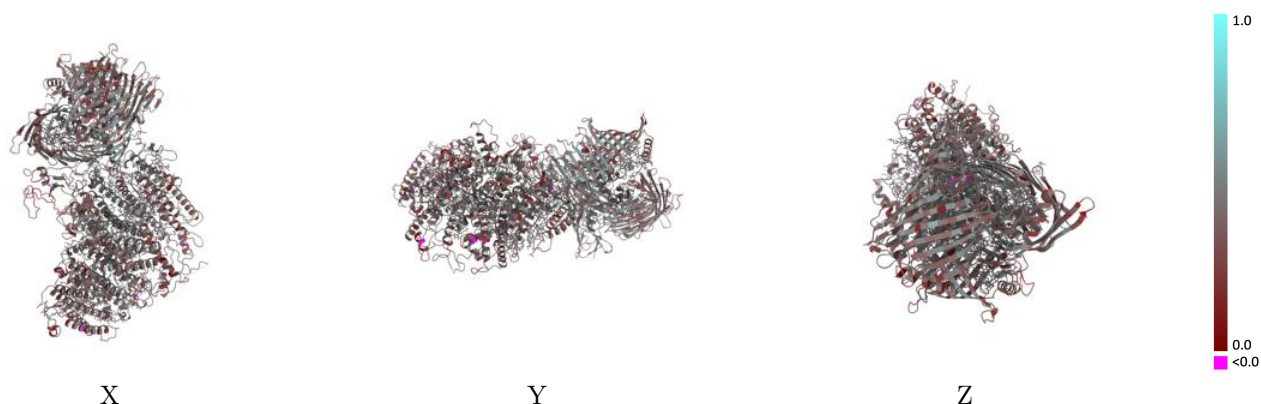
This section contains information regarding the fit between EMDB map EMD-26469 and PDB model 7UEA. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



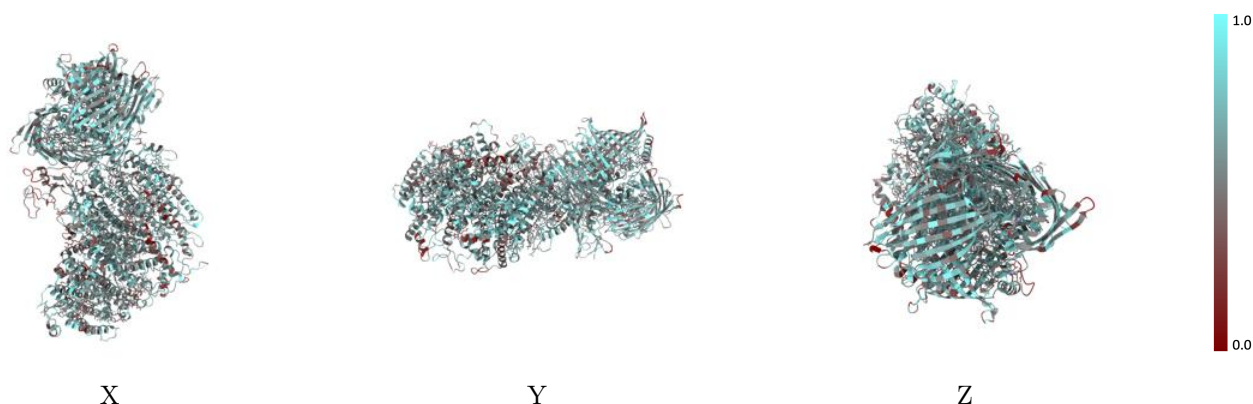
The images above show the 3D surface view of the map at the recommended contour level 0.352 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



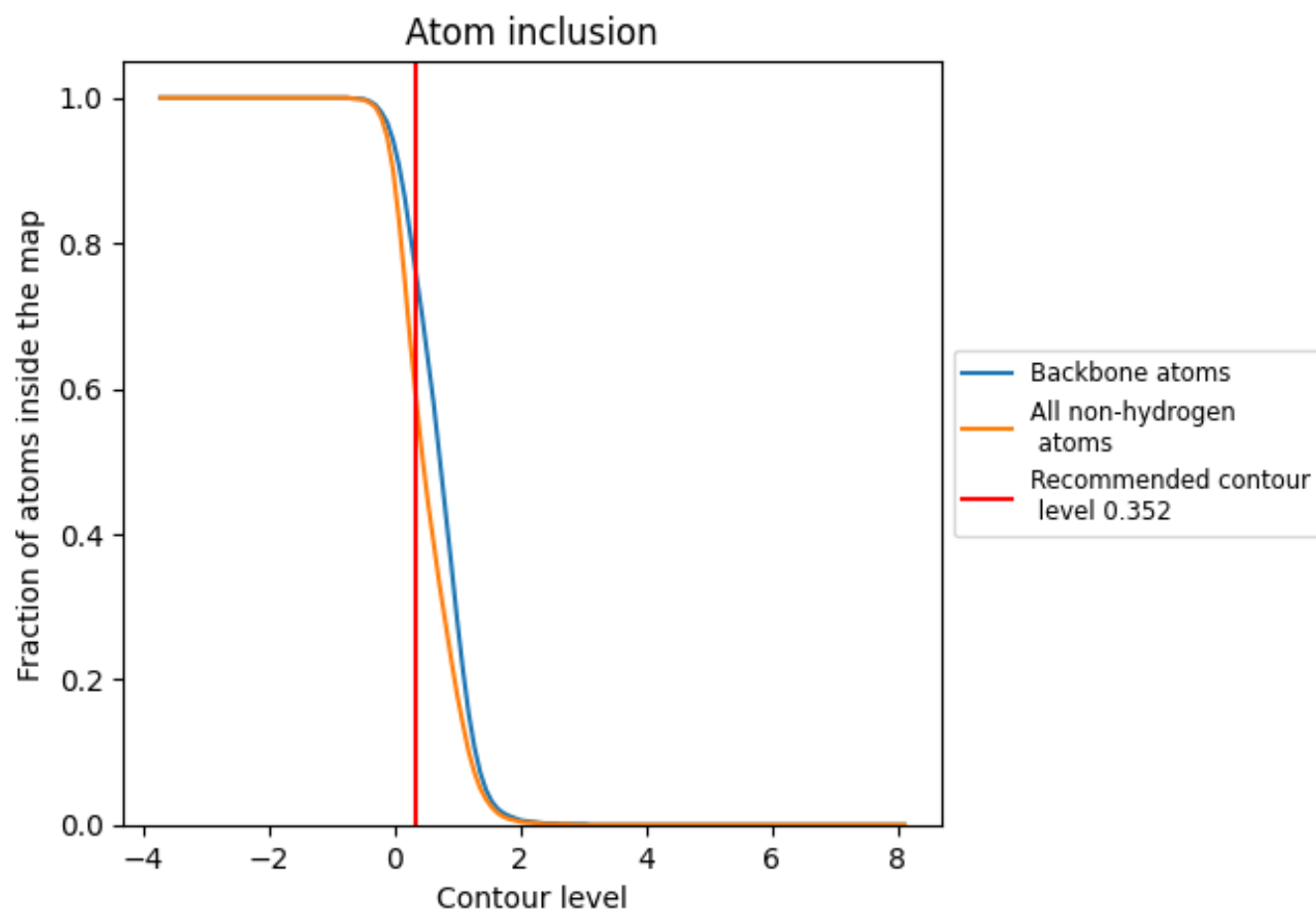
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.352).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 58% 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 (0.352) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5810	0.4060
A	0.6170	0.4250
B	0.5290	0.3720
C	0.3460	0.2920
D	0.3510	0.3080
U	0.6050	0.4160
V	0.6160	0.4350
W	0.6010	0.4070
a	0.5980	0.4080
c	0.4390	0.3380

1.0

0.0

<0.0