



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 09:58 AM EDT

PDB ID : 7UEB / pdb_00007ueb
EMDB ID : EMD-26471
Title : Photosynthetic assembly of Chlorobaculum tepidum (RC-FMO2)
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 : 3.08 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:

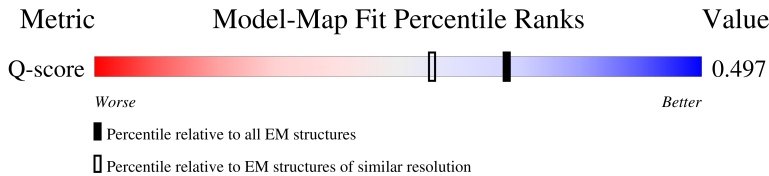
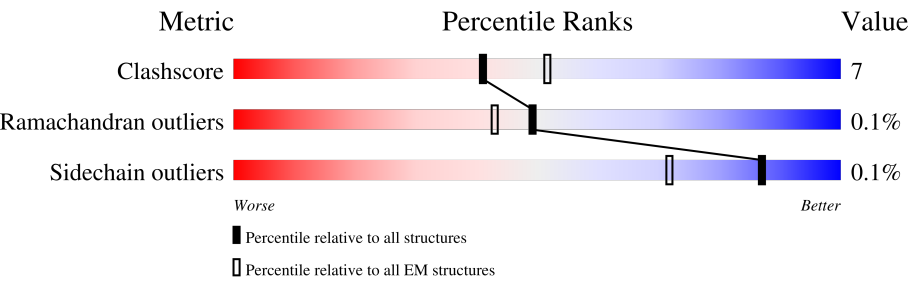
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.08 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.



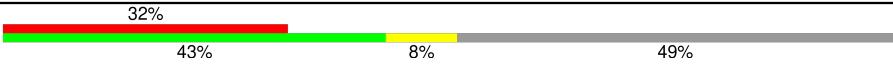
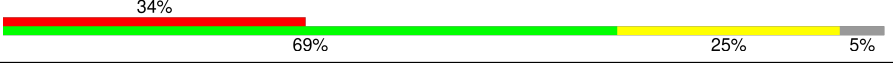
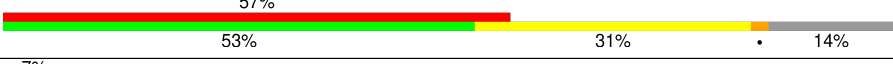
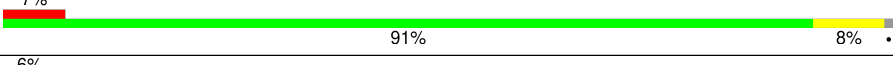
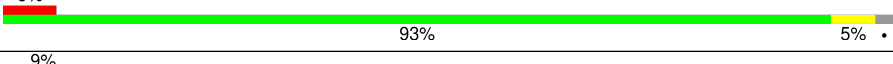
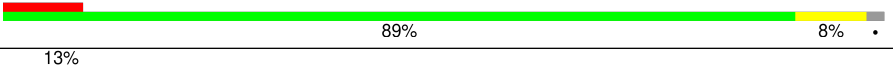
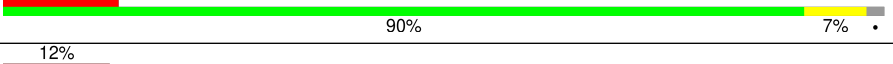
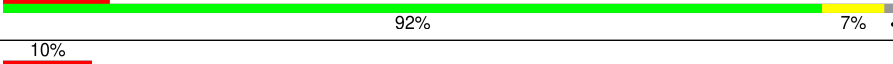
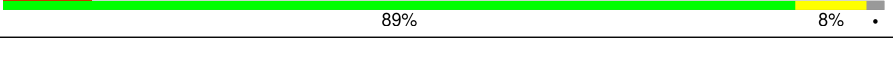
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14000 (2.58 - 3.58)

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	73%16%11%
1	a	731	75%14%11%
2	B	231	7%40%8%51%
3	C	206	9%50%9%41%

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Mol	Chain	Length	Quality of chain
3	c	206	
4	D	143	
5	E	59	
6	F	58	
7	U	366	
7	V	366	
7	W	366	
7	X	366	
7	Y	366	
7	Z	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
8	GS0	A	801	X	-	-	-
8	GS0	a	802	X	-	-	-
9	CLA	A	802	X	-	X	-
9	CLA	A	826	X	-	X	-
9	CLA	A	827	X	-	X	-
9	CLA	a	801	X	-	X	-

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 37570 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	650	Total	C	N	O	S	0	0
			5197	3469	827	875	26		
1	a	652	Total	C	N	O	S	0	0
			5214	3478	832	878	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	114	Total	C	N	O	S	0	0
			887	564	148	166	9		

- Molecule 3 is a protein called Cytochrome c.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	122	Total	C	N	O	S	0	0
			950	637	149	157	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	101	Total	C	N	O	S	0	0
			823	523	145	151	4		

- Molecule 5 is a protein called PscE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	56	Total	C	N	O	S	0	0
			441	280	75	83	3		

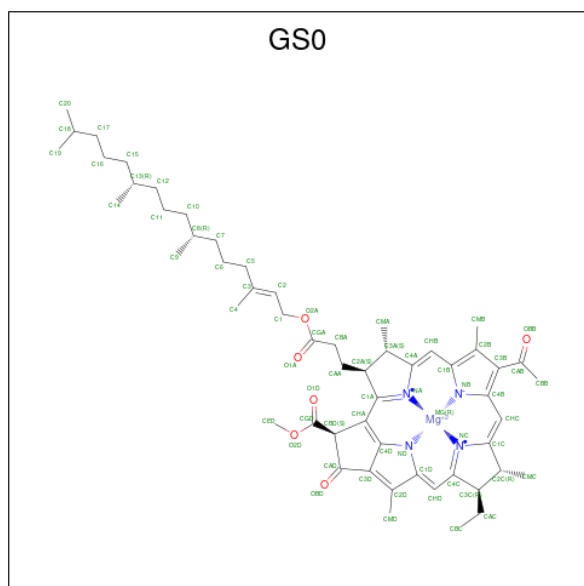
- Molecule 6 is a protein called PscF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	50	Total	C	N	O	S	0	0
			379	253	62	61	3		

- Molecule 7 is a protein called Bacteriochlorophyll a protein.

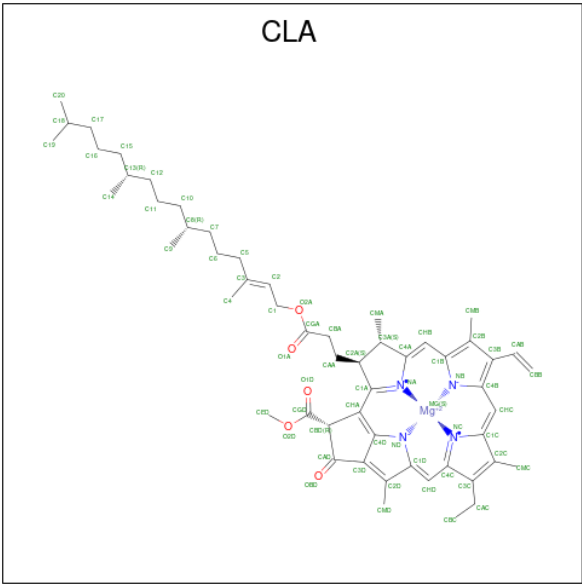
Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	363	Total	C	N	O	S	0	0
			2826	1792	502	525	7		
7	V	360	Total	C	N	O	S	0	0
			2805	1778	499	521	7		
7	W	358	Total	C	N	O	S	0	0
			2789	1770	496	516	7		
7	X	357	Total	C	N	O	S	0	0
			2782	1765	495	515	7		
7	Y	360	Total	C	N	O	S	0	0
			2805	1778	499	521	7		
7	Z	358	Total	C	N	O	S	0	0
			2789	1770	496	516	7		

- Molecule 8 is Bacteriochlorophyll A isomer (CCD ID: GS0) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



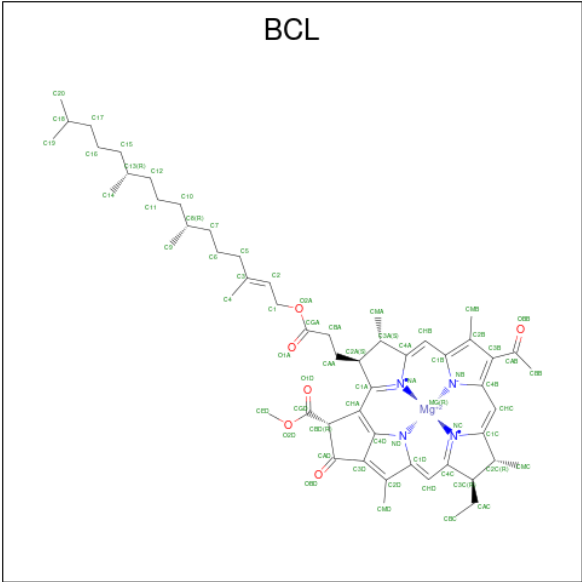
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 9 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



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

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

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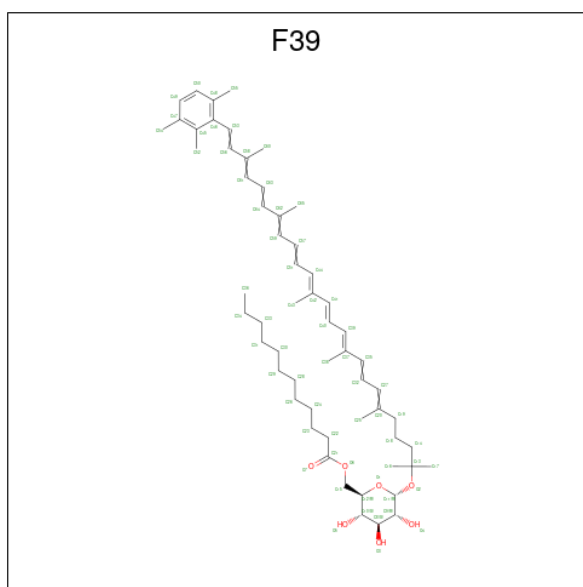
Mol	Chain	Residues	Atoms					AltConf
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10	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	V	1	Total 46	C 35	Mg 1	N 4	O 6	1
10	W	1	Total 66	C 55	Mg 1	N 4	O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

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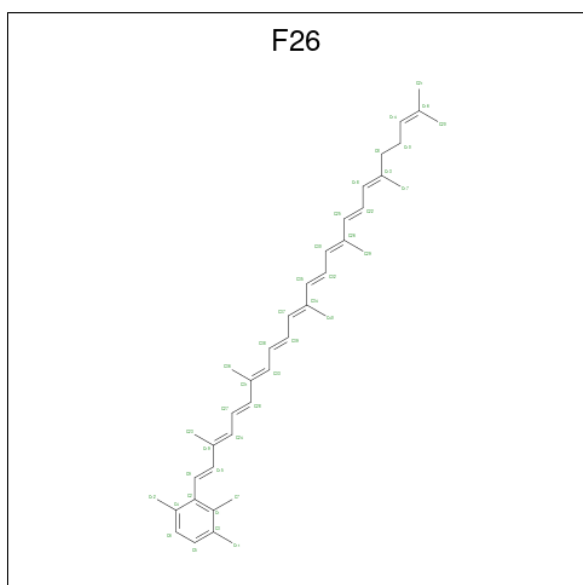
Mol	Chain	Residues	Atoms					AltConf
10	X	1	Total	C	Mg	N	O	1
			46	35	1	4	6	
10	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	Z	1	Total	C	Mg	N	O	1
			46	35	1	4	6	

- Molecule 11 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).



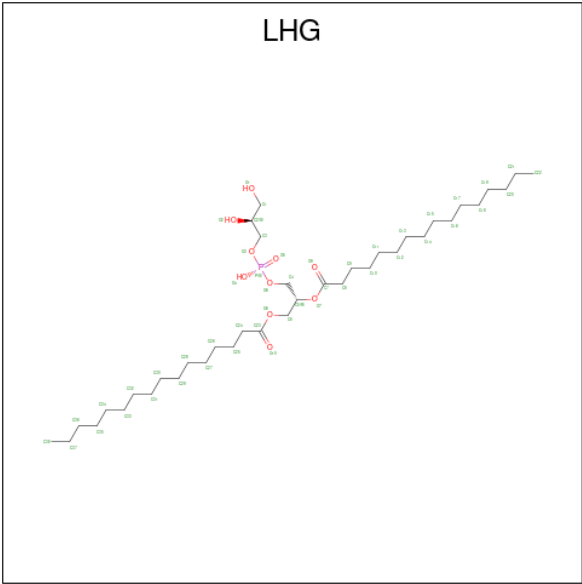
Mol	Chain	Residues	Atoms			AltConf
11	A	1	Total	C	O	0
			65	58	7	
11	a	1	Total	C	O	0
			65	58	7	
11	C	1	Total	C	O	0
			65	58	7	

- Molecule 12 is 2-[(1E,3E,5E,7E,9E,11E,13E,15E,17E,19E)-3,7,12,16,20,24-hexamethylpentacos-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
12	A	1	Total	C	0
			40	40	
12	a	1	Total	C	0
			40	40	
12	a	1	Total	C	0
			40	40	

- Molecule 13 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



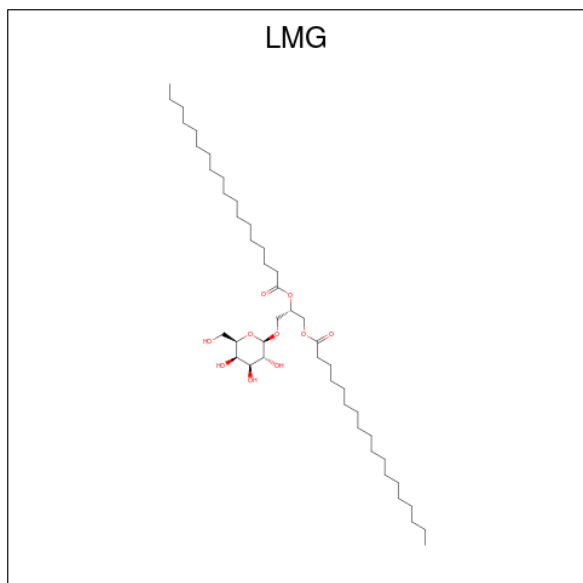
Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			37	26	10	1	
13	A	1	Total	C	O	P	0
			40	29	10	1	
13	A	1	Total	C	O	P	0
			34	23	10	1	
13	a	1	Total	C	O	P	0
			45	34	10	1	
13	a	1	Total	C	O	P	0
			34	23	10	1	
13	a	1	Total	C	O	P	0
			38	27	10	1	
13	a	1	Total	C	O	P	0
			38	27	10	1	
13	E	1	Total	C	O	P	0
			39	28	10	1	

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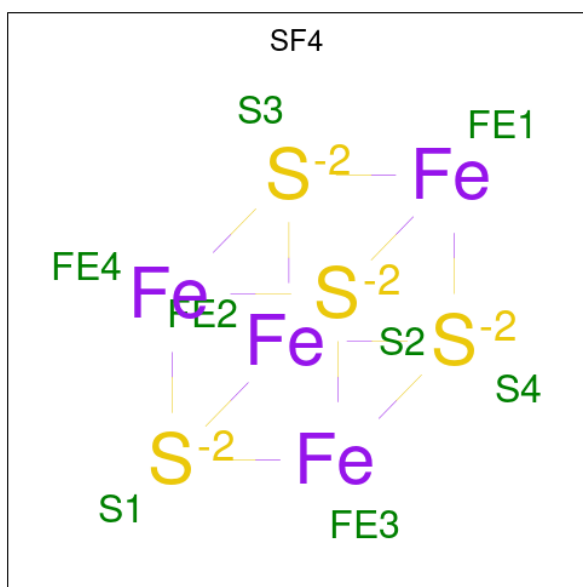
Mol	Chain	Residues	Atoms				AltConf
13	E	1	Total	C	O	P	0
			43	32	10	1	
13	Z	1	Total	C	O	P	0
			43	32	10	1	

- Molecule 14 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
14	A	1	Total	C	O	0
			42	32	10	
14	A	1	Total	C	O	0
			41	31	10	
14	A	1	Total	C	O	0
			42	32	10	
14	A	1	Total	C	O	0
			31	21	10	
14	a	1	Total	C	O	0
			45	35	10	
14	C	1	Total	C	O	0
			42	32	10	

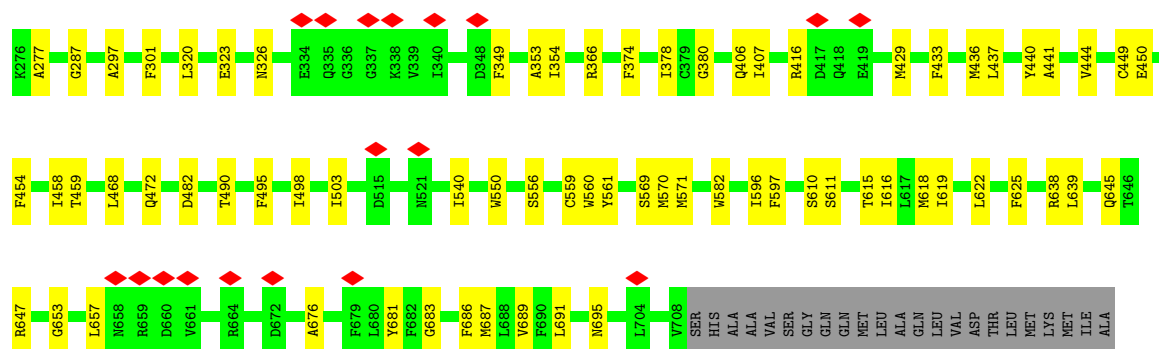
- Molecule 15 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



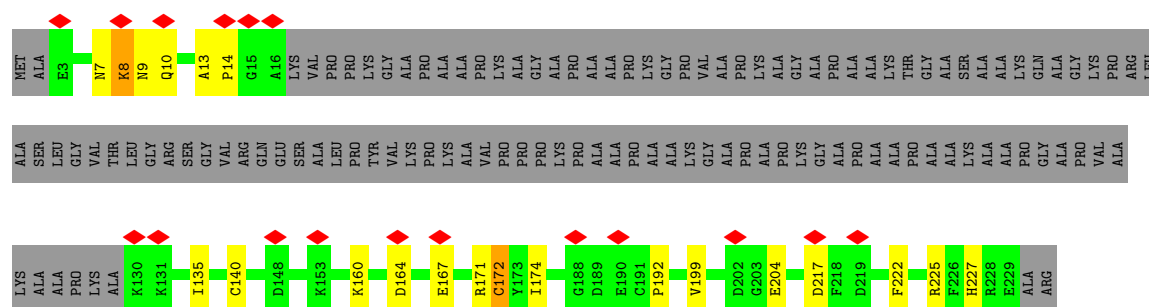
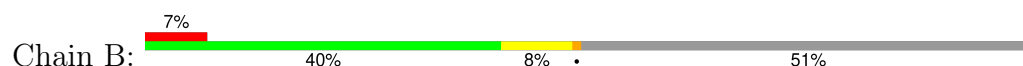
Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	Fe	S	0
			8	4	4	
15	B	1	Total	Fe	S	0
			8	4	4	
15	B	1	Total	Fe	S	0
			8	4	4	

- Molecule 16 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

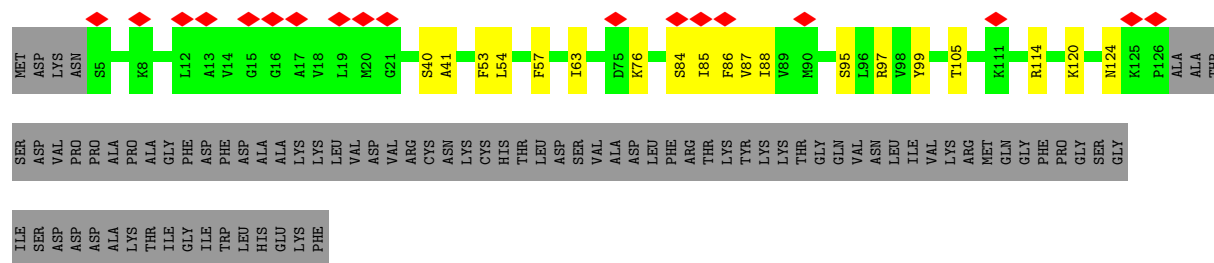
Mol	Chain	Residues	Atoms		AltConf
16	A	1	Total	Ca	0
			1	1	
16	a	1	Total	Ca	0
			1	1	



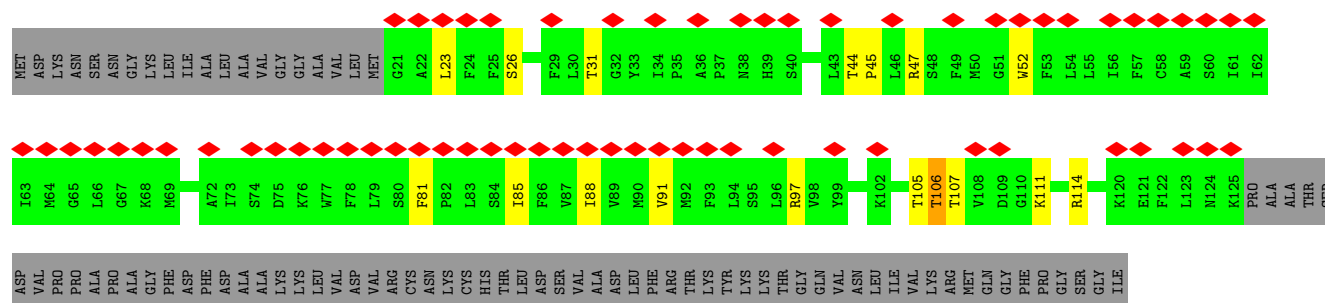
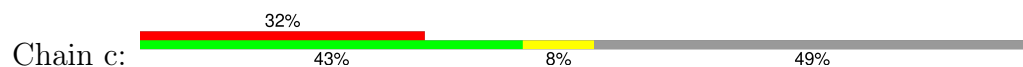
• Molecule 2: Photosystem P840 reaction center iron-sulfur protein



• Molecule 3: Cytochrome c

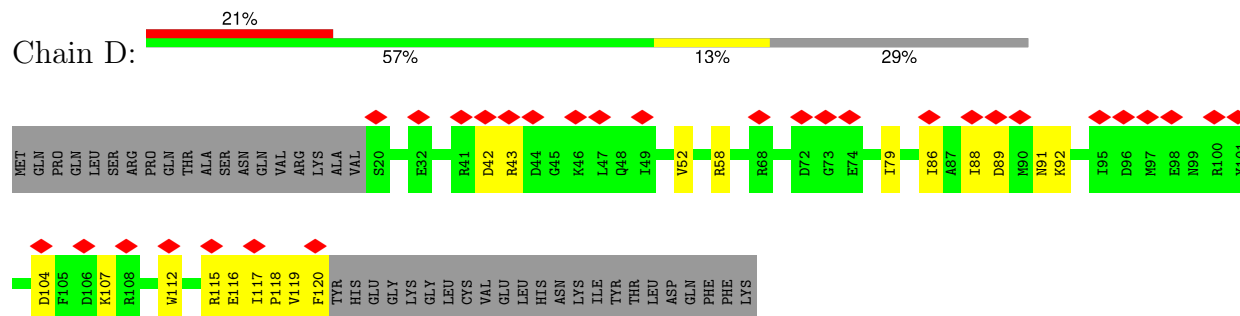


• Molecule 3: Cytochrome c

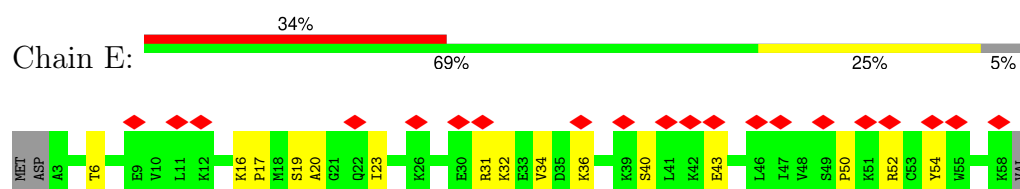


SER
ASP
ASP
ASP
ALA
LYS
THR
GLY
ILE
THR
TRP
LEU
HIS
GLU
LYS
PHE

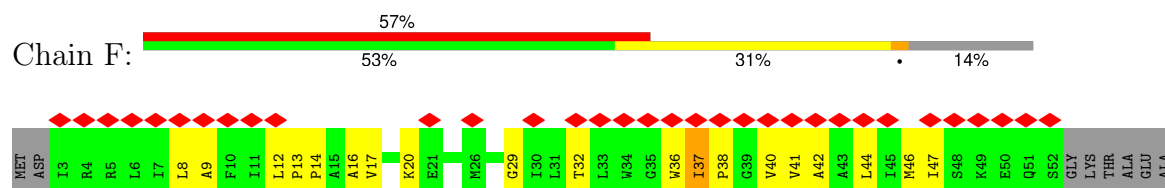
- Molecule 4: P840 reaction center 17 kDa protein



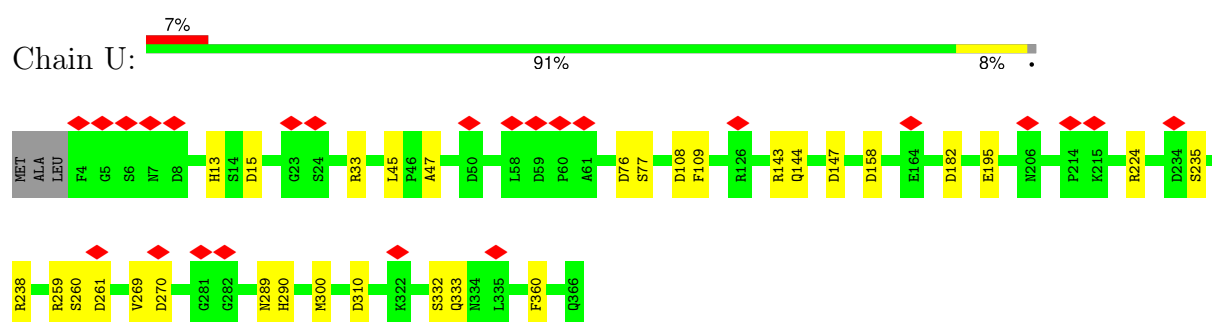
- Molecule 5: PscE



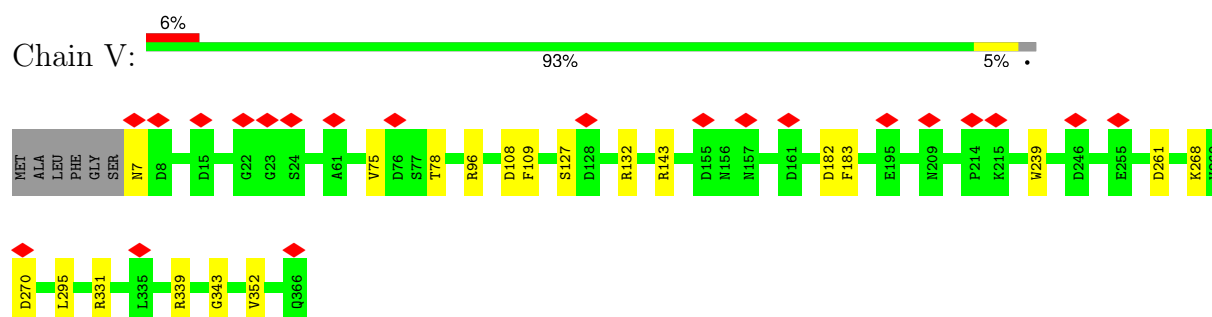
- Molecule 6: PscF



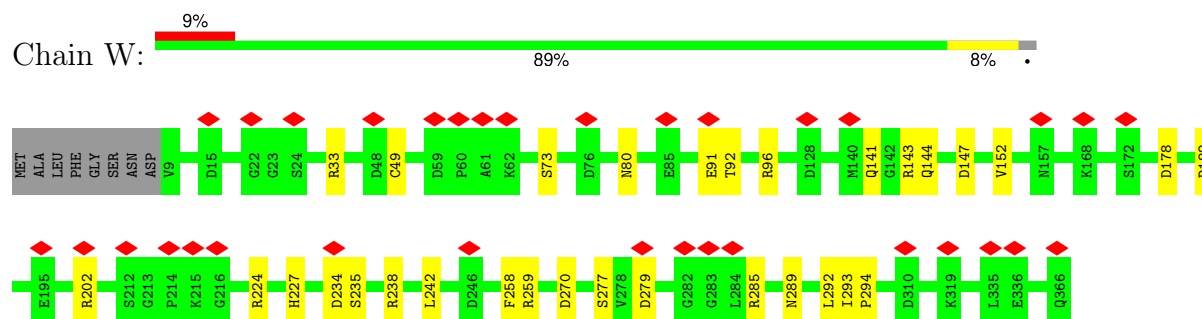
- Molecule 7: Bacteriochlorophyll a protein



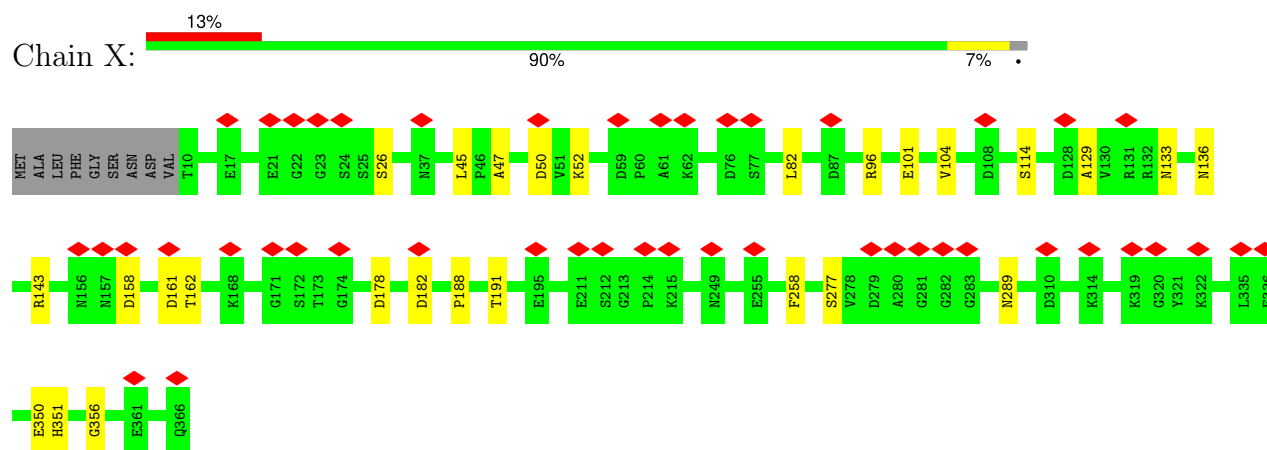
- Molecule 7: Bacteriochlorophyll a protein



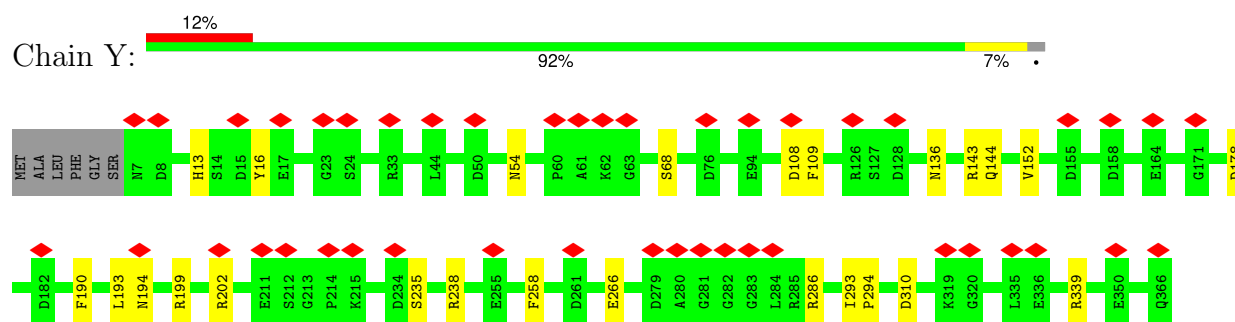
- Molecule 7: Bacteriochlorophyll a protein



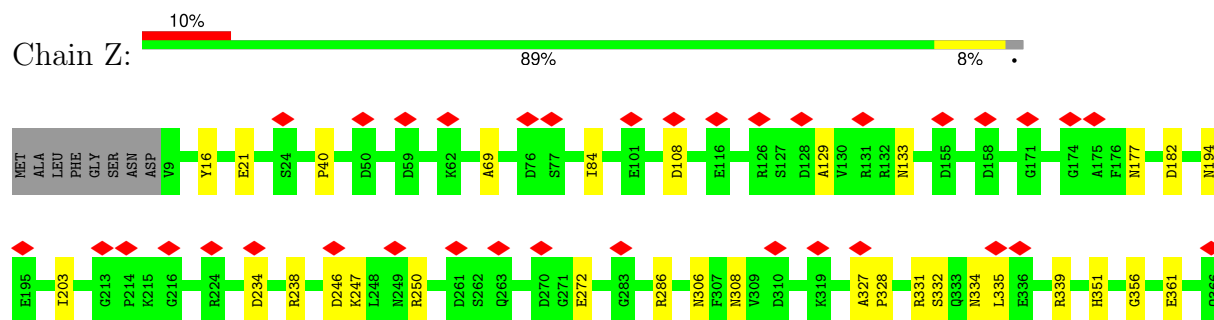
- Molecule 7: Bacteriochlorophyll a protein



- Molecule 7: Bacteriochlorophyll a protein



- Molecule 7: Bacteriochlorophyll a protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	157486	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	4.835	Depositor
Minimum map value	-2.409	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.112	Depositor
Recommended contour level	0.428	Depositor
Map size ($\text{\AA}$)	374.4, 374.4, 374.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.21	0/5379	0.32	0/7330
1	a	0.19	0/5396	0.32	0/7352
2	B	0.19	0/910	0.39	1/1230 (0.1%)
3	C	0.17	0/975	0.35	0/1319
3	c	0.17	0/863	0.39	0/1167
4	D	0.14	0/839	0.34	0/1130
5	E	0.23	0/446	0.52	0/593
6	F	0.22	0/386	0.47	0/525
7	U	0.18	0/2897	0.33	0/3926
7	V	0.18	0/2875	0.31	0/3897
7	W	0.17	0/2859	0.30	0/3875
7	X	0.16	0/2852	0.28	0/3865
7	Y	0.17	0/2875	0.31	0/3897
7	Z	0.18	0/2859	0.32	0/3875
All	All	0.18	0/32411	0.33	1/43981 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	172	CYS	CA-CB-SG	5.20	126.36	114.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5197	0	5090	108	0
1	a	5214	0	5107	99	0
2	B	887	0	833	19	0
3	C	950	0	996	17	0
3	c	839	0	870	16	0
4	D	823	0	839	12	0
5	E	441	0	476	11	0
6	F	379	0	419	21	0
7	U	2826	0	2759	24	0
7	V	2805	0	2742	15	0
7	W	2789	0	2732	22	0
7	X	2782	0	2723	20	0
7	Y	2805	0	2742	19	0
7	Z	2789	0	2732	23	0
8	A	66	0	0	3	0
8	a	66	0	0	0	0
9	A	195	0	207	95	0
9	a	65	0	69	29	0
10	A	791	0	884	30	0
10	B	66	0	74	3	0
10	U	442	0	479	7	0
10	V	574	0	627	4	0
10	W	508	0	553	13	0
10	X	554	0	588	10	0
10	Y	528	0	592	5	0
10	Z	442	0	479	10	0
10	a	772	0	849	24	0
11	A	65	0	0	0	0
11	C	65	0	0	0	0
11	a	65	0	0	0	0
12	A	40	0	0	0	0
12	a	80	0	0	0	0
13	A	111	0	135	9	0
13	E	82	0	104	6	0
13	Z	43	0	59	7	0
13	a	155	0	193	6	0
14	A	156	0	192	8	0
14	C	42	0	54	4	0
14	a	45	0	60	3	0
15	A	8	0	0	0	0
15	B	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	A	1	0	0	0	0
16	a	1	0	0	0	0
All	All	37570	0	37258	515	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 7.

All (515) 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)
9:A:827:CLA:HMB3	9:A:827:CLA:H101	1.44	0.97
9:A:827:CLA:HBA1	9:A:827:CLA:HED3	1.60	0.83
7:W:73:SER:OG	7:W:80:ASN:OD1	1.98	0.82
2:B:225:ARG:NH1	7:U:15:ASP:OD1	2.14	0.81
1:A:659:ARG:NH2	1:A:660:ASP:O	2.14	0.81
7:X:50:ASP:OD2	7:X:52:LYS:NZ	2.14	0.80
9:A:802:CLA:HAA1	9:A:802:CLA:CGD	2.12	0.78
3:C:99:TYR:OH	5:E:31:ARG:NH2	2.16	0.77
9:A:827:CLA:H72	9:A:827:CLA:HMB1	1.66	0.77
9:A:826:CLA:HAA1	9:A:826:CLA:CGD	2.15	0.77
10:A:804:BCL:HHD	10:A:809:BCL:OBB	1.86	0.76
13:a:820:LHG:HC91	13:Z:401:LHG:H132	1.66	0.76
7:V:96:ARG:NH1	10:V:407:BCL:OBD	2.20	0.75
7:X:143:ARG:NH2	7:Z:182:ASP:OD2	2.19	0.75
1:A:86:LEU:CD2	10:A:805:BCL:HHD	2.17	0.75
7:W:279:ASP:OD1	7:W:285:ARG:NH1	2.20	0.75
7:X:350:GLU:OE2	7:Z:306:ASN:ND2	2.20	0.74
9:A:827:CLA:O1D	9:A:827:CLA:HAA1	1.87	0.74
7:Y:16:TYR:OH	10:Y:404:BCL:OBB	2.06	0.74
7:Z:332:SER:OG	13:Z:401:LHG:O1	2.06	0.73
9:A:802:CLA:H203	9:a:801:CLA:H142	1.70	0.73
1:A:131:THR:O	3:c:114:ARG:NE	2.21	0.73
10:A:813:BCL:HHC	10:A:813:BCL:HBB3	1.70	0.72
9:A:802:CLA:H43	9:A:802:CLA:HMA3	1.70	0.72
10:a:809:BCL:HHC	10:a:809:BCL:HBB3	1.70	0.72
9:A:827:CLA:HAA1	9:A:827:CLA:CGD	2.20	0.71
7:X:96:ARG:NH1	10:X:405:BCL:OBD	2.24	0.71
5:E:52:ARG:NH2	13:E:101:LHG:O5	2.24	0.71
10:A:803:BCL:H191	10:A:810:BCL:HHD	1.73	0.71
1:A:539:SER:O	1:A:543:GLN:NE2	2.24	0.71
9:A:802:CLA:HAA1	9:A:802:CLA:O1D	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:CYS:SG	2:B:172:CYS:HB2	2.31	0.70
9:a:801:CLA:H43	9:a:801:CLA:H151	1.74	0.69
6:F:9:ALA:HB1	6:F:44:LEU:HD22	1.74	0.69
7:Y:144:GLN:NE2	7:Y:235:SER:O	2.25	0.69
1:A:570:MET:HE2	9:A:826:CLA:HBA2	1.75	0.69
9:A:802:CLA:HMB1	9:A:802:CLA:H112	1.75	0.69
1:A:625:PHE:CE2	9:A:802:CLA:HAB	2.28	0.69
7:Z:16:TYR:OH	10:Z:403:BCL:OBB	2.11	0.68
10:A:803:BCL:HHC	10:A:803:BCL:HBB3	1.76	0.68
7:Y:136:ASN:OD1	7:Y:286:ARG:NH1	2.26	0.68
7:U:144:GLN:NE2	7:U:235:SER:O	2.26	0.68
9:A:802:CLA:H8	9:A:802:CLA:HMB2	1.76	0.68
1:a:76:VAL:HG13	10:a:806:BCL:HBB2	1.75	0.67
1:A:440:TYR:CD2	9:A:826:CLA:H171	2.29	0.67
10:A:812:BCL:H93	10:A:812:BCL:H42	1.77	0.67
6:F:29:GLY:O	6:F:32:THR:OG1	2.10	0.67
10:A:809:BCL:HBB3	10:A:809:BCL:HHC	1.77	0.67
9:a:801:CLA:HED3	9:a:801:CLA:CAD	2.25	0.67
10:a:803:BCL:HHC	10:a:803:BCL:HBB3	1.76	0.66
9:A:826:CLA:H11	1:a:618:MET:HB3	1.77	0.66
6:F:32:THR:HG23	6:F:40:VAL:HG21	1.77	0.66
9:A:826:CLA:H141	9:A:827:CLA:H203	1.78	0.65
9:a:801:CLA:HHC	9:a:801:CLA:HBB1	1.79	0.65
2:B:135:ILE:HD13	2:B:172:CYS:HB3	1.79	0.65
9:A:802:CLA:HBC2	9:A:802:CLA:HHD	1.78	0.65
10:A:803:BCL:H202	10:A:811:BCL:HBB1	1.77	0.65
7:Z:129:ALA:O	7:Z:133:ASN:ND2	2.30	0.64
9:A:802:CLA:HBA1	9:A:802:CLA:HED2	1.79	0.64
9:A:827:CLA:HAB	1:a:625:PHE:CE1	2.32	0.64
1:A:515:ASP:OD2	1:a:647:ARG:NH2	2.31	0.64
9:A:827:CLA:H192	3:C:63:ILE:HG13	1.80	0.64
1:A:570:MET:CE	9:A:826:CLA:H12	2.28	0.64
1:a:472:GLN:OE1	1:a:472:GLN:N	2.30	0.64
5:E:50:PRO:O	5:E:54:TYR:N	2.30	0.64
1:A:86:LEU:HD21	10:A:805:BCL:HHD	1.79	0.63
7:U:182:ASP:OD2	7:V:143:ARG:NH2	2.31	0.63
1:A:378:ILE:HD12	1:A:555:LEU:HD13	1.80	0.63
1:a:683:GLY:O	1:a:687:MET:N	2.31	0.63
1:a:622:LEU:HD23	13:Z:401:LHG:H223	1.81	0.63
1:A:436:MET:HE2	9:A:827:CLA:H61	1.81	0.62
1:A:638:ARG:NE	13:A:818:LHG:O4	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:827:CLA:H172	3:C:63:ILE:HD11	1.82	0.62
7:U:238:ARG:NH2	7:U:289:ASN:O	2.29	0.62
10:A:803:BCL:C19	10:A:810:BCL:HHD	2.29	0.62
1:a:354:ILE:O	3:C:105:THR:HG21	1.99	0.62
10:A:811:BCL:HBB2	10:A:811:BCL:H72	1.82	0.62
2:B:140:CYS:O	2:B:171:ARG:NH1	2.32	0.62
6:F:8:LEU:O	6:F:12:LEU:N	2.32	0.61
9:A:827:CLA:HMB3	9:A:827:CLA:HBB1	1.82	0.61
1:a:436:MET:SD	9:a:801:CLA:HAB	2.40	0.61
6:F:9:ALA:HB2	6:F:16:ALA:HB2	1.81	0.61
7:Y:194:ASN:ND2	7:Z:194:ASN:OD1	2.32	0.61
7:Z:334:ASN:O	7:Z:335:LEU:HG	2.00	0.61
1:a:353:ALA:HB1	3:C:105:THR:HG23	1.83	0.61
1:a:561:TYR:HE2	14:a:822:LMG:HC72	1.66	0.61
9:A:802:CLA:HMB1	9:A:802:CLA:HBB1	1.82	0.61
2:B:174:ILE:N	4:D:116:GLU:OE1	2.34	0.60
9:A:826:CLA:H71	1:a:619:ILE:HD11	1.83	0.60
1:A:550:TRP:HA	9:A:826:CLA:HMC2	1.83	0.60
1:a:570:MET:HE3	9:a:801:CLA:H2	1.83	0.60
7:U:147:ASP:OD2	7:U:224:ARG:NH1	2.35	0.60
7:V:96:ARG:NH2	7:V:239:TRP:O	2.35	0.60
13:E:102:LHG:H261	13:E:102:LHG:H301	1.83	0.60
7:X:258:PHE:HZ	10:X:402:BCL:HED3	1.66	0.60
9:A:826:CLA:C14	9:A:827:CLA:H203	2.30	0.60
1:a:169:LEU:HD13	10:a:806:BCL:HMA3	1.82	0.60
9:A:802:CLA:H43	9:A:802:CLA:CMA	2.32	0.59
7:Z:234:ASP:OD1	7:Z:238:ARG:NH1	2.34	0.59
1:A:502:ARG:NH1	9:A:827:CLA:O2D	2.36	0.59
9:A:826:CLA:HAA1	9:A:826:CLA:O1D	2.02	0.59
7:Z:177:ASN:ND2	7:Z:203:ILE:O	2.35	0.59
7:Z:250:ARG:NH2	7:Z:272:GLU:OE2	2.35	0.59
1:A:564:GLY:O	1:A:593:THR:N	2.35	0.59
1:A:625:PHE:CZ	9:A:802:CLA:HAB	2.38	0.58
9:A:802:CLA:H112	9:A:802:CLA:CMB	2.32	0.58
7:U:158:ASP:OD2	7:V:132:ARG:NH2	2.36	0.58
1:A:195:ASN:OD1	7:V:7:ASN:N	2.37	0.58
1:A:321:TYR:HB3	10:A:814:BCL:HMA2	1.85	0.58
9:A:827:CLA:HMA3	9:A:827:CLA:C3	2.34	0.58
2:B:160:LYS:NZ	4:D:115:ARG:O	2.37	0.57
3:c:106:THR:O	3:c:107:THR:OG1	2.22	0.57
9:A:827:CLA:HHD	9:A:827:CLA:HBC2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:444:VAL:HG21	9:a:801:CLA:H162	1.85	0.57
7:W:91:GLU:OE1	7:W:92:THR:OG1	2.21	0.57
7:X:182:ASP:OD2	7:Y:143:ARG:NH2	2.37	0.57
10:X:402:BCL:HHC	10:X:402:BCL:HBB3	1.87	0.57
1:a:57:ARG:NH1	7:Z:331:ARG:O	2.37	0.57
7:W:178:ASP:OD2	7:W:202:ARG:NE	2.38	0.57
4:D:104:ASP:O	4:D:107:LYS:N	2.37	0.57
3:C:95:SER:OG	14:C:302:LMG:O10	2.22	0.57
14:A:823:LMG:HC62	7:U:13:HIS:HE1	1.68	0.57
1:A:692:PHE:CD2	8:A:801:GS0:OBD	2.58	0.56
1:A:615:THR:HG23	9:a:801:CLA:H62	1.86	0.56
2:B:9:ASN:OD1	2:B:10:GLN:N	2.38	0.56
7:Y:310:ASP:OD1	7:Y:310:ASP:N	2.38	0.56
1:A:130:SER:OG	1:A:132:LYS:NZ	2.37	0.56
1:A:635:ARG:NE	1:A:668:LEU:O	2.37	0.56
9:A:826:CLA:H152	9:A:827:CLA:C14	2.36	0.56
9:A:827:CLA:H72	9:A:827:CLA:CMB	2.34	0.56
1:a:444:VAL:CG1	9:a:801:CLA:H42	2.35	0.56
6:F:9:ALA:HB1	6:F:44:LEU:HD13	1.87	0.56
1:A:436:MET:HE1	9:A:827:CLA:H41	1.86	0.55
1:a:691:LEU:O	1:a:695:ASN:ND2	2.38	0.55
6:F:9:ALA:CB	6:F:44:LEU:HD13	2.35	0.55
10:W:402:BCL:H52	10:W:402:BCL:H93	1.88	0.55
1:A:546:PHE:CG	9:A:827:CLA:HMD2	2.42	0.55
13:E:101:LHG:HC61	13:E:101:LHG:H101	1.88	0.55
3:C:84:SER:O	3:C:87:VAL:HG12	2.06	0.55
1:a:366:ARG:NH1	14:a:822:LMG:O4	2.39	0.55
1:a:550:TRP:CD1	9:a:801:CLA:HMC3	2.42	0.55
1:A:86:LEU:HD23	10:A:805:BCL:HHD	1.89	0.54
1:A:183:PHE:CZ	10:A:806:BCL:HMB2	2.43	0.54
9:A:802:CLA:H93	1:a:437:LEU:HA	1.89	0.54
13:a:819:LHG:O1	13:Z:401:LHG:O6	2.24	0.54
9:A:802:CLA:H92	1:a:436:MET:HG2	1.88	0.54
1:a:76:VAL:CG1	10:a:806:BCL:HBB2	2.36	0.54
2:B:135:ILE:HD12	2:B:174:ILE:HG13	1.90	0.54
7:U:45:LEU:O	7:U:47:ALA:N	2.41	0.53
1:a:450:GLU:OE2	1:a:582:TRP:NE1	2.40	0.53
1:A:440:TYR:HE2	9:A:827:CLA:H142	1.73	0.53
4:D:42:ASP:OD1	4:D:43:ARG:N	2.42	0.53
1:A:595:GLY:O	1:A:599:TYR:N	2.40	0.53
10:B:301:BCL:H191	6:F:32:THR:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:37:ILE:HB	6:F:38:PRO:HD2	1.90	0.53
6:F:41:VAL:HA	6:F:44:LEU:HD23	1.91	0.53
7:Y:238:ARG:HB3	10:Y:406:BCL:HED1	1.91	0.53
7:W:234:ASP:OD2	7:W:292:LEU:N	2.39	0.53
10:W:403:BCL:HBC3	10:W:403:BCL:HHD	1.89	0.53
9:a:801:CLA:HAA1	9:a:801:CLA:CGD	2.39	0.53
7:U:290:HIS:NE2	10:U:403:BCL:ND	2.56	0.53
7:W:152:VAL:HG21	10:W:401:BCL:HHC	1.91	0.53
7:X:188:PRO:O	7:X:191:THR:OG1	2.23	0.53
1:A:621:HIS:HD2	9:a:801:CLA:HED1	1.72	0.53
1:a:202:TYR:CE1	1:a:274:ASP:OD1	2.62	0.53
1:A:621:HIS:CD2	9:a:801:CLA:HED1	2.43	0.52
9:A:826:CLA:H52	1:a:619:ILE:HG13	1.90	0.52
1:A:75:VAL:HG21	1:A:275:MET:HE3	1.91	0.52
1:A:444:VAL:HG12	9:A:826:CLA:H43	1.91	0.52
10:W:401:BCL:HHC	10:W:401:BCL:OBB	2.08	0.52
10:X:401:BCL:OBB	10:X:401:BCL:HHC	2.08	0.52
1:A:440:TYR:CE1	9:A:826:CLA:HMA2	2.44	0.52
1:a:459:THR:OG1	3:c:47:ARG:NH2	2.39	0.52
9:A:827:CLA:H202	13:Z:401:LHG:H221	1.91	0.52
3:c:107:THR:OG1	3:c:111:LYS:O	2.28	0.52
13:A:819:LHG:O5	14:A:823:LMG:O5	2.28	0.52
1:a:490:THR:HG21	10:a:813:BCL:HMA1	1.92	0.52
10:A:812:BCL:H91	3:c:81:PHE:HE2	1.74	0.52
6:F:37:ILE:HB	6:F:38:PRO:CD	2.40	0.52
7:Z:327:ALA:HB3	7:Z:328:PRO:CD	2.39	0.52
1:a:639:LEU:HD11	7:Z:335:LEU:HD22	1.92	0.52
10:V:402:BCL:HHC	10:V:402:BCL:OBB	2.10	0.52
9:A:802:CLA:H101	1:a:440:TYR:HD2	1.75	0.52
1:A:433:PHE:HB2	9:A:827:CLA:H2	1.92	0.52
10:a:810:BCL:C4	10:a:814:BCL:HHD	2.40	0.52
7:Y:13:HIS:ND1	7:Y:310:ASP:OD2	2.43	0.52
1:a:72:ASP:OD1	1:a:72:ASP:N	2.44	0.51
10:a:809:BCL:HHC	10:a:809:BCL:CBB	2.40	0.51
1:A:627:SER:OG	1:A:677:GLY:O	2.24	0.51
3:c:23:LEU:O	3:c:26:SER:OG	2.23	0.51
1:A:653:GLY:O	1:A:657:LEU:N	2.37	0.51
1:A:676:ALA:HB1	13:A:818:LHG:H252	1.92	0.51
9:A:827:CLA:HAB	1:a:625:PHE:CZ	2.46	0.51
9:A:802:CLA:HMA3	9:A:802:CLA:C4	2.40	0.51
1:a:681:TYR:OH	9:a:801:CLA:HMD1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:14:PRO:HA	6:F:17:VAL:HG22	1.92	0.51
7:Y:178:ASP:OD1	7:Y:202:ARG:NE	2.38	0.51
9:A:827:CLA:H161	13:Z:401:LHG:H161	1.93	0.50
10:A:809:BCL:HHC	10:A:809:BCL:CBB	2.41	0.50
10:Z:404:BCL:OBB	10:Z:404:BCL:HHC	2.10	0.50
1:A:561:TYR:CZ	14:A:820:LMG:HC61	2.46	0.50
2:B:7:ASN:O	2:B:8:LYS:CB	2.59	0.50
4:D:58:ARG:NH2	7:U:76:ASP:O	2.42	0.50
7:V:183:PHE:O	7:W:141:GLN:NE2	2.45	0.50
1:A:645:GLN:OE1	13:A:818:LHG:H182	2.12	0.50
7:W:242:LEU:CD2	10:W:406:BCL:HMD3	2.42	0.50
7:X:351:HIS:O	7:X:356:GLY:N	2.40	0.50
10:B:301:BCL:OBB	10:B:301:BCL:HHC	2.12	0.50
6:F:42:ALA:O	6:F:46:MET:HG2	2.12	0.50
7:V:331:ARG:N	7:V:339:ARG:O	2.44	0.50
1:A:514:ASP:OD1	1:A:515:ASP:N	2.44	0.50
9:A:802:CLA:HED3	9:A:802:CLA:O1A	2.12	0.50
10:X:409:BCL:H203	10:Z:406:BCL:HHB	1.93	0.50
1:a:570:MET:O	1:a:597:PHE:N	2.45	0.50
10:a:810:BCL:H42	10:a:814:BCL:HHD	1.93	0.50
10:V:405:BCL:OBB	10:V:405:BCL:HHC	2.11	0.50
7:X:45:LEU:O	7:X:47:ALA:N	2.45	0.49
1:A:481:ASN:OD1	1:A:567:ILE:N	2.44	0.49
10:W:403:BCL:HHC	10:W:403:BCL:HBB3	1.94	0.49
10:Z:402:BCL:OBB	10:Z:402:BCL:HHC	2.12	0.49
1:A:86:LEU:HD21	10:A:805:BCL:HMD1	1.93	0.49
1:A:444:VAL:CG1	9:A:826:CLA:H43	2.42	0.49
10:U:403:BCL:H2	10:U:404:BCL:H42	1.93	0.49
2:B:13:ALA:N	2:B:14:PRO:HD2	2.27	0.49
5:E:16:LYS:N	5:E:17:PRO:HD3	2.28	0.49
10:Z:403:BCL:HHC	10:Z:403:BCL:HBB3	1.93	0.49
1:A:404:TYR:O	1:A:416:ARG:NH2	2.45	0.49
1:a:561:TYR:CE2	14:a:822:LMG:HC72	2.48	0.49
9:A:827:CLA:HMA3	9:A:827:CLA:H42	1.95	0.49
1:a:450:GLU:OE2	1:a:569:SER:OG	2.28	0.49
7:Z:286:ARG:NE	7:Z:361:GLU:OE2	2.43	0.49
1:a:676:ALA:HB2	13:a:819:LHG:H251	1.94	0.49
10:Y:404:BCL:HHC	10:Y:404:BCL:HBB3	1.95	0.49
7:V:127:SER:N	10:V:409[B]:BCL:OBB	2.46	0.49
10:W:404:BCL:HBC3	10:W:404:BCL:HHD	1.94	0.49
7:X:82:LEU:HD13	10:X:406:BCL:H191	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ILE:CD1	1:a:615:THR:HG22	2.43	0.48
9:A:826:CLA:H152	9:A:827:CLA:H142	1.94	0.48
1:a:120:ARG:HB3	10:a:805:BCL:HED1	1.94	0.48
1:a:177:CYS:SG	1:a:178:GLY:N	2.86	0.48
7:Y:108:ASP:OD1	7:Y:109:PHE:N	2.45	0.48
1:A:265:PRO:HB2	13:A:819:LHG:HC82	1.95	0.48
7:V:182:ASP:OD2	7:W:143:ARG:NH2	2.46	0.48
1:A:645:GLN:NE2	9:A:802:CLA:HAA2	2.28	0.48
10:U:403:BCL:HHC	10:U:403:BCL:OB	2.12	0.48
10:X:402:BCL:HBB	10:X:403:BCL:H93	1.95	0.48
1:A:354:ILE:O	3:c:105:THR:OG1	2.25	0.48
1:A:621:HIS:HB3	9:a:801:CLA:CED	2.44	0.48
9:A:802:CLA:H101	1:a:440:TYR:CD2	2.48	0.48
9:A:802:CLA:H42	1:a:433:PHE:HB2	1.95	0.48
10:X:403:BCL:OB	10:X:403:BCL:HHC	2.13	0.48
9:A:826:CLA:H121	9:A:826:CLA:H51	1.96	0.48
1:a:297:ALA:HB1	1:a:301:PHE:CE2	2.49	0.48
9:A:802:CLA:HED1	1:a:498:ILE:HG21	1.96	0.48
13:A:819:LHG:O9	13:A:819:LHG:H242	2.13	0.48
9:A:827:CLA:H101	9:A:827:CLA:CMB	2.30	0.48
9:A:802:CLA:H142	13:A:818:LHG:H111	1.95	0.48
1:a:468:LEU:CD1	10:a:813:BCL:HMD2	2.44	0.48
1:A:490:THR:HG21	10:A:813:BCL:HMA1	1.94	0.48
1:a:406:GLN:N	1:a:406:GLN:OE1	2.47	0.48
2:B:199:VAL:HG23	2:B:199:VAL:O	2.14	0.48
10:U:401:BCL:HHC	10:U:401:BCL:OB	2.14	0.48
7:X:82:LEU:HD12	7:X:104:VAL:HG22	1.96	0.48
1:A:135:ASP:OD1	1:A:135:ASP:C	2.57	0.47
4:D:79:ILE:HG23	4:D:86:ILE:HD12	1.95	0.47
5:E:40:SER:O	5:E:43:GLU:HG2	2.14	0.47
7:Z:246:ASP:OD1	7:Z:247:LYS:N	2.47	0.47
7:Z:327:ALA:HB3	7:Z:328:PRO:HD3	1.96	0.47
1:A:163:ARG:NH2	1:A:170:THR:O	2.45	0.47
1:A:570:MET:HE1	9:A:826:CLA:H12	1.95	0.47
1:A:198:SER:OG	1:A:200:LYS:O	2.30	0.47
6:F:9:ALA:HB2	6:F:16:ALA:CB	2.43	0.47
9:A:826:CLA:H41	9:A:826:CLA:H62	1.68	0.47
5:E:31:ARG:O	5:E:36:LYS:HB2	2.15	0.47
14:C:302:LMG:H292	14:C:302:LMG:H111	1.96	0.47
10:X:409:BCL:H92	10:Z:407:BCL:H152	1.96	0.47
1:A:624:TRP:CD2	8:A:801:GS0:CMA	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:686:PHE:O	10:a:810:BCL:HBB2	2.15	0.47
3:C:85:ILE:O	3:C:88:ILE:HG22	2.14	0.47
9:a:801:CLA:HBC3	9:a:801:CLA:HHD	1.95	0.47
1:A:241:SER:OG	10:A:808:BCL:HHD	2.15	0.47
1:a:468:LEU:HD12	3:c:31:THR:HG22	1.96	0.47
7:W:144:GLN:OE1	7:W:227:HIS:NE2	2.46	0.47
7:Y:54:ASN:O	7:Y:68:SER:N	2.42	0.47
1:A:513:TRP:CZ2	1:A:538:VAL:HG11	2.50	0.47
8:A:801:GS0:CMB	9:a:801:CLA:OBD	2.63	0.47
10:a:804:BCL:HMD1	10:a:809:BCL:OBB	2.15	0.47
7:Y:190:PHE:O	7:Y:193:LEU:HB2	2.15	0.47
10:A:807:BCL:HBB2	10:A:807:BCL:HHC	1.97	0.46
13:E:102:LHG:H311	13:E:102:LHG:H282	1.76	0.46
1:a:611:SER:O	1:a:615:THR:HG23	2.15	0.46
9:a:801:CLA:CAD	9:a:801:CLA:CED	2.92	0.46
6:F:36:TRP:O	6:F:38:PRO:HD2	2.15	0.46
7:W:49:CYS:SG	10:W:404:BCL:H202	2.55	0.46
7:Z:331:ARG:N	7:Z:339:ARG:O	2.46	0.46
1:a:482:ASP:OD1	1:a:561:TYR:OH	2.33	0.46
1:a:638:ARG:NE	13:a:820:LHG:O4	2.38	0.46
1:A:405:ASN:OD1	7:U:259:ARG:NH1	2.49	0.46
1:A:374:PHE:O	1:A:378:ILE:HG22	2.15	0.46
14:A:823:LMG:HC62	7:U:13:HIS:CE1	2.50	0.46
1:a:160:GLY:HA3	10:a:806:BCL:HHD	1.97	0.46
1:A:250:ALA:O	1:A:254:PHE:N	2.44	0.46
1:a:98:ILE:HG23	1:a:98:ILE:O	2.16	0.46
7:Y:152:VAL:HG21	10:Y:402:BCL:HHC	1.98	0.46
1:A:597:PHE:HE2	9:A:826:CLA:HBA1	1.81	0.46
10:A:812:BCL:H91	3:c:81:PHE:CE2	2.51	0.46
1:a:653:GLY:HA2	1:a:657:LEU:HB3	1.98	0.46
1:A:348:ASP:OD2	1:A:348:ASP:C	2.59	0.46
1:A:408:LYS:NZ	7:U:261:ASP:OD2	2.38	0.46
7:X:162:THR:HA	10:X:408[B]:BCL:HBB2	1.98	0.46
7:Y:193:LEU:HD12	10:Y:408:BCL:HMB3	1.97	0.46
9:A:802:CLA:HED1	1:a:429:MET:HE2	1.97	0.46
14:A:820:LMG:HC2	14:A:820:LMG:HC72	1.28	0.46
9:A:826:CLA:H8	9:A:826:CLA:H122	1.53	0.46
7:X:136:ASN:OD1	7:X:289:ASN:ND2	2.45	0.46
1:A:511:PRO:O	1:A:514:ASP:OD1	2.34	0.45
9:A:826:CLA:H62	9:A:826:CLA:H102	1.77	0.45
1:A:436:MET:SD	9:A:826:CLA:HAB	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:23:ILE:O	5:E:23:ILE:HG22	2.15	0.45
5:E:32:LYS:O	5:E:34:VAL:N	2.48	0.45
7:U:143:ARG:NH2	7:W:182:ASP:OD2	2.49	0.45
7:U:269:VAL:HG11	10:U:404:BCL:H41	1.98	0.45
9:A:802:CLA:H61	1:a:436:MET:HB3	1.98	0.45
9:A:827:CLA:HBB1	9:A:827:CLA:H122	1.98	0.45
9:a:801:CLA:H41	9:a:801:CLA:H72	1.97	0.45
1:A:570:MET:SD	9:A:826:CLA:H12	2.56	0.45
9:A:826:CLA:HBB1	9:A:827:CLA:C4B	2.47	0.45
1:a:213:MET:HE1	10:a:807:BCL:CGA	2.47	0.45
7:W:147:ASP:OD2	7:W:224:ARG:NH2	2.49	0.45
10:Z:405:BCL:H202	10:Z:407:BCL:H201	1.98	0.45
1:A:440:TYR:HE1	9:A:826:CLA:HMA2	1.80	0.45
3:C:88:ILE:HD11	14:C:302:LMG:H392	1.99	0.45
3:c:105:THR:O	3:c:106:THR:C	2.59	0.45
1:A:287:GLY:HA2	1:A:380:GLY:HA2	1.98	0.45
10:W:404:BCL:OBB	10:W:404:BCL:HHC	2.16	0.45
1:a:270:HIS:HD1	1:a:277:ALA:HB1	1.82	0.45
9:a:801:CLA:H112	9:a:801:CLA:C4	2.47	0.45
6:F:37:ILE:O	6:F:38:PRO:C	2.60	0.45
1:A:440:TYR:CE2	9:A:826:CLA:H171	2.52	0.45
1:A:463:TYR:O	1:A:466:LYS:NZ	2.49	0.45
1:a:560:TRP:CZ3	1:a:596:ILE:HG23	2.53	0.45
1:A:618:MET:HE3	1:a:571:MET:HE3	1.99	0.44
1:a:374:PHE:O	1:a:378:ILE:HG22	2.17	0.44
10:B:301:BCL:H172	6:F:12:LEU:HD23	1.99	0.44
3:C:40:SER:OG	3:C:41:ALA:N	2.49	0.44
7:X:101:GLU:HA	7:X:114:SER:HA	1.98	0.44
1:A:378:ILE:HD11	1:A:682:PHE:HE2	1.82	0.44
2:B:135:ILE:CD1	2:B:174:ILE:HG13	2.47	0.44
7:U:33:ARG:NH2	7:U:270:ASP:OD1	2.51	0.44
9:A:802:CLA:HMB3	13:A:818:LHG:H112	2.00	0.44
9:A:827:CLA:HMA3	9:A:827:CLA:C4	2.47	0.44
10:a:814:BCL:O2A	10:a:814:BCL:H43	2.17	0.44
1:A:506:PHE:O	1:A:520:LYS:NZ	2.49	0.44
1:a:503:ILE:HG23	1:a:540:ILE:HG23	1.99	0.44
14:A:821:LMG:HC91	14:A:821:LMG:H111	2.00	0.44
9:a:801:CLA:H151	9:a:801:CLA:H112	1.69	0.44
9:A:827:CLA:H122	9:A:827:CLA:CBB	2.48	0.44
10:a:808:BCL:OBB	10:a:808:BCL:HHC	2.17	0.44
7:Z:351:HIS:O	7:Z:356:GLY:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:LEU:HD23	1:A:523:TYR:CB	2.47	0.44
2:B:225:ARG:NH2	7:U:310:ASP:O	2.51	0.44
14:C:302:LMG:H302	14:C:302:LMG:H331	1.46	0.44
10:W:401:BCL:OBD	10:W:402:BCL:HHB	2.17	0.44
3:C:53:PHE:O	3:C:54:LEU:C	2.61	0.44
9:A:802:CLA:H41	1:a:433:PHE:HD1	1.82	0.43
1:a:645:GLN:HE22	13:a:820:LHG:H162	1.82	0.43
1:A:473:TRP:CH2	13:A:817:LHG:HC91	2.52	0.43
9:A:826:CLA:H143	9:A:826:CLA:H161	1.74	0.43
2:B:13:ALA:N	2:B:14:PRO:CD	2.81	0.43
3:c:44:THR:HB	3:c:45:PRO:HD3	1.99	0.43
1:A:183:PHE:O	1:A:197:THR:HB	2.19	0.43
1:a:243:THR:O	1:a:246:SER:OG	2.35	0.43
2:B:164:ASP:O	2:B:167:GLU:N	2.46	0.43
4:D:88:ILE:O	4:D:89:ASP:HB3	2.19	0.43
5:E:19:SER:O	5:E:23:ILE:HG12	2.19	0.43
7:X:26:SER:OG	7:X:277:SER:N	2.45	0.43
7:X:133:ASN:OD1	7:Z:108:ASP:N	2.44	0.43
4:D:91:ASN:O	4:D:92:LYS:C	2.62	0.43
6:F:17:VAL:HG12	6:F:47:ILE:HG21	2.00	0.43
10:W:405:BCL:HBC2	10:W:406:BCL:H102	2.00	0.43
1:A:622:LEU:HD22	9:a:801:CLA:H11	2.00	0.43
9:A:826:CLA:H51	9:A:826:CLA:C12	2.48	0.43
1:a:441:ALA:HA	1:a:444:VAL:HG22	2.01	0.43
1:a:559:CYS:SG	1:a:689:VAL:HG13	2.58	0.43
6:F:17:VAL:O	6:F:20:LYS:N	2.51	0.43
7:U:76:ASP:O	7:U:77:SER:OG	2.31	0.43
7:W:96:ARG:NH1	10:W:406:BCL:OBD	2.44	0.43
1:A:383:TYR:OH	10:A:811:BCL:OBB	2.37	0.43
1:A:522:SER:O	1:A:523:TYR:CD1	2.71	0.43
7:W:238:ARG:NH2	7:W:289:ASN:O	2.50	0.43
7:W:258:PHE:O	7:W:259:ARG:C	2.61	0.43
1:A:378:ILE:HD11	1:A:682:PHE:CE2	2.53	0.43
1:a:111:ASN:OD1	1:a:111:ASN:N	2.51	0.43
3:C:76:LYS:NZ	7:Z:308:ASN:OD1	2.49	0.43
7:V:75:VAL:O	7:V:78:THR:OG1	2.32	0.43
10:A:808:BCL:CBB	10:A:808:BCL:HHC	2.49	0.43
1:a:287:GLY:HA2	1:a:380:GLY:HA2	2.01	0.43
9:a:801:CLA:HMA3	9:a:801:CLA:CGA	2.49	0.43
10:Z:403:BCL:HHB	10:Z:404:BCL:H93	2.00	0.43
1:A:601:TRP:O	1:A:605:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:802:CLA:H8	9:A:802:CLA:CMB	2.48	0.42
1:a:269:ILE:HD11	10:a:804:BCL:OBD	2.19	0.42
1:a:449:CYS:HB3	1:a:458:ILE:HA	2.01	0.42
1:a:625:PHE:CD1	1:a:625:PHE:C	2.96	0.42
7:W:238:ARG:NH1	7:W:289:ASN:O	2.50	0.42
9:A:826:CLA:H41	9:A:826:CLA:H102	2.01	0.42
1:a:444:VAL:HG12	9:a:801:CLA:H42	2.00	0.42
9:a:801:CLA:H141	9:a:801:CLA:H172	2.01	0.42
3:C:57:PHE:HD1	13:E:101:LHG:H171	1.83	0.42
9:A:827:CLA:H42	9:A:827:CLA:CMA	2.49	0.42
10:A:814:BCL:H191	1:a:454:PHE:H	1.84	0.42
1:a:115:LEU:HD12	1:a:320:LEU:HD21	2.02	0.42
1:a:441:ALA:HB3	3:c:52:TRP:NE1	2.34	0.42
3:C:85:ILE:O	3:C:86:PHE:C	2.62	0.42
7:U:360:PHE:HB3	10:U:403:BCL:HED3	2.01	0.42
1:A:450:GLU:OE1	1:A:582:TRP:NE1	2.43	0.42
1:a:90:MET:HE3	10:a:805:BCL:HMD2	2.00	0.42
1:a:622:LEU:HD12	1:a:625:PHE:CE2	2.54	0.42
10:a:809:BCL:O2A	10:a:809:BCL:H43	2.19	0.42
7:V:268:LYS:NZ	7:V:270:ASP:OD2	2.53	0.42
9:A:802:CLA:H92	9:A:802:CLA:H61	1.76	0.42
1:a:556:SER:O	1:a:560:TRP:CD1	2.72	0.42
13:E:102:LHG:HC5	13:E:102:LHG:HC81	1.60	0.42
7:X:129:ALA:O	7:X:133:ASN:ND2	2.51	0.42
1:A:271:LEU:O	7:V:343:GLY:HA3	2.19	0.42
1:A:679:PHE:HZ	14:A:821:LMG:H361	1.85	0.42
9:A:802:CLA:HED2	9:A:802:CLA:CBA	2.46	0.42
10:A:805:BCL:H111	10:A:809:BCL:H41	2.02	0.42
1:a:323:GLU:OE1	1:a:610:SER:OG	2.32	0.42
7:X:178:ASP:O	7:Y:199:ARG:NH2	2.53	0.42
1:A:297:ALA:HB1	1:A:301:PHE:CE2	2.55	0.42
1:A:625:PHE:O	9:A:802:CLA:HMC2	2.20	0.42
1:a:266:ASN:O	1:a:267:ALA:HB3	2.20	0.42
2:B:222:PHE:N	2:B:227:HIS:O	2.53	0.42
5:E:31:ARG:O	5:E:32:LYS:C	2.62	0.42
7:U:332:SER:OG	7:U:333:GLN:N	2.53	0.42
7:W:277:SER:OG	7:W:285:ARG:NH2	2.47	0.42
1:a:326:ASN:ND2	1:a:349:PHE:O	2.53	0.41
1:A:247:PHE:O	1:A:250:ALA:HB3	2.20	0.41
9:A:827:CLA:HMA1	9:A:827:CLA:O2A	2.20	0.41
1:a:182:ASP:OD2	7:Y:339:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:616:ILE:HB	1:a:691:LEU:HD21	2.02	0.41
3:c:85:ILE:HA	3:c:88:ILE:HG12	2.01	0.41
7:X:191:THR:HG22	7:Y:194:ASN:O	2.20	0.41
1:A:522:SER:C	1:A:524:SER:H	2.28	0.41
9:a:801:CLA:HED3	9:a:801:CLA:OBD	2.19	0.41
7:V:108:ASP:OD1	7:V:109:PHE:N	2.53	0.41
7:Z:21:GLU:OE2	7:Z:250:ARG:NH2	2.52	0.41
13:Z:401:LHG:H102	13:Z:401:LHG:H131	1.81	0.41
1:A:312:GLU:OE2	1:A:312:GLU:HA	2.21	0.41
1:A:444:VAL:O	1:A:448:ILE:HG12	2.21	0.41
1:A:593:THR:HG22	1:A:594:SER:N	2.35	0.41
4:D:119:VAL:O	4:D:120:PHE:C	2.63	0.41
7:U:260:SER:OG	10:U:402:BCL:HED2	2.20	0.41
7:W:144:GLN:NE2	7:W:235:SER:O	2.42	0.41
7:W:293:ILE:N	7:W:294:PRO:CD	2.84	0.41
5:E:17:PRO:HG2	5:E:20:ALA:HB3	2.03	0.41
7:U:108:ASP:OD1	7:U:109:PHE:N	2.53	0.41
7:U:195:GLU:HB2	7:U:300:MET:HE2	2.02	0.41
1:A:218:LEU:O	1:A:222:ILE:HG12	2.20	0.41
9:A:802:CLA:H203	9:a:801:CLA:C14	2.45	0.41
9:A:802:CLA:CMB	9:A:802:CLA:H72	2.51	0.41
9:A:827:CLA:H42	9:A:827:CLA:C3A	2.49	0.41
1:a:131:THR:O	3:C:114:ARG:NH2	2.53	0.41
1:A:571:MET:O	1:A:579:ALA:HB1	2.21	0.41
1:a:468:LEU:HD11	10:a:813:BCL:C19	2.51	0.41
7:V:261:ASP:OD1	7:V:261:ASP:N	2.49	0.41
10:Z:403:BCL:H201	10:Z:406:BCL:H2	2.02	0.41
1:A:383:TYR:OH	10:A:811:BCL:HBB1	2.21	0.41
1:A:526:PRO:CB	1:A:670:ILE:HB	2.51	0.41
1:a:101:PHE:HE2	3:C:97:ARG:HE	1.68	0.41
1:a:560:TRP:HZ3	1:a:596:ILE:HA	1.85	0.41
1:A:120:ARG:NH2	10:A:805:BCL:O1A	2.41	0.41
1:A:616:ILE:HB	1:A:691:LEU:HD21	2.01	0.41
9:A:826:CLA:HBB1	9:A:827:CLA:C3B	2.51	0.41
1:a:163:ARG:NH2	1:a:170:THR:O	2.47	0.41
1:a:270:HIS:O	1:a:274:ASP:N	2.54	0.41
4:D:79:ILE:O	4:D:112:TRP:N	2.52	0.41
7:Y:258:PHE:HA	7:Y:266:GLU:O	2.20	0.41
1:A:348:ASP:O	3:c:107:THR:HG23	2.21	0.41
1:a:99:GLN:O	1:a:107:GLY:N	2.52	0.41
13:a:821:LHG:H112	13:a:821:LHG:HC81	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:GLU:HB2	4:D:52:VAL:HG11	2.03	0.41
2:B:217:ASP:OD1	7:U:259:ARG:NE	2.50	0.41
1:A:681:TYR:CE2	9:A:826:CLA:HBC1	2.56	0.40
10:A:803:BCL:HHC	10:A:803:BCL:CBB	2.47	0.40
1:a:209:HIS:ND1	10:a:809:BCL:OBD	2.46	0.40
7:X:158:ASP:O	7:X:161:ASP:OD1	2.38	0.40
1:A:386:ALA:O	1:A:390:HIS:ND1	2.52	0.40
1:A:409:SER:OG	14:A:823:LMG:HC3	2.21	0.40
1:A:528:LEU:HD22	2:B:192:PRO:HG3	2.03	0.40
9:A:802:CLA:HED2	1:a:429:MET:SD	2.61	0.40
7:Y:293:ILE:N	7:Y:294:PRO:HD2	2.37	0.40
1:A:604:THR:HA	1:A:607:ILE:HB	2.04	0.40
10:A:808:BCL:HHC	10:A:808:BCL:HBB2	2.03	0.40
3:C:120:LYS:O	3:C:124:ASN:ND2	2.44	0.40
3:c:88:ILE:HA	3:c:91:VAL:HG22	2.03	0.40
4:D:117:ILE:N	4:D:118:PRO:CD	2.84	0.40
7:V:295:LEU:HD22	7:V:352:VAL:HB	2.03	0.40
7:W:235:SER:HB2	10:W:406:BCL:HMD1	2.02	0.40
1:A:101:PHE:HE2	3:c:97:ARG:HE	1.67	0.40
1:A:411:TRP:CH2	10:A:804:BCL:HBC2	2.57	0.40
1:A:635:ARG:O	1:A:635:ARG:HD2	2.22	0.40
1:a:407:ILE:O	1:a:416:ARG:NH1	2.49	0.40
1:a:440:TYR:CE2	9:a:801:CLA:H171	2.57	0.40
1:A:556:SER:O	1:A:560:TRP:HD1	2.05	0.40
1:a:67:THR:HG21	1:a:275:MET:O	2.22	0.40
1:a:120:ARG:NH2	10:a:805:BCL:O1A	2.41	0.40
1:a:185:PHE:HA	10:a:806:BCL:H42	2.04	0.40
1:a:495:PHE:CE2	9:a:801:CLA:HMC1	2.57	0.40
6:F:13:PRO:N	6:F:14:PRO:HD2	2.37	0.40
6:F:41:VAL:HA	6:F:44:LEU:CD2	2.52	0.40
7:W:33:ARG:NH2	7:W:270:ASP:OD2	2.52	0.40
7:Z:40:PRO:HA	10:Z:403:BCL:HMD2	2.04	0.40
7:Z:69:ALA:HB3	7:Z:84:ILE: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	648/731 (89%)	619 (96%)	29 (4%)	0	100	100
1	a	650/731 (89%)	616 (95%)	34 (5%)	0	100	100
2	B	110/231 (48%)	99 (90%)	10 (9%)	1 (1%)	14	41
3	C	120/206 (58%)	108 (90%)	12 (10%)	0	100	100
3	c	103/206 (50%)	91 (88%)	11 (11%)	1 (1%)	12	39
4	D	99/143 (69%)	88 (89%)	11 (11%)	0	100	100
5	E	54/59 (92%)	42 (78%)	12 (22%)	0	100	100
6	F	48/58 (83%)	46 (96%)	1 (2%)	1 (2%)	5	22
7	U	361/366 (99%)	340 (94%)	21 (6%)	0	100	100
7	V	358/366 (98%)	345 (96%)	13 (4%)	0	100	100
7	W	356/366 (97%)	338 (95%)	18 (5%)	0	100	100
7	X	355/366 (97%)	343 (97%)	12 (3%)	0	100	100
7	Y	358/366 (98%)	344 (96%)	14 (4%)	0	100	100
7	Z	356/366 (97%)	343 (96%)	13 (4%)	0	100	100
All	All	3976/4561 (87%)	3762 (95%)	211 (5%)	3 (0%)	49	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
6	F	37	ILE
3	c	106	THR

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	538/599 (90%)	536 (100%)	2 (0%)	84	84
1	a	540/599 (90%)	540 (100%)	0	100	100
2	B	96/162 (59%)	96 (100%)	0	100	100
3	C	103/173 (60%)	103 (100%)	0	100	100
3	c	92/173 (53%)	92 (100%)	0	100	100
4	D	90/128 (70%)	90 (100%)	0	100	100
5	E	49/52 (94%)	48 (98%)	1 (2%)	48	69
6	F	40/45 (89%)	40 (100%)	0	100	100
7	U	300/302 (99%)	300 (100%)	0	100	100
7	V	298/302 (99%)	298 (100%)	0	100	100
7	W	296/302 (98%)	296 (100%)	0	100	100
7	X	295/302 (98%)	295 (100%)	0	100	100
7	Y	298/302 (99%)	298 (100%)	0	100	100
7	Z	296/302 (98%)	296 (100%)	0	100	100
All	All	3331/3743 (89%)	3328 (100%)	3 (0%)	87	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	TRP
1	A	214	SER
5	E	6	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	HIS
1	A	266	ASN
1	A	543	GLN
1	a	272	ASN
1	a	303	GLN
1	a	541	GLN
1	a	662	ASN
1	a	699	GLN

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Mol	Chain	Res	Type
7	W	133	ASN
7	Y	334	ASN
7	Z	54	ASN
7	Z	141	GLN
7	Z	144	GLN
7	Z	198	GLN
7	Z	209	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 106 ligands modelled in this entry, 2 are monoatomic - leaving 104 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	$\# Z > 2$
10	BCL	a	805	1	69,74,74	1.11	6 (8%)	79,115,115	1.38	11 (13%)
10	BCL	W	401	-	69,74,74	1.10	5 (7%)	79,115,115	1.62	14 (17%)
10	BCL	V	408	-	69,74,74	1.08	4 (5%)	79,115,115	1.36	10 (12%)
10	BCL	U	403	7	69,74,74	1.05	5 (7%)	79,115,115	1.46	15 (18%)
10	BCL	U	404	7	69,74,74	1.09	4 (5%)	79,115,115	1.44	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	LHG	E	102	-	42,42,48	0.64	0	45,48,54	1.00	2 (4%)
10	BCL	Z	407	-	69,74,74	1.07	6 (8%)	79,115,115	1.43	11 (13%)
10	BCL	a	810	1	69,74,74	1.09	4 (5%)	79,115,115	1.51	13 (16%)
9	CLA	A	827	-	69,73,73	3.97	37 (53%)	82,113,113	2.86	21 (25%)
13	LHG	a	819	-	33,33,48	0.71	0	36,39,54	0.99	2 (5%)
9	CLA	A	802	-	69,73,73	3.93	36 (52%)	82,113,113	2.91	21 (25%)
10	BCL	a	813	1	69,74,74	1.12	4 (5%)	79,115,115	1.38	11 (13%)
10	BCL	a	804	-	69,74,74	1.12	5 (7%)	79,115,115	1.37	10 (12%)
12	F26	a	816	-	40,40,40	1.66	10 (25%)	49,50,50	2.22	13 (26%)
10	BCL	a	811	-	69,74,74	1.11	6 (8%)	79,115,115	1.39	12 (15%)
10	BCL	X	404	7	69,74,74	1.06	4 (5%)	79,115,115	1.33	10 (12%)
10	BCL	A	808	1	69,74,74	1.12	5 (7%)	79,115,115	1.38	10 (12%)
10	BCL	A	812	1	69,74,74	1.12	5 (7%)	79,115,115	1.76	14 (17%)
10	BCL	Y	402	-	69,74,74	1.08	4 (5%)	79,115,115	1.48	10 (12%)
10	BCL	a	814	1	69,74,74	1.12	5 (7%)	79,115,115	1.53	11 (13%)
10	BCL	A	814	1	68,73,74	1.12	4 (5%)	77,113,115	1.39	13 (16%)
14	LMG	A	821	-	41,41,55	0.82	0	49,49,63	1.16	4 (8%)
15	SF4	A	824	1	0,12,12	-	-	-	-	-
10	BCL	A	811	1	69,74,74	1.12	6 (8%)	79,115,115	1.44	11 (13%)
9	CLA	A	826	1	69,73,73	4.14	37 (53%)	82,113,113	2.98	21 (25%)
9	CLA	a	801	1	69,73,73	4.07	38 (55%)	82,113,113	2.88	21 (25%)
10	BCL	Z	404	7	69,74,74	1.04	5 (7%)	79,115,115	1.46	12 (15%)
14	LMG	A	820	-	42,42,55	0.84	1 (2%)	50,50,63	1.17	4 (8%)
10	BCL	A	813	1	69,74,74	1.13	6 (8%)	79,115,115	1.38	10 (12%)
10	BCL	Z	408[B]	7	49,54,74	1.25	5 (10%)	55,91,115	1.50	9 (16%)
10	BCL	X	401	-	69,74,74	1.09	4 (5%)	79,115,115	1.46	12 (15%)
10	BCL	Y	407	7	69,74,74	1.10	5 (7%)	79,115,115	1.46	10 (12%)
10	BCL	W	407	7	69,74,74	1.07	4 (5%)	79,115,115	1.37	11 (13%)
10	BCL	W	403	-	69,74,74	1.10	4 (5%)	79,115,115	1.44	10 (12%)
10	BCL	a	807	1,10	69,74,74	1.07	5 (7%)	79,115,115	1.47	10 (12%)
11	F39	A	815	-	66,66,66	2.74	19 (28%)	83,85,85	2.17	21 (25%)
10	BCL	a	803	1	69,74,74	1.10	5 (7%)	79,115,115	1.38	11 (13%)
10	BCL	B	301	14	69,74,74	1.14	6 (8%)	79,115,115	1.52	14 (17%)
10	BCL	X	407[B]	7	49,54,74	1.24	4 (8%)	55,91,115	1.36	7 (12%)
10	BCL	V	403	-	69,74,74	1.09	5 (7%)	79,115,115	1.33	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	BCL	A	806	1	69,74,74	1.15	4 (5%)	79,115,115	1.63	12 (15%)
14	LMG	A	823	10	31,31,55	0.90	1 (3%)	39,39,63	1.20	4 (10%)
10	BCL	X	402	-	69,74,74	1.10	5 (7%)	79,115,115	1.44	11 (13%)
10	BCL	A	803	1	69,74,74	1.13	5 (7%)	79,115,115	1.51	14 (17%)
13	LHG	a	818	-	44,44,48	0.64	1 (2%)	47,50,54	0.96	2 (4%)
10	BCL	V	406	7	69,74,74	1.08	4 (5%)	79,115,115	1.45	8 (10%)
10	BCL	A	807	1	69,74,74	1.09	6 (8%)	79,115,115	1.43	9 (11%)
15	SF4	B	303	2	0,12,12	-	-	-	-	-
10	BCL	V	405	7	69,74,74	1.06	4 (5%)	79,115,115	1.40	10 (12%)
10	BCL	Y	405	7	69,74,74	1.04	5 (7%)	79,115,115	1.40	11 (13%)
10	BCL	W	405	-	69,74,74	1.11	5 (7%)	79,115,115	1.33	8 (10%)
10	BCL	Z	403	-	69,74,74	1.09	5 (7%)	79,115,115	1.40	9 (11%)
10	BCL	a	808	1	49,54,74	1.21	4 (8%)	55,91,115	1.61	11 (20%)
10	BCL	U	406	-	69,74,74	1.10	5 (7%)	79,115,115	1.39	11 (13%)
13	LHG	Z	401	-	42,42,48	0.62	0	45,48,54	0.98	2 (4%)
10	BCL	V	402	7	69,74,74	1.10	6 (8%)	79,115,115	1.54	14 (17%)
10	BCL	Z	406	-	69,74,74	1.08	4 (5%)	79,115,115	1.43	9 (11%)
10	BCL	Y	404	7	69,74,74	1.08	5 (7%)	79,115,115	1.51	9 (11%)
8	GS0	A	801	1,8	69,74,74	2.23	15 (21%)	79,115,115	2.96	30 (37%)
10	BCL	W	406	-	69,74,74	1.10	4 (5%)	79,115,115	1.37	7 (8%)
10	BCL	X	409	-	69,74,74	1.09	6 (8%)	79,115,115	1.46	11 (13%)
10	BCL	A	804	-	69,74,74	1.14	4 (5%)	79,115,115	1.43	12 (15%)
10	BCL	X	408[B]	7	49,54,74	1.25	6 (12%)	55,91,115	1.40	7 (12%)
10	BCL	A	809	1	69,74,74	1.10	6 (8%)	79,115,115	1.45	11 (13%)
10	BCL	A	810	1	69,74,74	1.11	5 (7%)	79,115,115	1.57	10 (12%)
14	LMG	A	822	-	42,42,55	0.80	1 (2%)	50,50,63	1.12	4 (8%)
10	BCL	V	409[B]	7	49,54,74	1.24	6 (12%)	55,91,115	1.41	6 (10%)
8	GS0	a	802	1,8	69,74,74	2.38	15 (21%)	79,115,115	2.83	28 (35%)
12	F26	A	816	-	40,40,40	1.78	10 (25%)	49,50,50	2.31	15 (30%)
10	BCL	W	402	-	69,74,74	1.08	4 (5%)	79,115,115	1.38	9 (11%)
13	LHG	E	101	-	38,38,48	0.67	0	41,44,54	0.97	2 (4%)
10	BCL	X	403	7	69,74,74	1.07	5 (7%)	79,115,115	1.45	13 (16%)
10	BCL	X	405	-	69,74,74	1.10	5 (7%)	79,115,115	1.45	9 (11%)
13	LHG	A	819	-	33,33,48	0.74	1 (3%)	36,39,54	1.02	3 (8%)
10	BCL	Y	401	-	69,74,74	1.11	5 (7%)	79,115,115	1.48	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	LHG	A	817	-	36,36,48	0.73	1 (2%)	39,42,54	0.99	2 (5%)
12	F26	a	817	-	40,40,40	1.74	10 (25%)	49,50,50	2.27	15 (30%)
10	BCL	U	405	-	69,74,74	1.11	4 (5%)	79,115,115	1.33	8 (10%)
10	BCL	a	809	-	69,74,74	1.16	6 (8%)	79,115,115	1.34	7 (8%)
10	BCL	a	812	-	69,74,74	1.14	5 (7%)	79,115,115	1.42	12 (15%)
10	BCL	Y	408	-	69,74,74	1.09	4 (5%)	79,115,115	1.38	12 (15%)
10	BCL	Y	403	-	69,74,74	1.08	5 (7%)	79,115,115	1.40	12 (15%)
13	LHG	a	821	-	37,37,48	0.69	1 (2%)	40,43,54	0.99	2 (5%)
11	F39	a	815	-	66,66,66	2.80	19 (28%)	83,85,85	2.20	21 (25%)
13	LHG	a	820	-	37,37,48	0.65	0	40,43,54	0.97	2 (5%)
14	LMG	C	302	-	42,42,55	0.80	0	50,50,63	1.16	4 (8%)
10	BCL	X	406	7	69,74,74	1.07	5 (7%)	79,115,115	1.44	12 (15%)
10	BCL	V	401	-	69,74,74	1.09	5 (7%)	79,115,115	1.42	10 (12%)
10	BCL	Z	405	7	69,74,74	1.06	4 (5%)	79,115,115	1.40	10 (12%)
10	BCL	a	806	10	69,74,74	1.09	4 (5%)	79,115,115	1.57	12 (15%)
10	BCL	V	404	-	69,74,74	1.10	4 (5%)	79,115,115	1.45	9 (11%)
10	BCL	U	407[B]	7	49,54,74	1.29	6 (12%)	55,91,115	1.43	7 (12%)
10	BCL	Y	406	7	69,74,74	1.06	4 (5%)	79,115,115	1.37	11 (13%)
10	BCL	W	404	7	69,74,74	1.05	4 (5%)	79,115,115	1.37	11 (13%)
15	SF4	B	302	2	0,12,12	-	-	-	-	-
10	BCL	U	402	7	69,74,74	1.07	4 (5%)	79,115,115	1.39	10 (12%)
10	BCL	W	408[B]	7	49,54,74	1.23	6 (12%)	55,91,115	1.44	7 (12%)
11	F39	C	301	-	66,66,66	2.87	20 (30%)	83,85,85	2.12	24 (28%)
10	BCL	V	407	-	69,74,74	1.12	6 (8%)	79,115,115	1.51	12 (15%)
10	BCL	Z	402	-	69,74,74	1.09	4 (5%)	79,115,115	1.63	15 (18%)
14	LMG	a	822	-	45,45,55	0.77	0	53,53,63	1.16	4 (7%)
10	BCL	U	401	-	69,74,74	1.09	4 (5%)	79,115,115	1.55	11 (13%)
13	LHG	A	818	-	39,39,48	0.71	1 (2%)	42,45,54	1.02	3 (7%)
10	BCL	A	805	1	69,74,74	1.15	6 (8%)	79,115,115	1.48	12 (15%)

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
10	BCL	a	805	1	-	5/41/137/137	-
10	BCL	W	401	-	-	6/41/137/137	-
10	BCL	V	408	-	-	9/41/137/137	-
10	BCL	U	403	7	-	10/41/137/137	-
10	BCL	U	404	7	-	10/41/137/137	-
13	LHG	E	102	-	-	24/47/47/53	-
10	BCL	Z	407	-	-	7/41/137/137	-
10	BCL	a	810	1	-	13/41/137/137	-
9	CLA	A	827	-	3/3/15/20	12/39/115/115	-
13	LHG	a	819	-	-	19/38/38/53	-
9	CLA	A	802	-	3/3/15/20	18/39/115/115	-
10	BCL	a	813	1	-	19/41/137/137	-
10	BCL	a	804	-	-	12/41/137/137	-
12	F26	a	816	-	-	19/36/36/36	0/1/1/1
10	BCL	a	811	-	-	7/41/137/137	-
10	BCL	X	404	7	-	7/41/137/137	-
10	BCL	A	808	1	-	7/41/137/137	-
10	BCL	A	812	1	-	15/41/137/137	-
10	BCL	Y	402	-	-	7/41/137/137	-
10	BCL	a	814	1	-	13/41/137/137	-
10	BCL	A	814	1	-	16/40/136/137	-
14	LMG	A	821	-	-	23/36/56/70	0/1/1/1
15	SF4	A	824	1	-	-	0/6/5/5
10	BCL	A	811	1	-	6/41/137/137	-
9	CLA	A	826	1	3/3/15/20	21/39/115/115	-
9	CLA	a	801	1	3/3/15/20	19/39/115/115	-
10	BCL	Z	404	7	-	8/41/137/137	-
14	LMG	A	820	-	-	19/37/57/70	0/1/1/1
10	BCL	A	813	1	-	26/41/137/137	-
10	BCL	Z	408[B]	7	-	9/17/113/137	-
10	BCL	X	401	-	-	5/41/137/137	-
10	BCL	Y	407	7	-	11/41/137/137	-
10	BCL	W	407	7	-	7/41/137/137	-
10	BCL	W	403	-	-	14/41/137/137	-
10	BCL	a	807	1,10	-	14/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	F39	A	815	-	-	33/58/78/78	0/2/2/2
10	BCL	a	803	1	-	11/41/137/137	-
10	BCL	B	301	14	-	17/41/137/137	-
10	BCL	X	407[B]	7	-	8/17/113/137	-
10	BCL	V	403	-	-	7/41/137/137	-
10	BCL	A	806	1	-	16/41/137/137	-
14	LMG	A	823	10	-	4/26/46/70	0/1/1/1
10	BCL	X	402	-	-	13/41/137/137	-
10	BCL	A	803	1	-	14/41/137/137	-
13	LHG	a	818	-	-	23/49/49/53	-
10	BCL	V	406	7	-	7/41/137/137	-
10	BCL	A	807	1	-	13/41/137/137	-
15	SF4	B	303	2	-	-	0/6/5/5
10	BCL	V	405	7	-	9/41/137/137	-
10	BCL	Y	405	7	-	6/41/137/137	-
10	BCL	W	405	-	-	15/41/137/137	-
10	BCL	Z	403	-	-	15/41/137/137	-
10	BCL	a	808	1	-	6/17/113/137	-
10	BCL	U	406	-	-	5/41/137/137	-
13	LHG	Z	401	-	-	26/47/47/53	-
10	BCL	V	402	7	-	8/41/137/137	-
10	BCL	Z	406	-	-	9/41/137/137	-
10	BCL	Y	404	7	-	16/41/137/137	-
8	GS0	A	801	1,8	2/2/21/25	21/41/137/137	-
10	BCL	W	406	-	-	5/41/137/137	-
10	BCL	X	409	-	-	5/41/137/137	-
10	BCL	A	804	-	-	15/41/137/137	-
10	BCL	X	408[B]	7	-	8/17/113/137	-
10	BCL	A	809	1	-	15/41/137/137	-
10	BCL	A	810	1	-	7/41/137/137	-
14	LMG	A	822	-	-	25/37/57/70	0/1/1/1
10	BCL	V	409[B]	7	-	11/17/113/137	-
8	GS0	a	802	1,8	2/2/21/25	17/41/137/137	-
12	F26	A	816	-	-	19/36/36/36	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BCL	W	402	-	-	9/41/137/137	-
13	LHG	E	101	-	-	20/43/43/53	-
10	BCL	X	403	7	-	9/41/137/137	-
10	BCL	X	405	-	-	3/41/137/137	-
13	LHG	A	819	-	-	19/38/38/53	-
10	BCL	Y	401	-	-	10/41/137/137	-
13	LHG	A	817	-	-	17/41/41/53	-
12	F26	a	817	-	-	22/36/36/36	0/1/1/1
10	BCL	U	405	-	-	6/41/137/137	-
10	BCL	a	809	-	-	17/41/137/137	-
10	BCL	a	812	-	-	18/41/137/137	-
10	BCL	Y	408	-	-	5/41/137/137	-
10	BCL	Y	403	-	-	10/41/137/137	-
13	LHG	a	821	-	-	20/42/42/53	-
11	F39	a	815	-	-	39/58/78/78	0/2/2/2
13	LHG	a	820	-	-	25/42/42/53	-
14	LMG	C	302	-	-	19/37/57/70	0/1/1/1
10	BCL	X	406	7	-	5/41/137/137	-
10	BCL	V	401	-	-	12/41/137/137	-
10	BCL	Z	405	7	-	12/41/137/137	-
10	BCL	a	806	10	-	21/41/137/137	-
10	BCL	V	404	-	-	12/41/137/137	-
10	BCL	U	407[B]	7	-	9/17/113/137	-
10	BCL	Y	406	7	-	8/41/137/137	-
10	BCL	W	404	7	-	6/41/137/137	-
15	SF4	B	302	2	-	-	0/6/5/5
10	BCL	U	402	7	-	16/41/137/137	-
10	BCL	W	408[B]	7	-	11/17/113/137	-
11	F39	C	301	-	-	33/58/78/78	0/2/2/2
10	BCL	V	407	-	-	7/41/137/137	-
10	BCL	Z	402	-	-	6/41/137/137	-
14	LMG	a	822	-	-	20/40/60/70	0/1/1/1
10	BCL	U	401	-	-	7/41/137/137	-
13	LHG	A	818	-	-	22/44/44/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BCL	A	805	1	-	13/41/137/137	-

All (627) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	826	CLA	MG-ND	17.12	2.39	2.05
9	a	801	CLA	MG-ND	15.45	2.36	2.05
9	A	827	CLA	MG-ND	14.66	2.34	2.05
9	A	802	CLA	MG-ND	14.27	2.34	2.05
9	A	826	CLA	MG-NA	12.95	2.37	2.06
9	a	801	CLA	MG-NC	12.78	2.36	2.06
9	A	827	CLA	MG-NA	11.93	2.34	2.06
9	A	802	CLA	MG-NC	11.15	2.32	2.06
8	a	802	GS0	MG-NC	11.05	2.32	2.06
9	a	801	CLA	MG-NA	11.05	2.32	2.06
9	A	802	CLA	MG-NA	10.62	2.31	2.06
9	A	826	CLA	MG-NC	10.42	2.31	2.06
9	A	827	CLA	MG-NC	10.10	2.30	2.06
8	A	801	GS0	MG-NC	9.15	2.28	2.06
9	A	827	CLA	C4B-NB	8.77	1.49	1.37
9	A	802	CLA	C4B-NB	8.72	1.49	1.37
9	a	801	CLA	C4B-NB	8.41	1.48	1.37
9	A	826	CLA	C4B-NB	7.80	1.48	1.37
11	C	301	F39	C35-C37	7.59	1.62	1.46
11	a	815	F39	C35-C37	7.40	1.61	1.46
11	A	815	F39	C35-C37	7.24	1.61	1.46
11	C	301	F39	C56-C58	7.22	1.61	1.46
11	a	815	F39	C56-C58	7.18	1.61	1.46
9	A	802	CLA	CAA-C2A	-7.10	1.41	1.54
11	C	301	F39	C64-C62	7.08	1.61	1.46
9	A	826	CLA	CAA-C2A	-7.02	1.41	1.54
11	A	815	F39	C56-C58	7.00	1.60	1.46
9	A	827	CLA	CAA-C2A	-6.86	1.41	1.54
8	a	802	GS0	MG-NA	6.86	2.22	2.06
9	a	801	CLA	CAA-C2A	-6.80	1.41	1.54
8	a	802	GS0	MG-ND	-6.75	1.92	2.05
11	A	815	F39	C64-C62	6.67	1.60	1.46
11	a	815	F39	C64-C62	6.62	1.60	1.46
8	A	801	GS0	MG-NA	6.61	2.22	2.06
11	C	301	F39	C41-C42	6.46	1.59	1.46
11	a	815	F39	C41-C42	6.45	1.59	1.46
8	A	801	GS0	MG-ND	-6.38	1.93	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	815	F39	C41-C42	6.35	1.59	1.46
9	A	826	CLA	C1B-C2B	6.26	1.57	1.43
9	a	801	CLA	C1B-C2B	6.16	1.57	1.43
11	a	815	F39	C46-C53	6.06	1.60	1.47
9	A	802	CLA	C1B-C2B	5.96	1.57	1.43
9	A	827	CLA	C1B-C2B	5.93	1.57	1.43
11	C	301	F39	C46-C53	5.87	1.60	1.47
9	a	801	CLA	C1D-ND	5.82	1.45	1.37
11	A	815	F39	C46-C53	5.79	1.59	1.47
9	A	826	CLA	C1D-ND	5.74	1.45	1.37
9	A	827	CLA	C1D-ND	5.70	1.45	1.37
8	a	802	GS0	MG-NB	-5.60	1.94	2.05
9	A	802	CLA	C1D-ND	5.50	1.45	1.37
8	A	801	GS0	MG-NB	-5.43	1.95	2.05
11	C	301	F39	C51-C44	5.42	1.60	1.43
9	A	826	CLA	CHC-C1C	5.40	1.49	1.38
11	C	301	F39	C57-C59	5.40	1.59	1.43
11	C	301	F39	C32-C27	5.38	1.59	1.43
9	A	827	CLA	CHC-C1C	5.37	1.49	1.38
11	C	301	F39	C63-C61	5.36	1.59	1.43
11	A	815	F39	C51-C44	5.35	1.59	1.43
11	a	815	F39	C32-C27	5.33	1.59	1.43
9	A	802	CLA	CHC-C1C	5.30	1.49	1.38
11	a	815	F39	C51-C44	5.30	1.59	1.43
9	a	801	CLA	CHC-C1C	5.29	1.49	1.38
11	C	301	F39	C40-C39	5.27	1.59	1.43
11	a	815	F39	C40-C39	5.23	1.59	1.43
11	A	815	F39	C32-C27	5.23	1.59	1.43
11	A	815	F39	C63-C61	5.18	1.59	1.43
11	A	815	F39	C40-C39	5.18	1.59	1.43
9	A	826	CLA	CMA-C3A	-5.17	1.42	1.53
11	a	815	F39	C63-C61	5.12	1.59	1.43
11	A	815	F39	C57-C59	5.09	1.59	1.43
9	a	801	CLA	CMA-C3A	-5.09	1.42	1.53
11	a	815	F39	C57-C59	5.04	1.58	1.43
9	A	802	CLA	CMA-C3A	-5.01	1.42	1.53
9	A	827	CLA	CMA-C3A	-5.00	1.42	1.53
9	A	802	CLA	C3B-C4B	4.99	1.57	1.42
9	A	827	CLA	C3B-C4B	4.98	1.57	1.42
9	A	826	CLA	CHB-C4A	4.91	1.50	1.37
9	a	801	CLA	C3B-C4B	4.88	1.56	1.42
11	C	301	F39	C14-C13	4.86	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	826	CLA	C3B-C4B	4.83	1.56	1.42
9	A	827	CLA	C3C-C2C	4.77	1.47	1.36
9	a	801	CLA	CHB-C4A	4.75	1.49	1.37
9	A	827	CLA	CHB-C4A	4.73	1.49	1.37
9	A	802	CLA	C3C-C2C	4.72	1.47	1.36
9	A	826	CLA	C3C-C2C	4.71	1.46	1.36
9	A	802	CLA	CHB-C4A	4.63	1.49	1.37
9	a	801	CLA	C3C-C2C	4.62	1.46	1.36
11	a	815	F39	C14-C13	4.61	1.60	1.53
9	A	802	CLA	CBD-CGD	-4.56	1.38	1.52
11	C	301	F39	C19-C20	4.56	1.60	1.51
9	a	801	CLA	C1C-C2C	4.56	1.53	1.44
9	a	801	CLA	CBD-CGD	-4.55	1.38	1.52
9	A	802	CLA	C1C-C2C	4.51	1.53	1.44
10	Y	402	BCL	MG-NA	4.50	2.17	2.06
9	A	826	CLA	CBD-CGD	-4.50	1.38	1.52
9	A	827	CLA	CBD-CGD	-4.48	1.38	1.52
9	A	827	CLA	C1C-C2C	4.48	1.53	1.44
10	W	401	BCL	MG-NA	4.44	2.16	2.06
10	X	405	BCL	MG-NA	4.43	2.16	2.06
10	U	401	BCL	MG-NA	4.42	2.16	2.06
10	V	402	BCL	MG-NA	4.41	2.16	2.06
10	X	401	BCL	MG-NA	4.40	2.16	2.06
10	V	407	BCL	MG-NA	4.40	2.16	2.06
8	A	801	GS0	O1D-CGD	-4.40	1.10	1.21
10	a	813	BCL	MG-NA	4.36	2.16	2.06
10	Y	408	BCL	MG-NA	4.35	2.16	2.06
10	Z	408[B]	BCL	MG-NA	4.34	2.16	2.06
10	V	401	BCL	MG-NA	4.32	2.16	2.06
10	B	301	BCL	MG-NA	4.32	2.16	2.06
10	W	406	BCL	MG-NA	4.31	2.16	2.06
10	U	406	BCL	MG-NA	4.31	2.16	2.06
10	W	403	BCL	MG-NA	4.31	2.16	2.06
8	A	801	GS0	OBD-CAD	4.29	1.29	1.22
10	X	406	BCL	MG-NA	4.29	2.16	2.06
10	U	407[B]	BCL	MG-NA	4.29	2.16	2.06
10	Y	406	BCL	MG-NA	4.28	2.16	2.06
10	V	404	BCL	MG-NA	4.26	2.16	2.06
11	a	815	F39	C19-C20	4.26	1.60	1.51
10	A	808	BCL	MG-NA	4.24	2.16	2.06
10	V	409[B]	BCL	MG-NA	4.24	2.16	2.06
10	V	408	BCL	MG-NA	4.23	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	802	GS0	O1D-CGD	-4.23	1.10	1.21
10	Z	407	BCL	MG-NA	4.23	2.16	2.06
10	V	403	BCL	MG-NA	4.22	2.16	2.06
10	X	402	BCL	MG-NA	4.22	2.16	2.06
8	a	802	GS0	OBD-CAD	4.22	1.29	1.22
10	V	406	BCL	MG-NA	4.22	2.16	2.06
10	a	808	BCL	MG-NA	4.21	2.16	2.06
10	X	407[B]	BCL	MG-NA	4.21	2.16	2.06
10	Y	404	BCL	MG-NA	4.20	2.16	2.06
10	Z	402	BCL	MG-NA	4.20	2.16	2.06
11	A	815	F39	C19-C20	4.19	1.59	1.51
10	A	812	BCL	MG-NA	4.19	2.16	2.06
10	A	809	BCL	MG-NA	4.19	2.16	2.06
10	W	402	BCL	MG-NA	4.19	2.16	2.06
10	U	405	BCL	MG-NA	4.18	2.16	2.06
10	X	408[B]	BCL	MG-NA	4.18	2.16	2.06
10	Z	403	BCL	MG-NA	4.17	2.16	2.06
9	a	801	CLA	O2D-CGD	4.16	1.43	1.33
11	A	815	F39	C14-C13	4.16	1.59	1.53
10	Y	401	BCL	MG-NA	4.15	2.16	2.06
10	U	404	BCL	MG-NA	4.14	2.16	2.06
10	W	408[B]	BCL	MG-NA	4.14	2.16	2.06
10	Z	405	BCL	MG-NA	4.12	2.16	2.06
10	W	407	BCL	MG-NA	4.12	2.16	2.06
10	a	812	BCL	MG-NA	4.12	2.16	2.06
10	X	409	BCL	MG-NA	4.12	2.16	2.06
9	A	826	CLA	C1C-C2C	4.11	1.52	1.44
10	A	810	BCL	MG-NA	4.10	2.16	2.06
10	W	405	BCL	MG-NA	4.09	2.16	2.06
10	a	804	BCL	MG-NA	4.08	2.16	2.06
10	a	805	BCL	MG-NA	4.08	2.16	2.06
10	X	404	BCL	MG-NA	4.07	2.15	2.06
10	X	403	BCL	MG-NA	4.06	2.15	2.06
9	A	826	CLA	O2D-CGD	4.06	1.43	1.33
10	A	814	BCL	MG-NA	4.06	2.15	2.06
10	Y	403	BCL	MG-NA	4.06	2.15	2.06
10	W	404	BCL	MG-NA	4.05	2.15	2.06
10	Y	407	BCL	MG-NA	4.05	2.15	2.06
9	A	802	CLA	C4C-C3C	4.05	1.51	1.45
9	A	827	CLA	O2D-CGD	4.03	1.43	1.33
10	Z	406	BCL	MG-NA	4.03	2.15	2.06
10	A	807	BCL	MG-NA	4.03	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	a	809	BCL	MG-NA	4.02	2.15	2.06
10	A	804	BCL	MG-NA	4.02	2.15	2.06
10	a	807	BCL	MG-NA	4.01	2.15	2.06
10	U	402	BCL	MG-NA	4.01	2.15	2.06
10	a	814	BCL	MG-NA	3.99	2.15	2.06
10	A	805	BCL	MG-NA	3.99	2.15	2.06
9	A	827	CLA	C4C-C3C	3.98	1.51	1.45
10	U	403	BCL	MG-NA	3.97	2.15	2.06
10	a	810	BCL	MG-NA	3.96	2.15	2.06
10	Y	405	BCL	MG-NA	3.94	2.15	2.06
10	V	405	BCL	MG-NA	3.93	2.15	2.06
10	A	806	BCL	MG-NA	3.93	2.15	2.06
10	Z	404	BCL	MG-NA	3.89	2.15	2.06
9	A	826	CLA	O2A-CGA	3.87	1.44	1.33
10	A	813	BCL	MG-NA	3.87	2.15	2.06
10	A	803	BCL	MG-NA	3.87	2.15	2.06
10	a	806	BCL	MG-NA	3.86	2.15	2.06
9	A	827	CLA	O2A-CGA	3.86	1.44	1.33
9	a	801	CLA	O2A-CGA	3.84	1.44	1.33
9	A	827	CLA	CHD-C4C	3.84	1.47	1.39
9	a	801	CLA	C4C-C3C	3.84	1.51	1.45
9	A	802	CLA	O2D-CGD	3.83	1.42	1.33
10	a	811	BCL	MG-NA	3.81	2.15	2.06
10	A	811	BCL	MG-NA	3.81	2.15	2.06
9	A	802	CLA	CHD-C4C	3.81	1.47	1.39
9	A	802	CLA	O2A-CGA	3.80	1.44	1.33
10	a	803	BCL	MG-NA	3.76	2.15	2.06
9	A	826	CLA	C4C-C3C	3.76	1.51	1.45
9	a	801	CLA	CHB-C1B	3.75	1.47	1.39
9	A	826	CLA	CHB-C1B	3.73	1.47	1.39
9	A	826	CLA	CHD-C4C	3.70	1.47	1.39
9	A	827	CLA	CHB-C1B	3.64	1.47	1.39
8	a	802	GS0	O2D-CED	3.63	1.53	1.45
9	A	826	CLA	C2-C3	3.62	1.41	1.33
10	a	812	BCL	CHD-C1D	3.60	1.45	1.38
12	A	816	F26	C35-C34	3.59	1.53	1.46
10	A	806	BCL	CHD-C1D	3.58	1.45	1.38
9	a	801	CLA	CHD-C4C	3.57	1.47	1.39
9	A	827	CLA	C5-C3	3.55	1.58	1.51
12	A	816	F26	C25-C26	3.54	1.53	1.46
9	A	802	CLA	CHB-C1B	3.53	1.47	1.39
10	A	803	BCL	CHD-C1D	3.52	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	801	GS0	O2D-CED	3.52	1.53	1.45
10	W	405	BCL	CHD-C1D	3.51	1.45	1.38
10	B	301	BCL	CHD-C1D	3.51	1.45	1.38
10	A	806	BCL	MG-ND	-3.46	1.98	2.05
9	a	801	CLA	C5-C3	3.46	1.58	1.51
9	A	827	CLA	O1D-CGD	3.45	1.29	1.21
10	A	814	BCL	CHD-C1D	3.44	1.45	1.38
12	a	817	F26	C35-C34	3.42	1.53	1.46
9	a	801	CLA	C2-C3	3.42	1.40	1.33
10	a	814	BCL	CHD-C1D	3.42	1.45	1.38
12	A	816	F26	C28-C31	3.42	1.53	1.46
9	A	826	CLA	O1D-CGD	3.42	1.29	1.21
9	A	802	CLA	O1D-CGD	3.41	1.29	1.21
9	A	802	CLA	C5-C3	3.41	1.58	1.51
12	a	817	F26	C25-C26	3.41	1.53	1.46
9	A	827	CLA	OBD-CAD	3.40	1.28	1.22
10	a	804	BCL	CHD-C1D	3.40	1.45	1.38
10	U	406	BCL	CHD-C1D	3.38	1.45	1.38
9	A	802	CLA	C2-C3	3.37	1.40	1.33
10	U	404	BCL	CHD-C1D	3.37	1.45	1.38
9	A	827	CLA	C2-C3	3.37	1.40	1.33
10	A	805	BCL	CHD-C1D	3.37	1.45	1.38
10	A	811	BCL	CHD-C1D	3.35	1.44	1.38
9	a	801	CLA	O1D-CGD	3.35	1.29	1.21
10	A	812	BCL	CHD-C1D	3.35	1.44	1.38
12	a	817	F26	C28-C31	3.35	1.53	1.46
12	a	817	F26	C15-C19	3.34	1.53	1.46
9	A	826	CLA	C5-C3	3.34	1.58	1.51
9	A	802	CLA	OBD-CAD	3.34	1.28	1.22
10	V	408	BCL	CHD-C1D	3.31	1.44	1.38
9	A	802	CLA	C4D-CHA	3.30	1.49	1.38
10	Y	406	BCL	CHD-C1D	3.30	1.44	1.38
10	A	804	BCL	CHD-C1D	3.29	1.44	1.38
12	a	816	F26	C15-C19	3.29	1.53	1.46
10	a	811	BCL	CHD-C1D	3.29	1.44	1.38
10	W	401	BCL	CHD-C1D	3.28	1.44	1.38
9	a	801	CLA	C4D-CHA	3.28	1.49	1.38
10	Y	402	BCL	CHD-C1D	3.28	1.44	1.38
12	a	816	F26	C28-C31	3.27	1.53	1.46
9	A	826	CLA	OBD-CAD	3.26	1.28	1.22
12	A	816	F26	C15-C19	3.26	1.52	1.46
10	U	401	BCL	CHD-C1D	3.25	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	816	F26	C25-C26	3.25	1.52	1.46
10	U	407[B]	BCL	CHD-C1D	3.25	1.44	1.38
10	X	401	BCL	CHD-C1D	3.24	1.44	1.38
12	a	816	F26	C35-C34	3.24	1.52	1.46
10	Y	408	BCL	CHD-C1D	3.24	1.44	1.38
10	a	806	BCL	MG-ND	-3.23	1.99	2.05
10	X	404	BCL	CHD-C1D	3.22	1.44	1.38
10	a	806	BCL	CHD-C1D	3.22	1.44	1.38
10	X	408[B]	BCL	CHD-C1D	3.22	1.44	1.38
10	V	406	BCL	CHD-C1D	3.22	1.44	1.38
10	Y	407	BCL	CHD-C1D	3.21	1.44	1.38
10	V	402	BCL	CHD-C1D	3.20	1.44	1.38
10	Z	402	BCL	CHD-C1D	3.20	1.44	1.38
10	a	803	BCL	CHD-C1D	3.20	1.44	1.38
10	W	403	BCL	CHD-C1D	3.19	1.44	1.38
10	X	406	BCL	CHD-C1D	3.19	1.44	1.38
10	Z	405	BCL	CHD-C1D	3.19	1.44	1.38
10	a	808	BCL	CHD-C1D	3.17	1.44	1.38
9	A	827	CLA	C4D-CHA	3.17	1.49	1.38
10	U	403	BCL	CHD-C1D	3.17	1.44	1.38
10	X	407[B]	BCL	CHD-C1D	3.15	1.44	1.38
10	U	405	BCL	CHD-C1D	3.13	1.44	1.38
10	W	404	BCL	CHD-C1D	3.13	1.44	1.38
10	X	405	BCL	CHD-C1D	3.12	1.44	1.38
9	A	826	CLA	C4D-CHA	3.12	1.49	1.38
10	a	809	BCL	CHD-C1D	3.11	1.44	1.38
12	A	816	F26	C32-C30	3.11	1.52	1.43
10	A	808	BCL	CHD-C1D	3.11	1.44	1.38
10	W	407	BCL	CHD-C1D	3.11	1.44	1.38
10	V	409[B]	BCL	CHD-C1D	3.10	1.44	1.38
8	a	802	GS0	O2D-CGD	-3.09	1.25	1.33
10	W	406	BCL	CHD-C1D	3.09	1.44	1.38
9	A	827	CLA	CHD-C1D	3.09	1.44	1.38
10	X	403	BCL	CHD-C1D	3.09	1.44	1.38
10	Z	408[B]	BCL	CHD-C1D	3.08	1.44	1.38
10	V	404	BCL	CHD-C1D	3.08	1.44	1.38
10	a	810	BCL	CHD-C1D	3.06	1.44	1.38
10	V	403	BCL	CHD-C1D	3.05	1.44	1.38
10	Y	405	BCL	CHD-C1D	3.04	1.44	1.38
10	W	402	BCL	CHD-C1D	3.04	1.44	1.38
12	A	816	F26	C22-C18	3.04	1.52	1.43
10	A	809	BCL	CHD-C1D	3.03	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	816	F26	C27-C24	3.03	1.52	1.43
12	a	817	F26	C32-C30	3.03	1.52	1.43
10	V	401	BCL	CHD-C1D	3.03	1.44	1.38
10	A	807	BCL	CHD-C1D	3.03	1.44	1.38
8	a	802	GS0	O2A-CGA	-3.02	1.24	1.33
9	A	802	CLA	CHD-C1D	3.01	1.44	1.38
10	Z	407	BCL	CHD-C1D	3.01	1.44	1.38
12	A	816	F26	C39-C37	3.01	1.52	1.43
8	A	801	GS0	O2A-CGA	-3.00	1.24	1.33
10	A	811	BCL	MG-ND	-3.00	1.99	2.05
10	A	813	BCL	CHD-C1D	3.00	1.44	1.38
10	Z	406	BCL	CHD-C1D	3.00	1.44	1.38
10	a	805	BCL	CHD-C1D	2.99	1.44	1.38
10	A	810	BCL	CHD-C1D	2.99	1.44	1.38
10	Y	403	BCL	CHD-C1D	2.98	1.44	1.38
12	A	816	F26	C38-C33	2.98	1.52	1.43
12	a	817	F26	C39-C37	2.97	1.52	1.43
12	a	816	F26	C27-C24	2.97	1.52	1.43
8	A	801	GS0	O2D-CGD	-2.96	1.25	1.33
10	Y	401	BCL	CHD-C1D	2.96	1.44	1.38
10	V	407	BCL	CHD-C1D	2.96	1.44	1.38
12	a	817	F26	C38-C33	2.95	1.52	1.43
12	a	816	F26	C32-C30	2.94	1.52	1.43
10	V	404	BCL	MG-ND	-2.94	2.00	2.05
10	U	402	BCL	CHD-C1D	2.93	1.44	1.38
10	W	403	BCL	MG-ND	-2.92	2.00	2.05
9	A	826	CLA	CHD-C1D	2.92	1.44	1.38
10	A	809	BCL	MG-ND	-2.92	2.00	2.05
12	a	816	F26	C39-C37	2.91	1.52	1.43
10	Y	404	BCL	CHD-C1D	2.91	1.44	1.38
10	a	813	BCL	CHD-C1D	2.90	1.44	1.38
12	a	817	F26	C22-C18	2.89	1.52	1.43
12	a	816	F26	C38-C33	2.89	1.52	1.43
12	a	817	F26	C27-C24	2.89	1.52	1.43
9	a	801	CLA	CHD-C1D	2.89	1.44	1.38
10	V	405	BCL	CHD-C1D	2.89	1.44	1.38
10	Z	403	BCL	CHD-C1D	2.89	1.44	1.38
10	a	807	BCL	CHD-C1D	2.88	1.44	1.38
10	W	408[B]	BCL	CHD-C1D	2.88	1.44	1.38
10	a	811	BCL	MG-ND	-2.88	2.00	2.05
12	a	816	F26	C22-C18	2.87	1.52	1.43
10	W	406	BCL	MG-ND	-2.86	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	a	803	BCL	MG-ND	-2.86	2.00	2.05
10	a	809	BCL	MG-ND	-2.86	2.00	2.05
10	a	814	BCL	MG-ND	-2.85	2.00	2.05
10	X	409	BCL	CHD-C1D	2.85	1.44	1.38
10	Z	404	BCL	CHD-C1D	2.85	1.44	1.38
8	A	801	GS0	O1A-CGA	-2.84	1.14	1.22
12	a	817	F26	C8-C13	2.83	1.57	1.51
10	X	402	BCL	CHD-C1D	2.83	1.43	1.38
8	a	802	GS0	O1A-CGA	-2.81	1.14	1.22
10	Y	408	BCL	MG-ND	-2.81	2.00	2.05
10	X	404	BCL	MG-ND	-2.80	2.00	2.05
9	A	802	CLA	C3A-C2A	-2.80	1.46	1.54
10	U	404	BCL	MG-ND	-2.80	2.00	2.05
9	a	801	CLA	OBD-CAD	2.80	1.27	1.22
10	X	409	BCL	MG-ND	-2.79	2.00	2.05
8	a	802	GS0	C1D-C2D	-2.79	1.39	1.45
10	X	402	BCL	MG-ND	-2.78	2.00	2.05
10	U	405	BCL	MG-ND	-2.78	2.00	2.05
9	A	826	CLA	C6-C7	-2.77	1.40	1.52
9	A	827	CLA	C3A-C2A	-2.76	1.47	1.54
10	W	405	BCL	MG-ND	-2.76	2.00	2.05
9	A	802	CLA	C6-C7	-2.75	1.40	1.52
10	Y	407	BCL	MG-ND	-2.75	2.00	2.05
9	A	826	CLA	C3A-C2A	-2.75	1.47	1.54
10	X	405	BCL	MG-ND	-2.75	2.00	2.05
10	A	803	BCL	MG-ND	-2.75	2.00	2.05
10	Z	403	BCL	MG-ND	-2.75	2.00	2.05
10	Z	407	BCL	MG-ND	-2.74	2.00	2.05
10	a	810	BCL	MG-ND	-2.74	2.00	2.05
10	W	401	BCL	MG-ND	-2.74	2.00	2.05
10	A	808	BCL	MG-ND	-2.74	2.00	2.05
8	a	802	GS0	OBB-CAB	-2.74	1.17	1.23
10	V	405	BCL	MG-ND	-2.74	2.00	2.05
12	A	816	F26	C8-C13	2.74	1.56	1.51
10	A	814	BCL	MG-ND	-2.73	2.00	2.05
10	V	407	BCL	MG-ND	-2.73	2.00	2.05
10	Y	402	BCL	MG-ND	-2.73	2.00	2.05
10	B	301	BCL	MG-ND	-2.72	2.00	2.05
9	a	801	CLA	C6-C7	-2.72	1.40	1.52
10	a	813	BCL	MG-ND	-2.72	2.00	2.05
9	A	827	CLA	C6-C7	-2.72	1.40	1.52
10	V	408	BCL	MG-ND	-2.72	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	804	BCL	MG-ND	-2.71	2.00	2.05
10	Z	402	BCL	MG-ND	-2.70	2.00	2.05
11	C	301	F39	C11-C9	2.70	1.60	1.52
10	U	401	BCL	MG-ND	-2.70	2.00	2.05
10	A	805	BCL	C3D-C4D	-2.69	1.38	1.44
10	A	807	BCL	MG-ND	-2.69	2.00	2.05
9	A	802	CLA	C3D-C2D	2.67	1.46	1.39
10	Z	405	BCL	MG-ND	-2.67	2.00	2.05
10	U	402	BCL	MG-ND	-2.65	2.00	2.05
10	A	810	BCL	MG-ND	-2.65	2.00	2.05
10	V	402	BCL	MG-ND	-2.65	2.00	2.05
10	W	404	BCL	MG-ND	-2.65	2.00	2.05
10	A	813	BCL	MG-ND	-2.65	2.00	2.05
9	A	827	CLA	C3D-C2D	2.64	1.46	1.39
10	A	808	BCL	C3B-C4B	2.64	1.46	1.41
10	W	407	BCL	MG-ND	-2.64	2.00	2.05
10	W	402	BCL	MG-ND	-2.64	2.00	2.05
9	A	826	CLA	C3D-C2D	2.64	1.46	1.39
10	A	812	BCL	MG-ND	-2.64	2.00	2.05
10	a	812	BCL	MG-ND	-2.63	2.00	2.05
11	a	815	F39	C50-C49	2.63	1.43	1.38
9	A	802	CLA	O1A-CGA	2.63	1.30	1.22
8	A	801	GS0	C1B-C2B	-2.63	1.37	1.43
10	U	406	BCL	MG-ND	-2.63	2.00	2.05
10	a	804	BCL	MG-ND	-2.62	2.00	2.05
11	C	301	F39	C50-C49	2.62	1.43	1.38
10	Y	405	BCL	MG-ND	-2.61	2.00	2.05
11	A	815	F39	C50-C49	2.60	1.43	1.38
10	a	805	BCL	MG-ND	-2.60	2.00	2.05
11	a	815	F39	C46-C48	2.60	1.44	1.41
10	Y	401	BCL	MG-ND	-2.60	2.00	2.05
8	A	801	GS0	OBB-CAB	-2.59	1.17	1.23
10	V	403	BCL	MG-ND	-2.59	2.00	2.05
9	A	826	CLA	C1-C2	2.59	1.56	1.49
10	Z	408[B]	BCL	MG-ND	-2.59	2.00	2.05
9	a	801	CLA	CBA-CGA	2.59	1.58	1.50
9	A	827	CLA	C1-C2	2.59	1.56	1.49
10	Z	406	BCL	MG-ND	-2.58	2.00	2.05
9	A	827	CLA	O1A-CGA	2.58	1.30	1.22
10	A	805	BCL	MG-ND	-2.58	2.00	2.05
10	V	401	BCL	MG-ND	-2.58	2.00	2.05
10	X	403	BCL	MG-ND	-2.58	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	818	LHG	O7-C5	-2.57	1.40	1.46
9	a	801	CLA	O2D-CED	2.57	1.51	1.45
10	U	407[B]	BCL	MG-ND	-2.57	2.00	2.05
9	a	801	CLA	C3A-C2A	-2.57	1.47	1.54
10	Y	404	BCL	MG-ND	-2.57	2.00	2.05
10	Y	406	BCL	MG-ND	-2.56	2.00	2.05
9	A	826	CLA	O1A-CGA	2.56	1.30	1.22
10	X	406	BCL	MG-ND	-2.55	2.00	2.05
10	Z	404	BCL	MG-ND	-2.55	2.00	2.05
10	U	403	BCL	MG-ND	-2.55	2.00	2.05
10	V	406	BCL	MG-ND	-2.54	2.00	2.05
10	V	409[B]	BCL	MG-ND	-2.53	2.00	2.05
8	A	801	GS0	C1D-C2D	-2.53	1.40	1.45
10	X	407[B]	BCL	MG-ND	-2.53	2.00	2.05
9	A	827	CLA	CBA-CGA	2.52	1.58	1.50
9	A	802	CLA	CBA-CGA	2.52	1.58	1.50
9	a	801	CLA	O1A-CGA	2.51	1.30	1.22
10	W	408[B]	BCL	MG-ND	-2.51	2.00	2.05
10	X	408[B]	BCL	MG-ND	-2.50	2.00	2.05
10	Y	403	BCL	MG-ND	-2.50	2.00	2.05
9	A	802	CLA	C1-C2	2.50	1.56	1.49
10	a	808	BCL	MG-ND	-2.49	2.00	2.05
9	a	801	CLA	C1-C2	2.49	1.56	1.49
11	C	301	F39	O6-C21	2.48	1.40	1.33
9	A	826	CLA	CBA-CGA	2.48	1.57	1.50
10	a	807	BCL	MG-ND	-2.46	2.00	2.05
11	C	301	F39	C23-C22	2.45	1.61	1.52
11	C	301	F39	C46-C48	2.45	1.44	1.41
11	A	815	F39	C46-C48	2.43	1.44	1.41
10	X	401	BCL	MG-ND	-2.43	2.01	2.05
9	A	826	CLA	C4-C3	2.40	1.56	1.50
9	a	801	CLA	C3D-C2D	2.39	1.45	1.39
9	a	801	CLA	C1B-NB	2.38	1.41	1.37
11	a	815	F39	C23-C22	2.38	1.60	1.52
9	a	801	CLA	C4-C3	2.38	1.56	1.50
13	A	819	LHG	O7-C5	-2.37	1.41	1.46
11	a	815	F39	O6-C21	2.37	1.40	1.33
9	A	827	CLA	C4-C3	2.37	1.56	1.50
13	A	817	LHG	O7-C5	-2.36	1.41	1.46
9	A	802	CLA	C4-C3	2.36	1.56	1.50
11	a	815	F39	C47-C45	2.34	1.44	1.40
8	a	802	GS0	C1B-C2B	-2.33	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	301	F39	C47-C45	2.33	1.44	1.40
9	A	802	CLA	C1B-NB	2.32	1.40	1.37
10	U	407[B]	BCL	MG-NC	2.30	2.11	2.06
11	A	815	F39	O6-C21	2.30	1.40	1.33
9	A	827	CLA	C1D-C2D	2.29	1.49	1.45
10	a	809	BCL	C2A-C1A	-2.29	1.47	1.52
10	a	814	BCL	C3D-C4D	-2.28	1.39	1.44
10	Z	403	BCL	C1D-C2D	-2.28	1.40	1.45
10	a	804	BCL	C3D-C4D	-2.28	1.39	1.44
10	a	811	BCL	C2A-C1A	-2.28	1.47	1.52
10	A	807	BCL	C3B-C4B	2.28	1.45	1.41
10	a	810	BCL	C3D-C4D	-2.27	1.39	1.44
11	A	815	F39	C47-C45	2.27	1.44	1.40
10	V	405	BCL	C3D-C4D	-2.26	1.39	1.44
11	A	815	F39	C23-C22	2.26	1.60	1.52
10	a	811	BCL	C3D-C4D	-2.26	1.39	1.44
10	U	405	BCL	C3D-C4D	-2.26	1.39	1.44
10	A	803	BCL	C3D-C4D	-2.25	1.39	1.44
10	U	403	BCL	C3D-C4D	-2.25	1.39	1.44
9	A	802	CLA	C1D-C2D	2.25	1.49	1.45
10	W	407	BCL	C3D-C4D	-2.24	1.39	1.44
9	A	827	CLA	CAA-CBA	2.24	1.59	1.52
10	U	406	BCL	C3D-C4D	-2.24	1.39	1.44
10	B	301	BCL	C3D-C4D	-2.24	1.39	1.44
10	U	406	BCL	MG-NC	2.23	2.11	2.06
10	a	803	BCL	C3B-C4B	2.23	1.45	1.41
10	a	812	BCL	C3D-C4D	-2.23	1.39	1.44
10	A	813	BCL	CBD-CGD	-2.23	1.45	1.52
10	A	805	BCL	CBD-CGD	-2.23	1.45	1.52
10	A	804	BCL	C3D-C4D	-2.23	1.39	1.44
9	A	827	CLA	O2D-CED	2.22	1.50	1.45
9	A	826	CLA	CAA-CBA	2.21	1.59	1.52
10	a	804	BCL	C3B-C4B	2.21	1.45	1.41
10	a	808	BCL	C3D-C4D	-2.20	1.39	1.44
10	Y	401	BCL	C3D-C4D	-2.20	1.39	1.44
10	A	811	BCL	C3D-C4D	-2.20	1.39	1.44
10	A	803	BCL	C3B-C4B	2.20	1.45	1.41
10	a	809	BCL	C3D-C4D	-2.20	1.39	1.44
9	A	802	CLA	CAA-CBA	2.20	1.59	1.52
12	a	816	F26	C8-C13	2.20	1.55	1.51
10	W	403	BCL	C3D-C4D	-2.20	1.39	1.44
10	A	809	BCL	C3D-C4D	-2.20	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	820	LMG	O6-C5	-2.20	1.39	1.44
10	A	810	BCL	C3D-C4D	-2.19	1.39	1.44
10	X	403	BCL	C3D-C4D	-2.19	1.39	1.44
10	Z	404	BCL	C3D-C4D	-2.19	1.39	1.44
10	X	403	BCL	C3B-C4B	2.19	1.45	1.41
10	a	805	BCL	C3B-C4B	2.18	1.45	1.41
10	a	805	BCL	C3D-C4D	-2.18	1.39	1.44
10	A	805	BCL	C3B-C4B	2.18	1.45	1.41
10	A	812	BCL	C3D-C4D	-2.18	1.39	1.44
10	V	403	BCL	C3D-C4D	-2.18	1.39	1.44
13	a	821	LHG	O7-C5	-2.18	1.41	1.46
9	a	801	CLA	CAA-CBA	2.18	1.59	1.52
9	A	826	CLA	C1D-C2D	2.18	1.49	1.45
10	V	404	BCL	C3D-C4D	-2.18	1.39	1.44
10	Y	403	BCL	C3D-C4D	-2.18	1.39	1.44
10	A	814	BCL	C3D-C4D	-2.18	1.39	1.44
10	W	406	BCL	C3D-C4D	-2.17	1.39	1.44
10	A	813	BCL	C3D-C4D	-2.17	1.39	1.44
10	Z	404	BCL	C3B-C4B	2.17	1.45	1.41
10	a	806	BCL	MG-NC	2.16	2.11	2.06
10	A	808	BCL	C3D-C4D	-2.16	1.39	1.44
8	A	801	GS0	C3B-CAB	2.16	1.53	1.46
10	Y	405	BCL	C3D-C4D	-2.16	1.39	1.44
10	A	811	BCL	C2A-C1A	-2.16	1.47	1.52
10	W	408[B]	BCL	C3B-C4B	2.16	1.45	1.41
10	Y	408	BCL	C3D-C4D	-2.16	1.39	1.44
11	A	815	F39	C38-C37	2.15	1.55	1.50
10	V	408	BCL	C3D-C4D	-2.15	1.39	1.44
10	A	807	BCL	C3D-C4D	-2.15	1.39	1.44
10	V	401	BCL	C3D-C4D	-2.15	1.39	1.44
10	A	809	BCL	C1D-C2D	-2.15	1.41	1.45
11	a	815	F39	C38-C37	2.15	1.55	1.50
10	V	407	BCL	C3D-C4D	-2.14	1.39	1.44
10	Y	407	BCL	C3D-C4D	-2.14	1.39	1.44
10	X	409	BCL	C1D-C2D	-2.14	1.41	1.45
10	U	404	BCL	C3D-C4D	-2.14	1.39	1.44
10	Z	407	BCL	C3D-C4D	-2.14	1.39	1.44
9	A	827	CLA	C1B-NB	2.14	1.40	1.37
10	X	406	BCL	C3D-C4D	-2.14	1.39	1.44
11	a	815	F39	C18-C19	2.14	1.60	1.52
10	a	803	BCL	C3D-C4D	-2.14	1.39	1.44
10	X	409	BCL	C3D-C4D	-2.13	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	V	406	BCL	C3D-C4D	-2.13	1.39	1.44
10	X	408[B]	BCL	MG-NC	2.13	2.11	2.06
10	X	405	BCL	C3D-C4D	-2.13	1.39	1.44
10	Z	406	BCL	C3D-C4D	-2.12	1.39	1.44
10	X	404	BCL	C3D-C4D	-2.12	1.39	1.44
10	A	812	BCL	C3B-C4B	2.12	1.45	1.41
10	X	408[B]	BCL	C3B-C4B	2.12	1.45	1.41
10	V	401	BCL	MG-NC	2.12	2.11	2.06
10	Z	408[B]	BCL	MG-NC	2.12	2.11	2.06
9	A	826	CLA	O2D-CED	2.12	1.50	1.45
10	a	809	BCL	C3B-C4B	2.12	1.45	1.41
10	X	407[B]	BCL	C3D-C4D	-2.12	1.39	1.44
10	a	814	BCL	C3B-C4B	2.12	1.45	1.41
10	Z	405	BCL	C3D-C4D	-2.12	1.39	1.44
10	X	409	BCL	MG-NC	2.10	2.11	2.06
10	A	811	BCL	C3B-C4B	2.10	1.45	1.41
10	Y	402	BCL	C3D-C4D	-2.10	1.39	1.44
8	a	802	GS0	C3B-CAB	2.10	1.53	1.46
10	X	402	BCL	C3D-C4D	-2.10	1.39	1.44
13	a	818	LHG	O7-C5	-2.10	1.41	1.46
11	C	301	F39	C18-C19	2.10	1.59	1.52
10	W	404	BCL	C3D-C4D	-2.10	1.39	1.44
10	W	402	BCL	C3D-C4D	-2.10	1.39	1.44
10	U	402	BCL	C3D-C4D	-2.09	1.39	1.44
10	a	813	BCL	MG-NC	2.09	2.11	2.06
10	Z	402	BCL	C3D-C4D	-2.09	1.39	1.44
10	V	402	BCL	C3D-C4D	-2.09	1.39	1.44
10	B	301	BCL	C3B-C4B	2.09	1.45	1.41
11	C	301	F39	C38-C37	2.09	1.55	1.50
10	W	408[B]	BCL	MG-NC	2.08	2.11	2.06
10	V	409[B]	BCL	C3B-C4B	2.08	1.45	1.41
10	W	405	BCL	C3D-C4D	-2.08	1.39	1.44
10	V	403	BCL	MG-NC	2.08	2.11	2.06
10	Y	404	BCL	C3D-C4D	-2.08	1.39	1.44
10	a	807	BCL	C3B-C4B	2.08	1.45	1.41
10	X	406	BCL	MG-NC	2.08	2.11	2.06
14	A	823	LMG	O7-C8	-2.08	1.41	1.46
10	U	407[B]	BCL	C3D-C4D	-2.08	1.39	1.44
10	A	810	BCL	CBD-CGD	-2.07	1.46	1.52
10	U	401	BCL	C3D-C4D	-2.07	1.39	1.44
10	W	401	BCL	C3D-C4D	-2.07	1.39	1.44
10	V	409[B]	BCL	C3D-C4D	-2.07	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	a	805	BCL	CBD-CGD	-2.07	1.46	1.52
10	Z	403	BCL	C3D-C4D	-2.06	1.39	1.44
10	W	401	BCL	MG-NC	2.06	2.11	2.06
10	V	402	BCL	MG-NC	2.06	2.11	2.06
10	A	806	BCL	C3D-C4D	-2.06	1.39	1.44
11	A	815	F39	C18-C19	2.06	1.59	1.52
10	V	407	BCL	C3B-C4B	2.06	1.45	1.41
9	A	802	CLA	CBB-CAB	2.05	1.40	1.30
9	a	801	CLA	CBB-CAB	2.05	1.40	1.30
10	a	812	BCL	C3B-C4B	2.05	1.45	1.41
10	a	807	BCL	C3D-C4D	-2.05	1.39	1.44
10	X	405	BCL	CBD-CGD	-2.05	1.46	1.52
10	V	402	BCL	C3B-C4B	2.05	1.45	1.41
10	A	809	BCL	MG-NC	2.05	2.11	2.06
10	X	401	BCL	C3D-C4D	-2.05	1.39	1.44
10	X	408[B]	BCL	C3D-C4D	-2.05	1.39	1.44
10	a	811	BCL	C3B-C4B	2.05	1.45	1.41
9	A	827	CLA	CBB-CAB	2.04	1.40	1.30
10	V	409[B]	BCL	MG-NC	2.04	2.11	2.06
10	V	407	BCL	C1D-C2D	-2.04	1.41	1.45
10	U	403	BCL	C3B-C4B	2.04	1.45	1.41
8	A	801	GS0	C3D-C2D	-2.04	1.33	1.39
10	Y	401	BCL	CMC-C2C	-2.04	1.48	1.53
9	a	801	CLA	C1D-C2D	2.03	1.49	1.45
10	X	402	BCL	MG-NC	2.03	2.11	2.06
10	Y	403	BCL	MG-NC	2.03	2.11	2.06
10	A	807	BCL	MG-NC	2.03	2.11	2.06
10	A	813	BCL	C3B-C4B	2.03	1.45	1.41
9	a	801	CLA	O2A-C1	2.03	1.51	1.46
14	A	822	LMG	O7-C8	-2.02	1.41	1.46
10	Z	408[B]	BCL	C3D-C4D	-2.02	1.39	1.44
10	B	301	BCL	MG-NC	2.02	2.11	2.06
10	Y	406	BCL	C3D-C4D	-2.02	1.39	1.44
10	Y	404	BCL	MG-NC	2.02	2.11	2.06
10	U	407[B]	BCL	C3B-C4B	2.01	1.45	1.41
9	A	826	CLA	CBB-CAB	2.01	1.40	1.30
10	W	405	BCL	MG-NC	2.01	2.11	2.06
10	Y	407	BCL	C3B-C4B	2.01	1.45	1.41
10	Z	407	BCL	MG-NC	2.01	2.11	2.06
9	A	826	CLA	O2A-C1	2.01	1.51	1.46
10	W	408[B]	BCL	C3D-C4D	-2.01	1.39	1.44
8	a	802	GS0	C3B-C2B	-2.01	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Y	405	BCL	C1D-C2D	-2.01	1.41	1.45
10	Z	407	BCL	C1D-C2D	-2.00	1.41	1.45

All (1071) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	826	CLA	C4A-NA-C1A	19.27	115.47	106.68
9	A	802	CLA	C4A-NA-C1A	18.67	115.20	106.68
9	a	801	CLA	C4A-NA-C1A	18.38	115.06	106.68
9	A	827	CLA	C4A-NA-C1A	17.72	114.76	106.68
8	A	801	GS0	C4A-NA-C1A	13.32	112.76	106.68
8	a	802	GS0	C4A-NA-C1A	12.72	112.48	106.68
8	a	802	GS0	C1C-NC-C4C	8.39	110.51	106.68
8	A	801	GS0	C1C-NC-C4C	7.89	110.28	106.68
10	A	812	BCL	C1-C2-C3	-7.86	113.31	126.20
8	a	802	GS0	C4D-CHA-C1A	7.47	130.15	121.24
8	A	801	GS0	C4D-CHA-C1A	7.32	129.98	121.24
12	A	816	F26	C38-C33-C31	-7.09	117.34	127.28
9	A	827	CLA	C3B-C4B-NB	-6.45	104.78	110.53
9	A	802	CLA	C1D-ND-C4D	6.37	110.78	106.31
9	a	801	CLA	C3B-C4B-NB	-6.33	104.88	110.53
9	a	801	CLA	C1D-ND-C4D	6.31	110.74	106.31
9	A	826	CLA	C3B-C4B-NB	-6.23	104.97	110.53
9	A	802	CLA	C3B-C4B-NB	-6.16	105.03	110.53
8	A	801	GS0	O2D-CGD-O1D	-6.03	112.11	123.85
9	A	827	CLA	C1D-ND-C4D	5.93	110.47	106.31
12	a	816	F26	C38-C33-C31	-5.81	119.13	127.28
10	V	406	BCL	C4D-CHA-C1A	5.72	128.06	121.24
9	A	802	CLA	CMA-C3A-C4A	5.70	127.10	111.77
10	a	814	BCL	C4D-CHA-C1A	5.69	128.03	121.24
11	a	815	F39	C57-C59-C62	-5.68	119.31	127.28
10	a	808	BCL	C4D-CHA-C1A	5.68	128.02	121.24
10	X	405	BCL	C4D-CHA-C1A	5.67	128.01	121.24
9	A	827	CLA	CMA-C3A-C4A	5.65	126.97	111.77
10	A	810	BCL	C4D-CHA-C1A	5.65	127.98	121.24
12	a	817	F26	C22-C18-C13	-5.64	119.76	127.69
11	a	815	F39	C51-C44-C42	-5.63	119.38	127.28
12	a	817	F26	C23-C19-C15	-5.62	109.50	118.09
10	A	804	BCL	C4D-CHA-C1A	5.60	127.93	121.24
10	V	401	BCL	C4D-CHA-C1A	5.60	127.93	121.24
10	A	808	BCL	C4D-CHA-C1A	5.59	127.91	121.24
12	a	816	F26	C23-C19-C15	-5.59	109.55	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Z	402	BCL	C4D-CHA-C1A	5.57	127.89	121.24
10	a	804	BCL	C4D-CHA-C1A	5.57	127.89	121.24
10	Z	407	BCL	C4D-CHA-C1A	5.53	127.84	121.24
9	A	826	CLA	C1D-ND-C4D	5.53	110.19	106.31
11	a	815	F39	C11-O1-C12	5.52	124.51	113.72
10	A	807	BCL	C4D-CHA-C1A	5.51	127.81	121.24
10	B	301	BCL	C4D-CHA-C1A	5.50	127.80	121.24
10	U	404	BCL	C4D-CHA-C1A	5.48	127.78	121.24
10	U	406	BCL	C4D-CHA-C1A	5.48	127.78	121.24
10	Y	408	BCL	C4D-CHA-C1A	5.48	127.78	121.24
10	X	406	BCL	C4D-CHA-C1A	5.47	127.77	121.24
10	Y	404	BCL	C4D-CHA-C1A	5.47	127.77	121.24
10	W	401	BCL	C1-C2-C3	-5.46	117.25	126.20
11	C	301	F39	C32-C27-C20	-5.46	120.02	127.69
10	W	403	BCL	C4D-CHA-C1A	5.45	127.75	121.24
9	A	826	CLA	CMA-C3A-C4A	5.44	126.39	111.77
10	Z	403	BCL	C4D-CHA-C1A	5.44	127.73	121.24
10	A	812	BCL	C4D-CHA-C1A	5.43	127.72	121.24
11	a	815	F39	C32-C27-C20	-5.42	120.07	127.69
10	W	401	BCL	C4D-CHA-C1A	5.41	127.70	121.24
10	Y	407	BCL	C4D-CHA-C1A	5.41	127.69	121.24
10	a	812	BCL	C4D-CHA-C1A	5.40	127.69	121.24
10	V	403	BCL	C4D-CHA-C1A	5.40	127.68	121.24
10	V	404	BCL	C4D-CHA-C1A	5.39	127.67	121.24
10	V	407	BCL	C4D-CHA-C1A	5.38	127.67	121.24
10	V	402	BCL	C4D-CHA-C1A	5.36	127.64	121.24
10	a	809	BCL	C4D-CHA-C1A	5.36	127.64	121.24
10	W	407	BCL	C4D-CHA-C1A	5.35	127.62	121.24
10	Z	406	BCL	C4D-CHA-C1A	5.34	127.61	121.24
11	A	815	F39	C32-C27-C20	-5.33	120.20	127.69
11	A	815	F39	C40-C39-C37	-5.33	119.81	127.28
10	U	401	BCL	C4D-CHA-C1A	5.33	127.60	121.24
11	C	301	F39	C63-C61-C58	-5.31	119.83	127.28
9	a	801	CLA	CMA-C3A-C4A	5.27	125.94	111.77
10	W	406	BCL	C4D-CHA-C1A	5.27	127.53	121.24
10	X	404	BCL	C4D-CHA-C1A	5.26	127.52	121.24
8	A	801	GS0	C2A-C1A-CHA	5.26	133.00	123.87
10	Y	403	BCL	C4D-CHA-C1A	5.23	127.48	121.24
9	a	801	CLA	CAA-C2A-C3A	5.23	127.13	113.00
10	Z	405	BCL	C4D-CHA-C1A	5.21	127.46	121.24
10	X	409	BCL	C4D-CHA-C1A	5.20	127.45	121.24
10	a	807	BCL	C4D-CHA-C1A	5.20	127.45	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	U	405	BCL	C4D-CHA-C1A	5.19	127.43	121.24
10	V	408	BCL	C4D-CHA-C1A	5.18	127.42	121.24
10	Z	408[B]	BCL	C4D-CHA-C1A	5.18	127.42	121.24
10	a	810	BCL	C4D-CHA-C1A	5.18	127.42	121.24
11	a	815	F39	C63-C61-C58	-5.17	120.02	127.28
10	A	805	BCL	C4D-CHA-C1A	5.17	127.41	121.24
10	U	403	BCL	C4D-CHA-C1A	5.17	127.41	121.24
10	Y	401	BCL	C4D-CHA-C1A	5.15	127.39	121.24
10	W	405	BCL	C4D-CHA-C1A	5.15	127.39	121.24
12	A	816	F26	C32-C30-C26	-5.15	120.06	127.28
11	a	815	F39	C40-C39-C37	-5.14	120.06	127.28
11	A	815	F39	C11-O1-C12	5.14	123.76	113.72
10	A	806	BCL	C4A-NA-C1A	5.13	109.02	106.68
10	a	806	BCL	C4A-NA-C1A	5.12	109.02	106.68
10	A	803	BCL	C4D-CHA-C1A	5.11	127.34	121.24
8	a	802	GS0	O2D-CGD-O1D	-5.10	113.92	123.85
10	A	809	BCL	C4D-CHA-C1A	5.10	127.32	121.24
12	a	817	F26	C32-C30-C26	-5.09	120.14	127.28
11	A	815	F39	C57-C59-C62	-5.09	120.14	127.28
10	A	811	BCL	C4D-CHA-C1A	5.08	127.31	121.24
10	Z	404	BCL	C4D-CHA-C1A	5.08	127.31	121.24
10	U	404	BCL	C1-C2-C3	-5.08	117.87	126.20
8	a	802	GS0	C2A-C1A-CHA	5.07	132.67	123.87
10	A	814	BCL	C4D-CHA-C1A	5.07	127.29	121.24
10	X	402	BCL	C4D-CHA-C1A	5.06	127.28	121.24
10	U	402	BCL	C4D-CHA-C1A	5.06	127.28	121.24
11	A	815	F39	C63-C61-C58	-5.06	120.19	127.28
10	a	811	BCL	C4D-CHA-C1A	5.05	127.27	121.24
8	A	801	GS0	O2D-CGD-CBD	5.05	120.06	111.23
8	A	801	GS0	CMB-C2B-C1B	-5.04	117.74	125.42
11	A	815	F39	C51-C44-C42	-5.03	120.22	127.28
9	A	802	CLA	CAA-C2A-C1A	5.03	128.45	111.97
9	A	827	CLA	CAA-C2A-C1A	5.02	128.43	111.97
9	A	826	CLA	CAA-C2A-C1A	5.01	128.40	111.97
12	A	816	F26	C23-C19-C15	-5.00	110.45	118.09
10	Y	406	BCL	C4D-CHA-C1A	4.99	127.19	121.24
10	V	405	BCL	C4D-CHA-C1A	4.98	127.18	121.24
10	A	806	BCL	C4D-CHA-C1A	4.97	127.17	121.24
10	Y	402	BCL	C4D-CHA-C1A	4.94	127.14	121.24
10	X	405	BCL	C4A-NA-C1A	4.94	108.93	106.68
12	A	816	F26	C22-C18-C13	-4.90	120.80	127.69
9	A	827	CLA	CAA-C2A-C3A	4.90	126.24	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	301	F39	C40-C39-C37	-4.89	120.41	127.28
10	X	403	BCL	C4D-CHA-C1A	4.88	127.06	121.24
10	X	401	BCL	C4D-CHA-C1A	4.88	127.06	121.24
9	A	826	CLA	CAA-C2A-C3A	4.86	126.13	113.00
12	a	817	F26	C38-C33-C31	-4.85	120.47	127.28
12	a	816	F26	C22-C18-C13	-4.85	120.87	127.69
12	a	817	F26	C27-C24-C19	-4.85	120.48	127.28
10	Y	405	BCL	C4D-CHA-C1A	4.85	127.02	121.24
10	X	408[B]	BCL	C4D-CHA-C1A	4.84	127.02	121.24
11	C	301	F39	C57-C59-C62	-4.83	120.50	127.28
9	a	801	CLA	CAA-C2A-C1A	4.82	127.75	111.97
10	a	813	BCL	C4D-CHA-C1A	4.81	126.98	121.24
10	W	402	BCL	C4D-CHA-C1A	4.78	126.94	121.24
11	A	815	F39	O6-C21-C22	4.75	126.31	111.83
10	A	806	BCL	CHD-C1D-ND	-4.73	118.15	124.80
11	C	301	F39	C51-C44-C42	-4.73	120.65	127.28
8	A	801	GS0	CMA-C3A-C4A	-4.71	99.12	111.77
12	a	817	F26	C39-C37-C34	-4.70	120.69	127.28
12	a	816	F26	C27-C24-C19	-4.70	120.69	127.28
9	A	802	CLA	CAA-C2A-C3A	4.69	125.67	113.00
10	W	404	BCL	C4D-CHA-C1A	4.68	126.83	121.24
10	A	813	BCL	C4D-CHA-C1A	4.67	126.82	121.24
10	W	408[B]	BCL	C4D-CHA-C1A	4.67	126.81	121.24
10	a	805	BCL	C4D-CHA-C1A	4.66	126.81	121.24
12	A	816	F26	C39-C37-C34	-4.66	120.74	127.28
10	Y	404	BCL	C4A-NA-C1A	4.66	108.81	106.68
10	a	803	BCL	C4D-CHA-C1A	4.66	126.80	121.24
10	V	401	BCL	C1-C2-C3	-4.65	118.57	126.20
9	a	801	CLA	C2A-C1A-CHA	4.63	131.90	123.87
11	a	815	F39	O6-C21-C22	4.61	125.88	111.83
10	a	806	BCL	C4D-CHA-C1A	4.60	126.73	121.24
10	A	810	BCL	C1-C2-C3	-4.60	118.67	126.20
10	X	402	BCL	C4A-NA-C1A	4.57	108.76	106.68
10	A	805	BCL	CHD-C1D-ND	-4.55	118.39	124.80
10	U	407[B]	BCL	C4D-CHA-C1A	4.54	126.67	121.24
10	Y	404	BCL	C1-C2-C3	-4.54	118.76	126.20
10	a	803	BCL	C1C-NC-C4C	4.53	108.74	106.68
10	X	407[B]	BCL	C4D-CHA-C1A	4.48	126.59	121.24
10	Z	402	BCL	C4A-NA-C1A	4.48	108.72	106.68
10	V	409[B]	BCL	C4D-CHA-C1A	4.45	126.55	121.24
8	a	802	GS0	O2D-CGD-CBD	4.45	119.01	111.23
11	C	301	F39	O6-C21-C22	4.45	125.39	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	816	F26	C27-C24-C19	-4.44	121.05	127.28
9	A	802	CLA	C2A-C1A-CHA	4.41	131.52	123.87
10	V	405	BCL	C4A-NA-C1A	4.40	108.69	106.68
10	Y	407	BCL	CHD-C1D-ND	-4.39	118.63	124.80
9	A	826	CLA	CHB-C4A-NA	4.38	130.72	124.40
10	A	812	BCL	C4A-NA-C1A	4.35	108.67	106.68
10	Y	402	BCL	C1-C2-C3	-4.35	119.07	126.20
10	a	806	BCL	CHD-C1D-ND	-4.35	118.69	124.80
10	U	401	BCL	C4-C3-C5	-4.33	107.71	115.23
10	W	402	BCL	C1-C2-C3	-4.30	119.15	126.20
10	Y	405	BCL	CHD-C1D-ND	-4.30	118.75	124.80
8	A	801	GS0	CHB-C1B-NB	4.29	130.49	124.05
10	a	814	BCL	C1C-NC-C4C	4.28	108.63	106.68
10	Z	404	BCL	CHD-C1D-ND	-4.28	118.78	124.80
9	A	827	CLA	C2A-C1A-CHA	4.26	131.27	123.87
8	a	802	GS0	CMB-C2B-C1B	-4.26	118.94	125.42
10	A	810	BCL	C1C-NC-C4C	4.24	108.61	106.68
12	a	816	F26	C39-C37-C34	-4.24	121.33	127.28
10	X	403	BCL	CHD-C1D-ND	-4.24	118.84	124.80
10	a	808	BCL	CHD-C1D-ND	-4.23	118.85	124.80
9	A	827	CLA	CHB-C4A-NA	4.23	130.50	124.40
10	A	806	BCL	C1-C2-C3	-4.22	119.28	126.20
12	a	816	F26	C32-C30-C26	-4.22	121.36	127.28
10	V	406	BCL	C4A-NA-C1A	4.22	108.60	106.68
10	a	814	BCL	CHD-C1D-ND	-4.22	118.86	124.80
10	a	804	BCL	C1C-NC-C4C	4.21	108.60	106.68
10	a	810	BCL	CHD-C1D-ND	-4.21	118.88	124.80
10	Z	402	BCL	C4-C3-C5	-4.19	107.95	115.23
10	B	301	BCL	C1-C2-C3	-4.18	119.34	126.20
10	Z	406	BCL	C4A-NA-C1A	4.18	108.59	106.68
10	A	803	BCL	CHD-C1D-ND	-4.18	118.92	124.80
9	A	826	CLA	C2A-C1A-CHA	4.17	131.10	123.87
10	Z	406	BCL	CHD-C1D-ND	-4.16	118.95	124.80
10	a	814	BCL	C4-C3-C5	-4.16	108.01	115.23
10	Z	402	BCL	C1-C2-C3	-4.15	119.39	126.20
10	Y	401	BCL	C1-C2-C3	-4.15	119.41	126.20
10	Z	407	BCL	C4A-NA-C1A	4.13	108.56	106.68
10	U	403	BCL	CHD-C1D-ND	-4.13	118.99	124.80
10	Y	403	BCL	CHD-C1D-ND	-4.11	119.02	124.80
10	X	409	BCL	CHD-C1D-ND	-4.10	119.04	124.80
10	A	810	BCL	CHD-C1D-ND	-4.10	119.04	124.80
10	V	405	BCL	CHD-C1D-ND	-4.09	119.05	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	402	BCL	CHD-C1D-ND	-4.07	119.07	124.80
10	B	301	BCL	C4A-NA-C1A	4.07	108.53	106.68
10	U	402	BCL	CHD-C1D-ND	-4.07	119.08	124.80
10	X	401	BCL	CHD-C1D-ND	-4.06	119.09	124.80
10	a	807	BCL	C4-C3-C5	-4.05	108.19	115.23
12	a	816	F26	C2-C9-C15	-4.05	119.32	128.50
9	A	826	CLA	C2C-C1C-NC	-4.03	105.75	109.98
10	Z	406	BCL	C1C-NC-C4C	4.03	108.52	106.68
10	Z	403	BCL	C4A-NA-C1A	4.01	108.51	106.68
10	Y	404	BCL	CHD-C1D-ND	-4.01	119.16	124.80
10	W	401	BCL	C4A-NA-C1A	4.01	108.51	106.68
10	V	407	BCL	CHD-C1D-ND	-4.00	119.17	124.80
8	A	801	GS0	CGD-CBD-CAD	3.99	123.77	110.85
10	X	405	BCL	CHD-C1D-ND	-3.98	119.20	124.80
10	W	403	BCL	C4A-NA-C1A	3.98	108.50	106.68
10	a	803	BCL	CHD-C1D-ND	-3.98	119.21	124.80
10	A	808	BCL	CHD-C1D-ND	-3.97	119.21	124.80
10	a	813	BCL	CHD-C1D-ND	-3.97	119.21	124.80
10	Y	407	BCL	C1C-NC-C4C	3.97	108.49	106.68
10	a	805	BCL	CHD-C1D-ND	-3.96	119.23	124.80
10	Y	406	BCL	CHD-C1D-ND	-3.95	119.24	124.80
10	X	409	BCL	C4A-NA-C1A	3.94	108.48	106.68
10	V	401	BCL	CHD-C1D-ND	-3.94	119.25	124.80
10	A	812	BCL	CHD-C1D-ND	-3.94	119.26	124.80
10	A	809	BCL	C1C-NC-C4C	3.94	108.47	106.68
8	a	802	GS0	OBB-CAB-CBB	-3.93	110.96	119.77
8	a	802	GS0	CHB-C1B-NB	3.93	129.94	124.05
10	a	806	BCL	C1-C2-C3	-3.93	119.77	126.20
10	V	403	BCL	CHD-C1D-ND	-3.92	119.29	124.80
10	X	401	BCL	C1-C2-C3	-3.92	119.78	126.20
8	A	801	GS0	OBB-CAB-CBB	-3.91	111.01	119.77
11	C	301	F39	C11-O1-C12	3.91	121.35	113.72
10	a	814	BCL	C4A-NA-C1A	3.91	108.46	106.68
10	a	810	BCL	C1-C2-C3	-3.90	119.80	126.20
11	A	815	F39	O6-C21-O7	-3.90	113.88	123.63
10	U	406	BCL	CHD-C1D-ND	-3.90	119.32	124.80
10	a	807	BCL	CHD-C1D-ND	-3.89	119.32	124.80
10	W	402	BCL	C4A-NA-C1A	3.89	108.45	106.68
10	A	811	BCL	CHD-C1D-ND	-3.89	119.33	124.80
10	X	401	BCL	C4A-NA-C1A	3.88	108.45	106.68
10	V	404	BCL	C1-C2-C3	-3.88	119.84	126.20
10	Z	402	BCL	CHD-C1D-ND	-3.87	119.36	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	V	408	BCL	CHD-C1D-ND	-3.86	119.37	124.80
10	V	402	BCL	C1-C2-C3	-3.86	119.87	126.20
10	V	402	BCL	C1C-NC-C4C	3.86	108.44	106.68
11	a	815	F39	O6-C21-O7	-3.86	113.98	123.63
10	U	402	BCL	C4A-NA-C1A	3.85	108.44	106.68
10	V	402	BCL	CHD-C1D-ND	-3.85	119.38	124.80
10	W	408[B]	BCL	CHD-C1D-ND	-3.85	119.39	124.80
10	A	814	BCL	CHD-C1D-ND	-3.84	119.39	124.80
8	a	802	GS0	CHA-C1A-NA	-3.84	117.69	126.39
10	A	813	BCL	CHD-C1D-ND	-3.84	119.40	124.80
11	C	301	F39	C46-C53-C56	-3.83	119.81	128.50
10	X	406	BCL	C4A-NA-C1A	3.83	108.43	106.68
11	C	301	F39	C41-C42-C44	-3.83	112.99	119.01
9	A	802	CLA	CHB-C4A-NA	3.83	129.92	124.40
9	A	827	CLA	C2D-C1D-ND	-3.82	106.34	110.13
10	A	810	BCL	C4A-NA-C1A	3.81	108.42	106.68
10	a	812	BCL	CHD-C1D-ND	-3.81	119.44	124.80
10	a	808	BCL	C4A-NA-C1A	3.80	108.41	106.68
10	Y	405	BCL	C4A-NA-C1A	3.80	108.41	106.68
11	A	815	F39	C56-C58-C61	-3.79	113.04	119.01
9	A	826	CLA	O2D-CGD-O1D	-3.79	116.47	123.85
11	C	301	F39	O6-C21-O7	-3.79	114.16	123.63
10	V	409[B]	BCL	CHD-C1D-ND	-3.78	119.48	124.80
10	Z	405	BCL	CHD-C1D-ND	-3.78	119.48	124.80
10	X	406	BCL	CHD-C1D-ND	-3.78	119.48	124.80
10	X	403	BCL	C4A-NA-C1A	3.78	108.40	106.68
10	a	809	BCL	CHD-C1D-ND	-3.78	119.48	124.80
10	W	403	BCL	C1-C2-C3	-3.78	120.01	126.20
10	a	807	BCL	C4A-NA-C1A	3.78	108.40	106.68
10	X	408[B]	BCL	CHD-C1D-ND	-3.76	119.51	124.80
10	V	404	BCL	CHD-C1D-ND	-3.75	119.52	124.80
10	V	406	BCL	CHD-C1D-ND	-3.75	119.52	124.80
10	U	404	BCL	C1C-NC-C4C	3.75	108.39	106.68
10	Y	402	BCL	C4A-NA-C1A	3.75	108.39	106.68
10	W	405	BCL	C1C-NC-C4C	3.75	108.39	106.68
10	U	405	BCL	C4A-NA-C1A	3.74	108.39	106.68
8	A	801	GS0	CHA-C1A-NA	-3.74	117.92	126.39
10	U	405	BCL	CHD-C1D-ND	-3.74	119.54	124.80
8	a	802	GS0	CGD-CBD-CAD	3.73	122.93	110.85
10	A	804	BCL	CHD-C1D-ND	-3.73	119.55	124.80
8	a	802	GS0	CMA-C3A-C4A	-3.73	101.75	111.77
9	A	802	CLA	C2D-C1D-ND	-3.73	106.44	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	W	402	BCL	CHD-C1D-ND	-3.73	119.56	124.80
10	B	301	BCL	CHD-C1D-ND	-3.72	119.56	124.80
11	A	815	F39	C41-C42-C44	-3.72	113.16	119.01
10	W	407	BCL	C1C-NC-C4C	3.71	108.37	106.68
10	Y	408	BCL	CHD-C1D-ND	-3.71	119.58	124.80
10	U	401	BCL	CHD-C1D-ND	-3.70	119.59	124.80
10	V	408	BCL	C4A-NA-C1A	3.70	108.37	106.68
10	Y	401	BCL	CHD-C1D-ND	-3.70	119.60	124.80
10	a	811	BCL	CHD-C1D-ND	-3.69	119.61	124.80
10	Y	402	BCL	CHD-C1D-ND	-3.69	119.61	124.80
10	a	804	BCL	CHD-C1D-ND	-3.69	119.61	124.80
10	Y	401	BCL	C4A-NA-C1A	3.68	108.36	106.68
10	U	407[B]	BCL	CHD-C1D-ND	-3.68	119.63	124.80
10	U	404	BCL	CHD-C1D-ND	-3.67	119.63	124.80
10	A	809	BCL	C1-C2-C3	-3.67	120.19	126.20
10	W	408[B]	BCL	C1C-NC-C4C	3.66	108.35	106.68
9	A	827	CLA	CGD-CBD-CAD	3.66	122.68	110.85
10	A	807	BCL	C1C-NC-C4C	3.65	108.35	106.68
10	W	406	BCL	C4A-NA-C1A	3.65	108.35	106.68
10	W	406	BCL	CHD-C1D-ND	-3.65	119.66	124.80
10	Z	404	BCL	C4A-NA-C1A	3.65	108.34	106.68
11	a	815	F39	C46-C53-C56	-3.64	120.25	128.50
10	Z	407	BCL	CHD-C1D-ND	-3.63	119.69	124.80
10	a	809	BCL	C4A-NA-C1A	3.63	108.33	106.68
10	V	404	BCL	C4A-NA-C1A	3.63	108.33	106.68
11	a	815	F39	C35-C37-C39	-3.63	113.31	119.01
10	A	807	BCL	CHD-C1D-ND	-3.62	119.70	124.80
10	V	407	BCL	C4A-NA-C1A	3.62	108.33	106.68
10	X	404	BCL	CHD-C1D-ND	-3.62	119.70	124.80
10	A	809	BCL	CHD-C1D-ND	-3.62	119.71	124.80
9	a	801	CLA	CGD-CBD-CAD	3.62	122.55	110.85
10	U	403	BCL	C4A-NA-C1A	3.61	108.33	106.68
10	Z	402	BCL	C1C-NC-C4C	3.61	108.33	106.68
10	W	407	BCL	CHD-C1D-ND	-3.61	119.72	124.80
8	a	802	GS0	C3B-C4B-NB	-3.60	105.00	109.76
10	Z	403	BCL	C1-C2-C3	-3.60	120.30	126.20
10	U	401	BCL	C4A-NA-C1A	3.60	108.32	106.68
10	Y	407	BCL	C4A-NA-C1A	3.60	108.32	106.68
12	a	817	F26	C2-C9-C15	-3.59	120.36	128.50
10	W	405	BCL	CHD-C1D-ND	-3.59	119.75	124.80
10	A	803	BCL	C1C-NC-C4C	3.58	108.31	106.68
10	V	402	BCL	C4A-NA-C1A	3.58	108.31	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	W	401	BCL	CHD-C1D-ND	-3.58	119.77	124.80
10	A	807	BCL	C1-C2-C3	-3.57	120.35	126.20
10	U	401	BCL	C1-C2-C3	-3.57	120.35	126.20
10	V	403	BCL	C4A-NA-C1A	3.57	108.31	106.68
10	Z	408[B]	BCL	C4A-NA-C1A	3.57	108.31	106.68
8	A	801	GS0	C3B-C4B-NB	-3.56	105.06	109.76
10	A	813	BCL	C1C-NC-C4C	3.56	108.31	106.68
10	X	405	BCL	C1C-NC-C4C	3.56	108.31	106.68
11	a	815	F39	C41-C42-C44	-3.55	113.43	119.01
10	X	407[B]	BCL	CHD-C1D-ND	-3.54	119.83	124.80
10	Z	403	BCL	CHD-C1D-ND	-3.53	119.83	124.80
10	W	403	BCL	CHD-C1D-ND	-3.53	119.83	124.80
9	A	826	CLA	C2B-C1B-NB	-3.53	106.66	110.33
9	A	802	CLA	CGD-CBD-CAD	3.53	122.28	110.85
9	A	826	CLA	C3C-C4C-NC	-3.53	105.91	110.43
9	a	801	CLA	C2D-C1D-ND	-3.53	106.63	110.13
10	V	401	BCL	C4A-NA-C1A	3.53	108.29	106.68
10	W	404	BCL	C4A-NA-C1A	3.52	108.29	106.68
10	a	803	BCL	C1-C2-C3	-3.52	120.42	126.20
10	a	806	BCL	C4-C3-C5	-3.51	109.13	115.23
10	A	806	BCL	C1C-NC-C4C	3.51	108.28	106.68
10	U	407[B]	BCL	C1C-NC-C4C	3.51	108.28	106.68
10	A	804	BCL	C4A-NA-C1A	3.49	108.27	106.68
10	a	810	BCL	C4-C3-C5	-3.49	109.17	115.23
10	W	404	BCL	CHD-C1D-ND	-3.48	119.90	124.80
9	A	826	CLA	CGD-CBD-CAD	3.48	122.11	110.85
10	Y	408	BCL	C4A-NA-C1A	3.47	108.26	106.68
8	a	802	GS0	C2B-C1B-NB	-3.47	106.73	110.33
10	A	809	BCL	C4A-NA-C1A	3.47	108.26	106.68
10	U	402	BCL	C1C-NC-C4C	3.46	108.26	106.68
9	a	801	CLA	CHB-C4A-NA	3.46	129.39	124.40
10	a	810	BCL	C4A-NA-C1A	3.46	108.26	106.68
10	X	404	BCL	C1C-NC-C4C	3.46	108.26	106.68
8	A	801	GS0	CBB-CAB-C3B	3.46	127.69	120.40
10	Z	408[B]	BCL	CHD-C1D-ND	-3.45	119.94	124.80
10	V	402	BCL	CHA-C1A-NA	-3.45	118.58	126.39
9	a	801	CLA	CMA-C3A-C2A	3.42	127.21	113.98
10	W	406	BCL	C1C-NC-C4C	3.42	108.24	106.68
10	W	404	BCL	C1C-NC-C4C	3.41	108.24	106.68
11	a	815	F39	C56-C58-C61	-3.40	113.66	119.01
10	a	806	BCL	CHA-C1A-NA	-3.40	118.70	126.39
10	Z	407	BCL	C1C-NC-C4C	3.39	108.23	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	806	BCL	CHA-C1A-NA	-3.39	118.71	126.39
8	A	801	GS0	CMA-C3A-C2A	-3.39	100.87	113.98
10	V	406	BCL	C1C-NC-C4C	3.38	108.22	106.68
10	V	409[B]	BCL	C2A-C1A-CHA	3.38	129.73	123.87
11	A	815	F39	C46-C53-C56	-3.37	120.86	128.50
10	a	813	BCL	CHA-C1A-NA	-3.36	118.77	126.39
10	a	805	BCL	C1-C2-C3	-3.36	120.69	126.20
9	A	826	CLA	C2D-C1D-ND	-3.35	106.81	110.13
10	Y	402	BCL	CHA-C1A-NA	-3.34	118.82	126.39
11	a	815	F39	C32-C35-C37	-3.34	117.20	126.36
10	V	404	BCL	C1C-NC-C4C	3.34	108.20	106.68
8	a	802	GS0	C16-C15-C13	-3.33	104.91	115.97
10	W	401	BCL	CHA-C1A-NA	-3.33	118.86	126.39
10	U	401	BCL	CHA-C1A-NA	-3.32	118.86	126.39
10	a	807	BCL	C5-C3-C2	-3.32	113.71	121.17
10	A	806	BCL	C1-O2A-CGA	3.32	124.69	116.65
10	a	813	BCL	C1C-NC-C4C	3.32	108.19	106.68
10	X	406	BCL	C1C-NC-C4C	3.31	108.19	106.68
11	A	815	F39	C32-C35-C37	-3.31	117.29	126.36
9	A	826	CLA	C2A-C3A-C4A	3.30	107.20	101.87
10	A	810	BCL	C4-C3-C5	-3.29	109.51	115.23
10	A	805	BCL	C4A-NA-C1A	3.29	108.18	106.68
10	V	404	BCL	CHA-C1A-NA	-3.28	118.96	126.39
11	C	301	F39	C32-C35-C37	-3.27	117.39	126.36
10	A	808	BCL	CHA-C1A-NA	-3.27	118.98	126.39
10	X	402	BCL	C1-C2-C3	-3.27	120.84	126.20
10	V	406	BCL	C1-C2-C3	-3.27	120.84	126.20
10	A	808	BCL	C4A-NA-C1A	3.25	108.16	106.68
10	a	812	BCL	C4A-NA-C1A	3.24	108.16	106.68
9	A	802	CLA	CMA-C3A-C2A	3.24	126.51	113.98
14	A	820	LMG	O6-C1-O1	-3.24	102.39	110.04
10	A	809	BCL	CHA-C1A-NA	-3.24	119.06	126.39
10	Y	408	BCL	C1C-NC-C4C	3.24	108.16	106.68
11	C	301	F39	C35-C37-C39	-3.23	113.92	119.01
8	A	801	GS0	CMC-C2C-C3C	-3.22	101.52	113.98
10	Y	402	BCL	CAB-C3B-C2B	3.22	134.44	127.74
9	A	826	CLA	CMA-C3A-C2A	3.22	126.41	113.98
10	U	405	BCL	C1C-NC-C4C	3.21	108.14	106.68
9	A	827	CLA	C3C-C4C-NC	-3.21	106.31	110.43
8	A	801	GS0	C2B-C1B-NB	-3.21	107.00	110.33
8	A	801	GS0	C16-C15-C13	-3.20	105.32	115.97
10	A	811	BCL	CHA-C1A-NA	-3.20	119.14	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	805	BCL	C1D-ND-C4D	-3.20	104.07	106.31
8	a	802	GS0	C7-C6-C5	-3.20	104.74	113.26
10	Z	402	BCL	CHA-C1A-NA	-3.20	119.15	126.39
10	A	813	BCL	CHA-C1A-NA	-3.20	119.15	126.39
10	U	401	BCL	C1C-NC-C4C	3.20	108.14	106.68
10	a	805	BCL	C1C-NC-C4C	3.19	108.14	106.68
10	Z	405	BCL	C1C-NC-C4C	3.18	108.13	106.68
10	V	407	BCL	CHA-C1A-NA	-3.18	119.20	126.39
11	C	301	F39	C56-C58-C61	-3.18	114.01	119.01
10	A	805	BCL	C1-C2-C3	-3.17	121.00	126.20
10	A	803	BCL	C16-C15-C13	-3.16	105.45	115.97
10	W	401	BCL	C1C-NC-C4C	3.16	108.12	106.68
11	A	815	F39	C35-C37-C39	-3.15	114.05	119.01
9	A	827	CLA	CMA-C3A-C2A	3.15	126.16	113.98
10	A	814	BCL	CHA-C1A-NA	-3.15	119.27	126.39
10	X	401	BCL	CHA-C1A-NA	-3.14	119.28	126.39
10	a	809	BCL	CHA-C1A-NA	-3.12	119.32	126.39
10	W	401	BCL	C2A-C1A-CHA	3.11	129.27	123.87
10	W	406	BCL	CHA-C1A-NA	-3.11	119.34	126.39
11	C	301	F39	C25-C20-C27	-3.11	109.07	122.50
10	Z	405	BCL	C2A-C1A-CHA	3.11	129.26	123.87
10	U	403	BCL	CHA-C1A-NA	-3.10	119.36	126.39
10	Y	403	BCL	C1-C2-C3	-3.10	121.11	126.20
8	A	801	GS0	C7-C6-C5	-3.10	105.00	113.26
8	a	802	GS0	O2A-CGA-O1A	-3.10	115.87	123.63
10	X	401	BCL	C1D-ND-C4D	-3.10	104.14	106.31
10	a	805	BCL	C1D-ND-C4D	-3.10	104.14	106.31
11	A	815	F39	C53-C56-C58	-3.10	118.90	126.25
9	A	827	CLA	C2A-C3A-C4A	3.10	106.87	101.87
10	W	407	BCL	C4A-NA-C1A	3.10	108.09	106.68
11	A	815	F39	C25-C20-C27	-3.10	109.11	122.50
11	a	815	F39	C25-C20-C27	-3.09	109.15	122.50
10	a	813	BCL	C1D-ND-C4D	-3.08	104.15	106.31
9	a	801	CLA	C2A-C3A-C4A	3.08	106.85	101.87
10	a	810	BCL	C16-C15-C13	-3.08	105.73	115.97
10	U	403	BCL	C2A-C1A-CHA	3.08	129.20	123.87
9	A	827	CLA	C2B-C1B-NB	-3.07	107.14	110.33
10	A	805	BCL	CHA-C1A-NA	-3.07	119.44	126.39
10	W	403	BCL	CHA-C1A-NA	-3.07	119.44	126.39
10	V	401	BCL	CHA-C1A-NA	-3.06	119.46	126.39
10	Z	407	BCL	C1-C2-C3	-3.06	121.19	126.20
10	Y	407	BCL	CHA-C1A-NA	-3.05	119.48	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	V	401	BCL	C1C-NC-C4C	3.05	108.07	106.68
10	U	402	BCL	CHA-C1A-NA	-3.05	119.49	126.39
10	a	804	BCL	CHA-C1A-NA	-3.05	119.49	126.39
10	a	810	BCL	C2A-C1A-CHA	3.04	129.15	123.87
10	U	402	BCL	C1-C2-C3	-3.04	121.22	126.20
10	X	409	BCL	C1-C2-C3	-3.03	121.23	126.20
10	A	810	BCL	CHA-C1A-NA	-3.03	119.52	126.39
9	A	802	CLA	C3A-C2A-C1A	3.03	105.88	101.34
10	a	805	BCL	C4A-NA-C1A	3.03	108.06	106.68
10	A	807	BCL	C4D-C3D-CAD	-3.03	104.81	108.11
10	Z	408[B]	BCL	C1C-NC-C4C	3.03	108.06	106.68
10	W	408[B]	BCL	CHA-C1A-NA	-3.02	119.55	126.39
10	Y	401	BCL	CAB-C3B-C2B	3.02	134.02	127.74
10	V	409[B]	BCL	CHA-C1A-NA	-3.02	119.55	126.39
10	Z	408[B]	BCL	CHA-C1A-NA	-3.02	119.55	126.39
10	X	409	BCL	C1C-NC-C4C	3.02	108.06	106.68
9	A	802	CLA	C4D-CHA-C1A	3.02	124.84	121.24
10	A	806	BCL	C2A-C1A-CHA	3.02	129.10	123.87
10	W	401	BCL	CAB-C3B-C2B	3.01	134.00	127.74
10	X	405	BCL	CHA-C1A-NA	-3.01	119.57	126.39
10	A	813	BCL	C2A-C1A-CHA	3.01	129.09	123.87
10	X	402	BCL	CHA-C1A-NA	-3.01	119.58	126.39
10	a	808	BCL	CHA-C1A-NA	-3.01	119.58	126.39
10	Y	405	BCL	C1-C2-C3	-3.00	121.28	126.20
8	A	801	GS0	O2A-CGA-O1A	-3.00	116.13	123.63
10	a	811	BCL	C1-C2-C3	-3.00	121.28	126.20
10	Z	405	BCL	CHA-C1A-NA	-2.99	119.61	126.39
10	W	404	BCL	C1-C2-C3	-2.99	121.30	126.20
10	A	803	BCL	CHA-C1A-NA	-2.99	119.62	126.39
10	a	806	BCL	C2A-C1A-CHA	2.99	129.05	123.87
10	a	814	BCL	CHA-C1A-NA	-2.99	119.63	126.39
10	A	807	BCL	CHA-C1A-NA	-2.98	119.64	126.39
10	A	812	BCL	C11-C10-C8	2.98	125.88	115.97
8	A	801	GS0	C11-C10-C8	-2.98	106.05	115.97
10	U	406	BCL	CHA-C1A-NA	-2.98	119.64	126.39
10	X	409	BCL	CHA-C1A-NA	-2.98	119.64	126.39
10	U	404	BCL	CHA-C1A-NA	-2.98	119.64	126.39
10	X	408[B]	BCL	CHA-C1A-NA	-2.98	119.64	126.39
10	X	402	BCL	C1C-NC-C4C	2.98	108.04	106.68
9	A	827	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
10	X	403	BCL	CHA-C1A-NA	-2.97	119.66	126.39
10	a	810	BCL	CHA-C1A-NA	-2.97	119.66	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	V	407	BCL	C16-C15-C13	-2.97	106.09	115.97
9	A	802	CLA	C3C-C4C-NC	-2.97	106.63	110.43
10	a	807	BCL	C1C-NC-C4C	2.97	108.03	106.68
10	V	403	BCL	C1-C2-C3	-2.97	121.34	126.20
10	V	407	BCL	C2A-C1A-CHA	2.97	129.01	123.87
10	Z	404	BCL	CHA-C1A-NA	-2.97	119.67	126.39
9	a	801	CLA	C2B-C1B-NB	-2.96	107.25	110.33
10	U	406	BCL	C4A-NA-C1A	2.96	108.03	106.68
10	Y	404	BCL	CHA-C1A-NA	-2.96	119.69	126.39
10	a	812	BCL	C1-C2-C3	-2.96	121.35	126.20
10	a	803	BCL	C2A-C1A-CHA	2.96	129.00	123.87
10	Y	408	BCL	CHA-C1A-NA	-2.96	119.70	126.39
10	W	403	BCL	C1C-NC-C4C	2.95	108.03	106.68
10	Z	406	BCL	C2A-C1A-CHA	2.95	128.99	123.87
8	a	802	GS0	CBB-CAB-C3B	2.95	126.62	120.40
10	X	404	BCL	CHA-C1A-NA	-2.95	119.72	126.39
10	X	401	BCL	CAB-C3B-C2B	2.95	133.86	127.74
10	a	803	BCL	CHA-C1A-NA	-2.94	119.73	126.39
10	X	409	BCL	C1D-ND-C4D	-2.94	104.25	106.31
10	Z	406	BCL	CHA-C1A-NA	-2.94	119.74	126.39
10	V	406	BCL	CHA-C1A-NA	-2.93	119.75	126.39
10	Y	403	BCL	CHA-C1A-NA	-2.93	119.75	126.39
10	Z	404	BCL	C2A-C1A-CHA	2.93	128.96	123.87
10	a	811	BCL	CHA-C1A-NA	-2.93	119.75	126.39
10	a	807	BCL	CHA-C1A-NA	-2.93	119.76	126.39
10	U	407[B]	BCL	CHA-C1A-NA	-2.93	119.77	126.39
10	A	805	BCL	CHD-C1D-C2D	2.92	131.57	125.49
10	W	407	BCL	CHA-C1A-NA	-2.92	119.77	126.39
10	W	405	BCL	C4A-NA-C1A	2.92	108.01	106.68
10	A	812	BCL	CHA-C1A-NA	-2.92	119.78	126.39
10	Z	403	BCL	CHA-C1A-NA	-2.92	119.78	126.39
10	A	814	BCL	C2A-C1A-CHA	2.91	128.93	123.87
10	V	408	BCL	CHA-C1A-NA	-2.91	119.79	126.39
10	Z	404	BCL	C4-C3-C5	-2.91	110.17	115.23
14	A	823	LMG	O6-C1-O1	-2.91	103.17	110.04
10	A	813	BCL	C1-C2-C3	-2.91	121.43	126.20
10	A	807	BCL	C2A-C1A-CHA	2.90	128.91	123.87
10	X	409	BCL	C2A-C1A-CHA	2.90	128.91	123.87
10	V	404	BCL	C2A-C1A-CHA	2.90	128.90	123.87
10	V	404	BCL	C1D-ND-C4D	-2.90	104.28	106.31
10	Y	406	BCL	C2A-C1A-CHA	2.90	128.89	123.87
10	X	403	BCL	C1C-NC-C4C	2.90	108.00	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	U	405	BCL	CHA-C1A-NA	-2.89	119.84	126.39
9	A	826	CLA	CHD-C4C-C3C	2.89	128.99	124.77
10	a	807	BCL	C1D-ND-C4D	-2.89	104.28	106.31
10	Y	406	BCL	CHA-C1A-NA	-2.89	119.84	126.39
10	Z	405	BCL	C1-C2-C3	-2.89	121.46	126.20
10	Y	405	BCL	C2A-C1A-CHA	2.89	128.88	123.87
10	Y	405	BCL	CHA-C1A-NA	-2.89	119.85	126.39
10	Z	407	BCL	CHA-C1A-NA	-2.89	119.85	126.39
10	Y	407	BCL	C2A-C1A-CHA	2.89	128.88	123.87
10	Y	406	BCL	C4A-NA-C1A	2.88	108.00	106.68
10	Z	403	BCL	C1C-NC-C4C	2.88	108.00	106.68
10	Y	403	BCL	C2A-C1A-CHA	2.88	128.87	123.87
10	a	812	BCL	CHA-C1A-NA	-2.88	119.86	126.39
10	A	811	BCL	CAC-C3C-C4C	2.88	118.98	112.58
10	Y	403	BCL	C4A-NA-C1A	2.88	107.99	106.68
10	A	812	BCL	C2A-C1A-CHA	2.88	128.86	123.87
10	X	406	BCL	CHA-C1A-NA	-2.88	119.88	126.39
10	Z	402	BCL	CAB-C3B-C2B	2.87	133.71	127.74
10	V	403	BCL	CHA-C1A-NA	-2.87	119.89	126.39
10	V	408	BCL	C1D-ND-C4D	-2.87	104.30	106.31
10	a	811	BCL	O2A-CGA-O1A	-2.87	116.45	123.63
8	A	801	GS0	C3C-C2C-C1C	2.87	106.50	101.87
10	V	405	BCL	CAB-C3B-C2B	2.87	133.70	127.74
10	A	804	BCL	CHA-C1A-NA	-2.86	119.91	126.39
10	X	407[B]	BCL	CHA-C1A-NA	-2.86	119.92	126.39
10	U	403	BCL	C1D-ND-C4D	-2.85	104.31	106.31
10	W	405	BCL	CHA-C1A-NA	-2.85	119.93	126.39
10	A	803	BCL	C11-C10-C8	-2.85	106.49	115.97
10	V	402	BCL	CAB-C3B-C2B	2.85	133.66	127.74
10	B	301	BCL	CHA-C1A-NA	-2.84	119.96	126.39
10	a	805	BCL	CHA-C1A-NA	-2.84	119.96	126.39
12	A	816	F26	C27-C28-C31	-2.84	118.58	126.36
10	A	809	BCL	C4-C3-C5	-2.84	110.30	115.23
10	a	807	BCL	C2A-C1A-CHA	2.84	128.79	123.87
10	Z	406	BCL	C1-C2-C3	-2.84	121.55	126.20
10	A	809	BCL	C2A-C1A-CHA	2.84	128.79	123.87
10	U	403	BCL	C1C-NC-C4C	2.83	107.97	106.68
10	W	401	BCL	C4-C3-C5	-2.83	110.31	115.23
10	W	404	BCL	CHA-C1A-NA	-2.83	119.98	126.39
10	A	803	BCL	C1D-ND-C4D	-2.83	104.33	106.31
10	V	402	BCL	C4-C3-C5	-2.83	110.32	115.23
10	V	405	BCL	C1C-NC-C4C	2.83	107.97	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	a	803	BCL	C4A-NA-C1A	2.82	107.97	106.68
10	V	408	BCL	C2A-C1A-CHA	2.82	128.76	123.87
13	A	818	LHG	O8-C23-C24	2.82	120.43	111.83
10	Y	401	BCL	C4-C3-C5	-2.82	110.34	115.23
10	A	814	BCL	C1C-NC-C4C	2.81	107.96	106.68
10	a	809	BCL	C4-C3-C5	-2.81	110.34	115.23
10	X	403	BCL	C2A-C1A-CHA	2.81	128.75	123.87
10	A	813	BCL	C5-C3-C2	-2.81	114.86	121.17
10	V	407	BCL	C1C-NC-C4C	2.81	107.96	106.68
10	V	405	BCL	CHA-C1A-NA	-2.81	120.03	126.39
12	A	816	F26	C17-C13-C8	2.81	120.10	115.23
10	U	401	BCL	C2A-C1A-CHA	2.81	128.74	123.87
10	V	402	BCL	C2A-C1A-CHA	2.81	128.74	123.87
10	U	402	BCL	C2A-C1A-CHA	2.80	128.73	123.87
10	A	807	BCL	C4A-NA-C1A	2.80	107.96	106.68
9	A	827	CLA	C2C-C1C-NC	-2.80	107.04	109.98
9	A	802	CLA	C2A-C3A-C4A	2.80	106.39	101.87
10	W	408[B]	BCL	C2A-C1A-CHA	2.80	128.72	123.87
10	X	407[B]	BCL	C4A-NA-C1A	2.79	107.95	106.68
12	a	817	F26	C9-C15-C19	-2.79	119.63	126.25
10	A	804	BCL	C1C-NC-C4C	2.79	107.95	106.68
10	a	810	BCL	C1C-NC-C4C	2.79	107.95	106.68
10	U	406	BCL	C1-C2-C3	-2.79	121.63	126.20
10	V	409[B]	BCL	C1C-NC-C4C	2.79	107.95	106.68
10	W	404	BCL	CAB-C3B-C2B	2.79	133.53	127.74
10	Y	401	BCL	CHA-C1A-NA	-2.79	120.08	126.39
14	a	822	LMG	O6-C1-O1	-2.79	103.46	110.04
10	W	405	BCL	C2A-C1A-CHA	2.79	128.70	123.87
10	a	805	BCL	C2A-C1A-CHA	2.78	128.70	123.87
10	X	407[B]	BCL	C1C-NC-C4C	2.78	107.95	106.68
10	U	406	BCL	C2A-C1A-CHA	2.78	128.69	123.87
10	W	406	BCL	C2A-C1A-CHA	2.78	128.69	123.87
8	a	802	GS0	C11-C10-C8	-2.78	106.73	115.97
10	V	407	BCL	C6-C5-C3	2.78	120.24	113.47
12	A	816	F26	C36-C31-C33	-2.78	118.32	122.82
9	A	802	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
10	Y	404	BCL	O2D-CGD-O1D	-2.78	118.44	123.85
10	X	403	BCL	CAB-C3B-C2B	2.77	133.51	127.74
10	Z	404	BCL	C1-C2-C3	-2.77	121.66	126.20
10	a	809	BCL	C1D-ND-C4D	-2.76	104.37	106.31
10	a	811	BCL	O2A-CGA-CBA	2.76	120.26	111.83
10	A	803	BCL	C2A-C1A-CHA	2.76	128.66	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	811	BCL	O2A-CGA-O1A	-2.76	116.71	123.63
10	W	402	BCL	CHA-C1A-NA	-2.76	120.13	126.39
10	A	811	BCL	CMB-C2B-C1B	-2.76	121.22	125.42
9	A	826	CLA	C3A-C2A-C1A	2.76	105.47	101.34
10	Z	407	BCL	C1D-ND-C4D	-2.75	104.38	106.31
10	a	812	BCL	C2A-C1A-CHA	2.75	128.65	123.87
10	X	409	BCL	CAB-C3B-C2B	2.75	133.46	127.74
10	Y	401	BCL	C2A-C1A-CHA	2.75	128.64	123.87
10	X	406	BCL	CAB-C3B-C2B	2.74	133.44	127.74
10	A	806	BCL	CHD-C1D-C2D	2.74	131.19	125.49
10	a	806	BCL	C1C-NC-C4C	2.74	107.93	106.68
13	a	820	LHG	O8-C23-C24	2.74	120.19	111.83
10	Y	404	BCL	C2A-C1A-CHA	2.74	128.62	123.87
10	X	404	BCL	C2A-C1A-CHA	2.74	128.62	123.87
11	A	815	F39	C25-C20-C19	2.74	119.98	115.23
10	A	811	BCL	C1-C2-C3	-2.73	121.73	126.20
14	C	302	LMG	O6-C1-O1	-2.73	103.60	110.04
10	U	404	BCL	C2A-C1A-CHA	2.72	128.59	123.87
10	Y	404	BCL	C1D-ND-C4D	-2.72	104.40	106.31
10	X	408[B]	BCL	C2A-C1A-CHA	2.72	128.59	123.87
10	a	808	BCL	C1D-ND-C4D	-2.72	104.40	106.31
13	a	819	LHG	O8-C23-C24	2.72	120.13	111.83
10	U	401	BCL	CAB-C3B-C2B	2.71	133.38	127.74
9	a	801	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
13	E	102	LHG	O8-C23-C24	2.71	120.10	111.83
13	E	101	LHG	O8-C23-C24	2.71	120.10	111.83
10	B	301	BCL	CAB-C3B-C2B	2.71	133.37	127.74
12	a	816	F26	C17-C13-C8	2.71	119.93	115.23
10	X	402	BCL	C1D-ND-C4D	-2.71	104.41	106.31
8	a	802	GS0	C3C-C2C-C1C	2.70	106.23	101.87
10	Y	403	BCL	C1D-ND-C4D	-2.70	104.42	106.31
10	Z	402	BCL	C1D-ND-C4D	-2.70	104.42	106.31
10	V	403	BCL	C2A-C1A-CHA	2.70	128.55	123.87
10	V	409[B]	BCL	C1D-ND-C4D	-2.70	104.42	106.31
10	X	402	BCL	C2A-C1A-CHA	2.70	128.55	123.87
12	a	817	F26	C17-C13-C8	2.69	119.90	115.23
10	Y	405	BCL	C1D-ND-C4D	-2.69	104.42	106.31
10	V	401	BCL	C1D-ND-C4D	-2.69	104.42	106.31
10	V	406	BCL	C2A-C1A-CHA	2.69	128.53	123.87
10	V	405	BCL	C2A-C1A-CHA	2.69	128.53	123.87
10	Y	404	BCL	C1C-NC-C4C	2.69	107.90	106.68
10	W	402	BCL	CAB-C3B-C2B	2.68	133.32	127.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	a	808	BCL	C2A-C1A-CHA	2.68	128.52	123.87
10	a	809	BCL	C1C-NC-C4C	2.68	107.90	106.68
10	A	805	BCL	C1C-NC-C4C	2.68	107.90	106.68
10	Z	402	BCL	C2A-C1A-CHA	2.68	128.51	123.87
10	V	402	BCL	C1D-ND-C4D	-2.68	104.43	106.31
10	X	406	BCL	C2A-C1A-CHA	2.67	128.50	123.87
10	W	402	BCL	C1C-NC-C4C	2.67	107.90	106.68
8	a	802	GS0	CMA-C3A-C2A	-2.67	103.68	113.98
11	C	301	F39	C25-C20-C19	2.66	119.85	115.23
9	A	827	CLA	C3A-C2A-C1A	2.66	105.32	101.34
10	X	409	BCL	C4-C3-C5	-2.66	110.61	115.23
10	X	406	BCL	C1D-ND-C4D	-2.66	104.45	106.31
10	W	404	BCL	C2A-C1A-CHA	2.65	128.47	123.87
13	Z	401	LHG	O8-C23-C24	2.65	119.92	111.83
10	W	406	BCL	C1D-ND-C4D	-2.65	104.45	106.31
10	A	804	BCL	C2A-C1A-CHA	2.65	128.46	123.87
10	X	408[B]	BCL	C1C-NC-C4C	2.65	107.89	106.68
10	A	812	BCL	CAC-C3C-C4C	2.65	118.46	112.58
10	A	808	BCL	C1D-ND-C4D	-2.65	104.46	106.31
11	a	815	F39	C25-C20-C19	2.64	119.81	115.23
10	A	804	BCL	C11-C10-C8	2.64	124.73	115.97
11	A	815	F39	O5-C10-C12	-2.64	102.83	109.32
14	A	822	LMG	O6-C1-O1	-2.64	103.82	110.04
10	Y	405	BCL	CAB-C3B-C2B	2.63	133.21	127.74
10	Z	408[B]	BCL	C2A-C1A-CHA	2.63	128.44	123.87
10	Z	404	BCL	CAB-C3B-C2B	2.63	133.21	127.74
10	Y	407	BCL	C1-C2-C3	-2.63	121.89	126.20
10	A	803	BCL	C16-C17-C18	-2.62	104.23	115.94
10	A	810	BCL	C1D-ND-C4D	-2.62	104.47	106.31
10	U	404	BCL	C4A-NA-C1A	2.62	107.87	106.68
10	A	814	BCL	O2D-CGD-O1D	-2.62	118.75	123.85
11	a	815	F39	C53-C56-C58	-2.62	120.04	126.25
11	C	301	F39	C46-C45-C47	2.61	121.59	118.96
10	U	405	BCL	C2A-C1A-CHA	2.61	128.40	123.87
13	A	817	LHG	O8-C23-C24	2.61	119.80	111.83
10	Y	401	BCL	C1C-NC-C4C	2.61	107.87	106.68
10	Y	408	BCL	C2A-C1A-CHA	2.61	128.40	123.87
10	A	803	BCL	C4A-NA-C1A	2.60	107.87	106.68
10	X	407[B]	BCL	C2A-C1A-CHA	2.60	128.38	123.87
10	X	401	BCL	C2A-C1A-CHA	2.60	128.38	123.87
13	A	819	LHG	C11-C10-C9	-2.60	101.22	114.37
10	Y	406	BCL	C1C-NC-C4C	2.60	107.86	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	801	GS0	C11-C12-C13	-2.60	107.33	115.97
11	C	301	F39	O4-C9-C11	-2.59	103.89	110.08
10	A	811	BCL	C1C-NC-C4C	2.59	107.86	106.68
10	A	805	BCL	C2A-C1A-CHA	2.59	128.37	123.87
10	U	407[B]	BCL	C4A-NA-C1A	2.59	107.86	106.68
10	A	811	BCL	C2A-C1A-CHA	2.59	128.35	123.87
10	A	810	BCL	C2A-C1A-CHA	2.58	128.35	123.87
9	A	802	CLA	C2B-C1B-NB	-2.58	107.65	110.33
13	E	101	LHG	C11-C10-C9	-2.58	101.32	114.37
9	a	801	CLA	O2A-CGA-O1A	-2.58	117.18	123.63
13	E	102	LHG	C11-C10-C9	-2.58	101.35	114.37
10	W	407	BCL	C2A-C1A-CHA	2.57	128.33	123.87
13	a	821	LHG	O8-C23-C24	2.57	119.68	111.83
11	C	301	F39	C53-C56-C58	-2.57	120.14	126.25
10	a	814	BCL	C5-C3-C2	-2.57	115.40	121.17
11	a	815	F39	C46-C45-C47	2.57	121.55	118.96
10	A	813	BCL	C1D-ND-C4D	-2.57	104.51	106.31
10	U	405	BCL	C1D-ND-C4D	-2.56	104.51	106.31
8	A	801	GS0	CMD-C2D-C1D	2.56	129.24	124.73
10	a	813	BCL	C1-C2-C3	-2.56	122.00	126.20
10	W	407	BCL	C5-C3-C2	-2.56	115.42	121.17
12	a	817	F26	C22-C25-C26	-2.56	119.36	126.36
10	X	405	BCL	C2A-C1A-CHA	2.55	128.29	123.87
10	W	402	BCL	C1D-ND-C4D	-2.55	104.52	106.31
10	Z	403	BCL	O2D-CGD-O1D	-2.55	118.89	123.85
10	Z	403	BCL	C2A-C1A-CHA	2.55	128.29	123.87
10	a	804	BCL	C2A-C1A-CHA	2.55	128.28	123.87
10	a	812	BCL	CAC-C3C-C4C	2.54	118.23	112.58
10	V	408	BCL	CAB-C3B-C2B	2.54	133.02	127.74
9	a	801	CLA	C4D-CHA-C1A	2.54	124.27	121.24
13	A	818	LHG	C11-C10-C9	-2.54	101.55	114.37
10	A	806	BCL	C4D-C3D-CAD	-2.54	105.35	108.11
14	A	821	LMG	C1-O6-C5	-2.53	108.77	113.72
10	A	814	BCL	C1-C2-C3	-2.53	122.05	126.20
10	Z	404	BCL	C1D-ND-C4D	-2.53	104.53	106.31
9	a	801	CLA	C2C-C1C-NC	-2.53	107.32	109.98
10	U	403	BCL	C5-C3-C2	-2.53	115.49	121.17
10	U	406	BCL	C5-C3-C2	-2.53	115.49	121.17
10	a	813	BCL	C2A-C1A-CHA	2.53	128.25	123.87
13	A	819	LHG	O8-C23-C24	2.52	119.52	111.83
9	a	801	CLA	C3A-C2A-C1A	2.52	105.11	101.34
10	A	808	BCL	C1-C2-C3	-2.52	122.07	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Z	407	BCL	C2A-C1A-CHA	2.52	128.24	123.87
12	a	816	F26	C20-C16-C21	2.51	120.37	114.59
10	U	402	BCL	C1D-ND-C4D	-2.51	104.55	106.31
10	Y	402	BCL	C2A-C1A-CHA	2.51	128.22	123.87
10	Z	406	BCL	C1D-ND-C4D	-2.51	104.55	106.31
10	Y	402	BCL	C1C-NC-C4C	2.50	107.82	106.68
10	U	406	BCL	C1D-ND-C4D	-2.50	104.56	106.31
10	a	806	BCL	CHC-C1C-NC	-2.50	120.80	124.40
10	U	407[B]	BCL	C1D-ND-C4D	-2.50	104.56	106.31
10	Y	408	BCL	C1D-ND-C4D	-2.50	104.56	106.31
10	B	301	BCL	C1C-NC-C4C	2.49	107.82	106.68
10	A	812	BCL	O2A-CGA-O1A	-2.49	117.39	123.63
10	U	406	BCL	O2A-CGA-O1A	-2.49	117.39	123.63
10	a	810	BCL	C1D-ND-C4D	-2.49	104.56	106.31
10	W	408[B]	BCL	C1D-ND-C4D	-2.49	104.56	106.31
10	U	403	BCL	CAB-C3B-C2B	2.49	132.92	127.74
10	a	808	BCL	CAB-C3B-C2B	2.49	132.91	127.74
10	a	808	BCL	C1C-NC-C4C	2.49	107.81	106.68
10	a	814	BCL	C1D-ND-C4D	-2.48	104.57	106.31
10	Z	404	BCL	CMB-C2B-C1B	-2.48	121.64	125.42
10	a	814	BCL	CAC-C3C-C4C	2.48	118.09	112.58
13	Z	401	LHG	C11-C10-C9	-2.48	101.82	114.37
10	Y	403	BCL	C5-C3-C2	-2.48	115.60	121.17
12	a	817	F26	C27-C28-C31	-2.48	119.57	126.36
10	Z	405	BCL	C4A-NA-C1A	2.48	107.81	106.68
10	W	402	BCL	C2A-C1A-CHA	2.47	128.16	123.87
10	A	814	BCL	C4A-NA-C1A	2.47	107.81	106.68
10	X	404	BCL	C4A-NA-C1A	2.47	107.81	106.68
10	V	408	BCL	C5-C3-C2	-2.47	115.63	121.17
10	a	811	BCL	C1C-NC-C4C	2.47	107.80	106.68
10	V	405	BCL	C1D-ND-C4D	-2.47	104.58	106.31
14	A	821	LMG	O2-C2-C1	-2.46	104.21	110.08
10	a	803	BCL	C1D-ND-C4D	-2.46	104.59	106.31
10	Z	403	BCL	C1D-ND-C4D	-2.46	104.59	106.31
11	a	815	F39	C63-C64-C62	-2.46	119.62	126.36
10	V	407	BCL	C1D-ND-C4D	-2.45	104.59	106.31
10	U	406	BCL	C11-C10-C8	-2.45	107.82	115.97
14	a	822	LMG	O1-C1-C2	-2.45	104.55	108.27
10	B	301	BCL	C2A-C1A-CHA	2.45	128.12	123.87
13	a	819	LHG	C11-C10-C9	-2.45	102.00	114.37
14	A	823	LMG	O3-C3-C2	-2.45	104.61	110.38
13	a	820	LHG	C11-C10-C9	-2.44	102.01	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	821	LMG	O6-C1-O1	-2.44	104.27	110.04
10	X	406	BCL	C1-C2-C3	-2.44	122.20	126.20
10	Z	405	BCL	CAB-C3B-C2B	2.44	132.81	127.74
11	C	301	F39	O1-C12-C10	-2.44	105.31	109.70
13	A	817	LHG	C11-C10-C9	-2.43	102.06	114.37
8	a	802	GS0	CMC-C2C-C3C	-2.43	104.57	113.98
10	Y	407	BCL	C16-C15-C13	-2.43	107.88	115.97
10	V	403	BCL	C1D-ND-C4D	-2.43	104.61	106.31
10	a	814	BCL	C2A-C1A-CHA	2.43	128.08	123.87
12	A	816	F26	C32-C35-C34	-2.42	119.72	126.36
9	A	802	CLA	C2C-C1C-NC	-2.42	107.44	109.98
8	a	802	GS0	C11-C12-C13	-2.42	107.92	115.97
13	a	818	LHG	O8-C23-C24	2.42	119.21	111.83
10	V	401	BCL	C4-C3-C5	-2.42	111.03	115.23
10	a	812	BCL	C1C-NC-C4C	2.42	107.78	106.68
10	a	803	BCL	O2D-CGD-O1D	-2.42	119.14	123.85
10	A	814	BCL	CAC-C3C-C4C	2.42	117.94	112.58
10	X	403	BCL	C1D-ND-C4D	-2.41	104.62	106.31
9	a	801	CLA	C3C-C4C-NC	-2.41	107.34	110.43
8	a	802	GS0	CMC-C2C-C1C	-2.41	105.30	111.77
10	X	408[B]	BCL	C1D-ND-C4D	-2.41	104.62	106.31
10	V	401	BCL	C2A-C1A-CHA	2.41	128.04	123.87
10	a	812	BCL	C11-C10-C8	2.41	123.96	115.97
14	A	822	LMG	O2-C2-C1	-2.41	104.34	110.08
11	A	815	F39	C46-C45-C47	2.40	121.38	118.96
10	Y	405	BCL	C4-C3-C5	-2.40	111.06	115.23
10	Y	406	BCL	C1-C2-C3	-2.40	122.27	126.20
11	A	815	F39	C63-C64-C62	-2.39	119.80	126.36
10	A	809	BCL	C1D-ND-C4D	-2.39	104.63	106.31
14	a	822	LMG	O2-C2-C1	-2.39	104.38	110.08
10	Y	408	BCL	C1-C2-C3	-2.39	122.28	126.20
10	A	808	BCL	O2D-CGD-O1D	-2.39	119.20	123.85
10	X	405	BCL	C1D-ND-C4D	-2.38	104.64	106.31
10	Y	407	BCL	CHD-C1D-C2D	2.38	130.44	125.49
10	W	403	BCL	C2A-C1A-CHA	2.38	127.99	123.87
9	A	826	CLA	C4D-CHA-C1A	2.37	124.07	121.24
13	a	821	LHG	C11-C10-C9	-2.37	102.38	114.37
10	a	804	BCL	C1D-ND-C4D	-2.37	104.65	106.31
10	X	404	BCL	C1-C2-C3	-2.37	122.32	126.20
10	X	403	BCL	C1-C2-C3	-2.37	122.32	126.20
10	X	406	BCL	O2A-CGA-O1A	-2.36	117.72	123.63
10	V	402	BCL	CBA-CAA-C2A	2.36	120.83	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	U	407[B]	BCL	C2A-C1A-CHA	2.36	127.97	123.87
10	U	401	BCL	C1D-ND-C4D	-2.36	104.66	106.31
10	Y	402	BCL	C1D-ND-C4D	-2.36	104.66	106.31
10	a	805	BCL	C4D-C3D-CAD	-2.35	105.55	108.11
12	a	816	F26	C10-C14-C16	-2.35	119.81	127.64
10	V	404	BCL	O2D-CGD-O1D	-2.35	119.28	123.85
13	a	818	LHG	C11-C10-C9	-2.34	102.52	114.37
10	Y	407	BCL	C1D-ND-C4D	-2.34	104.67	106.31
10	W	407	BCL	C1-C2-C3	-2.34	122.36	126.20
10	a	811	BCL	C2A-C1A-CHA	2.34	127.93	123.87
10	U	404	BCL	O2A-CGA-O1A	-2.34	117.77	123.63
9	A	802	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
10	W	401	BCL	CBA-CAA-C2A	2.34	120.75	113.79
10	a	807	BCL	CAB-C3B-C2B	2.34	132.60	127.74
10	V	405	BCL	C6-C5-C3	2.34	119.16	113.47
8	A	801	GS0	CHC-C4B-NB	2.34	127.55	124.05
10	a	806	BCL	C4D-C3D-CAD	-2.33	105.57	108.11
10	W	401	BCL	C1D-ND-C4D	-2.33	104.67	106.31
10	W	404	BCL	C4-C3-C5	-2.33	111.18	115.23
8	a	802	GS0	CHC-C4B-NB	2.33	127.55	124.05
8	A	801	GS0	CMB-C2B-C3B	2.33	133.03	125.67
12	a	816	F26	C38-C39-C37	-2.33	118.75	123.52
11	C	301	F39	C63-C64-C62	-2.33	119.99	126.36
12	A	816	F26	C10-C14-C16	-2.32	119.89	127.64
10	a	806	BCL	C1D-ND-C4D	-2.32	104.68	106.31
9	A	827	CLA	C4-C3-C2	-2.32	117.67	123.63
10	A	805	BCL	C5-C3-C2	-2.32	115.97	121.17
10	W	407	BCL	C1D-ND-C4D	-2.32	104.69	106.31
10	a	813	BCL	CBA-CAA-C2A	2.32	120.68	113.79
10	Y	401	BCL	C1D-ND-C4D	-2.31	104.69	106.31
10	A	807	BCL	C1D-ND-C4D	-2.31	104.69	106.31
12	a	817	F26	C32-C35-C34	-2.31	120.03	126.36
14	A	823	LMG	O7-C10-O9	-2.31	118.31	123.70
10	a	814	BCL	CHD-C1D-C2D	2.30	130.28	125.49
12	A	816	F26	C38-C39-C37	-2.30	118.81	123.52
10	A	808	BCL	C5-C3-C2	-2.30	116.01	121.17
14	C	302	LMG	O3-C3-C2	-2.30	104.96	110.38
10	A	812	BCL	O2D-CGD-O1D	-2.30	119.38	123.85
10	V	407	BCL	CMB-C2B-C1B	-2.30	121.92	125.42
10	A	812	BCL	C6-C5-C3	2.30	119.06	113.47
11	a	815	F39	O4-C9-C11	-2.29	104.61	110.08
10	U	403	BCL	O2D-CGD-O1D	-2.29	119.39	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	815	F39	O4-C9-C11	-2.29	104.63	110.08
10	Y	408	BCL	C5-C3-C2	-2.28	116.04	121.17
10	A	804	BCL	C6-C5-C3	2.28	119.03	113.47
10	X	407[B]	BCL	C1D-ND-C4D	-2.28	104.71	106.31
10	Y	406	BCL	CAB-C3B-C2B	2.28	132.48	127.74
10	W	403	BCL	O2D-CGD-O1D	-2.28	119.41	123.85
11	a	815	F39	O5-C10-C12	-2.27	103.72	109.32
10	X	406	BCL	C5-C3-C2	-2.27	116.06	121.17
10	a	813	BCL	CAA-C2A-C1A	2.27	119.42	111.97
10	A	804	BCL	C1D-ND-C4D	-2.27	104.72	106.31
10	X	402	BCL	O2D-CGD-O1D	-2.27	119.43	123.85
14	C	302	LMG	O1-C1-C2	-2.27	104.83	108.27
10	A	813	BCL	C4D-C3D-CAD	-2.27	105.64	108.11
10	W	407	BCL	CAB-C3B-C2B	2.27	132.45	127.74
10	A	813	BCL	O2A-CGA-O1A	-2.26	117.97	123.63
11	C	301	F39	C40-C41-C42	-2.26	120.18	126.36
12	A	816	F26	C20-C16-C21	2.25	119.77	114.59
11	C	301	F39	O2-C11-C9	2.25	114.69	108.42
12	a	816	F26	C9-C15-C19	-2.25	120.91	126.25
10	Y	406	BCL	C1D-ND-C4D	-2.25	104.73	106.31
10	B	301	BCL	CBA-CAA-C2A	2.25	120.48	113.79
10	V	407	BCL	CAB-C3B-C2B	2.25	132.41	127.74
10	a	806	BCL	CHD-C1D-C2D	2.24	130.16	125.49
8	A	801	GS0	C3D-C2D-C1D	-2.24	102.77	105.83
10	Y	408	BCL	CAB-C3B-C2B	2.24	132.40	127.74
14	A	821	LMG	O1-C7-C8	-2.24	105.37	110.82
12	a	817	F26	C10-C14-C16	-2.24	120.17	127.64
10	a	803	BCL	C4D-C3D-CAD	-2.23	105.68	108.11
8	a	802	GS0	CHB-C4A-NA	-2.23	121.18	124.40
10	A	805	BCL	CMD-C2D-C1D	2.23	128.66	124.73
10	A	803	BCL	CHD-C1D-C2D	2.23	130.13	125.49
10	a	813	BCL	C4D-C3D-CAD	-2.23	105.69	108.11
10	Y	403	BCL	CAB-C3B-C2B	2.23	132.37	127.74
10	Y	406	BCL	C4D-C3D-CAD	-2.23	105.69	108.11
9	A	826	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
10	X	404	BCL	CAB-C3B-C2B	2.23	132.37	127.74
10	A	806	BCL	O2A-CGA-CBA	-2.23	105.05	111.83
10	Z	408[B]	BCL	C1D-ND-C4D	-2.22	104.75	106.31
10	a	810	BCL	C1-O2A-CGA	-2.22	111.27	116.65
10	A	808	BCL	C2A-C1A-CHA	2.22	127.72	123.87
10	B	301	BCL	CMB-C2B-C1B	-2.22	122.04	125.42
8	A	801	GS0	C2D-C1D-ND	2.22	112.32	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	815	F39	C40-C41-C42	-2.22	120.29	126.36
10	W	403	BCL	C16-C15-C13	2.21	123.33	115.97
8	a	802	GS0	C2D-C1D-ND	2.21	112.32	110.13
9	A	827	CLA	C1-C2-C3	-2.21	122.57	126.20
10	a	804	BCL	C4-C3-C5	-2.21	111.39	115.23
14	A	820	LMG	C3-C4-C5	-2.21	106.22	110.23
9	A	802	CLA	CHD-C1D-C2D	2.21	130.08	125.49
12	a	816	F26	C27-C28-C31	-2.21	120.31	126.36
10	U	405	BCL	C6-C5-C3	2.21	118.84	113.47
10	X	403	BCL	CHD-C1D-C2D	2.21	130.07	125.49
10	Y	408	BCL	O2A-CGA-O1A	-2.21	118.11	123.63
8	A	801	GS0	C1D-ND-C4D	-2.20	104.77	106.31
10	A	804	BCL	C17-C16-C15	2.20	123.16	113.28
10	a	808	BCL	CHD-C1D-C2D	2.20	130.07	125.49
10	Z	407	BCL	CAB-C3B-C2B	2.20	132.32	127.74
10	W	401	BCL	O2A-CGA-O1A	-2.20	118.13	123.63
10	U	402	BCL	O2D-CGD-O1D	-2.20	119.57	123.85
10	a	813	BCL	C4A-NA-C1A	2.19	107.68	106.68
10	Z	404	BCL	C1C-NC-C4C	2.19	107.68	106.68
10	B	301	BCL	C1D-ND-C4D	-2.19	104.77	106.31
10	Z	404	BCL	CHD-C1D-C2D	2.19	130.05	125.49
10	W	404	BCL	C1D-ND-C4D	-2.19	104.78	106.31
9	a	801	CLA	CHD-C1D-C2D	2.19	130.04	125.49
10	U	404	BCL	C4D-C3D-CAD	-2.19	105.73	108.11
10	V	403	BCL	C1C-NC-C4C	2.19	107.68	106.68
10	A	811	BCL	C4D-C3D-CAD	-2.19	105.73	108.11
14	a	822	LMG	O3-C3-C2	-2.19	105.22	110.38
10	X	403	BCL	C4-C3-C5	-2.19	111.44	115.23
11	a	815	F39	C40-C41-C42	-2.18	120.38	126.36
14	C	302	LMG	O2-C2-C1	-2.18	104.88	110.08
14	A	823	LMG	O2-C2-C1	-2.18	104.88	110.08
10	Z	405	BCL	C1D-ND-C4D	-2.18	104.78	106.31
10	A	803	BCL	C17-C16-C15	2.18	123.03	113.28
11	C	301	F39	O5-C10-C12	-2.17	103.98	109.32
10	V	406	BCL	C1D-ND-C4D	-2.17	104.79	106.31
8	A	801	GS0	C12-C11-C10	-2.17	103.56	113.28
10	a	805	BCL	C4-C3-C5	-2.17	111.47	115.23
10	Z	402	BCL	CBA-CAA-C2A	2.17	120.24	113.79
10	a	810	BCL	CHD-C1D-C2D	2.17	129.99	125.49
10	A	814	BCL	O2A-CGA-O1A	-2.17	118.21	123.63
10	a	812	BCL	O2D-CGD-O1D	-2.16	119.64	123.85
10	a	812	BCL	C1D-ND-C4D	-2.16	104.80	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	W	408[B]	BCL	C4A-NA-C1A	2.16	107.66	106.68
10	Z	402	BCL	CMB-C2B-C1B	-2.16	122.13	125.42
10	B	301	BCL	O2D-CGD-O1D	-2.16	119.65	123.85
10	U	401	BCL	CBA-CAA-C2A	2.16	120.21	113.79
10	Y	405	BCL	CHD-C1D-C2D	2.15	129.97	125.49
10	A	803	BCL	O2A-CGA-O1A	-2.15	118.25	123.63
10	A	812	BCL	C6-C7-C8	2.15	123.10	115.97
10	a	804	BCL	C4A-NA-C1A	2.14	107.66	106.68
9	A	827	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
10	W	401	BCL	CAA-C2A-C1A	2.14	119.00	111.97
10	U	403	BCL	C6-C5-C3	2.14	118.68	113.47
10	a	804	BCL	C1-C2-C3	-2.14	122.69	126.20
10	W	405	BCL	C1D-ND-C4D	-2.14	104.81	106.31
10	X	405	BCL	C6-C5-C3	2.14	118.67	113.47
10	W	403	BCL	C1D-ND-C4D	-2.13	104.81	106.31
9	a	801	CLA	CHA-C4D-ND	2.13	136.94	132.55
10	Z	406	BCL	CHD-C1D-C2D	2.13	129.91	125.49
10	Z	405	BCL	C4D-C3D-CAD	-2.13	105.80	108.11
8	a	802	GS0	C3D-C2D-C1D	-2.13	102.93	105.83
10	U	403	BCL	CHD-C1D-C2D	2.12	129.90	125.49
10	X	402	BCL	C5-C3-C2	-2.12	116.41	121.17
10	a	811	BCL	C4A-NA-C1A	2.12	107.64	106.68
10	U	403	BCL	CMB-C2B-C1B	-2.11	122.20	125.42
10	Y	402	BCL	C4D-C3D-CAD	-2.11	105.81	108.11
12	a	817	F26	C20-C16-C21	2.11	119.45	114.59
10	Z	407	BCL	O2A-CGA-O1A	-2.11	118.35	123.63
10	A	805	BCL	O2A-CGA-O1A	-2.11	118.35	123.63
10	W	401	BCL	CMB-C2B-C1B	-2.11	122.21	125.42
10	A	812	BCL	CHD-C1D-C2D	2.11	129.87	125.49
10	V	405	BCL	CHD-C1D-C2D	2.11	129.87	125.49
10	a	811	BCL	O2D-CGD-O1D	-2.10	119.75	123.85
10	Z	408[B]	BCL	O2D-CGD-O1D	-2.10	119.75	123.85
10	A	814	BCL	C1D-ND-C4D	-2.10	104.84	106.31
14	A	820	LMG	O3-C3-C2	-2.10	105.44	110.38
10	Z	402	BCL	C4D-C3D-CAD	-2.10	105.83	108.11
10	U	403	BCL	C1-O2A-CGA	2.10	121.72	116.65
10	W	405	BCL	CAB-C3B-C2B	2.09	132.09	127.74
10	U	404	BCL	C1D-ND-C4D	-2.09	104.84	106.31
10	V	401	BCL	O2D-CGD-O1D	-2.09	119.77	123.85
10	X	405	BCL	CHD-C1D-C2D	2.09	129.84	125.49
10	X	401	BCL	C1C-NC-C4C	2.09	107.63	106.68
10	A	803	BCL	C1-C2-C3	-2.09	122.77	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	820	LMG	O2-C2-C1	-2.09	105.10	110.08
10	W	404	BCL	CMB-C2B-C1B	-2.09	122.24	125.42
10	Y	403	BCL	C1C-NC-C4C	2.09	107.63	106.68
10	A	811	BCL	CHD-C1D-C2D	2.09	129.83	125.49
11	C	301	F39	C14-C18-C19	2.09	117.34	112.33
10	U	406	BCL	CAB-C3B-C2B	2.09	132.08	127.74
10	Y	405	BCL	C4D-C3D-CAD	-2.09	105.84	108.11
10	V	408	BCL	C1C-NC-C4C	2.08	107.63	106.68
10	X	408[B]	BCL	C4A-NA-C1A	2.08	107.63	106.68
10	Y	403	BCL	CHD-C1D-C2D	2.08	129.82	125.49
10	X	404	BCL	C4-C3-C5	-2.08	111.62	115.23
10	A	809	BCL	C4D-C3D-CAD	-2.08	105.85	108.11
10	a	811	BCL	C1D-ND-C4D	-2.08	104.86	106.31
10	Z	402	BCL	C6-C5-C3	2.07	118.52	113.47
10	A	814	BCL	CHD-C1D-C2D	2.07	129.79	125.49
10	V	402	BCL	OBb-CAB-CBB	-2.07	115.13	119.77
10	a	812	BCL	CHD-C1D-C2D	2.07	129.79	125.49
10	V	402	BCL	CAA-C2A-C1A	2.07	118.75	111.97
10	X	403	BCL	CMB-C2B-C1B	-2.07	122.27	125.42
10	X	403	BCL	O2D-CGD-O1D	-2.06	119.83	123.85
9	A	826	CLA	CHD-C1D-C2D	2.06	129.78	125.49
10	Y	403	BCL	C6-C5-C3	2.06	118.48	113.47
10	A	804	BCL	O2D-CGD-O1D	-2.06	119.85	123.85
10	A	812	BCL	C1D-ND-C4D	-2.05	104.87	106.31
14	A	822	LMG	O3-C3-C2	-2.05	105.54	110.38
10	X	404	BCL	C1D-ND-C4D	-2.05	104.87	106.31
10	Y	408	BCL	O2D-CGD-O1D	-2.05	119.86	123.85
12	a	817	F26	C23-C19-C24	-2.05	119.49	122.82
10	A	809	BCL	O2D-CGD-O1D	-2.05	119.86	123.85
10	a	805	BCL	CHD-C1D-C2D	2.05	129.75	125.49
10	Y	406	BCL	CHD-C1D-C2D	2.05	129.75	125.49
10	A	806	BCL	OBb-CAB-C3B	2.05	124.05	120.43
10	W	407	BCL	O2A-CGA-O1A	-2.04	118.51	123.63
10	Y	401	BCL	C11-C10-C8	2.04	122.76	115.97
10	a	808	BCL	O2D-CGD-O1D	-2.04	119.87	123.85
13	A	819	LHG	C5-O7-C7	-2.04	112.91	117.80
10	a	808	BCL	C4D-C3D-CAD	-2.04	105.89	108.11
10	X	402	BCL	O2A-CGA-O1A	-2.04	118.52	123.63
10	A	810	BCL	CHD-C1D-C2D	2.04	129.73	125.49
10	V	407	BCL	C11-C10-C8	-2.04	109.18	115.97
10	V	403	BCL	CHD-C1D-C2D	2.04	129.73	125.49
10	V	403	BCL	CAB-C3B-C2B	2.04	131.98	127.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	401	BCL	OBB-CAB-CBB	-2.04	115.20	119.77
9	A	802	CLA	C1-C2-C3	-2.03	122.86	126.20
10	U	403	BCL	CAC-C3C-C4C	2.03	117.10	112.58
10	Z	408[B]	BCL	C4D-C3D-CAD	-2.03	105.90	108.11
10	X	406	BCL	C11-C10-C8	-2.03	109.21	115.97
14	A	822	LMG	O7-C10-O9	-2.03	118.96	123.70
12	A	816	F26	C22-C25-C26	-2.03	120.81	126.36
10	A	804	BCL	C16-C15-C13	2.03	122.70	115.97
10	A	814	BCL	C6-C5-C3	2.03	118.40	113.47
10	a	803	BCL	CHD-C1D-C2D	2.02	129.70	125.49
10	B	301	BCL	CHD-C1D-C2D	2.02	129.70	125.49
13	A	818	LHG	C5-O7-C7	-2.02	112.95	117.80
10	B	301	BCL	C4-C3-C5	-2.02	111.72	115.23
10	a	810	BCL	C6-C5-C3	2.02	118.39	113.47
10	X	409	BCL	O2D-CGD-O1D	-2.02	119.92	123.85
9	A	827	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
10	X	401	BCL	CHD-C1D-C2D	2.02	129.69	125.49
12	A	816	F26	C23-C19-C24	-2.02	119.55	122.82
10	A	808	BCL	CHD-C1D-C2D	2.02	129.68	125.49
10	Z	402	BCL	OBB-CAB-CBB	-2.02	115.25	119.77
10	V	408	BCL	O2D-CGD-O1D	-2.01	119.93	123.85
10	V	402	BCL	CMB-C2B-C1B	-2.01	122.36	125.42
10	U	402	BCL	C5-C3-C2	-2.01	116.66	121.17
10	X	401	BCL	C4-C3-C5	-2.00	111.75	115.23
10	Z	407	BCL	O2D-CGD-O1D	-2.00	119.95	123.85
10	a	811	BCL	CMB-C2B-C1B	-2.00	122.37	125.42
10	a	804	BCL	CHD-C1D-C2D	2.00	129.65	125.49

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	801	GS0	C13
8	A	801	GS0	CBD
8	a	802	GS0	C3C
8	a	802	GS0	CBD
9	A	802	CLA	CBD
9	A	802	CLA	C3A
9	A	802	CLA	C2A
9	A	826	CLA	CBD
9	A	826	CLA	C3A
9	A	826	CLA	C2A
9	A	827	CLA	CBD

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Mol	Chain	Res	Type	Atom
9	A	827	CLA	C3A
9	A	827	CLA	C2A
9	a	801	CLA	CBD
9	a	801	CLA	C3A
9	a	801	CLA	C2A

All (1354) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	801	GS0	C1-C2-C3-C4
8	A	801	GS0	C1-C2-C3-C5
8	A	801	GS0	C3A-C2A-CAA-CBA
8	A	801	GS0	CBD-CGD-O2D-CED
8	A	801	GS0	O1D-CGD-O2D-CED
8	a	802	GS0	C1-C2-C3-C4
8	a	802	GS0	C1-C2-C3-C5
8	a	802	GS0	C3A-C2A-CAA-CBA
8	a	802	GS0	C2C-C3C-CAC-CBC
8	a	802	GS0	C4C-C3C-CAC-CBC
9	A	802	CLA	CBD-CGD-O2D-CED
9	A	826	CLA	CAD-CBD-CGD-O2D
9	A	826	CLA	CBD-CGD-O2D-CED
9	A	826	CLA	O1D-CGD-O2D-CED
9	A	826	CLA	C1-C2-C3-C5
9	A	826	CLA	C14-C13-C15-C16
9	A	827	CLA	C1A-C2A-CAA-CBA
9	a	801	CLA	CBD-CGD-O2D-CED
9	a	801	CLA	O1D-CGD-O2D-CED
9	a	801	CLA	C1-C2-C3-C4
9	a	801	CLA	C1-C2-C3-C5
10	A	805	BCL	C2B-C3B-CAB-OBB
10	A	805	BCL	C2B-C3B-CAB-CBB
10	A	805	BCL	C4B-C3B-CAB-OBB
10	A	805	BCL	C4B-C3B-CAB-CBB
10	A	805	BCL	C4C-C3C-CAC-CBC
10	A	806	BCL	C2B-C3B-CAB-OBB
10	A	806	BCL	C2B-C3B-CAB-CBB
10	A	807	BCL	C4C-C3C-CAC-CBC
10	A	808	BCL	CHA-CBD-CGD-O1D
10	A	809	BCL	CAD-CBD-CGD-O1D
10	A	809	BCL	CAD-CBD-CGD-O2D
10	A	812	BCL	C2B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
10	A	812	BCL	C2B-C3B-CAB-CBB
10	A	812	BCL	C1-C2-C3-C4
10	A	813	BCL	C1A-C2A-CAA-CBA
10	A	813	BCL	C4C-C3C-CAC-CBC
10	A	814	BCL	C2B-C3B-CAB-OBB
10	A	814	BCL	C2B-C3B-CAB-CBB
10	A	814	BCL	C4B-C3B-CAB-OBB
10	A	814	BCL	CAD-CBD-CGD-O2D
10	a	803	BCL	C4C-C3C-CAC-CBC
10	a	803	BCL	CHA-CBD-CGD-O1D
10	a	804	BCL	C2B-C3B-CAB-OBB
10	a	804	BCL	C2B-C3B-CAB-CBB
10	a	804	BCL	C4B-C3B-CAB-CBB
10	a	805	BCL	C4C-C3C-CAC-CBC
10	a	806	BCL	C2B-C3B-CAB-OBB
10	a	806	BCL	C2B-C3B-CAB-CBB
10	a	806	BCL	C4B-C3B-CAB-OBB
10	a	806	BCL	C4B-C3B-CAB-CBB
10	a	806	BCL	C2C-C3C-CAC-CBC
10	a	806	BCL	C4C-C3C-CAC-CBC
10	a	807	BCL	C2C-C3C-CAC-CBC
10	a	807	BCL	C4C-C3C-CAC-CBC
10	a	807	BCL	C1-C2-C3-C4
10	a	808	BCL	CHA-CBD-CGD-O1D
10	a	809	BCL	CAD-CBD-CGD-O2D
10	a	809	BCL	O2A-C1-C2-C3
10	a	810	BCL	C2C-C3C-CAC-CBC
10	a	810	BCL	C4C-C3C-CAC-CBC
10	a	812	BCL	C2B-C3B-CAB-OBB
10	a	812	BCL	C2B-C3B-CAB-CBB
10	a	812	BCL	C4B-C3B-CAB-OBB
10	a	812	BCL	C4B-C3B-CAB-CBB
10	a	812	BCL	CAD-CBD-CGD-O2D
10	a	813	BCL	C1A-C2A-CAA-CBA
10	a	813	BCL	C3A-C2A-CAA-CBA
10	a	813	BCL	C2B-C3B-CAB-OBB
10	a	813	BCL	C4B-C3B-CAB-OBB
10	a	813	BCL	C2C-C3C-CAC-CBC
10	a	813	BCL	C4C-C3C-CAC-CBC
10	a	813	BCL	CAD-CBD-CGD-O2D
10	a	814	BCL	C2B-C3B-CAB-OBB
10	a	814	BCL	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
10	a	814	BCL	C4C-C3C-CAC-CBC
10	a	814	BCL	O2A-C1-C2-C3
10	a	814	BCL	C2-C3-C5-C6
10	B	301	BCL	C1A-C2A-CAA-CBA
10	B	301	BCL	C4C-C3C-CAC-CBC
10	B	301	BCL	CAD-CBD-CGD-O1D
10	B	301	BCL	CAD-CBD-CGD-O2D
10	U	402	BCL	C2B-C3B-CAB-OB
10	U	402	BCL	C2B-C3B-CAB-CB
10	U	402	BCL	C4B-C3B-CAB-OB
10	U	402	BCL	C4B-C3B-CAB-CB
10	U	402	BCL	C4C-C3C-CAC-CBC
10	U	402	BCL	CAD-CBD-CGD-O1D
10	U	402	BCL	CAD-CBD-CGD-O2D
10	U	404	BCL	CAD-CBD-CGD-O2D
10	U	405	BCL	C2B-C3B-CAB-OB
10	U	405	BCL	C2B-C3B-CAB-CB
10	U	407[B]	BCL	C2C-C3C-CAC-CBC
10	U	407[B]	BCL	CAD-CBD-CGD-O2D
10	V	404	BCL	C2B-C3B-CAB-OB
10	V	404	BCL	C2B-C3B-CAB-CB
10	V	404	BCL	C4B-C3B-CAB-OB
10	V	404	BCL	C4B-C3B-CAB-CB
10	V	404	BCL	C2C-C3C-CAC-CBC
10	V	404	BCL	C4C-C3C-CAC-CBC
10	V	405	BCL	C2C-C3C-CAC-CBC
10	V	405	BCL	C4C-C3C-CAC-CBC
10	V	409[B]	BCL	C1A-C2A-CAA-CBA
10	V	409[B]	BCL	C2B-C3B-CAB-OB
10	W	402	BCL	C2C-C3C-CAC-CBC
10	W	402	BCL	C4C-C3C-CAC-CBC
10	W	403	BCL	C2B-C3B-CAB-OB
10	W	403	BCL	C2B-C3B-CAB-CB
10	W	403	BCL	C4B-C3B-CAB-OB
10	W	403	BCL	C4B-C3B-CAB-CB
10	W	403	BCL	C4C-C3C-CAC-CBC
10	W	404	BCL	C2C-C3C-CAC-CBC
10	W	404	BCL	C4C-C3C-CAC-CBC
10	W	405	BCL	C2C-C3C-CAC-CBC
10	W	408[B]	BCL	C4C-C3C-CAC-CBC
10	X	402	BCL	C4B-C3B-CAB-CB
10	X	402	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
10	X	402	BCL	C4-C3-C5-C6
10	X	403	BCL	C2C-C3C-CAC-CBC
10	X	403	BCL	C4C-C3C-CAC-CBC
10	X	407[B]	BCL	C2B-C3B-CAB-OBB
10	X	408[B]	BCL	CAD-CBD-CGD-O2D
10	Y	404	BCL	C2B-C3B-CAB-OBB
10	Y	404	BCL	C2B-C3B-CAB-CBB
10	Y	404	BCL	C4B-C3B-CAB-OBB
10	Y	404	BCL	C4B-C3B-CAB-CBB
10	Y	404	BCL	C4C-C3C-CAC-CBC
10	Y	404	BCL	CAD-CBD-CGD-O1D
10	Y	404	BCL	CAD-CBD-CGD-O2D
10	Y	407	BCL	C2B-C3B-CAB-OBB
10	Y	407	BCL	C2B-C3B-CAB-CBB
10	Y	407	BCL	C4B-C3B-CAB-OBB
10	Y	407	BCL	C4B-C3B-CAB-CBB
10	Z	403	BCL	C2B-C3B-CAB-OBB
10	Z	403	BCL	C2B-C3B-CAB-CBB
10	Z	403	BCL	C4B-C3B-CAB-OBB
10	Z	403	BCL	C4B-C3B-CAB-CBB
10	Z	403	BCL	C4C-C3C-CAC-CBC
10	Z	403	BCL	CAD-CBD-CGD-O1D
10	Z	403	BCL	CAD-CBD-CGD-O2D
10	Z	404	BCL	C4C-C3C-CAC-CBC
10	Z	406	BCL	C2B-C3B-CAB-OBB
10	Z	406	BCL	C2B-C3B-CAB-CBB
10	Z	406	BCL	C4B-C3B-CAB-OBB
10	Z	408[B]	BCL	CAD-CBD-CGD-O1D
10	Z	408[B]	BCL	CAD-CBD-CGD-O2D
11	A	815	F39	C17-C13-C14-C18
11	A	815	F39	C25-C20-C27-C32
11	A	815	F39	C32-C35-C37-C38
11	A	815	F39	C38-C37-C39-C40
11	A	815	F39	C37-C39-C40-C41
11	A	815	F39	C39-C40-C41-C42
11	A	815	F39	C40-C41-C42-C44
11	A	815	F39	C41-C42-C44-C51
11	A	815	F39	C44-C51-C57-C59
11	A	815	F39	C56-C58-C61-C63
11	A	815	F39	C60-C58-C61-C63
11	A	815	F39	C57-C59-C62-C64
11	A	815	F39	C57-C59-C62-C65

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Mol	Chain	Res	Type	Atoms
11	A	815	F39	C58-C61-C63-C64
11	A	815	F39	C59-C62-C64-C63
11	A	815	F39	C65-C62-C64-C63
11	a	815	F39	O2-C13-C14-C18
11	a	815	F39	C19-C20-C27-C32
11	a	815	F39	C22-C21-O6-C15
11	a	815	F39	O7-C21-O6-C15
11	a	815	F39	C37-C39-C40-C41
11	a	815	F39	C39-C40-C41-C42
11	a	815	F39	C40-C41-C42-C43
11	a	815	F39	C41-C42-C44-C51
11	a	815	F39	C43-C42-C44-C51
11	a	815	F39	C44-C51-C57-C59
11	a	815	F39	C53-C56-C58-C60
11	a	815	F39	C56-C58-C61-C63
11	a	815	F39	C60-C58-C61-C63
11	a	815	F39	C57-C59-C62-C64
11	a	815	F39	C57-C59-C62-C65
11	a	815	F39	C61-C63-C64-C62
11	C	301	F39	C19-C20-C27-C32
11	C	301	F39	C25-C20-C27-C32
11	C	301	F39	C22-C21-O6-C15
11	C	301	F39	C27-C32-C35-C37
11	C	301	F39	C32-C35-C37-C38
11	C	301	F39	C32-C35-C37-C39
11	C	301	F39	C37-C39-C40-C41
11	C	301	F39	C40-C41-C42-C43
11	C	301	F39	C43-C42-C44-C51
11	C	301	F39	C42-C44-C51-C57
11	C	301	F39	C44-C51-C57-C59
11	C	301	F39	C51-C57-C59-C62
11	C	301	F39	C56-C58-C61-C63
11	C	301	F39	C60-C58-C61-C63
11	C	301	F39	C59-C62-C64-C63
11	C	301	F39	C65-C62-C64-C63
12	A	816	F26	C17-C13-C18-C22
12	A	816	F26	C8-C13-C18-C22
12	A	816	F26	C9-C15-C19-C24
12	A	816	F26	C23-C19-C24-C27
12	A	816	F26	C15-C19-C24-C27
12	A	816	F26	C22-C25-C26-C29
12	A	816	F26	C22-C25-C26-C30

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Mol	Chain	Res	Type	Atoms
12	A	816	F26	C25-C26-C30-C32
12	A	816	F26	C29-C26-C30-C32
12	A	816	F26	C26-C30-C32-C35
12	A	816	F26	C35-C34-C37-C39
12	A	816	F26	C40-C34-C37-C39
12	a	816	F26	C17-C13-C18-C22
12	a	816	F26	C8-C13-C18-C22
12	a	816	F26	C9-C15-C19-C24
12	a	816	F26	C23-C19-C24-C27
12	a	816	F26	C15-C19-C24-C27
12	a	816	F26	C10-C14-C16-C21
12	a	816	F26	C10-C14-C16-C20
12	a	816	F26	C25-C26-C30-C32
12	a	816	F26	C29-C26-C30-C32
12	a	817	F26	C17-C13-C18-C22
12	a	817	F26	C8-C13-C18-C22
12	a	817	F26	C23-C19-C24-C27
12	a	817	F26	C15-C19-C24-C27
12	a	817	F26	C25-C26-C30-C32
12	a	817	F26	C29-C26-C30-C32
12	a	817	F26	C27-C28-C31-C33
12	a	817	F26	C27-C28-C31-C36
12	a	817	F26	C31-C33-C38-C39
13	A	817	LHG	C3-O3-P-O4
13	A	817	LHG	C3-O3-P-O5
13	A	817	LHG	C3-O3-P-O6
13	A	817	LHG	O9-C7-O7-C5
13	A	817	LHG	C8-C7-O7-C5
13	A	818	LHG	C3-O3-P-O5
13	A	818	LHG	C4-O6-P-O3
13	A	818	LHG	C4-O6-P-O4
13	A	818	LHG	C4-O6-P-O5
13	A	819	LHG	O1-C1-C2-C3
13	A	819	LHG	C4-O6-P-O3
13	A	819	LHG	C4-O6-P-O4
13	a	818	LHG	C1-C2-C3-O3
13	a	818	LHG	C3-O3-P-O5
13	a	818	LHG	C3-O3-P-O6
13	a	818	LHG	O9-C7-O7-C5
13	a	818	LHG	C8-C7-O7-C5
13	a	819	LHG	C4-O6-P-O3
13	a	819	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
13	a	820	LHG	O1-C1-C2-C3
13	a	820	LHG	C4-O6-P-O3
13	a	820	LHG	C4-O6-P-O5
13	a	821	LHG	O9-C7-O7-C5
13	a	821	LHG	C8-C7-O7-C5
13	a	821	LHG	O10-C23-O8-C6
13	E	101	LHG	O1-C1-C2-C3
13	E	101	LHG	C3-O3-P-O5
13	E	102	LHG	O1-C1-C2-O2
13	E	102	LHG	O1-C1-C2-C3
13	E	102	LHG	O9-C7-O7-C5
13	Z	401	LHG	O1-C1-C2-C3
13	Z	401	LHG	C3-O3-P-O4
13	Z	401	LHG	C3-O3-P-O5
13	Z	401	LHG	C3-O3-P-O6
13	Z	401	LHG	C8-C7-O7-C5
14	A	820	LMG	C2-C1-O1-C7
14	A	822	LMG	O9-C10-O7-C8
14	a	822	LMG	C2-C1-O1-C7
14	a	822	LMG	O6-C1-O1-C7
14	C	302	LMG	O9-C10-O7-C8
8	a	802	GS0	CBD-CGD-O2D-CED
8	A	801	GS0	O1A-CGA-O2A-C1
8	a	802	GS0	O1A-CGA-O2A-C1
9	A	826	CLA	O1A-CGA-O2A-C1
11	C	301	F39	O7-C21-O6-C15
9	A	802	CLA	O1D-CGD-O2D-CED
12	A	816	F26	C10-C14-C16-C21
12	a	817	F26	C10-C14-C16-C21
12	a	817	F26	C10-C14-C16-C20
9	A	826	CLA	CBA-CGA-O2A-C1
13	A	819	LHG	O10-C23-O8-C6
13	a	819	LHG	O10-C23-O8-C6
13	Z	401	LHG	O10-C23-O8-C6
14	C	302	LMG	O10-C28-O8-C9
9	A	802	CLA	C13-C15-C16-C17
9	A	827	CLA	O1D-CGD-O2D-CED
9	A	826	CLA	C8-C10-C11-C12
11	A	815	F39	O1-C12-C15-O6
11	a	815	F39	O1-C12-C15-O6
14	A	821	LMG	O10-C28-O8-C9
13	a	820	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
13	Z	401	LHG	O9-C7-O7-C5
14	A	821	LMG	O9-C10-O7-C8
9	A	802	CLA	C3-C5-C6-C7
9	A	827	CLA	C3-C5-C6-C7
8	a	802	GS0	CBA-CGA-O2A-C1
13	a	821	LHG	C24-C23-O8-C6
13	Z	401	LHG	C24-C23-O8-C6
14	C	302	LMG	C29-C28-O8-C9
9	A	827	CLA	CBD-CGD-O2D-CED
13	E	102	LHG	C8-C7-O7-C5
14	A	821	LMG	C11-C10-O7-C8
14	A	822	LMG	C11-C10-O7-C8
14	C	302	LMG	C11-C10-O7-C8
9	A	802	CLA	C2C-C3C-CAC-CBC
9	a	801	CLA	C2C-C3C-CAC-CBC
9	A	826	CLA	C4-C3-C5-C6
10	A	804	BCL	C4-C3-C5-C6
10	U	403	BCL	C4-C3-C5-C6
10	V	407	BCL	C4-C3-C5-C6
11	A	815	F39	C18-C19-C20-C25
9	A	802	CLA	C2-C3-C5-C6
10	U	402	BCL	C2-C3-C5-C6
10	V	407	BCL	C2-C3-C5-C6
10	W	403	BCL	C2-C3-C5-C6
10	Y	403	BCL	C2-C3-C5-C6
9	A	802	CLA	C2A-CAA-CBA-CGA
9	A	827	CLA	C2A-CAA-CBA-CGA
8	A	801	GS0	CBA-CGA-O2A-C1
13	A	818	LHG	C24-C23-O8-C6
13	A	819	LHG	C24-C23-O8-C6
13	a	819	LHG	C24-C23-O8-C6
13	E	102	LHG	C24-C23-O8-C6
14	A	820	LMG	C29-C28-O8-C9
14	A	821	LMG	C29-C28-O8-C9
11	A	815	F39	C10-C12-C15-O6
11	C	301	F39	C20-C27-C32-C35
12	a	817	F26	C34-C37-C39-C38
13	E	102	LHG	O10-C23-O8-C6
13	a	819	LHG	O9-C7-O7-C5
11	C	301	F39	C46-C53-C56-C58
9	A	826	CLA	C3-C5-C6-C7
9	a	801	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
13	A	819	LHG	O2-C2-C3-O3
13	a	819	LHG	O2-C2-C3-O3
13	a	820	LHG	C24-C23-O8-C6
9	a	801	CLA	O1A-CGA-O2A-C1
11	A	815	F39	O7-C21-O6-C15
9	A	827	CLA	C2C-C3C-CAC-CBC
10	W	406	BCL	C3-C5-C6-C7
11	A	815	F39	C22-C21-O6-C15
10	A	804	BCL	C2-C3-C5-C6
10	V	404	BCL	C2-C3-C5-C6
10	V	405	BCL	C2-C3-C5-C6
10	X	402	BCL	C2-C3-C5-C6
14	A	820	LMG	O6-C1-O1-C7
14	C	302	LMG	O6-C1-O1-C7
11	a	815	F39	C10-C12-C15-O6
13	E	101	LHG	O9-C7-O7-C5
13	A	819	LHG	C1-C2-C3-O3
9	a	801	CLA	CBA-CGA-O2A-C1
14	A	822	LMG	C29-C28-O8-C9
9	A	802	CLA	C4-C3-C5-C6
10	V	405	BCL	C4-C3-C5-C6
11	a	815	F39	C18-C19-C20-C25
9	A	826	CLA	C2-C3-C5-C6
10	Y	404	BCL	C2-C3-C5-C6
10	Z	403	BCL	C2-C3-C5-C6
9	A	802	CLA	C4C-C3C-CAC-CBC
9	a	801	CLA	C11-C10-C8-C9
9	a	801	CLA	C14-C13-C15-C16
10	A	803	BCL	C11-C12-C13-C14
10	A	804	BCL	C6-C7-C8-C9
10	A	805	BCL	C11-C10-C8-C9
10	A	811	BCL	C11-C12-C13-C14
10	a	809	BCL	C11-C10-C8-C9
10	a	812	BCL	C6-C7-C8-C9
10	a	814	BCL	C11-C10-C8-C9
14	C	302	LMG	C2-C1-O1-C7
13	A	818	LHG	C23-C24-C25-C26
13	a	818	LHG	O2-C2-C3-O3
14	A	823	LMG	O6-C5-C6-O5
11	A	815	F39	C40-C41-C42-C43
11	A	815	F39	C53-C56-C58-C60
11	a	815	F39	C65-C62-C64-C63

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Mol	Chain	Res	Type	Atoms
12	A	816	F26	C9-C15-C19-C23
12	a	816	F26	C22-C25-C26-C29
12	a	816	F26	C27-C28-C31-C36
12	a	817	F26	C9-C15-C19-C23
11	a	815	F39	C32-C35-C37-C39
11	a	815	F39	C40-C41-C42-C44
11	C	301	F39	C40-C41-C42-C44
11	C	301	F39	C53-C56-C58-C61
12	a	816	F26	C22-C25-C26-C30
12	a	817	F26	C9-C15-C19-C24
12	a	817	F26	C37-C34-C35-C32
14	C	302	LMG	C30-C31-C32-C33
14	A	822	LMG	C28-C29-C30-C31
13	A	818	LHG	O10-C23-O8-C6
14	A	820	LMG	O10-C28-O8-C9
10	a	813	BCL	C2-C1-O2A-CGA
10	U	403	BCL	C13-C15-C16-C17
10	X	405	BCL	C10-C11-C12-C13
12	A	816	F26	C10-C14-C16-C20
10	A	804	BCL	C11-C10-C8-C7
10	A	813	BCL	C6-C7-C8-C10
10	a	812	BCL	C11-C10-C8-C7
13	A	818	LHG	C25-C26-C27-C28
12	a	817	F26	C17-C13-C8-C10
12	a	817	F26	C19-C24-C27-C28
12	a	816	F26	C14-C10-C8-C13
10	X	402	BCL	O1D-CGD-O2D-CED
10	Y	401	BCL	C8-C10-C11-C12
13	A	817	LHG	C2-C3-O3-P
10	a	808	BCL	C2A-CAA-CBA-CGA
9	A	827	CLA	C4C-C3C-CAC-CBC
10	A	804	BCL	C5-C6-C7-C8
10	X	409	BCL	C5-C6-C7-C8
11	a	815	F39	C46-C53-C56-C58
14	a	822	LMG	C28-C29-C30-C31
10	A	813	BCL	C8-C10-C11-C12
10	a	806	BCL	C13-C15-C16-C17
10	a	814	BCL	C13-C15-C16-C17
13	A	818	LHG	O2-C2-C3-O3
13	a	820	LHG	O2-C2-C3-O3
13	a	820	LHG	O10-C23-O8-C6
13	a	820	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
14	A	820	LMG	C10-C11-C12-C13
9	A	827	CLA	C13-C15-C16-C17
13	a	818	LHG	C7-C8-C9-C10
10	a	803	BCL	O1D-CGD-O2D-CED
9	a	801	CLA	C5-C6-C7-C8
14	a	822	LMG	C29-C28-O8-C9
13	A	819	LHG	C8-C7-O7-C5
13	E	101	LHG	C8-C7-O7-C5
11	C	301	F39	C58-C61-C63-C64
12	A	816	F26	C19-C24-C27-C28
14	A	823	LMG	O9-C10-O7-C8
13	a	820	LHG	C1-C2-C3-O3
10	a	814	BCL	C2A-CAA-CBA-CGA
8	A	801	GS0	C13-C15-C16-C17
10	a	803	BCL	C13-C15-C16-C17
10	a	813	BCL	C15-C16-C17-C18
10	V	408	BCL	C13-C15-C16-C17
11	C	301	F39	O1-C12-C15-O6
10	A	810	BCL	C8-C10-C11-C12
10	V	403	BCL	C10-C11-C12-C13
14	A	823	LMG	C4-C5-C6-O5
10	A	812	BCL	C5-C6-C7-C8
10	Y	404	BCL	C4-C3-C5-C6
11	C	301	F39	C10-C12-C15-O6
10	A	812	BCL	C4B-C3B-CAB-CBB
10	A	814	BCL	C4B-C3B-CAB-CBB
10	a	804	BCL	C4B-C3B-CAB-OB
10	a	813	BCL	C4B-C3B-CAB-CBB
10	a	814	BCL	C4B-C3B-CAB-OB
10	U	405	BCL	C4B-C3B-CAB-OB
10	U	405	BCL	C4B-C3B-CAB-CBB
10	V	401	BCL	C4B-C3B-CAB-OB
10	V	409[B]	BCL	C4B-C3B-CAB-OB
10	X	402	BCL	C4B-C3B-CAB-OB
10	X	407[B]	BCL	C4B-C3B-CAB-OB
10	X	409	BCL	C14-C13-C15-C16
10	a	805	BCL	O1D-CGD-O2D-CED
13	a	819	LHG	C23-C24-C25-C26
14	A	820	LMG	C4-C5-C6-O5
11	a	815	F39	C38-C37-C39-C40
12	A	816	F26	C36-C31-C33-C38
12	a	816	F26	C36-C31-C33-C38

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Mol	Chain	Res	Type	Atoms
12	a	816	F26	C40-C34-C37-C39
12	a	817	F26	C40-C34-C37-C39
11	C	301	F39	C53-C56-C58-C60
12	a	817	F26	C40-C34-C35-C32
14	A	820	LMG	O6-C5-C6-O5
11	A	815	F39	C53-C56-C58-C61
11	a	815	F39	C53-C56-C58-C61
12	a	816	F26	C27-C28-C31-C33
10	A	803	BCL	C2A-CAA-CBA-CGA
10	A	814	BCL	C2A-CAA-CBA-CGA
13	A	817	LHG	O1-C1-C2-C3
13	a	818	LHG	O1-C1-C2-C3
13	a	819	LHG	O1-C1-C2-C3
10	A	806	BCL	O2A-C1-C2-C3
10	a	806	BCL	O2A-C1-C2-C3
10	B	301	BCL	O2A-C1-C2-C3
10	V	401	BCL	C2B-C3B-CAB-OB
10	X	402	BCL	C2B-C3B-CAB-OB
10	X	402	BCL	C2B-C3B-CAB-CB
13	a	819	LHG	C6-C5-O7-C7
10	Y	403	BCL	C16-C17-C18-C19
10	A	814	BCL	O1D-CGD-O2D-CED
10	Y	403	BCL	C10-C11-C12-C13
11	A	815	F39	C35-C37-C39-C40
11	C	301	F39	C35-C37-C39-C40
12	A	816	F26	C28-C31-C33-C38
12	a	816	F26	C28-C31-C33-C38
12	a	816	F26	C35-C34-C37-C39
12	a	817	F26	C35-C34-C37-C39
13	A	818	LHG	O9-C7-O7-C5
10	A	808	BCL	O1D-CGD-O2D-CED
10	V	404	BCL	O1D-CGD-O2D-CED
14	A	822	LMG	O6-C5-C6-O5
10	A	813	BCL	O1D-CGD-O2D-CED
9	A	802	CLA	C5-C6-C7-C8
13	a	821	LHG	C23-C24-C25-C26
10	A	813	BCL	C16-C17-C18-C20
10	Y	403	BCL	C16-C17-C18-C20
13	E	101	LHG	C14-C15-C16-C17
13	Z	401	LHG	C15-C16-C17-C18
14	a	822	LMG	C32-C33-C34-C35
13	a	818	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
11	a	815	F39	C24-C26-C28-C29
14	A	821	LMG	C13-C14-C15-C16
13	A	819	LHG	O1-C1-C2-O2
13	a	820	LHG	O1-C1-C2-O2
13	E	101	LHG	O1-C1-C2-O2
13	A	818	LHG	C10-C11-C12-C13
13	a	820	LHG	C13-C14-C15-C16
10	Y	404	BCL	O1D-CGD-O2D-CED
13	E	102	LHG	C7-C8-C9-C10
14	A	820	LMG	C28-C29-C30-C31
8	a	802	GS0	O1D-CGD-O2D-CED
14	C	302	LMG	C31-C32-C33-C34
14	A	821	LMG	C12-C13-C14-C15
10	A	811	BCL	C6-C7-C8-C10
10	a	811	BCL	C11-C10-C8-C7
13	Z	401	LHG	O2-C2-C3-O3
13	A	819	LHG	C7-C8-C9-C10
13	A	818	LHG	C17-C18-C19-C20
13	a	818	LHG	C25-C26-C27-C28
14	A	822	LMG	C13-C14-C15-C16
10	A	813	BCL	C3A-C2A-CAA-CBA
10	a	807	BCL	C3A-C2A-CAA-CBA
10	B	301	BCL	C3A-C2A-CAA-CBA
14	A	820	LMG	C30-C31-C32-C33
11	C	301	F39	C28-C29-C30-C31
13	A	817	LHG	C24-C25-C26-C27
9	A	802	CLA	C8-C10-C11-C12
14	A	822	LMG	C8-C9-O8-C28
10	W	404	BCL	O1D-CGD-O2D-CED
13	E	102	LHG	C31-C32-C33-C34
14	A	820	LMG	C32-C33-C34-C35
11	a	815	F39	C42-C44-C51-C57
10	A	813	BCL	C16-C17-C18-C19
10	W	401	BCL	C16-C17-C18-C19
13	a	821	LHG	C18-C19-C20-C21
13	A	818	LHG	C1-C2-C3-O3
13	A	818	LHG	C24-C25-C26-C27
13	a	820	LHG	C10-C11-C12-C13
11	a	815	F39	C21-C22-C23-C24
10	A	809	BCL	C5-C6-C7-C8
10	A	814	BCL	C15-C16-C17-C18
13	A	817	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
14	C	302	LMG	C34-C35-C36-C37
10	U	403	BCL	O1D-CGD-O2D-CED
10	Z	408[B]	BCL	O1D-CGD-O2D-CED
11	A	815	F39	C26-C28-C29-C30
13	A	818	LHG	C8-C7-O7-C5
13	a	820	LHG	C8-C7-O7-C5
10	A	812	BCL	C3-C5-C6-C7
8	A	801	GS0	C2A-CAA-CBA-CGA
13	A	817	LHG	C25-C26-C27-C28
14	A	821	LMG	C32-C33-C34-C35
14	a	822	LMG	C31-C32-C33-C34
13	E	102	LHG	C30-C31-C32-C33
10	U	403	BCL	C2-C3-C5-C6
12	a	817	F26	C18-C13-C8-C10
13	a	821	LHG	C17-C18-C19-C20
13	Z	401	LHG	C25-C26-C27-C28
14	C	302	LMG	C11-C12-C13-C14
13	Z	401	LHG	C18-C19-C20-C21
14	A	821	LMG	C11-C12-C13-C14
13	E	102	LHG	C24-C25-C26-C27
13	a	819	LHG	C11-C12-C13-C14
14	C	302	LMG	C13-C14-C15-C16
10	V	401	BCL	C16-C17-C18-C19
13	a	818	LHG	C23-C24-C25-C26
13	E	102	LHG	C15-C16-C17-C18
11	a	815	F39	C59-C62-C64-C63
10	A	804	BCL	C16-C17-C18-C20
10	W	405	BCL	C16-C17-C18-C20
10	U	404	BCL	C4-C3-C5-C6
10	Z	403	BCL	C4-C3-C5-C6
13	Z	401	LHG	C26-C27-C28-C29
13	A	818	LHG	C18-C19-C20-C21
14	A	822	LMG	O10-C28-O8-C9
10	W	404	BCL	C8-C10-C11-C12
13	E	102	LHG	C27-C28-C29-C30
10	a	808	BCL	O1D-CGD-O2D-CED
13	a	818	LHG	C11-C10-C9-C8
10	A	804	BCL	C16-C17-C18-C19
10	V	401	BCL	C16-C17-C18-C20
10	W	405	BCL	C16-C17-C18-C19
14	A	820	LMG	C17-C18-C19-C20
10	A	812	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	A	819	LHG	C25-C26-C27-C28
13	a	818	LHG	C14-C15-C16-C17
13	a	821	LHG	C7-C8-C9-C10
14	A	821	LMG	C28-C29-C30-C31
14	A	822	LMG	C33-C34-C35-C36
10	Z	403	BCL	O1D-CGD-O2D-CED
10	A	805	BCL	O1D-CGD-O2D-CED
13	a	820	LHG	C16-C17-C18-C19
13	E	102	LHG	C10-C11-C12-C13
14	a	822	LMG	C16-C17-C18-C19
14	a	822	LMG	O6-C5-C6-O5
10	A	812	BCL	O1D-CGD-O2D-CED
10	X	409	BCL	O1D-CGD-O2D-CED
10	W	401	BCL	C16-C17-C18-C20
14	A	821	LMG	C35-C36-C37-C38
13	A	819	LHG	O9-C7-O7-C5
14	C	302	LMG	C36-C37-C38-C39
10	A	809	BCL	O1D-CGD-O2D-CED
10	V	403	BCL	C15-C16-C17-C18
13	A	817	LHG	O1-C1-C2-O2
13	a	819	LHG	O1-C1-C2-O2
13	Z	401	LHG	O1-C1-C2-O2
8	A	801	GS0	C1A-C2A-CAA-CBA
8	a	802	GS0	C1A-C2A-CAA-CBA
9	A	802	CLA	C1A-C2A-CAA-CBA
9	A	826	CLA	C1A-C2A-CAA-CBA
9	a	801	CLA	C1A-C2A-CAA-CBA
10	A	809	BCL	C1A-C2A-CAA-CBA
10	a	807	BCL	C1A-C2A-CAA-CBA
10	a	810	BCL	C1A-C2A-CAA-CBA
10	a	806	BCL	O1A-CGA-O2A-C1
13	E	101	LHG	C25-C26-C27-C28
14	A	822	LMG	C36-C37-C38-C39
13	A	817	LHG	O6-C4-C5-C6
13	a	821	LHG	O6-C4-C5-C6
8	A	801	GS0	C11-C10-C8-C7
8	a	802	GS0	C11-C12-C13-C15
9	a	801	CLA	C11-C10-C8-C7
9	a	801	CLA	C11-C12-C13-C15
10	A	805	BCL	C11-C10-C8-C7
10	A	806	BCL	C12-C13-C15-C16
10	a	806	BCL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
10	a	813	BCL	C11-C12-C13-C15
10	Y	406	BCL	C11-C10-C8-C7
10	A	803	BCL	C16-C17-C18-C20
10	V	403	BCL	C5-C6-C7-C8
10	A	813	BCL	C2C-C3C-CAC-CBC
10	B	301	BCL	C2C-C3C-CAC-CBC
10	U	402	BCL	C2C-C3C-CAC-CBC
10	X	402	BCL	C2C-C3C-CAC-CBC
10	Y	404	BCL	C2C-C3C-CAC-CBC
10	Z	403	BCL	C2C-C3C-CAC-CBC
10	Z	404	BCL	C2C-C3C-CAC-CBC
13	Z	401	LHG	C12-C13-C14-C15
10	a	809	BCL	C4-C3-C5-C6
10	a	812	BCL	C2-C3-C5-C6
10	U	401	BCL	C2-C3-C5-C6
11	A	815	F39	C46-C53-C56-C58
10	A	806	BCL	C4B-C3B-CAB-OBB
10	A	806	BCL	C4B-C3B-CAB-CBB
10	A	810	BCL	C4B-C3B-CAB-OBB
10	A	812	BCL	C4B-C3B-CAB-OBB
10	a	814	BCL	C4B-C3B-CAB-CBB
10	U	407[B]	BCL	C4B-C3B-CAB-OBB
10	V	401	BCL	C4B-C3B-CAB-CBB
10	V	409[B]	BCL	C4B-C3B-CAB-CBB
10	W	408[B]	BCL	C4B-C3B-CAB-OBB
10	X	407[B]	BCL	C4B-C3B-CAB-CBB
10	Z	406	BCL	C4B-C3B-CAB-CBB
10	Z	408[B]	BCL	C4B-C3B-CAB-OBB
14	A	823	LMG	C11-C10-O7-C8
9	a	801	CLA	C2A-CAA-CBA-CGA
10	A	804	BCL	C11-C10-C8-C9
10	A	806	BCL	C14-C13-C15-C16
10	a	809	BCL	C6-C7-C8-C9
10	U	403	BCL	C14-C13-C15-C16
10	U	405	BCL	C11-C10-C8-C9
10	X	402	BCL	C11-C10-C8-C9
10	Y	401	BCL	C11-C10-C8-C9
10	Y	406	BCL	C11-C10-C8-C9
13	E	101	LHG	C24-C25-C26-C27
13	Z	401	LHG	C11-C12-C13-C14
14	a	822	LMG	C18-C19-C20-C21
10	W	402	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	C	302	LMG	O6-C5-C6-O5
14	A	821	LMG	C7-C8-C9-O8
14	a	822	LMG	C7-C8-C9-O8
10	A	806	BCL	C13-C15-C16-C17
13	Z	401	LHG	C7-C8-C9-C10
13	a	821	LHG	C15-C16-C17-C18
10	A	805	BCL	O1A-CGA-O2A-C1
10	W	401	BCL	O1A-CGA-O2A-C1
10	A	807	BCL	C2-C3-C5-C6
10	Y	401	BCL	C2-C3-C5-C6
10	V	405	BCL	C10-C11-C12-C13
10	V	407	BCL	C15-C16-C17-C18
11	a	815	F39	C32-C35-C37-C38
14	a	822	LMG	C33-C34-C35-C36
11	A	815	F39	C32-C35-C37-C39
13	E	101	LHG	O10-C23-O8-C6
9	a	801	CLA	C13-C15-C16-C17
10	a	809	BCL	C13-C15-C16-C17
10	a	811	BCL	C2A-CAA-CBA-CGA
11	C	301	F39	C30-C31-C33-C34
10	B	301	BCL	C15-C16-C17-C18
14	C	302	LMG	C32-C33-C34-C35
10	B	301	BCL	O1D-CGD-O2D-CED
10	X	405	BCL	O1D-CGD-O2D-CED
10	A	808	BCL	O2A-C1-C2-C3
13	E	101	LHG	C6-C5-O7-C7
13	a	820	LHG	C9-C10-C11-C12
10	A	803	BCL	C16-C17-C18-C19
10	V	408	BCL	O1D-CGD-O2D-CED
13	E	101	LHG	O6-C4-C5-O7
10	a	806	BCL	C10-C11-C12-C13
14	a	822	LMG	C14-C15-C16-C17
13	Z	401	LHG	C17-C18-C19-C20
10	A	806	BCL	C4-C3-C5-C6
13	a	821	LHG	C19-C20-C21-C22
13	a	820	LHG	C12-C13-C14-C15
13	a	820	LHG	O7-C5-C6-O8
10	V	403	BCL	O1D-CGD-O2D-CED
14	a	822	LMG	C36-C37-C38-C39
13	Z	401	LHG	C19-C20-C21-C22
10	Y	406	BCL	O1D-CGD-O2D-CED
10	a	813	BCL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
13	E	101	LHG	C16-C17-C18-C19
14	a	822	LMG	C30-C31-C32-C33
10	W	403	BCL	O1D-CGD-O2D-CED
14	C	302	LMG	C37-C38-C39-C40
10	a	804	BCL	C15-C16-C17-C18
10	a	806	BCL	O1D-CGD-O2D-CED
10	a	810	BCL	C4-C3-C5-C6
10	a	812	BCL	C4-C3-C5-C6
10	a	813	BCL	C4-C3-C5-C6
10	W	407	BCL	C4-C3-C5-C6
13	A	817	LHG	C24-C23-O8-C6
13	a	818	LHG	C30-C31-C32-C33
8	A	801	GS0	C11-C10-C8-C9
10	A	806	BCL	C6-C7-C8-C9
10	a	806	BCL	C11-C12-C13-C14
10	B	301	BCL	C14-C13-C15-C16
10	V	406	BCL	C11-C10-C8-C9
10	W	405	BCL	C11-C12-C13-C14
10	a	809	BCL	O1D-CGD-O2D-CED
10	A	803	BCL	O1A-CGA-O2A-C1
10	A	810	BCL	O1D-CGD-O2D-CED
14	A	822	LMG	C15-C16-C17-C18
10	A	804	BCL	C10-C11-C12-C13
13	a	818	LHG	C13-C14-C15-C16
10	A	806	BCL	O1A-CGA-O2A-C1
10	Z	407	BCL	C2A-CAA-CBA-CGA
13	A	817	LHG	C9-C10-C11-C12
10	A	804	BCL	C15-C16-C17-C18
13	A	818	LHG	O6-C4-C5-C6
11	A	815	F39	C16-C13-C14-C18
11	a	815	F39	C17-C13-C14-C18
14	a	822	LMG	C12-C13-C14-C15
9	A	826	CLA	C11-C10-C8-C7
9	a	801	CLA	C12-C13-C15-C16
10	A	806	BCL	C6-C7-C8-C10
10	A	813	BCL	C12-C13-C15-C16
10	U	403	BCL	C12-C13-C15-C16
10	U	405	BCL	C11-C10-C8-C7
10	V	406	BCL	C11-C10-C8-C7
10	X	402	BCL	C11-C10-C8-C7
10	U	403	BCL	C5-C6-C7-C8
14	A	822	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
13	a	820	LHG	C25-C26-C27-C28
13	A	818	LHG	C9-C10-C11-C12
10	a	807	BCL	O1A-CGA-O2A-C1
10	a	807	BCL	C4-C3-C5-C6
10	U	406	BCL	C4-C3-C5-C6
10	a	807	BCL	O1D-CGD-O2D-CED
10	U	402	BCL	O1D-CGD-O2D-CED
10	a	813	BCL	C2-C3-C5-C6
10	X	401	BCL	C2-C3-C5-C6
14	a	822	LMG	O10-C28-O8-C9
10	A	814	BCL	O1A-CGA-O2A-C1
10	V	406	BCL	O1A-CGA-O2A-C1
8	A	801	GS0	C8-C10-C11-C12
14	C	302	LMG	C16-C17-C18-C19
10	X	408[B]	BCL	O1D-CGD-O2D-CED
10	Y	403	BCL	C8-C10-C11-C12
13	E	102	LHG	C4-C5-C6-O8
14	C	302	LMG	C7-C8-C9-O8
14	A	821	LMG	C37-C38-C39-C40
10	a	812	BCL	C10-C11-C12-C13
14	A	820	LMG	C15-C16-C17-C18
9	A	802	CLA	C1-C2-C3-C4
9	A	826	CLA	C1-C2-C3-C4
10	A	803	BCL	C1-C2-C3-C4
10	A	806	BCL	C1-C2-C3-C4
10	A	808	BCL	C1-C2-C3-C4
10	A	809	BCL	C1-C2-C3-C4
10	A	810	BCL	C1-C2-C3-C4
10	A	811	BCL	C1-C2-C3-C4
10	A	813	BCL	C1-C2-C3-C4
10	a	805	BCL	C1-C2-C3-C4
10	a	806	BCL	C1-C2-C3-C4
10	a	810	BCL	C1-C2-C3-C4
10	a	814	BCL	C1-C2-C3-C4
10	B	301	BCL	C1-C2-C3-C4
10	U	401	BCL	C1-C2-C3-C4
10	U	406	BCL	C1-C2-C3-C4
10	V	403	BCL	C1-C2-C3-C4
10	V	408	BCL	C1-C2-C3-C4
10	W	402	BCL	C1-C2-C3-C4
10	W	407	BCL	C1-C2-C3-C4
10	X	403	BCL	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
10	X	406	BCL	C1-C2-C3-C4
10	Y	401	BCL	C1-C2-C3-C4
10	Y	403	BCL	C1-C2-C3-C4
10	Y	408	BCL	C1-C2-C3-C4
10	Z	404	BCL	C1-C2-C3-C4
10	Z	407	BCL	C1-C2-C3-C4
10	A	809	BCL	C4-C3-C5-C6
10	a	804	BCL	C4-C3-C5-C6
10	V	402	BCL	C4-C3-C5-C6
10	Y	402	BCL	C4-C3-C5-C6
10	Z	402	BCL	C4-C3-C5-C6
10	a	804	BCL	C2-C3-C5-C6
10	W	402	BCL	C2-C3-C5-C6
10	A	813	BCL	O1A-CGA-O2A-C1
10	U	407[B]	BCL	O1D-CGD-O2D-CED
10	Y	408	BCL	O1D-CGD-O2D-CED
13	Z	401	LHG	C2-C3-O3-P
9	A	826	CLA	C13-C15-C16-C17
10	Z	407	BCL	O1D-CGD-O2D-CED
10	A	808	BCL	C2A-CAA-CBA-CGA
13	a	819	LHG	O7-C5-C6-O8
13	E	102	LHG	O7-C5-C6-O8
14	a	822	LMG	O7-C8-C9-O8
14	C	302	LMG	O7-C8-C9-O8
13	E	102	LHG	C14-C15-C16-C17
10	Y	402	BCL	C2-C3-C5-C6
14	A	820	LMG	C31-C32-C33-C34
9	A	802	CLA	C1-C2-C3-C5
10	A	812	BCL	C1-C2-C3-C5
13	A	818	LHG	C11-C10-C9-C8
13	A	818	LHG	C11-C12-C13-C14
10	A	803	BCL	C4B-C3B-CAB-CBB
10	A	807	BCL	C4B-C3B-CAB-OB
10	A	807	BCL	C4B-C3B-CAB-CBB
10	A	813	BCL	C4B-C3B-CAB-OB
10	A	813	BCL	C4B-C3B-CAB-CBB
10	X	408[B]	BCL	C4B-C3B-CAB-OB
10	Z	408[B]	BCL	C4B-C3B-CAB-CBB
9	A	802	CLA	C6-C7-C8-C9
10	A	813	BCL	C14-C13-C15-C16
10	a	812	BCL	C11-C10-C8-C9
10	a	813	BCL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
10	W	403	BCL	C11-C10-C8-C9
10	Z	405	BCL	C11-C10-C8-C9
10	V	401	BCL	O1D-CGD-O2D-CED
14	A	821	LMG	C38-C39-C40-C41
10	A	805	BCL	C5-C6-C7-C8
13	a	819	LHG	C13-C14-C15-C16
13	E	101	LHG	C10-C11-C12-C13
10	A	804	BCL	O1D-CGD-O2D-CED
10	Y	402	BCL	O1D-CGD-O2D-CED
10	A	809	BCL	C4C-C3C-CAC-CBC
10	A	810	BCL	C4C-C3C-CAC-CBC
10	U	407[B]	BCL	C4C-C3C-CAC-CBC
10	W	405	BCL	C4C-C3C-CAC-CBC
10	W	406	BCL	C4C-C3C-CAC-CBC
11	A	815	F39	O2-C13-C14-C18
10	A	807	BCL	C4-C3-C5-C6
13	a	819	LHG	C14-C15-C16-C17
13	a	819	LHG	C1-C2-C3-O3
10	a	807	BCL	C5-C6-C7-C8
13	A	819	LHG	O6-C4-C5-C6
13	a	820	LHG	O6-C4-C5-C6
13	E	101	LHG	O6-C4-C5-C6
10	W	408[B]	BCL	O1D-CGD-O2D-CED
10	Y	406	BCL	O1A-CGA-O2A-C1
14	A	822	LMG	C35-C36-C37-C38
8	A	801	GS0	C11-C12-C13-C15
9	A	802	CLA	C12-C13-C15-C16
9	A	826	CLA	C6-C7-C8-C10
10	a	810	BCL	C12-C13-C15-C16
10	W	403	BCL	C11-C10-C8-C7
10	X	404	BCL	C11-C10-C8-C7
10	Y	407	BCL	C11-C10-C8-C7
10	Z	403	BCL	C11-C10-C8-C7
10	Z	405	BCL	C11-C10-C8-C7
11	C	301	F39	C26-C28-C29-C30
14	A	822	LMG	C14-C15-C16-C17
10	a	805	BCL	O1A-CGA-O2A-C1
10	a	814	BCL	C5-C6-C7-C8
10	V	406	BCL	C16-C17-C18-C19
10	a	809	BCL	O1A-CGA-O2A-C1
10	V	407	BCL	O1A-CGA-O2A-C1
10	V	408	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
10	A	803	BCL	C2B-C3B-CAB-OBB
10	A	803	BCL	C2B-C3B-CAB-CBB
10	A	807	BCL	C2B-C3B-CAB-OBB
10	A	807	BCL	C2B-C3B-CAB-CBB
10	A	813	BCL	C2B-C3B-CAB-OBB
10	A	813	BCL	C2B-C3B-CAB-CBB
13	Z	401	LHG	C6-C5-O7-C7
14	A	821	LMG	C9-C8-O7-C10
10	Z	406	BCL	O1A-CGA-O2A-C1
13	A	817	LHG	O6-C4-C5-O7
13	A	818	LHG	O6-C4-C5-O7
13	a	821	LHG	O6-C4-C5-O7
13	a	819	LHG	C4-C5-C6-O8
14	A	820	LMG	O1-C7-C8-C9
10	V	406	BCL	C16-C17-C18-C20
14	A	820	LMG	C33-C34-C35-C36
10	U	401	BCL	C15-C16-C17-C18
10	A	809	BCL	C2-C3-C5-C6
13	a	821	LHG	C11-C10-C9-C8
13	E	102	LHG	C11-C12-C13-C14
14	A	820	LMG	O1-C7-C8-O7
14	A	822	LMG	O1-C7-C8-O7
9	A	826	CLA	C11-C10-C8-C9
10	A	813	BCL	C6-C7-C8-C9
10	A	814	BCL	C6-C7-C8-C9
10	X	404	BCL	C11-C10-C8-C9
10	Y	401	BCL	C6-C7-C8-C9
14	A	821	LMG	C34-C35-C36-C37
13	E	101	LHG	C27-C28-C29-C30
11	C	301	F39	C13-C14-C18-C19
10	W	406	BCL	C10-C11-C12-C13
14	a	822	LMG	C13-C14-C15-C16
14	A	821	LMG	C33-C34-C35-C36
13	A	819	LHG	C13-C14-C15-C16
10	A	813	BCL	C4-C3-C5-C6
10	W	407	BCL	C10-C11-C12-C13
10	Y	403	BCL	O1A-CGA-O2A-C1
10	Z	405	BCL	O1A-CGA-O2A-C1
10	V	409[B]	BCL	O1D-CGD-O2D-CED
12	A	816	F26	C19-C15-C9-C2
9	A	826	CLA	C4B-C3B-CAB-CBB
10	X	406	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	A	820	LMG	C19-C20-C21-C22
10	U	404	BCL	O1A-CGA-O2A-C1
10	A	804	BCL	C11-C12-C13-C15
10	a	810	BCL	C6-C7-C8-C10
10	a	812	BCL	C6-C7-C8-C10
10	U	401	BCL	C12-C13-C15-C16
10	U	402	BCL	C11-C10-C8-C7
10	V	402	BCL	C12-C13-C15-C16
10	V	404	BCL	C11-C10-C8-C7
10	Y	401	BCL	C12-C13-C15-C16
10	Y	404	BCL	C11-C10-C8-C7
10	Z	402	BCL	C12-C13-C15-C16
10	Z	404	BCL	C11-C12-C13-C15
10	W	407	BCL	C16-C17-C18-C19
10	A	807	BCL	C2C-C3C-CAC-CBC
10	W	403	BCL	C2C-C3C-CAC-CBC
10	W	408[B]	BCL	C2C-C3C-CAC-CBC
10	A	806	BCL	O1D-CGD-O2D-CED
10	B	301	BCL	C13-C15-C16-C17
13	E	101	LHG	C2-C3-O3-P
11	A	815	F39	C22-C23-C24-C26
11	C	301	F39	C14-C13-O2-C11
13	A	819	LHG	O6-C4-C5-O7
13	a	820	LHG	O6-C4-C5-O7
13	A	818	LHG	C26-C27-C28-C29
8	A	801	GS0	C4B-C3B-CAB-OBB
10	A	803	BCL	C4B-C3B-CAB-OBB
10	A	810	BCL	C4B-C3B-CAB-CBB
10	U	407[B]	BCL	C4B-C3B-CAB-CBB
10	W	408[B]	BCL	C4B-C3B-CAB-CBB
8	a	802	GS0	C2A-CAA-CBA-CGA
10	Y	401	BCL	C14-C13-C15-C16
10	Z	403	BCL	C11-C10-C8-C9
11	a	815	F39	C58-C61-C63-C64
10	A	812	BCL	C13-C15-C16-C17
14	A	822	LMG	C11-C12-C13-C14
13	a	819	LHG	C25-C26-C27-C28
10	Y	401	BCL	O1A-CGA-O2A-C1
14	A	821	LMG	O7-C8-C9-O8
9	A	827	CLA	C5-C6-C7-C8
9	a	801	CLA	C10-C11-C12-C13
10	X	406	BCL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
14	A	822	LMG	O1-C7-C8-C9
11	C	301	F39	C29-C30-C31-C33
10	B	301	BCL	C5-C6-C7-C8
10	A	803	BCL	CAD-CBD-CGD-O2D
10	A	813	BCL	CAD-CBD-CGD-O2D
10	V	406	BCL	CAD-CBD-CGD-O2D
10	V	409[B]	BCL	CAD-CBD-CGD-O2D
10	W	405	BCL	CAD-CBD-CGD-O2D
10	W	408[B]	BCL	CAD-CBD-CGD-O2D
10	X	404	BCL	CAD-CBD-CGD-O2D
10	X	407[B]	BCL	CAD-CBD-CGD-O2D
10	Y	406	BCL	CAD-CBD-CGD-O2D
10	Z	405	BCL	CAD-CBD-CGD-O2D
14	C	302	LMG	C14-C15-C16-C17
9	A	826	CLA	C2A-CAA-CBA-CGA
10	X	408[B]	BCL	C2A-CAA-CBA-CGA
10	W	406	BCL	C8-C10-C11-C12
10	X	405	BCL	O1A-CGA-O2A-C1
8	A	801	GS0	CAD-CBD-CGD-O1D
8	a	802	GS0	CAD-CBD-CGD-O1D
10	A	807	BCL	CAD-CBD-CGD-O1D
10	A	808	BCL	CHA-CBD-CGD-O2D
10	a	809	BCL	CAD-CBD-CGD-O1D
10	a	812	BCL	CAD-CBD-CGD-O1D
10	a	813	BCL	CAD-CBD-CGD-O1D
10	U	403	BCL	CAD-CBD-CGD-O1D
10	W	404	BCL	CHA-CBD-CGD-O1D
10	X	404	BCL	CAD-CBD-CGD-O1D
10	X	408[B]	BCL	CAD-CBD-CGD-O1D
11	a	815	F39	C20-C27-C32-C35
13	a	818	LHG	C3-O3-P-O4
13	a	819	LHG	C4-O6-P-O5
13	a	821	LHG	C4-O6-P-O5
13	E	101	LHG	C3-O3-P-O6
13	E	102	LHG	C3-O3-P-O6
9	A	826	CLA	C2B-C3B-CAB-CBB
13	A	819	LHG	C2-C3-O3-P
10	Z	405	BCL	C13-C15-C16-C17
13	a	818	LHG	C11-C12-C13-C14
10	a	811	BCL	O1D-CGD-O2D-CED
10	U	406	BCL	O1A-CGA-O2A-C1
10	a	809	BCL	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
10	a	813	BCL	C2B-C3B-CAB-CBB
13	a	820	LHG	C6-C5-O7-C7
8	A	801	GS0	C4-C3-C5-C6
14	A	820	LMG	C14-C15-C16-C17
10	X	409	BCL	C10-C11-C12-C13
10	Y	407	BCL	C15-C16-C17-C18
10	W	405	BCL	C2-C3-C5-C6
9	A	802	CLA	C14-C13-C15-C16
10	A	804	BCL	C11-C12-C13-C14
10	a	803	BCL	C11-C12-C13-C14
10	a	804	BCL	C14-C13-C15-C16
10	a	810	BCL	C14-C13-C15-C16
10	V	408	BCL	C14-C13-C15-C16
14	a	822	LMG	C11-C12-C13-C14
10	X	403	BCL	O1D-CGD-O2D-CED
10	B	301	BCL	O1A-CGA-O2A-C1
10	X	404	BCL	O1A-CGA-O2A-C1
10	W	401	BCL	C5-C6-C7-C8
10	X	407[B]	BCL	O1D-CGD-O2D-CED
13	E	101	LHG	C24-C23-O8-C6
10	A	811	BCL	C2A-CAA-CBA-CGA
10	Z	407	BCL	O1A-CGA-O2A-C1
10	A	814	BCL	C4-C3-C5-C6
10	Y	408	BCL	C4-C3-C5-C6
13	a	820	LHG	C4-C5-C6-O8
14	A	822	LMG	C4-C5-C6-O5
10	A	813	BCL	C3-C5-C6-C7
10	A	814	BCL	C3-C5-C6-C7
10	a	811	BCL	CAA-CBA-CGA-O2A
10	U	404	BCL	CAA-CBA-CGA-O2A
14	A	821	LMG	C8-C7-O1-C1
11	a	815	F39	C51-C57-C59-C62
13	E	102	LHG	C12-C13-C14-C15
10	a	810	BCL	C2-C3-C5-C6
8	a	802	GS0	C4B-C3B-CAB-OBB
10	a	803	BCL	C4B-C3B-CAB-OBB
10	a	809	BCL	C4B-C3B-CAB-OBB
10	a	810	BCL	C4B-C3B-CAB-OBB
10	X	408[B]	BCL	C4B-C3B-CAB-CBB
13	a	821	LHG	O1-C1-C2-O2
8	A	801	GS0	C16-C17-C18-C19
10	U	406	BCL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
10	V	404	BCL	C11-C10-C8-C9
10	W	402	BCL	C11-C12-C13-C14
10	Y	404	BCL	C11-C10-C8-C9
10	Z	404	BCL	C11-C12-C13-C14
10	Y	408	BCL	C16-C17-C18-C19
10	U	403	BCL	C8-C10-C11-C12
10	a	813	BCL	C2A-CAA-CBA-CGA
13	Z	401	LHG	C14-C15-C16-C17
10	a	806	BCL	C16-C17-C18-C19
10	Z	405	BCL	C16-C17-C18-C19
10	Z	404	BCL	O1D-CGD-O2D-CED
13	A	819	LHG	C24-C25-C26-C27
10	A	803	BCL	C11-C12-C13-C15
10	a	811	BCL	C11-C12-C13-C15
10	X	403	BCL	O1A-CGA-O2A-C1
11	a	815	F39	C30-C31-C33-C34
10	a	808	BCL	CAA-CBA-CGA-O2A
10	X	403	BCL	C10-C11-C12-C13
13	Z	401	LHG	C24-C25-C26-C27
10	V	409[B]	BCL	C3A-C2A-CAA-CBA
13	A	819	LHG	C9-C10-C11-C12
10	U	404	BCL	C2-C3-C5-C6
13	a	821	LHG	C14-C15-C16-C17
10	W	401	BCL	C8-C10-C11-C12
10	W	406	BCL	C5-C6-C7-C8
13	a	818	LHG	C24-C25-C26-C27
13	A	817	LHG	C1-C2-C3-O3
10	W	408[B]	BCL	CAA-CBA-CGA-O1A
10	a	806	BCL	C6-C7-C8-C9
10	Y	403	BCL	C6-C7-C8-C9
13	E	101	LHG	C13-C14-C15-C16
10	U	407[B]	BCL	CAA-CBA-CGA-O1A
10	A	809	BCL	C2B-C3B-CAB-OB
10	A	809	BCL	C2B-C3B-CAB-CB
10	a	803	BCL	C2B-C3B-CAB-OB
10	a	803	BCL	C2B-C3B-CAB-CB
10	a	809	BCL	C2B-C3B-CAB-OB
10	V	409[B]	BCL	C2B-C3B-CAB-CB
10	X	407[B]	BCL	C2B-C3B-CAB-CB
10	Z	408[B]	BCL	C2B-C3B-CAB-OB
13	a	821	LHG	C4-C5-O7-C7
14	A	822	LMG	C9-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
10	A	805	BCL	C1-C2-C3-C4
10	A	807	BCL	C1-C2-C3-C4
10	a	809	BCL	C1-C2-C3-C4
10	U	402	BCL	C1-C2-C3-C4
10	U	404	BCL	C1-C2-C3-C4
10	V	401	BCL	C1-C2-C3-C4
10	V	402	BCL	C1-C2-C3-C4
10	V	404	BCL	C1-C2-C3-C4
10	W	401	BCL	C1-C2-C3-C4
10	W	403	BCL	C1-C2-C3-C4
10	W	404	BCL	C1-C2-C3-C4
10	W	405	BCL	C1-C2-C3-C4
10	X	401	BCL	C1-C2-C3-C4
10	X	404	BCL	C1-C2-C3-C4
10	X	409	BCL	C1-C2-C3-C4
10	Y	402	BCL	C1-C2-C3-C4
10	Y	405	BCL	C1-C2-C3-C4
10	Y	406	BCL	C1-C2-C3-C4
10	Y	407	BCL	C1-C2-C3-C4
10	Z	402	BCL	C1-C2-C3-C4
10	Z	405	BCL	C1-C2-C3-C4
10	Z	406	BCL	C1-C2-C3-C4
12	a	816	F26	C31-C33-C38-C39
14	A	821	LMG	C10-C11-C12-C13
10	Y	406	BCL	CAA-CBA-CGA-O2A
10	A	805	BCL	C2-C3-C5-C6
10	V	408	BCL	C2-C3-C5-C6
13	a	820	LHG	C18-C19-C20-C21
10	a	804	BCL	CAA-CBA-CGA-O2A
11	a	815	F39	C23-C24-C26-C28
10	V	403	BCL	O1A-CGA-O2A-C1
13	A	819	LHG	C5-C4-O6-P
13	a	818	LHG	C32-C33-C34-C35
13	a	821	LHG	C12-C13-C14-C15
10	U	404	BCL	O1D-CGD-O2D-CED
10	Z	408[B]	BCL	CAA-CBA-CGA-O1A
10	W	402	BCL	C4-C3-C5-C6
10	A	812	BCL	C2-C3-C5-C6
10	A	803	BCL	C12-C13-C15-C16
10	a	804	BCL	C12-C13-C15-C16
10	V	405	BCL	C11-C12-C13-C15
10	V	408	BCL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
10	W	402	BCL	C11-C12-C13-C15
10	Y	405	BCL	C11-C12-C13-C15
10	Z	405	BCL	CAA-CBA-CGA-O1A
10	V	401	BCL	C15-C16-C17-C18
10	X	407[B]	BCL	CAA-CBA-CGA-O1A
13	a	820	LHG	C11-C12-C13-C14
10	a	811	BCL	C16-C17-C18-C20
10	B	301	BCL	C4-C3-C5-C6
10	Z	407	BCL	C4-C3-C5-C6
10	A	808	BCL	C2-C3-C5-C6
10	A	811	BCL	C2-C3-C5-C6
13	a	821	LHG	C13-C14-C15-C16
10	A	813	BCL	C13-C15-C16-C17
10	A	809	BCL	C4B-C3B-CAB-OBB
10	a	803	BCL	C4B-C3B-CAB-CBB
10	a	809	BCL	C4B-C3B-CAB-CBB
10	A	809	BCL	C14-C13-C15-C16
10	W	405	BCL	C6-C7-C8-C9
10	Y	406	BCL	C5-C6-C7-C8
10	a	803	BCL	C4-C3-C5-C6
10	Z	402	BCL	C15-C16-C17-C18
10	W	405	BCL	O1D-CGD-O2D-CED
13	a	818	LHG	C33-C34-C35-C36
10	A	803	BCL	C4C-C3C-CAC-CBC
10	V	409[B]	BCL	C4C-C3C-CAC-CBC
10	V	401	BCL	C13-C15-C16-C17
13	a	818	LHG	O1-C1-C2-O2
13	a	818	LHG	O6-C4-C5-O7
10	V	403	BCL	C4-C3-C5-C6
8	A	801	GS0	C16-C17-C18-C20
10	a	812	BCL	C8-C10-C11-C12
10	W	403	BCL	C10-C11-C12-C13
10	X	407[B]	BCL	CAA-CBA-CGA-O2A
10	Y	404	BCL	C16-C17-C18-C19
10	a	812	BCL	O1D-CGD-O2D-CED
12	a	817	F26	C36-C31-C33-C38
10	A	806	BCL	CAA-CBA-CGA-O2A
9	A	826	CLA	C12-C13-C15-C16
10	X	403	BCL	C11-C12-C13-C15
10	V	407	BCL	O1D-CGD-O2D-CED
10	a	806	BCL	CAA-CBA-CGA-O2A
11	a	815	F39	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
10	A	813	BCL	C11-C12-C13-C14
10	U	401	BCL	C14-C13-C15-C16
10	Z	405	BCL	C14-C13-C15-C16
14	A	821	LMG	C14-C15-C16-C17
10	V	402	BCL	C15-C16-C17-C18
10	B	301	BCL	C2-C1-O2A-CGA
10	Z	407	BCL	C16-C17-C18-C19
13	E	102	LHG	C11-C10-C9-C8
10	W	408[B]	BCL	CAA-CBA-CGA-O2A
10	V	406	BCL	CAA-CBA-CGA-O2A
10	W	405	BCL	O1A-CGA-O2A-C1
10	U	404	BCL	C13-C15-C16-C17
10	A	812	BCL	O2A-C1-C2-C3
10	U	407[B]	BCL	C2B-C3B-CAB-OBB
10	V	401	BCL	C2B-C3B-CAB-CBB
10	W	408[B]	BCL	C2B-C3B-CAB-OBB
14	A	822	LMG	C7-C8-O7-C10
11	A	815	F39	C27-C32-C35-C37
11	a	815	F39	C27-C32-C35-C37
11	A	815	F39	C24-C26-C28-C29
10	W	407	BCL	C16-C17-C18-C20
13	E	101	LHG	O2-C2-C3-O3
11	a	815	F39	C22-C23-C24-C26
10	Z	405	BCL	C16-C17-C18-C20
10	U	407[B]	BCL	CAA-CBA-CGA-O2A
13	a	819	LHG	C11-C10-C9-C8
10	a	808	BCL	CAA-CBA-CGA-O1A
10	U	404	BCL	C16-C17-C18-C20
10	a	812	BCL	C13-C15-C16-C17
10	Z	408[B]	BCL	CAA-CBA-CGA-O2A
10	U	401	BCL	CAA-CBA-CGA-O2A
10	U	403	BCL	CAA-CBA-CGA-O2A
10	A	809	BCL	C4B-C3B-CAB-CBB
10	A	812	BCL	C6-C7-C8-C9
10	a	810	BCL	C6-C7-C8-C9
10	U	402	BCL	C11-C10-C8-C9
10	V	407	BCL	C14-C13-C15-C16
10	X	403	BCL	C11-C12-C13-C14
10	Y	402	BCL	C14-C13-C15-C16
10	Y	405	BCL	C11-C12-C13-C14
10	Z	402	BCL	C14-C13-C15-C16
10	a	806	BCL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
10	U	406	BCL	CAA-CBA-CGA-O2A
10	A	804	BCL	C6-C7-C8-C10
10	A	809	BCL	C12-C13-C15-C16
10	A	813	BCL	C11-C12-C13-C15
10	a	807	BCL	C11-C12-C13-C15
10	a	807	BCL	C12-C13-C15-C16
10	W	405	BCL	C6-C7-C8-C10
9	A	802	CLA	C2B-C3B-CAB-CBB
13	A	817	LHG	C31-C32-C33-C34
13	Z	401	LHG	O8-C23-C24-C25
10	a	806	BCL	C2-C1-O2A-CGA
10	V	408	BCL	C2-C1-O2A-CGA
10	Z	404	BCL	C2-C1-O2A-CGA
10	A	806	BCL	CAA-CBA-CGA-O1A
10	Y	407	BCL	CAA-CBA-CGA-O2A
14	A	821	LMG	C29-C30-C31-C32
10	V	402	BCL	CAA-CBA-CGA-O2A
10	X	401	BCL	CAA-CBA-CGA-O2A
10	Y	402	BCL	CAA-CBA-CGA-O2A
10	A	813	BCL	C2A-CAA-CBA-CGA
10	Y	402	BCL	C8-C10-C11-C12
10	Z	406	BCL	C10-C11-C12-C13
10	Z	406	BCL	CAA-CBA-CGA-O2A
14	A	822	LMG	C31-C32-C33-C34
10	V	409[B]	BCL	CAA-CBA-CGA-O1A
10	V	401	BCL	O1A-CGA-O2A-C1
9	A	827	CLA	CAA-CBA-CGA-O2A
10	A	814	BCL	CAA-CBA-CGA-O2A
10	V	408	BCL	CAA-CBA-CGA-O2A
10	Y	408	BCL	CAA-CBA-CGA-O2A
10	Z	402	BCL	CAA-CBA-CGA-O2A
14	a	822	LMG	C35-C36-C37-C38
10	X	401	BCL	C4-C3-C5-C6
10	V	405	BCL	CAA-CBA-CGA-O2A
10	X	406	BCL	CAA-CBA-CGA-O2A
10	Z	404	BCL	CAA-CBA-CGA-O2A
14	A	821	LMG	O8-C28-C29-C30
13	Z	401	LHG	C29-C30-C31-C32
10	a	806	BCL	C2-C3-C5-C6
9	a	801	CLA	C11-C12-C13-C14
10	V	405	BCL	C11-C12-C13-C14
10	B	301	BCL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
10	Y	405	BCL	CAA-CBA-CGA-O2A
10	X	406	BCL	O1A-CGA-O2A-C1
10	X	402	BCL	C16-C17-C18-C19
10	U	402	BCL	CAA-CBA-CGA-O2A
10	W	405	BCL	CAA-CBA-CGA-O2A
13	a	820	LHG	C11-C10-C9-C8
10	V	409[B]	BCL	CAA-CBA-CGA-O2A
10	X	403	BCL	CAA-CBA-CGA-O2A
10	Z	407	BCL	CAA-CBA-CGA-O2A
10	W	407	BCL	CAA-CBA-CGA-O2A
10	Z	403	BCL	CAA-CBA-CGA-O2A
10	a	804	BCL	CAA-CBA-CGA-O1A
10	A	805	BCL	C2-C1-O2A-CGA
10	A	812	BCL	C2-C1-O2A-CGA
10	Y	407	BCL	C2-C1-O2A-CGA
10	A	807	BCL	CAA-CBA-CGA-O2A
13	E	102	LHG	O8-C23-C24-C25
10	A	811	BCL	C11-C12-C13-C15
10	a	809	BCL	C11-C10-C8-C7
10	a	814	BCL	C11-C10-C8-C7
10	V	407	BCL	C11-C10-C8-C7
10	Z	405	BCL	C12-C13-C15-C16
10	U	402	BCL	C16-C17-C18-C19
8	A	801	GS0	C2B-C3B-CAB-OB
10	A	807	BCL	O2A-C1-C2-C3
10	A	810	BCL	C2B-C3B-CAB-OB
10	W	408[B]	BCL	C2B-C3B-CAB-CB
10	X	408[B]	BCL	C2B-C3B-CAB-OB
10	Z	408[B]	BCL	C2B-C3B-CAB-CB
10	a	805	BCL	C8-C10-C11-C12
10	a	811	BCL	C10-C11-C12-C13
10	a	804	BCL	C8-C10-C11-C12
10	V	402	BCL	C5-C6-C7-C8
14	A	822	LMG	C32-C33-C34-C35
10	a	813	BCL	C5-C6-C7-C8
10	Z	405	BCL	CAA-CBA-CGA-O2A
8	a	802	GS0	C10-C11-C12-C13
10	Y	401	BCL	C5-C6-C7-C8
10	X	408[B]	BCL	CAA-CBA-CGA-O2A
10	A	814	BCL	C3A-C2A-CAA-CBA
10	A	813	BCL	C10-C11-C12-C13
10	Y	403	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
10	W	407	BCL	O1D-CGD-O2D-CED
10	W	403	BCL	CAA-CBA-CGA-O1A
10	Y	405	BCL	CAA-CBA-CGA-O1A
13	E	102	LHG	O10-C23-C24-C25
14	A	822	LMG	C12-C13-C14-C15
14	A	822	LMG	O6-C1-O1-C7
10	X	402	BCL	CAA-CBA-CGA-O1A
10	Y	401	BCL	CAA-CBA-CGA-O1A
10	a	810	BCL	C4B-C3B-CAB-CBB
10	a	807	BCL	C10-C11-C12-C13
10	a	809	BCL	C2A-CAA-CBA-CGA
10	W	408[B]	BCL	C2A-CAA-CBA-CGA
10	V	402	BCL	C14-C13-C15-C16
10	Y	407	BCL	C11-C10-C8-C9
10	V	404	BCL	CAA-CBA-CGA-O1A
10	W	405	BCL	CAA-CBA-CGA-O1A
10	Y	407	BCL	O1A-CGA-O2A-C1
10	Y	404	BCL	CAA-CBA-CGA-O1A
10	Z	403	BCL	CAA-CBA-CGA-O1A
10	V	402	BCL	CAA-CBA-CGA-O1A
10	a	807	BCL	C13-C15-C16-C17
10	W	405	BCL	C5-C6-C7-C8
13	E	102	LHG	O7-C7-C8-C9
10	U	404	BCL	C8-C10-C11-C12
10	a	806	BCL	CAA-CBA-CGA-O1A
10	U	402	BCL	CAA-CBA-CGA-O1A
10	X	401	BCL	CAA-CBA-CGA-O1A
14	A	822	LMG	C8-C7-O1-C1
10	U	401	BCL	O1A-CGA-O2A-C1
8	a	802	GS0	CAA-CBA-CGA-O1A
10	Y	404	BCL	CAA-CBA-CGA-O2A
10	W	402	BCL	C2A-CAA-CBA-CGA
8	A	801	GS0	CAA-CBA-CGA-O1A
14	A	820	LMG	O10-C28-C29-C30
14	A	821	LMG	O10-C28-C29-C30
11	C	301	F39	C21-C22-C23-C24
10	A	804	BCL	CAA-CBA-CGA-O2A
13	a	818	LHG	C17-C18-C19-C20
10	a	803	BCL	CAD-CBD-CGD-O2D
10	a	808	BCL	CAD-CBD-CGD-O2D
10	V	405	BCL	O1D-CGD-O2D-CED
10	a	812	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
10	a	807	BCL	C2-C1-O2A-CGA
10	Y	405	BCL	C2-C1-O2A-CGA
10	Z	406	BCL	C2-C1-O2A-CGA
10	Y	403	BCL	CAA-CBA-CGA-O1A
10	W	403	BCL	CAA-CBA-CGA-O2A
10	X	404	BCL	CAA-CBA-CGA-O2A
9	A	827	CLA	C1-C2-C3-C4
10	A	814	BCL	C1-C2-C3-C4
10	a	812	BCL	C1-C2-C3-C4
13	a	821	LHG	C9-C10-C11-C12
10	A	807	BCL	CAA-CBA-CGA-O1A
10	A	814	BCL	C10-C11-C12-C13
9	A	827	CLA	C4-C3-C5-C6
10	a	809	BCL	CAA-CBA-CGA-O2A
10	a	810	BCL	CAA-CBA-CGA-O2A
8	a	802	GS0	C15-C16-C17-C18
10	V	401	BCL	CAA-CBA-CGA-O1A
13	Z	401	LHG	O10-C23-C24-C25
13	E	102	LHG	C16-C17-C18-C19

There are no ring outliers.

73 monomers are involved in 264 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	a	805	BCL	3	0
10	W	401	BCL	3	0
10	U	403	BCL	4	0
10	U	404	BCL	2	0
13	E	102	LHG	3	0
10	Z	407	BCL	2	0
10	a	810	BCL	3	0
9	A	827	CLA	35	0
13	a	819	LHG	2	0
9	A	802	CLA	34	0
10	a	813	BCL	3	0
10	a	804	BCL	2	0
10	A	808	BCL	3	0
10	A	812	BCL	3	0
10	Y	402	BCL	1	0
10	a	814	BCL	3	0
10	A	814	BCL	2	0
14	A	821	LMG	2	0

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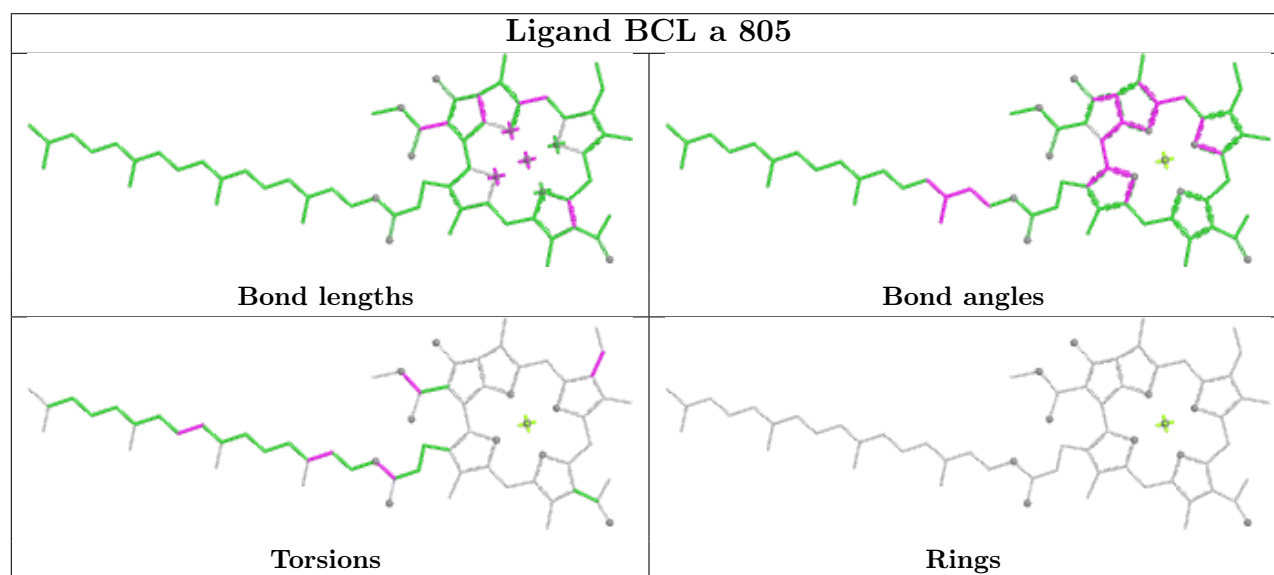
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	811	BCL	4	0
9	A	826	CLA	32	0
9	a	801	CLA	29	0
10	Z	404	BCL	2	0
14	A	820	LMG	2	0
10	A	813	BCL	2	0
10	X	401	BCL	1	0
10	W	403	BCL	2	0
10	a	807	BCL	1	0
10	a	803	BCL	1	0
10	B	301	BCL	3	0
10	A	806	BCL	1	0
14	A	823	LMG	4	0
10	X	402	BCL	3	0
10	A	803	BCL	5	0
10	A	807	BCL	1	0
10	V	405	BCL	1	0
10	W	405	BCL	1	0
10	Z	403	BCL	5	0
10	a	808	BCL	1	0
13	Z	401	LHG	7	0
10	V	402	BCL	1	0
10	Z	406	BCL	2	0
10	Y	404	BCL	2	0
8	A	801	GS0	3	0
10	W	406	BCL	4	0
10	X	409	BCL	2	0
10	A	804	BCL	2	0
10	X	408[B]	BCL	1	0
10	A	809	BCL	4	0
10	A	810	BCL	2	0
10	V	409[B]	BCL	1	0
10	W	402	BCL	2	0
13	E	101	LHG	3	0
10	X	403	BCL	2	0
10	X	405	BCL	1	0
13	A	819	LHG	3	0
13	A	817	LHG	1	0
10	a	809	BCL	5	0
10	Y	408	BCL	1	0
13	a	821	LHG	1	0
13	a	820	LHG	3	0

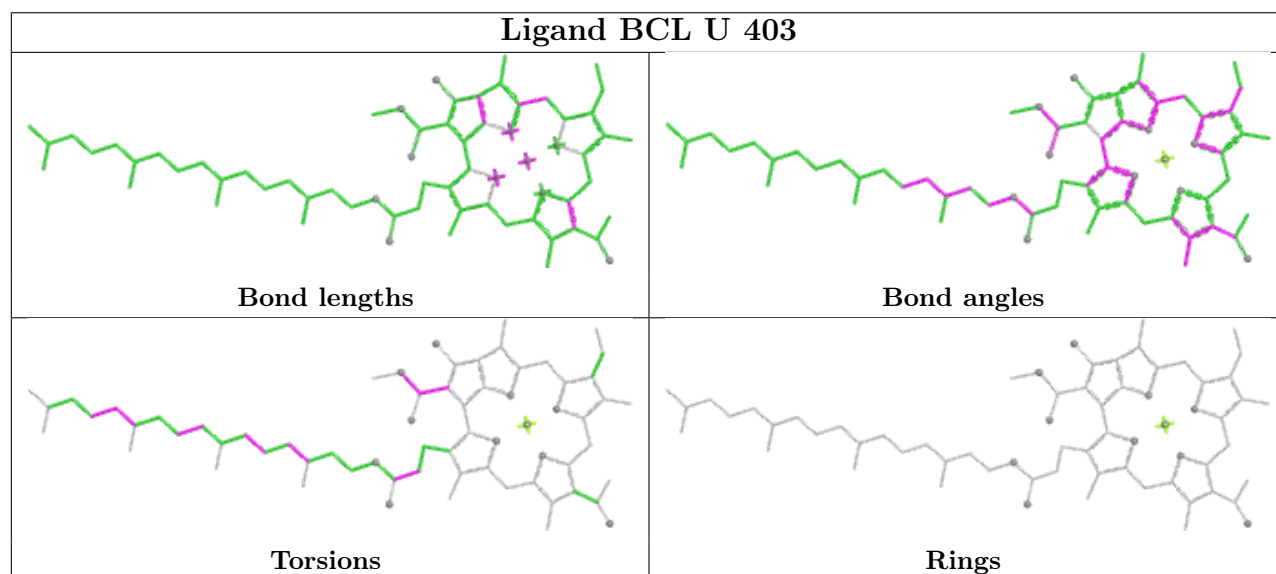
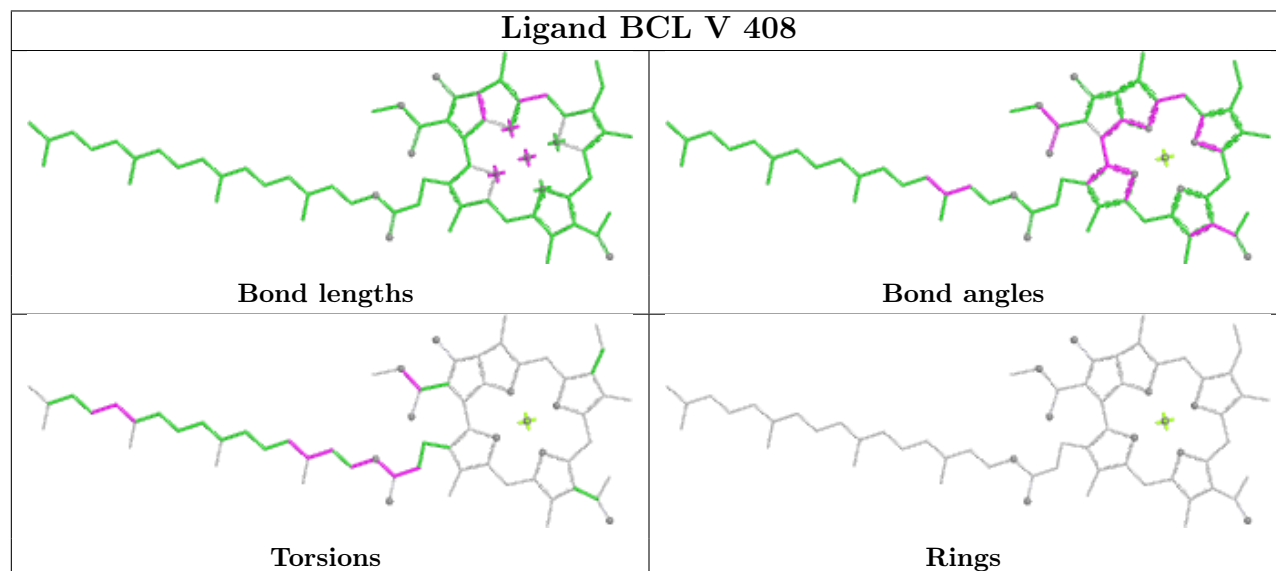
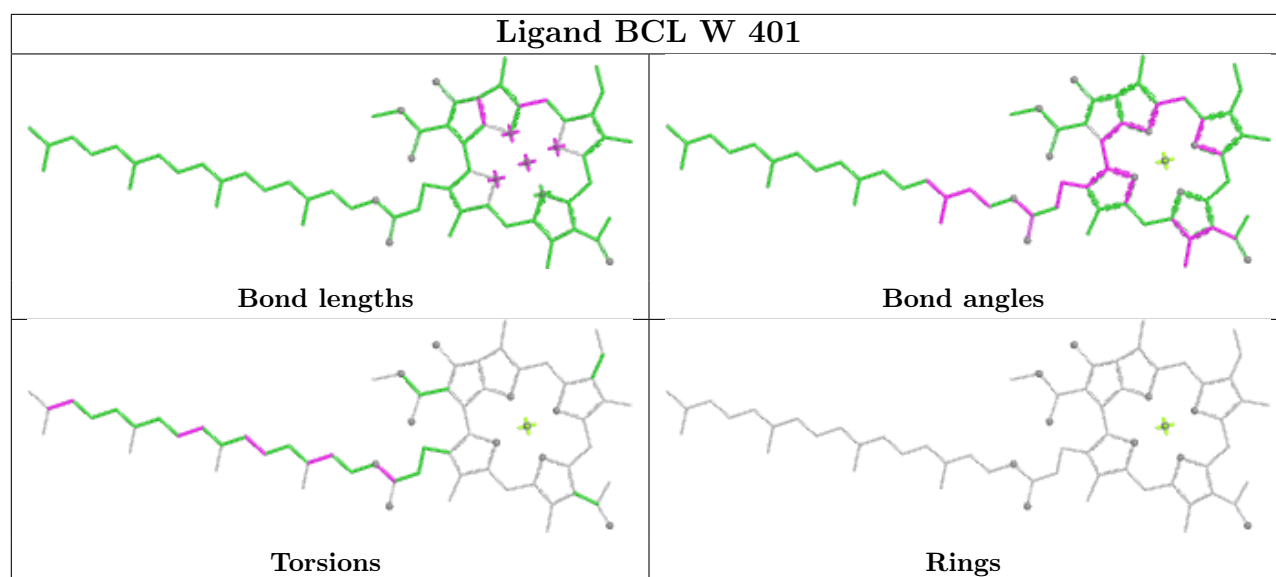
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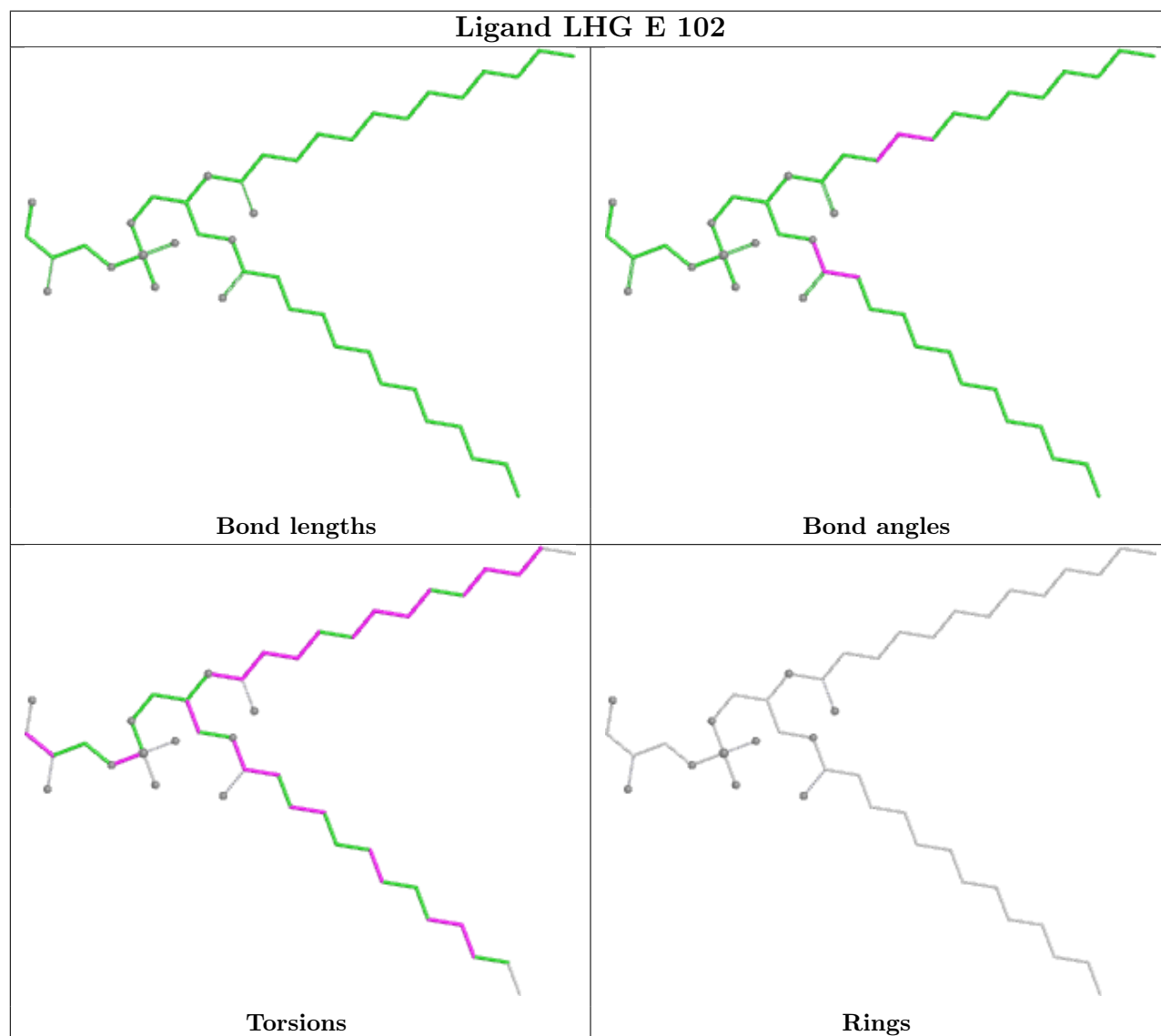
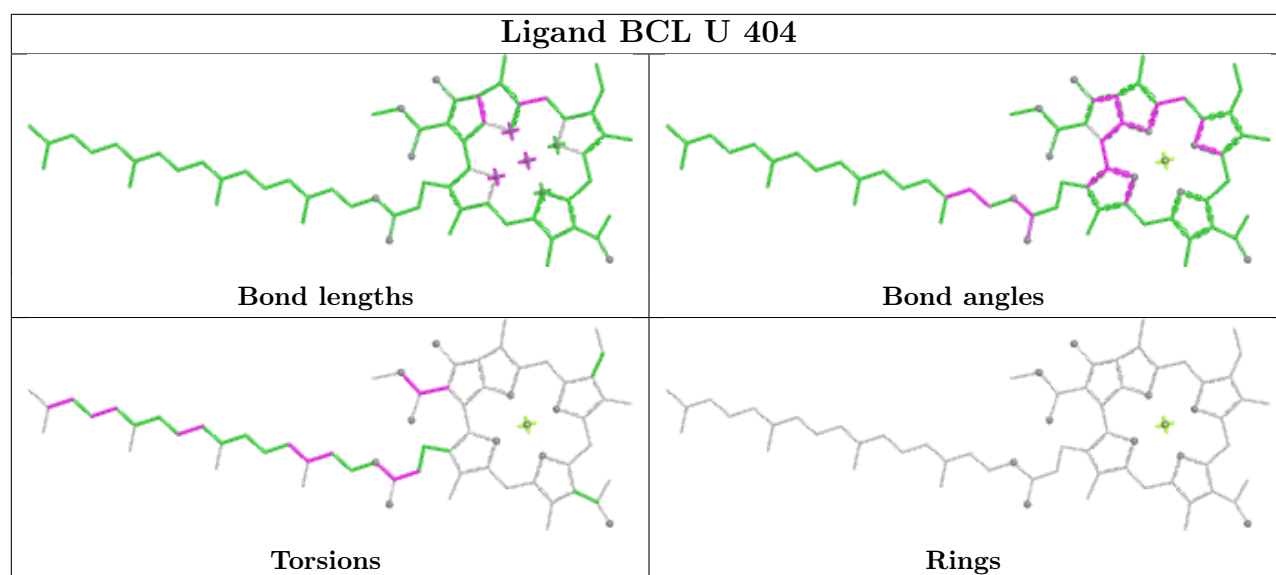
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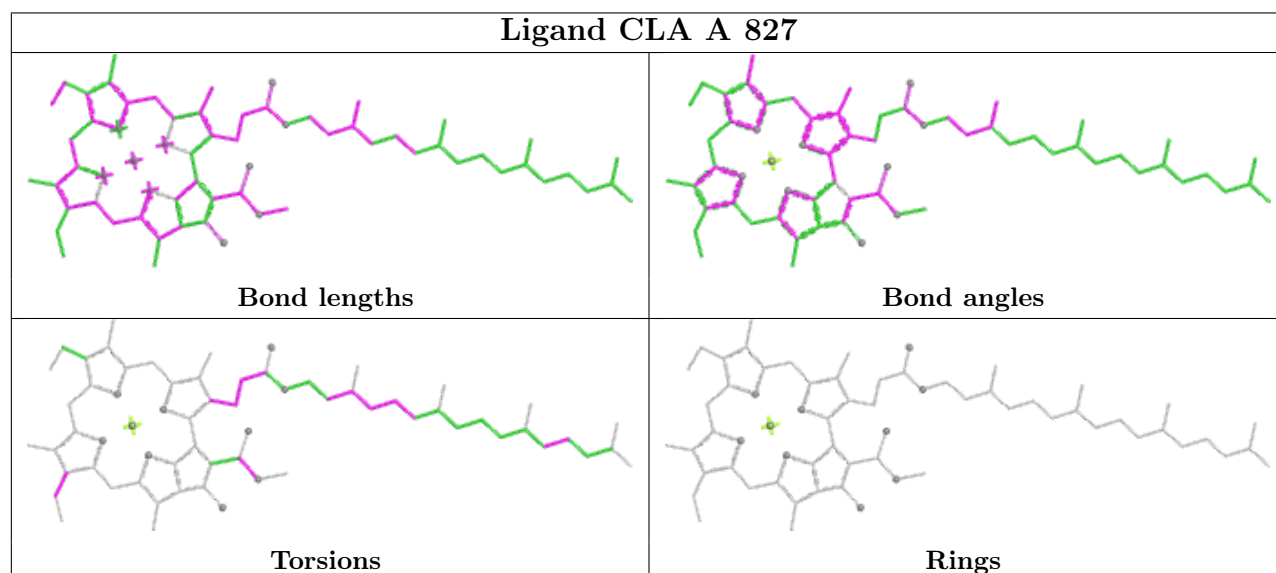
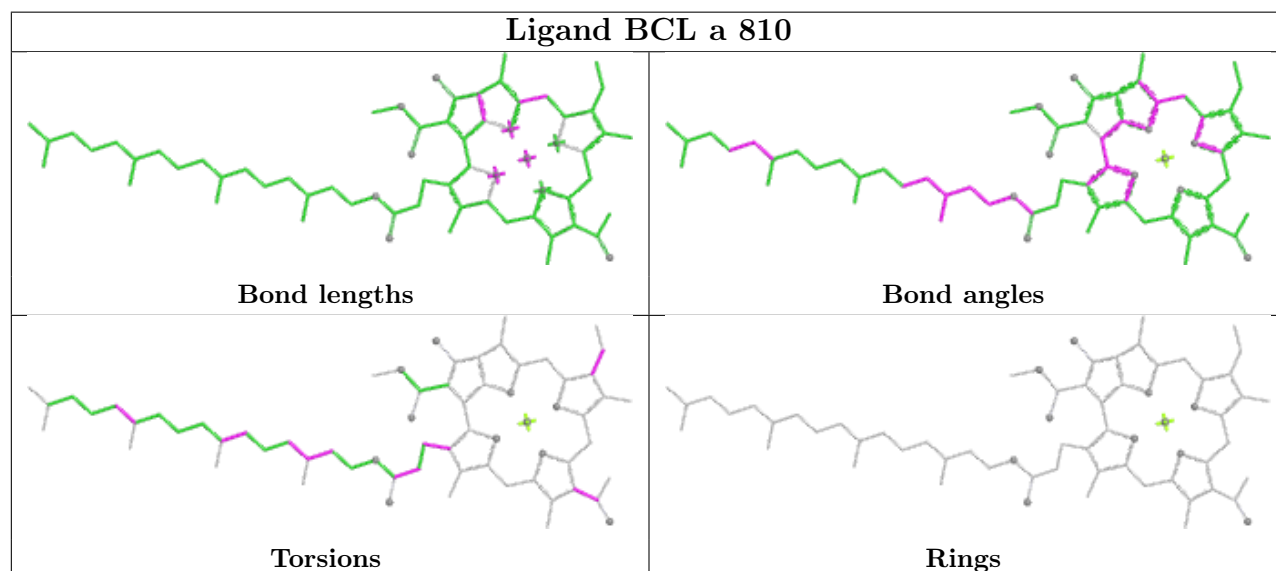
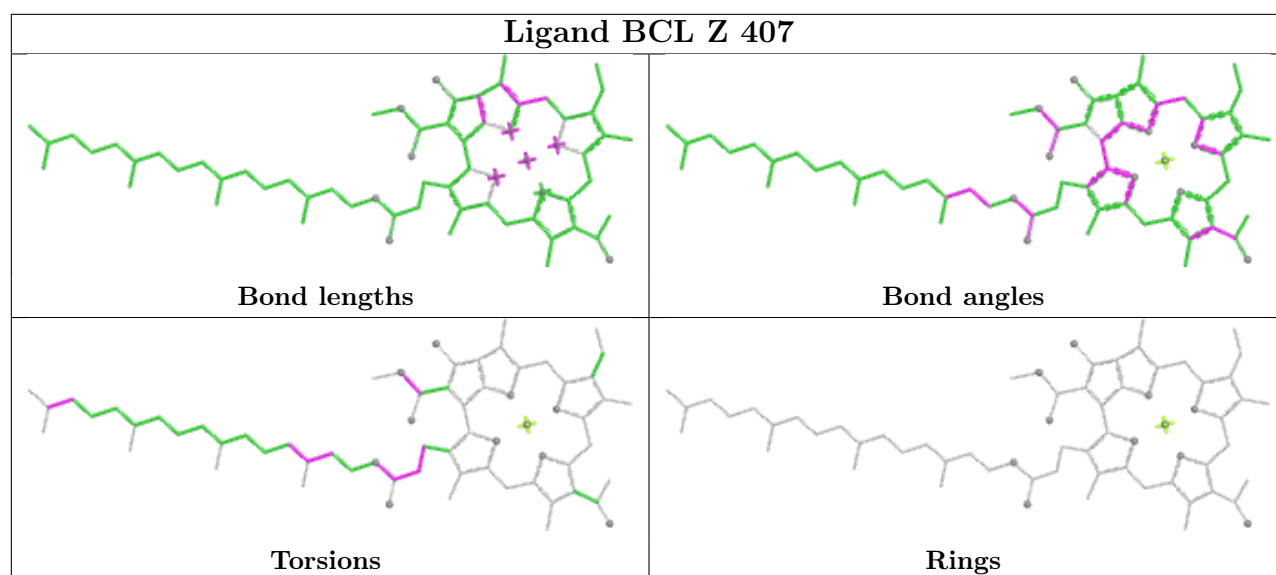
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	C	302	LMG	4	0
10	X	406	BCL	1	0
10	Z	405	BCL	1	0
10	a	806	BCL	5	0
10	Y	406	BCL	1	0
10	W	404	BCL	3	0
10	U	402	BCL	1	0
10	V	407	BCL	1	0
10	Z	402	BCL	1	0
14	a	822	LMG	3	0
10	U	401	BCL	1	0
13	A	818	LHG	5	0
10	A	805	BCL	6	0

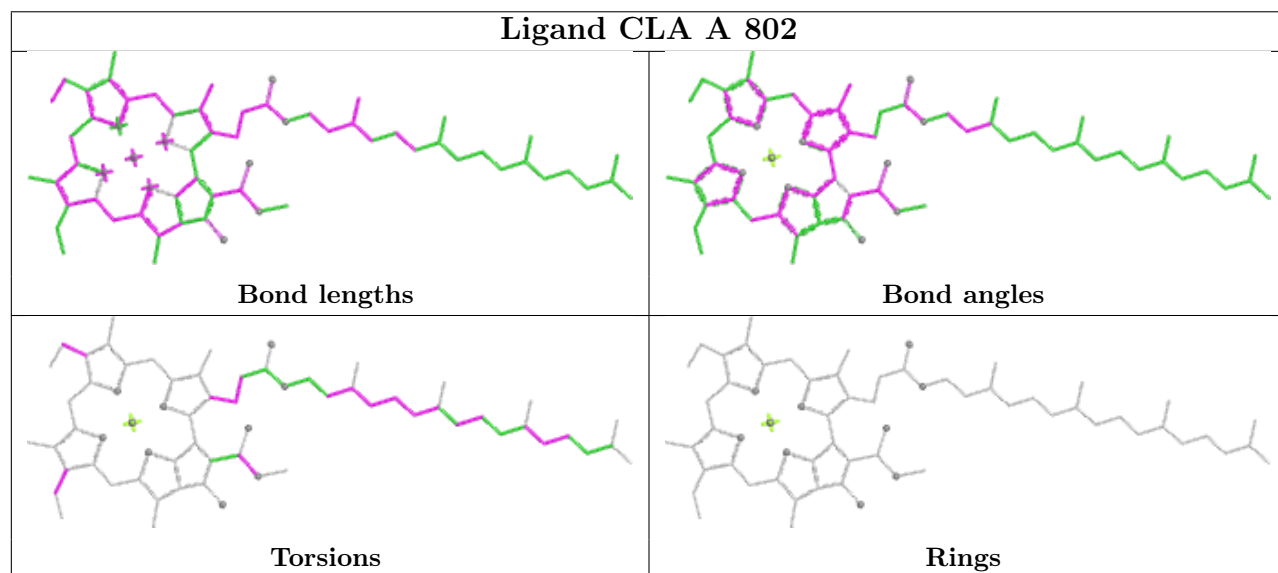
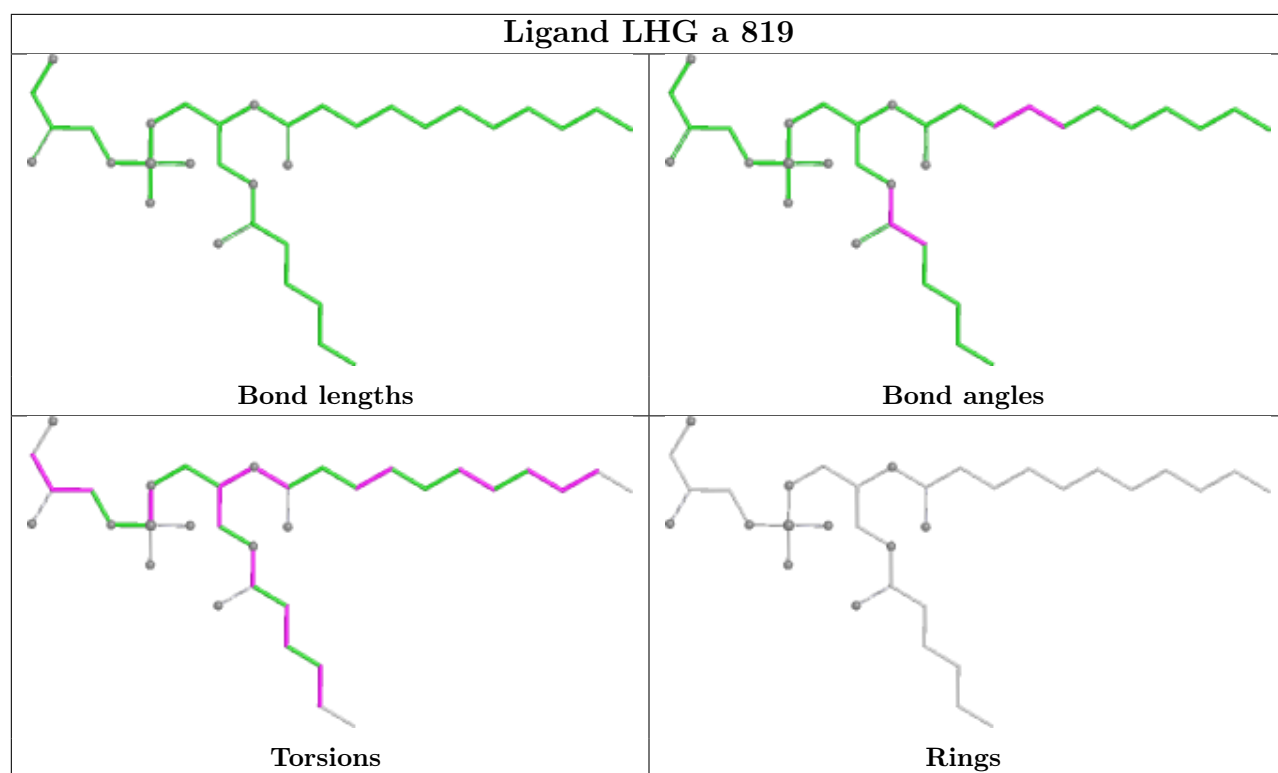
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

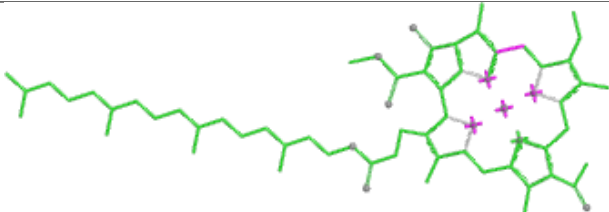
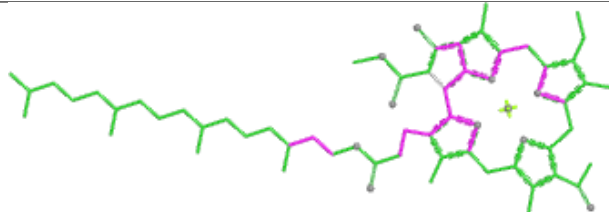
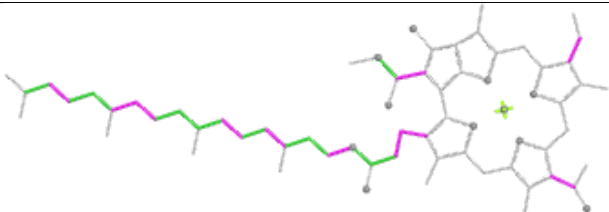
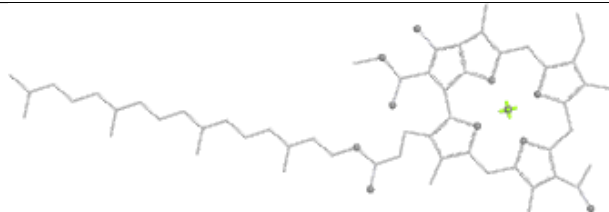


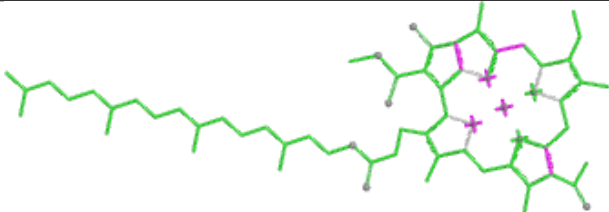
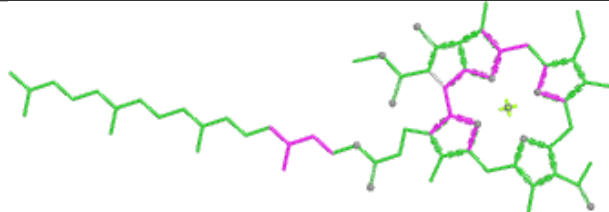
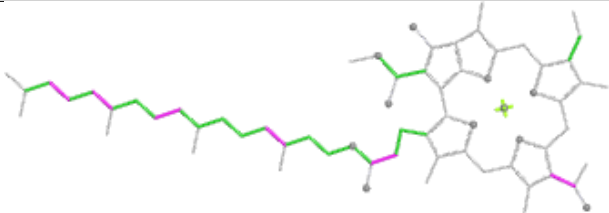
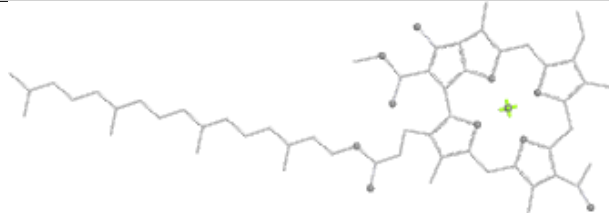


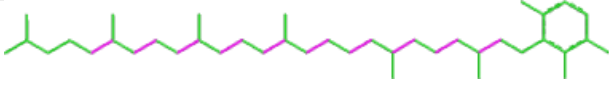
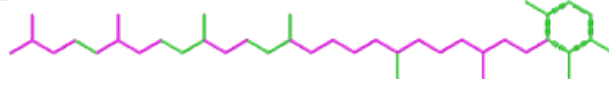
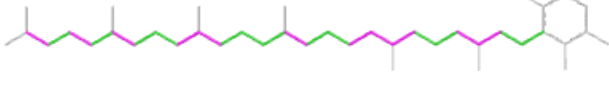
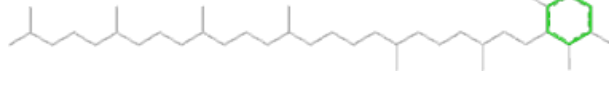


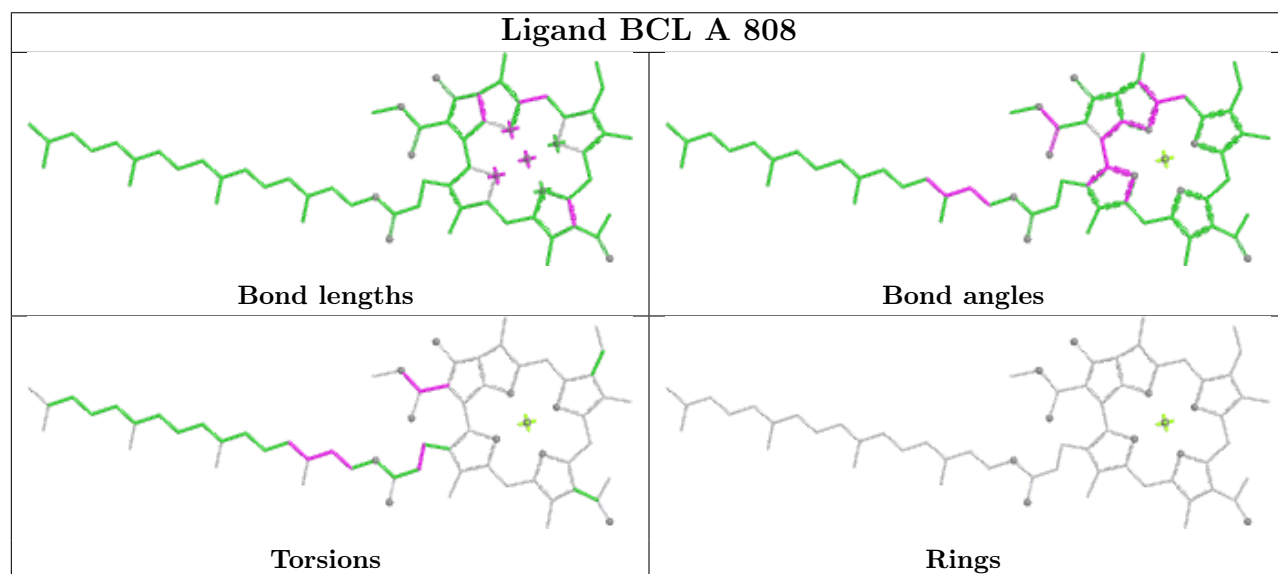
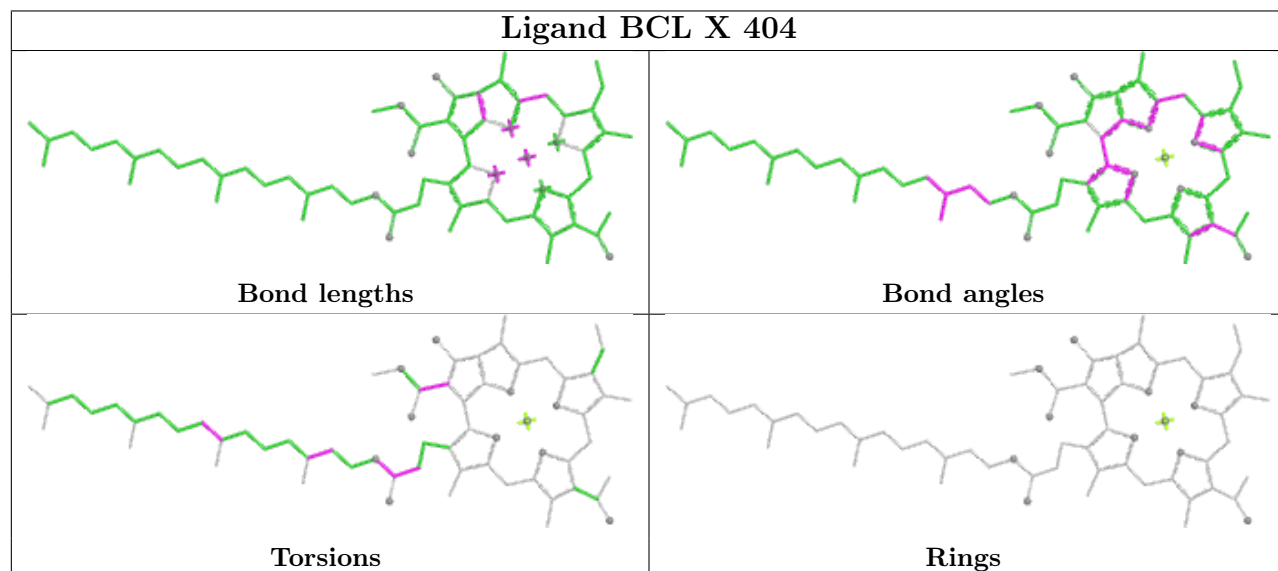
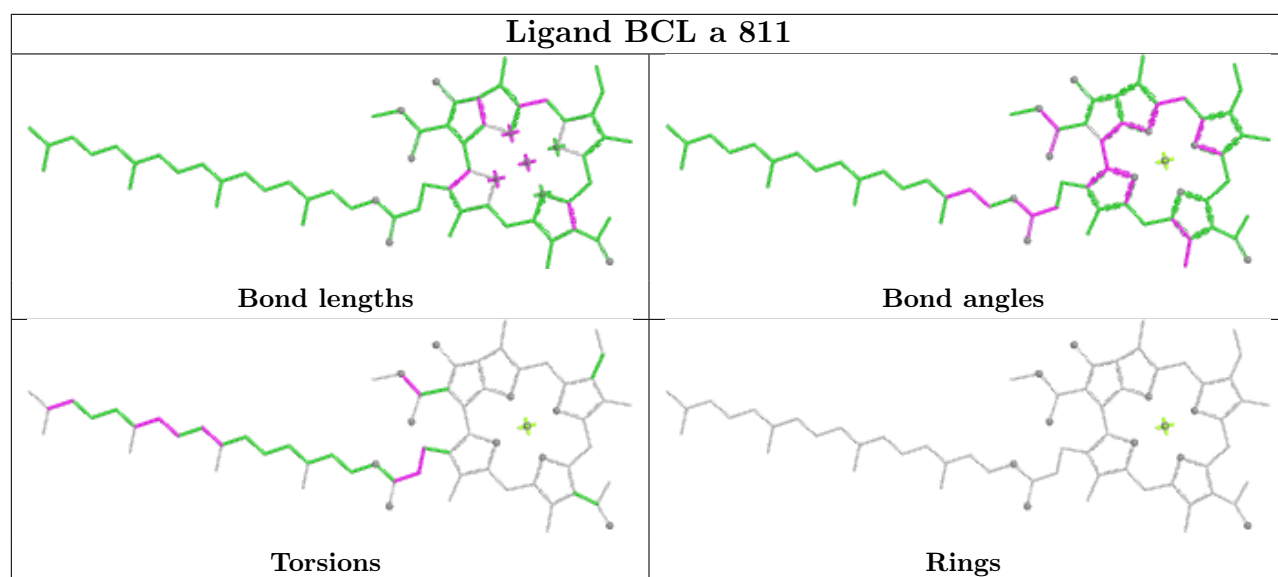


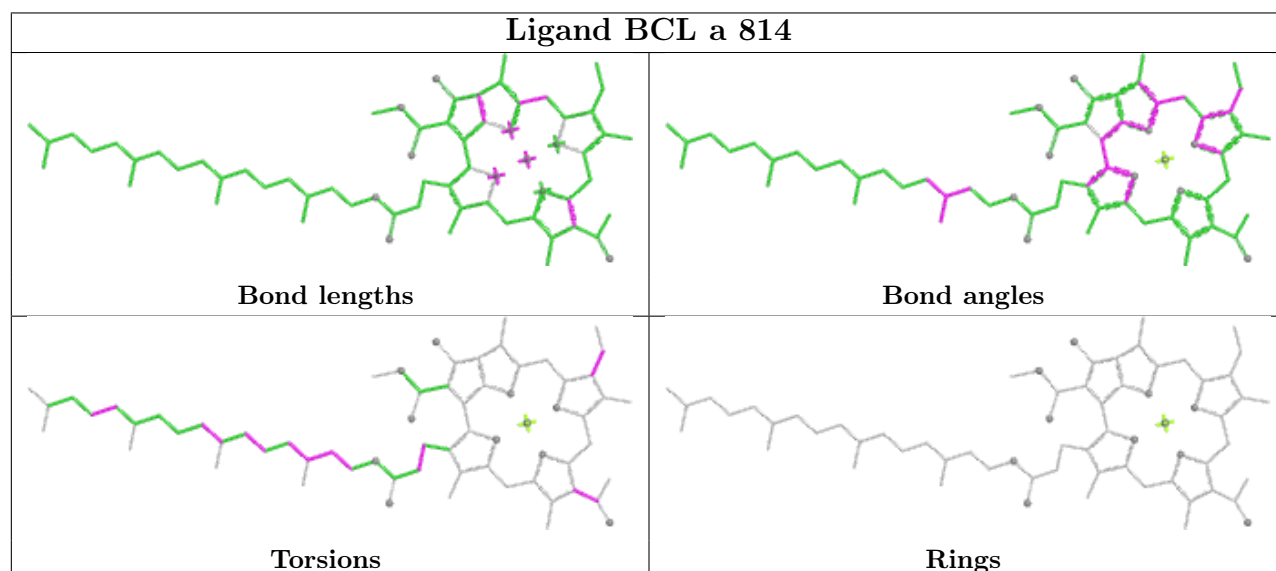
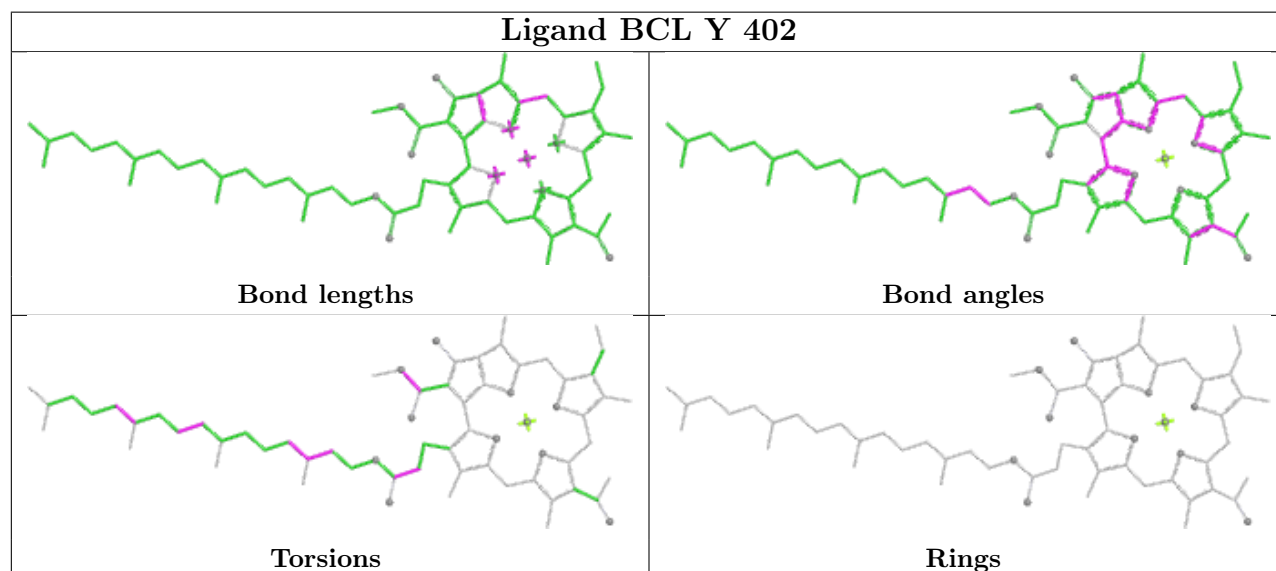
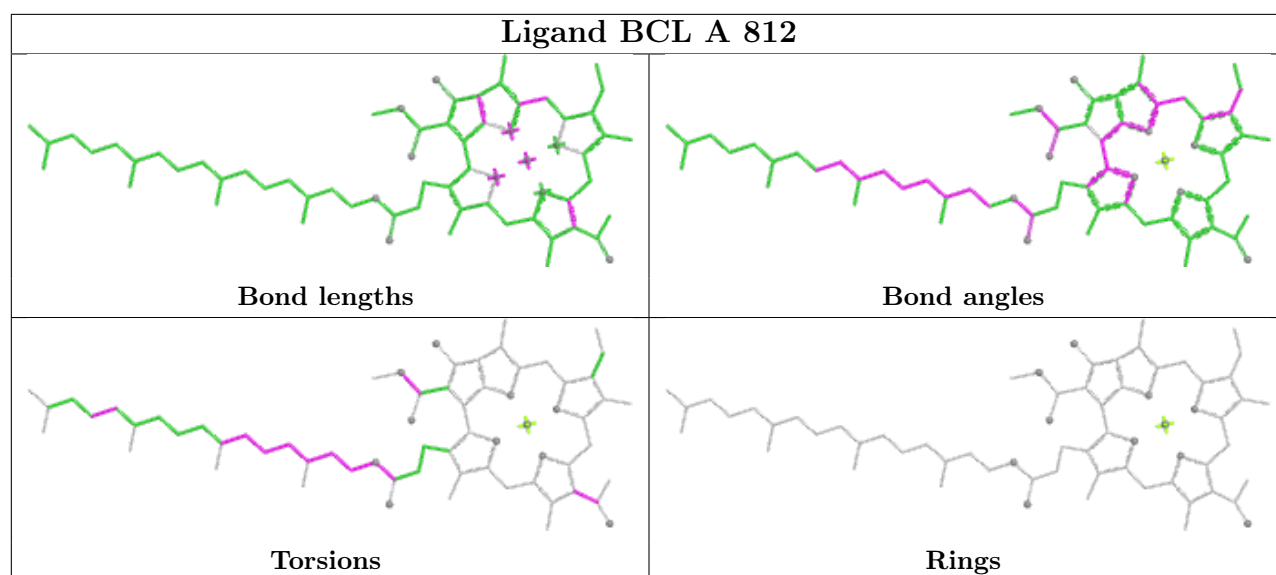


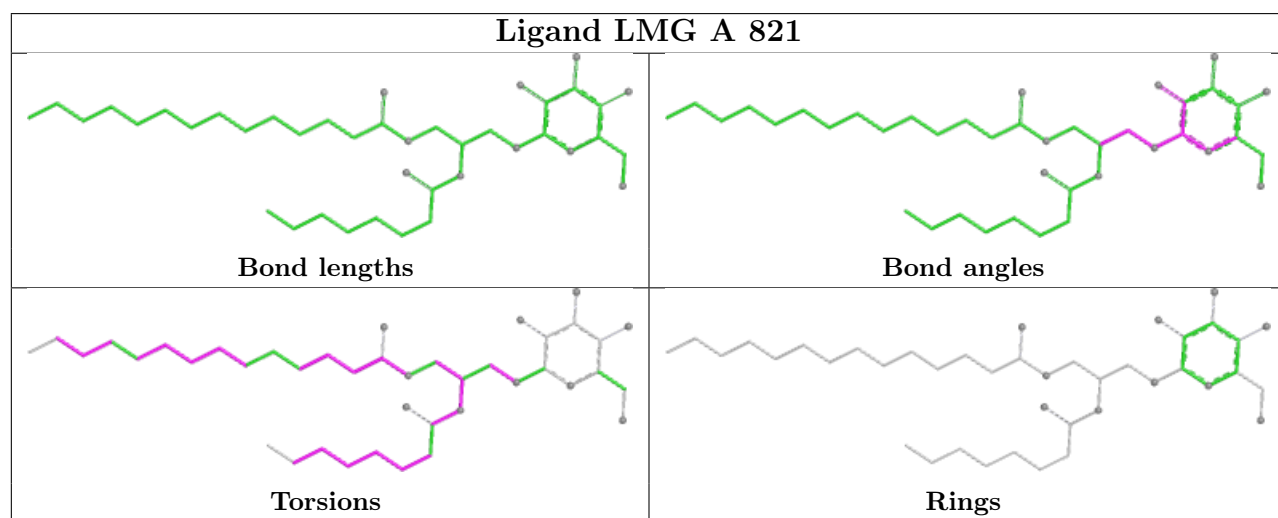
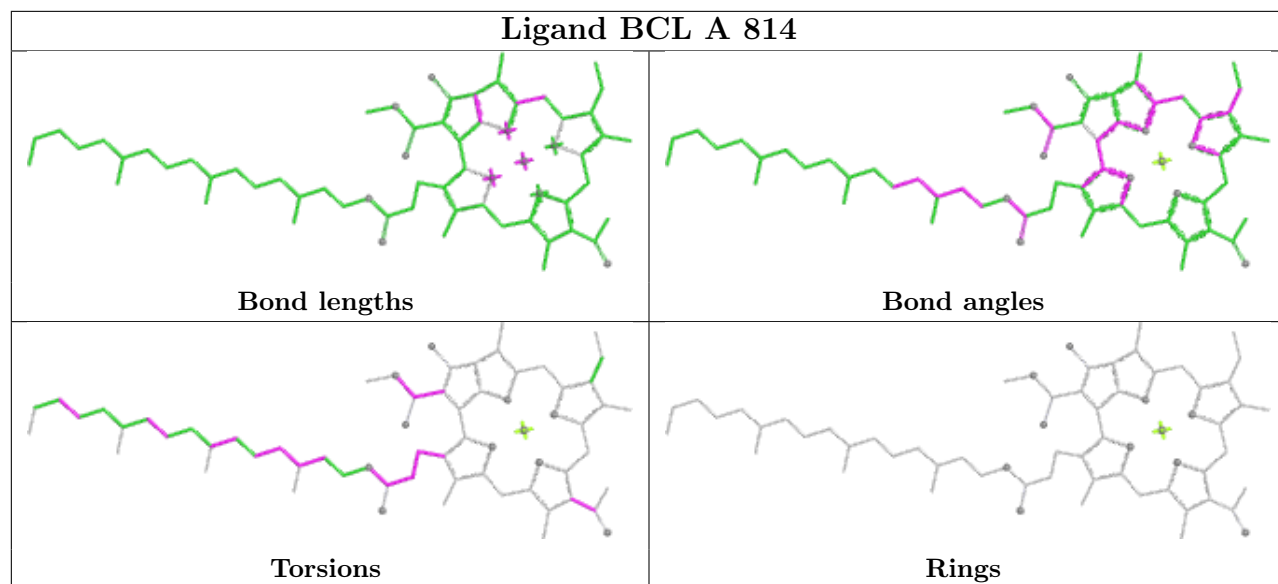
Ligand BCL a 813	
	
Bond lengths	Bond angles
	
Torsions	Rings

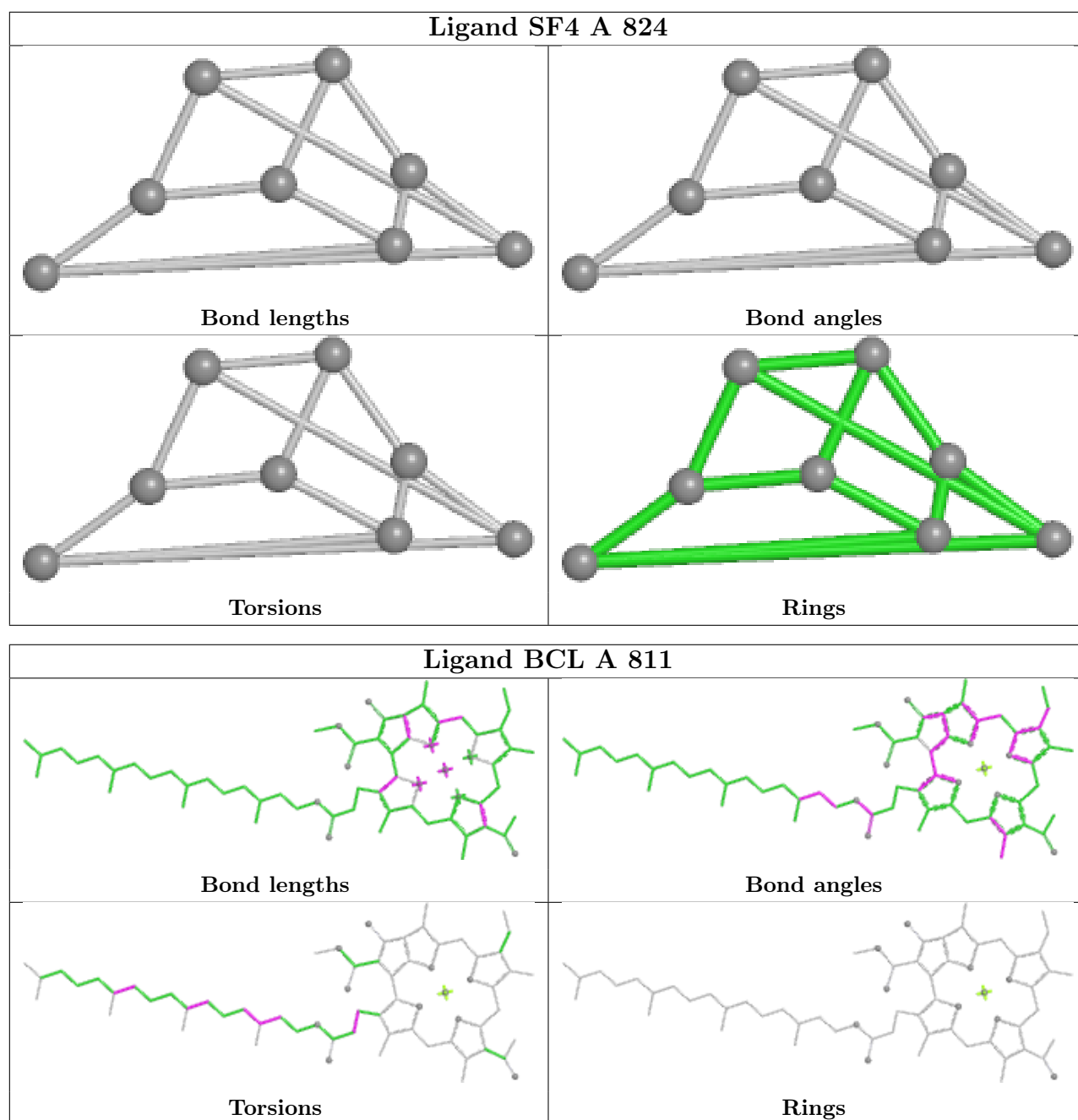
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Bond lengths	Bond angles
	
Torsions	Rings

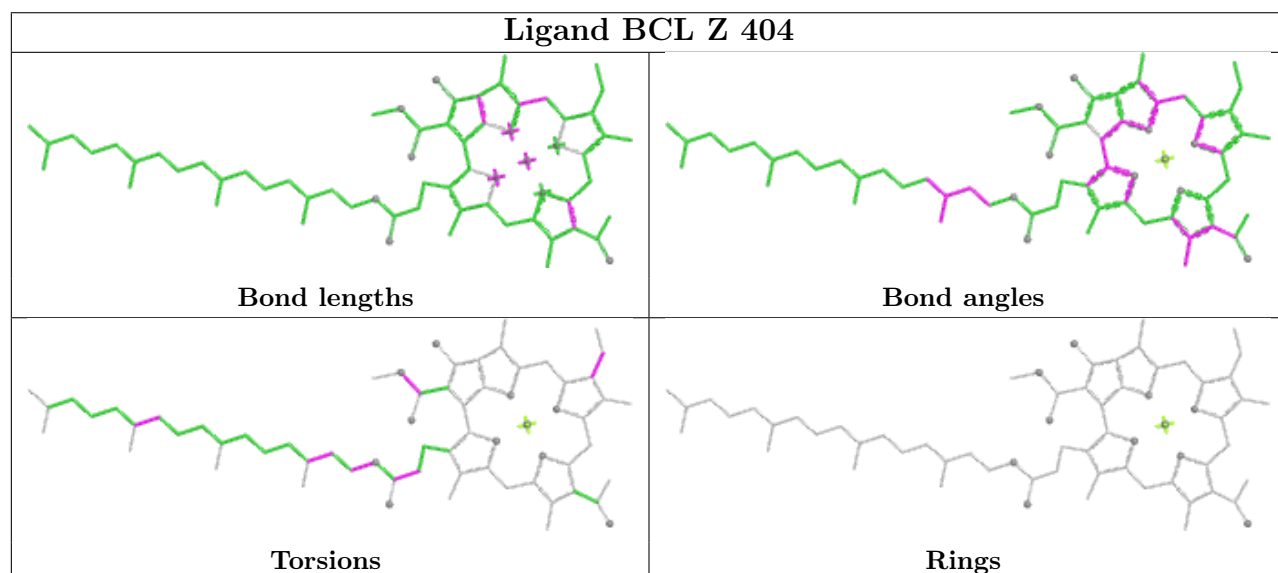
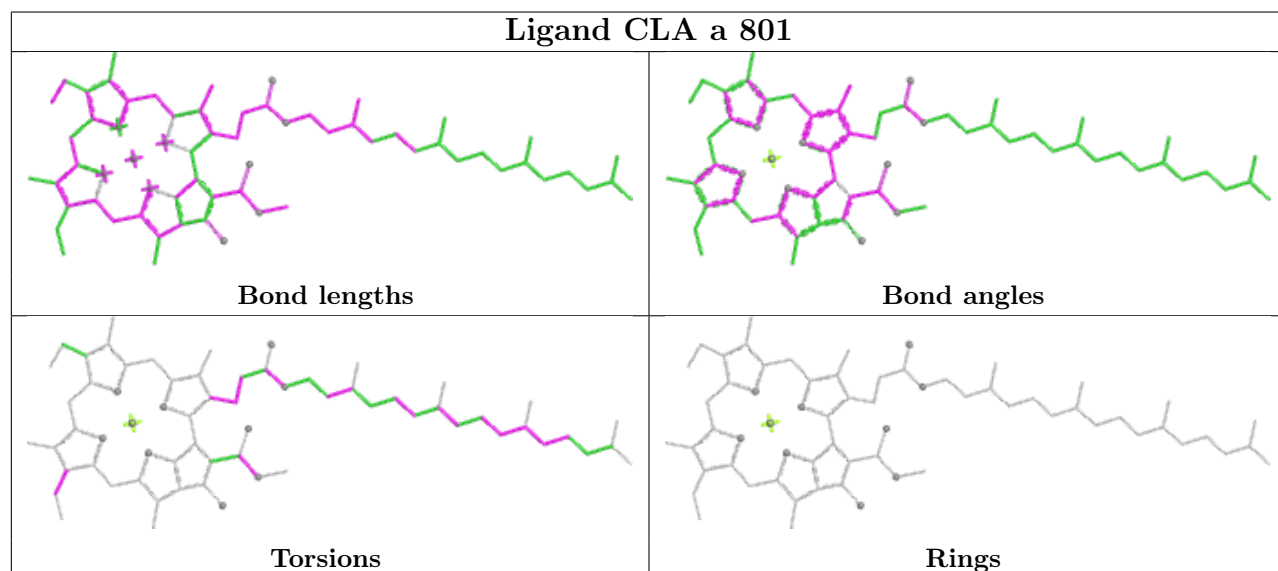
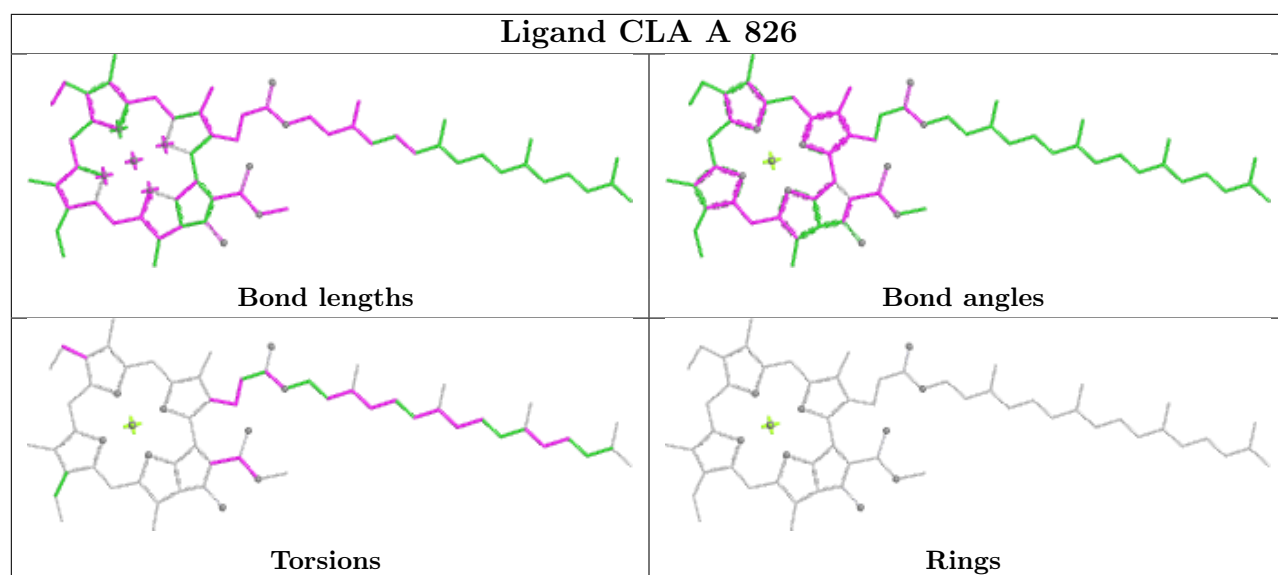
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Bond lengths	Bond angles
	
Torsions	Rings

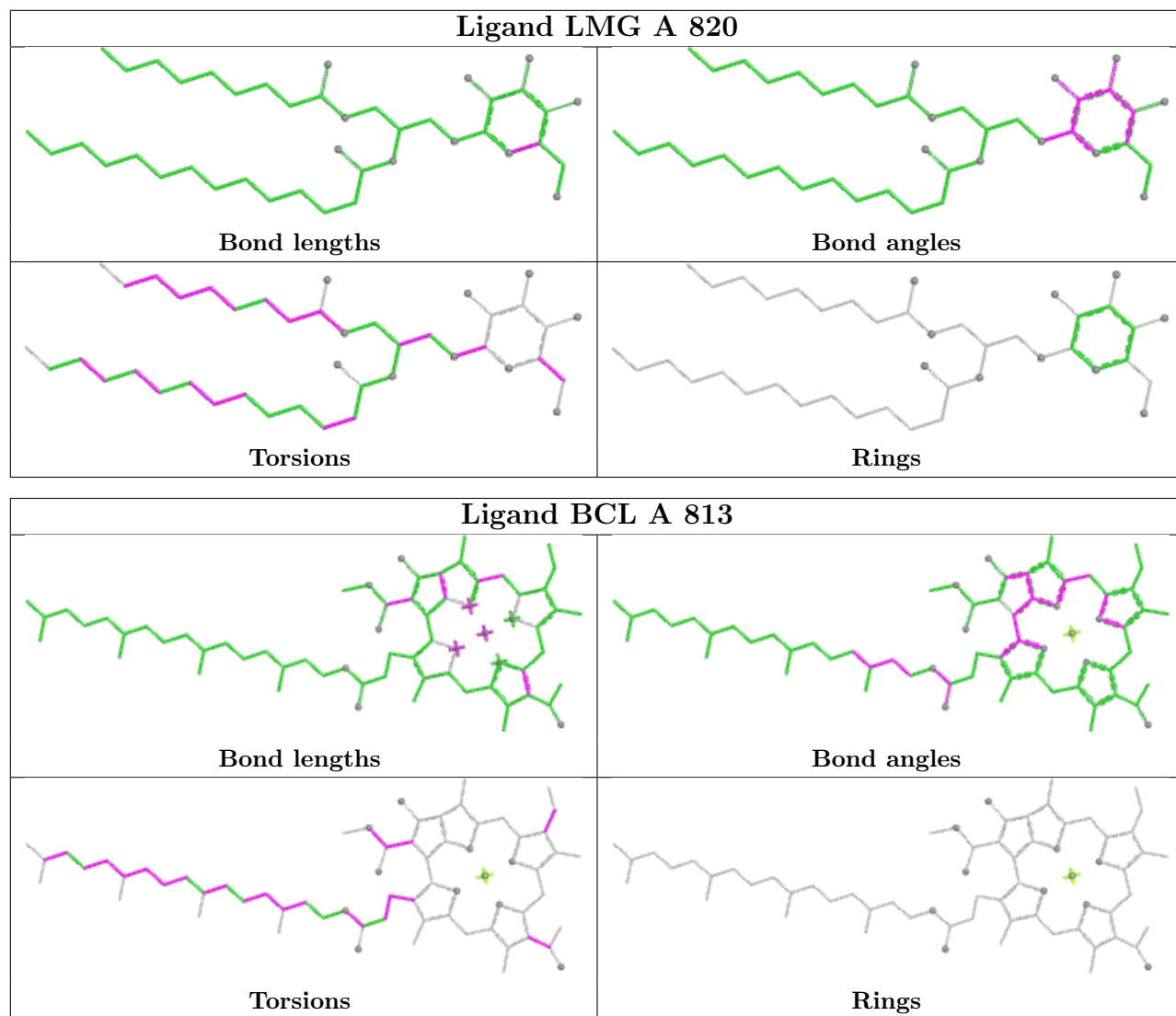




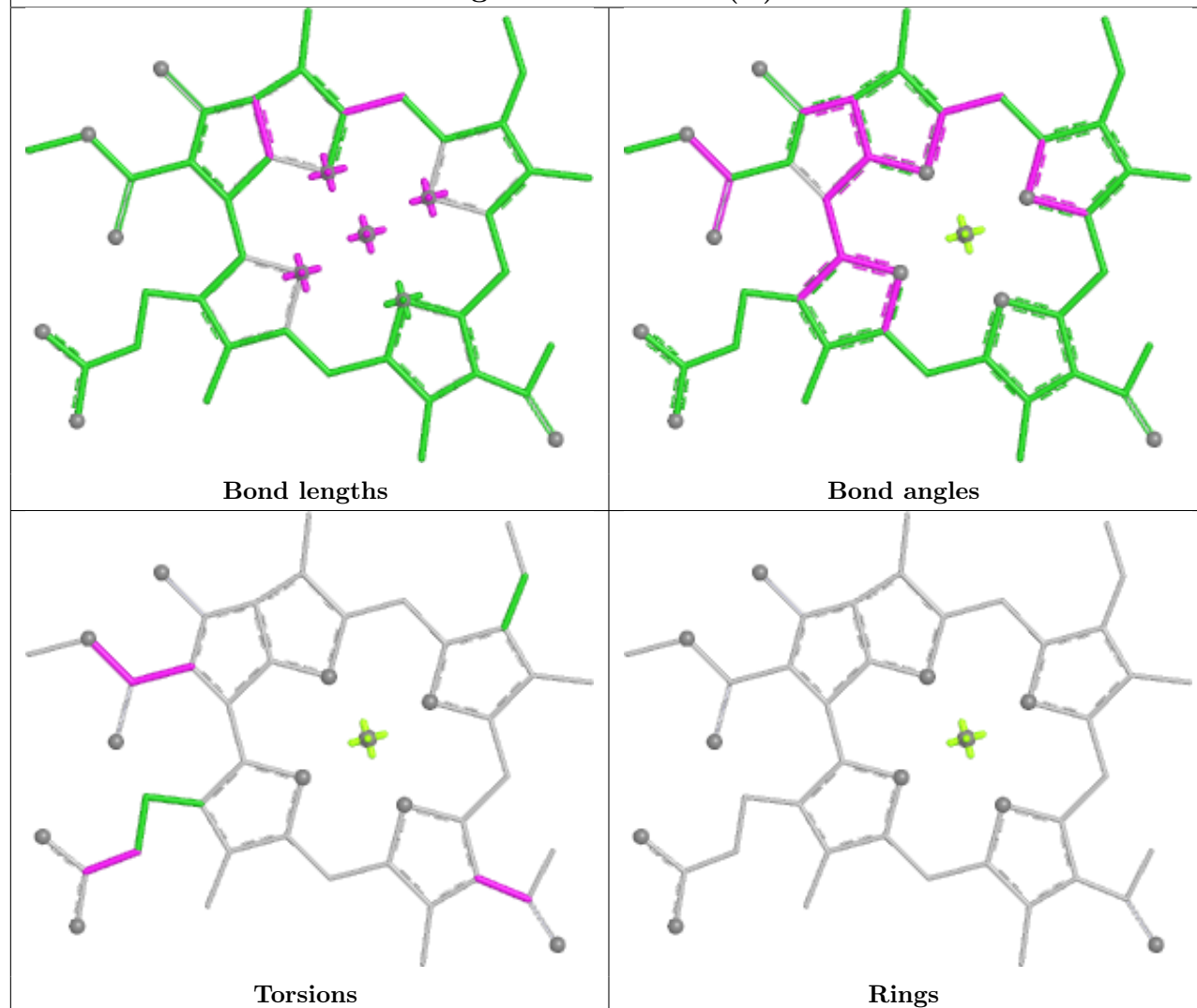




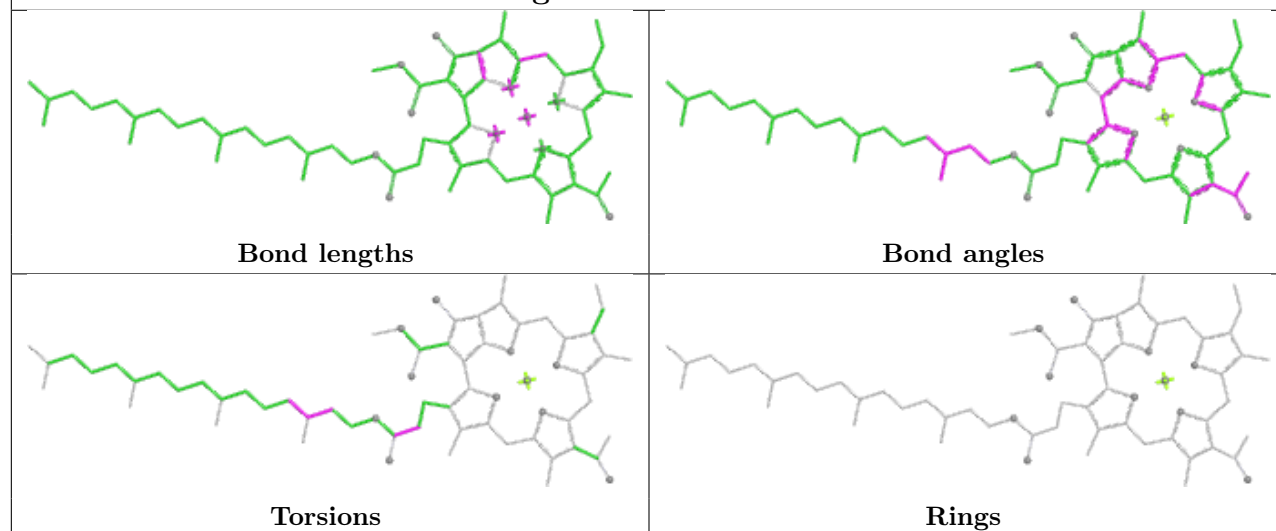


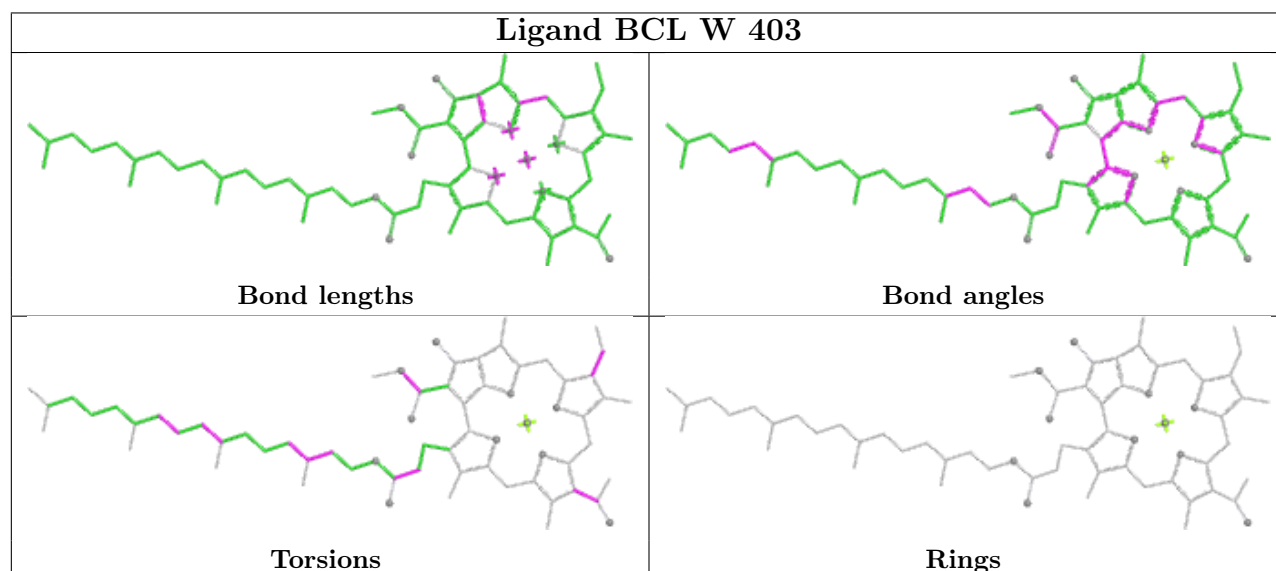
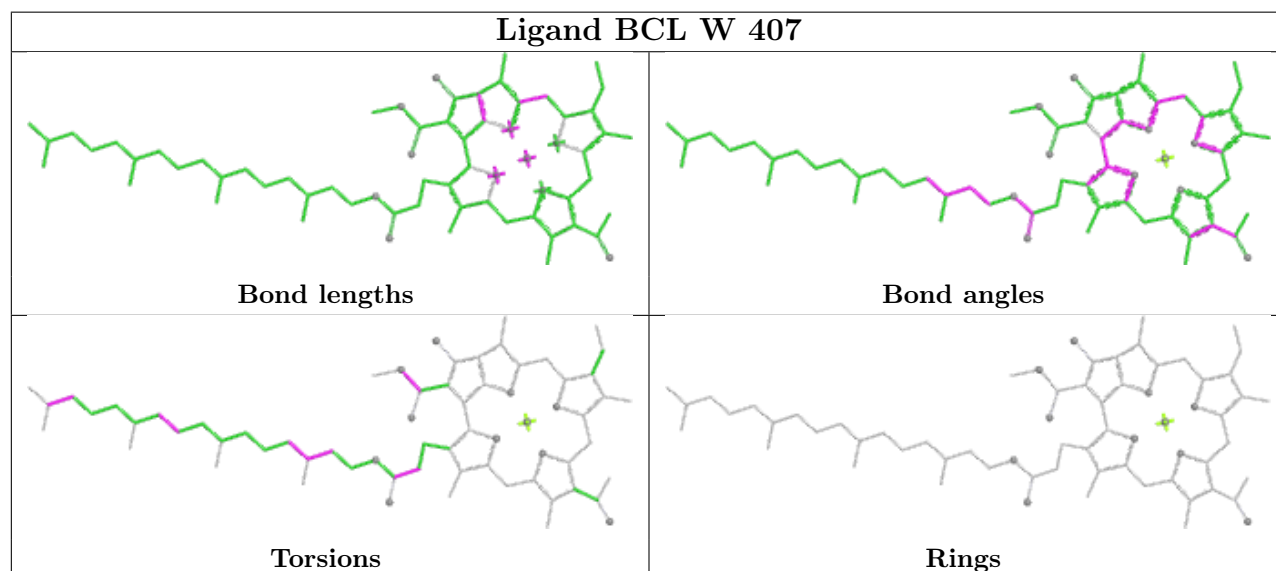
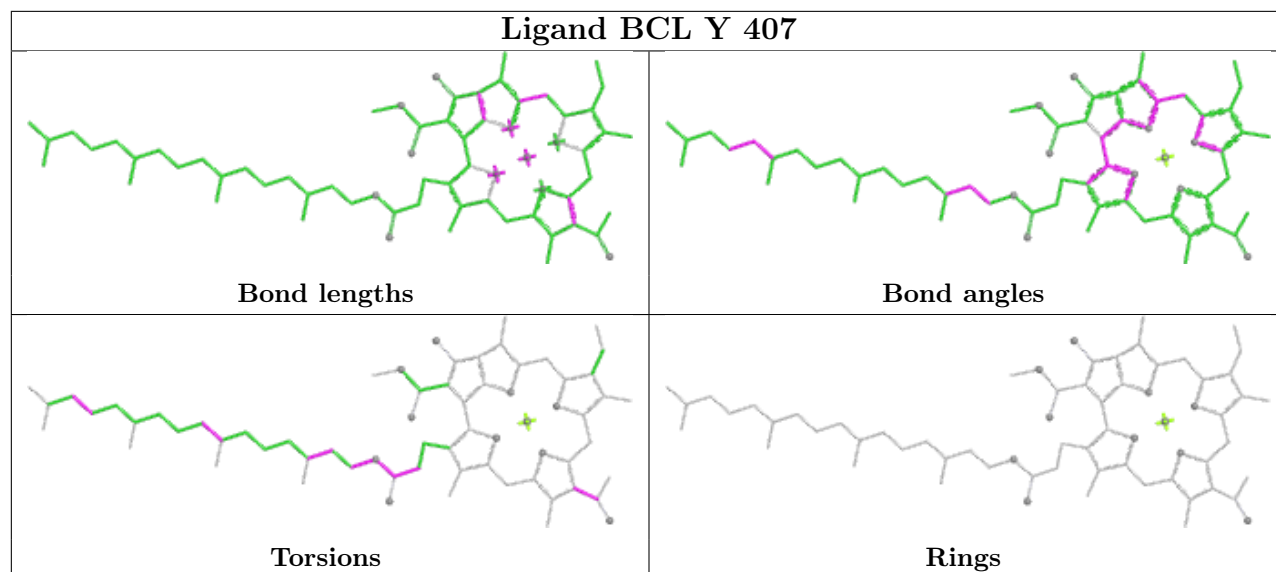


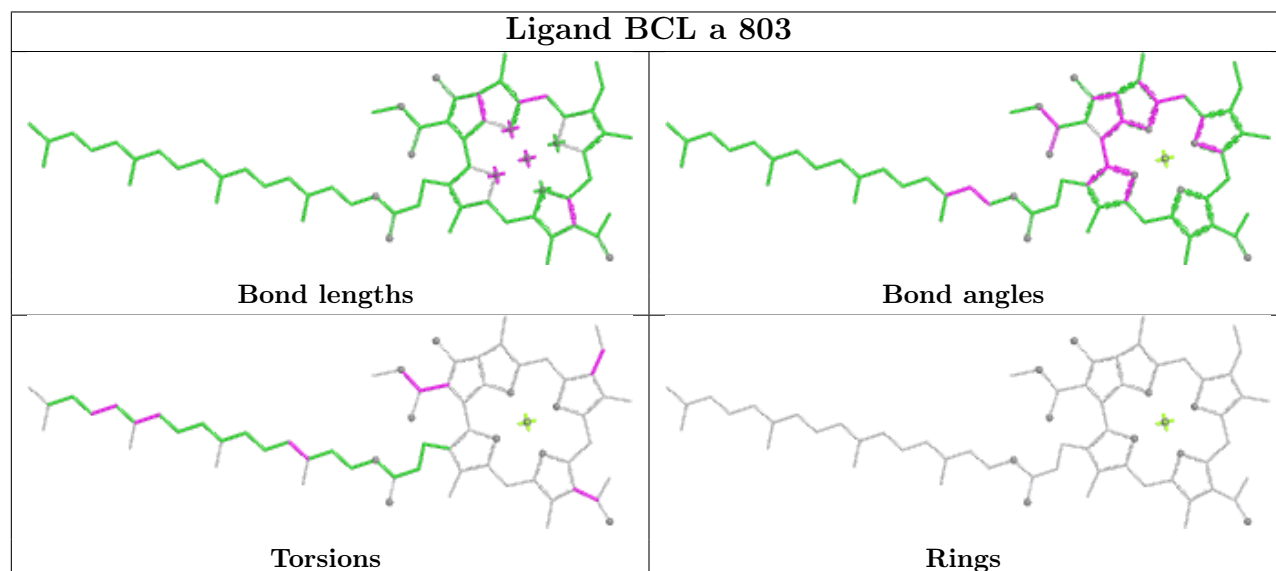
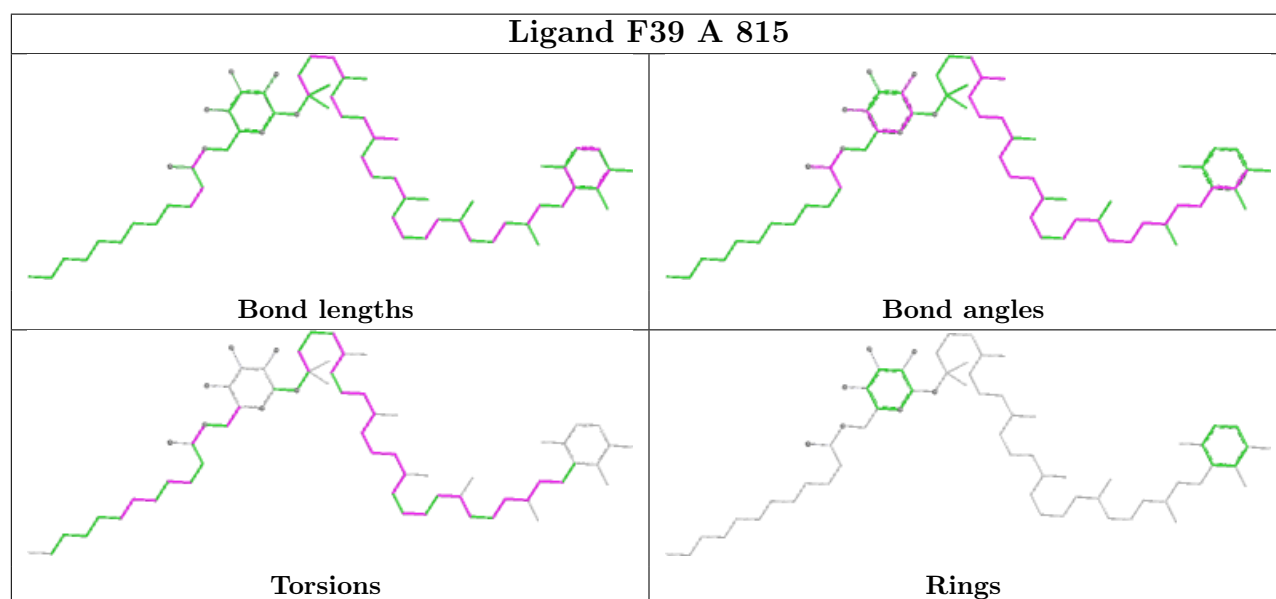
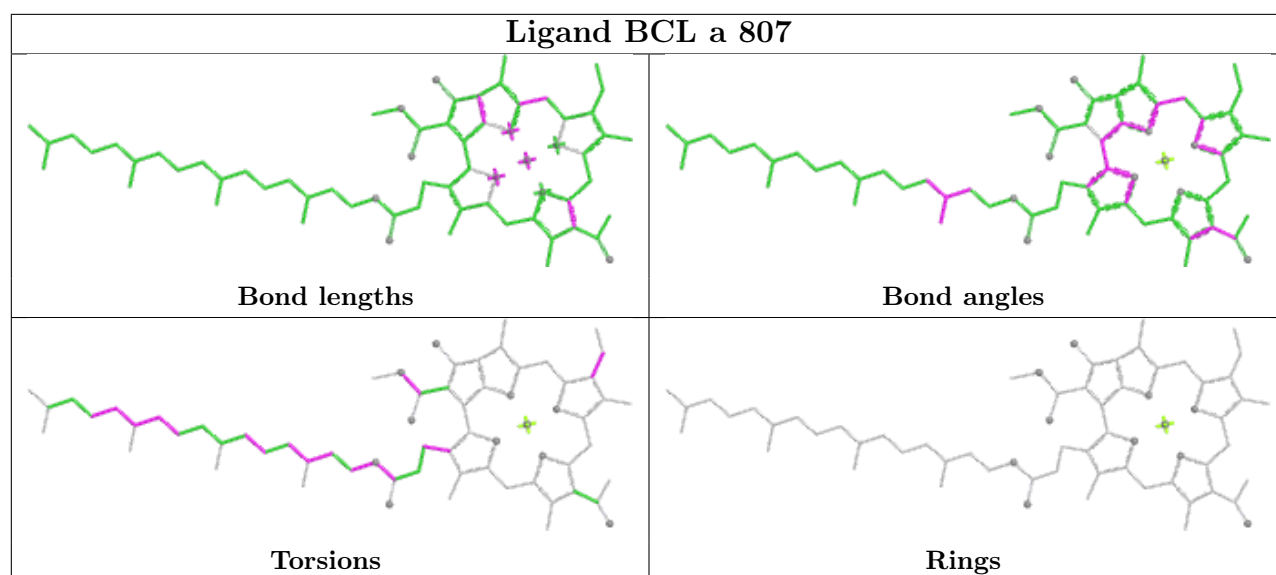
Ligand BCL Z 408 (B)

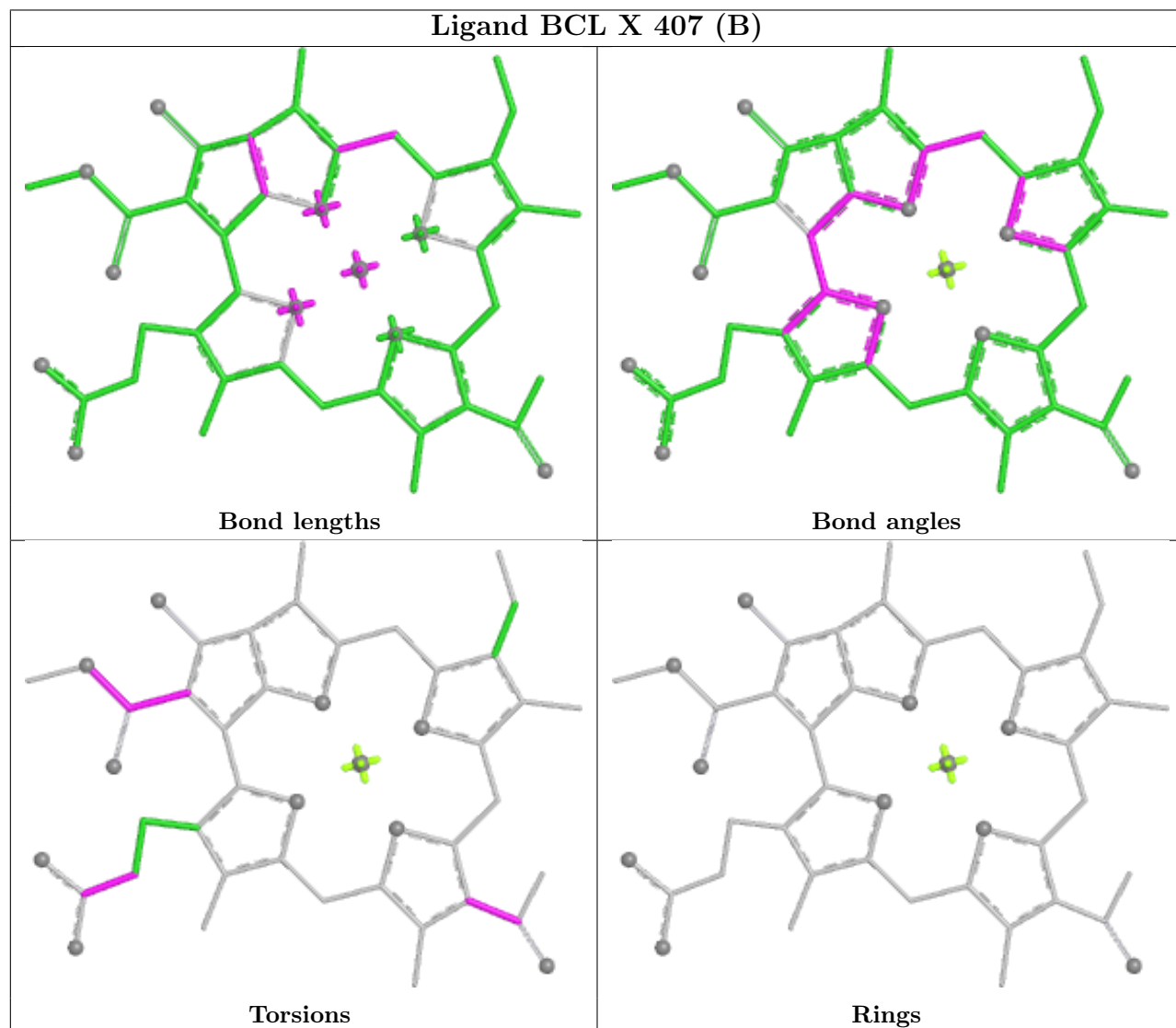
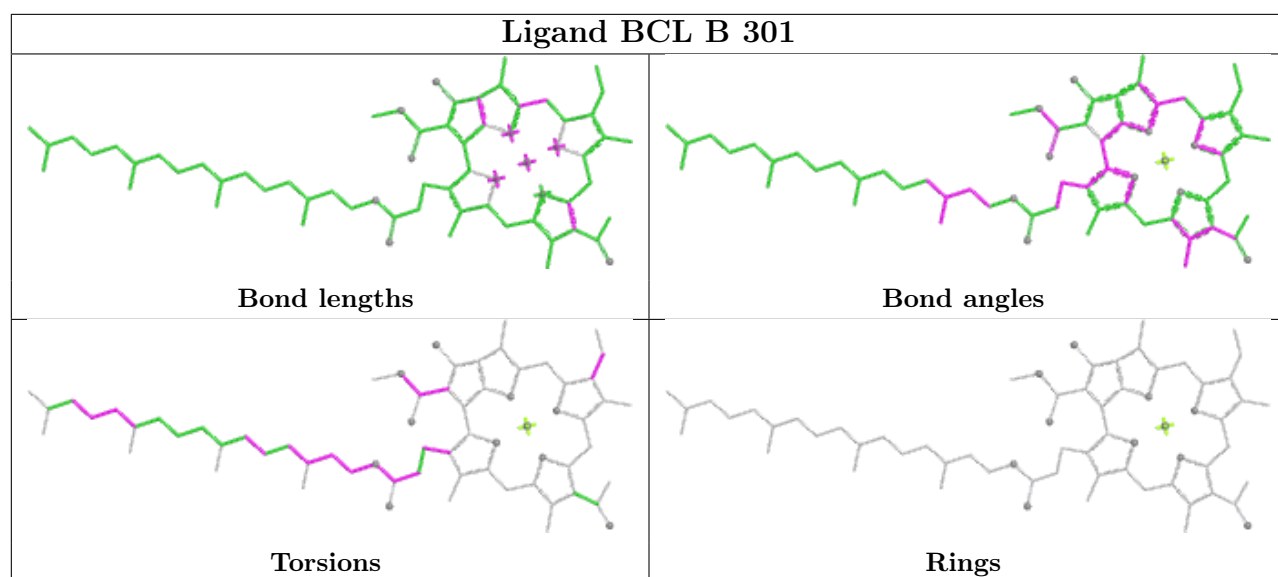


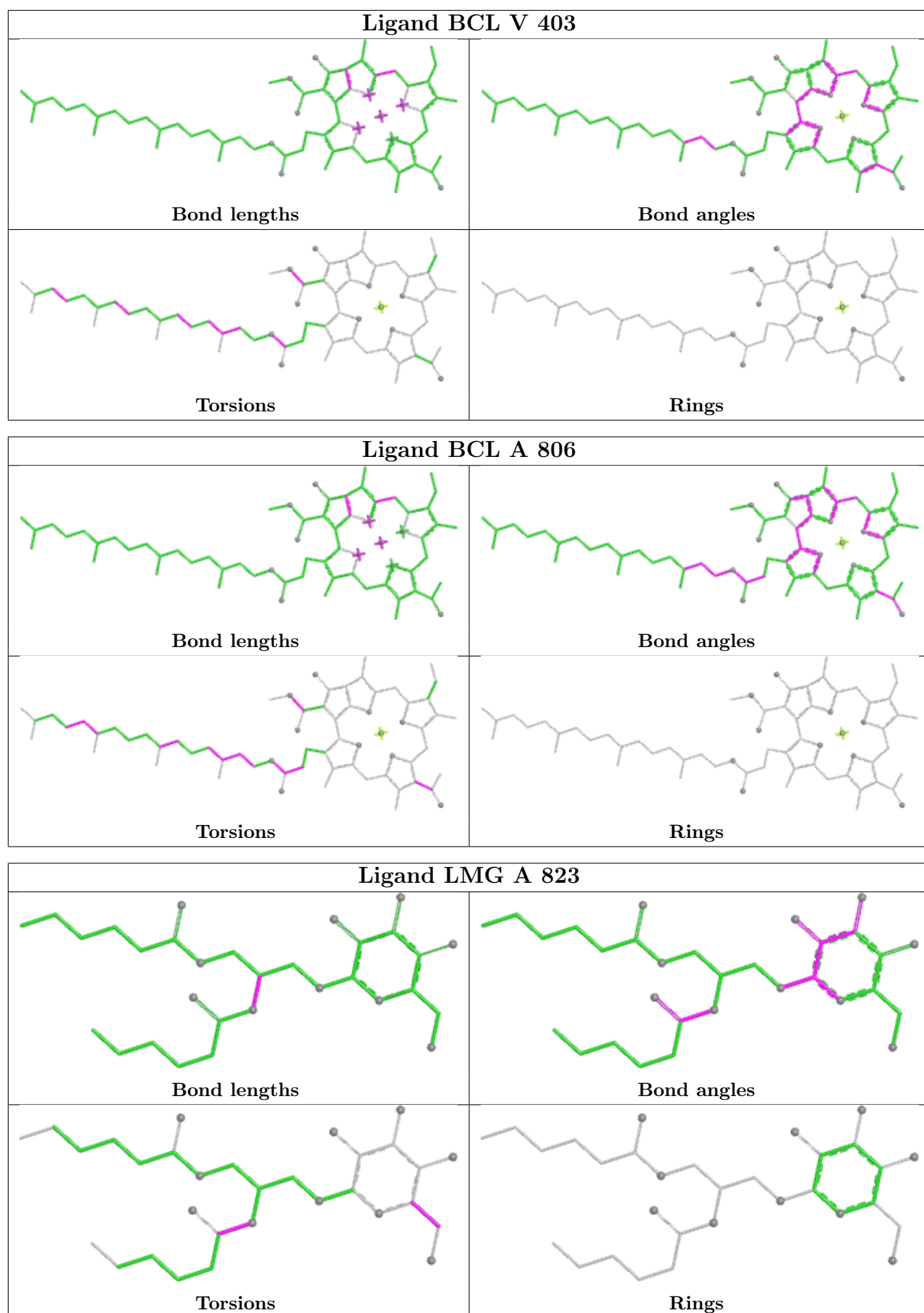
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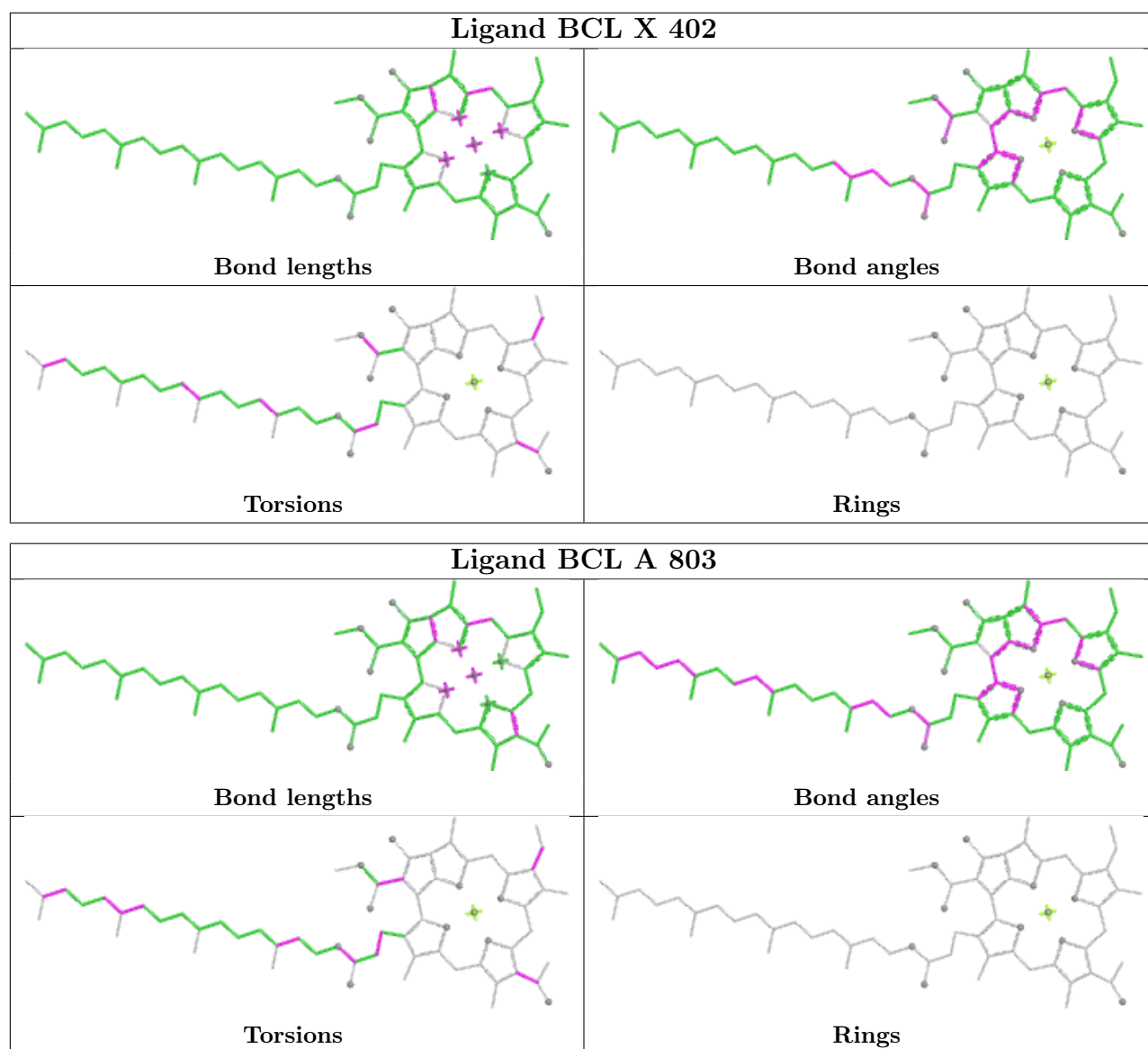


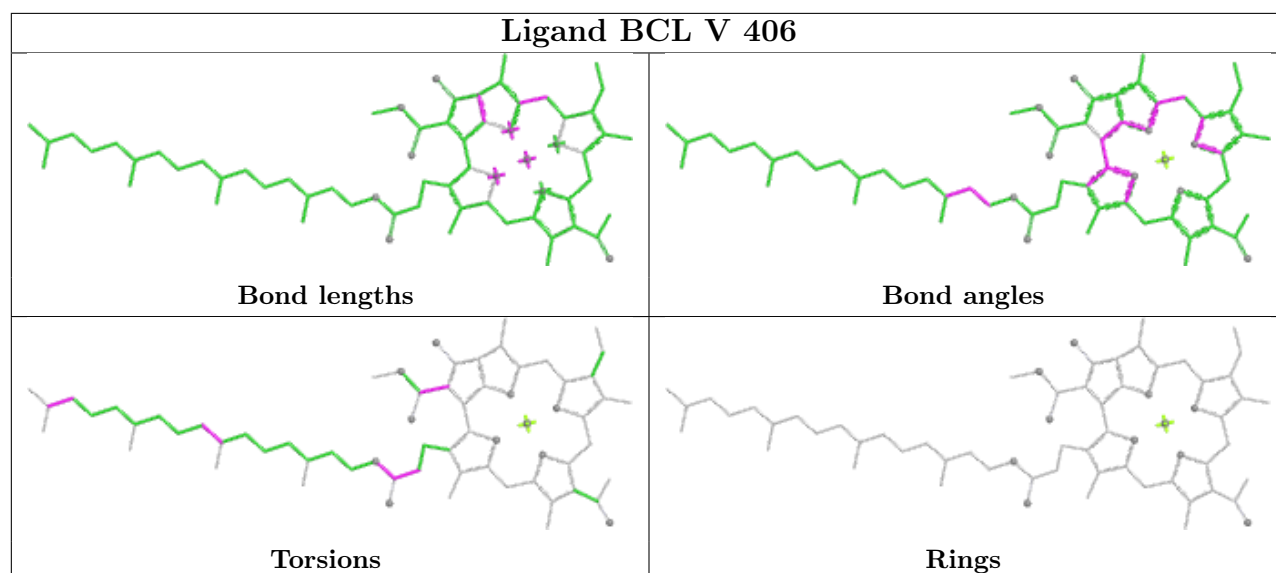
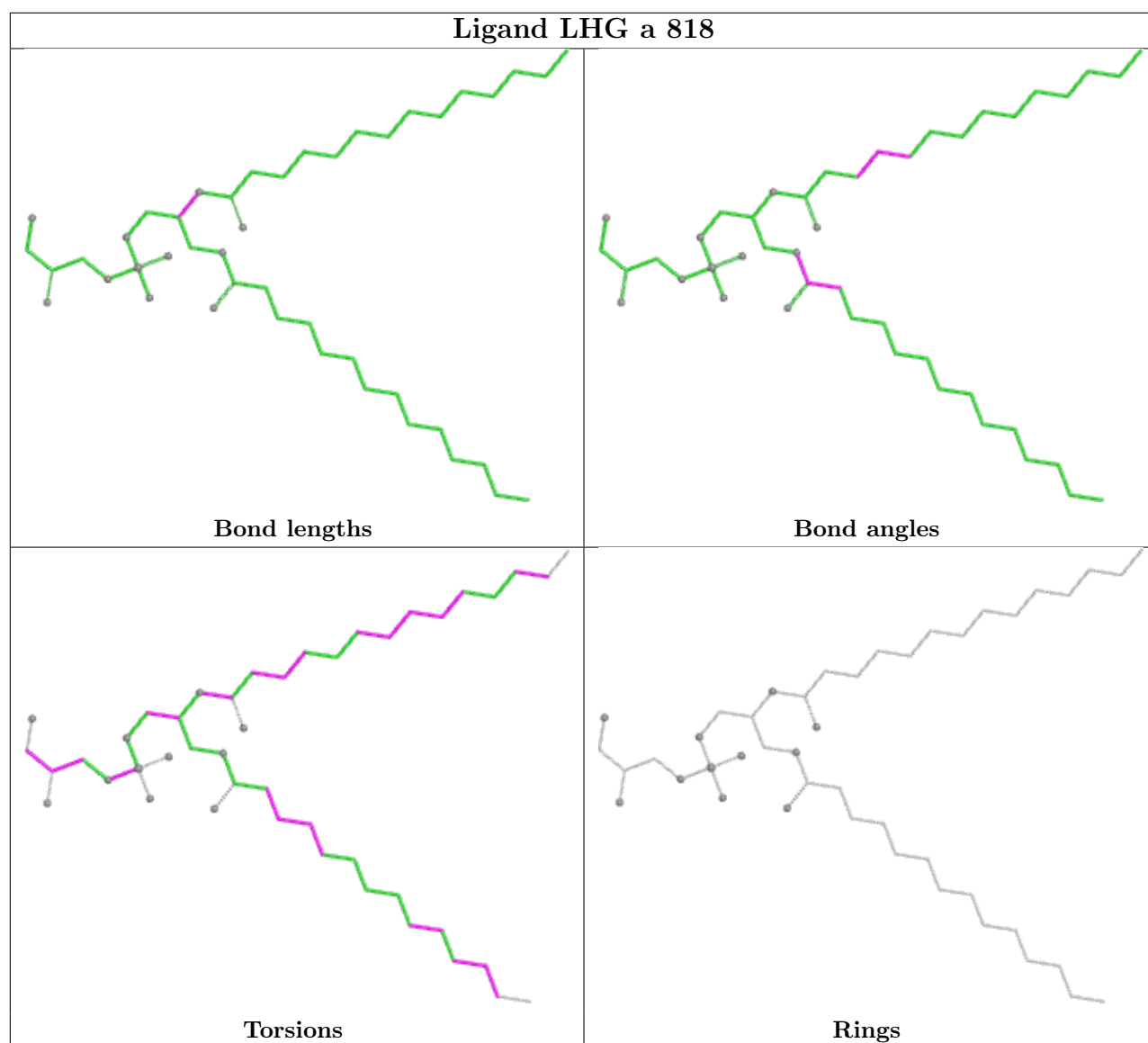


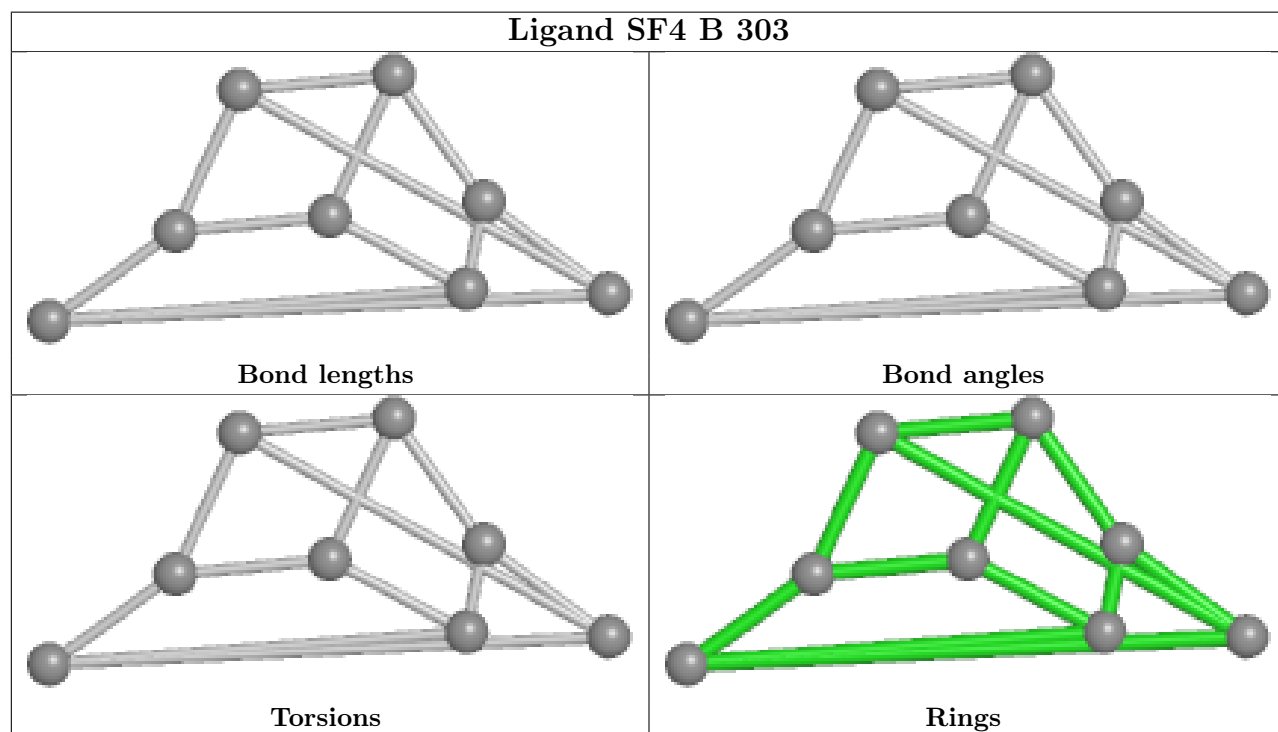
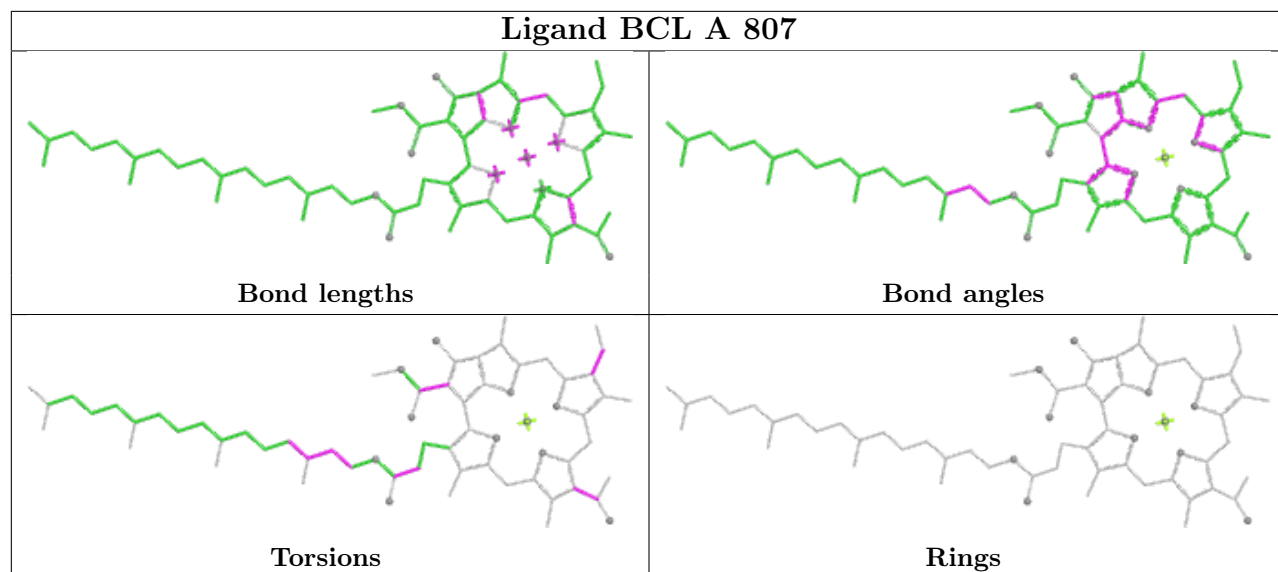


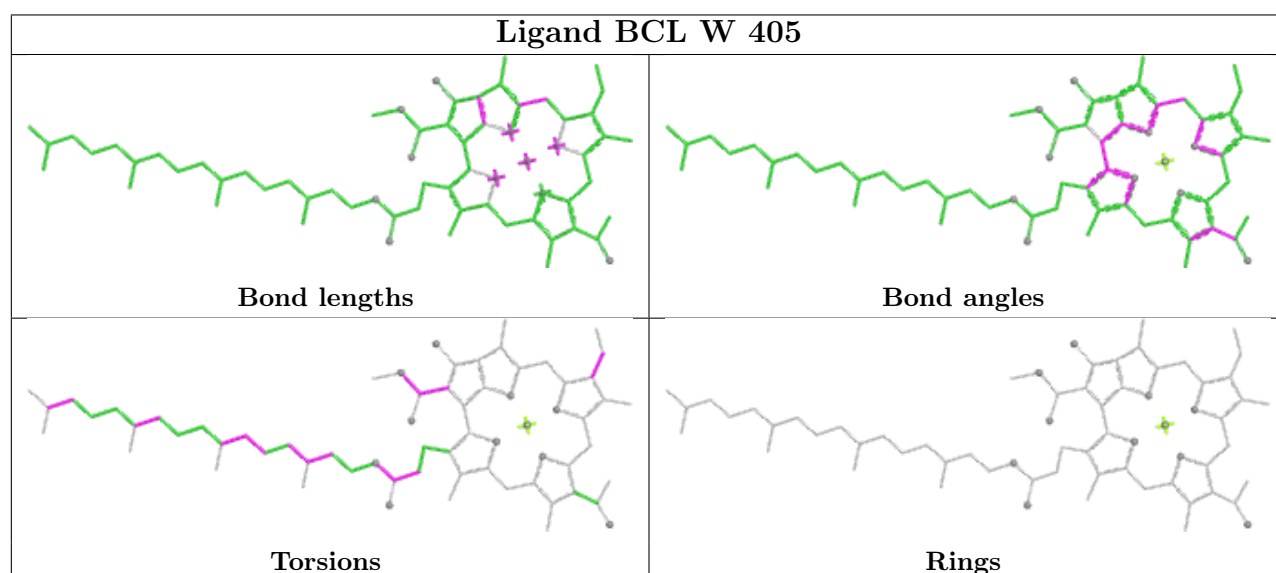
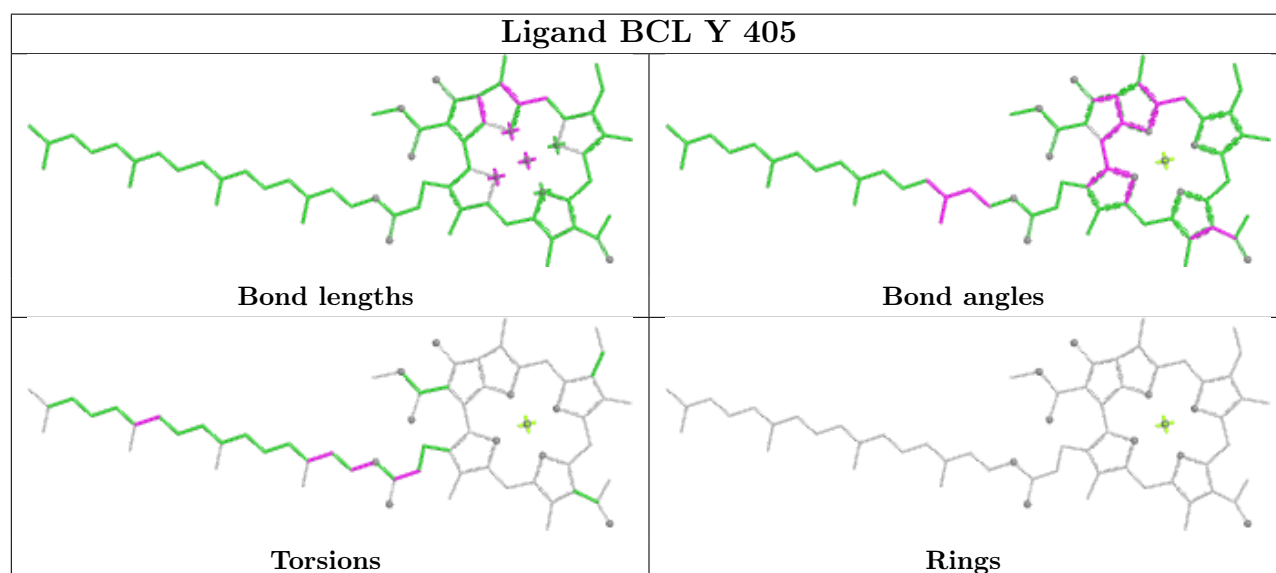
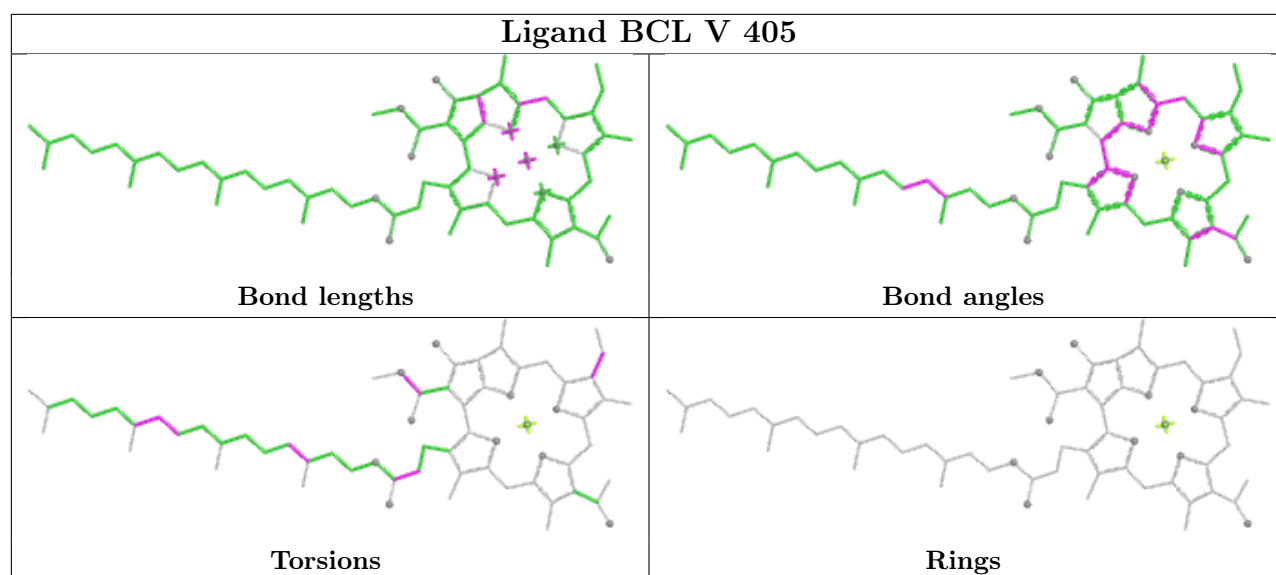


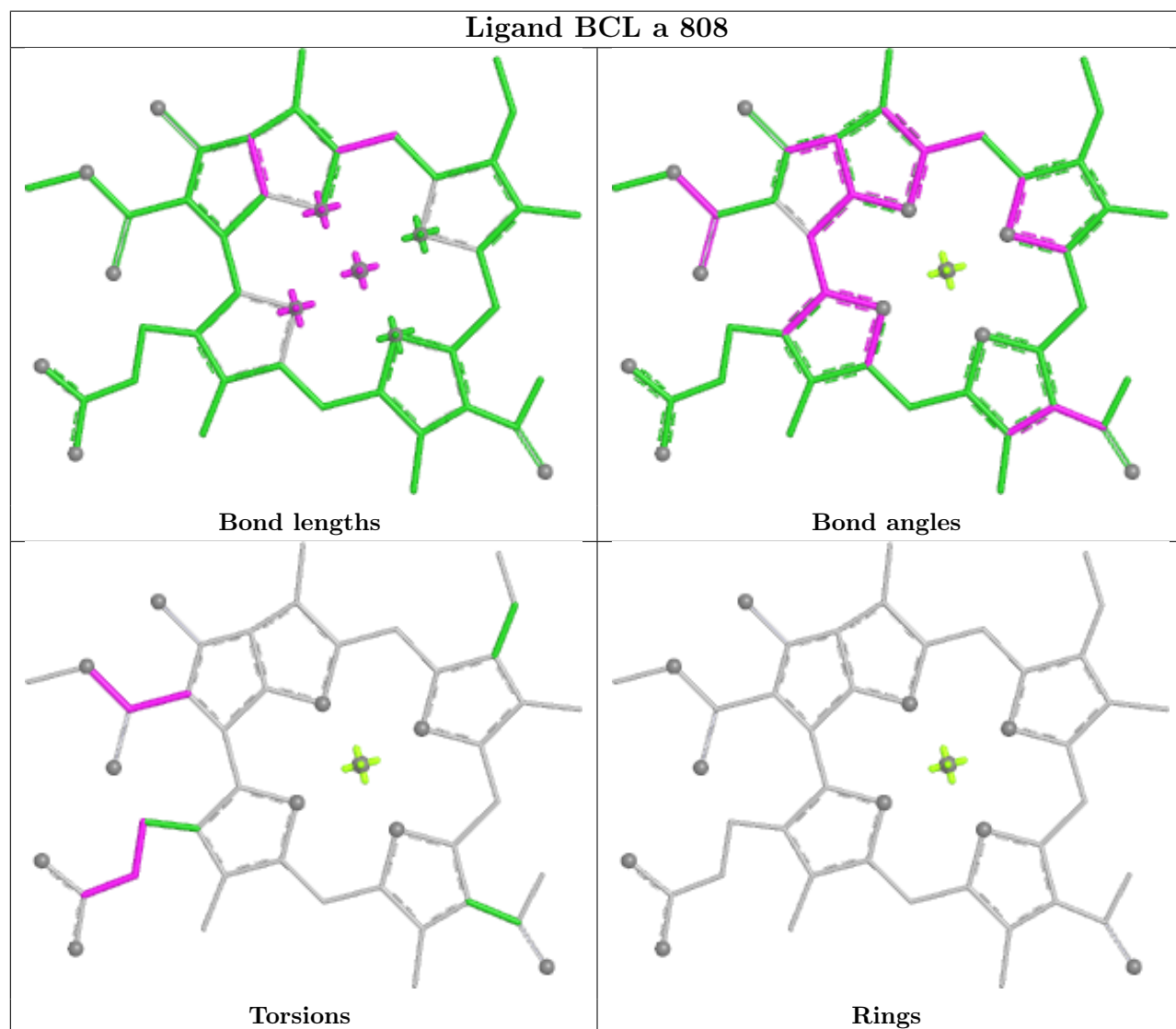
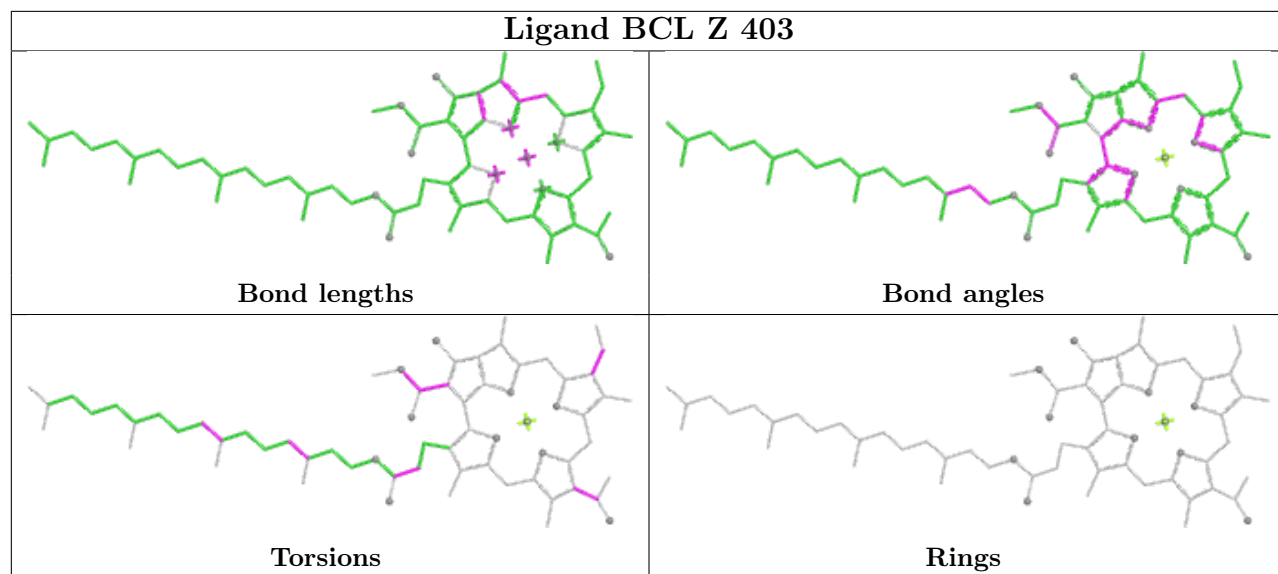


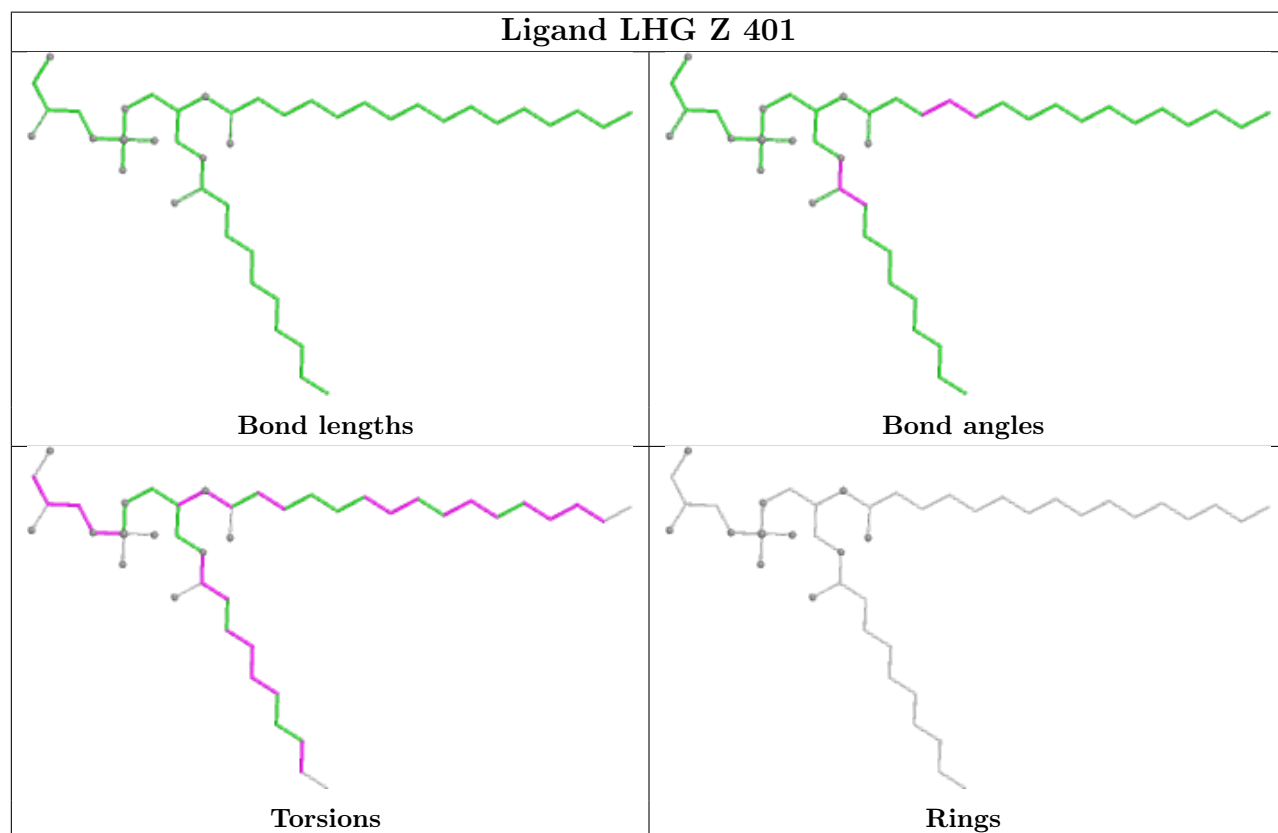
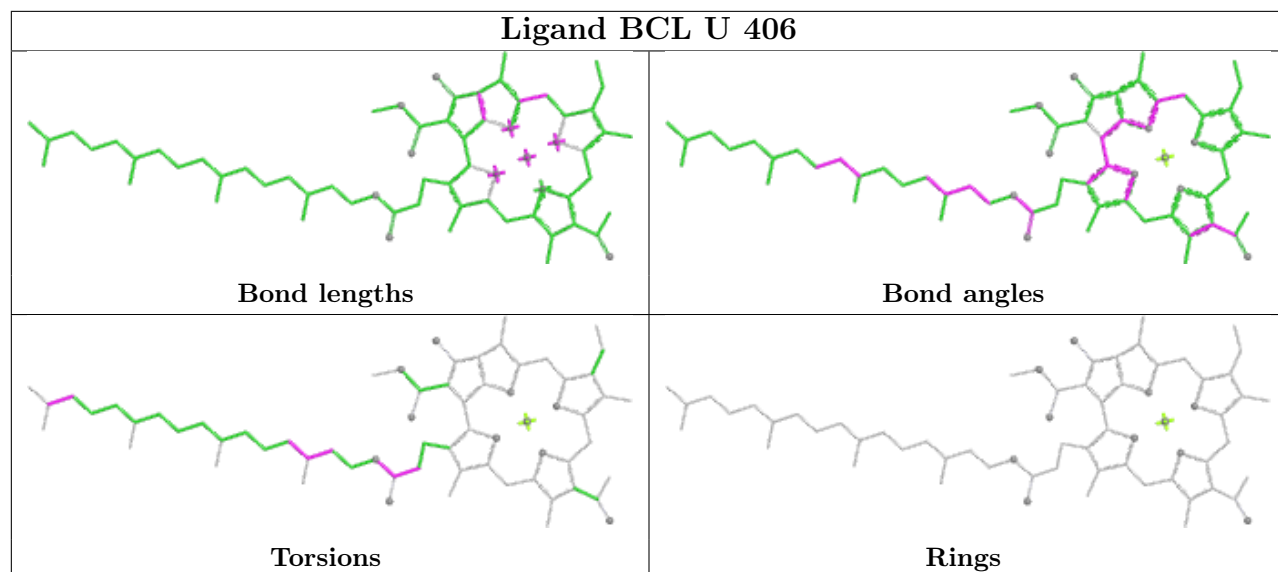


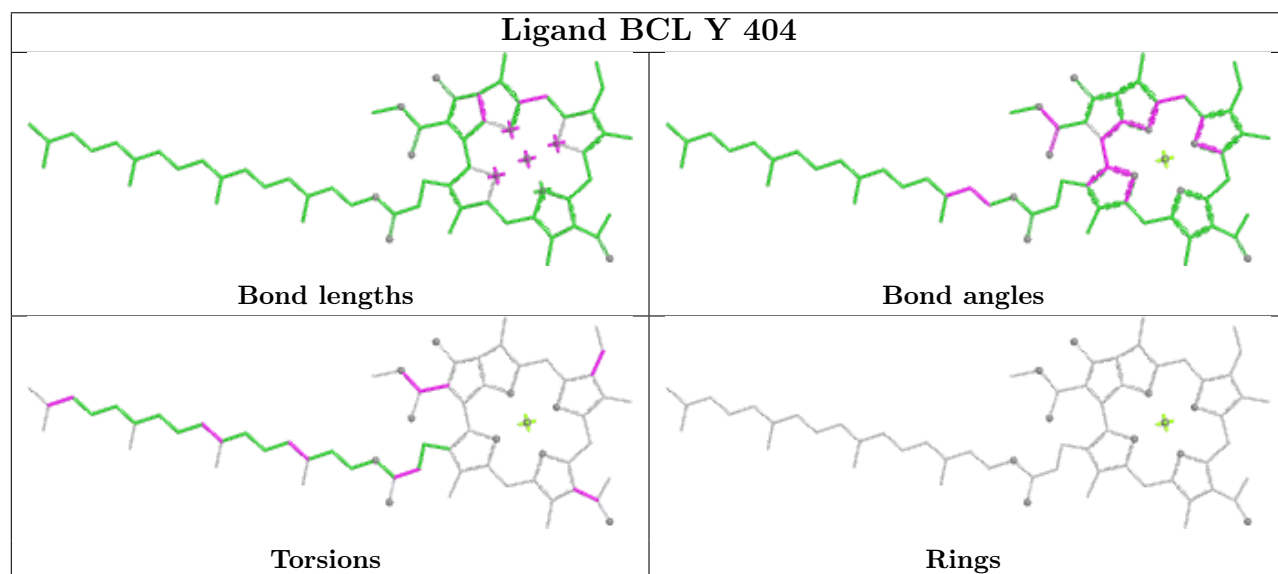
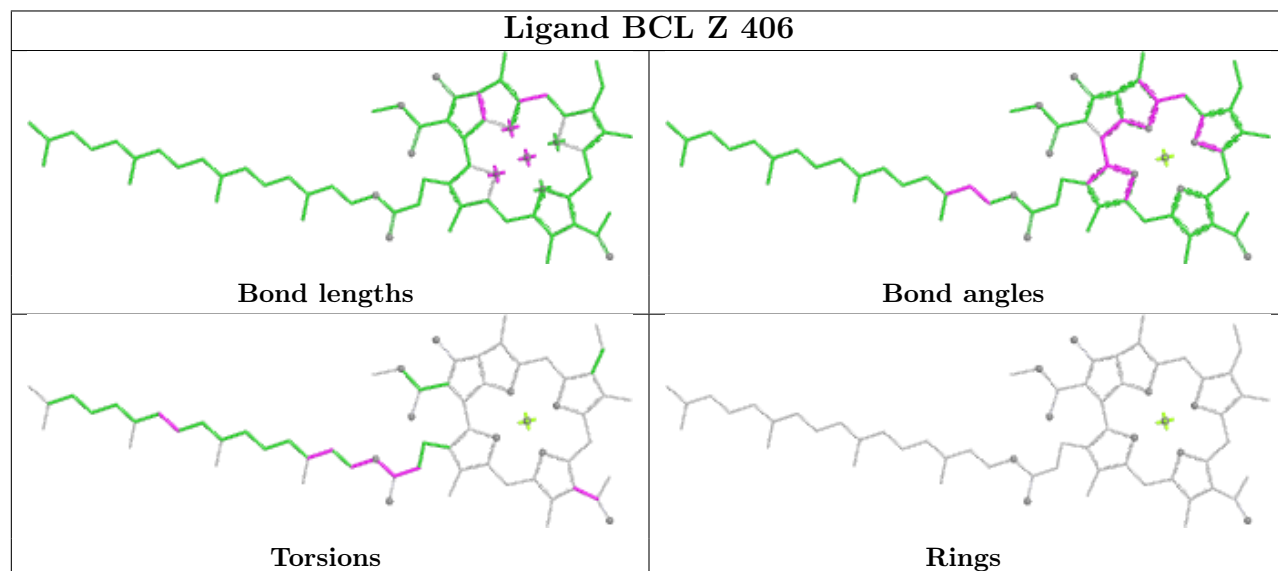
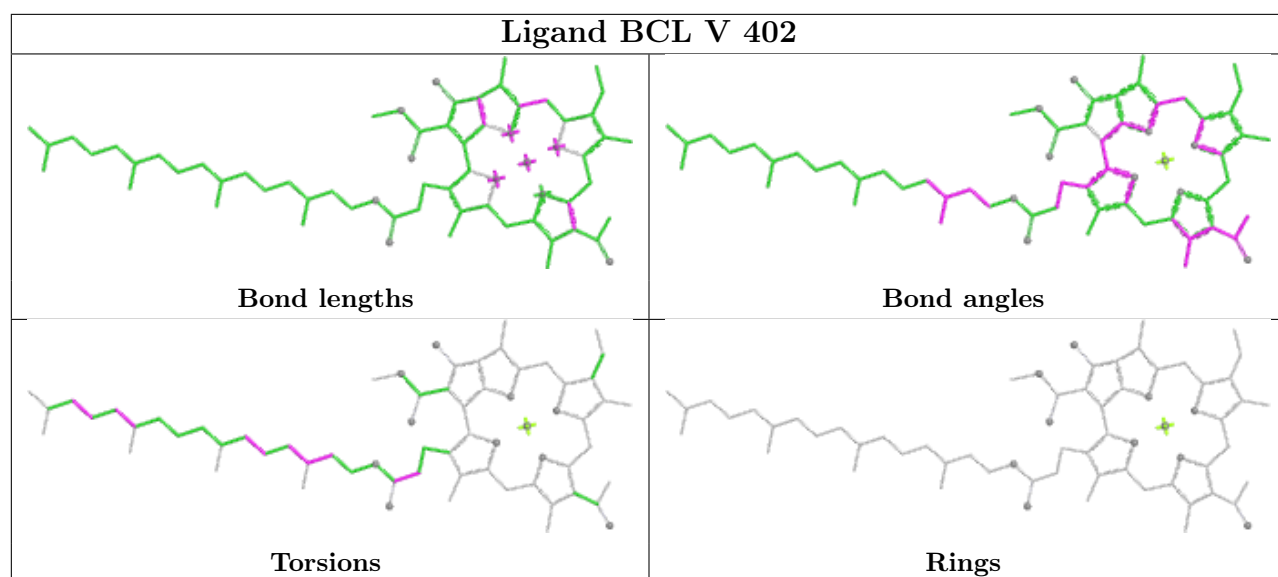


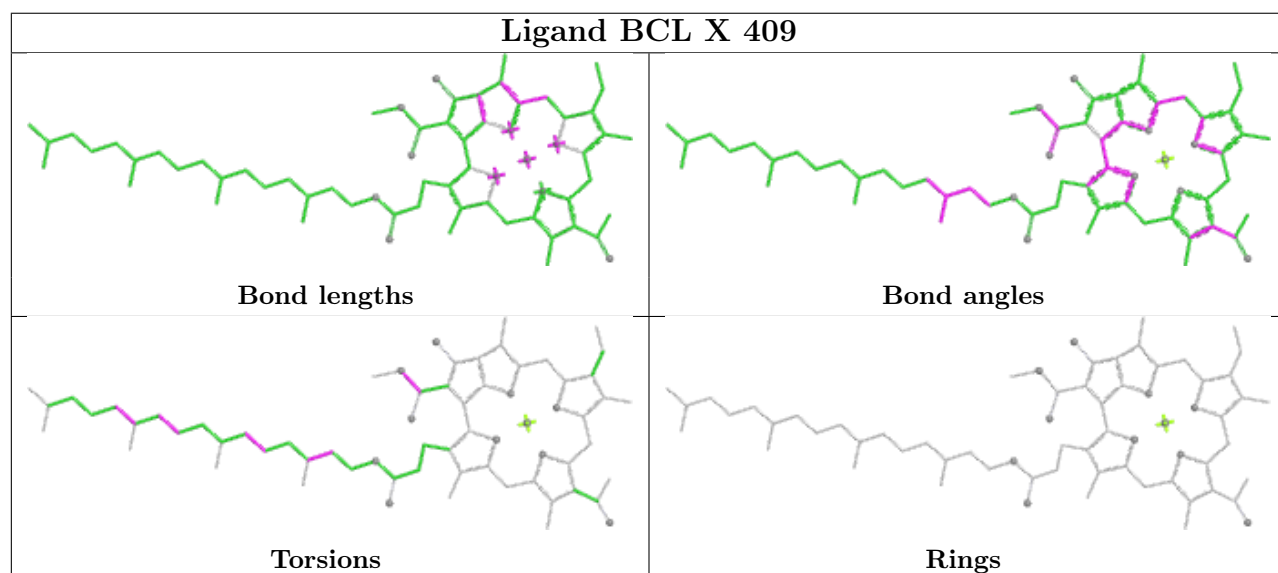
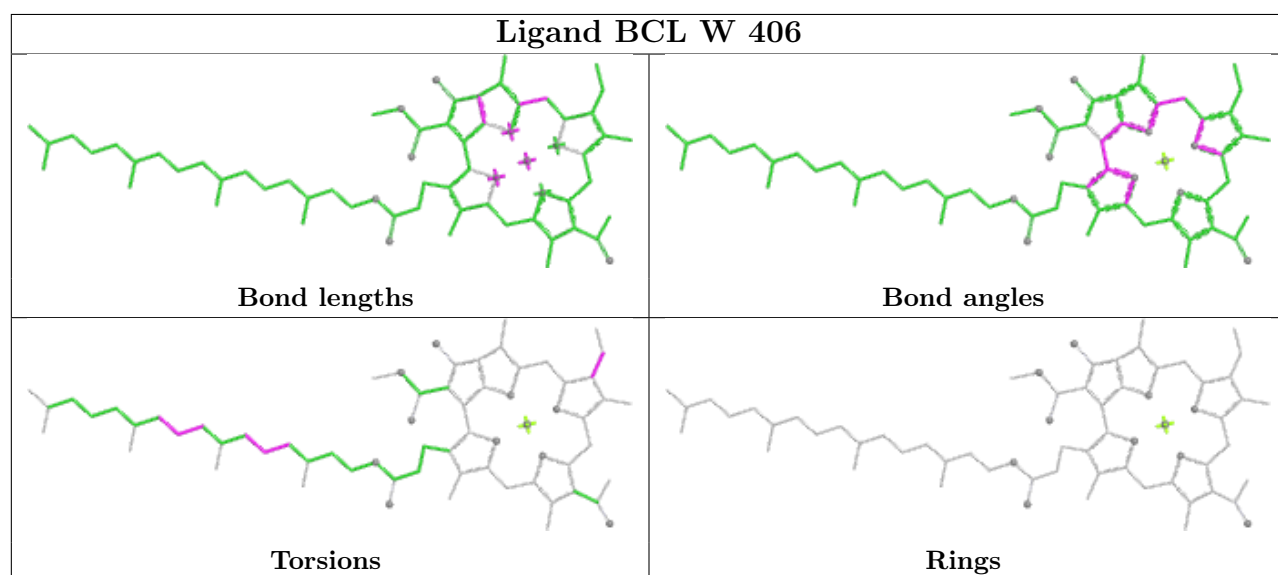
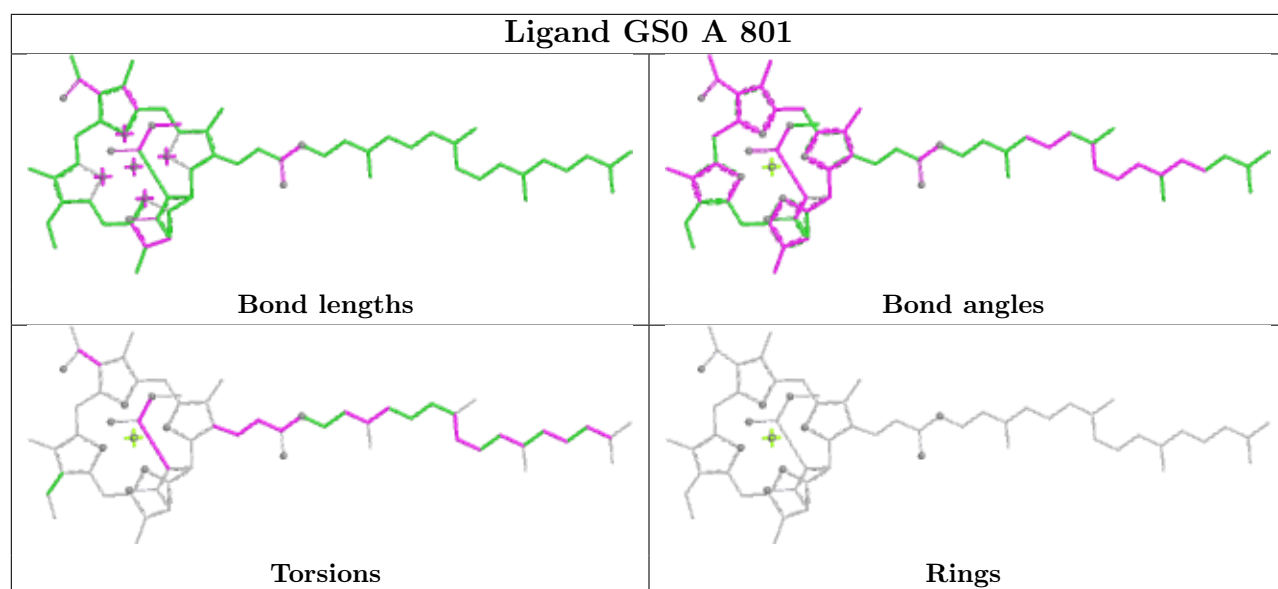


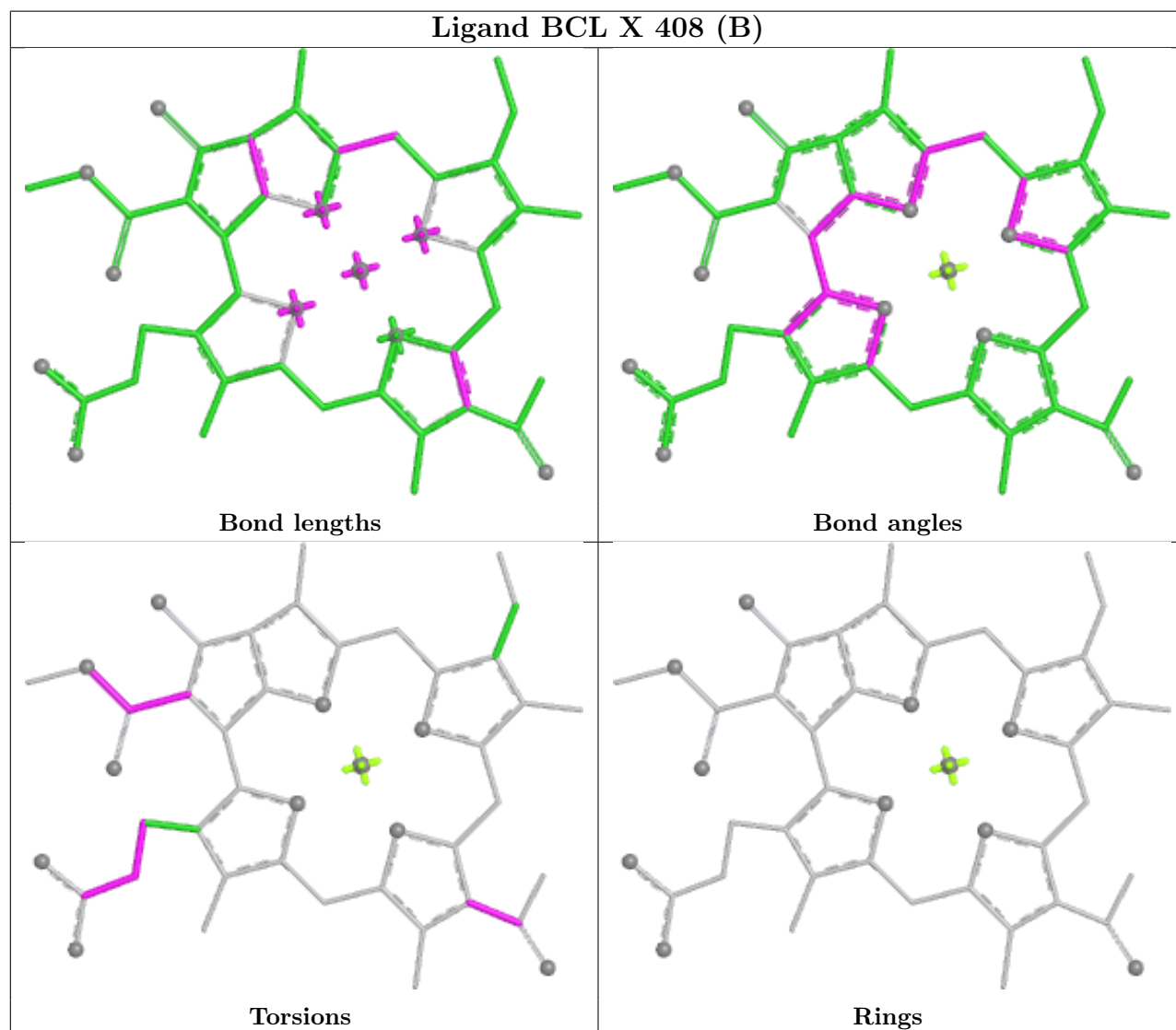
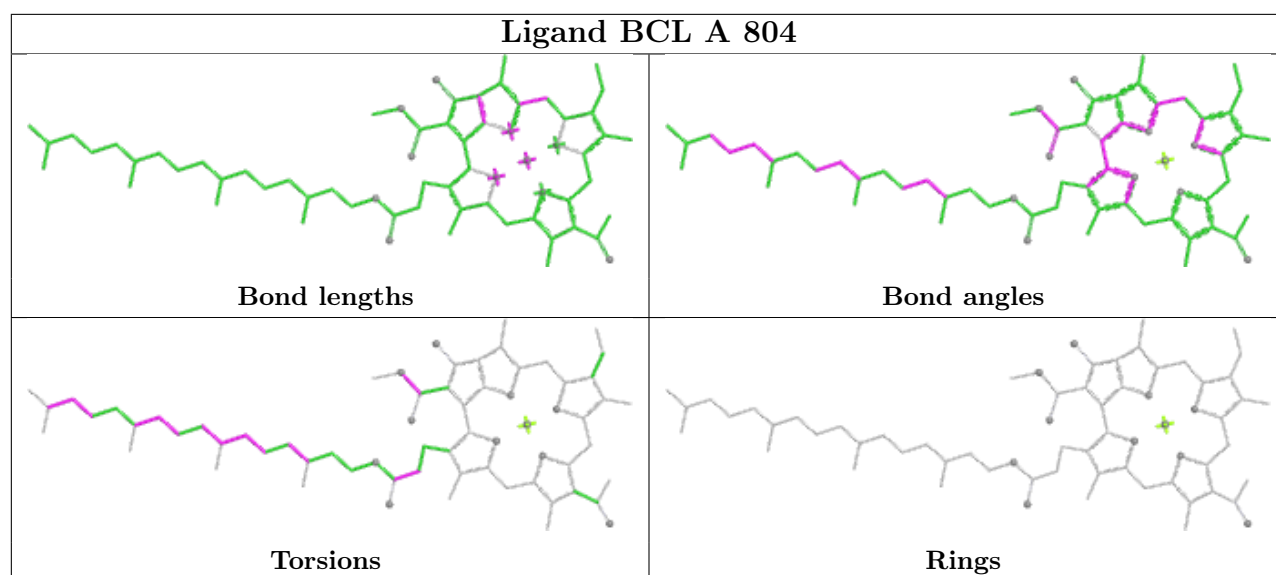


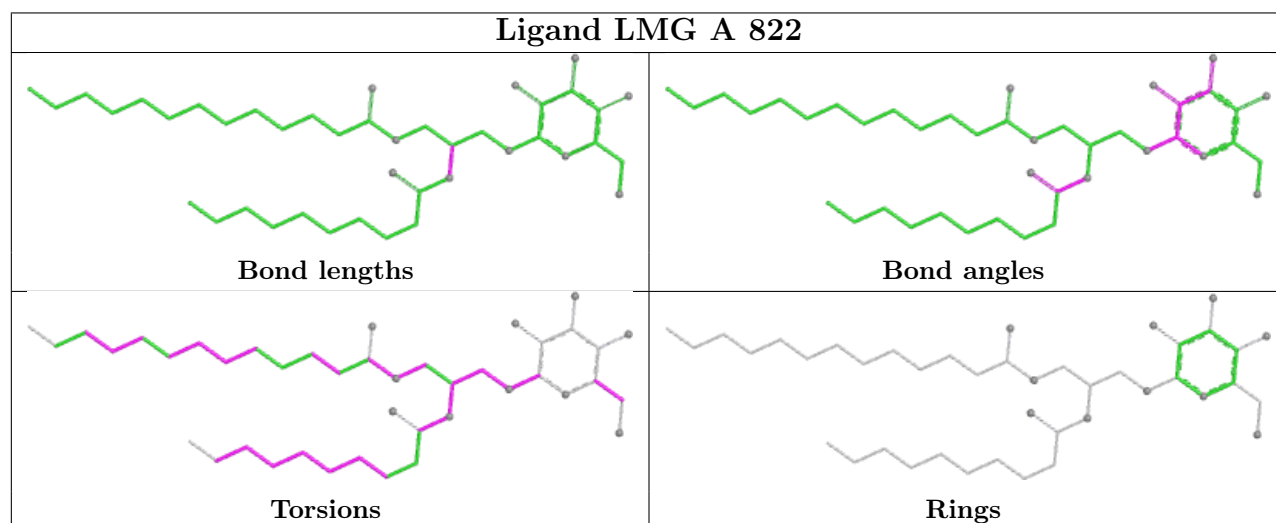
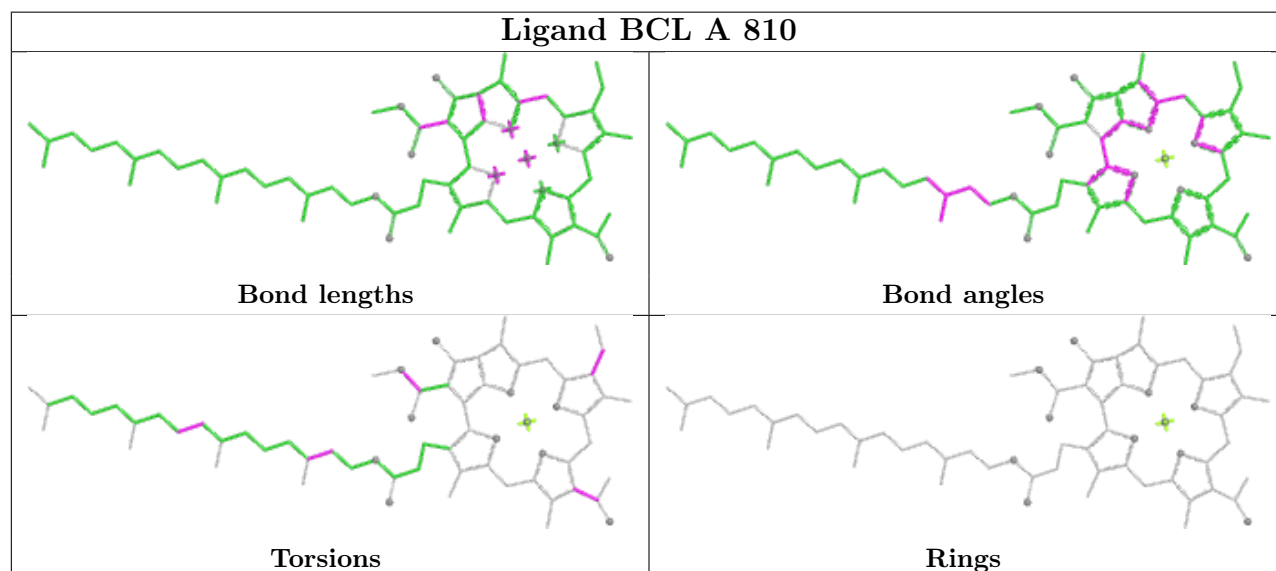
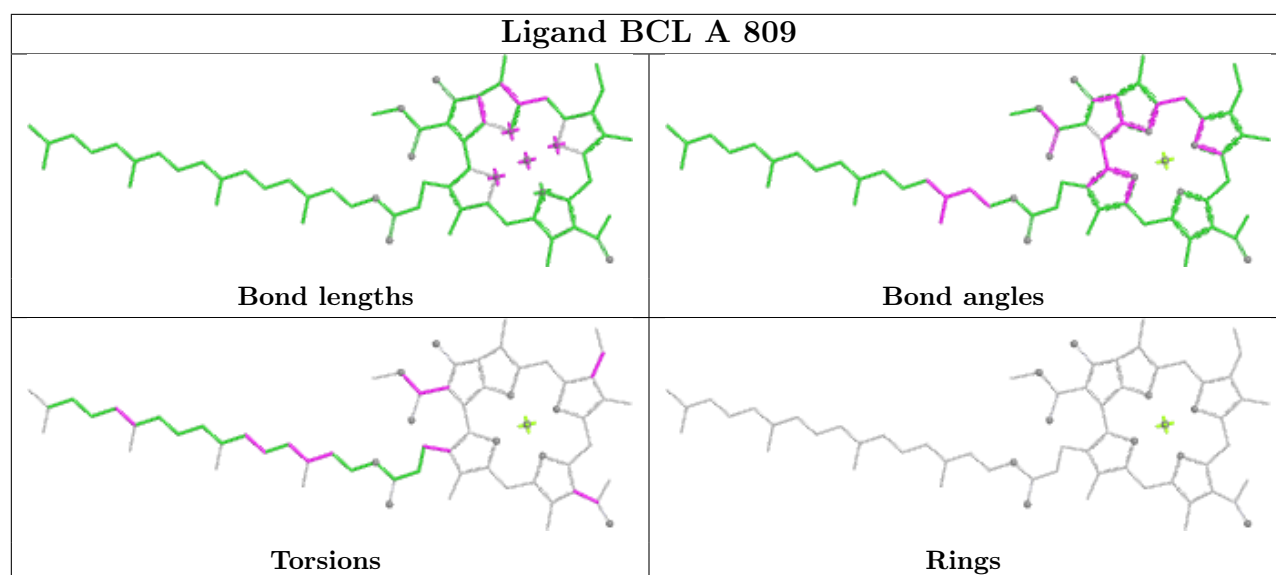




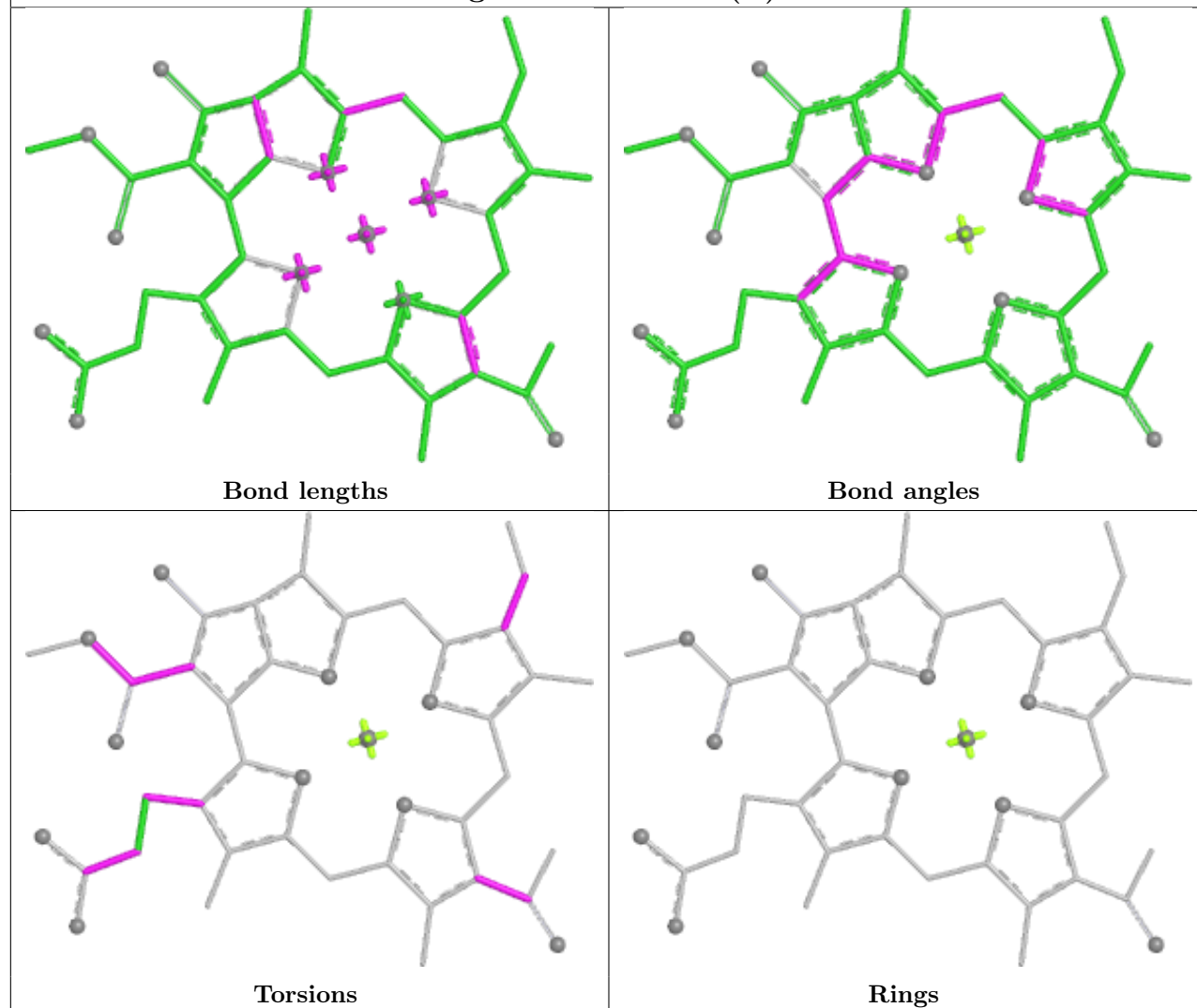




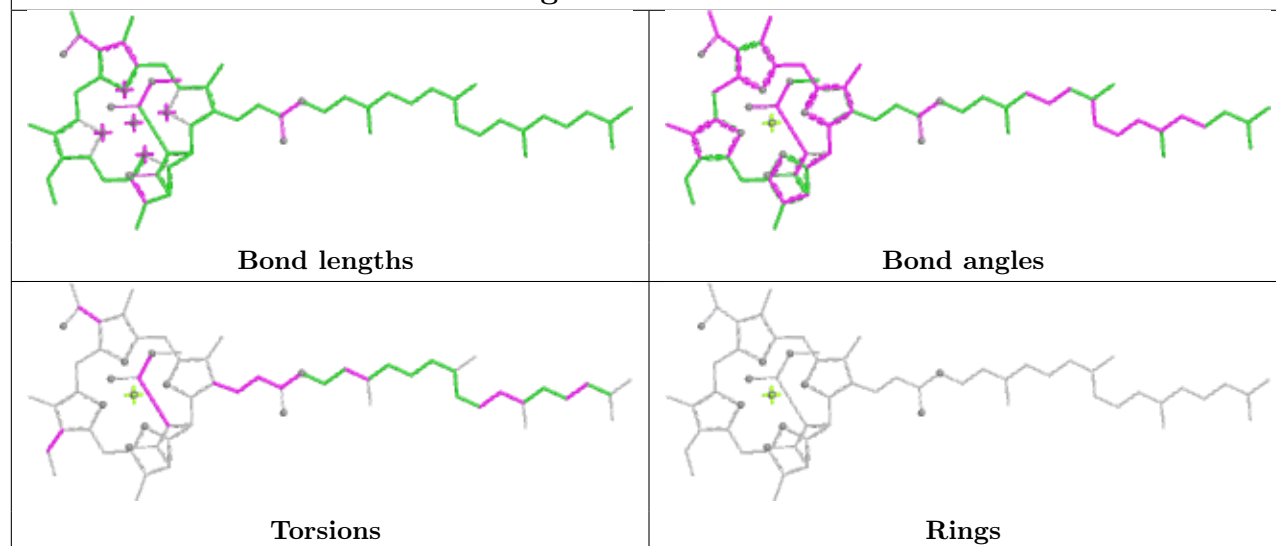


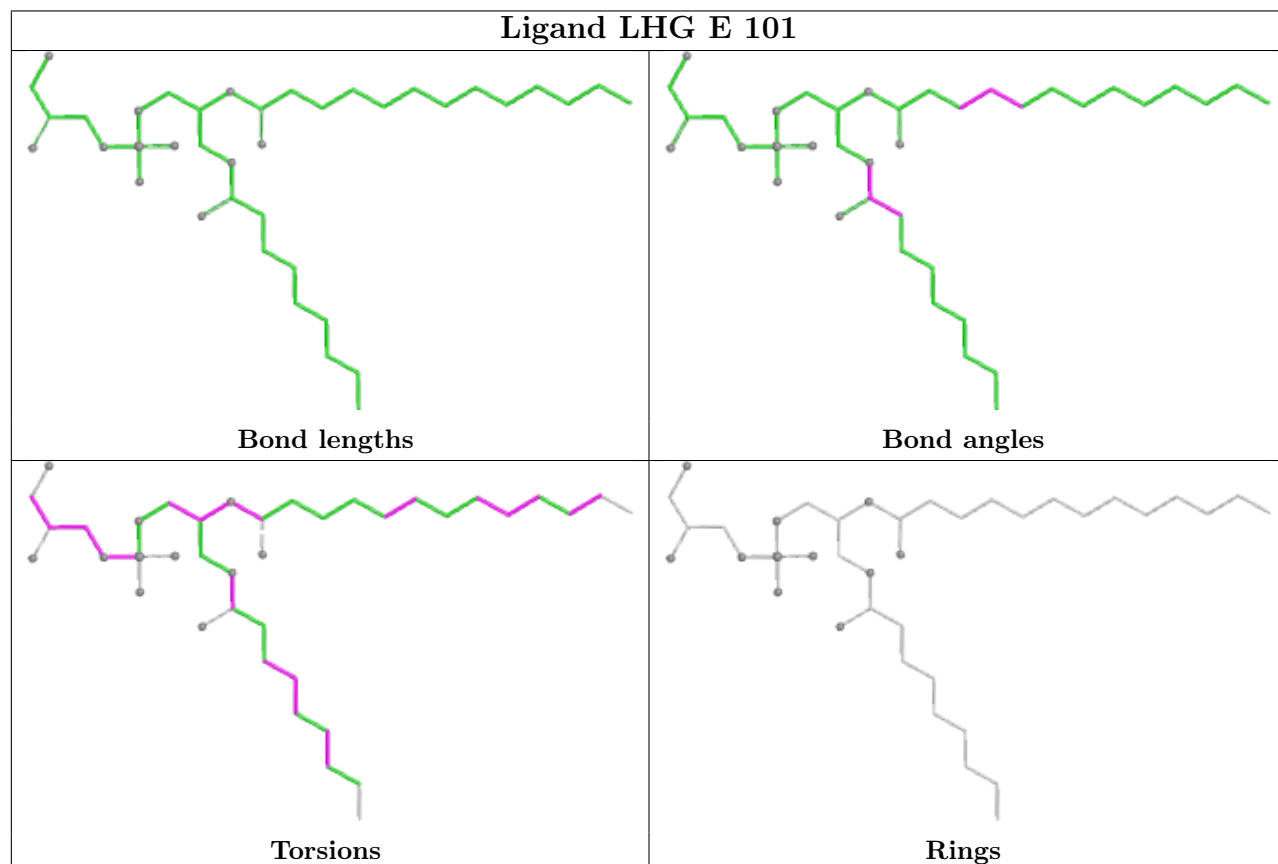
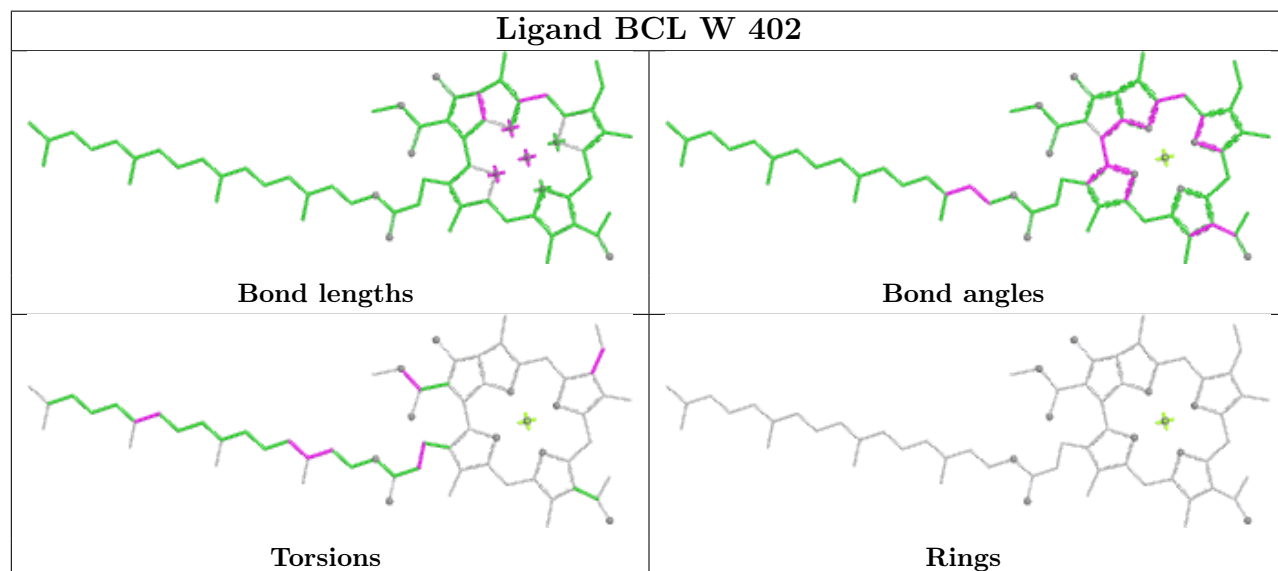
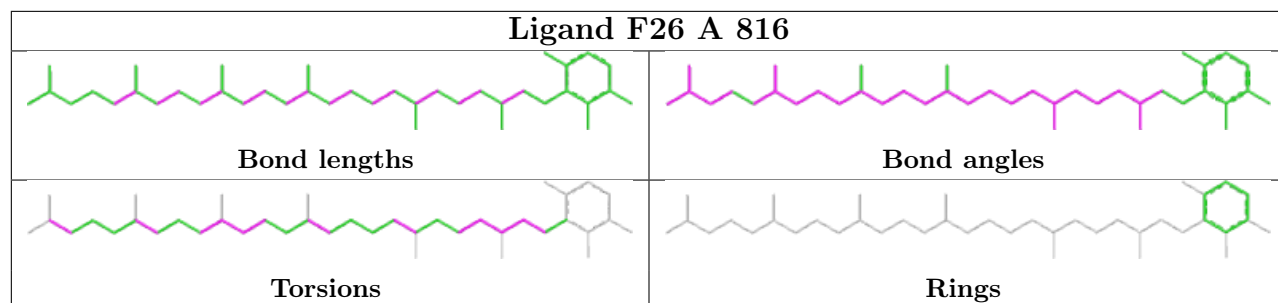


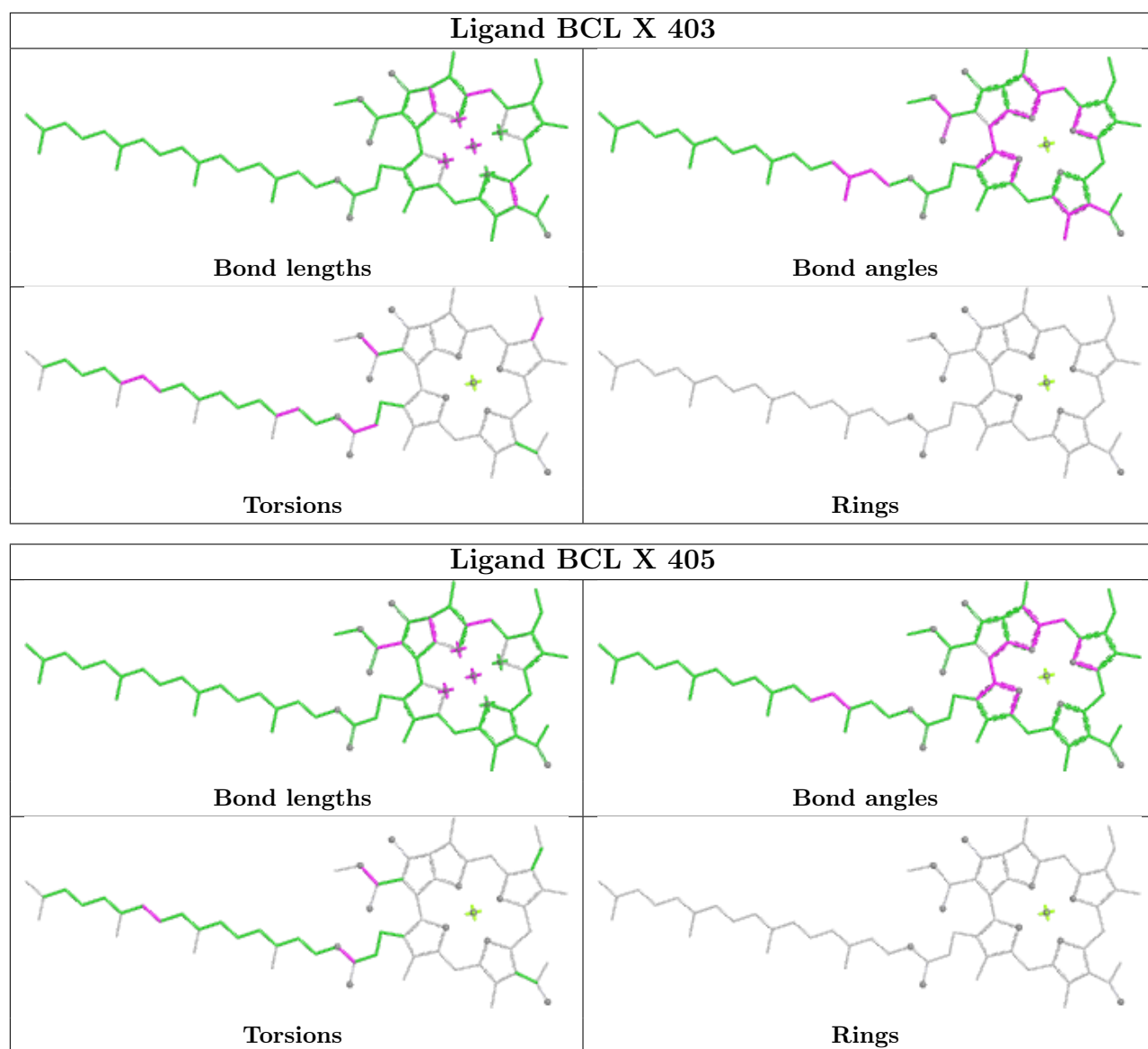
Ligand BCL V 409 (B)

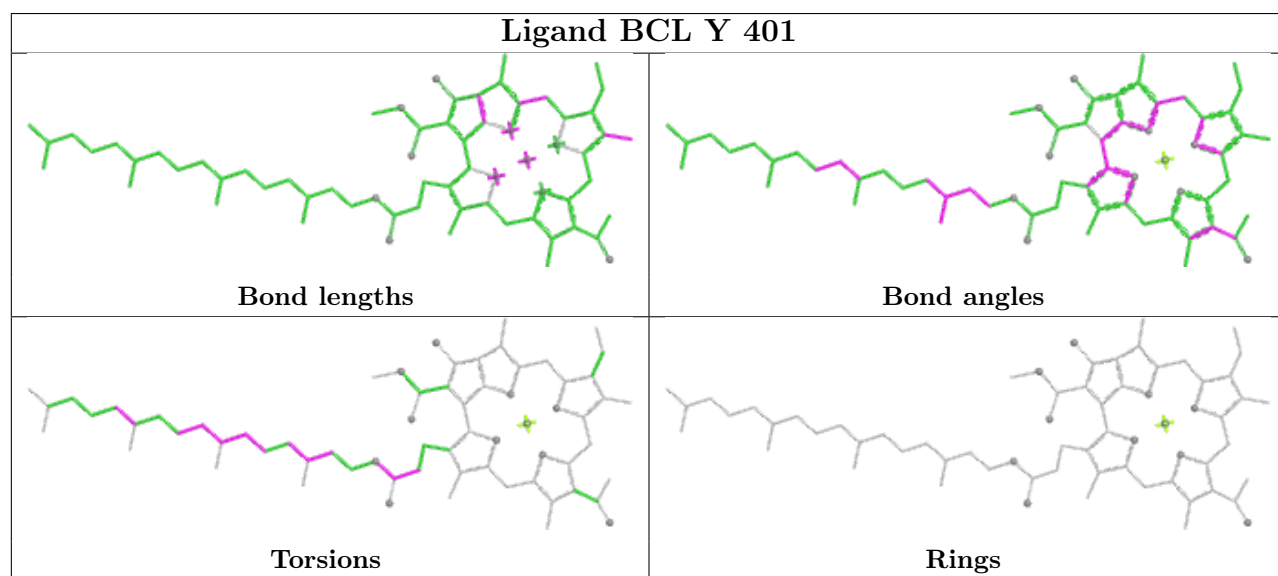
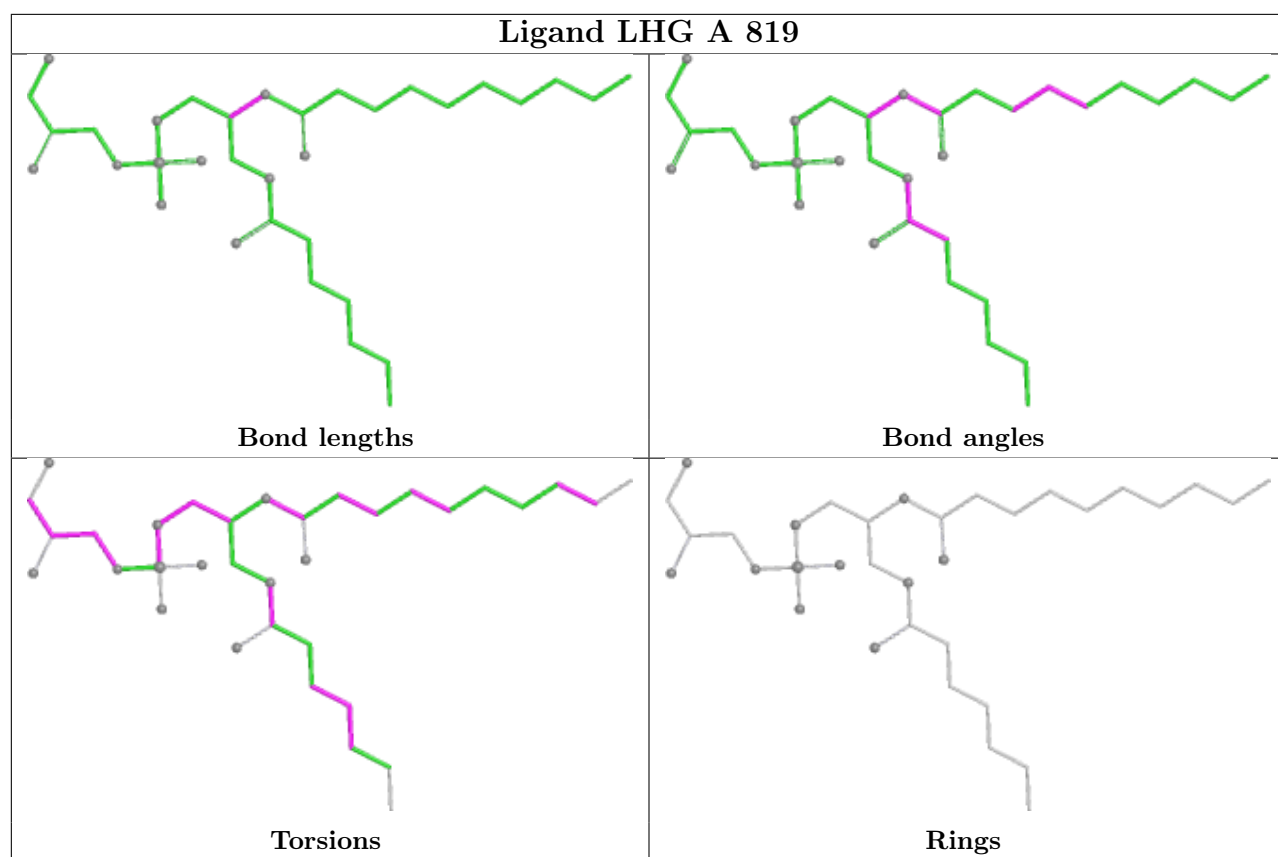


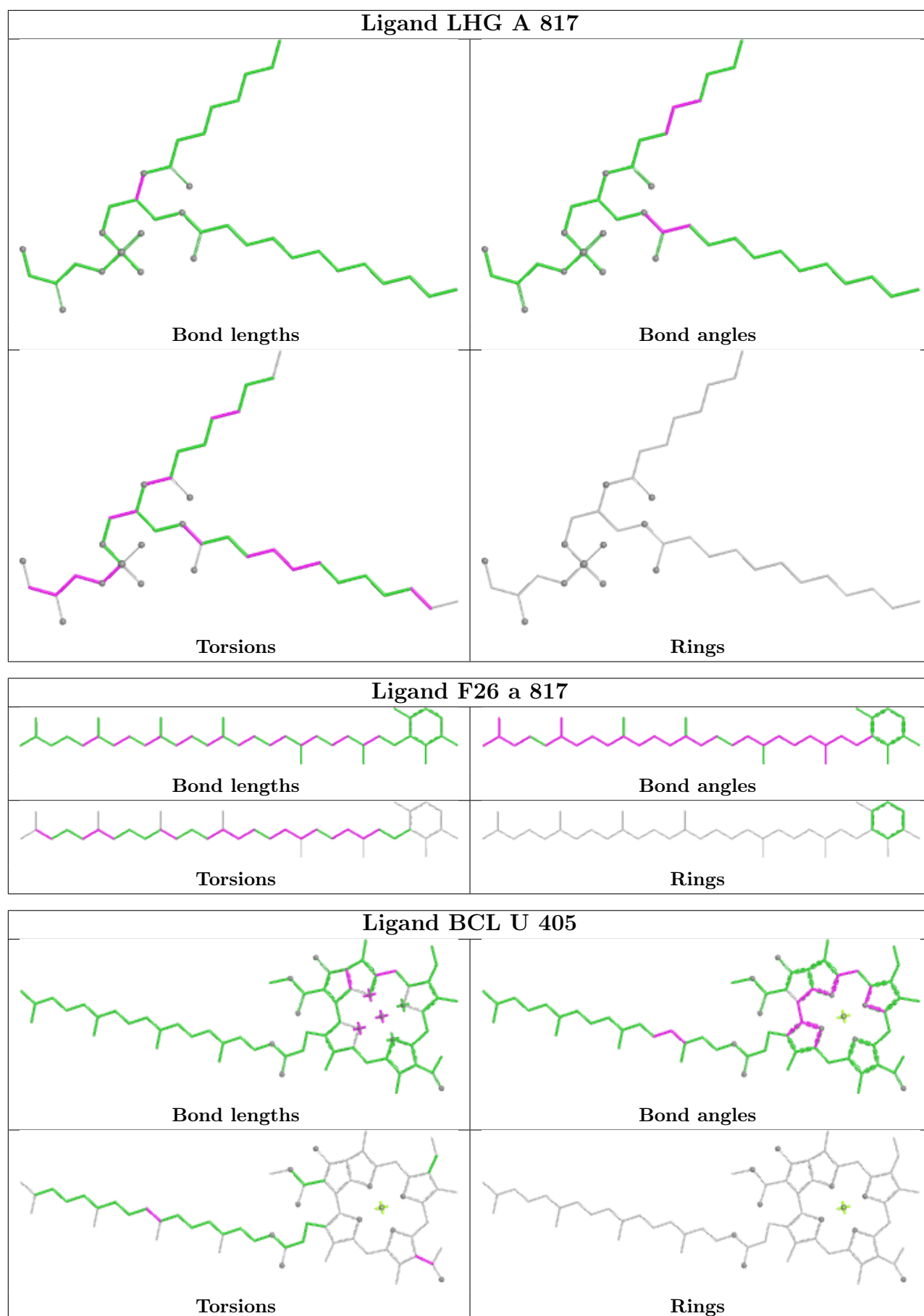
Ligand GS0 a 802

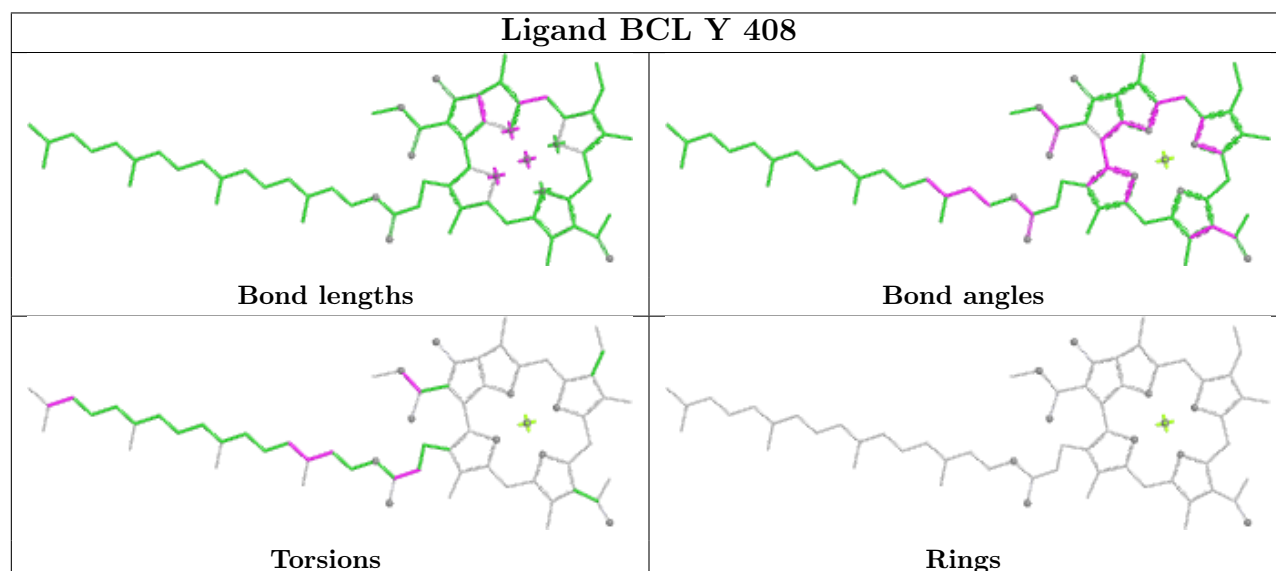
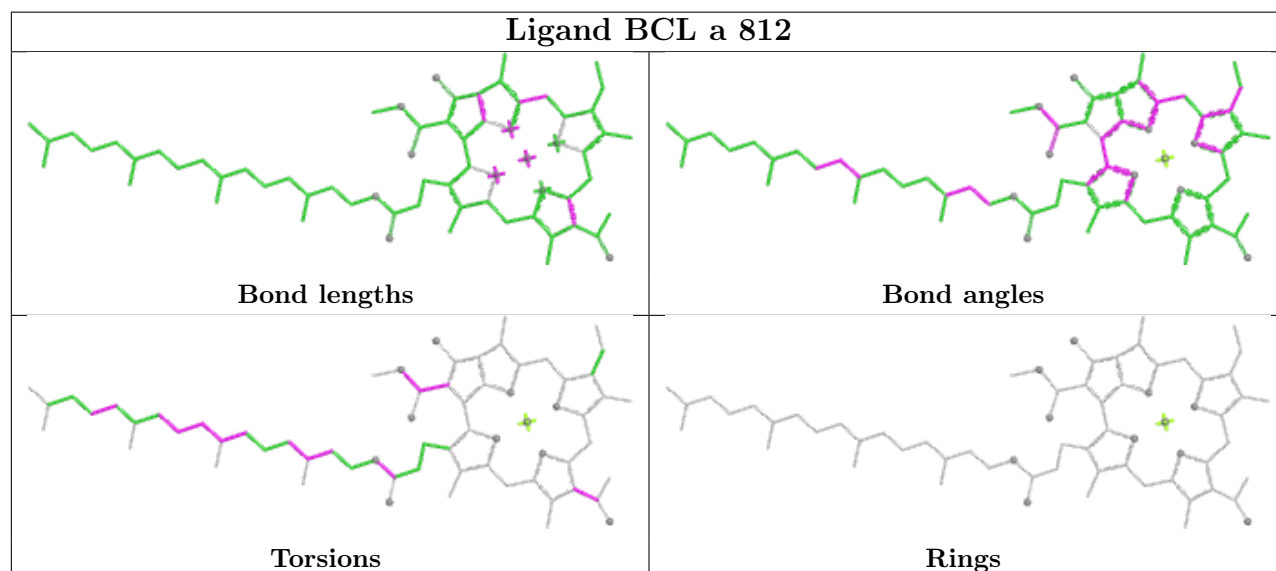
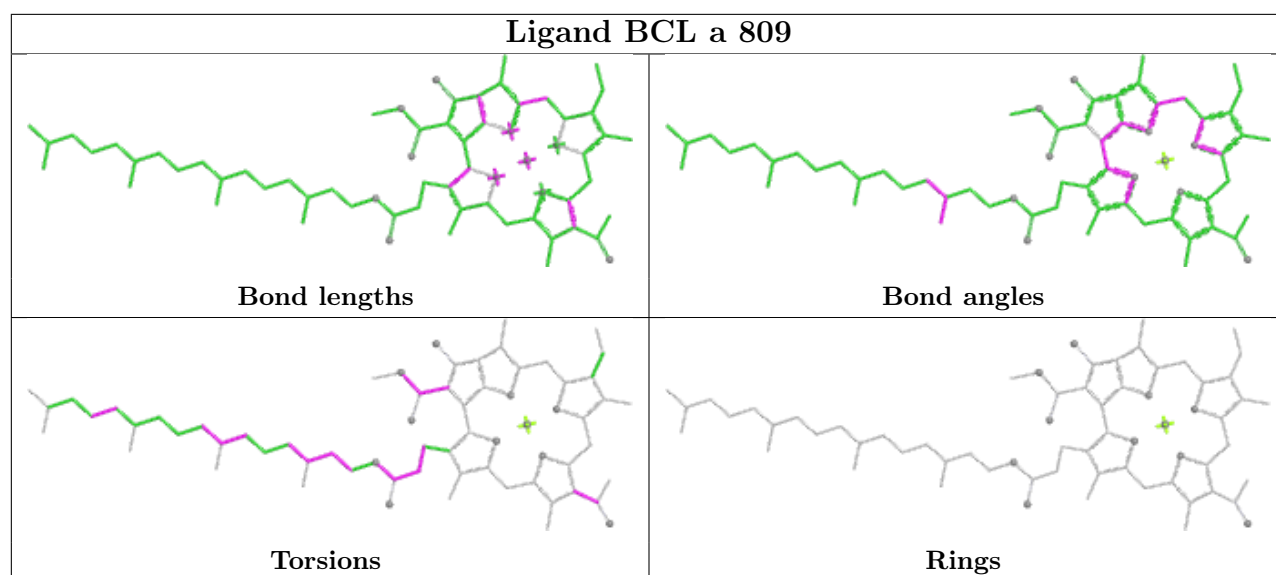


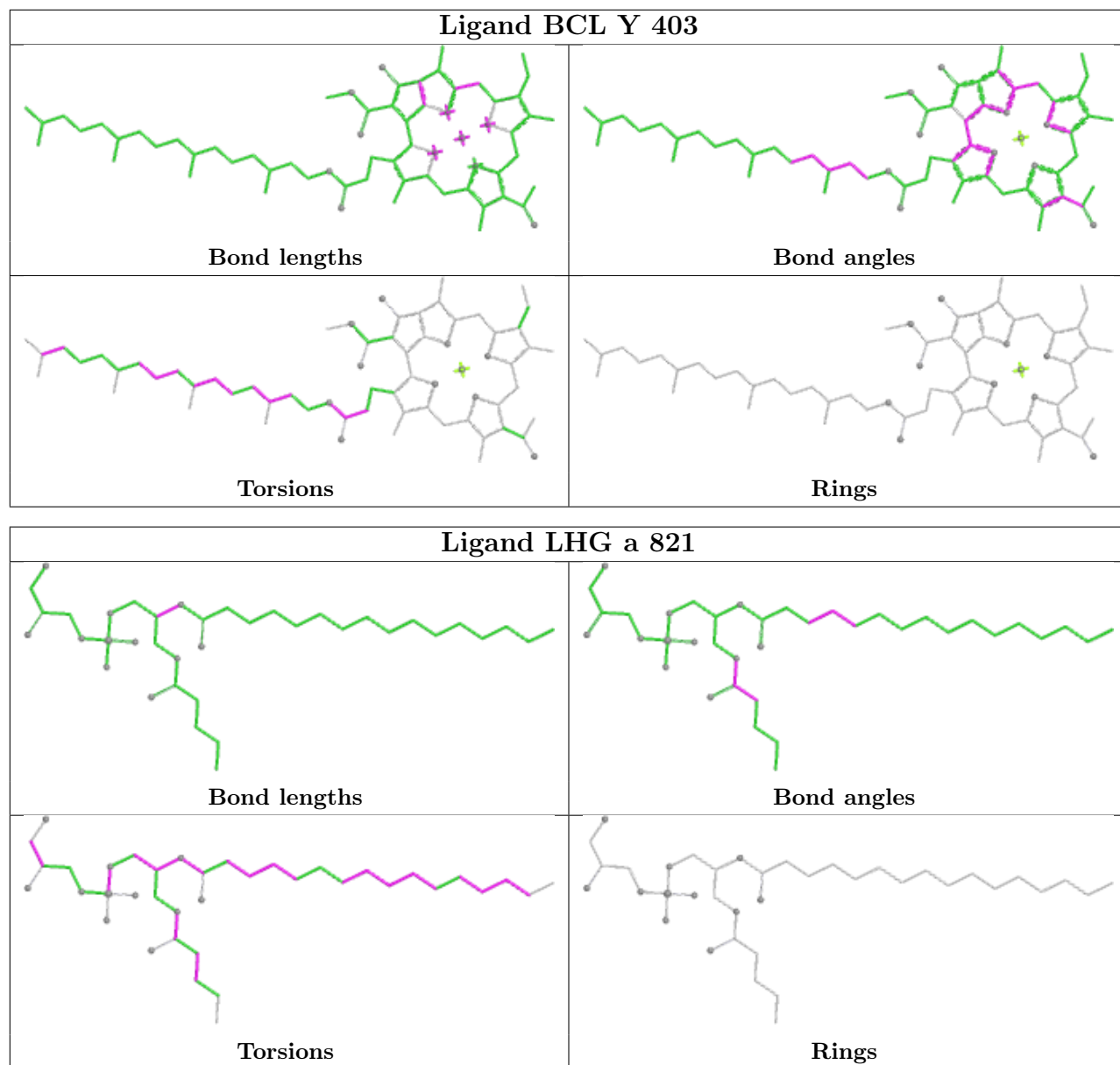


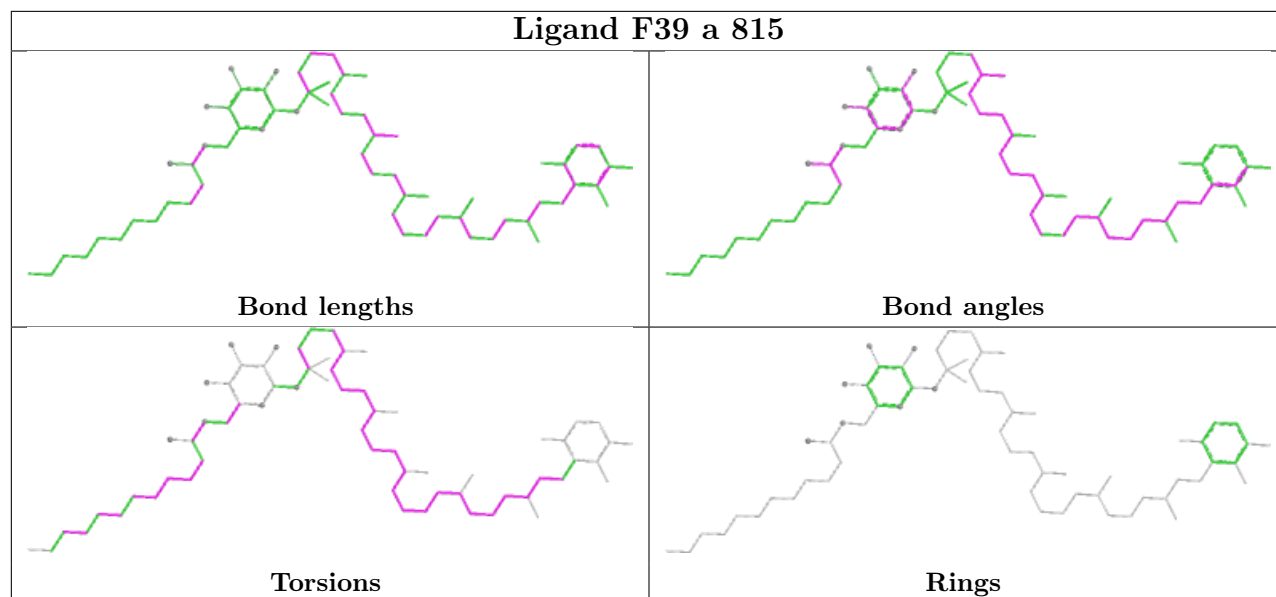
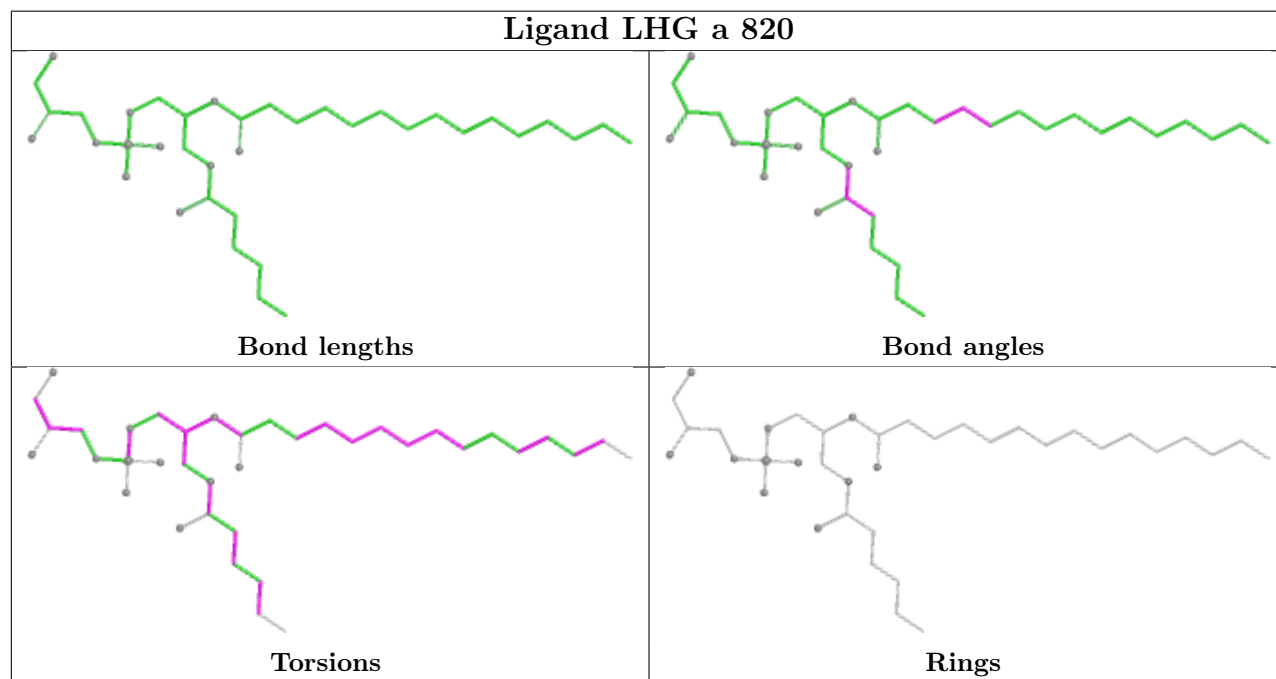


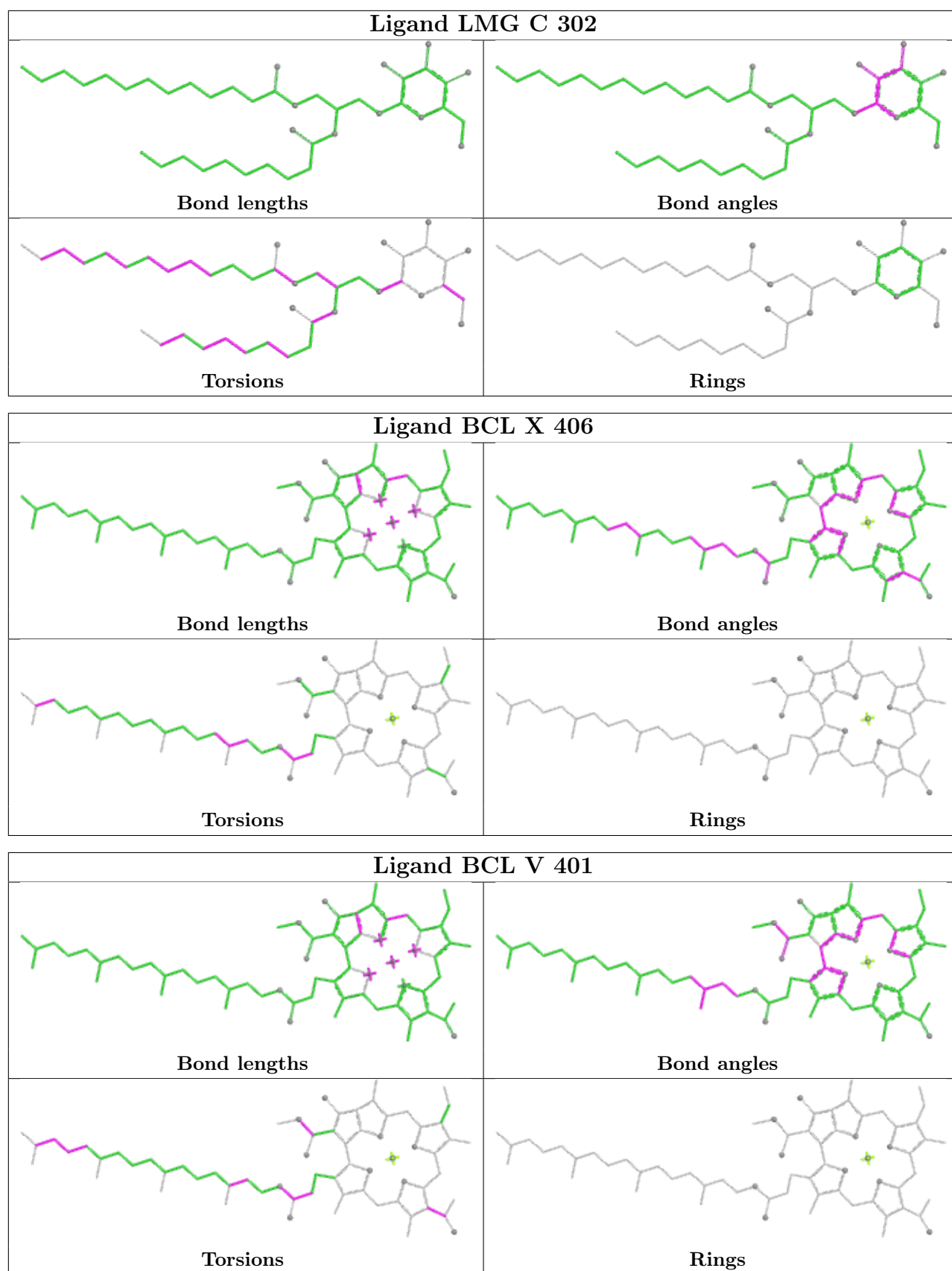


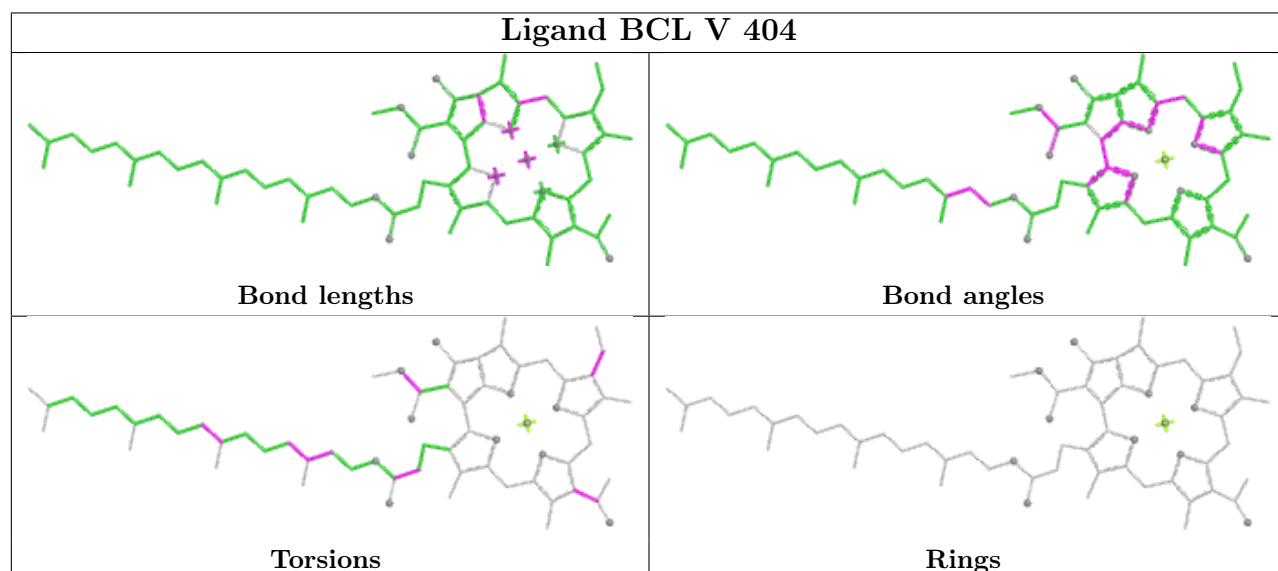
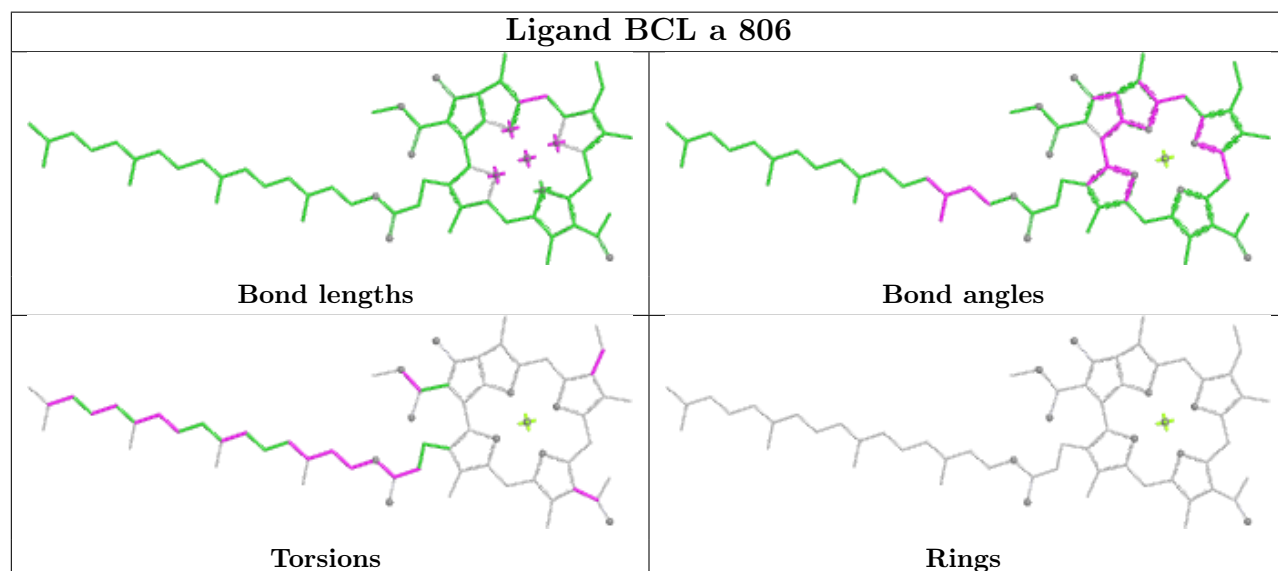
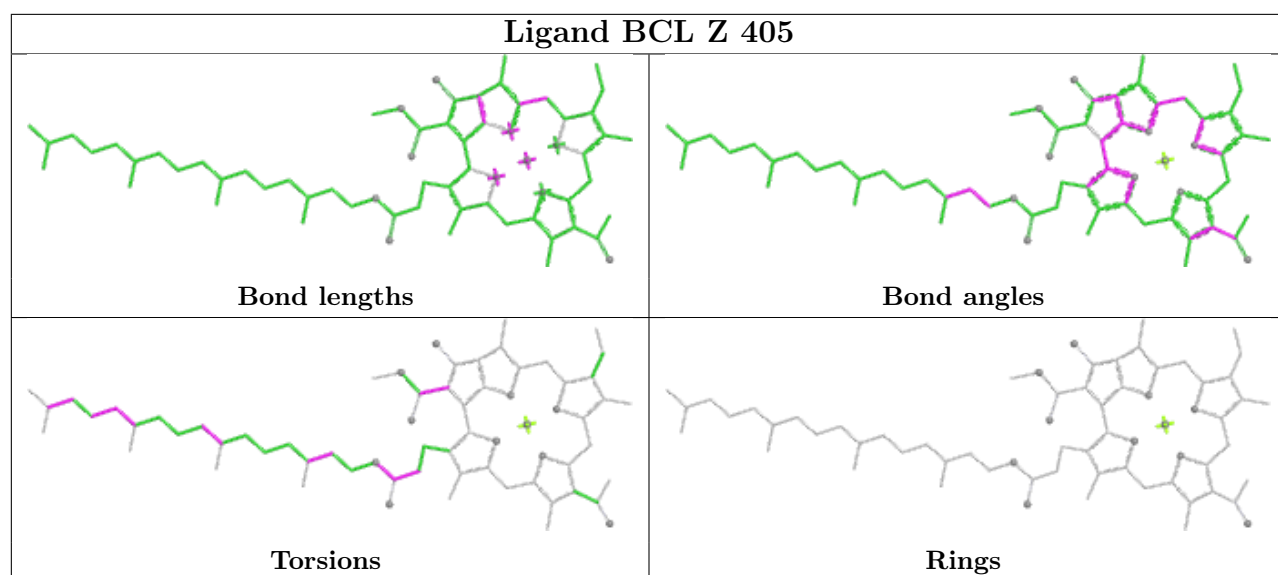




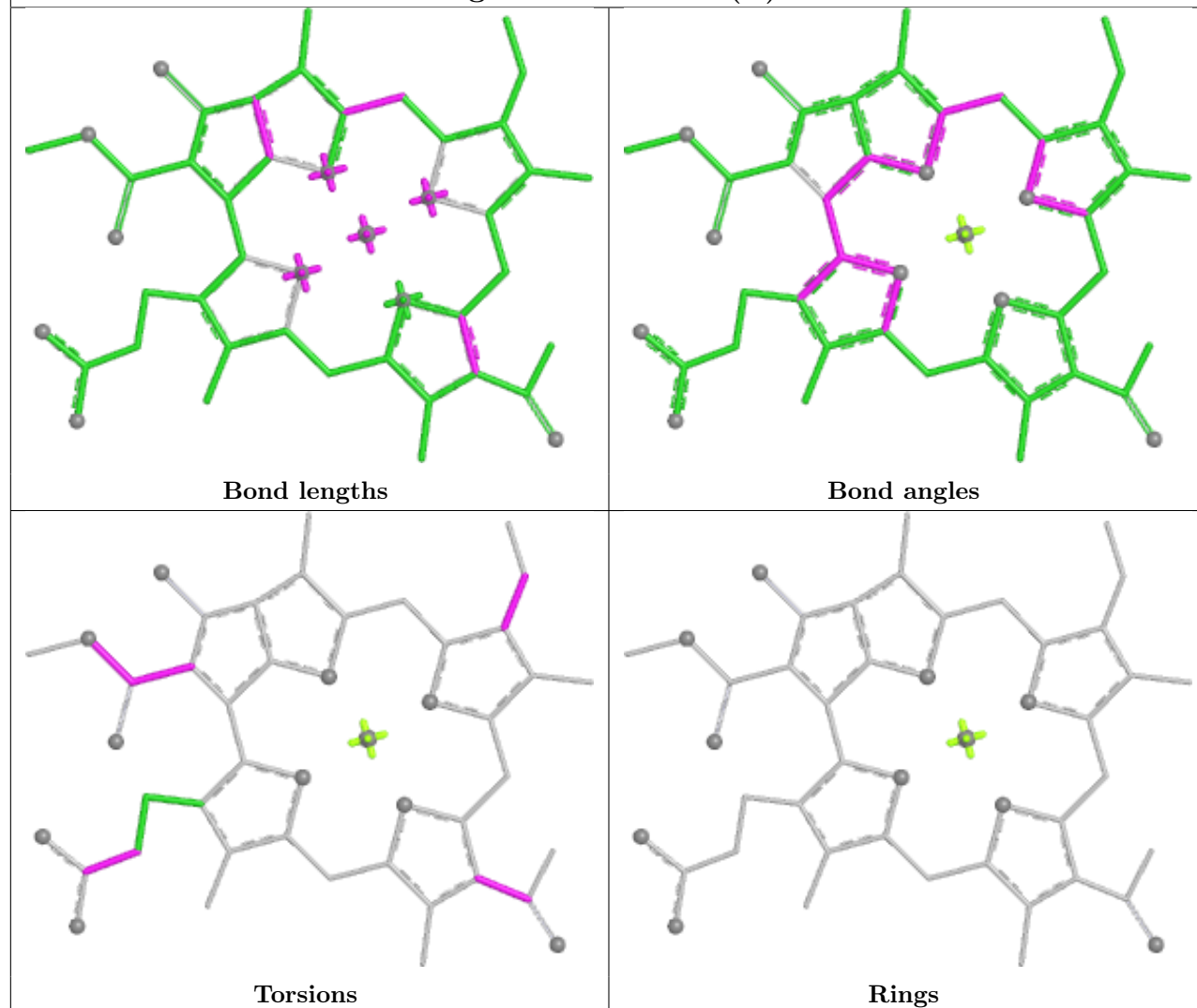


Ligand F39 a 815**Ligand LHG a 820**

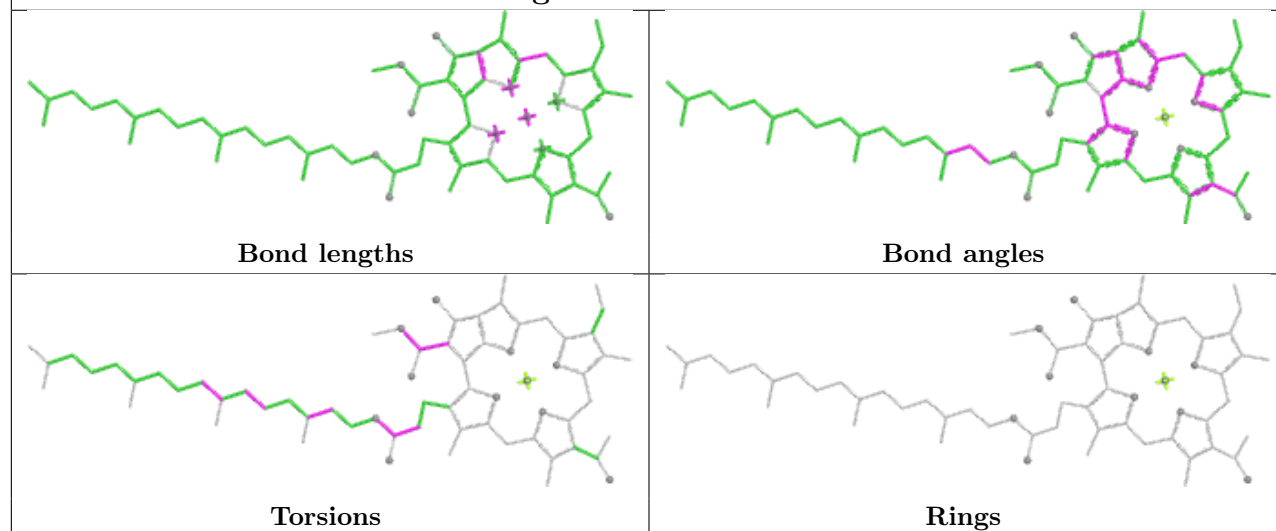


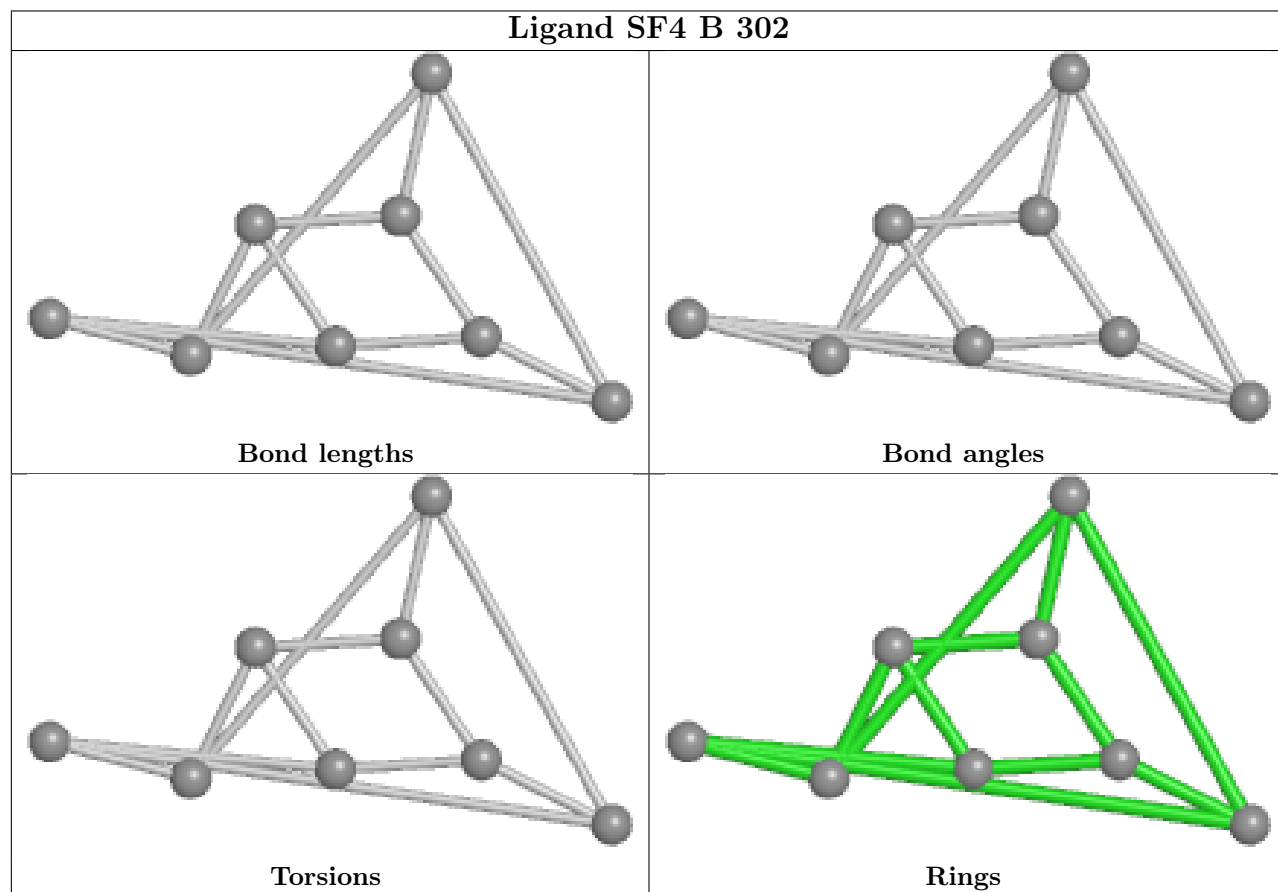
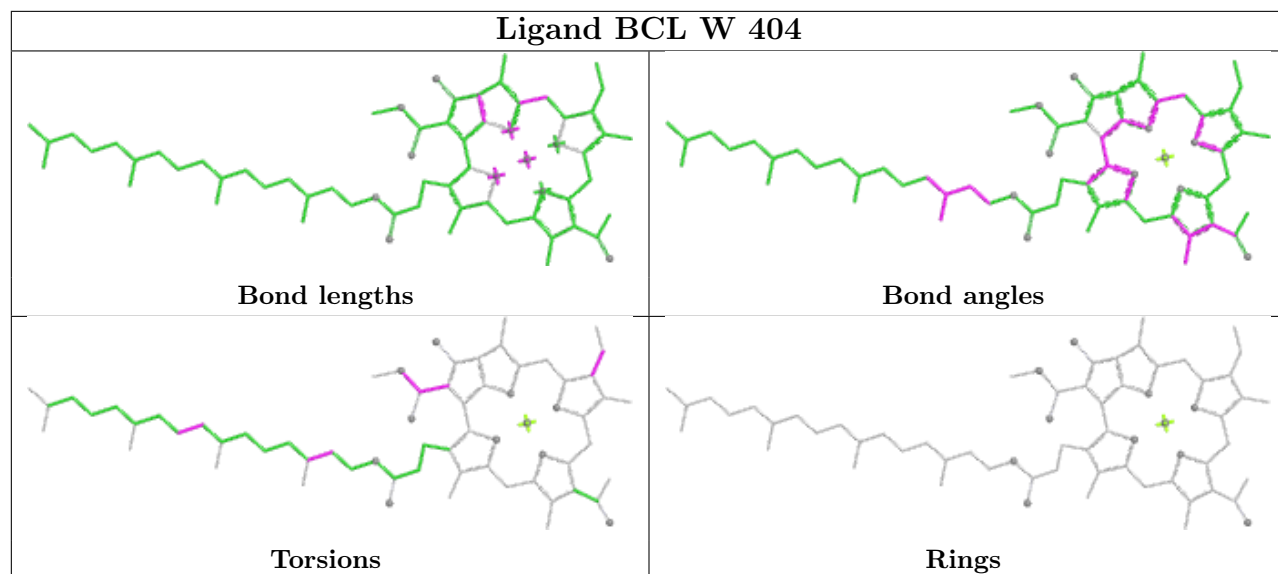


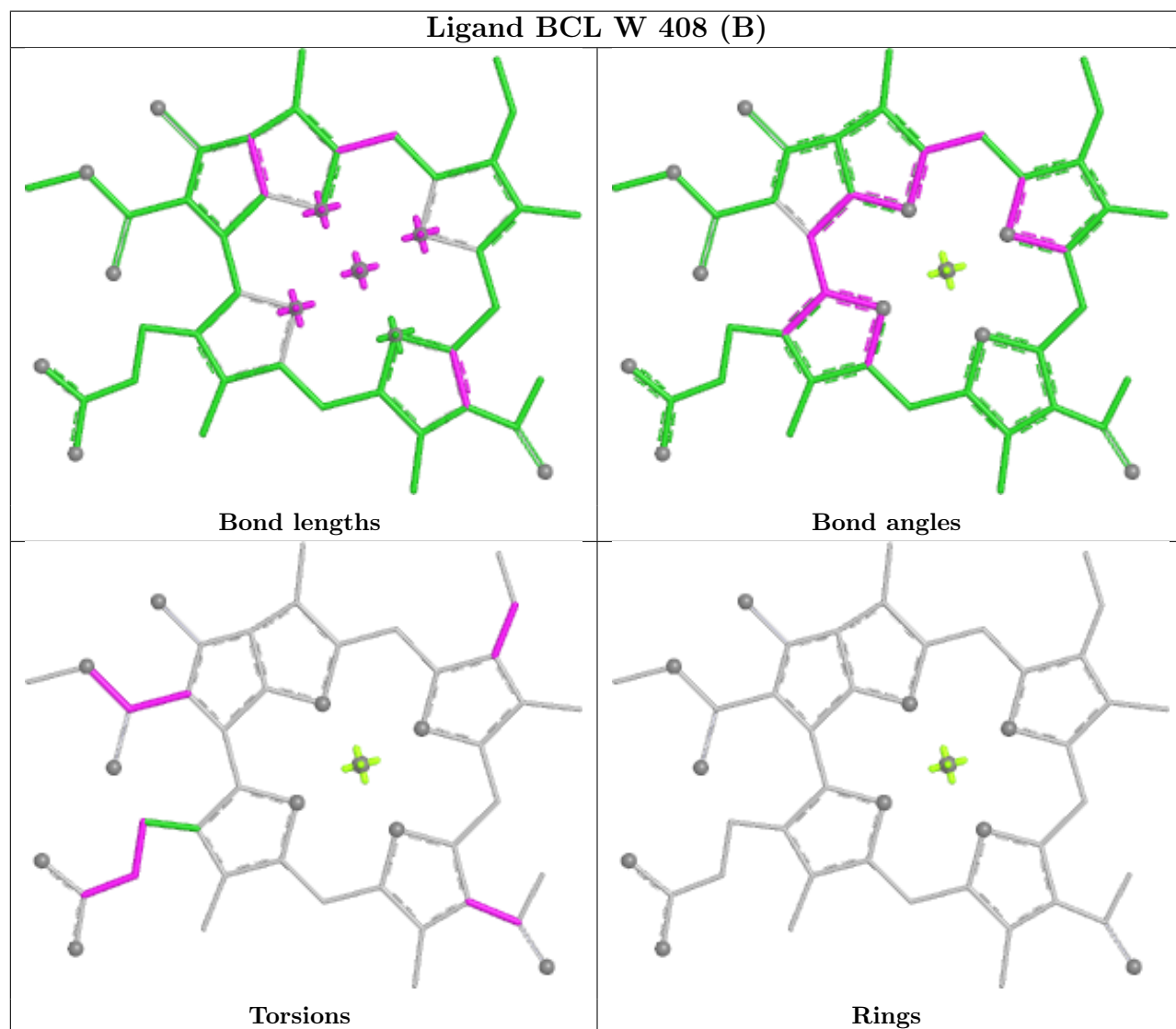
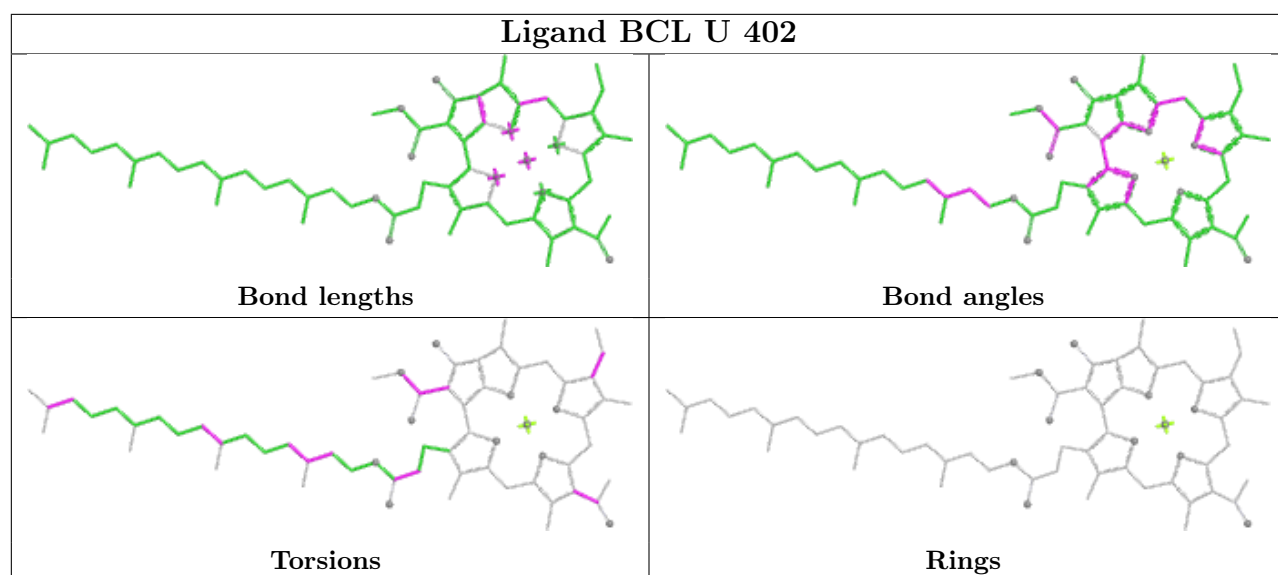
Ligand BCL U 407 (B)

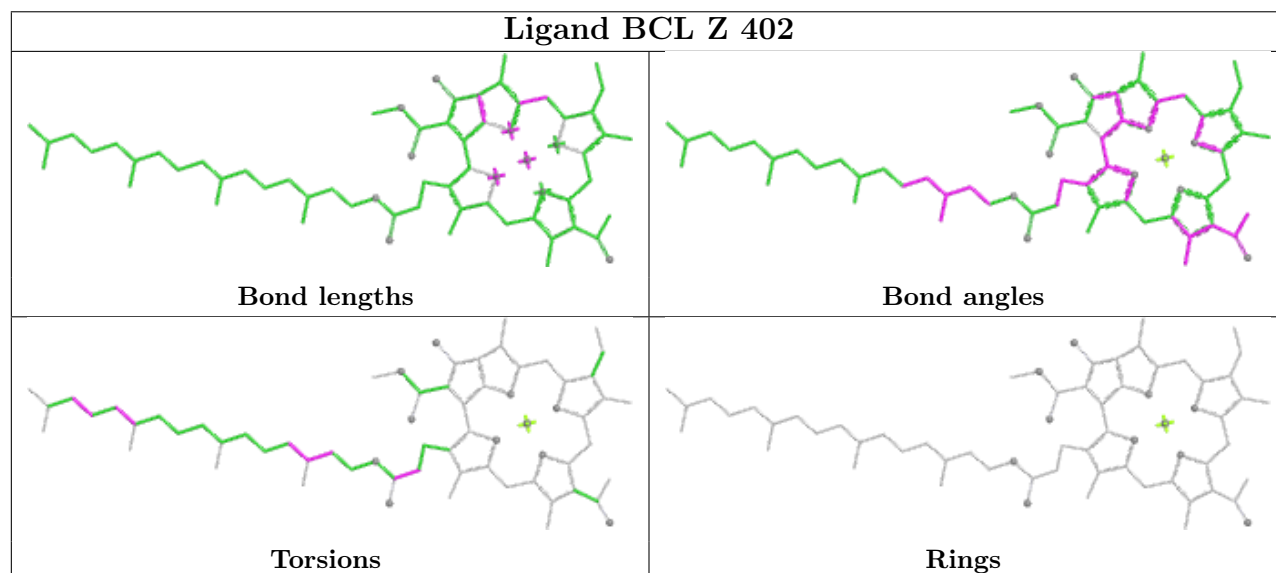
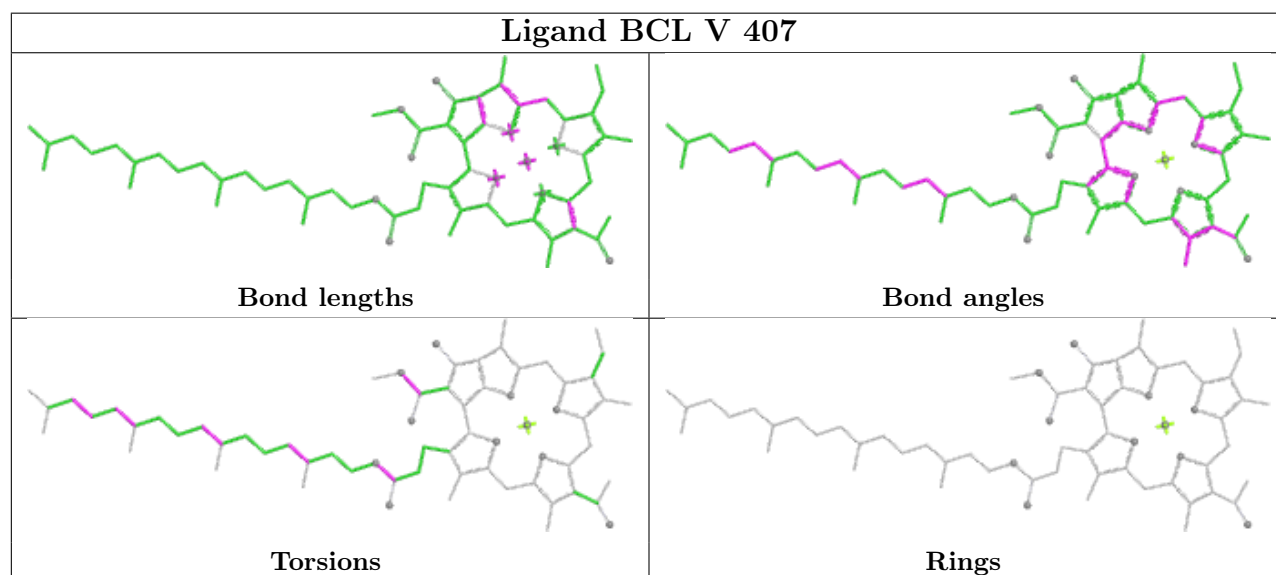
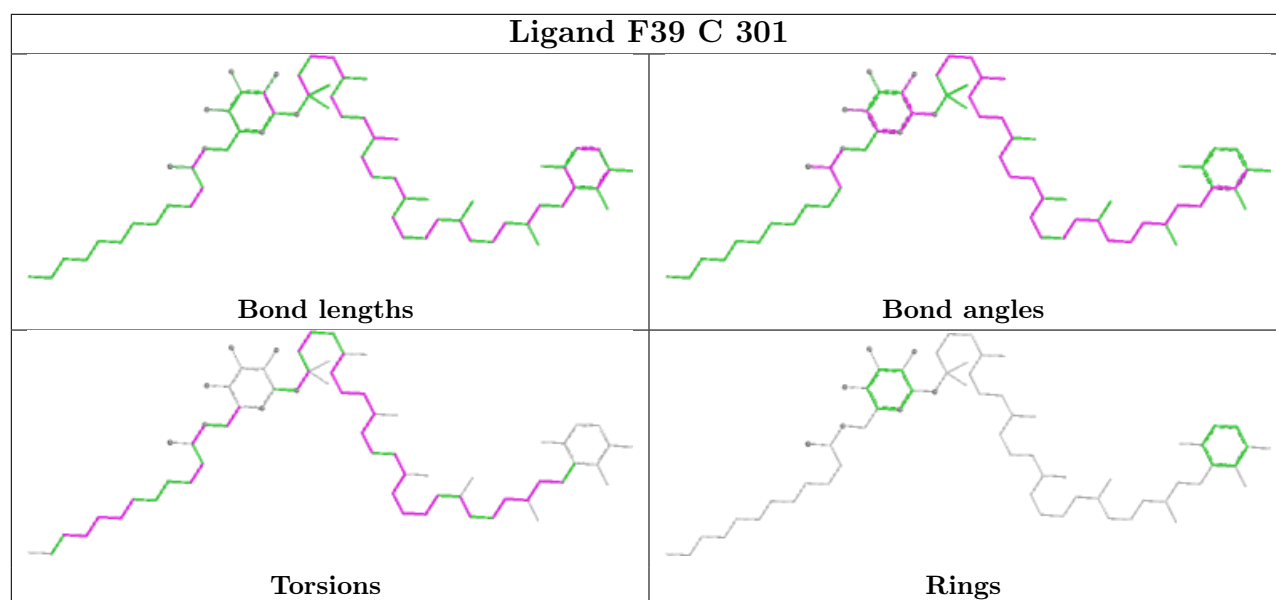


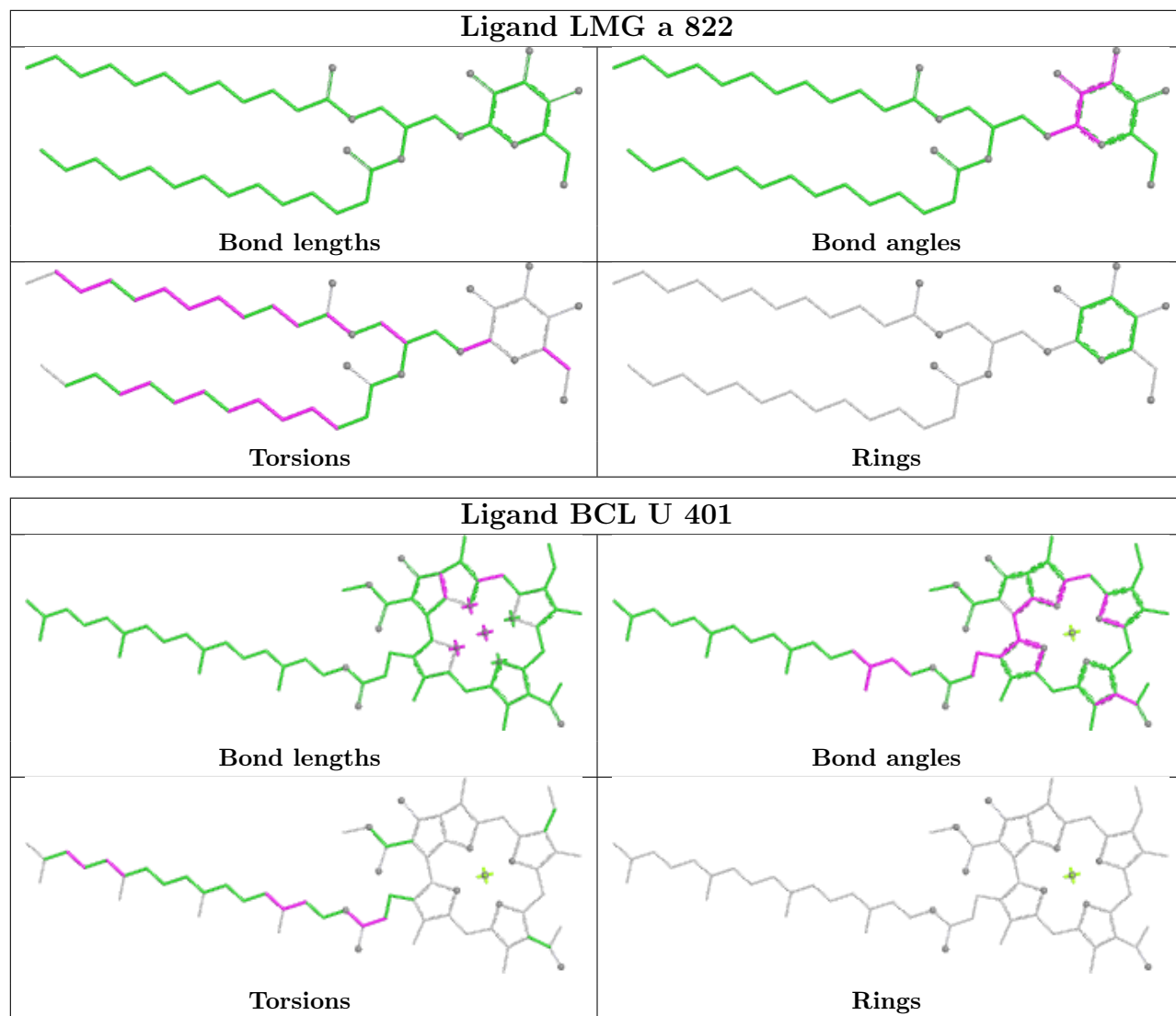
Ligand BCL Y 406

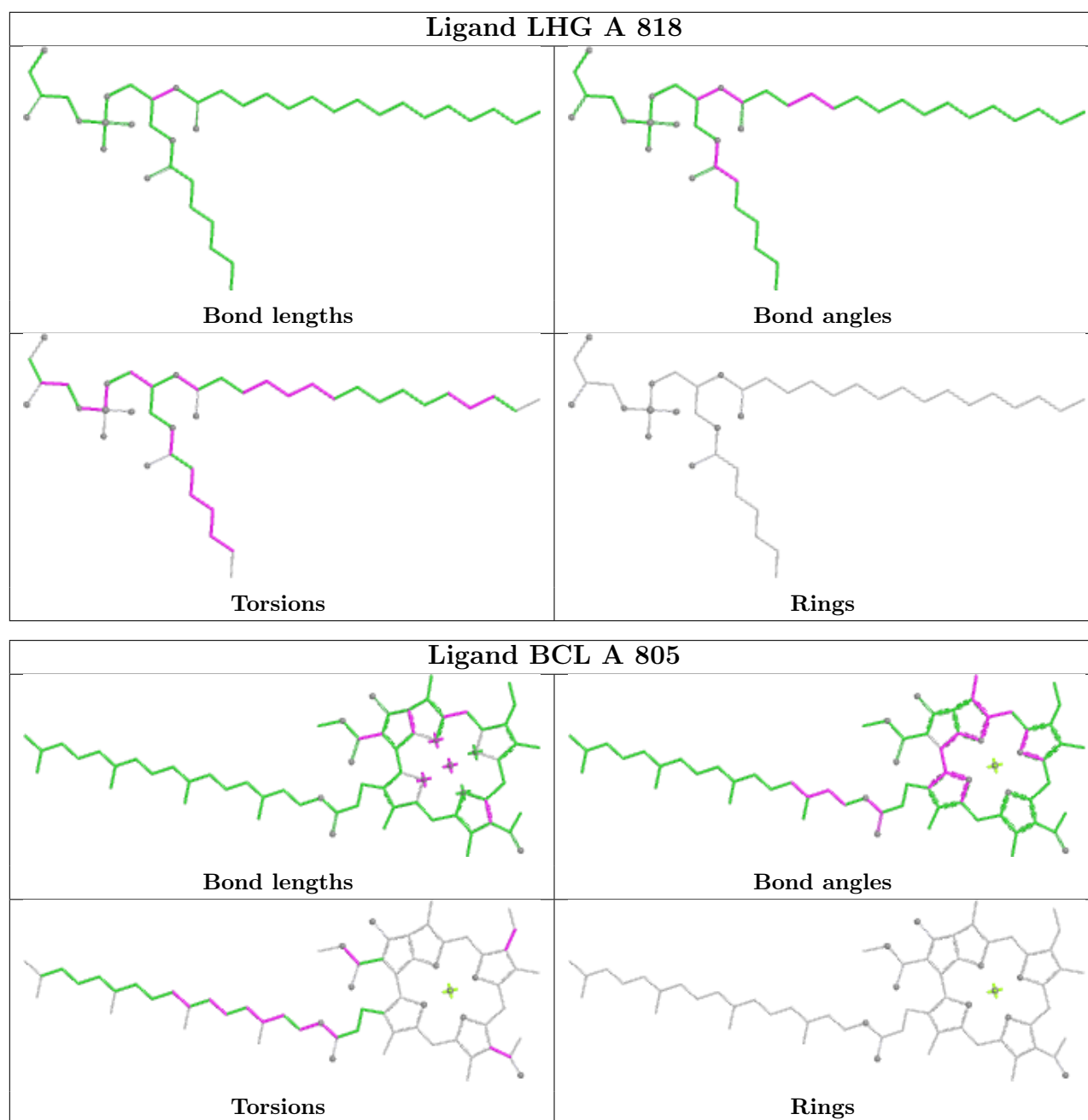












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

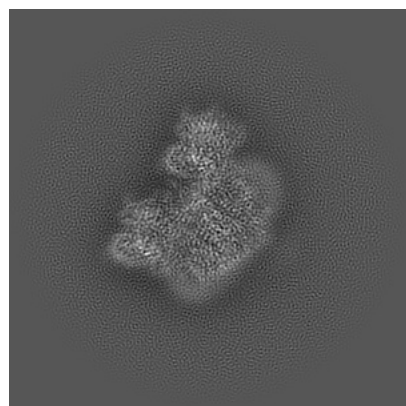
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26471. These allow visual inspection of the internal detail of the map and identification of artifacts.

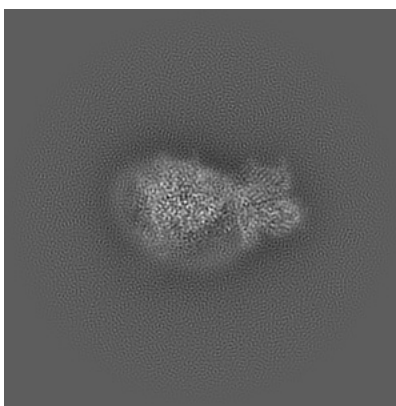
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

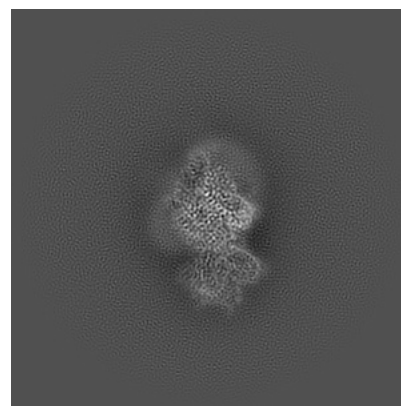
6.1.1 Primary map



X

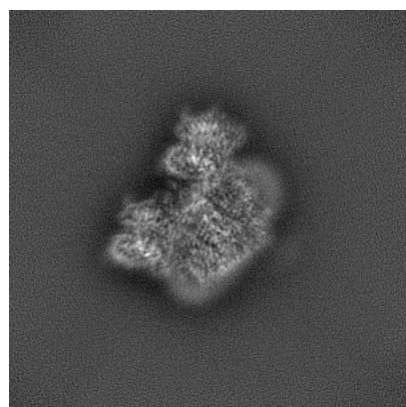


Y

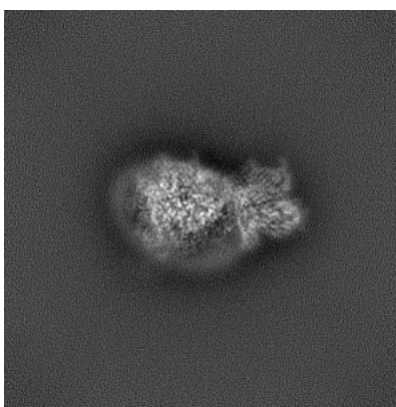


Z

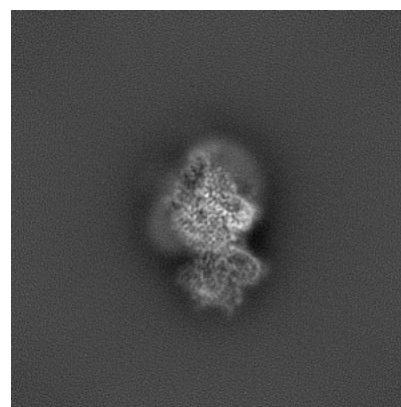
6.1.2 Raw map



X



Y

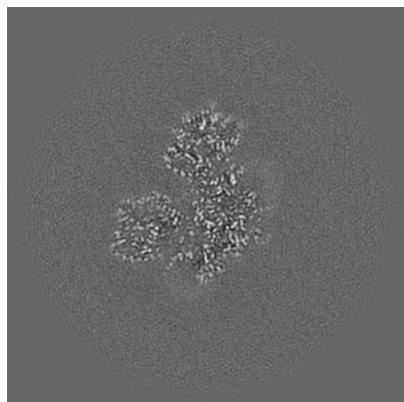


Z

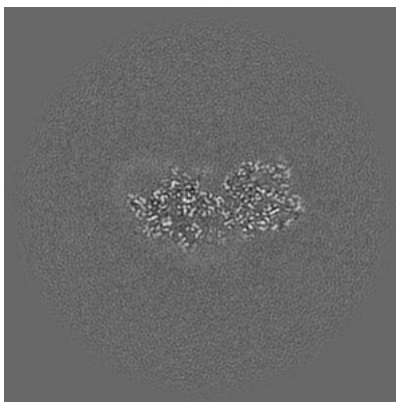
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

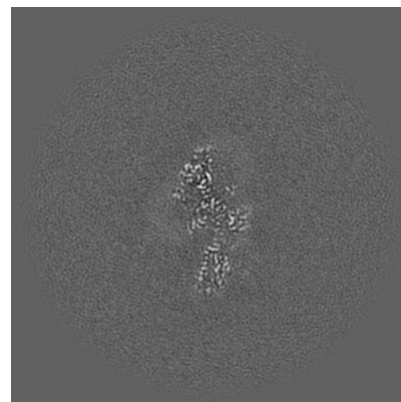
6.2.1 Primary map



X Index: 180

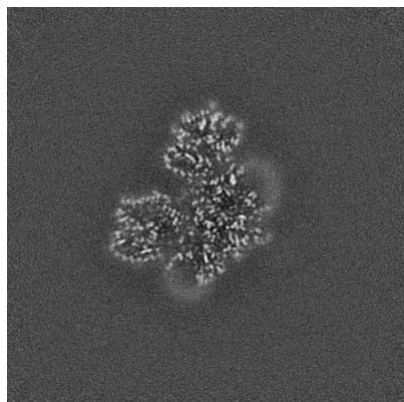


Y Index: 180

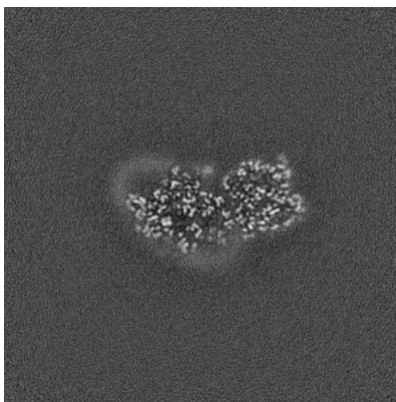


Z Index: 180

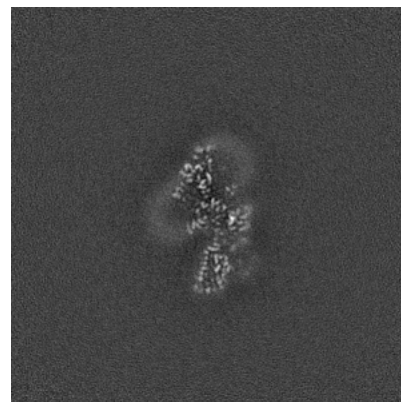
6.2.2 Raw map



X Index: 180



Y Index: 180

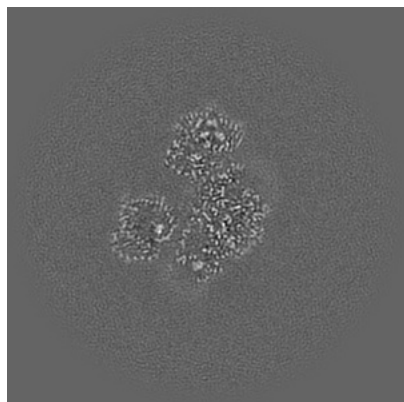


Z Index: 180

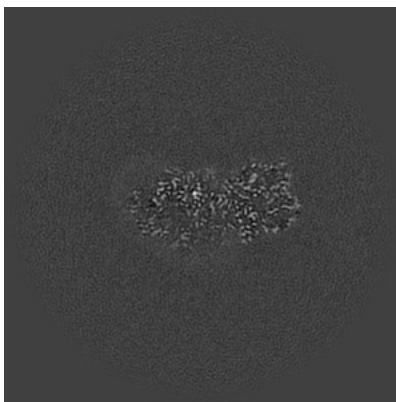
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

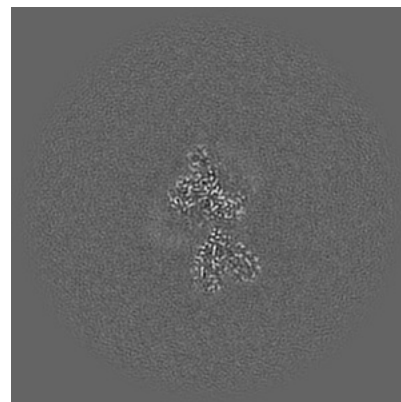
6.3.1 Primary map



X Index: 177

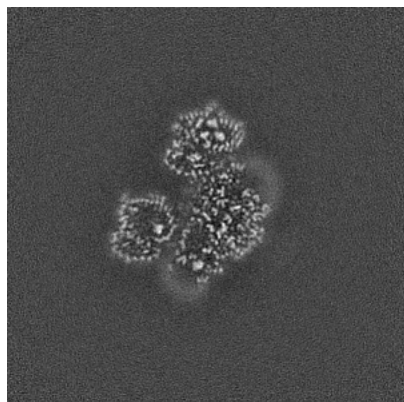


Y Index: 176

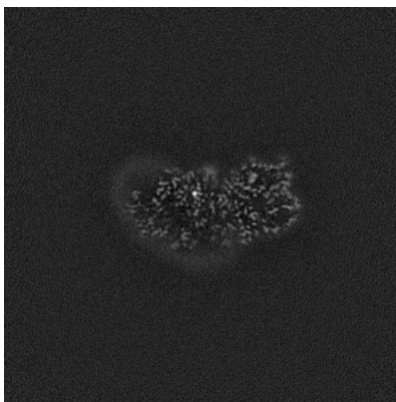


Z Index: 165

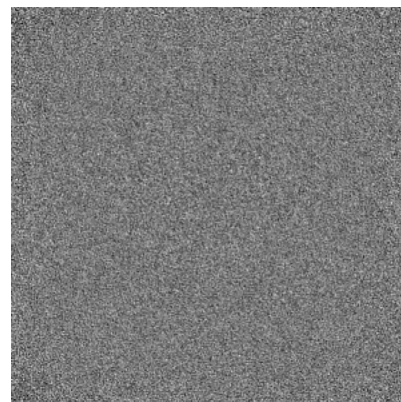
6.3.2 Raw map



X Index: 177



Y Index: 176

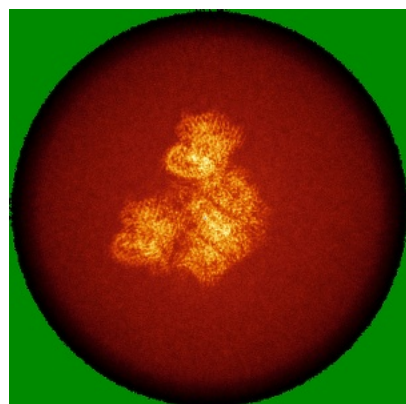


Z Index: 359

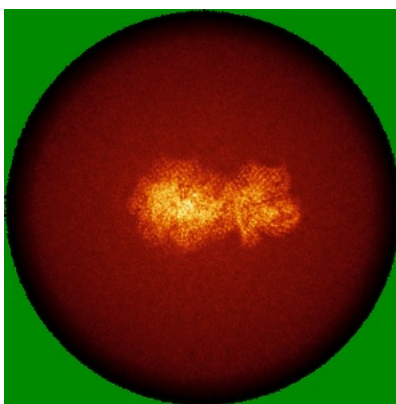
The images above show the largest variance slices of the map in three orthogonal directions.

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

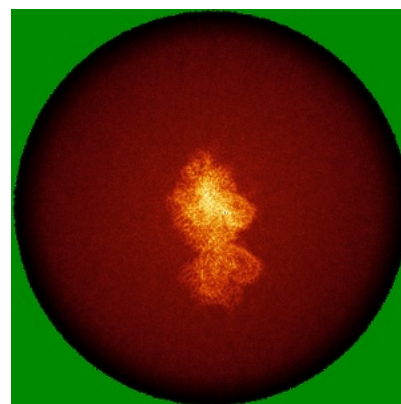
6.4.1 Primary map



X

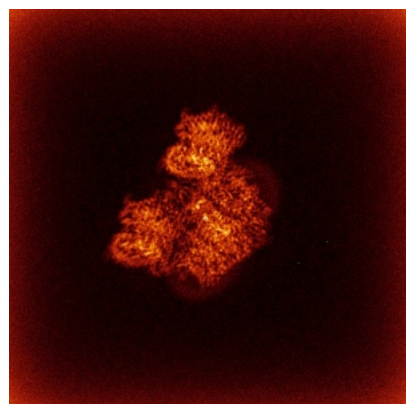


Y

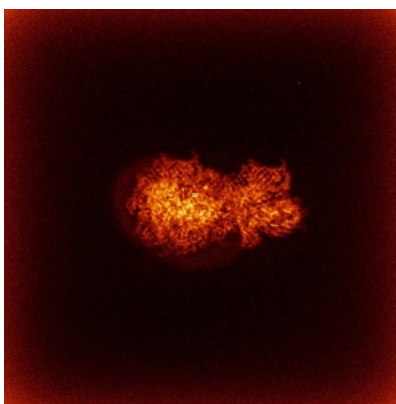


Z

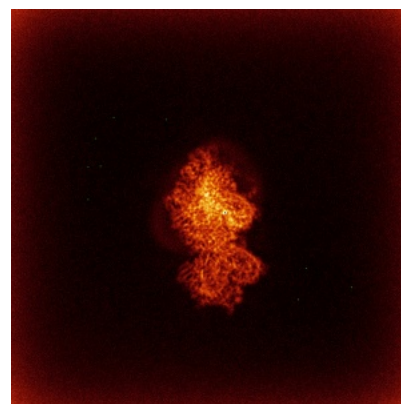
6.4.2 Raw map



X



Y

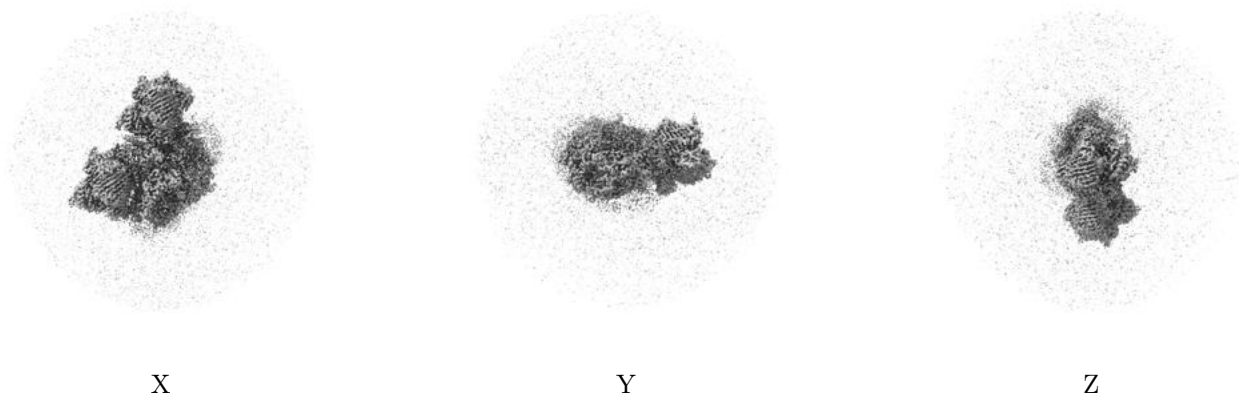


Z

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.

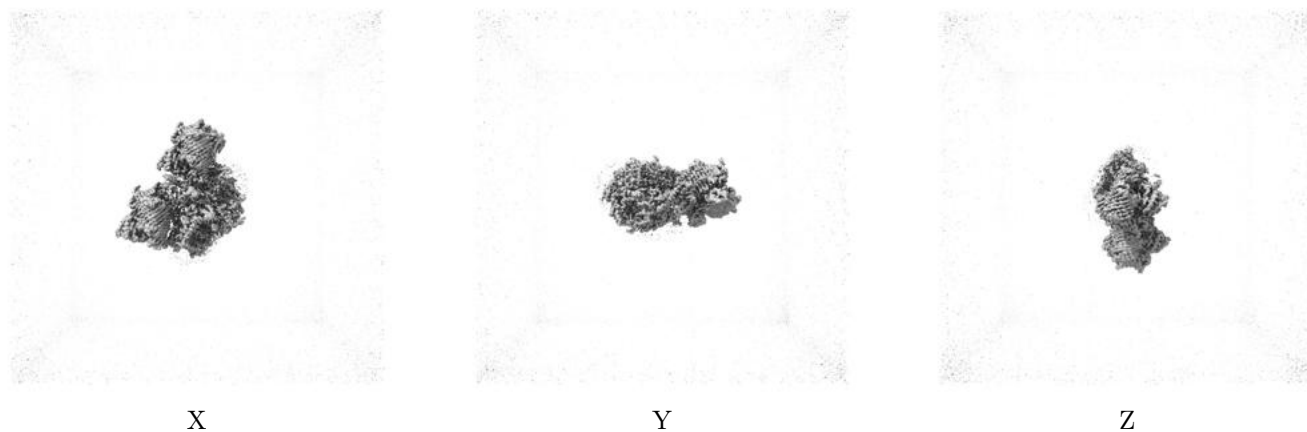
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.428. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

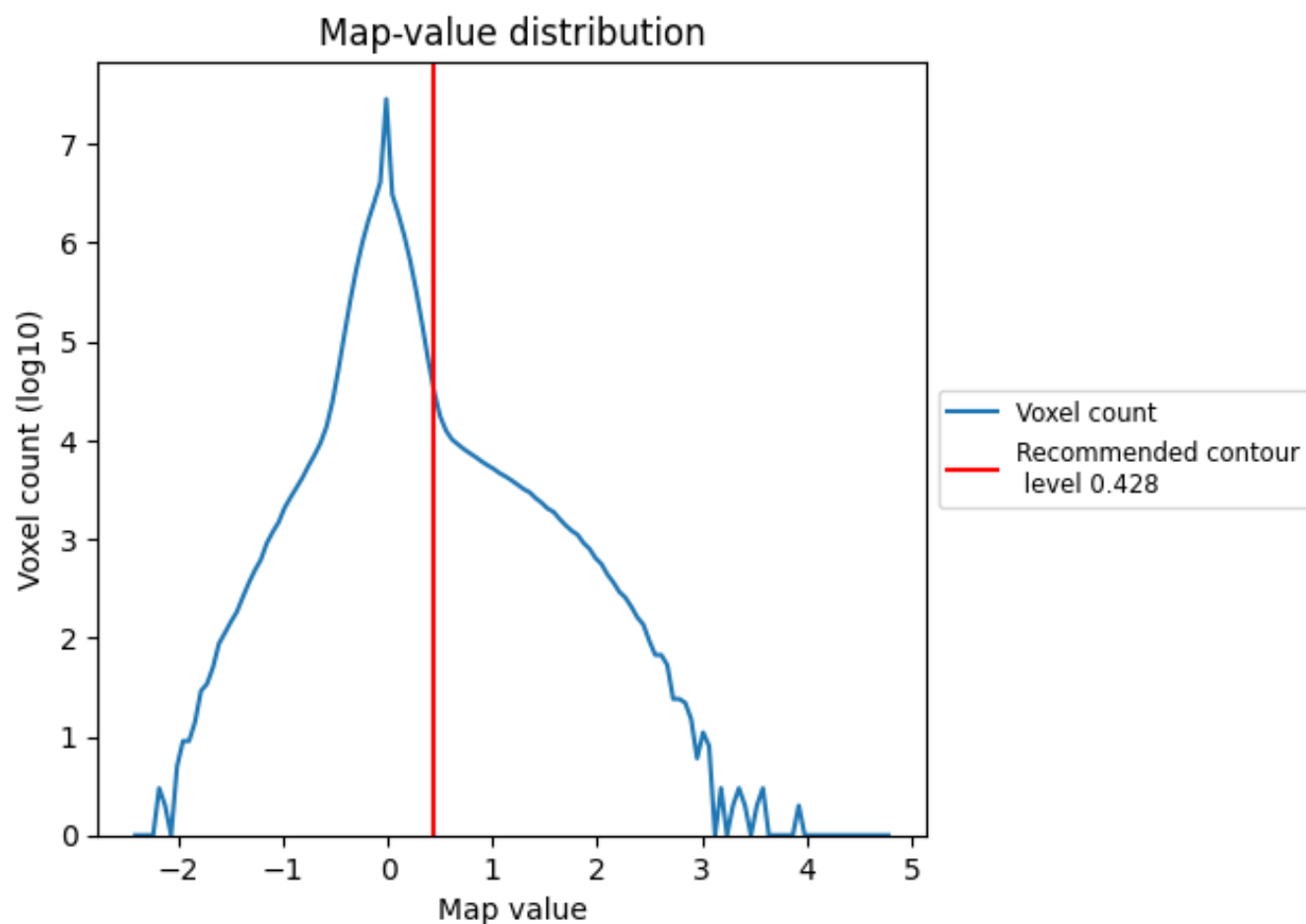
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

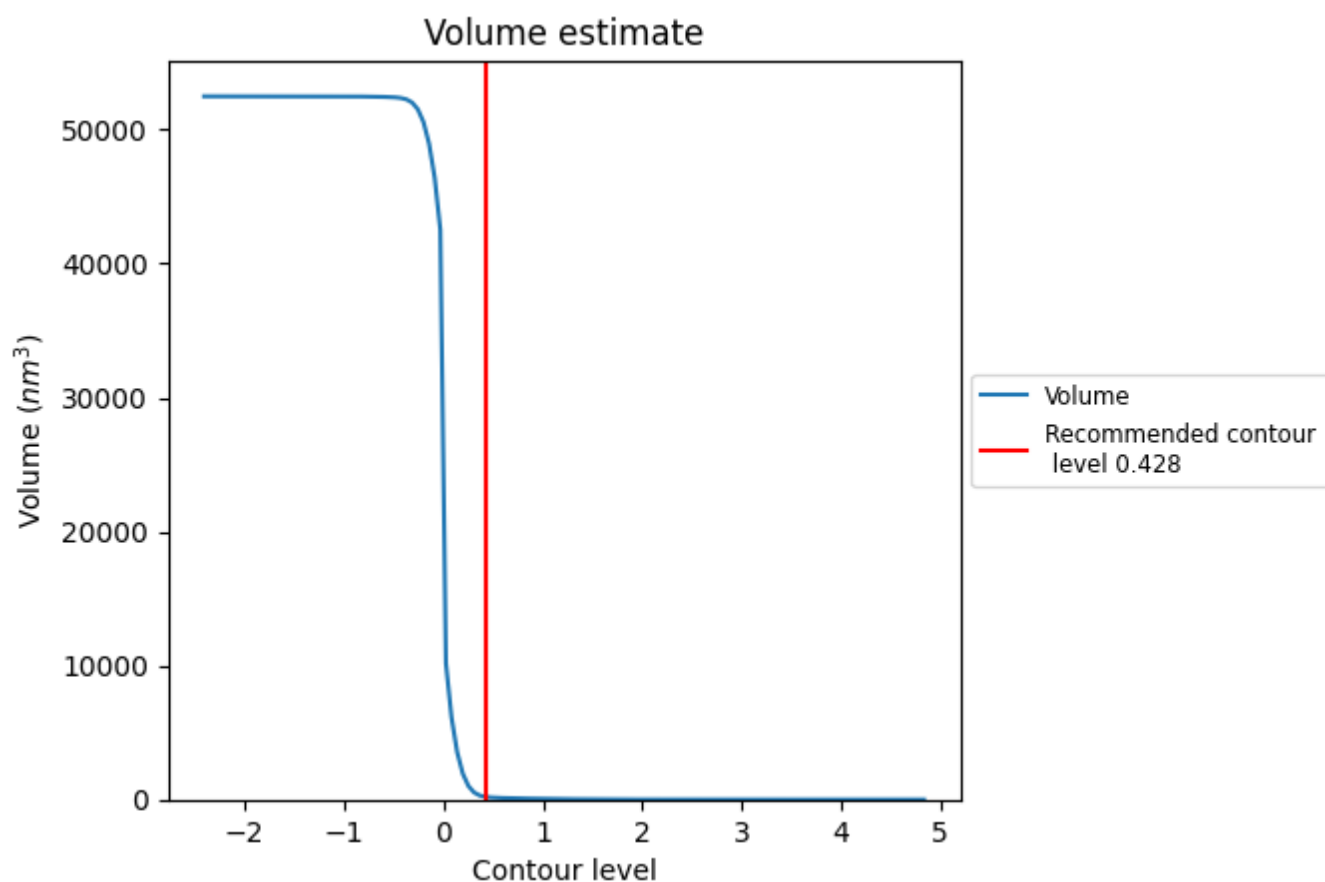
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

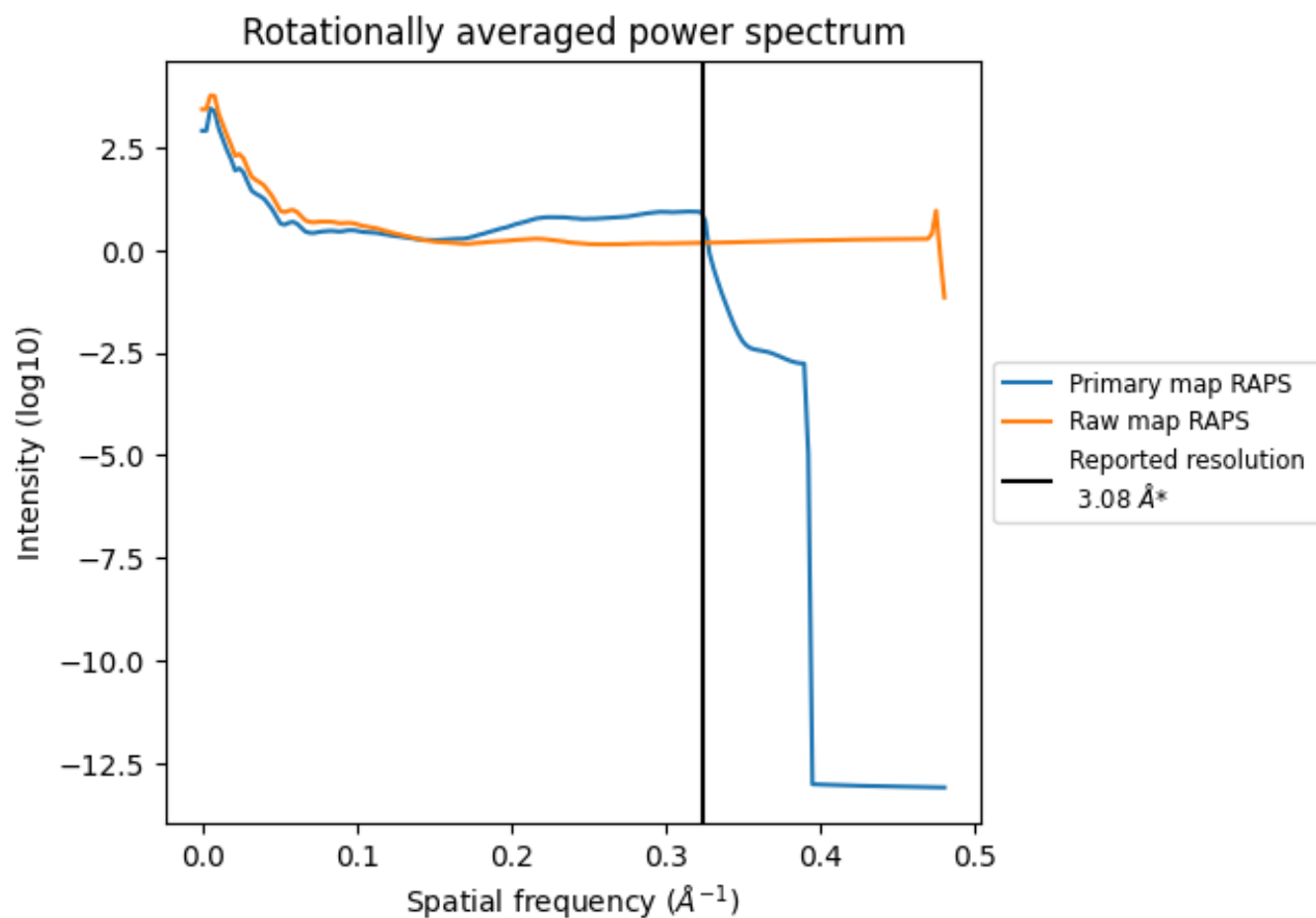
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 198 nm³; this corresponds to an approximate mass of 179 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 ⓘ

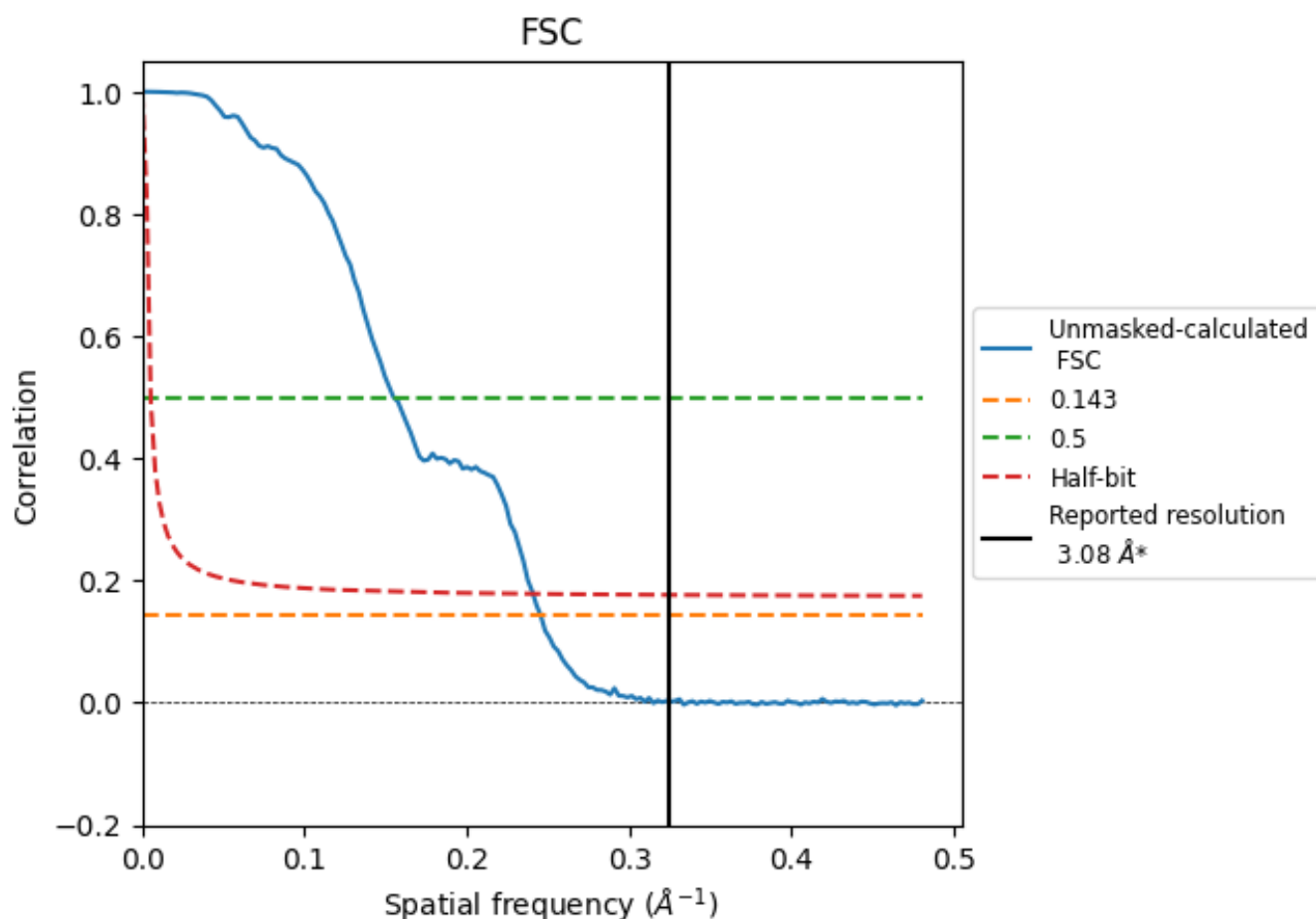


*Reported resolution corresponds to spatial frequency of 0.325 $\text{\AA}^{-1}$

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 0.325 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

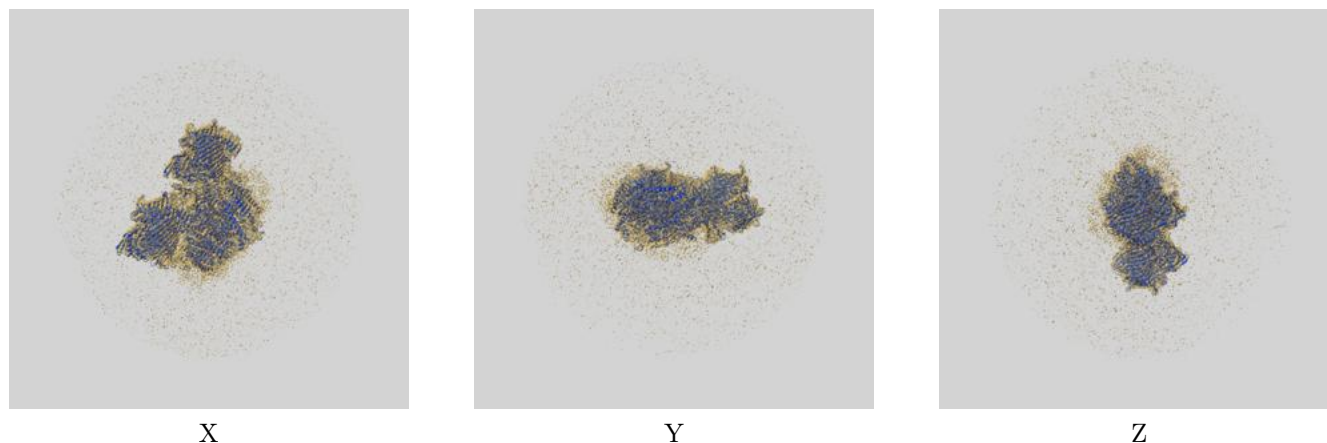
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.07	6.46	4.15

*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 4.07 differs from the reported value 3.08 by more than 10 %

9 Map-model fit [i](#)

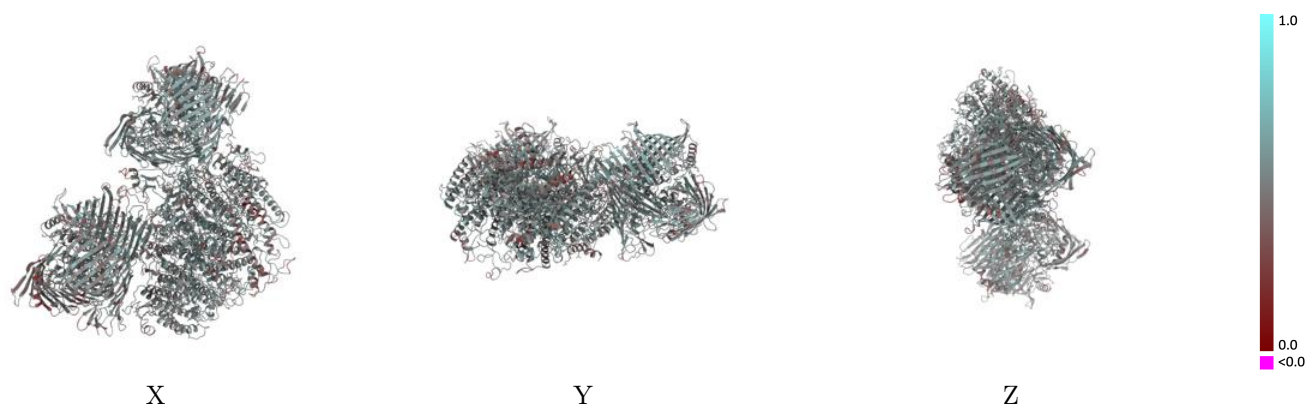
This section contains information regarding the fit between EMDB map EMD-26471 and PDB model 7UEB. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



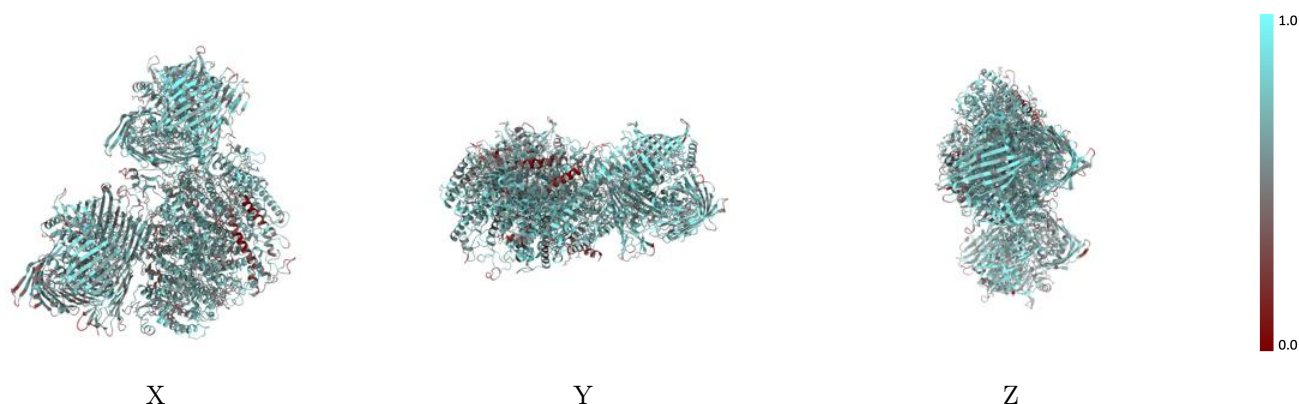
The images above show the 3D surface view of the map at the recommended contour level 0.428 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



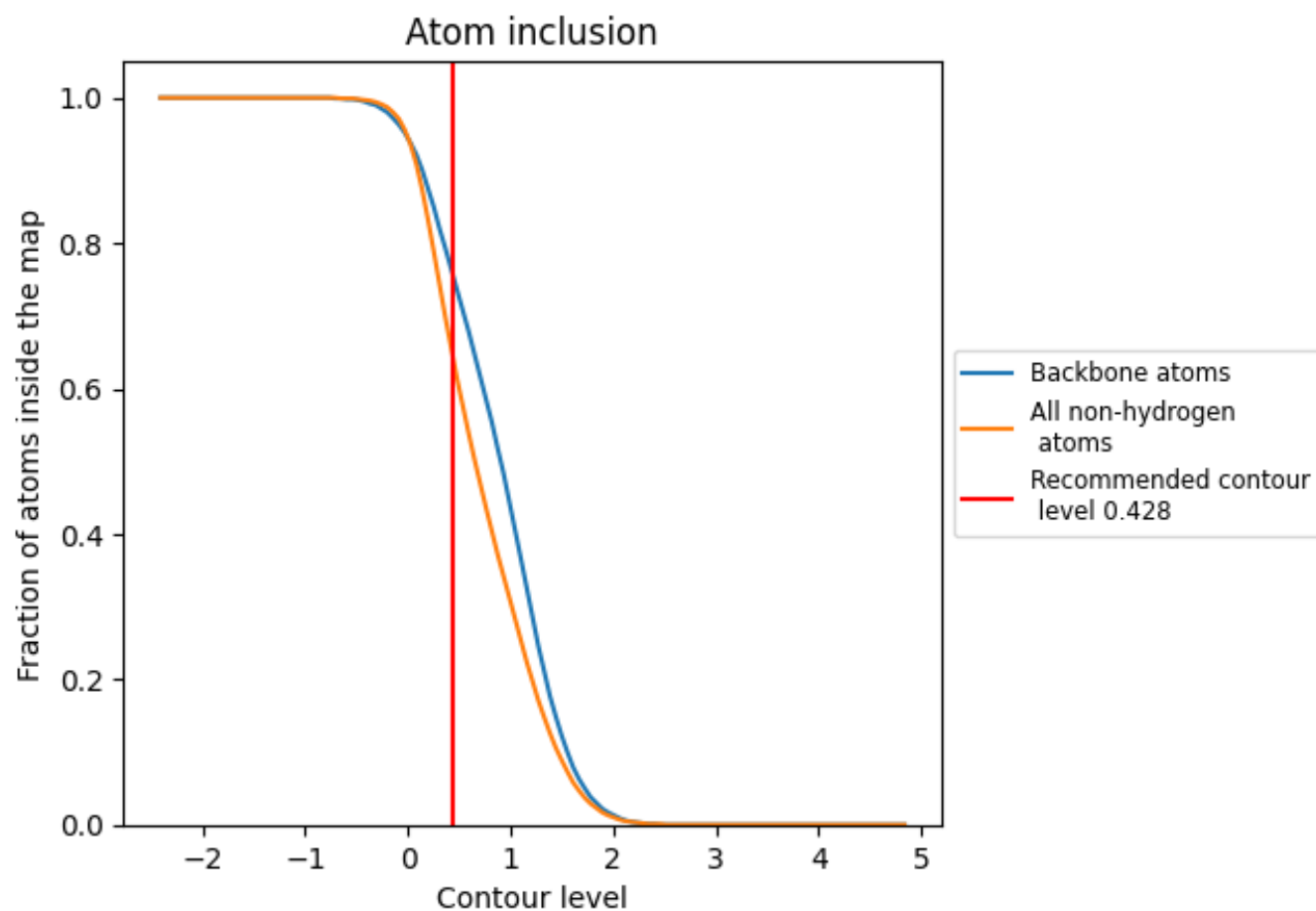
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.428).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 65% 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 (0.428) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6500	0.4970
A	0.6790	0.5170
B	0.6410	0.4920
C	0.5490	0.4680
D	0.5260	0.4370
E	0.4120	0.3720
F	0.3410	0.3920
U	0.7040	0.5110
V	0.7100	0.5230
W	0.6780	0.4930
X	0.6250	0.4710
Y	0.6320	0.4870
Z	0.6690	0.5120
a	0.6680	0.5140
c	0.3480	0.3940

1.0

0.0

<0.0