



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 01:05 AM UTC

PDB ID : 7YML / pdb_00007yml
EMDB ID : EMD-33931
Title : Structure of photosynthetic LH1-RC super-complex of Rhodobacter capsulatus
Authors : Tani, K.; Kanno, R.; Ji, X.-C.; Satoh, I.; Kobayashi, Y.; Nagashima, K.V.P.; Hall, M.; Yu, L.-J.; Kimura, Y.; Mizoguchi, A.; Humbel, B.M.; Madigan, M.T.; Wang-Otomo, Z.-Y.
Deposited on : 2022-07-28
Resolution : 2.60 Å (reported)
Based on initial model : 7F0L

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

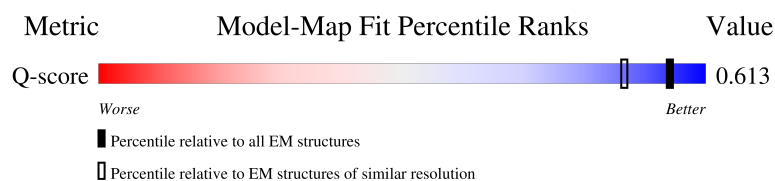
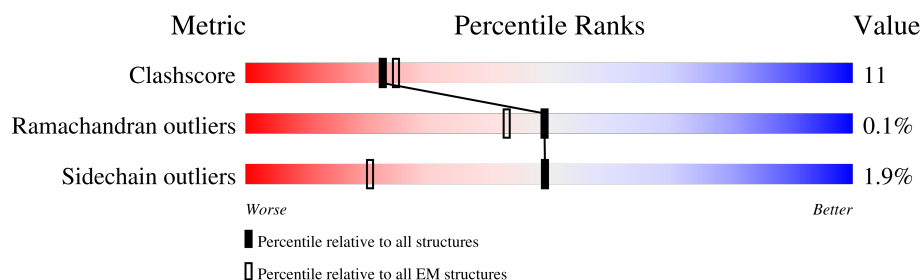
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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

Mol	Chain	Length	Quality of chain
1	L	282	
2	M	307	
3	H	253	

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Mol	Chain	Length	Quality of chain
4	A	58	
4	D	58	
4	F	58	
4	I	58	
4	K	58	
4	O	58	
4	Q	58	
4	S	58	
4	V	58	
4	Y	58	
5	B	49	
5	E	49	
5	G	49	
5	J	49	
5	N	49	
5	P	49	
5	R	49	
5	T	49	
5	W	49	
5	Z	49	
6	X	78	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 18554 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 Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	281	Total	C	N	O	S	1	0
			2239	1501	356	365	17		

- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	304	Total	C	N	O	S	0	0
			2417	1608	392	404	13		

- Molecule 3 is a protein called Photosynthetic reaction center H subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	248	Total	C	N	O	S	0	0
			1956	1246	329	371	10		

- Molecule 4 is a protein called Light-harvesting protein B-870 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	44	Total	C	N	O	S	0	0
			374	262	58	53	1		
4	D	56	Total	C	N	O	S	0	0
			457	315	73	68	1		
4	F	54	Total	C	N	O	S	0	0
			447	309	71	66	1		
4	I	56	Total	C	N	O	S	0	0
			457	315	73	68	1		
4	K	55	Total	C	N	O	S	0	0
			452	312	72	67	1		
4	O	56	Total	C	N	O	S	0	0
			453	312	72	68	1		
4	Q	56	Total	C	N	O	S	0	0
			457	315	73	68	1		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	S	56	Total	C	N	O	1	0
			462	318	76	68		
4	V	56	Total	C	N	O	0	0
			457	315	73	68		
4	Y	42	Total	C	N	O	0	0
			335	228	56	51		

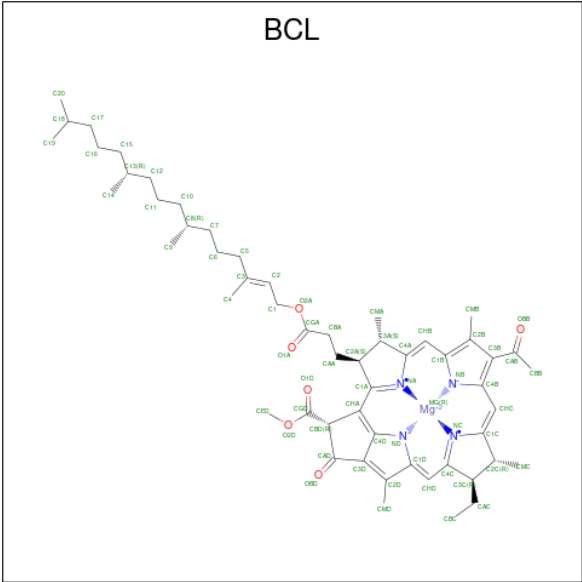
- Molecule 5 is a protein called Light-harvesting protein B-870 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	44	Total	C	N	O	S	0	0
			346	229	55	60	2		
5	E	44	Total	C	N	O	S	0	0
			346	229	55	60	2		
5	G	43	Total	C	N	O	S	0	0
			338	225	54	57	2		
5	J	44	Total	C	N	O	S	0	0
			346	229	55	60	2		
5	N	43	Total	C	N	O	S	0	0
			338	225	54	57	2		
5	P	43	Total	C	N	O	S	0	0
			338	225	54	57	2		
5	R	43	Total	C	N	O	S	0	0
			334	223	54	55	2		
5	T	43	Total	C	N	O	S	0	0
			338	225	54	57	2		
5	W	41	Total	C	N	O	S	0	0
			309	204	52	51	2		
5	Z	31	Total	C	N	O	S	0	0
			224	150	36	36	2		

- Molecule 6 is a protein called Photosynthetic reaction center PufX protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	65	Total	C	N	O	S	0	0
			502	333	79	86	4		

- Molecule 7 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



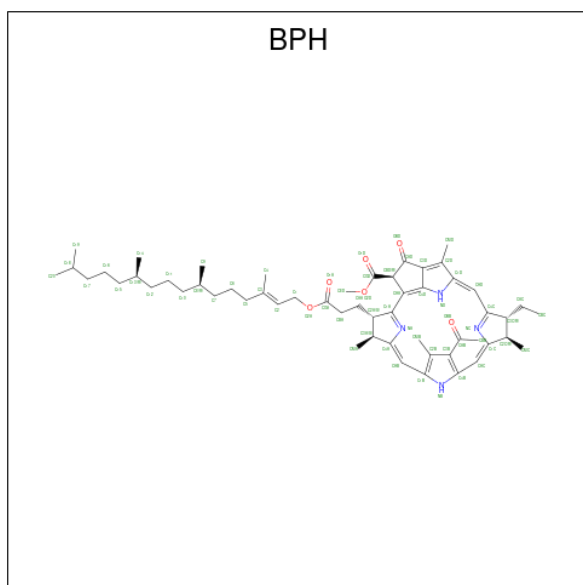
Mol	Chain	Residues	Atoms					AltConf
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	A	1	Total 61	C 50	Mg 1	N 4	O 6	0
7	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	K	1	Total 66	C 55	Mg 1	N 4	O 6	0

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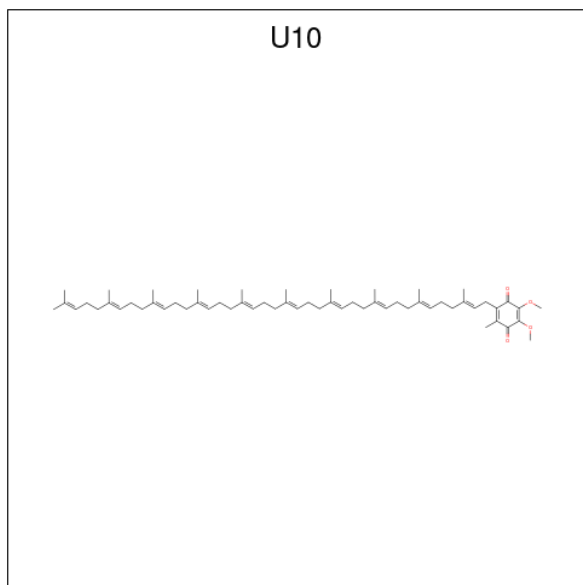
Mol	Chain	Residues	Atoms					AltConf
7	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	T	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 8 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



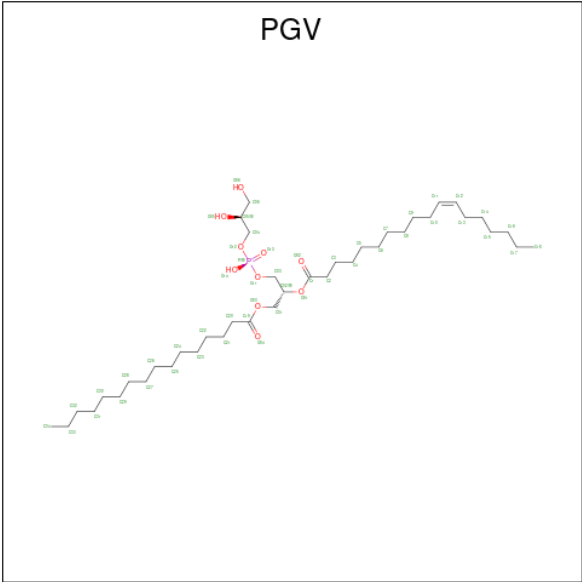
Mol	Chain	Residues	Atoms				AltConf
8	L	1	Total	C	N	O	0
			65	55	4	6	
8	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 9 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).



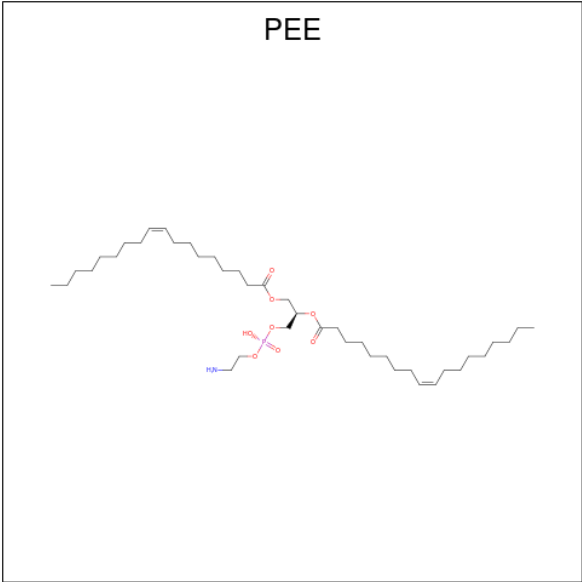
Mol	Chain	Residues	Atoms			AltConf
9	L	1	Total	C	O	0
			48	44	4	
9	L	1	Total	C	O	0
			63	59	4	
9	M	1	Total	C	O	0
			20	16	4	
9	M	1	Total	C	O	0
			48	44	4	

- Molecule 10 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



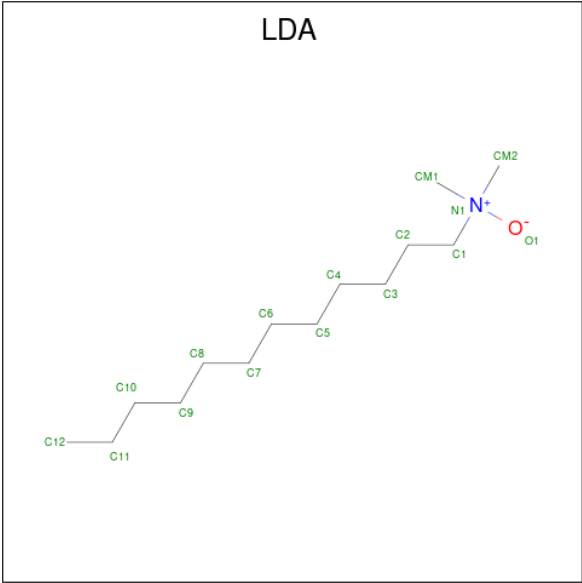
Mol	Chain	Residues	Atoms				AltConf
10	L	1	Total	C	O	P	0
			39	28	10	1	
10	M	1	Total	C	O	P	0
			36	25	10	1	
10	M	1	Total	C	O	P	0
			45	34	10	1	
10	M	1	Total	C	O	P	0
			35	24	10	1	
10	M	1	Total	C	O	P	0
			38	27	10	1	
10	H	1	Total	C	O	P	0
			43	32	10	1	
10	H	1	Total	C	O	P	0
			34	23	10	1	
10	Q	1	Total	C	O	P	0
			35	24	10	1	

- Molecule 11 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C₄₁H₇₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
11	L	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 12 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).



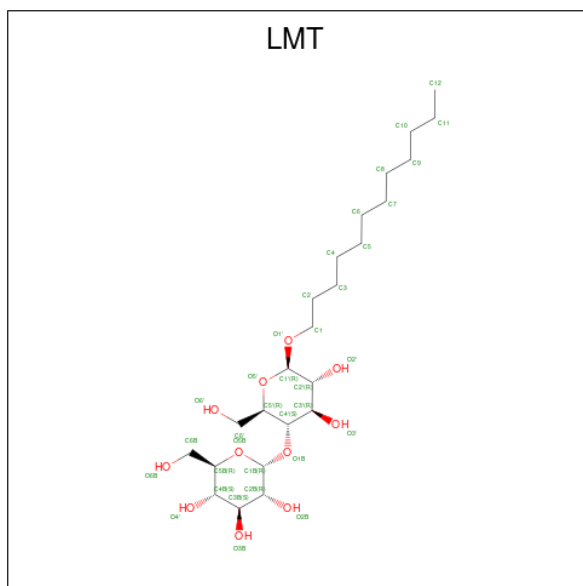
Mol	Chain	Residues	Atoms				AltConf
12	L	1	Total	C	N	O	0
			16	14	1	1	
12	M	1	Total	C	N	O	0
			16	14	1	1	

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Mol	Chain	Residues	Atoms				AltConf
12	M	1	Total	C	N	O	0
			16	14	1	1	
12	M	1	Total	C	N	O	0
			16	14	1	1	
12	M	1	Total	C	N	O	0
			16	14	1	1	
12	H	1	Total	C	N	O	0
			16	14	1	1	
12	H	1	Total	C	N	O	0
			14	12	1	1	
12	D	1	Total	C	N	O	0
			16	14	1	1	
12	O	1	Total	C	N	O	0
			16	14	1	1	
12	Q	1	Total	C	N	O	0
			9	7	1	1	
12	Q	1	Total	C	N	O	0
			12	10	1	1	

- Molecule 13 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
13	L	1	Total	C	O	0
			35	24	11	
13	L	1	Total	C	O	0
			34	23	11	

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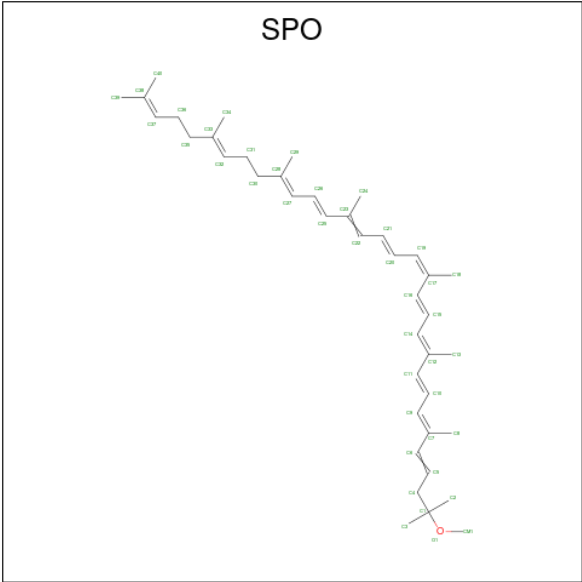
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Mol	Chain	Residues	Atoms			AltConf
13	L	1	Total	C	O	0
			35	24	11	
13	M	1	Total	C	O	0
			24	13	11	
13	M	1	Total	C	O	0
			35	24	11	
13	M	1	Total	C	O	0
			35	24	11	
13	M	1	Total	C	O	0
			32	21	11	
13	M	1	Total	C	O	0
			33	22	11	
13	A	1	Total	C	O	0
			32	21	11	
13	I	1	Total	C	O	0
			35	24	11	
13	K	1	Total	C	O	0
			35	24	11	
13	Q	1	Total	C	O	0
			35	24	11	
13	S	1	Total	C	O	0
			26	15	11	
13	S	1	Total	C	O	0
			33	22	11	
13	Y	1	Total	C	O	0
			28	17	11	
13	Y	1	Total	C	O	0
			27	16	11	
13	X	1	Total	C	O	0
			35	24	11	
13	X	1	Total	C	O	0
			35	24	11	

- Molecule 14 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
14	M	1	Total	Fe	0
			1	1	

- Molecule 15 is SPHEROIDENE (CCD ID: SPO) (formula: C₄₁H₆₀O).



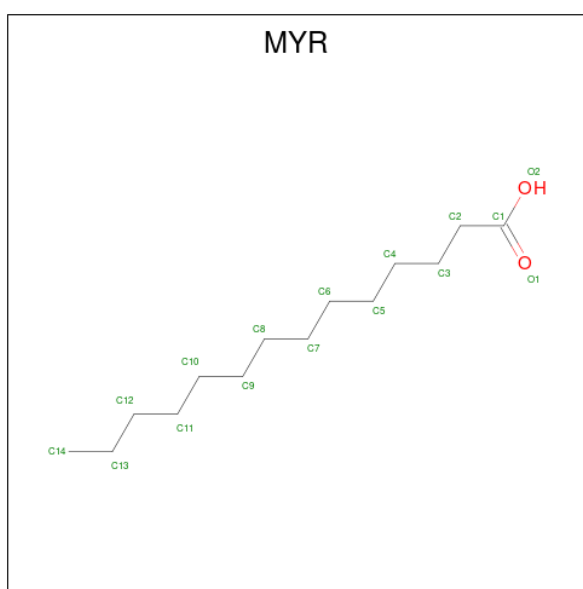
Mol	Chain	Residues	Atoms			AltConf
15	M	1	Total	C	O	0
			42	41	1	
15	D	1	Total	C	O	0
			42	41	1	
15	D	1	Total	C	O	0
			42	41	1	
15	D	1	Total	C	O	0
			42	41	1	
15	E	1	Total	C	O	0
			42	41	1	
15	F	1	Total	C	O	0
			42	41	1	
15	G	1	Total	C	O	0
			42	41	1	
15	I	1	Total	C	O	0
			42	41	1	
15	I	1	Total	C	O	0
			42	41	1	
15	N	1	Total	C	O	0
			42	41	1	
15	O	1	Total	C	O	0
			42	41	1	
15	O	1	Total	C	O	0
			42	41	1	
15	P	1	Total	C	O	0
			42	41	1	
15	R	1	Total	C	O	0
			42	41	1	

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Mol	Chain	Residues	Atoms			AltConf
15	S	1	Total	C	O	0
			42	41	1	
15	S	1	Total	C	O	0
			42	41	1	
15	T	1	Total	C	O	0
			42	41	1	
15	W	1	Total	C	O	0
			42	41	1	

- Molecule 16 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			AltConf
16	F	1	Total	C	O	0
			16	14	2	

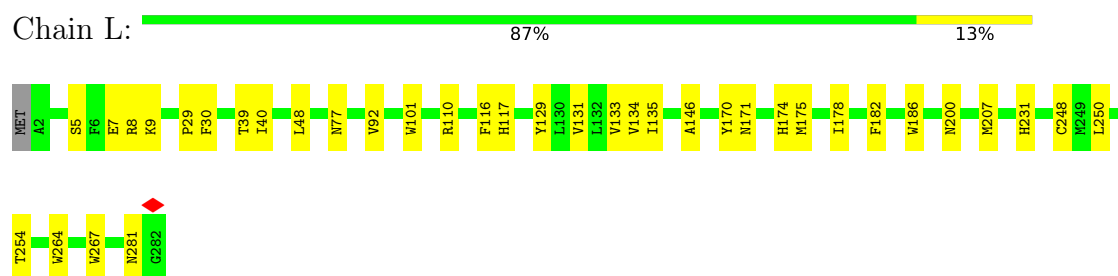
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		AltConf
17	L	4	Total	O	0
			4	4	
17	M	3	Total	O	0
			3	3	

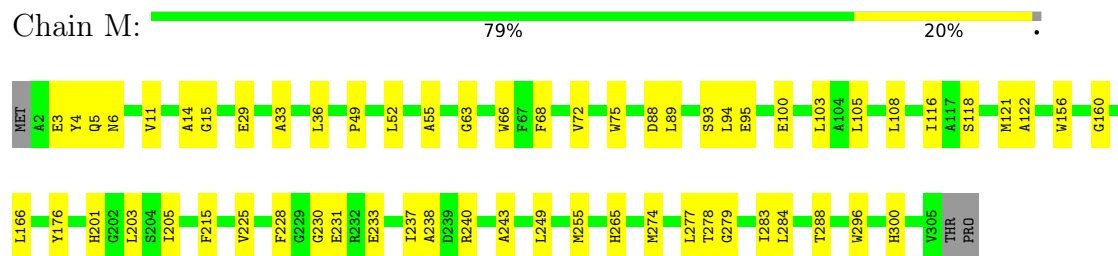
3 Residue-property plots

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

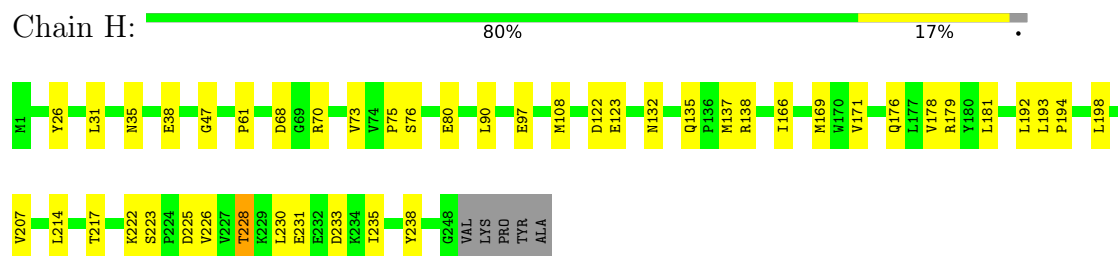
• Molecule 1: Reaction center protein L chain



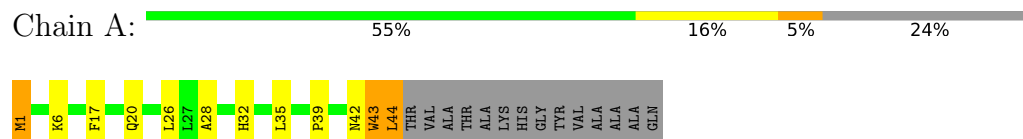
• Molecule 2: Reaction center protein M chain



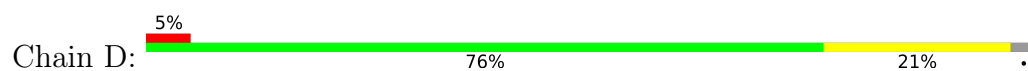
• Molecule 3: Photosynthetic reaction center H subunit



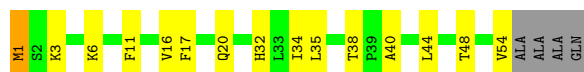
• Molecule 4: Light-harvesting protein B-870 alpha chain



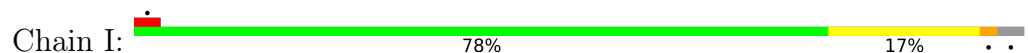
- Molecule 4: Light-harvesting protein B-870 alpha chain



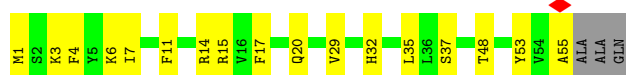
- Molecule 4: Light-harvesting protein B-870 alpha chain



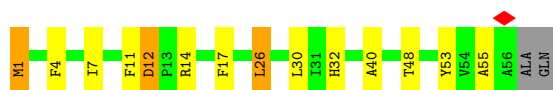
- Molecule 4: Light-harvesting protein B-870 alpha chain



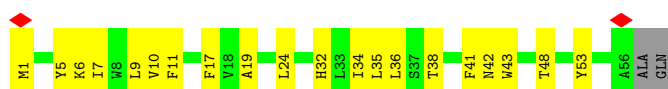
- Molecule 4: Light-harvesting protein B-870 alpha chain



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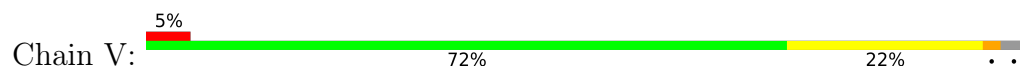


- Molecule 4: Light-harvesting protein B-870 alpha chain





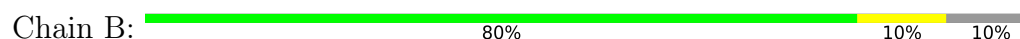
- Molecule 4: Light-harvesting protein B-870 alpha chain



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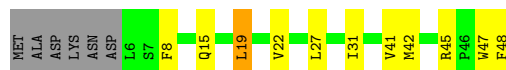
- Molecule 5: Light-harvesting protein B-870 beta chain



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- Molecule 5: Light-harvesting protein B-870 beta chain



- Molecule 5: Light-harvesting protein B-870 beta chain



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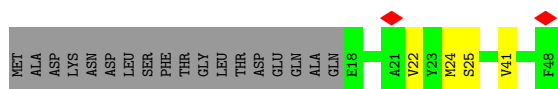
- Molecule 5: Light-harvesting protein B-870 beta chain



- Molecule 5: Light-harvesting protein B-870 beta chain



- Molecule 5: Light-harvesting protein B-870 beta chain



- Molecule 6: Photosynthetic reaction center PufX protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	224431	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.191	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.019	Depositor
Map size ($\text{\AA}$)	328.0, 328.0, 328.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MYR, BPH, FME, LMT, PGV, LDA, SPO, FE, BCL, U10, PEE

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	L	0.28	0/2328	0.29	0/3180
2	M	0.27	0/2507	0.28	0/3425
3	H	0.22	0/2006	0.25	0/2728
4	A	0.25	0/377	0.26	0/514
4	D	0.28	0/462	0.27	0/631
4	F	0.28	0/452	0.25	0/617
4	I	0.26	0/462	0.25	0/631
4	K	0.25	0/457	0.24	0/624
4	O	0.22	0/458	0.21	0/627
4	Q	0.19	0/462	0.21	0/631
4	S	0.18	0/473	0.26	0/645
4	V	0.15	0/462	0.24	0/631
4	Y	0.08	0/345	0.22	0/472
5	B	0.20	0/356	0.22	0/486
5	E	0.23	0/356	0.25	0/486
5	G	0.22	0/348	0.24	0/475
5	J	0.24	0/356	0.22	0/486
5	N	0.22	0/348	0.23	0/475
5	P	0.21	0/348	0.25	0/475
5	R	0.17	0/344	0.21	0/470
5	T	0.17	0/348	0.21	0/475
5	W	0.13	0/318	0.23	0/435
5	Z	0.07	0/229	0.22	0/313
6	X	0.21	0/519	0.25	0/700
All	All	0.24	0/15121	0.26	0/20632

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2239	0	2184	33	0
2	M	2417	0	2327	54	0
3	H	1956	0	1923	31	0
4	A	374	0	396	9	0
4	D	457	0	480	13	0
4	F	447	0	470	12	0
4	I	457	0	480	11	0
4	K	452	0	475	17	0
4	O	453	0	469	15	0
4	Q	457	0	480	14	0
4	S	462	0	486	16	0
4	V	457	0	480	13	0
4	Y	335	0	351	12	0
5	B	346	0	337	5	0
5	E	346	0	337	8	0
5	G	338	0	333	12	0
5	J	346	0	337	8	0
5	N	338	0	333	10	0
5	P	338	0	333	9	0
5	R	334	0	329	8	0
5	T	338	0	333	7	0
5	W	309	0	292	8	0
5	Z	224	0	217	3	0
6	X	502	0	488	4	0
7	A	61	0	61	3	0
7	B	66	0	74	4	0
7	D	66	0	74	8	0
7	E	66	0	74	3	0
7	F	132	0	148	8	0
7	G	66	0	74	8	0
7	I	66	0	74	6	0
7	J	66	0	74	6	0
7	K	66	0	74	7	0
7	L	132	0	148	2	0
7	M	132	0	148	8	0
7	N	66	0	74	7	0
7	O	66	0	74	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	P	66	0	74	8	0
7	Q	66	0	74	0	0
7	R	66	0	74	4	0
7	S	66	0	74	5	0
7	T	66	0	74	5	0
7	V	66	0	74	6	0
7	W	66	0	74	6	0
7	Y	66	0	74	3	0
7	Z	66	0	74	3	0
8	L	65	0	76	3	0
8	M	65	0	76	8	0
9	L	111	0	153	10	0
9	M	68	0	82	6	0
10	H	77	0	92	5	0
10	L	39	0	47	5	0
10	M	154	0	188	14	0
10	Q	35	0	40	5	0
11	L	46	0	69	3	0
12	D	16	0	31	3	0
12	H	30	0	55	3	0
12	L	16	0	31	2	0
12	M	64	0	124	5	0
12	O	16	0	31	1	0
12	Q	21	0	34	3	0
13	A	32	0	37	3	0
13	I	35	0	46	3	0
13	K	35	0	46	2	0
13	L	104	0	133	6	0
13	M	159	0	189	15	0
13	Q	35	0	46	2	0
13	S	59	0	64	8	0
13	X	70	0	92	1	0
13	Y	55	0	56	2	0
14	M	1	0	0	0	0
15	D	126	0	180	17	0
15	E	42	0	60	6	0
15	F	42	0	60	5	0
15	G	42	0	60	3	0
15	I	84	0	120	13	0
15	M	42	0	60	6	0
15	N	42	0	60	6	0
15	O	84	0	120	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	P	42	0	60	5	0
15	R	42	0	60	6	0
15	S	84	0	120	14	0
15	T	42	0	60	3	0
15	W	42	0	60	8	0
16	F	16	0	27	2	0
17	L	4	0	0	0	0
17	M	3	0	0	0	0
All	All	18554	0	19452	429	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 11.

All (429) 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)
4:D:11:PHE:HZ	4:F:17:PHE:HD2	1.21	0.85
4:F:1:FME:HCN	4:F:3:LYS:H	1.41	0.84
4:D:25:PHE:HB2	7:D:102:BCL:H43	1.61	0.81
4:O:40:ALA:O	5:P:45:ARG:NH1	2.18	0.77
10:L:305:PGV:H51	10:L:305:PGV:H232	1.67	0.76
4:Y:15:ARG:HE	13:Y:103:LMT:H6'2	1.50	0.76
13:M:410:LMT:H82	13:S:102:LMT:H62	1.69	0.75
2:M:231:GLU:OE2	3:H:179:ARG:NH1	2.20	0.74
15:I:104:SPO:H37	5:N:22:VAL:HG21	1.67	0.74
15:O:104:SPO:H293	15:R:101:SPO:H37	1.70	0.74
4:V:10:VAL:HG12	4:Y:14:ARG:HB3	1.72	0.71
2:M:240:ARG:NH1	3:H:38:GLU:OE1	2.22	0.71
4:S:35:LEU:HD11	7:T:102:BCL:HHD	1.73	0.71
2:M:233:GLU:OE1	2:M:265:HIS:CE1	2.46	0.69
1:L:231:HIS:CE1	2:M:233:GLU:OE2	2.46	0.69
12:M:418:LDA:H82	12:M:419:LDA:H31	1.73	0.69
1:L:133:VAL:HG23	1:L:134:VAL:HG23	1.76	0.68
15:S:104:SPO:H37	5:T:22:VAL:HG11	1.74	0.68
5:Z:41:VAL:HG11	7:Z:101:BCL:HBC1	1.76	0.68
5:G:31:ILE:HD12	7:G:101:BCL:H11	1.74	0.68
2:M:55:ALA:HB2	10:M:415:PGV:H012	1.74	0.68
15:G:102:SPO:H37	15:I:103:SPO:H293	1.77	0.67
3:H:31:LEU:O	3:H:35:ASN:ND2	2.27	0.67
7:W:102:BCL:HHB	7:W:102:BCL:H8	1.77	0.67
15:I:104:SPO:H401	5:J:6:LEU:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:68:ASP:OD2	3:H:70:ARG:NH1	2.28	0.66
13:S:101:LMT:H5'	13:S:102:LMT:H12	1.77	0.66
1:L:77:ASN:HD22	13:A:102:LMT:H6D	1.60	0.66
4:D:19:ALA:HB2	12:D:104:LDA:H51	1.79	0.65
5:G:42:MET:HE2	7:G:101:BCL:H203	1.78	0.65
4:O:7:ILE:HB	15:O:104:SPO:H343	1.79	0.65
11:L:306:PEE:H29	6:X:36:PRO:HB3	1.78	0.65
7:P:102:BCL:HBB2	7:P:102:BCL:H122	1.80	0.64
4:I:7:ILE:HB	15:I:104:SPO:H343	1.79	0.64
4:O:12:ASP:OD1	4:O:12:ASP:N	2.29	0.64
4:I:40:ALA:O	5:J:45:ARG:NH1	2.30	0.64
2:M:279:GLY:HA2	7:M:404:BCL:HED2	1.80	0.64
2:M:118:SER:HB3	15:M:408:SPO:H311	1.80	0.63
4:O:1:FME:SD	4:O:1:FME:N	2.71	0.63
4:Y:12:ASP:HB3	4:Y:15:ARG:HB2	1.80	0.62
13:M:409:LMT:O6'	12:H:301:LDA:O1	2.17	0.62
4:Q:35:LEU:HD11	7:R:102:BCL:HHD	1.82	0.62
13:L:311:LMT:H42	10:H:303:PGV:H011	1.82	0.62
4:S:45:THR:HA	4:S:48:THR:HG22	1.82	0.61
1:L:267:TRP:HB2	9:M:401:U10:H4M3	1.83	0.61
15:O:104:SPO:H402	5:R:19:LEU:HA	1.81	0.61
8:M:405:BPH:HBB3	8:M:405:BPH:HHC	1.83	0.61
4:Q:7:ILE:HB	15:S:104:SPO:H343	1.81	0.61
3:H:198:LEU:HD22	3:H:207:VAL:HG22	1.83	0.61
7:O:102:BCL:H111	15:P:101:SPO:H341	1.83	0.61
4:A:43:TRP:H	4:A:43:TRP:CD1	2.18	0.61
7:M:403:BCL:H193	12:M:419:LDA:H82	1.82	0.60
4:I:20:GLN:NE2	5:J:23:TYR:OH	2.31	0.60
4:I:40:ALA:HB2	4:K:55:ALA:HB2	1.84	0.60
7:K:102:BCL:HED3	15:N:101:SPO:H25	1.83	0.60
4:S:40:ALA:O	5:T:45:ARG:NH1	2.35	0.59
10:H:304:PGV:H012	4:K:15:ARG:HG2	1.84	0.59
4:D:40:ALA:O	5:E:45:ARG:NH1	2.36	0.59
7:V:101:BCL:H41	15:W:101:SPO:H352	1.84	0.59
15:S:104:SPO:HM11	4:V:29:VAL:HG13	1.85	0.59
13:M:409:LMT:O3'	13:S:101:LMT:H6D	2.02	0.59
10:H:304:PGV:H031	4:K:15:ARG:HG2	1.83	0.59
4:Y:43:TRP:CZ2	7:Y:102:BCL:HHC	2.38	0.59
13:M:409:LMT:H6D	12:H:301:LDA:H31	1.84	0.59
4:Q:10:VAL:HG23	4:Q:11:PHE:HD1	1.68	0.59
15:S:105:SPO:H31	7:Y:102:BCL:HBB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:63:GLY:HA3	8:M:405:BPH:H5C1	1.86	0.58
5:E:27:LEU:O	5:E:31:ILE:HG12	2.02	0.58
2:M:300:HIS:ND1	10:M:402:PGV:O14	2.27	0.58
3:H:70:ARG:NH2	3:H:123:GLU:OE1	2.31	0.58
4:K:37:SER:HA	13:K:101:LMT:H5B	1.86	0.58
4:I:6:LYS:HD3	15:I:104:SPO:H403	1.85	0.57
5:B:31:ILE:HG12	7:B:101:BCL:H2	1.87	0.57
7:N:102:BCL:H42	15:P:101:SPO:H293	1.86	0.57
10:M:415:PGV:H251	10:M:415:PGV:H91	1.87	0.57
13:M:417:LMT:O3'	13:M:417:LMT:O2B	2.22	0.57
2:M:75:TRP:HE1	15:M:408:SPO:HM12	1.68	0.57
15:D:101:SPO:H132	7:D:102:BCL:H42	1.87	0.57
15:D:105:SPO:H182	7:I:102:BCL:H8	1.87	0.57
7:M:403:BCL:H142	8:M:405:BPH:HED2	1.86	0.56
4:D:11:PHE:CZ	4:F:17:PHE:HD2	2.13	0.56
10:L:305:PGV:H222	10:M:402:PGV:H41	1.88	0.56
4:D:32:HIS:CE1	7:E:102:BCL:HMD3	2.40	0.56
15:D:105:SPO:H32	5:G:22:VAL:HG12	1.88	0.56
4:V:35:LEU:HD11	7:W:102:BCL:HHD	1.88	0.56
10:M:415:PGV:H061	4:V:14:ARG:HD2	1.88	0.56
3:H:138:ARG:NH1	3:H:225:ASP:OD1	2.37	0.56
4:S:37:SER:HB3	13:S:102:LMT:H2'	1.86	0.56
5:R:6:LEU:HD21	15:S:104:SPO:H401	1.87	0.56
4:F:40:ALA:O	5:G:45:ARG:NH1	2.39	0.56
8:L:302:BPH:HHC	8:L:302:BPH:HBB3	1.88	0.55
15:O:103:SPO:H32	5:P:22:VAL:HG12	1.88	0.55
2:M:75:TRP:HE1	15:M:408:SPO:H22A	1.70	0.55
4:F:6:LYS:HD3	15:I:103:SPO:H393	1.88	0.55
15:O:104:SPO:H391	5:P:6:LEU:HD13	1.87	0.55
2:M:228:PHE:HB2	2:M:243:ALA:HB2	1.89	0.55
8:M:405:BPH:HBC3	8:M:405:BPH:HHD	1.87	0.55
2:M:72:VAL:HG21	13:M:412:LMT:H81	1.88	0.55
1:L:8[B]:ARG:NH2	3:H:47:GLY:HA2	2.23	0.54
2:M:166:LEU:HD11	13:Q:101:LMT:H82	1.89	0.54
4:O:48:THR:HG23	4:O:53:TYR:HB2	1.90	0.54
1:L:174:HIS:CE1	1:L:178:ILE:HD11	2.42	0.54
2:M:108:LEU:HD23	13:M:412:LMT:H6'1	1.88	0.54
4:K:35:LEU:HD11	7:N:102:BCL:HHD	1.89	0.54
15:S:105:SPO:H392	5:W:19:LEU:HA	1.89	0.54
7:M:403:BCL:H13	8:M:405:BPH:HMA1	1.90	0.54
1:L:110:ARG:NH1	11:L:306:PEE:O1P	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:193:LEU:HB3	3:H:198:LEU:HD21	1.89	0.54
7:P:102:BCL:H202	15:R:101:SPO:H9	1.90	0.54
4:D:11:PHE:HZ	4:F:17:PHE:CD2	2.13	0.53
15:I:104:SPO:H32	4:K:17:PHE:CZ	2.43	0.53
7:D:102:BCL:H52	15:E:101:SPO:H351	1.90	0.53
1:L:92:VAL:HG11	9:L:304:U10:H53	1.90	0.53
5:T:7:SER:OG	5:T:11:LEU:N	2.37	0.53
5:W:47:TRP:CE2	7:W:102:BCL:H2C	2.44	0.53
2:M:68:PHE:HB3	13:M:412:LMT:H82	1.92	0.53
15:I:104:SPO:H32	4:K:17:PHE:CE1	2.44	0.53
3:H:166:ILE:HD12	3:H:181:LEU:HB3	1.90	0.52
15:D:105:SPO:H6	7:I:102:BCL:HMB1	1.92	0.52
15:O:103:SPO:H352	5:P:22:VAL:HB	1.90	0.52
7:P:102:BCL:H42	15:R:101:SPO:H293	1.91	0.52
10:Q:103:PGV:H201	12:Q:104:LDA:H52	1.91	0.52
8:L:302:BPH:HHC	8:L:302:BPH:CBB	2.39	0.52
2:M:15:GLY:H	3:H:176:GLN:HE22	1.57	0.52
13:Q:101:LMT:H6'	13:Q:101:LMT:H2O1	1.58	0.52
2:M:116:ILE:HG21	13:M:412:LMT:H11	1.90	0.52
1:L:9:LYS:HA	3:H:90:LEU:HD11	1.91	0.52
1:L:171:ASN:HB3	1:L:174:HIS:HB2	1.90	0.52
4:Q:48:THR:HG23	4:Q:53:TYR:HB2	1.92	0.52
7:J:101:BCL:H43	15:N:101:SPO:H292	1.91	0.52
4:F:44:LEU:O	4:F:48:THR:HG23	2.11	0.51
15:O:104:SPO:H41	4:S:32:HIS:CG	2.46	0.51
5:P:27:LEU:O	5:P:31:ILE:HG12	2.10	0.51
4:Y:48:THR:HG23	4:Y:53:TYR:HB2	1.90	0.51
15:O:103:SPO:H351	5:P:19:LEU:HD22	1.92	0.51
4:V:3:LYS:HD3	5:Z:22:VAL:HG22	1.93	0.51
1:L:182:PHE:HB3	8:M:405:BPH:HBB2	1.92	0.51
5:T:8:PHE:HB3	4:V:14:ARG:NH2	2.26	0.51
4:S:11:PHE:HE2	4:V:17:PHE:HD2	1.59	0.51
2:M:288:THR:HB	12:H:301:LDA:H72	1.93	0.50
10:Q:103:PGV:H32	7:S:103:BCL:H72	1.92	0.50
4:Y:33:LEU:HD23	4:Y:36:LEU:HD12	1.92	0.50
4:K:11:PHE:HZ	4:O:17:PHE:HB2	1.76	0.50
2:M:29:GLU:HG3	4:V:15:ARG:HH21	1.76	0.50
1:L:117:HIS:HE1	2:M:5:GLN:O	1.94	0.50
4:K:20:GLN:OE1	5:N:23:TYR:OH	2.24	0.50
5:N:20:HIS:HE1	7:O:102:BCL:H191	1.75	0.50
7:V:101:BCL:H43	15:W:101:SPO:H32	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:6:LEU:HD23	15:D:103:SPO:H403	1.94	0.50
5:T:42:MET:HE1	5:T:48:PHE:HB2	1.94	0.50
9:L:304:U10:H4M1	4:A:20:GLN:HG2	1.92	0.50
7:E:102:BCL:H42	15:F:104:SPO:H293	1.94	0.50
4:F:20:GLN:HE21	15:F:104:SPO:H392	1.77	0.50
5:N:42:MET:HE2	7:N:102:BCL:H193	1.93	0.50
1:L:40:ILE:HG21	12:D:104:LDA:H111	1.93	0.50
12:L:307:LDA:H21	2:M:3:GLU:HG2	1.93	0.49
4:I:35:LEU:HD11	7:J:101:BCL:HHD	1.93	0.49
7:F:101:BCL:HBB3	16:F:102:MYR:H81	1.93	0.49
7:P:102:BCL:H172	15:R:101:SPO:H11	1.94	0.49
4:Q:19:ALA:HB2	12:Q:104:LDA:H12	1.94	0.49
2:M:255:MET:HE1	9:M:407:U10:H102	1.94	0.49
2:M:36:LEU:HD13	13:M:417:LMT:H5'	1.95	0.49
1:L:29:PRO:HD3	13:L:311:LMT:H2'	1.93	0.49
4:F:35:LEU:HD11	7:G:101:BCL:HHD	1.95	0.49
4:K:29:VAL:HG11	13:K:101:LMT:H111	1.95	0.49
7:J:101:BCL:H92	7:J:101:BCL:HAA1	1.93	0.49
1:L:281:ASN:ND2	2:M:88:ASP:OD1	2.37	0.49
7:B:101:BCL:HBA1	7:B:101:BCL:H71	1.94	0.49
1:L:30:PHE:CD1	9:M:407:U10:H312	2.47	0.49
2:M:66:TRP:CD1	2:M:121:MET:HB2	2.48	0.49
13:M:410:LMT:H62	13:S:102:LMT:H42	1.95	0.48
2:M:284:LEU:O	2:M:288:THR:OG1	2.26	0.48
2:M:94:LEU:HB3	2:M:176:TYR:HB2	1.95	0.48
2:M:225:VAL:HG23	2:M:230:GLY:HA3	1.96	0.48
5:E:48:PHE:HB3	15:F:104:SPO:H82	1.94	0.48
4:K:11:PHE:CZ	4:O:17:PHE:HB2	2.49	0.48
4:I:10:VAL:HG13	4:K:14:ARG:HG2	1.95	0.48
7:W:102:BCL:HBB3	7:Y:102:BCL:NB	2.28	0.48
4:Y:27:LEU:HD23	7:Z:101:BCL:HED2	1.94	0.48
15:D:105:SPO:H392	5:G:19:LEU:HA	1.96	0.48
4:O:48:THR:HG21	4:O:55:ALA:HB2	1.95	0.48
11:L:306:PEE:H34	13:X:101:LMT:H112	1.96	0.48
1:L:267:TRP:HB3	9:M:401:U10:H3M3	1.96	0.48
3:H:171:VAL:HG12	3:H:178:VAL:HG22	1.96	0.48
4:Q:32:HIS:CE1	7:R:102:BCL:HMD1	2.49	0.47
1:L:48:LEU:HD13	4:D:30:LEU:HD22	1.96	0.47
15:D:103:SPO:H26	15:E:101:SPO:H37	1.97	0.47
4:S:12:ASP:HB3	4:S:15[A]:ARG:HH11	1.79	0.47
4:S:36:LEU:O	4:S:42:ASN:ND2	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:413:PGV:H212	3:H:26:TYR:HE2	1.79	0.47
3:H:108:MET:HE2	3:H:214:LEU:HD13	1.96	0.47
10:H:304:PGV:H62	10:H:304:PGV:H31	1.73	0.47
7:O:102:BCL:H192	7:O:102:BCL:H161	1.73	0.47
2:M:156:TRP:CD1	7:M:403:BCL:HBB1	2.49	0.47
5:T:27:LEU:O	5:T:31:ILE:HG12	2.14	0.47
10:M:413:PGV:H202	10:M:413:PGV:H231	1.65	0.47
4:D:15:ARG:HD2	12:D:104:LDA:H21	1.95	0.47
5:W:12:THR:HG23	5:W:15:GLN:H	1.79	0.47
2:M:93:SER:OG	2:M:95:GLU:OE2	2.29	0.47
4:I:29:VAL:HG11	13:I:101:LMT:H92	1.96	0.47
7:A:101:BCL:H121	15:D:101:SPO:H292	1.97	0.47
3:H:122:ASP:OD1	3:H:228:THR:HG21	2.15	0.46
7:K:102:BCL:O1D	15:N:101:SPO:H22	2.14	0.46
7:V:101:BCL:H52	7:V:101:BCL:H8	1.61	0.46
4:Q:36:LEU:O	4:Q:42:ASN:ND2	2.48	0.46
4:S:32:HIS:CE1	7:T:102:BCL:HMD1	2.50	0.46
4:S:43:TRP:CD2	7:S:103:BCL:H2C	2.50	0.46
15:S:105:SPO:HM13	4:Y:33:LEU:HG	1.98	0.46
15:I:104:SPO:H37	5:N:22:VAL:CG2	2.41	0.46
4:Y:34:ILE:O	4:Y:37:SER:OG	2.22	0.46
9:L:304:U10:H1M2	4:D:21:GLY:HA3	1.98	0.46
15:I:104:SPO:H391	5:J:6:LEU:HD11	1.98	0.46
15:S:105:SPO:H41	4:Y:32:HIS:CG	2.51	0.46
2:M:103:LEU:HB2	13:S:102:LMT:H11	1.96	0.46
12:M:420:LDA:H82	10:Q:103:PGV:H212	1.96	0.46
3:H:97:GLU:O	4:D:15:ARG:NH2	2.33	0.46
5:B:47:TRP:CD2	7:B:101:BCL:H2C	2.51	0.46
13:M:412:LMT:H52	4:Y:26:LEU:HD22	1.98	0.46
3:H:228:THR:HG22	3:H:230:LEU:H	1.81	0.46
5:G:42:MET:HE1	5:G:48:PHE:HB2	1.97	0.46
2:M:231:GLU:OE1	2:M:231:GLU:N	2.40	0.46
7:D:102:BCL:H2A	15:E:101:SPO:H25	1.96	0.46
7:D:102:BCL:H151	7:D:102:BCL:H111	1.52	0.46
5:P:47:TRP:CE2	7:P:102:BCL:H2C	2.51	0.46
4:K:32:HIS:CE1	7:N:102:BCL:HMD1	2.51	0.45
2:M:201:HIS:CE1	2:M:205:ILE:HD11	2.51	0.45
10:M:415:PGV:H041	4:V:15:ARG:HH12	1.81	0.45
15:D:105:SPO:H403	5:E:6:LEU:HD21	1.98	0.45
5:G:47:TRP:CE2	7:G:101:BCL:H2C	2.51	0.45
4:O:32:HIS:CE1	7:P:102:BCL:HMD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z:24:MET:SD	5:Z:25:SER:N	2.90	0.45
1:L:5:SER:OG	3:H:80:GLU:OE2	2.31	0.45
5:G:8:PHE:HZ	5:J:11:LEU:HD11	1.82	0.45
4:K:48:THR:HG23	4:K:53:TYR:HB2	1.98	0.45
4:O:30:LEU:HD12	12:O:101:LDA:H123	1.97	0.45
5:J:27:LEU:O	5:J:31:ILE:HG12	2.17	0.45
5:P:12:THR:C	5:P:14:GLU:H	2.25	0.45
7:T:102:BCL:H92	7:T:102:BCL:HAA1	1.98	0.45
4:D:35:LEU:HD11	7:E:102:BCL:HHD	1.98	0.45
15:O:104:SPO:H20	15:O:104:SPO:H181	1.80	0.45
5:R:31:ILE:HD12	7:R:102:BCL:H2	1.98	0.45
5:R:44:TRP:HB2	15:R:101:SPO:H10	1.99	0.45
15:R:101:SPO:H341	15:R:101:SPO:H361	1.68	0.45
7:F:101:BCL:HAC1	7:I:102:BCL:H101	1.98	0.45
16:F:102:MYR:H82	16:F:102:MYR:H122	1.99	0.45
4:I:32:HIS:CE1	7:J:101:BCL:HMD1	2.51	0.45
15:I:104:SPO:H41	4:O:32:HIS:CG	2.52	0.45
15:O:104:SPO:H341	15:O:104:SPO:H362	1.72	0.45
5:W:42:MET:HE2	5:W:47:TRP:CE2	2.52	0.45
7:Z:101:BCL:H192	7:Z:101:BCL:H162	1.82	0.45
9:L:303:U10:H312	9:L:303:U10:H372	1.98	0.45
2:M:4:TYR:CZ	2:M:6:ASN:HA	2.52	0.45
7:M:403:BCL:HHC	7:M:404:BCL:H42	1.98	0.45
15:D:101:SPO:H6	7:D:102:BCL:HMB2	1.98	0.45
13:M:411:LMT:H11	13:M:411:LMT:H42	1.76	0.44
5:N:47:TRP:CE2	7:N:102:BCL:H2C	2.52	0.44
10:L:305:PGV:H21	10:L:305:PGV:H52	1.81	0.44
7:L:310:BCL:HMD2	2:M:205:ILE:HD13	1.98	0.44
13:L:311:LMT:H51	13:L:311:LMT:H22	1.58	0.44
2:M:29:GLU:HG3	4:V:15:ARG:NH2	2.32	0.44
4:A:1:FME:HE1	5:E:29:ALA:HB2	1.99	0.44
4:A:28:ALA:O	4:A:32:HIS:ND1	2.32	0.44
15:G:102:SPO:H25	7:I:102:BCL:HED3	1.97	0.44
15:O:104:SPO:H26	15:O:104:SPO:H241	1.81	0.44
10:L:305:PGV:H11	13:I:101:LMT:H123	1.99	0.44
15:I:103:SPO:H20	15:I:103:SPO:H181	1.82	0.44
15:S:105:SPO:H293	15:W:101:SPO:H392	1.99	0.44
7:W:102:BCL:H112	7:W:102:BCL:H72	1.80	0.44
1:L:116:PHE:CE2	12:L:307:LDA:H12	2.52	0.44
1:L:207:MET:HE1	2:M:238:ALA:HB2	1.98	0.44
7:A:101:BCL:H62	7:A:101:BCL:H41	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:31:ILE:HD12	7:T:102:BCL:H2	2.00	0.44
9:L:304:U10:H261	4:A:26:LEU:HD22	1.99	0.44
2:M:89:LEU:HB3	9:M:401:U10:H1M3	1.99	0.44
12:M:420:LDA:H52	12:M:420:LDA:H21	1.78	0.44
15:D:101:SPO:H133	15:E:101:SPO:H301	1.98	0.44
10:Q:103:PGV:H32	7:S:103:BCL:H93	1.99	0.44
15:O:103:SPO:H26	15:O:103:SPO:H241	1.86	0.44
15:P:101:SPO:H20	15:P:101:SPO:H181	1.89	0.44
5:W:42:MET:HE1	5:W:48:PHE:HB2	2.00	0.44
15:W:101:SPO:H15	15:W:101:SPO:H131	1.89	0.44
4:A:39:PRO:HA	4:A:42:ASN:HB2	2.00	0.44
4:S:17:PHE:CE2	15:S:104:SPO:H351	2.53	0.44
7:J:101:BCL:H162	7:J:101:BCL:H141	1.76	0.44
7:V:101:BCL:H2A	15:W:101:SPO:H25	2.00	0.44
2:M:296:TRP:O	2:M:300:HIS:HD2	2.01	0.44
4:Q:36:LEU:HG	12:Q:102:LDA:H41	2.00	0.44
5:W:42:MET:HE2	5:W:47:TRP:CZ2	2.53	0.44
15:F:104:SPO:H20	15:F:104:SPO:H181	1.84	0.43
15:P:101:SPO:H10	15:P:101:SPO:H81	1.89	0.43
4:S:1:FME:HA	4:S:4:PHE:CE2	2.53	0.43
3:H:228:THR:HG22	3:H:230:LEU:N	2.33	0.43
15:D:103:SPO:H392	5:E:19:LEU:HA	2.01	0.43
7:F:101:BCL:H2A	7:F:101:BCL:HED3	1.99	0.43
4:K:4:PHE:O	4:K:7:ILE:HG22	2.18	0.43
15:M:408:SPO:H10	15:M:408:SPO:H81	1.91	0.43
4:V:1:FME:HA	4:V:4:PHE:HE1	1.82	0.43
2:M:160:GLY:HA3	15:M:408:SPO:H292	2.01	0.43
4:A:6:LYS:HD3	15:D:103:SPO:H393	2.00	0.43
7:G:101:BCL:H93	7:G:101:BCL:H61	1.81	0.43
7:O:102:BCL:HED3	15:P:101:SPO:H27	2.01	0.43
7:A:101:BCL:H93	7:A:101:BCL:H61	1.77	0.43
7:K:102:BCL:H41	7:K:102:BCL:H62	1.66	0.43
15:S:105:SPO:H20	15:S:105:SPO:H181	1.79	0.43
10:L:305:PGV:H51	10:L:305:PGV:H261	2.00	0.43
2:M:33:ALA:HB2	2:M:49:PRO:HD3	2.01	0.43
2:M:274:MET:O	2:M:278:THR:OG1	2.32	0.43
13:L:308:LMT:H5B	13:L:308:LMT:H6E	2.00	0.43
15:M:408:SPO:H15	15:M:408:SPO:H131	1.93	0.43
10:M:415:PGV:H72	4:S:22:VAL:HG11	2.01	0.43
5:N:6:LEU:HD11	15:O:103:SPO:H391	2.01	0.43
7:F:103:BCL:HHD	5:G:41:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:102:BCL:HED3	15:N:101:SPO:H27	2.01	0.43
15:N:101:SPO:H15	15:N:101:SPO:H131	1.77	0.43
4:O:1:FME:HA	4:O:4:PHE:CE1	2.53	0.43
13:L:311:LMT:O2'	7:F:101:BCL:HED2	2.18	0.43
7:D:102:BCL:H202	7:D:102:BCL:H162	1.73	0.43
5:G:27:LEU:O	5:G:31:ILE:HG12	2.18	0.43
4:K:3:LYS:NZ	4:K:6:LYS:HD2	2.34	0.43
15:W:101:SPO:H20	15:W:101:SPO:H181	1.89	0.43
15:W:101:SPO:H291	15:W:101:SPO:H312	1.85	0.43
9:L:304:U10:H403	13:A:102:LMT:H82	2.01	0.43
1:L:146:ALA:O	6:X:65:TYR:OH	2.28	0.42
2:M:284:LEU:HD23	2:M:284:LEU:HA	1.91	0.42
13:I:101:LMT:O6B	13:I:101:LMT:O3'	2.31	0.42
15:S:104:SPO:H10	15:S:104:SPO:H81	1.93	0.42
2:M:122:ALA:HA	2:M:156:TRP:HH2	1.84	0.42
2:M:203:LEU:HD23	10:M:402:PGV:H241	2.01	0.42
5:W:48:PHE:HD2	7:W:102:BCL:H171	1.84	0.42
2:M:100:GLU:O	13:S:102:LMT:H6'1	2.19	0.42
2:M:105:LEU:HB3	13:Y:101:LMT:O2'	2.19	0.42
3:H:137:MET:HG3	3:H:169:MET:HB2	2.01	0.42
4:Q:34:ILE:O	4:Q:38:THR:HG23	2.19	0.42
3:H:194:PRO:O	3:H:198:LEU:HG	2.20	0.42
7:D:102:BCL:HHH	5:E:41:VAL:HG21	2.01	0.42
7:F:101:BCL:C4B	4:I:22:VAL:HG22	2.49	0.42
5:N:47:TRP:CD2	7:N:102:BCL:H2C	2.54	0.42
1:L:250:LEU:HD12	1:L:250:LEU:HA	1.83	0.42
2:M:283:ILE:HG12	7:M:404:BCL:HED3	2.02	0.42
7:K:102:BCL:H161	7:K:102:BCL:H141	1.75	0.42
3:H:192:LEU:HB2	3:H:235:ILE:HD13	2.02	0.42
5:B:22:VAL:HG13	15:D:101:SPO:H362	2.01	0.42
15:F:104:SPO:H15	15:F:104:SPO:H131	1.96	0.42
13:M:410:LMT:H6'2	4:S:38:THR:HB	2.02	0.42
15:G:102:SPO:H22	7:I:102:BCL:O1D	2.20	0.42
4:Q:5:TYR:CZ	4:Q:6:LYS:HE3	2.54	0.42
5:R:6:LEU:HB3	5:R:7:SER:H	1.71	0.42
15:D:105:SPO:H241	15:D:105:SPO:H26	1.78	0.42
4:F:32:HIS:CE1	7:G:101:BCL:HMD1	2.53	0.42
4:O:11:PHE:HE2	4:Q:17:PHE:HD2	1.67	0.42
15:O:104:SPO:H15	15:O:104:SPO:H131	1.94	0.42
1:L:186:TRP:CZ3	9:L:303:U10:H153	2.55	0.42
4:A:44:LEU:HD11	13:A:102:LMT:O2'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:7:GLU:HA	2:M:249:LEU:HD11	2.02	0.42
1:L:178:ILE:HD13	7:M:403:BCL:HMD2	2.02	0.42
10:H:303:PGV:H21	10:H:303:PGV:H52	1.86	0.42
15:E:101:SPO:H42	15:E:101:SPO:H83	2.02	0.42
5:J:47:TRP:CE2	7:J:101:BCL:H2C	2.55	0.42
4:Q:24:LEU:HD23	4:Q:24:LEU:HA	1.90	0.42
5:R:27:LEU:O	5:R:31:ILE:HG12	2.20	0.42
7:S:103:BCL:H122	15:T:101:SPO:H341	2.02	0.42
9:L:304:U10:C43	9:L:304:U10:H401	2.49	0.41
4:D:7:ILE:HD11	15:D:105:SPO:H311	2.01	0.41
5:G:47:TRP:CD2	7:G:101:BCL:H2C	2.54	0.41
15:O:104:SPO:H10	15:O:104:SPO:H81	1.94	0.41
6:X:8:PHE:HB2	6:X:21:TRP:CE2	2.55	0.41
1:L:200:ASN:HB3	10:M:413:PGV:H041	2.02	0.41
1:L:264:TRP:HH2	9:L:303:U10:H351	1.85	0.41
8:M:405:BPH:HBA2	8:M:405:BPH:H3A	1.73	0.41
5:B:31:ILE:HD13	7:B:101:BCL:H51	2.02	0.41
7:R:102:BCL:H52	15:T:101:SPO:H243	2.02	0.41
15:T:101:SPO:H20	15:T:101:SPO:H181	1.82	0.41
4:V:40:ALA:O	5:W:45:ARG:NH1	2.53	0.41
9:L:304:U10:H521	9:L:304:U10:H501	1.71	0.41
2:M:14:ALA:HA	3:H:176:GLN:HE21	1.86	0.41
3:H:217:THR:OG1	3:H:238:TYR:OH	2.29	0.41
4:K:11:PHE:CZ	4:O:14:ARG:HA	2.54	0.41
5:N:42:MET:HE1	5:N:48:PHE:HB2	2.03	0.41
10:M:413:PGV:H252	10:M:414:PGV:H201	2.01	0.41
15:S:104:SPO:H132	7:V:101:BCL:H61	2.02	0.41
9:M:407:U10:H301	9:M:407:U10:H321	1.74	0.41
15:E:101:SPO:H10	15:E:101:SPO:H81	1.64	0.41
7:F:101:BCL:H191	4:I:33:LEU:HD12	2.03	0.41
7:G:101:BCL:H61	7:G:101:BCL:H2	1.66	0.41
7:K:102:BCL:HHD	7:K:102:BCL:HAC1	1.86	0.41
5:P:42:MET:HE3	7:P:102:BCL:H161	2.01	0.41
7:P:102:BCL:H93	7:P:102:BCL:H62	1.75	0.41
7:V:101:BCL:H162	7:V:101:BCL:H141	1.84	0.41
1:L:131:VAL:HA	1:L:135:ILE:HB	2.03	0.41
1:L:250:LEU:O	1:L:254:THR:OG1	2.28	0.41
4:O:26:LEU:HD13	4:O:26:LEU:HA	1.93	0.41
5:R:36:LEU:HD13	5:R:36:LEU:HA	1.91	0.41
15:S:104:SPO:H20	15:S:104:SPO:H181	1.78	0.41
7:I:102:BCL:H162	7:I:102:BCL:H192	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:20:GLN:HE21	4:V:20:GLN:HB3	1.66	0.41
1:L:129:TYR:O	1:L:133:VAL:HG22	2.20	0.41
2:M:233:GLU:O	2:M:237:ILE:HG13	2.21	0.41
12:M:420:LDA:H92	12:M:420:LDA:H61	1.87	0.41
4:F:34:ILE:O	4:F:38:THR:HG23	2.20	0.41
5:J:6:LEU:HD21	5:N:19:LEU:HD12	2.02	0.41
7:N:102:BCL:H162	7:N:102:BCL:H202	1.70	0.41
15:W:101:SPO:H10	15:W:101:SPO:H81	1.81	0.41
1:L:39:THR:HG21	1:L:101:TRP:HE3	1.85	0.41
2:M:277:LEU:HD21	10:M:414:PGV:H261	2.03	0.41
8:M:405:BPH:H6C2	8:M:405:BPH:H4C1	1.82	0.41
13:M:412:LMT:H6E	4:Y:33:LEU:HB3	2.02	0.41
5:E:6:LEU:H	5:G:15:GLN:NE2	2.19	0.41
3:H:132:ASN:HB2	3:H:135:GLN:HE21	1.86	0.40
3:H:222:LYS:HG2	3:H:231:GLU:OE2	2.20	0.40
3:H:223:SER:HB2	3:H:226:VAL:HB	2.02	0.40
4:A:17:PHE:CE2	6:X:22:ILE:HG12	2.55	0.40
15:D:101:SPO:H26	15:D:101:SPO:H241	1.86	0.40
4:Q:36:LEU:HD13	4:Q:43:TRP:CH2	2.56	0.40
7:T:102:BCL:H162	7:T:102:BCL:H192	1.73	0.40
13:L:308:LMT:H121	13:L:308:LMT:H92	1.88	0.40
3:H:73:VAL:O	3:H:76:SER:OG	2.37	0.40
4:F:11:PHE:HB3	4:F:16:VAL:HG21	2.02	0.40
4:Q:41:PHE:CE2	5:R:45:ARG:HG2	2.56	0.40
10:Q:103:PGV:H242	4:S:22:VAL:HG23	2.03	0.40
4:S:37:SER:HA	13:S:101:LMT:H1B	2.03	0.40
7:S:103:BCL:H161	7:S:103:BCL:H202	1.80	0.40
1:L:170:TYR:HA	1:L:175:MET:HE3	2.02	0.40
10:M:413:PGV:H131	10:M:413:PGV:H102	1.77	0.40
3:H:61:PRO:HA	3:H:75:PRO:HD2	2.03	0.40
15:I:103:SPO:H6	7:K:102:BCL:HMB2	2.03	0.40
7:F:101:BCL:H93	7:F:101:BCL:H111	1.95	0.40
8:L:302:BPH:H141	7:L:310:BCL:HBB3	2.03	0.40
2:M:11:VAL:HG11	3:H:169:MET:HE1	2.04	0.40
15:N:101:SPO:H10	15:N:101:SPO:H81	1.90	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	L	280/282 (99%)	274 (98%)	6 (2%)	0	100	100
2	M	302/307 (98%)	293 (97%)	9 (3%)	0	100	100
3	H	246/253 (97%)	240 (98%)	6 (2%)	0	100	100
4	A	42/58 (72%)	41 (98%)	1 (2%)	0	100	100
4	D	54/58 (93%)	52 (96%)	2 (4%)	0	100	100
4	F	52/58 (90%)	52 (100%)	0	0	100	100
4	I	54/58 (93%)	52 (96%)	2 (4%)	0	100	100
4	K	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
4	O	54/58 (93%)	52 (96%)	2 (4%)	0	100	100
4	Q	54/58 (93%)	53 (98%)	1 (2%)	0	100	100
4	S	55/58 (95%)	51 (93%)	4 (7%)	0	100	100
4	V	54/58 (93%)	51 (94%)	2 (4%)	1 (2%)	6	13
4	Y	40/58 (69%)	40 (100%)	0	0	100	100
5	B	42/49 (86%)	40 (95%)	2 (5%)	0	100	100
5	E	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
5	G	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	J	42/49 (86%)	40 (95%)	2 (5%)	0	100	100
5	N	41/49 (84%)	41 (100%)	0	0	100	100
5	P	41/49 (84%)	39 (95%)	2 (5%)	0	100	100
5	R	41/49 (84%)	41 (100%)	0	0	100	100
5	T	41/49 (84%)	41 (100%)	0	0	100	100
5	W	39/49 (80%)	38 (97%)	1 (3%)	0	100	100
5	Z	29/49 (59%)	29 (100%)	0	0	100	100
6	X	63/78 (81%)	60 (95%)	3 (5%)	0	100	100
All	All	1802/1990 (91%)	1753 (97%)	48 (3%)	1 (0%)	49	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	V	2	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	227/227 (100%)	226 (100%)	1 (0%)	84	93
2	M	236/239 (99%)	234 (99%)	2 (1%)	73	88
3	H	213/217 (98%)	211 (99%)	2 (1%)	70	87
4	A	39/47 (83%)	36 (92%)	3 (8%)	12	27
4	D	46/47 (98%)	45 (98%)	1 (2%)	45	72
4	F	46/47 (98%)	45 (98%)	1 (2%)	45	72
4	I	46/47 (98%)	45 (98%)	1 (2%)	45	72
4	K	46/47 (98%)	46 (100%)	0	100	100
4	O	45/47 (96%)	43 (96%)	2 (4%)	25	50
4	Q	46/47 (98%)	45 (98%)	1 (2%)	45	72
4	S	47/47 (100%)	47 (100%)	0	100	100
4	V	46/47 (98%)	44 (96%)	2 (4%)	26	51
4	Y	35/47 (74%)	33 (94%)	2 (6%)	18	40
5	B	35/39 (90%)	34 (97%)	1 (3%)	37	65
5	E	35/39 (90%)	34 (97%)	1 (3%)	37	65
5	G	34/39 (87%)	33 (97%)	1 (3%)	37	65
5	J	35/39 (90%)	33 (94%)	2 (6%)	18	40
5	N	34/39 (87%)	34 (100%)	0	100	100
5	P	34/39 (87%)	33 (97%)	1 (3%)	37	65
5	R	33/39 (85%)	31 (94%)	2 (6%)	17	37
5	T	34/39 (87%)	34 (100%)	0	100	100
5	W	28/39 (72%)	28 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Z	20/39 (51%)	20 (100%)	0	100	100
6	X	50/62 (81%)	48 (96%)	2 (4%)	28	55
All	All	1490/1605 (93%)	1462 (98%)	28 (2%)	49	75

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	248	CYS
2	M	52	LEU
2	M	215	PHE
3	H	228	THR
3	H	233	ASP
4	A	35	LEU
4	A	43	TRP
4	A	44	LEU
5	B	18	GLU
4	D	33	LEU
5	E	6	LEU
4	F	54	VAL
5	G	19	LEU
4	I	10	VAL
5	J	6	LEU
5	J	42	MET
4	O	12	ASP
4	O	26	LEU
5	P	19	LEU
4	Q	9	LEU
5	R	19	LEU
5	R	36	LEU
4	V	5	TYR
4	V	34	ILE
4	Y	31	ILE
4	Y	32	HIS
6	X	20	ILE
6	X	53	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	63	GLN

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Mol	Chain	Res	Type
1	L	77	ASN
1	L	117	HIS
2	M	12	GLN
2	M	44	ASN
2	M	144	HIS
2	M	258	ASN
3	H	44	ASN
3	H	135	GLN
3	H	176	GLN
4	D	51	HIS
5	E	17	GLN
4	I	20	GLN
5	J	17	GLN
5	N	15	GLN
4	O	51	HIS
4	V	20	GLN
5	W	17	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
4	FME	F	1	4	8,9,10	0.52	0	8,9,11	1.12	1 (12%)
4	FME	S	1	4	5,6,10	0.82	0	4,6,11	1.08	0
4	FME	Q	1	4	8,9,10	0.56	0	8,9,11	0.92	1 (12%)
4	FME	D	1	4	8,9,10	0.55	0	8,9,11	0.98	1 (12%)
4	FME	K	1	4	8,9,10	0.57	0	8,9,11	0.93	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FME	I	1	4	8,9,10	0.56	0	8,9,11	0.91	1 (12%)
4	FME	V	1	4	8,9,10	0.58	0	8,9,11	0.89	1 (12%)
4	FME	O	1	4	8,9,10	0.55	0	8,9,11	1.02	1 (12%)
4	FME	A	1	4	8,9,10	0.56	0	8,9,11	0.89	1 (12%)

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
4	FME	F	1	4	-	1/7/9/11	-
4	FME	S	1	4	-	2/3/5/11	-
4	FME	Q	1	4	-	0/7/9/11	-
4	FME	D	1	4	-	0/7/9/11	-
4	FME	K	1	4	-	1/7/9/11	-
4	FME	I	1	4	-	1/7/9/11	-
4	FME	V	1	4	-	1/7/9/11	-
4	FME	O	1	4	-	1/7/9/11	-
4	FME	A	1	4	-	1/7/9/11	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	1	FME	O-C-CA	-2.63	118.00	124.77
4	F	1	FME	O-C-CA	-2.57	118.16	124.77
4	D	1	FME	O-C-CA	-2.56	118.18	124.77
4	I	1	FME	O-C-CA	-2.50	118.35	124.77
4	V	1	FME	O-C-CA	-2.47	118.42	124.77
4	K	1	FME	O-C-CA	-2.45	118.47	124.77
4	Q	1	FME	O-C-CA	-2.45	118.47	124.77
4	A	1	FME	O-C-CA	-2.39	118.63	124.77

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	FME	O1-CN-N-CA
4	F	1	FME	O1-CN-N-CA

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Mol	Chain	Res	Type	Atoms
4	O	1	FME	O1-CN-N-CA
4	S	1	FME	O1-CN-N-CA
4	S	1	FME	O-C-CA-CB
4	I	1	FME	N-CA-CB-CG
4	V	1	FME	N-CA-CB-CG
4	K	1	FME	N-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	FME	1	0
4	S	1	FME	1	0
4	V	1	FME	1	0
4	O	1	FME	2	0
4	A	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 89 ligands modelled in this entry, 1 is monoatomic - leaving 88 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	$\# Z > 2$
15	SPO	E	101	-	41,41,41	0.62	0	47,50,50	2.12	15 (31%)
15	SPO	P	101	-	41,41,41	0.59	0	47,50,50	1.91	17 (36%)
10	PGV	H	303	-	42,42,50	0.98	2 (4%)	45,48,56	1.16	5 (11%)
12	LDA	O	101	-	13,15,15	2.19	2 (15%)	14,17,17	0.53	0
15	SPO	S	105	-	41,41,41	0.57	0	47,50,50	2.02	15 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BCL	R	102	-	69,74,74	1.80	18 (26%)	79,115,115	2.17	23 (29%)
10	PGV	M	402	-	35,35,50	1.07	2 (5%)	38,41,56	1.15	3 (7%)
9	U10	L	304	-	63,63,63	0.65	2 (3%)	78,79,79	0.61	0
7	BCL	G	101	-	69,74,74	1.79	18 (26%)	79,115,115	2.12	20 (25%)
7	BCL	L	310	-	69,74,74	1.78	17 (24%)	79,115,115	2.19	22 (27%)
8	BPH	M	405	-	59,70,70	0.80	3 (5%)	59,101,101	0.95	4 (6%)
13	LMT	M	410	-	36,36,36	0.36	0	47,47,47	0.87	3 (6%)
13	LMT	X	102	-	36,36,36	0.41	0	47,47,47	0.74	1 (2%)
10	PGV	L	305	-	38,38,50	1.05	2 (5%)	41,44,56	1.12	2 (4%)
8	BPH	L	302	-	59,70,70	0.86	3 (5%)	59,101,101	0.95	3 (5%)
13	LMT	I	101	-	36,36,36	0.33	0	47,47,47	1.04	3 (6%)
7	BCL	E	102	-	69,74,74	1.79	19 (27%)	79,115,115	2.19	22 (27%)
13	LMT	S	102	-	34,34,36	0.38	0	45,45,47	0.73	1 (2%)
7	BCL	K	102	-	69,74,74	1.79	18 (26%)	79,115,115	2.31	25 (31%)
15	SPO	R	101	-	41,41,41	0.64	0	47,50,50	2.04	17 (36%)
7	BCL	V	101	-	69,74,74	1.78	18 (26%)	79,115,115	2.27	23 (29%)
13	LMT	Q	101	-	36,36,36	0.45	0	47,47,47	0.84	1 (2%)
12	LDA	D	104	-	13,15,15	2.20	2 (15%)	14,17,17	0.61	0
7	BCL	S	103	-	69,74,74	1.79	19 (27%)	79,115,115	2.35	23 (29%)
13	LMT	Y	101	-	29,29,36	0.43	0	40,40,47	0.76	1 (2%)
7	BCL	L	301	-	69,74,74	1.78	18 (26%)	79,115,115	2.27	23 (29%)
16	MYR	F	102	7	15,15,15	0.58	0	15,15,15	0.55	0
15	SPO	I	103	-	41,41,41	0.57	0	47,50,50	1.99	15 (31%)
15	SPO	M	408	-	41,41,41	0.58	0	47,50,50	1.97	13 (27%)
13	LMT	M	412	-	33,33,36	0.38	0	44,44,47	0.82	1 (2%)
13	LMT	L	309	-	35,35,36	0.39	0	46,46,47	0.73	1 (2%)
13	LMT	M	409	-	25,25,36	0.48	0	36,36,47	1.01	1 (2%)
15	SPO	D	105	-	41,41,41	0.58	0	47,50,50	2.02	14 (29%)
13	LMT	L	311	-	36,36,36	0.38	0	47,47,47	0.94	1 (2%)
12	LDA	M	419	-	13,15,15	2.18	2 (15%)	14,17,17	0.45	0
7	BCL	F	101	16	69,74,74	1.84	17 (24%)	79,115,115	2.18	22 (27%)
7	BCL	M	403	-	69,74,74	1.81	18 (26%)	79,115,115	2.13	20 (25%)
10	PGV	M	414	-	34,34,50	1.09	2 (5%)	37,40,56	1.17	3 (8%)
7	BCL	J	101	-	69,74,74	1.79	18 (26%)	79,115,115	2.13	23 (29%)
13	LMT	K	101	-	36,36,36	0.41	0	47,47,47	0.85	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	SPO	S	104	-	41,41,41	0.58	0	47,50,50	2.09	16 (34%)
10	PGV	H	304	-	33,33,50	1.11	2 (6%)	36,39,56	1.16	3 (8%)
13	LMT	S	101	-	27,27,36	0.44	0	38,38,47	0.88	2 (5%)
12	LDA	M	416	-	13,15,15	2.17	2 (15%)	14,17,17	0.46	0
7	BCL	P	102	-	69,74,74	1.77	18 (26%)	79,115,115	2.17	23 (29%)
12	LDA	M	418	-	13,15,15	2.21	2 (15%)	14,17,17	0.53	0
10	PGV	M	415	-	37,37,50	1.06	2 (5%)	40,43,56	1.13	3 (7%)
15	SPO	D	101	-	41,41,41	0.58	0	47,50,50	1.92	13 (27%)
12	LDA	Q	104	-	9,11,15	2.64	2 (22%)	10,13,17	0.44	0
9	U10	L	303	-	48,48,63	0.70	2 (4%)	60,61,79	0.68	1 (1%)
7	BCL	I	102	-	69,74,74	1.77	19 (27%)	79,115,115	2.33	25 (31%)
7	BCL	B	101	-	69,74,74	1.80	19 (27%)	79,115,115	2.16	23 (29%)
7	BCL	N	102	-	69,74,74	1.78	17 (24%)	79,115,115	2.17	21 (26%)
15	SPO	N	101	-	41,41,41	0.62	0	47,50,50	2.00	17 (36%)
13	LMT	M	411	-	36,36,36	0.35	0	47,47,47	0.74	1 (2%)
12	LDA	H	301	-	13,15,15	2.21	2 (15%)	14,17,17	0.49	0
10	PGV	Q	103	-	34,34,50	1.11	2 (5%)	37,40,56	1.16	3 (8%)
11	PEE	L	306	-	45,45,50	0.79	2 (4%)	48,50,55	0.55	0
12	LDA	L	307	-	13,15,15	2.15	2 (15%)	14,17,17	0.49	0
7	BCL	A	101	-	64,69,74	1.90	17 (26%)	73,109,115	2.29	23 (31%)
9	U10	M	401	-	20,20,63	1.00	2 (10%)	25,27,79	0.96	1 (4%)
7	BCL	Q	105	-	69,74,74	1.78	19 (27%)	79,115,115	2.31	25 (31%)
12	LDA	M	420	-	13,15,15	2.19	2 (15%)	14,17,17	0.58	0
15	SPO	T	101	-	41,41,41	0.59	0	47,50,50	1.90	15 (31%)
7	BCL	F	103	-	69,74,74	1.78	19 (27%)	79,115,115	2.28	22 (27%)
15	SPO	D	103	-	41,41,41	0.57	0	47,50,50	2.13	16 (34%)
15	SPO	O	104	-	41,41,41	0.58	0	47,50,50	2.16	17 (36%)
15	SPO	O	103	-	41,41,41	0.57	0	47,50,50	1.92	12 (25%)
15	SPO	G	102	-	41,41,41	0.58	0	47,50,50	2.07	17 (36%)
12	LDA	Q	102	-	6,8,15	3.30	2 (33%)	7,10,17	0.34	0
15	SPO	F	104	-	41,41,41	0.60	0	47,50,50	2.01	15 (31%)
15	SPO	W	101	-	41,41,41	0.60	0	47,50,50	1.90	14 (29%)
7	BCL	Z	101	-	69,74,74	1.88	17 (24%)	79,115,115	2.14	22 (27%)
13	LMT	L	308	-	36,36,36	0.35	0	47,47,47	0.72	0
7	BCL	M	404	-	69,74,74	1.80	19 (27%)	79,115,115	2.29	23 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BCL	W	102	-	69,74,74	1.82	17 (24%)	79,115,115	2.12	21 (26%)
7	BCL	T	102	-	69,74,74	1.81	17 (24%)	79,115,115	2.16	21 (26%)
10	PGV	M	413	-	44,44,50	0.97	2 (4%)	47,50,56	1.12	2 (4%)
9	U10	M	407	-	48,48,63	0.73	2 (4%)	60,61,79	0.68	2 (3%)
7	BCL	Y	102	-	69,74,74	1.85	17 (24%)	79,115,115	2.16	23 (29%)
12	LDA	H	302	-	11,13,15	2.41	2 (18%)	12,15,17	0.46	0
13	LMT	A	102	-	33,33,36	0.47	0	44,44,47	0.98	2 (4%)
13	LMT	Y	103	-	28,28,36	0.45	0	39,39,47	0.75	1 (2%)
7	BCL	O	102	-	69,74,74	1.77	19 (27%)	79,115,115	2.32	24 (30%)
7	BCL	D	102	-	69,74,74	1.79	20 (28%)	79,115,115	2.33	23 (29%)
13	LMT	M	417	-	34,34,36	0.39	0	45,45,47	0.69	1 (2%)
13	LMT	X	101	-	36,36,36	0.43	0	47,47,47	0.91	2 (4%)
15	SPO	I	104	-	41,41,41	0.57	0	47,50,50	2.07	18 (38%)

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
15	SPO	E	101	-	-	14/47/47/47	-
15	SPO	P	101	-	-	5/47/47/47	-
10	PGV	H	303	-	-	8/47/47/55	-
12	LDA	O	101	-	-	2/13/13/13	-
15	SPO	S	105	-	-	5/47/47/47	-
7	BCL	R	102	-	-	14/41/137/137	-
10	PGV	M	402	-	-	16/40/40/55	-
9	U10	L	304	-	-	17/63/87/87	0/1/1/1
7	BCL	G	101	-	-	14/41/137/137	-
7	BCL	L	310	-	-	8/41/137/137	-
8	BPH	M	405	-	-	3/37/105/105	0/5/6/6
13	LMT	M	410	-	-	4/21/61/61	0/2/2/2
13	LMT	X	102	-	-	4/21/61/61	0/2/2/2
10	PGV	L	305	-	-	13/43/43/55	-
8	BPH	L	302	-	-	4/37/105/105	0/5/6/6
13	LMT	I	101	-	-	6/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	E	102	-	-	14/41/137/137	-
13	LMT	S	102	-	-	4/19/59/61	0/2/2/2
7	BCL	K	102	-	-	10/41/137/137	-
15	SPO	R	101	-	-	9/47/47/47	-
7	BCL	V	101	-	-	11/41/137/137	-
13	LMT	Q	101	-	-	7/21/61/61	0/2/2/2
12	LDA	D	104	-	-	9/13/13/13	-
7	BCL	S	103	-	-	7/41/137/137	-
13	LMT	Y	101	-	-	4/14/54/61	0/2/2/2
7	BCL	L	301	-	-	7/41/137/137	-
16	MYR	F	102	7	-	5/13/13/13	-
15	SPO	I	103	-	-	4/47/47/47	-
15	SPO	M	408	-	-	4/47/47/47	-
13	LMT	M	412	-	-	1/18/58/61	0/2/2/2
13	LMT	L	309	-	-	8/20/60/61	0/2/2/2
13	LMT	M	409	-	-	1/10/50/61	0/2/2/2
15	SPO	D	105	-	-	4/47/47/47	-
13	LMT	L	311	-	-	6/21/61/61	0/2/2/2
12	LDA	M	419	-	-	2/13/13/13	-
7	BCL	F	101	16	-	14/41/137/137	-
7	BCL	M	403	-	-	14/41/137/137	-
10	PGV	M	414	-	-	5/39/39/55	-
7	BCL	J	101	-	-	11/41/137/137	-
13	LMT	K	101	-	-	5/21/61/61	0/2/2/2
15	SPO	S	104	-	-	4/47/47/47	-
10	PGV	H	304	-	-	18/38/38/55	-
13	LMT	S	101	-	-	6/12/52/61	0/2/2/2
12	LDA	M	416	-	-	1/13/13/13	-
7	BCL	P	102	-	-	10/41/137/137	-
12	LDA	M	418	-	-	2/13/13/13	-
10	PGV	M	415	-	-	8/42/42/55	-
15	SPO	D	101	-	-	5/47/47/47	-
12	LDA	Q	104	-	-	2/9/9/13	-
9	U10	L	303	-	-	11/45/69/87	0/1/1/1
7	BCL	I	102	-	-	9/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	B	101	-	-	9/41/137/137	-
7	BCL	N	102	-	-	15/41/137/137	-
15	SPO	N	101	-	-	9/47/47/47	-
13	LMT	M	411	-	-	3/21/61/61	0/2/2/2
12	LDA	H	301	-	-	7/13/13/13	-
10	PGV	Q	103	-	-	11/39/39/55	-
11	PEE	L	306	-	-	10/49/49/54	-
12	LDA	L	307	-	-	2/13/13/13	-
7	BCL	A	101	-	-	11/35/131/137	-
9	U10	M	401	-	-	4/12/36/87	0/1/1/1
7	BCL	Q	105	-	-	15/41/137/137	-
12	LDA	M	420	-	-	3/13/13/13	-
15	SPO	T	101	-	-	4/47/47/47	-
7	BCL	F	103	-	-	9/41/137/137	-
15	SPO	D	103	-	-	6/47/47/47	-
15	SPO	O	104	-	-	4/47/47/47	-
15	SPO	O	103	-	-	1/47/47/47	-
15	SPO	G	102	-	-	12/47/47/47	-
12	LDA	Q	102	-	-	0/6/6/13	-
15	SPO	F	104	-	-	10/47/47/47	-
15	SPO	W	101	-	-	3/47/47/47	-
7	BCL	Z	101	-	-	11/41/137/137	-
13	LMT	L	308	-	-	1/21/61/61	0/2/2/2
7	BCL	M	404	-	-	8/41/137/137	-
7	BCL	W	102	-	-	14/41/137/137	-
7	BCL	T	102	-	-	9/41/137/137	-
10	PGV	M	413	-	-	15/49/49/55	-
9	U10	M	407	-	-	5/45/69/87	0/1/1/1
7	BCL	Y	102	-	-	7/41/137/137	-
12	LDA	H	302	-	-	2/11/11/13	-
13	LMT	A	102	-	-	6/18/58/61	0/2/2/2
13	LMT	Y	103	-	-	6/13/53/61	0/2/2/2
7	BCL	O	102	-	-	11/41/137/137	-
7	BCL	D	102	-	-	14/41/137/137	-
13	LMT	M	417	-	-	7/19/59/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	LMT	X	101	-	-	6/21/61/61	0/2/2/2
15	SPO	I	104	-	-	4/47/47/47	-

All (506) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	301	LDA	O1-N1	-6.96	1.25	1.42
12	M	420	LDA	O1-N1	-6.91	1.25	1.42
12	M	419	LDA	O1-N1	-6.88	1.25	1.42
12	Q	102	LDA	O1-N1	-6.88	1.25	1.42
12	M	416	LDA	O1-N1	-6.87	1.25	1.42
12	L	307	LDA	O1-N1	-6.86	1.25	1.42
12	M	418	LDA	O1-N1	-6.86	1.25	1.42
12	H	302	LDA	O1-N1	-6.84	1.25	1.42
12	Q	104	LDA	O1-N1	-6.84	1.25	1.42
12	O	101	LDA	O1-N1	-6.80	1.25	1.42
12	D	104	LDA	O1-N1	-6.79	1.25	1.42
7	A	101	BCL	O2D-CGD	5.06	1.45	1.33
7	Z	101	BCL	O2D-CGD	5.06	1.45	1.33
7	M	404	BCL	O2D-CGD	5.06	1.45	1.33
7	B	101	BCL	O2D-CGD	5.05	1.45	1.33
7	Y	102	BCL	O2D-CGD	5.05	1.45	1.33
7	F	101	BCL	O2D-CGD	5.03	1.45	1.33
7	W	102	BCL	O2D-CGD	5.02	1.45	1.33
7	L	301	BCL	C3D-C4D	-5.01	1.32	1.44
7	L	301	BCL	O2D-CGD	4.99	1.45	1.33
7	M	403	BCL	C3D-C4D	-4.98	1.33	1.44
7	R	102	BCL	O2D-CGD	4.97	1.45	1.33
7	J	101	BCL	C3D-C4D	-4.97	1.33	1.44
7	J	101	BCL	O2D-CGD	4.95	1.45	1.33
7	N	102	BCL	O2D-CGD	4.94	1.45	1.33
7	M	404	BCL	C3D-C4D	-4.93	1.33	1.44
7	F	103	BCL	O2D-CGD	4.93	1.45	1.33
7	T	102	BCL	O2D-CGD	4.93	1.45	1.33
7	D	102	BCL	O2D-CGD	4.92	1.45	1.33
7	P	102	BCL	O2D-CGD	4.92	1.45	1.33
7	L	310	BCL	C3D-C4D	-4.92	1.33	1.44
7	G	101	BCL	C3D-C4D	-4.92	1.33	1.44
7	S	103	BCL	O2D-CGD	4.90	1.45	1.33
7	Q	105	BCL	O2D-CGD	4.90	1.45	1.33
7	E	102	BCL	C3D-C4D	-4.89	1.33	1.44
7	K	102	BCL	C3D-C4D	-4.89	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	103	BCL	C3D-C4D	-4.89	1.33	1.44
7	N	102	BCL	C3D-C4D	-4.89	1.33	1.44
7	I	102	BCL	C3D-C4D	-4.88	1.33	1.44
7	P	102	BCL	C3D-C4D	-4.88	1.33	1.44
7	O	102	BCL	O2D-CGD	4.88	1.45	1.33
7	G	101	BCL	O2D-CGD	4.88	1.45	1.33
7	V	101	BCL	O2D-CGD	4.87	1.45	1.33
7	K	102	BCL	O2D-CGD	4.87	1.45	1.33
7	B	101	BCL	C3D-C4D	-4.85	1.33	1.44
7	A	101	BCL	C3D-C4D	-4.85	1.33	1.44
7	E	102	BCL	O2D-CGD	4.85	1.45	1.33
7	I	102	BCL	O2D-CGD	4.84	1.45	1.33
7	T	102	BCL	C3D-C4D	-4.84	1.33	1.44
7	S	103	BCL	C3D-C4D	-4.84	1.33	1.44
7	R	102	BCL	C3D-C4D	-4.83	1.33	1.44
7	F	101	BCL	C3D-C4D	-4.81	1.33	1.44
7	Z	101	BCL	C3D-C4D	-4.80	1.33	1.44
7	O	102	BCL	C3D-C4D	-4.79	1.33	1.44
7	M	403	BCL	O2D-CGD	4.78	1.45	1.33
7	Q	105	BCL	C3D-C4D	-4.78	1.33	1.44
7	D	102	BCL	C3D-C4D	-4.76	1.33	1.44
7	L	310	BCL	O2D-CGD	4.74	1.44	1.33
7	V	101	BCL	C3D-C4D	-4.74	1.33	1.44
7	W	102	BCL	C3D-C4D	-4.72	1.33	1.44
7	Y	102	BCL	C3D-C4D	-4.62	1.33	1.44
7	Z	101	BCL	CHD-C1D	4.38	1.47	1.38
7	Z	101	BCL	O2A-CGA	4.30	1.45	1.33
10	L	305	PGV	O03-C19	4.30	1.45	1.33
7	G	101	BCL	O2A-CGA	4.29	1.45	1.33
7	L	310	BCL	O2A-CGA	4.27	1.45	1.33
10	Q	103	PGV	O03-C19	4.26	1.45	1.33
7	Y	102	BCL	CHD-C1D	4.25	1.46	1.38
7	V	101	BCL	O2A-CGA	4.25	1.45	1.33
7	Y	102	BCL	O2A-CGA	4.24	1.45	1.33
7	A	101	BCL	CHD-C1D	4.24	1.46	1.38
10	M	413	PGV	O03-C19	4.23	1.45	1.33
7	W	102	BCL	O2A-CGA	4.22	1.45	1.33
7	F	101	BCL	O2A-CGA	4.22	1.45	1.33
10	H	304	PGV	O03-C19	4.20	1.45	1.33
7	M	403	BCL	O2A-CGA	4.20	1.45	1.33
12	Q	102	LDA	C1-N1	-4.20	1.47	1.51
7	Q	105	BCL	O2A-CGA	4.19	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	414	PGV	O03-C19	4.19	1.45	1.33
7	D	102	BCL	O2A-CGA	4.18	1.45	1.33
10	M	415	PGV	O03-C19	4.17	1.45	1.33
10	H	303	PGV	O03-C19	4.14	1.45	1.33
7	E	102	BCL	O2A-CGA	4.13	1.45	1.33
7	S	103	BCL	O2A-CGA	4.13	1.45	1.33
10	M	402	PGV	O03-C19	4.12	1.45	1.33
7	F	103	BCL	O2A-CGA	4.11	1.45	1.33
7	J	101	BCL	O2A-CGA	4.11	1.45	1.33
7	A	101	BCL	O2A-CGA	4.10	1.45	1.33
10	M	413	PGV	O01-C1	4.10	1.45	1.34
7	B	101	BCL	O2A-CGA	4.09	1.45	1.33
7	R	102	BCL	O2A-CGA	4.08	1.45	1.33
12	D	104	LDA	C1-N1	-4.08	1.47	1.51
7	T	102	BCL	O2A-CGA	4.08	1.45	1.33
7	L	301	BCL	O2A-CGA	4.08	1.45	1.33
12	H	302	LDA	C1-N1	-4.06	1.47	1.51
10	L	305	PGV	O01-C1	4.06	1.45	1.34
7	O	102	BCL	O2A-CGA	4.06	1.45	1.33
7	K	102	BCL	O2A-CGA	4.04	1.45	1.33
7	P	102	BCL	O2A-CGA	4.04	1.45	1.33
7	N	102	BCL	O2A-CGA	4.04	1.45	1.33
10	M	415	PGV	O01-C1	4.03	1.45	1.34
10	Q	103	PGV	O01-C1	4.03	1.45	1.34
7	I	102	BCL	O2A-CGA	4.03	1.45	1.33
10	M	402	PGV	O01-C1	4.01	1.45	1.34
7	M	404	BCL	O2A-CGA	4.01	1.45	1.33
12	M	418	LDA	C1-N1	-4.01	1.47	1.51
10	M	414	PGV	O01-C1	3.98	1.45	1.34
12	Q	104	LDA	C1-N1	-3.97	1.47	1.51
10	H	304	PGV	O01-C1	3.97	1.45	1.34
7	F	101	BCL	CHD-C1D	3.96	1.46	1.38
10	H	303	PGV	O01-C1	3.96	1.45	1.34
12	O	101	LDA	C1-N1	-3.95	1.47	1.51
7	K	102	BCL	C3B-C4B	3.93	1.48	1.41
7	W	102	BCL	CHD-C1D	3.86	1.45	1.38
7	L	301	BCL	C3B-C4B	3.86	1.48	1.41
7	F	103	BCL	C3B-C4B	3.84	1.48	1.41
7	Q	105	BCL	C3B-C4B	3.81	1.48	1.41
7	S	103	BCL	C3B-C4B	3.80	1.48	1.41
12	H	301	LDA	C1-N1	-3.80	1.47	1.51
7	T	102	BCL	C3B-C4B	3.80	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	404	BCL	C3B-C4B	3.79	1.48	1.41
7	Y	102	BCL	C3B-C4B	3.78	1.48	1.41
7	V	101	BCL	CHD-C1D	3.77	1.45	1.38
7	Y	102	BCL	CHB-C1B	3.77	1.47	1.39
12	M	419	LDA	C1-N1	-3.76	1.47	1.51
12	M	420	LDA	C1-N1	-3.74	1.47	1.51
7	F	101	BCL	C3B-C4B	3.74	1.48	1.41
7	Z	101	BCL	C3B-C4B	3.73	1.48	1.41
7	O	102	BCL	C3B-C4B	3.72	1.48	1.41
7	A	101	BCL	CHB-C1B	3.70	1.47	1.39
7	Z	101	BCL	CHB-C1B	3.70	1.47	1.39
7	I	102	BCL	C3B-C4B	3.68	1.48	1.41
12	M	416	LDA	C1-N1	-3.68	1.47	1.51
7	Z	101	BCL	CHC-C4B	3.66	1.47	1.39
7	D	102	BCL	C3B-C4B	3.66	1.48	1.41
7	R	102	BCL	C3B-C4B	3.65	1.48	1.41
7	N	102	BCL	C3B-C4B	3.64	1.48	1.41
7	Y	102	BCL	OBD-CAD	3.63	1.28	1.22
7	W	102	BCL	C3B-C4B	3.63	1.48	1.41
7	G	101	BCL	C3B-C4B	3.62	1.48	1.41
7	F	101	BCL	OBD-CAD	3.62	1.28	1.22
7	M	403	BCL	C4B-NB	-3.60	1.33	1.37
7	J	101	BCL	C3B-C4B	3.60	1.48	1.41
7	E	102	BCL	C3B-C4B	3.57	1.48	1.41
7	M	403	BCL	C3B-C4B	3.57	1.48	1.41
7	Z	101	BCL	OBD-CAD	3.56	1.28	1.22
7	S	103	BCL	CHD-C1D	3.55	1.45	1.38
12	L	307	LDA	C1-N1	-3.54	1.47	1.51
7	V	101	BCL	C3B-C4B	3.54	1.48	1.41
7	W	102	BCL	OBD-CAD	3.51	1.28	1.22
7	F	101	BCL	CHB-C1B	3.51	1.47	1.39
7	A	101	BCL	OBD-CAD	3.49	1.28	1.22
7	B	101	BCL	C3B-C4B	3.48	1.48	1.41
7	L	310	BCL	C3B-C4B	3.47	1.48	1.41
7	R	102	BCL	OBD-CAD	3.47	1.28	1.22
11	L	306	PEE	C39-C38	3.47	1.51	1.31
7	B	101	BCL	CHD-C1D	3.47	1.45	1.38
7	V	101	BCL	OBD-CAD	3.46	1.28	1.22
7	P	102	BCL	C3B-C4B	3.46	1.47	1.41
7	G	101	BCL	CHD-C1D	3.46	1.45	1.38
7	W	102	BCL	CHB-C1B	3.45	1.47	1.39
7	M	403	BCL	OBD-CAD	3.45	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	306	PEE	C18-C19	3.43	1.51	1.31
7	Y	102	BCL	CHC-C4B	3.42	1.47	1.39
7	M	403	BCL	CHD-C1D	3.42	1.45	1.38
7	L	310	BCL	CHB-C1B	3.40	1.47	1.39
7	A	101	BCL	C3B-C4B	3.39	1.47	1.41
7	S	103	BCL	OBD-CAD	3.39	1.28	1.22
7	B	101	BCL	OBD-CAD	3.38	1.28	1.22
7	M	404	BCL	OBD-CAD	3.38	1.28	1.22
7	R	102	BCL	CHD-C1D	3.36	1.45	1.38
7	P	102	BCL	OBD-CAD	3.36	1.28	1.22
7	N	102	BCL	OBD-CAD	3.35	1.28	1.22
7	T	102	BCL	OBD-CAD	3.35	1.28	1.22
7	G	101	BCL	OBD-CAD	3.35	1.28	1.22
7	T	102	BCL	CHD-C1D	3.34	1.44	1.38
7	Q	105	BCL	CHD-C1D	3.34	1.44	1.38
7	M	403	BCL	CHB-C1B	3.33	1.46	1.39
7	Q	105	BCL	OBD-CAD	3.33	1.28	1.22
7	T	102	BCL	CHB-C1B	3.33	1.46	1.39
7	J	101	BCL	CHD-C1D	3.33	1.44	1.38
7	R	102	BCL	CHC-C4B	3.33	1.46	1.39
7	G	101	BCL	CHB-C1B	3.32	1.46	1.39
7	T	102	BCL	CHC-C4B	3.32	1.46	1.39
7	R	102	BCL	CHB-C1B	3.32	1.46	1.39
7	L	310	BCL	C1D-ND	-3.32	1.33	1.37
7	F	103	BCL	CHD-C1D	3.31	1.44	1.38
7	N	102	BCL	CHD-C1D	3.31	1.44	1.38
7	K	102	BCL	OBD-CAD	3.30	1.28	1.22
7	L	310	BCL	CHD-C1D	3.28	1.44	1.38
7	F	103	BCL	OBD-CAD	3.28	1.28	1.22
7	F	101	BCL	CHC-C4B	3.27	1.46	1.39
7	O	102	BCL	OBD-CAD	3.27	1.28	1.22
7	M	403	BCL	C1D-ND	-3.27	1.33	1.37
7	Z	101	BCL	C3D-C2D	3.26	1.47	1.39
7	E	102	BCL	OBD-CAD	3.26	1.28	1.22
7	Z	101	BCL	CHD-C4C	3.26	1.48	1.39
7	P	102	BCL	CHD-C1D	3.26	1.44	1.38
7	V	101	BCL	CHB-C1B	3.26	1.46	1.39
7	M	404	BCL	CHD-C1D	3.26	1.44	1.38
7	J	101	BCL	OBD-CAD	3.25	1.28	1.22
7	D	102	BCL	OBD-CAD	3.25	1.28	1.22
7	K	102	BCL	CHB-C1B	3.25	1.46	1.39
7	A	101	BCL	CHC-C4B	3.25	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	310	BCL	OBD-CAD	3.24	1.28	1.22
7	K	102	BCL	CHD-C1D	3.24	1.44	1.38
7	N	102	BCL	CHC-C4B	3.24	1.46	1.39
7	L	301	BCL	CHD-C1D	3.23	1.44	1.38
7	O	102	BCL	CHD-C1D	3.23	1.44	1.38
7	L	301	BCL	OBD-CAD	3.23	1.28	1.22
7	J	101	BCL	C1D-ND	-3.23	1.33	1.37
7	D	102	BCL	C4B-NB	-3.23	1.33	1.37
7	M	404	BCL	CHC-C4B	3.23	1.46	1.39
7	T	102	BCL	C1D-ND	-3.22	1.33	1.37
7	I	102	BCL	OBD-CAD	3.22	1.28	1.22
7	E	102	BCL	CHB-C1B	3.21	1.46	1.39
7	F	101	BCL	C4B-NB	-3.21	1.33	1.37
7	M	404	BCL	CHB-C1B	3.21	1.46	1.39
7	D	102	BCL	CHB-C1B	3.21	1.46	1.39
7	P	102	BCL	CHB-C1B	3.20	1.46	1.39
7	J	101	BCL	CHB-C1B	3.20	1.46	1.39
7	E	102	BCL	C1D-ND	-3.20	1.33	1.37
7	N	102	BCL	C1D-ND	-3.18	1.33	1.37
7	R	102	BCL	C1D-ND	-3.18	1.33	1.37
7	B	101	BCL	CHB-C1B	3.18	1.46	1.39
7	N	102	BCL	CHB-C1B	3.18	1.46	1.39
7	I	102	BCL	C4B-NB	-3.17	1.33	1.37
7	D	102	BCL	CHD-C1D	3.17	1.44	1.38
7	P	102	BCL	C4B-NB	-3.15	1.33	1.37
7	L	301	BCL	CHC-C4B	3.15	1.46	1.39
7	I	102	BCL	CHB-C1B	3.15	1.46	1.39
7	L	301	BCL	CHB-C1B	3.14	1.46	1.39
7	W	102	BCL	CHC-C4B	3.14	1.46	1.39
7	E	102	BCL	CHD-C1D	3.14	1.44	1.38
7	M	403	BCL	CHC-C4B	3.13	1.46	1.39
7	J	101	BCL	CHC-C4B	3.12	1.46	1.39
7	Y	102	BCL	C3D-C2D	3.11	1.47	1.39
7	E	102	BCL	CHC-C4B	3.10	1.46	1.39
7	G	101	BCL	C4B-NB	-3.10	1.33	1.37
7	I	102	BCL	CHD-C1D	3.09	1.44	1.38
7	B	101	BCL	C1D-ND	-3.09	1.33	1.37
7	Q	105	BCL	CHB-C1B	3.09	1.46	1.39
7	L	310	BCL	C4B-NB	-3.09	1.33	1.37
7	O	102	BCL	CHB-C1B	3.08	1.46	1.39
7	J	101	BCL	C4B-NB	-3.08	1.33	1.37
7	G	101	BCL	CHC-C4B	3.08	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	101	BCL	CHC-C4B	3.08	1.46	1.39
7	F	101	BCL	CHD-C4C	3.07	1.47	1.39
7	K	102	BCL	CHC-C4B	3.07	1.46	1.39
7	P	102	BCL	C1D-ND	-3.07	1.33	1.37
7	W	102	BCL	C4B-NB	-3.07	1.33	1.37
7	O	102	BCL	C4B-NB	-3.06	1.33	1.37
7	Q	105	BCL	CHC-C4B	3.06	1.46	1.39
7	B	101	BCL	C4B-NB	-3.05	1.33	1.37
7	I	102	BCL	C1D-ND	-3.05	1.33	1.37
7	D	102	BCL	C1D-ND	-3.05	1.33	1.37
7	Z	101	BCL	MG-NC	-3.04	1.99	2.06
7	G	101	BCL	C1D-ND	-3.04	1.33	1.37
7	W	102	BCL	C3D-C2D	3.04	1.47	1.39
7	F	103	BCL	CHC-C4B	3.04	1.46	1.39
7	L	301	BCL	C4B-NB	-3.03	1.33	1.37
7	F	101	BCL	C3D-C2D	3.03	1.47	1.39
7	A	101	BCL	CHD-C4C	3.03	1.47	1.39
7	S	103	BCL	CHB-C1B	3.03	1.46	1.39
7	F	103	BCL	CHB-C1B	3.02	1.46	1.39
7	M	403	BCL	C3D-C2D	3.02	1.47	1.39
7	A	101	BCL	MG-NC	-3.02	1.99	2.06
7	M	404	BCL	C4B-NB	-3.02	1.33	1.37
7	K	102	BCL	C4B-NB	-3.01	1.33	1.37
7	Z	101	BCL	C1D-C2D	3.01	1.51	1.45
7	A	101	BCL	C3D-C2D	3.00	1.47	1.39
7	P	102	BCL	CHC-C4B	3.00	1.46	1.39
7	A	101	BCL	C4B-NB	-2.99	1.33	1.37
7	T	102	BCL	C3D-C2D	2.99	1.47	1.39
7	Y	102	BCL	CHD-C4C	2.99	1.47	1.39
7	Q	105	BCL	C4B-NB	-2.99	1.33	1.37
7	L	310	BCL	C3D-C2D	2.98	1.47	1.39
7	R	102	BCL	C3D-C2D	2.98	1.47	1.39
7	Y	102	BCL	MG-NC	-2.98	1.99	2.06
7	O	102	BCL	C1D-ND	-2.98	1.33	1.37
8	M	405	BPH	C4D-CHA	2.97	1.44	1.39
7	E	102	BCL	C4B-NB	-2.97	1.34	1.37
7	Y	102	BCL	C1D-C2D	2.96	1.51	1.45
7	N	102	BCL	C4B-NB	-2.96	1.34	1.37
7	T	102	BCL	C4B-NB	-2.95	1.34	1.37
7	N	102	BCL	C3D-C2D	2.95	1.47	1.39
7	K	102	BCL	C1D-ND	-2.95	1.34	1.37
7	F	103	BCL	C1B-NB	-2.94	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	V	101	BCL	C4B-NB	-2.94	1.34	1.37
7	B	101	BCL	C3D-C2D	2.92	1.47	1.39
7	P	102	BCL	C3D-C2D	2.92	1.46	1.39
7	G	101	BCL	C3D-C2D	2.91	1.46	1.39
7	E	102	BCL	C3D-C2D	2.91	1.46	1.39
7	L	310	BCL	CHC-C4B	2.91	1.45	1.39
7	D	102	BCL	C3D-C2D	2.90	1.46	1.39
7	F	103	BCL	C4B-NB	-2.90	1.34	1.37
7	V	101	BCL	CHC-C4B	2.90	1.45	1.39
7	S	103	BCL	CHC-C4B	2.89	1.45	1.39
7	I	102	BCL	CHC-C4B	2.89	1.45	1.39
7	O	102	BCL	CHC-C4B	2.89	1.45	1.39
7	M	404	BCL	C1D-ND	-2.88	1.34	1.37
7	S	103	BCL	C4B-NB	-2.87	1.34	1.37
7	Y	102	BCL	C4B-NB	-2.87	1.34	1.37
7	S	103	BCL	C1B-NB	-2.86	1.34	1.37
7	V	101	BCL	C3D-C2D	2.86	1.46	1.39
7	D	102	BCL	C1B-NB	-2.86	1.34	1.37
7	F	103	BCL	C1D-ND	-2.86	1.34	1.37
7	Z	101	BCL	MG-NA	-2.85	1.99	2.06
7	Q	105	BCL	C1D-ND	-2.85	1.34	1.37
7	R	102	BCL	C4B-NB	-2.84	1.34	1.37
7	O	102	BCL	C3D-C2D	2.84	1.46	1.39
7	I	102	BCL	C3D-C2D	2.84	1.46	1.39
7	J	101	BCL	C3D-C2D	2.83	1.46	1.39
7	K	102	BCL	C3D-C2D	2.83	1.46	1.39
7	M	404	BCL	C3D-C2D	2.83	1.46	1.39
7	Q	105	BCL	C1B-NB	-2.82	1.34	1.37
7	F	103	BCL	C3D-C2D	2.82	1.46	1.39
8	M	405	BPH	C3A-C2A	-2.82	1.52	1.54
7	Q	105	BCL	C3D-C2D	2.82	1.46	1.39
7	M	404	BCL	C1B-NB	-2.81	1.34	1.37
7	L	301	BCL	C1D-ND	-2.80	1.34	1.37
7	A	101	BCL	C1D-C2D	2.79	1.50	1.45
7	F	101	BCL	C1D-C2D	2.79	1.50	1.45
9	L	303	U10	C4-C5	-2.78	1.40	1.48
7	W	102	BCL	C1D-ND	-2.78	1.34	1.37
7	Z	101	BCL	C1B-C2B	2.77	1.49	1.43
7	V	101	BCL	CHD-C4C	2.77	1.47	1.39
7	F	101	BCL	MG-NC	-2.77	1.99	2.06
8	L	302	BPH	C4D-CHA	2.77	1.43	1.39
7	W	102	BCL	CHD-C4C	2.77	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	403	BCL	C1B-NB	-2.75	1.34	1.37
7	A	101	BCL	MG-NA	-2.74	1.99	2.06
7	Z	101	BCL	C4B-NB	-2.74	1.34	1.37
7	S	103	BCL	CHD-C4C	2.73	1.46	1.39
7	L	301	BCL	C3D-C2D	2.73	1.46	1.39
9	M	407	U10	C4-C5	-2.71	1.41	1.48
7	D	102	BCL	CHC-C4B	2.71	1.45	1.39
7	S	103	BCL	C3D-C2D	2.71	1.46	1.39
7	I	102	BCL	C1B-NB	-2.70	1.34	1.37
7	W	102	BCL	MG-NC	-2.69	1.99	2.06
8	L	302	BPH	CBD-CGD	-2.67	1.49	1.52
8	L	302	BPH	C3A-C2A	-2.67	1.52	1.54
9	L	304	U10	C3-C2	-2.67	1.41	1.48
7	A	101	BCL	C1B-C2B	2.66	1.49	1.43
7	E	102	BCL	C1B-NB	-2.66	1.34	1.37
7	Q	105	BCL	CHD-C4C	2.66	1.46	1.39
7	F	101	BCL	C1D-ND	-2.65	1.34	1.37
7	S	103	BCL	C1D-ND	-2.63	1.34	1.37
7	O	102	BCL	C1B-NB	-2.63	1.34	1.37
7	K	102	BCL	C1B-NB	-2.62	1.34	1.37
7	R	102	BCL	CHD-C4C	2.62	1.46	1.39
7	W	102	BCL	MG-NA	-2.61	2.00	2.06
7	V	101	BCL	C1D-C2D	2.60	1.50	1.45
7	Y	102	BCL	MG-NA	-2.59	2.00	2.06
7	F	101	BCL	MG-NA	-2.59	2.00	2.06
7	W	102	BCL	C1B-C2B	2.59	1.49	1.43
7	B	101	BCL	C1B-NB	-2.59	1.34	1.37
7	J	101	BCL	C1B-NB	-2.59	1.34	1.37
7	L	310	BCL	C1B-NB	-2.58	1.34	1.37
7	L	301	BCL	C1B-NB	-2.58	1.34	1.37
7	Z	101	BCL	C1D-ND	-2.57	1.34	1.37
7	V	101	BCL	C1B-NB	-2.56	1.34	1.37
7	T	102	BCL	CHD-C4C	2.56	1.46	1.39
7	Y	102	BCL	C1B-C2B	2.56	1.49	1.43
7	T	102	BCL	C1B-NB	-2.56	1.34	1.37
9	M	401	U10	C4-C5	-2.56	1.41	1.48
7	B	101	BCL	CHD-C4C	2.55	1.46	1.39
7	S	103	BCL	C1D-C2D	2.55	1.50	1.45
7	M	403	BCL	CHD-C4C	2.55	1.46	1.39
7	T	102	BCL	MG-NA	-2.54	2.00	2.06
7	K	102	BCL	CHD-C4C	2.54	1.46	1.39
7	J	101	BCL	CHD-C4C	2.53	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	102	BCL	C1B-NB	-2.52	1.34	1.37
7	G	101	BCL	CHD-C4C	2.51	1.46	1.39
7	P	102	BCL	C1B-NB	-2.50	1.34	1.37
7	F	103	BCL	CHD-C4C	2.49	1.46	1.39
7	N	102	BCL	CHD-C4C	2.49	1.46	1.39
7	D	102	BCL	CHD-C4C	2.49	1.46	1.39
7	M	404	BCL	CHD-C4C	2.48	1.46	1.39
7	R	102	BCL	MG-NA	-2.48	2.00	2.06
7	D	102	BCL	MG-NA	-2.48	2.00	2.06
9	M	407	U10	C3-C2	-2.47	1.41	1.48
7	O	102	BCL	CHD-C4C	2.47	1.46	1.39
7	P	102	BCL	CHD-C4C	2.45	1.46	1.39
7	B	101	BCL	MG-NA	-2.45	2.00	2.06
7	O	102	BCL	MG-NA	-2.45	2.00	2.06
7	V	101	BCL	C1D-ND	-2.45	1.34	1.37
7	B	101	BCL	MG-NC	-2.43	2.00	2.06
7	L	310	BCL	CHD-C4C	2.43	1.46	1.39
7	R	102	BCL	C1B-C2B	2.42	1.48	1.43
7	L	310	BCL	MG-NA	-2.42	2.00	2.06
7	I	102	BCL	CHD-C4C	2.42	1.46	1.39
7	I	102	BCL	MG-NA	-2.41	2.00	2.06
7	T	102	BCL	C1B-C2B	2.41	1.48	1.43
9	L	304	U10	C4-C5	-2.41	1.41	1.48
7	M	403	BCL	MG-NA	-2.41	2.00	2.06
7	E	102	BCL	MG-NA	-2.41	2.00	2.06
7	T	102	BCL	MG-NC	-2.40	2.00	2.06
7	M	404	BCL	C1D-C2D	2.40	1.50	1.45
7	E	102	BCL	CHD-C4C	2.40	1.45	1.39
7	F	101	BCL	C1B-NB	-2.39	1.34	1.37
7	K	102	BCL	MG-NA	-2.39	2.00	2.06
7	L	301	BCL	CHD-C4C	2.39	1.45	1.39
7	F	101	BCL	C1B-C2B	2.39	1.48	1.43
7	Q	105	BCL	C1D-C2D	2.38	1.50	1.45
7	D	102	BCL	C3C-C4C	-2.38	1.48	1.51
7	K	102	BCL	C3C-C4C	-2.38	1.48	1.51
7	W	102	BCL	C1B-NB	-2.37	1.34	1.37
7	W	102	BCL	C1D-C2D	2.37	1.50	1.45
7	A	101	BCL	C1D-ND	-2.37	1.34	1.37
7	I	102	BCL	C3C-C4C	-2.37	1.48	1.51
7	V	101	BCL	MG-NC	-2.37	2.00	2.06
7	P	102	BCL	C1B-C2B	2.36	1.48	1.43
8	M	405	BPH	CBD-CGD	-2.36	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	101	BCL	C1B-NB	-2.33	1.34	1.37
7	V	101	BCL	MG-NA	-2.33	2.00	2.06
7	M	403	BCL	MG-NC	-2.32	2.00	2.06
7	Q	105	BCL	MG-NA	-2.32	2.00	2.06
7	E	102	BCL	MG-NC	-2.31	2.00	2.06
7	E	102	BCL	C3C-C4C	-2.31	1.48	1.51
7	S	103	BCL	MG-NC	-2.30	2.00	2.06
7	B	101	BCL	C1B-C2B	2.30	1.48	1.43
7	G	101	BCL	C1B-C2B	2.29	1.48	1.43
7	R	102	BCL	C1B-NB	-2.29	1.34	1.37
7	Y	102	BCL	C1D-ND	-2.27	1.34	1.37
7	P	102	BCL	MG-NA	-2.27	2.00	2.06
7	M	404	BCL	MG-NA	-2.27	2.00	2.06
7	R	102	BCL	MG-NC	-2.27	2.00	2.06
7	L	310	BCL	C1B-C2B	2.27	1.48	1.43
9	L	303	U10	C3-C2	-2.26	1.42	1.48
7	S	103	BCL	MG-NA	-2.26	2.00	2.06
7	F	103	BCL	MG-NA	-2.25	2.00	2.06
7	L	301	BCL	C1D-C2D	2.25	1.49	1.45
7	L	301	BCL	C3C-C4C	-2.23	1.48	1.51
7	L	301	BCL	MG-NC	-2.23	2.01	2.06
7	K	102	BCL	C1D-C2D	2.23	1.49	1.45
7	J	101	BCL	MG-NA	-2.21	2.01	2.06
7	A	101	BCL	C1B-NB	-2.21	1.35	1.37
7	N	102	BCL	MG-NA	-2.20	2.01	2.06
7	L	301	BCL	C1B-C2B	2.19	1.48	1.43
7	J	101	BCL	C1B-C2B	2.19	1.48	1.43
7	L	310	BCL	CHC-C1C	-2.19	1.32	1.37
7	D	102	BCL	CHC-C1C	-2.18	1.32	1.37
7	N	102	BCL	C1B-C2B	2.18	1.48	1.43
7	S	103	BCL	C1B-C2B	2.18	1.48	1.43
9	M	401	U10	C3-C2	-2.18	1.42	1.48
7	G	101	BCL	MG-NA	-2.17	2.01	2.06
7	M	404	BCL	MG-NC	-2.17	2.01	2.06
7	V	101	BCL	C1B-C2B	2.17	1.48	1.43
7	R	102	BCL	C1D-C2D	2.17	1.49	1.45
7	P	102	BCL	C3C-C4C	-2.16	1.48	1.51
7	I	102	BCL	C1D-C2D	2.16	1.49	1.45
7	O	102	BCL	C1D-C2D	2.16	1.49	1.45
7	P	102	BCL	MG-NC	-2.16	2.01	2.06
7	L	310	BCL	MG-NC	-2.16	2.01	2.06
7	F	103	BCL	CHB-C4A	-2.15	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	404	BCL	C3C-C4C	-2.15	1.48	1.51
7	Y	102	BCL	C1B-NB	-2.15	1.35	1.37
7	I	102	BCL	C1B-C2B	2.14	1.48	1.43
7	F	103	BCL	C3C-C4C	-2.14	1.48	1.51
7	G	101	BCL	C3C-C4C	-2.14	1.48	1.51
7	Q	105	BCL	MG-NC	-2.14	2.01	2.06
7	J	101	BCL	MG-NC	-2.14	2.01	2.06
7	Z	101	BCL	C1B-NB	-2.13	1.35	1.37
7	E	102	BCL	C1B-C2B	2.12	1.48	1.43
7	F	103	BCL	MG-NC	-2.12	2.01	2.06
7	G	101	BCL	MG-NC	-2.12	2.01	2.06
7	M	403	BCL	C1B-C2B	2.12	1.48	1.43
7	O	102	BCL	CHC-C1C	-2.12	1.32	1.37
7	F	103	BCL	C1D-C2D	2.12	1.49	1.45
7	P	102	BCL	CHC-C1C	-2.11	1.32	1.37
7	N	102	BCL	MG-NC	-2.10	2.01	2.06
7	S	103	BCL	CHB-C4A	-2.10	1.32	1.37
7	B	101	BCL	C3C-C4C	-2.10	1.49	1.51
7	J	101	BCL	C3C-C4C	-2.10	1.49	1.51
7	V	101	BCL	CHC-C1C	-2.10	1.32	1.37
7	L	301	BCL	CHB-C4A	-2.09	1.32	1.37
7	O	102	BCL	MG-NC	-2.08	2.01	2.06
7	T	102	BCL	C1D-C2D	2.08	1.49	1.45
7	M	404	BCL	C1B-C2B	2.08	1.48	1.43
7	D	102	BCL	C1D-C2D	2.08	1.49	1.45
7	B	101	BCL	C1D-C2D	2.08	1.49	1.45
7	O	102	BCL	C3C-C4C	-2.08	1.49	1.51
7	I	102	BCL	MG-NC	-2.08	2.01	2.06
7	E	102	BCL	CHC-C1C	-2.07	1.32	1.37
7	O	102	BCL	CHB-C4A	-2.07	1.32	1.37
7	K	102	BCL	MG-NC	-2.05	2.01	2.06
7	M	404	BCL	CHC-C1C	-2.04	1.32	1.37
7	Q	105	BCL	CHC-C1C	-2.04	1.32	1.37
7	G	101	BCL	C1D-C2D	2.04	1.49	1.45
7	M	403	BCL	C3C-C4C	-2.04	1.49	1.51
7	Q	105	BCL	CHB-C4A	-2.04	1.32	1.37
7	Q	105	BCL	C3C-C4C	-2.03	1.49	1.51
7	R	102	BCL	C3C-C4C	-2.03	1.49	1.51
7	J	101	BCL	CHC-C1C	-2.03	1.32	1.37
7	F	103	BCL	CHC-C1C	-2.03	1.32	1.37
7	B	101	BCL	CHC-C1C	-2.03	1.32	1.37
7	I	102	BCL	CHC-C1C	-2.03	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	102	BCL	CHB-C4A	-2.02	1.32	1.37
7	E	102	BCL	CHB-C4A	-2.01	1.32	1.37
7	D	102	BCL	C1B-C2B	2.01	1.47	1.43
7	S	103	BCL	CHC-C1C	-2.01	1.32	1.37
7	N	102	BCL	CHB-C4A	-2.01	1.32	1.37
7	K	102	BCL	C1B-C2B	2.01	1.47	1.43
7	D	102	BCL	MG-NC	-2.01	2.01	2.06
7	M	403	BCL	CHC-C1C	-2.00	1.32	1.37

All (900) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	101	BCL	CMD-C2D-C1D	8.36	139.44	124.73
7	V	101	BCL	CMD-C2D-C1D	8.29	139.34	124.73
7	S	103	BCL	CMD-C2D-C1D	8.28	139.32	124.73
7	F	101	BCL	CMD-C2D-C1D	8.16	139.10	124.73
7	L	301	BCL	CMD-C2D-C1D	8.16	139.10	124.73
7	Y	102	BCL	CMD-C2D-C1D	8.11	139.01	124.73
7	Z	101	BCL	CMD-C2D-C1D	8.05	138.91	124.73
7	M	404	BCL	CMD-C2D-C1D	8.03	138.86	124.73
7	F	103	BCL	CMD-C2D-C1D	7.87	138.58	124.73
7	Q	105	BCL	CMD-C2D-C1D	7.83	138.51	124.73
7	K	102	BCL	CMD-C2D-C1D	7.76	138.39	124.73
7	I	102	BCL	CMD-C2D-C1D	7.68	138.26	124.73
7	O	102	BCL	CMD-C2D-C1D	7.58	138.07	124.73
15	E	101	SPO	C10-C9-C7	-7.55	116.69	127.28
7	D	102	BCL	CMD-C2D-C1D	7.44	137.83	124.73
7	W	102	BCL	CMD-C2D-C1D	7.26	137.51	124.73
7	S	103	BCL	C2B-C1B-NB	6.97	117.55	110.33
7	G	101	BCL	CMD-C2D-C1D	6.94	136.95	124.73
7	R	102	BCL	CMD-C2D-C1D	6.93	136.94	124.73
7	F	103	BCL	C2B-C1B-NB	6.93	117.51	110.33
7	P	102	BCL	CMD-C2D-C1D	6.90	136.89	124.73
7	O	102	BCL	C2B-C1B-NB	6.89	117.47	110.33
7	B	101	BCL	CMD-C2D-C1D	6.88	136.84	124.73
7	T	102	BCL	CMD-C2D-C1D	6.84	136.77	124.73
7	Q	105	BCL	C2B-C1B-NB	6.78	117.36	110.33
7	M	403	BCL	CMD-C2D-C1D	6.77	136.64	124.73
7	J	101	BCL	CMD-C2D-C1D	6.72	136.57	124.73
7	D	102	BCL	C2B-C1B-NB	6.70	117.28	110.33
7	K	102	BCL	C2B-C1B-NB	6.69	117.26	110.33
7	I	102	BCL	C2B-C1B-NB	6.64	117.21	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	301	BCL	C2B-C1B-NB	6.59	117.16	110.33
7	M	404	BCL	C2B-C1B-NB	6.59	117.16	110.33
7	N	102	BCL	CMD-C2D-C1D	6.56	136.29	124.73
7	L	310	BCL	CMD-C2D-C1D	6.54	136.25	124.73
7	N	102	BCL	C2B-C1B-NB	6.52	117.09	110.33
7	J	101	BCL	C2B-C1B-NB	6.52	117.09	110.33
7	B	101	BCL	C2B-C1B-NB	6.50	117.07	110.33
7	E	102	BCL	C2B-C1B-NB	6.48	117.04	110.33
7	E	102	BCL	CMD-C2D-C1D	6.47	136.12	124.73
7	G	101	BCL	C2B-C1B-NB	6.40	116.96	110.33
7	V	101	BCL	C2B-C1B-NB	6.37	116.93	110.33
7	P	102	BCL	C2B-C1B-NB	6.34	116.90	110.33
7	T	102	BCL	C2B-C1B-NB	6.24	116.80	110.33
15	D	103	SPO	C4-C5-C6	-6.22	116.18	124.91
7	Z	101	BCL	CHD-C1D-ND	-6.19	116.09	124.80
7	M	403	BCL	C2B-C1B-NB	6.10	116.65	110.33
7	L	310	BCL	O2D-CGD-CBD	6.08	121.86	111.23
7	R	102	BCL	C2B-C1B-NB	6.08	116.63	110.33
7	F	101	BCL	CHD-C1D-ND	-6.05	116.29	124.80
7	L	310	BCL	C2B-C1B-NB	6.02	116.57	110.33
7	W	102	BCL	C2B-C1B-NB	5.98	116.52	110.33
7	M	403	BCL	O2D-CGD-CBD	5.97	121.67	111.23
15	F	104	SPO	C5-C6-C7	-5.96	116.89	125.89
7	Y	102	BCL	CHD-C1D-ND	-5.86	116.55	124.80
7	M	404	BCL	CHD-C1D-ND	-5.86	116.56	124.80
7	V	101	BCL	CHD-C1D-ND	-5.86	116.56	124.80
7	S	103	BCL	CHD-C1D-ND	-5.78	116.67	124.80
7	Q	105	BCL	CHD-C1D-ND	-5.75	116.71	124.80
15	O	103	SPO	C4-C5-C6	-5.72	116.89	124.91
7	D	102	BCL	CHD-C1D-ND	-5.71	116.77	124.80
7	O	102	BCL	CHD-C1D-ND	-5.69	116.79	124.80
7	F	103	BCL	CHD-C1D-ND	-5.69	116.80	124.80
7	Y	102	BCL	O2D-CGD-CBD	5.66	121.12	111.23
7	A	101	BCL	CHD-C1D-ND	-5.65	116.86	124.80
15	I	104	SPO	C4-C5-C6	-5.63	117.00	124.91
7	L	301	BCL	CHD-C1D-ND	-5.63	116.88	124.80
7	K	102	BCL	CHD-C1D-ND	-5.61	116.90	124.80
15	I	103	SPO	C4-C5-C6	-5.57	117.09	124.91
7	I	102	BCL	CHD-C1D-ND	-5.57	116.97	124.80
7	F	101	BCL	C2B-C1B-NB	5.56	116.10	110.33
15	O	104	SPO	C4-C5-C6	-5.55	117.11	124.91
7	R	102	BCL	CHD-C1D-ND	-5.46	117.11	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	D	101	SPO	C26-C27-C28	-5.42	120.06	127.69
15	S	104	SPO	C26-C27-C28	-5.42	120.07	127.69
15	R	101	SPO	C3-C1-C2	5.37	120.24	110.43
7	Y	102	BCL	C2B-C1B-NB	5.35	115.88	110.33
7	T	102	BCL	CHD-C1D-ND	-5.32	117.31	124.80
15	O	104	SPO	C21-C22-C23	-5.32	119.81	127.28
7	Z	101	BCL	C2B-C1B-NB	5.28	115.80	110.33
7	L	301	BCL	C3D-C2D-C1D	-5.26	98.65	105.83
15	D	105	SPO	C4-C5-C6	-5.25	117.55	124.91
15	D	101	SPO	C4-C5-C6	-5.23	117.57	124.91
7	B	101	BCL	CHD-C1D-ND	-5.22	117.45	124.80
7	A	101	BCL	C2B-C1B-NB	5.22	115.74	110.33
7	W	102	BCL	CHD-C1D-ND	-5.21	117.46	124.80
7	L	310	BCL	CHD-C1D-ND	-5.20	117.48	124.80
15	G	102	SPO	C15-C14-C12	-5.16	120.04	127.28
7	M	404	BCL	C3D-C2D-C1D	-5.14	98.81	105.83
7	M	403	BCL	CHD-C1D-ND	-5.14	117.58	124.80
7	Q	105	BCL	O2D-CGD-CBD	5.10	120.14	111.23
7	V	101	BCL	O2D-CGD-CBD	5.07	120.09	111.23
7	G	101	BCL	CHD-C1D-ND	-5.04	117.70	124.80
7	N	102	BCL	CHD-C1D-ND	-5.04	117.72	124.80
7	D	102	BCL	C3D-C2D-C1D	-5.02	98.98	105.83
7	I	102	BCL	C3D-C2D-C1D	-5.01	98.99	105.83
7	S	103	BCL	C3D-C2D-C1D	-5.01	98.99	105.83
7	S	103	BCL	O2D-CGD-CBD	5.01	119.99	111.23
7	K	102	BCL	C3C-C4C-CHD	-4.99	112.88	123.39
7	P	102	BCL	CHD-C1D-ND	-4.97	117.81	124.80
7	J	101	BCL	CHD-C1D-ND	-4.96	117.81	124.80
15	M	408	SPO	C20-C19-C17	-4.96	120.32	127.28
7	E	102	BCL	CHD-C1D-ND	-4.95	117.83	124.80
7	O	102	BCL	C3D-C2D-C1D	-4.94	99.09	105.83
7	K	102	BCL	C3D-C2D-C1D	-4.92	99.11	105.83
7	K	102	BCL	O2D-CGD-CBD	4.92	119.83	111.23
7	D	102	BCL	C3C-C4C-CHD	-4.91	113.04	123.39
7	F	103	BCL	C3D-C2D-C1D	-4.91	99.13	105.83
7	O	102	BCL	O2D-CGD-CBD	4.89	119.78	111.23
7	I	102	BCL	C3C-C4C-CHD	-4.89	113.08	123.39
7	I	102	BCL	O2D-CGD-CBD	4.87	119.75	111.23
7	A	101	BCL	C4A-NA-C1A	4.86	108.90	106.68
7	V	101	BCL	C3D-C2D-C1D	-4.86	99.20	105.83
7	O	102	BCL	C3C-C4C-CHD	-4.85	113.16	123.39
15	O	104	SPO	C26-C27-C28	-4.84	120.88	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	103	BCL	O2D-CGD-CBD	4.84	119.68	111.23
7	Z	101	BCL	O2D-CGD-CBD	4.83	119.67	111.23
7	F	101	BCL	O2D-CGD-CBD	4.83	119.67	111.23
7	Q	105	BCL	C3D-C2D-C1D	-4.82	99.25	105.83
15	M	408	SPO	C4-C5-C6	-4.81	118.16	124.91
7	N	102	BCL	O2D-CGD-CBD	4.77	119.57	111.23
7	R	102	BCL	C3D-C2D-C1D	-4.77	99.32	105.83
7	T	102	BCL	O2D-CGD-CBD	4.76	119.55	111.23
7	P	102	BCL	C3D-C2D-C1D	-4.75	99.34	105.83
7	F	101	BCL	C3D-C2D-C1D	-4.75	99.35	105.83
7	F	103	BCL	C3C-C4C-CHD	-4.75	113.38	123.39
15	S	105	SPO	C20-C19-C17	-4.75	120.62	127.28
15	M	408	SPO	C21-C22-C23	-4.71	120.67	127.28
7	L	310	BCL	C3D-C2D-C1D	-4.71	99.41	105.83
7	A	101	BCL	O2D-CGD-CBD	4.70	119.45	111.23
7	T	102	BCL	C3D-C2D-C1D	-4.70	99.42	105.83
7	D	102	BCL	C1-C2-C3	-4.64	118.60	126.20
7	E	102	BCL	C3C-C4C-CHD	-4.63	113.62	123.39
7	N	102	BCL	C3D-C2D-C1D	-4.62	99.52	105.83
7	G	101	BCL	C3D-C2D-C1D	-4.62	99.53	105.83
15	S	104	SPO	C21-C22-C23	-4.62	120.80	127.28
15	R	101	SPO	C5-C6-C7	-4.61	118.92	125.89
7	Q	105	BCL	C3C-C4C-CHD	-4.61	113.67	123.39
15	I	103	SPO	C26-C27-C28	-4.61	121.21	127.69
7	A	101	BCL	C3D-C2D-C1D	-4.60	99.55	105.83
7	W	102	BCL	C3D-C2D-C1D	-4.60	99.56	105.83
7	M	403	BCL	C3D-C2D-C1D	-4.60	99.56	105.83
7	L	301	BCL	C3C-C4C-CHD	-4.59	113.70	123.39
7	P	102	BCL	C3C-C4C-CHD	-4.59	113.71	123.39
7	N	102	BCL	C3C-C4C-CHD	-4.57	113.76	123.39
7	R	102	BCL	O2D-CGD-CBD	4.56	119.20	111.23
7	E	102	BCL	O2D-CGD-CBD	4.56	119.20	111.23
7	J	101	BCL	C3D-C2D-C1D	-4.55	99.62	105.83
7	E	102	BCL	C3D-C2D-C1D	-4.55	99.62	105.83
7	Y	102	BCL	C3D-C2D-C1D	-4.55	99.62	105.83
15	G	102	SPO	C5-C6-C7	-4.54	119.03	125.89
7	G	101	BCL	C3C-C4C-CHD	-4.53	113.84	123.39
7	J	101	BCL	C3C-C4C-CHD	-4.53	113.84	123.39
7	B	101	BCL	C3D-C2D-C1D	-4.53	99.65	105.83
15	S	104	SPO	C4-C5-C6	-4.52	118.56	124.91
7	M	404	BCL	O2D-CGD-CBD	4.51	119.12	111.23
7	M	404	BCL	C3C-C4C-CHD	-4.51	113.89	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	D	103	SPO	C26-C27-C28	-4.50	121.36	127.69
7	R	102	BCL	C3C-C4C-CHD	-4.50	113.90	123.39
7	Z	101	BCL	C3D-C2D-C1D	-4.49	99.71	105.83
10	M	413	PGV	O01-C1-C2	4.48	121.17	111.48
15	D	105	SPO	C21-C22-C23	-4.45	121.04	127.28
7	T	102	BCL	C3C-C4C-CHD	-4.39	114.14	123.39
7	D	102	BCL	O2D-CGD-CBD	4.37	118.88	111.23
7	B	101	BCL	O2D-CGD-CBD	4.37	118.87	111.23
10	H	303	PGV	O01-C1-C2	4.35	120.89	111.48
15	D	105	SPO	C26-C27-C28	-4.35	121.57	127.69
7	B	101	BCL	C3C-C4C-CHD	-4.32	114.29	123.39
7	S	103	BCL	C3B-C4B-NB	4.31	115.45	109.76
7	S	103	BCL	C3C-C4C-CHD	-4.29	114.35	123.39
7	G	101	BCL	O2D-CGD-CBD	4.27	118.70	111.23
7	W	102	BCL	O2D-CGD-CBD	4.26	118.68	111.23
15	S	104	SPO	C20-C19-C17	-4.26	121.30	127.28
7	L	310	BCL	C3C-C4C-CHD	-4.23	114.46	123.39
7	J	101	BCL	O2D-CGD-CBD	4.23	118.63	111.23
15	D	103	SPO	C21-C22-C23	-4.22	121.36	127.28
15	S	105	SPO	C26-C27-C28	-4.20	121.79	127.69
7	P	102	BCL	O2D-CGD-CBD	4.19	118.56	111.23
15	R	101	SPO	C21-C22-C23	-4.18	121.41	127.28
10	L	305	PGV	O01-C1-C2	4.17	120.50	111.48
15	O	103	SPO	C26-C27-C28	-4.15	121.85	127.69
7	M	404	BCL	C1D-ND-C4D	-4.14	103.40	106.31
15	S	105	SPO	C4-C5-C6	-4.14	119.09	124.91
10	M	402	PGV	O01-C1-C2	4.14	120.44	111.48
13	Q	101	LMT	O1B-C4'-C3'	4.11	117.67	107.23
7	K	102	BCL	C1D-ND-C4D	-4.10	103.43	106.31
15	P	101	SPO	C5-C6-C7	-4.10	119.69	125.89
15	N	101	SPO	C8-C7-C6	4.10	124.35	118.09
7	L	301	BCL	O2D-CGD-CBD	4.08	118.37	111.23
7	B	101	BCL	C1D-ND-C4D	-4.08	103.45	106.31
7	V	101	BCL	C3B-C4B-NB	4.08	115.14	109.76
15	O	104	SPO	C20-C19-C17	-4.06	121.58	127.28
15	I	104	SPO	C26-C27-C28	-4.06	121.98	127.69
15	W	101	SPO	C10-C9-C7	-4.06	121.58	127.28
15	D	103	SPO	C20-C19-C17	-4.06	121.59	127.28
15	M	408	SPO	C26-C27-C28	-4.05	121.99	127.69
8	L	302	BPH	C4D-CHA-CBD	-4.04	106.52	108.45
15	T	101	SPO	C21-C22-C23	-4.03	121.62	127.28
7	E	102	BCL	C1D-ND-C4D	-4.03	103.49	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	102	BCL	C1D-ND-C4D	-4.03	103.49	106.31
15	I	104	SPO	C21-C22-C23	-4.03	121.63	127.28
15	N	101	SPO	C15-C14-C12	-4.03	121.63	127.28
15	I	103	SPO	C20-C19-C17	-4.02	121.64	127.28
15	E	101	SPO	C20-C19-C17	-4.00	121.67	127.28
7	S	103	BCL	C1-C2-C3	-3.98	119.67	126.20
7	I	102	BCL	C3B-C4B-NB	3.98	115.01	109.76
15	W	101	SPO	C4-C5-C6	-3.98	119.32	124.91
7	A	101	BCL	CHB-C1B-NB	-3.98	118.08	124.05
15	T	101	SPO	C4-C5-C6	-3.97	119.33	124.91
7	Q	105	BCL	C1D-ND-C4D	-3.97	103.53	106.31
15	I	104	SPO	C20-C19-C17	-3.96	121.72	127.28
7	D	102	BCL	C2D-C1D-ND	3.96	114.05	110.13
7	E	102	BCL	C3B-C4B-NB	3.96	114.98	109.76
7	B	101	BCL	C3B-C4B-NB	3.96	114.98	109.76
7	A	101	BCL	C1-C2-C3	-3.93	119.75	126.20
15	O	103	SPO	C21-C22-C23	-3.93	121.77	127.28
10	H	304	PGV	O01-C1-C2	3.92	119.97	111.48
15	W	101	SPO	C21-C22-C23	-3.92	121.78	127.28
7	D	102	BCL	C3B-C4B-NB	3.91	114.92	109.76
7	L	301	BCL	C1D-ND-C4D	-3.91	103.57	106.31
15	G	102	SPO	C20-C19-C17	-3.90	121.80	127.28
7	L	310	BCL	C3B-C4B-NB	3.90	114.91	109.76
7	M	403	BCL	C3C-C4C-CHD	-3.89	115.18	123.39
7	V	101	BCL	C1-C2-C3	-3.89	119.83	126.20
7	G	101	BCL	C1D-ND-C4D	-3.88	103.59	106.31
10	Q	103	PGV	O01-C1-C2	3.88	119.87	111.48
15	S	105	SPO	C21-C22-C23	-3.87	121.85	127.28
7	L	301	BCL	C2D-C1D-ND	3.87	113.96	110.13
7	T	102	BCL	C1D-ND-C4D	-3.87	103.59	106.31
7	O	102	BCL	C3B-C4B-NB	3.87	114.87	109.76
7	D	102	BCL	O2A-CGA-CBA	3.87	123.63	111.83
7	I	102	BCL	C2D-C1D-ND	3.87	113.95	110.13
7	M	404	BCL	C2D-C1D-ND	3.87	113.95	110.13
7	G	101	BCL	C3B-C4B-NB	3.86	114.86	109.76
7	F	103	BCL	C1D-ND-C4D	-3.86	103.60	106.31
15	D	105	SPO	C20-C19-C17	-3.85	121.87	127.28
7	I	102	BCL	C1D-ND-C4D	-3.85	103.61	106.31
7	K	102	BCL	C2D-C1D-ND	3.85	113.94	110.13
7	S	103	BCL	C1D-ND-C4D	-3.85	103.61	106.31
7	N	102	BCL	C1D-ND-C4D	-3.85	103.61	106.31
7	Q	105	BCL	C3B-C4B-NB	3.84	114.83	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	102	BCL	C3B-C4B-NB	3.84	114.83	109.76
15	F	104	SPO	C10-C9-C7	-3.83	121.90	127.28
7	O	102	BCL	C2D-C1D-ND	3.83	113.91	110.13
7	O	102	BCL	C1-C2-C3	-3.82	119.93	126.20
7	P	102	BCL	C1D-ND-C4D	-3.82	103.63	106.31
7	L	301	BCL	C3B-C4B-NB	3.82	114.80	109.76
7	R	102	BCL	C2D-C1D-ND	3.81	113.90	110.13
7	O	102	BCL	C1D-ND-C4D	-3.80	103.64	106.31
15	E	101	SPO	C14-C15-C16	-3.80	112.18	123.20
10	M	414	PGV	O01-C1-C2	3.80	119.71	111.48
10	M	415	PGV	O01-C1-C2	3.80	119.70	111.48
7	F	103	BCL	C3B-C4B-NB	3.80	114.77	109.76
15	N	101	SPO	C5-C6-C7	3.79	131.62	125.89
7	L	310	BCL	C1-C2-C3	-3.78	120.01	126.20
15	O	103	SPO	C20-C19-C17	-3.78	121.98	127.28
7	J	101	BCL	C3B-C4B-NB	3.78	114.74	109.76
7	Y	102	BCL	C4A-NA-C1A	3.77	108.40	106.68
7	P	102	BCL	C3B-C4B-NB	3.77	114.74	109.76
7	E	102	BCL	C2D-C1D-ND	3.77	113.86	110.13
7	J	101	BCL	C1D-ND-C4D	-3.77	103.67	106.31
15	P	101	SPO	C4-C5-C6	-3.76	119.64	124.91
15	N	101	SPO	C21-C22-C23	-3.75	122.02	127.28
15	D	105	SPO	C31-C32-C33	-3.75	119.05	127.62
7	F	103	BCL	C2D-C1D-ND	3.74	113.83	110.13
15	F	104	SPO	C21-C22-C23	-3.73	122.05	127.28
7	T	102	BCL	C3B-C4B-NB	3.73	114.67	109.76
7	D	102	BCL	C1D-ND-C4D	-3.72	103.70	106.31
7	T	102	BCL	C2D-C1D-ND	3.71	113.80	110.13
7	P	102	BCL	C2D-C1D-ND	3.71	113.79	110.13
15	D	101	SPO	C21-C22-C23	-3.70	122.09	127.28
15	G	102	SPO	C21-C22-C23	-3.70	122.09	127.28
7	L	310	BCL	C1D-ND-C4D	-3.69	103.73	106.31
7	N	102	BCL	C2D-C1D-ND	3.68	113.77	110.13
15	T	101	SPO	C20-C19-C17	-3.68	122.11	127.28
7	Q	105	BCL	C1-C2-C3	-3.67	120.18	126.20
7	N	102	BCL	C3B-C4B-NB	3.67	114.60	109.76
15	N	101	SPO	C20-C19-C17	-3.67	122.14	127.28
7	Q	105	BCL	C2D-C1D-ND	3.66	113.75	110.13
7	L	301	BCL	O2A-CGA-CBA	3.66	123.00	111.83
7	M	404	BCL	C3B-C4B-NB	3.66	114.59	109.76
7	W	102	BCL	CHB-C1B-NB	-3.64	118.58	124.05
15	O	104	SPO	C31-C32-C33	-3.64	119.30	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	310	BCL	C2D-C1D-ND	3.63	113.72	110.13
7	B	101	BCL	C3D-C4D-ND	3.63	115.89	109.99
7	B	101	BCL	C2D-C1D-ND	3.60	113.69	110.13
8	M	405	BPH	C4D-CHA-CBD	-3.59	106.73	108.45
15	S	105	SPO	C31-C32-C33	-3.57	119.44	127.62
7	W	102	BCL	C3B-C4B-NB	3.57	114.47	109.76
7	S	103	BCL	C2D-C1D-ND	3.56	113.65	110.13
7	R	102	BCL	C3B-C4B-NB	3.56	114.45	109.76
7	J	101	BCL	C2D-C1D-ND	3.56	113.65	110.13
7	G	101	BCL	C2D-C1D-ND	3.55	113.64	110.13
15	F	104	SPO	C20-C19-C17	-3.54	122.31	127.28
7	R	102	BCL	C3D-C4D-ND	3.53	115.72	109.99
7	M	403	BCL	C3B-C4B-NB	3.52	114.40	109.76
7	V	101	BCL	C3C-C4C-CHD	-3.51	115.98	123.39
7	F	101	BCL	C4A-NA-C1A	3.51	108.28	106.68
7	V	101	BCL	C1D-ND-C4D	-3.51	103.85	106.31
15	D	103	SPO	C31-C32-C33	-3.49	119.62	127.62
7	T	102	BCL	C3D-C4D-ND	3.48	115.64	109.99
7	E	102	BCL	C3D-C4D-ND	3.46	115.61	109.99
7	E	102	BCL	C4-C3-C5	3.46	121.23	115.23
7	G	101	BCL	C3D-C4D-ND	3.46	115.61	109.99
7	L	310	BCL	C3D-C4D-ND	3.45	115.59	109.99
15	S	104	SPO	C31-C32-C33	-3.44	119.74	127.62
7	Z	101	BCL	CHB-C1B-NB	-3.43	118.91	124.05
7	M	403	BCL	C3D-C4D-ND	3.42	115.55	109.99
7	N	102	BCL	C3D-C4D-ND	3.42	115.55	109.99
7	Z	101	BCL	C1C-NC-C4C	3.42	108.24	106.68
15	W	101	SPO	C5-C6-C7	-3.42	120.73	125.89
7	N	102	BCL	C1-C2-C3	-3.42	120.60	126.20
15	T	101	SPO	C26-C27-C28	-3.42	122.89	127.69
7	M	404	BCL	C3D-C4D-ND	3.41	115.53	109.99
15	G	102	SPO	C34-C33-C35	3.41	121.14	115.23
7	M	403	BCL	C1D-ND-C4D	-3.39	103.93	106.31
15	T	101	SPO	C5-C6-C7	-3.39	120.77	125.89
7	Y	102	BCL	C3D-C4D-ND	3.39	115.50	109.99
7	M	403	BCL	C2D-C1D-ND	3.38	113.47	110.13
13	M	412	LMT	C1B-O1B-C4'	-3.38	109.97	117.98
7	P	102	BCL	C1-C2-C3	-3.38	120.66	126.20
7	K	102	BCL	C4-C3-C5	3.37	121.08	115.23
7	Y	102	BCL	C1-C2-C3	-3.37	120.67	126.20
7	P	102	BCL	C3D-C4D-ND	3.37	115.47	109.99
7	F	101	BCL	C3D-C4D-ND	3.37	115.47	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	102	BCL	C1-C2-C3	-3.37	120.67	126.20
15	D	105	SPO	C9-C10-C11	-3.36	113.48	123.20
15	T	101	SPO	C29-C28-C30	3.35	121.05	115.23
7	L	310	BCL	O2D-CGD-O1D	-3.35	117.33	123.85
7	S	103	BCL	C4-C3-C5	3.34	121.03	115.23
7	J	101	BCL	C3D-C4D-ND	3.34	115.41	109.99
7	Q	105	BCL	C3D-C4D-ND	3.34	115.41	109.99
13	M	409	LMT	C1B-O1B-C4'	-3.33	110.09	117.98
7	V	101	BCL	C2D-C1D-ND	3.31	113.40	110.13
15	E	101	SPO	C21-C22-C23	-3.31	122.64	127.28
7	K	102	BCL	C3D-C4D-ND	3.30	115.35	109.99
15	P	101	SPO	C21-C22-C23	-3.30	122.66	127.28
7	Z	101	BCL	C1-C2-C3	-3.27	120.84	126.20
15	I	103	SPO	C31-C32-C33	-3.27	120.14	127.62
15	P	101	SPO	C29-C28-C30	3.26	120.89	115.23
7	Y	102	BCL	CHC-C4B-NB	-3.26	119.16	124.05
7	D	102	BCL	C1C-NC-C4C	-3.25	105.19	106.68
7	I	102	BCL	O2A-CGA-CBA	3.24	121.72	111.83
7	P	102	BCL	O2A-CGA-CBA	3.24	121.72	111.83
7	S	103	BCL	CHC-C1C-NC	3.23	129.07	124.40
7	Z	101	BCL	C3D-C4D-ND	3.23	115.23	109.99
7	A	101	BCL	CHC-C4B-NB	-3.23	119.21	124.05
7	E	102	BCL	C1-C2-C3	-3.22	120.92	126.20
7	S	103	BCL	C3D-C4D-ND	3.22	115.22	109.99
7	F	101	BCL	CHC-C4B-NB	-3.21	119.23	124.05
7	V	101	BCL	C3D-C4D-ND	3.21	115.21	109.99
15	F	104	SPO	C29-C28-C30	3.21	120.80	115.23
7	F	103	BCL	C3D-C4D-ND	3.20	115.19	109.99
7	M	404	BCL	C1-C2-C3	-3.20	120.96	126.20
15	E	101	SPO	C13-C12-C11	3.19	122.97	118.09
13	X	101	LMT	C1B-O1B-C4'	-3.19	110.42	117.98
7	A	101	BCL	C3B-C4B-NB	3.18	113.96	109.76
15	M	408	SPO	C31-C32-C33	-3.18	120.35	127.62
7	I	102	BCL	C3D-C4D-ND	3.18	115.15	109.99
15	F	104	SPO	C14-C15-C16	-3.18	114.00	123.20
15	P	101	SPO	C10-C9-C7	-3.18	122.83	127.28
7	O	102	BCL	C3D-C4D-ND	3.17	115.15	109.99
15	E	101	SPO	C29-C28-C30	3.17	120.73	115.23
7	A	101	BCL	C3D-C4D-ND	3.17	115.13	109.99
7	W	102	BCL	C3D-C4D-ND	3.17	115.13	109.99
7	D	102	BCL	C4A-NA-C1A	3.16	108.12	106.68
7	J	101	BCL	O2A-CGA-CBA	3.16	121.47	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	P	101	SPO	C34-C33-C35	3.16	120.71	115.23
15	D	103	SPO	C9-C10-C11	-3.15	114.06	123.20
15	F	104	SPO	C34-C33-C35	3.15	120.69	115.23
7	F	101	BCL	CHB-C1B-NB	-3.15	119.33	124.05
7	N	102	BCL	C4-C3-C5	3.15	120.69	115.23
15	G	102	SPO	C26-C27-C28	-3.14	123.27	127.69
7	W	102	BCL	CHC-C4B-NB	-3.14	119.34	124.05
7	D	102	BCL	CHC-C1C-NC	3.14	128.93	124.40
15	I	103	SPO	C21-C22-C23	-3.13	122.88	127.28
15	R	101	SPO	C15-C14-C12	-3.13	122.89	127.28
7	L	301	BCL	C3D-C4D-ND	3.12	115.07	109.99
15	R	101	SPO	C20-C19-C17	-3.12	122.90	127.28
7	T	102	BCL	C4-C3-C5	3.12	120.64	115.23
15	D	101	SPO	C31-C32-C33	-3.11	120.50	127.62
7	W	102	BCL	C1-C2-C3	-3.11	121.11	126.20
7	D	102	BCL	C3D-C4D-ND	3.10	115.03	109.99
7	I	102	BCL	C1-C2-C3	-3.10	121.11	126.20
15	P	101	SPO	C14-C15-C16	-3.10	114.22	123.20
15	G	102	SPO	C29-C28-C30	3.09	120.60	115.23
15	S	105	SPO	C5-C6-C7	-3.09	121.22	125.89
7	M	403	BCL	O2A-CGA-CBA	3.09	121.25	111.83
15	I	104	SPO	C29-C28-C30	3.08	120.57	115.23
15	S	105	SPO	C29-C28-C30	3.08	120.57	115.23
15	R	101	SPO	C29-C28-C30	3.08	120.57	115.23
7	O	102	BCL	CHC-C1C-NC	3.07	128.84	124.40
7	E	102	BCL	O2A-CGA-CBA	3.07	121.19	111.83
7	Y	102	BCL	C3B-C4B-NB	3.06	113.80	109.76
15	I	103	SPO	C9-C10-C11	-3.06	114.32	123.20
15	S	105	SPO	C10-C9-C7	-3.06	122.98	127.28
13	A	102	LMT	O1B-C1B-C2B	3.06	115.61	108.09
15	F	104	SPO	C13-C12-C11	3.06	122.75	118.09
15	I	104	SPO	C9-C10-C11	-3.05	114.36	123.20
7	F	103	BCL	CHC-C1C-NC	3.05	128.80	124.40
15	N	101	SPO	C34-C33-C35	3.04	120.51	115.23
7	W	102	BCL	C2D-C1D-ND	3.04	113.13	110.13
7	Y	102	BCL	CHB-C1B-NB	-3.03	119.50	124.05
7	M	403	BCL	O2D-CGD-O1D	-3.03	117.95	123.85
7	Q	105	BCL	O2A-CGA-CBA	3.03	121.08	111.83
15	N	101	SPO	C26-C27-C28	-3.03	123.43	127.69
7	P	102	BCL	C4-C3-C5	3.02	120.48	115.23
15	O	104	SPO	C15-C14-C12	-3.02	123.04	127.28
15	P	101	SPO	C27-C26-C25	-3.01	114.48	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	D	103	SPO	C29-C28-C30	3.01	120.45	115.23
7	T	102	BCL	O2A-CGA-CBA	3.00	121.00	111.83
15	I	104	SPO	C31-C32-C33	-3.00	120.75	127.62
15	R	101	SPO	C34-C33-C35	3.00	120.44	115.23
15	T	101	SPO	C31-C32-C33	-3.00	120.77	127.62
15	S	104	SPO	C9-C10-C11	-2.99	114.52	123.20
7	L	301	BCL	C4-C3-C5	2.99	120.42	115.23
15	D	101	SPO	C14-C15-C16	-2.99	114.53	123.20
7	R	102	BCL	O2A-CGA-CBA	2.98	120.94	111.83
15	E	101	SPO	C34-C33-C35	2.98	120.41	115.23
7	I	102	BCL	C4-C3-C5	2.98	120.40	115.23
7	G	101	BCL	O2A-CGA-CBA	2.98	120.92	111.83
7	O	102	BCL	C4-C3-C5	2.98	120.39	115.23
7	F	103	BCL	C1-C2-C3	-2.97	121.33	126.20
7	W	102	BCL	C3C-C4C-CHD	-2.97	117.12	123.39
7	F	101	BCL	C3B-C4B-NB	2.97	113.68	109.76
15	D	103	SPO	C15-C14-C12	-2.97	123.11	127.28
15	W	101	SPO	C29-C28-C30	2.97	120.38	115.23
7	Z	101	BCL	C3B-C4B-NB	2.97	113.68	109.76
15	O	104	SPO	C9-C10-C11	-2.97	114.61	123.20
7	B	101	BCL	CHB-C4A-NA	2.96	128.67	124.40
15	O	103	SPO	C9-C10-C11	-2.96	114.63	123.20
7	M	403	BCL	C1-C2-C3	-2.95	121.36	126.20
7	S	103	BCL	O2A-CGA-CBA	2.95	120.83	111.83
10	M	414	PGV	C02-O01-C1	-2.95	110.74	117.80
15	E	101	SPO	C26-C27-C28	-2.95	123.54	127.69
7	I	102	BCL	C4A-NA-C1A	2.95	108.02	106.68
15	W	101	SPO	C21-C20-C19	-2.94	117.49	123.52
7	F	101	BCL	C1D-ND-C4D	-2.94	104.25	106.31
7	W	102	BCL	C4A-NA-C1A	2.94	108.02	106.68
7	W	102	BCL	O2A-CGA-CBA	2.94	120.81	111.83
15	P	101	SPO	C20-C19-C17	-2.94	123.15	127.28
15	E	101	SPO	C31-C32-C33	-2.92	120.93	127.62
10	H	303	PGV	O03-C19-C20	2.92	120.75	111.83
7	Q	105	BCL	CHC-C1C-NC	2.92	128.61	124.40
7	A	101	BCL	CMD-C2D-C3D	-2.91	121.01	127.69
7	W	102	BCL	C4-C3-C5	2.91	120.28	115.23
7	I	102	BCL	CHC-C4B-NB	-2.90	119.70	124.05
7	K	102	BCL	CHC-C4B-NB	-2.90	119.70	124.05
7	F	101	BCL	C2D-C1D-ND	2.89	112.99	110.13
15	W	101	SPO	C26-C27-C28	-2.89	123.63	127.69
10	H	304	PGV	O03-C19-C20	2.88	120.63	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	F	104	SPO	C27-C26-C25	-2.88	114.85	123.20
15	D	101	SPO	C9-C10-C11	-2.87	114.87	123.20
7	O	102	BCL	O2A-CGA-CBA	2.87	120.60	111.83
7	R	102	BCL	C4-C3-C5	2.87	120.22	115.23
7	Z	101	BCL	CHD-C1D-C2D	2.87	131.46	125.49
10	M	413	PGV	O03-C19-C20	2.87	120.59	111.83
7	F	103	BCL	C4-C3-C5	2.86	120.20	115.23
15	S	104	SPO	C34-C33-C35	2.86	120.19	115.23
7	N	102	BCL	O2D-CGD-O1D	-2.86	118.28	123.85
15	I	103	SPO	C29-C28-C30	2.86	120.19	115.23
15	W	101	SPO	C31-C32-C33	-2.85	121.09	127.62
7	M	403	BCL	C4-C3-C5	2.85	120.18	115.23
7	F	101	BCL	C3C-C4C-CHD	-2.85	117.38	123.39
7	W	102	BCL	C1D-ND-C4D	-2.85	104.31	106.31
7	O	102	BCL	C1C-NC-C4C	-2.85	105.38	106.68
7	M	403	BCL	CHC-C4B-NB	-2.84	119.79	124.05
7	F	101	BCL	O2A-CGA-CBA	2.84	120.49	111.83
7	I	102	BCL	CHC-C1C-NC	2.84	128.49	124.40
7	T	102	BCL	C1-C2-C3	-2.84	121.55	126.20
7	E	102	BCL	CHC-C1C-NC	2.83	128.48	124.40
7	K	102	BCL	CHC-C1C-NC	2.83	128.48	124.40
13	L	309	LMT	C1B-O1B-C4'	-2.83	111.28	117.98
7	Q	105	BCL	CHC-C4B-NB	-2.82	119.81	124.05
15	N	101	SPO	C29-C28-C30	2.82	120.13	115.23
7	L	301	BCL	C1-C2-C3	-2.82	121.57	126.20
7	N	102	BCL	O2A-CGA-CBA	2.82	120.44	111.83
15	P	101	SPO	C21-C20-C19	-2.82	117.75	123.52
7	I	102	BCL	O2D-CGD-O1D	-2.82	118.36	123.85
7	A	101	BCL	C4-C3-C5	2.82	120.12	115.23
15	D	101	SPO	C20-C19-C17	-2.82	123.33	127.28
7	K	102	BCL	O2D-CGD-O1D	-2.82	118.36	123.85
7	Y	102	BCL	C1D-ND-C4D	-2.82	104.34	106.31
7	Q	105	BCL	C4-C3-C5	2.82	120.12	115.23
15	I	104	SPO	C14-C15-C16	-2.82	115.04	123.20
10	Q	103	PGV	O03-C19-C20	2.81	120.42	111.83
7	F	103	BCL	CHC-C4B-NB	-2.81	119.83	124.05
7	S	103	BCL	CHC-C4B-NB	-2.81	119.84	124.05
13	X	102	LMT	C1B-O1B-C4'	-2.81	111.33	117.98
7	F	101	BCL	C1-C2-C3	-2.81	121.60	126.20
15	G	102	SPO	C4-C5-C6	-2.80	120.98	124.91
15	R	101	SPO	C26-C27-C28	-2.80	123.75	127.69
7	B	101	BCL	C4-C3-C5	2.80	120.08	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	102	BCL	O2A-CGA-CBA	2.79	120.35	111.83
7	K	102	BCL	C1-C2-C3	-2.79	121.62	126.20
7	O	102	BCL	CHC-C4B-NB	-2.79	119.87	124.05
13	I	101	LMT	O1B-C4'-C5'	-2.79	102.17	109.48
15	W	101	SPO	C34-C33-C35	2.78	120.06	115.23
7	F	103	BCL	O2A-CGA-CBA	2.77	120.27	111.83
15	R	101	SPO	C10-C9-C7	-2.76	123.40	127.28
7	Z	101	BCL	O2A-CGA-CBA	2.76	120.25	111.83
7	Y	102	BCL	C4-C3-C5	2.76	120.02	115.23
7	Y	102	BCL	CMD-C2D-C3D	-2.76	121.36	127.69
7	Q	105	BCL	O2D-CGD-O1D	-2.75	118.49	123.85
15	D	105	SPO	C29-C28-C30	2.75	120.00	115.23
7	Z	101	BCL	CMD-C2D-C3D	-2.75	121.38	127.69
7	S	103	BCL	CHB-C4A-NA	2.75	128.36	124.40
7	G	101	BCL	CHB-C4A-NA	2.74	128.36	124.40
7	B	101	BCL	C1-C2-C3	-2.74	121.71	126.20
10	M	415	PGV	O03-C19-C20	2.74	120.18	111.83
7	V	101	BCL	CHB-C4A-NA	2.73	128.35	124.40
7	L	310	BCL	O2A-CGA-CBA	2.73	120.15	111.83
15	W	101	SPO	C15-C14-C12	-2.72	123.46	127.28
15	N	101	SPO	C9-C10-C11	-2.72	115.32	123.20
7	V	101	BCL	CMD-C2D-C3D	-2.72	121.46	127.69
8	L	302	BPH	CMA-C3A-C4A	-2.71	108.77	114.61
15	I	104	SPO	C34-C33-C35	2.71	119.93	115.23
15	M	408	SPO	C34-C33-C35	2.71	119.93	115.23
15	P	101	SPO	C31-C32-C33	-2.71	121.43	127.62
7	G	101	BCL	C4-C3-C5	2.70	119.92	115.23
7	L	310	BCL	C4-C3-C5	2.70	119.91	115.23
7	P	102	BCL	CHB-C4A-NA	2.70	128.29	124.40
7	Z	101	BCL	C4-C3-C5	2.70	119.91	115.23
7	I	102	BCL	CAC-C3C-C4C	-2.70	106.60	112.58
10	M	402	PGV	O03-C19-C20	2.69	120.05	111.83
8	L	302	BPH	C2B-C1B-NB	-2.69	107.48	109.43
15	S	104	SPO	C29-C28-C30	2.69	119.90	115.23
15	G	102	SPO	C31-C32-C33	-2.69	121.46	127.62
15	N	101	SPO	C27-C26-C25	-2.69	115.40	123.20
7	M	404	BCL	CED-O2D-CGD	2.69	122.01	115.92
7	Q	105	BCL	CMB-C2B-C3B	2.68	134.14	125.67
15	O	103	SPO	C14-C15-C16	-2.68	115.42	123.20
7	F	101	BCL	CMD-C2D-C3D	-2.68	121.55	127.69
7	M	404	BCL	C4-C3-C5	2.68	119.88	115.23
7	V	101	BCL	O2A-CGA-CBA	2.68	119.99	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	404	BCL	O2A-CGA-CBA	2.67	119.99	111.83
15	S	105	SPO	C15-C14-C12	-2.67	123.53	127.28
15	T	101	SPO	C9-C10-C11	-2.67	115.46	123.20
13	M	410	LMT	O1'-C1'-C2'	2.67	112.33	108.27
15	T	101	SPO	C14-C15-C16	-2.67	115.47	123.20
7	B	101	BCL	CHC-C1C-NC	2.67	128.25	124.40
7	F	101	BCL	C4-C3-C5	2.67	119.86	115.23
15	I	103	SPO	C14-C15-C16	-2.67	115.47	123.20
7	Z	101	BCL	C3C-C4C-CHD	-2.66	117.78	123.39
10	M	414	PGV	O03-C19-C20	2.66	119.95	111.83
7	E	102	BCL	CHB-C4A-NA	2.66	128.24	124.40
10	Q	103	PGV	C02-O01-C1	-2.66	111.43	117.80
7	M	404	BCL	CAA-C2A-C3A	-2.66	105.82	113.00
8	M	405	BPH	C2B-C1B-NB	-2.66	107.51	109.43
15	M	408	SPO	C9-C10-C11	-2.65	115.51	123.20
7	T	102	BCL	CHC-C4B-NB	-2.65	120.07	124.05
7	V	101	BCL	CHC-C1C-NC	2.65	128.23	124.40
15	D	105	SPO	C14-C15-C16	-2.65	115.51	123.20
10	M	415	PGV	C02-O01-C1	-2.65	111.45	117.80
7	L	310	BCL	C1C-NC-C4C	-2.65	105.47	106.68
10	H	303	PGV	C02-O01-C1	-2.65	111.46	117.80
15	G	102	SPO	C27-C26-C25	-2.65	115.53	123.20
15	D	105	SPO	C8-C7-C6	2.64	122.12	118.09
7	Y	102	BCL	C2D-C1D-ND	2.64	112.74	110.13
7	V	101	BCL	O2D-CGD-O1D	-2.64	118.71	123.85
7	J	101	BCL	CHC-C1C-NC	2.64	128.21	124.40
7	F	103	BCL	CHB-C4A-NA	2.64	128.21	124.40
7	D	102	BCL	CHC-C4B-NB	-2.64	120.09	124.05
7	N	102	BCL	CHB-C4A-NA	2.64	128.20	124.40
7	E	102	BCL	C2A-C1A-CHA	-2.64	119.29	123.87
15	D	103	SPO	C8-C7-C6	2.63	122.11	118.09
7	V	101	BCL	C4-C3-C5	2.63	119.79	115.23
15	T	101	SPO	C34-C33-C35	2.63	119.79	115.23
7	G	101	BCL	C2A-C1A-CHA	-2.62	119.31	123.87
7	K	102	BCL	CMB-C2B-C3B	2.62	133.93	125.67
7	L	301	BCL	O2A-CGA-O1A	-2.62	117.08	123.63
7	S	103	BCL	CMD-C2D-C3D	-2.61	121.69	127.69
15	W	101	SPO	C20-C19-C17	-2.61	123.61	127.28
15	E	101	SPO	C27-C26-C25	-2.61	115.63	123.20
15	F	104	SPO	C9-C10-C11	-2.61	115.63	123.20
7	J	101	BCL	C2A-C1A-CHA	-2.61	119.34	123.87
7	Z	101	BCL	O2D-CGD-O1D	-2.61	118.78	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	103	SPO	C29-C28-C30	2.60	119.75	115.23
7	L	301	BCL	CED-O2D-CGD	2.60	121.82	115.92
7	F	103	BCL	CMB-C2B-C3B	2.60	133.88	125.67
7	O	102	BCL	O2D-CGD-O1D	-2.60	118.78	123.85
15	O	104	SPO	C21-C20-C19	-2.60	118.20	123.52
15	I	103	SPO	C34-C33-C35	2.60	119.74	115.23
13	S	101	LMT	O1B-C4'-C3'	2.60	113.84	107.23
15	N	101	SPO	C21-C20-C19	-2.59	118.21	123.52
15	G	102	SPO	C9-C10-C11	-2.59	115.69	123.20
7	E	102	BCL	O2D-CGD-O1D	-2.59	118.80	123.85
7	A	101	BCL	O2A-CGA-CBA	2.59	119.74	111.83
7	K	102	BCL	CAC-C3C-C4C	-2.59	106.84	112.58
10	L	305	PGV	O03-C19-C20	2.58	119.69	111.83
7	J	101	BCL	C4-C3-C5	2.57	119.69	115.23
7	J	101	BCL	CHB-C4A-NA	2.57	128.11	124.40
7	D	102	BCL	O2A-CGA-O1A	-2.57	117.20	123.63
7	T	102	BCL	CHB-C4A-NA	2.57	128.11	124.40
7	K	102	BCL	CHB-C4A-NA	2.57	128.10	124.40
7	V	101	BCL	CHC-C4B-NB	-2.57	120.20	124.05
7	B	101	BCL	O2D-CGD-O1D	-2.56	118.86	123.85
15	D	103	SPO	C34-C33-C35	2.56	119.67	115.23
7	M	404	BCL	CHC-C4B-NB	-2.56	120.21	124.05
7	F	103	BCL	O2D-CGD-O1D	-2.56	118.87	123.85
7	K	102	BCL	C4A-NA-C1A	2.56	107.85	106.68
7	L	301	BCL	CHC-C1C-NC	2.56	128.09	124.40
7	I	102	BCL	CMB-C2B-C3B	2.55	133.73	125.67
7	J	101	BCL	O2D-CGD-O1D	-2.55	118.89	123.85
7	L	310	BCL	CHC-C1C-NC	2.55	128.08	124.40
7	A	101	BCL	C3C-C2C-C1C	-2.55	97.76	101.87
7	O	102	BCL	CMB-C2B-C3B	2.55	133.70	125.67
7	R	102	BCL	CHB-C4A-NA	2.54	128.07	124.40
7	B	101	BCL	C2A-C1A-CHA	-2.54	119.46	123.87
13	L	311	LMT	O1B-C4'-C3'	2.54	113.69	107.23
7	I	102	BCL	C1C-NC-C4C	-2.54	105.52	106.68
7	Y	102	BCL	C1D-CHD-C4C	-2.53	120.51	126.62
7	I	102	BCL	CHB-C4A-NA	2.53	128.05	124.40
7	S	103	BCL	O2D-CGD-O1D	-2.53	118.92	123.85
7	Y	102	BCL	O2D-CGD-O1D	-2.53	118.92	123.85
7	O	102	BCL	C4A-NA-C1A	2.53	107.83	106.68
7	M	404	BCL	CHB-C4A-NA	2.52	128.04	124.40
15	M	408	SPO	C10-C9-C7	-2.52	123.75	127.28
15	D	103	SPO	C14-C15-C16	-2.52	115.91	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	103	BCL	CAC-C3C-C4C	-2.52	107.00	112.58
7	F	101	BCL	CHD-C1D-C2D	2.52	130.72	125.49
7	L	301	BCL	CHC-C4B-NB	-2.52	120.28	124.05
13	M	417	LMT	C1B-O1B-C4'	-2.51	112.02	117.98
15	O	104	SPO	C34-C33-C35	2.51	119.59	115.23
7	Y	102	BCL	CHD-C1D-C2D	2.51	130.71	125.49
15	W	101	SPO	C14-C15-C16	-2.51	115.93	123.20
15	O	104	SPO	C14-C15-C16	-2.51	115.93	123.20
7	L	301	BCL	C1D-CHD-C4C	-2.51	120.57	126.62
7	N	102	BCL	C2A-C1A-CHA	-2.51	119.52	123.87
15	G	102	SPO	C40-C38-C39	2.50	120.35	114.59
8	M	405	BPH	CMA-C3A-C4A	-2.50	109.23	114.61
15	S	104	SPO	C5-C6-C7	-2.50	122.12	125.89
15	S	104	SPO	C40-C38-C39	2.50	120.33	114.59
7	T	102	BCL	O2D-CGD-O1D	-2.49	119.01	123.85
10	M	402	PGV	C02-O01-C1	-2.49	111.85	117.80
15	M	408	SPO	C40-C38-C39	2.49	120.31	114.59
7	D	102	BCL	CHB-C4A-NA	2.48	127.98	124.40
7	Z	101	BCL	C4D-CHA-C1A	-2.48	118.29	121.24
7	B	101	BCL	C4D-CHA-C1A	-2.48	118.29	121.24
7	M	404	BCL	CMB-C2B-C3B	2.48	133.48	125.67
15	S	104	SPO	C13-C12-C11	2.47	121.87	118.09
7	P	102	BCL	C2A-C1A-CHA	-2.47	119.58	123.87
15	G	102	SPO	C21-C20-C19	-2.47	118.46	123.52
13	M	410	LMT	C1-O1'-C1'	-2.47	109.46	113.68
15	D	101	SPO	C29-C28-C30	2.47	119.52	115.23
7	P	102	BCL	C1D-CHD-C4C	-2.47	120.67	126.62
7	A	101	BCL	CHD-C1D-C2D	2.46	130.61	125.49
7	G	101	BCL	CHC-C1C-NC	2.46	127.95	124.40
7	R	102	BCL	CHC-C4B-NB	-2.46	120.36	124.05
15	D	105	SPO	C34-C33-C35	2.46	119.49	115.23
7	Z	101	BCL	CHC-C4B-NB	-2.46	120.37	124.05
15	N	101	SPO	C31-C32-C33	-2.45	122.02	127.62
15	R	101	SPO	C21-C20-C19	-2.45	118.51	123.52
15	N	101	SPO	C14-C15-C16	-2.45	116.11	123.20
15	O	103	SPO	C34-C33-C35	2.45	119.47	115.23
15	O	104	SPO	C29-C28-C30	2.45	119.47	115.23
15	I	104	SPO	C13-C12-C11	2.44	121.82	118.09
7	O	102	BCL	CHB-C4A-NA	2.44	127.92	124.40
9	L	303	U10	C7-C6-C1	-2.44	120.71	124.89
15	O	103	SPO	C8-C7-C6	2.44	121.81	118.09
7	E	102	BCL	CHC-C4B-NB	-2.44	120.40	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Y	102	BCL	O2A-CGA-CBA	2.43	119.26	111.83
7	M	404	BCL	CHC-C1C-NC	2.43	127.91	124.40
13	Y	103	LMT	O1B-C4'-C3'	2.43	113.42	107.23
7	N	102	BCL	CMB-C2B-C3B	2.43	133.33	125.67
7	A	101	BCL	C2D-C1D-ND	2.43	112.53	110.13
15	P	101	SPO	C13-C12-C11	2.43	121.80	118.09
15	S	104	SPO	C14-C15-C16	-2.43	116.17	123.20
7	G	101	BCL	CHC-C4B-NB	-2.42	120.42	124.05
7	I	102	BCL	C1D-CHD-C4C	-2.42	120.78	126.62
7	K	102	BCL	C1C-NC-C4C	-2.42	105.58	106.68
7	S	103	BCL	CMB-C2B-C3B	2.42	133.30	125.67
7	E	102	BCL	C1D-CHD-C4C	-2.41	120.80	126.62
7	D	102	BCL	CMB-C2B-C3B	2.41	133.28	125.67
7	K	102	BCL	C1D-CHD-C4C	-2.41	120.80	126.62
15	I	104	SPO	C10-C9-C7	-2.41	123.89	127.28
7	J	101	BCL	C1-C2-C3	-2.41	122.25	126.20
15	T	101	SPO	C27-C26-C25	-2.41	116.22	123.20
7	L	310	BCL	C1D-CHD-C4C	-2.41	120.82	126.62
15	T	101	SPO	C21-C20-C19	-2.40	118.61	123.52
15	O	104	SPO	C13-C12-C11	2.40	121.76	118.09
7	A	101	BCL	CMB-C2B-C1B	2.40	129.07	125.42
7	Q	105	BCL	CHB-C4A-NA	2.40	127.86	124.40
7	R	102	BCL	O2D-CGD-O1D	-2.40	119.18	123.85
15	I	104	SPO	C21-C20-C19	-2.40	118.62	123.52
7	A	101	BCL	C1D-ND-C4D	-2.39	104.63	106.31
7	L	301	BCL	CMB-C2B-C3B	2.39	133.22	125.67
7	E	102	BCL	CMB-C2B-C3B	2.39	133.22	125.67
7	D	102	BCL	C1D-CHD-C4C	-2.39	120.86	126.62
7	O	102	BCL	C1D-CHD-C4C	-2.39	120.86	126.62
15	I	103	SPO	C20-C21-C22	-2.39	118.63	123.52
7	L	310	BCL	C2A-C1A-CHA	-2.39	119.73	123.87
7	G	101	BCL	O2D-CGD-O1D	-2.39	119.20	123.85
15	S	105	SPO	C9-C10-C11	-2.38	116.29	123.20
7	M	404	BCL	O2D-CGD-O1D	-2.38	119.21	123.85
15	D	103	SPO	C13-C12-C11	2.38	121.73	118.09
15	E	101	SPO	C8-C7-C9	-2.38	118.96	122.82
15	I	104	SPO	C8-C7-C6	2.38	121.72	118.09
7	G	101	BCL	CMB-C2B-C3B	2.38	133.17	125.67
7	Q	105	BCL	CMD-C2D-C3D	-2.38	122.24	127.69
15	F	104	SPO	C21-C20-C19	-2.38	118.66	123.52
15	S	104	SPO	C10-C9-C7	-2.38	123.94	127.28
15	W	101	SPO	C27-C26-C25	-2.37	116.32	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	301	BCL	CMD-C2D-C3D	-2.37	122.25	127.69
7	M	403	BCL	C1D-CHD-C4C	-2.37	120.91	126.62
15	D	101	SPO	C5-C6-C7	-2.37	122.32	125.89
15	G	102	SPO	C8-C7-C6	2.36	121.69	118.09
7	F	103	BCL	CMD-C2D-C3D	-2.36	122.29	127.69
15	D	105	SPO	C21-C20-C19	-2.35	118.71	123.52
7	J	101	BCL	C1D-CHD-C4C	-2.35	120.95	126.62
15	S	105	SPO	C14-C15-C16	-2.35	116.40	123.20
7	Z	101	BCL	C2D-C1D-ND	2.35	112.45	110.13
7	N	102	BCL	CHC-C1C-NC	2.34	127.78	124.40
15	T	101	SPO	C40-C38-C39	2.34	119.98	114.59
7	M	404	BCL	CMD-C2D-C3D	-2.34	122.32	127.69
7	M	403	BCL	CMB-C2B-C3B	2.34	133.03	125.67
7	G	101	BCL	C1D-CHD-C4C	-2.34	120.99	126.62
15	N	101	SPO	C1-C4-C5	-2.33	106.94	112.98
15	I	104	SPO	C40-C38-C39	2.33	119.94	114.59
7	D	102	BCL	CAC-C3C-C4C	-2.33	107.42	112.58
15	S	105	SPO	C20-C21-C22	-2.33	118.76	123.52
9	M	401	U10	C7-C6-C1	-2.32	120.91	124.89
7	T	102	BCL	C2A-C1A-CHA	-2.32	119.84	123.87
7	W	102	BCL	C1D-CHD-C4C	-2.32	121.02	126.62
7	V	101	BCL	CMB-C2B-C3B	2.32	132.98	125.67
15	R	101	SPO	C4-C5-C6	-2.32	121.66	124.91
15	R	101	SPO	C40-C38-C39	2.32	119.92	114.59
7	F	103	BCL	CHB-C1B-C2B	-2.32	120.70	127.43
15	F	104	SPO	C31-C32-C33	-2.31	122.33	127.62
15	D	101	SPO	C40-C38-C39	2.31	119.91	114.59
7	Y	102	BCL	O1D-CGD-CBD	-2.31	119.96	124.52
15	R	101	SPO	C31-C32-C33	-2.31	122.33	127.62
7	Q	105	BCL	CHB-C1B-C2B	-2.31	120.72	127.43
7	R	102	BCL	C1D-CHD-C4C	-2.31	121.05	126.62
7	N	102	BCL	CHC-C4B-NB	-2.31	120.58	124.05
7	T	102	BCL	CMB-C2B-C3B	2.31	132.94	125.67
15	D	101	SPO	C34-C33-C35	2.31	119.23	115.23
15	P	101	SPO	C40-C38-C39	2.30	119.89	114.59
7	J	101	BCL	CMB-C2B-C3B	2.30	132.93	125.67
7	F	101	BCL	C1D-CHD-C4C	-2.30	121.07	126.62
7	M	403	BCL	C2A-C1A-CHA	-2.30	119.88	123.87
15	M	408	SPO	C15-C14-C12	-2.30	124.05	127.28
7	I	102	BCL	O2A-CGA-O1A	-2.30	117.88	123.63
15	I	104	SPO	C27-C26-C25	-2.30	116.54	123.20
7	P	102	BCL	CHC-C1C-NC	2.30	127.71	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	101	BCL	CHC-C4B-NB	-2.29	120.61	124.05
7	J	101	BCL	CHC-C4B-NB	-2.29	120.61	124.05
7	N	102	BCL	C1D-CHD-C4C	-2.29	121.11	126.62
15	M	408	SPO	C8-C7-C6	2.29	121.58	118.09
7	L	310	BCL	CHC-C4B-NB	-2.29	120.62	124.05
15	S	105	SPO	C40-C38-C39	2.28	119.84	114.59
15	E	101	SPO	C40-C38-C39	2.28	119.84	114.59
15	P	101	SPO	C15-C14-C12	-2.28	124.08	127.28
15	M	408	SPO	C5-C6-C7	-2.28	122.45	125.89
15	I	103	SPO	C13-C12-C11	2.27	121.55	118.09
7	K	102	BCL	CMD-C2D-C3D	-2.27	122.49	127.69
15	I	104	SPO	C15-C14-C12	-2.27	124.10	127.28
7	T	102	BCL	CHB-C1B-NB	-2.27	120.65	124.05
7	F	103	BCL	C1D-CHD-C4C	-2.27	121.16	126.62
7	O	102	BCL	CHB-C1B-C2B	-2.26	120.86	127.43
15	N	101	SPO	C40-C38-C39	2.26	119.80	114.59
15	O	104	SPO	C40-C38-C39	2.26	119.79	114.59
7	P	102	BCL	O2D-CGD-O1D	-2.26	119.45	123.85
7	R	102	BCL	C2A-C1A-CHA	-2.26	119.94	123.87
7	V	101	BCL	C1D-CHD-C4C	-2.26	121.18	126.62
7	F	101	BCL	O2D-CGD-O1D	-2.25	119.47	123.85
15	W	101	SPO	C40-C38-C39	2.25	119.76	114.59
7	B	101	BCL	C1D-CHD-C4C	-2.24	121.21	126.62
13	S	102	LMT	C1B-O1B-C4'	-2.24	112.66	117.98
7	L	310	BCL	C1-O2A-CGA	2.24	122.06	116.65
15	D	103	SPO	C21-C20-C19	-2.24	118.94	123.52
7	W	102	BCL	CBC-CAC-C3C	-2.24	108.67	113.41
7	D	102	BCL	O2D-CGD-O1D	-2.23	119.50	123.85
15	D	105	SPO	C26-C25-C23	-2.23	120.25	126.36
7	P	102	BCL	CHC-C4B-NB	-2.23	120.70	124.05
7	L	310	BCL	CMB-C2B-C3B	2.23	132.70	125.67
13	I	101	LMT	O1B-C4'-C3'	2.23	112.90	107.23
7	A	101	BCL	C1D-CHD-C4C	-2.23	121.25	126.62
7	B	101	BCL	CMB-C2B-C3B	2.23	132.69	125.67
15	R	101	SPO	C14-C15-C16	-2.23	116.75	123.20
7	D	102	BCL	CHB-C1B-C2B	-2.22	120.97	127.43
7	Z	101	BCL	CMB-C2B-C1B	2.22	128.80	125.42
7	M	404	BCL	C1D-CHD-C4C	-2.22	121.26	126.62
15	O	104	SPO	C10-C9-C7	-2.22	124.17	127.28
7	Y	102	BCL	CAC-C3C-C4C	-2.22	107.66	112.58
15	O	104	SPO	C8-C7-C6	2.22	121.47	118.09
7	K	102	BCL	CHB-C1B-C2B	-2.21	121.00	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	I	104	SPO	C20-C21-C22	-2.21	118.99	123.52
15	M	408	SPO	C14-C15-C16	-2.21	116.80	123.20
7	T	102	BCL	C1D-CHD-C4C	-2.21	121.29	126.62
7	L	301	BCL	CHB-C4A-NA	2.21	127.59	124.40
7	S	103	BCL	C1D-CHD-C4C	-2.20	121.31	126.62
7	L	310	BCL	CHB-C4A-NA	2.20	127.58	124.40
15	E	101	SPO	C21-C20-C19	-2.20	119.02	123.52
13	K	101	LMT	C1B-O1B-C4'	-2.20	112.76	117.98
7	E	102	BCL	C4D-CHA-C1A	-2.19	118.63	121.24
13	Y	101	LMT	C1B-O1B-C4'	-2.19	112.78	117.98
7	S	103	BCL	CHB-C1B-C2B	-2.19	121.06	127.43
15	E	101	SPO	C9-C10-C11	2.19	129.55	123.20
15	I	103	SPO	C8-C7-C6	2.19	121.43	118.09
15	D	103	SPO	C20-C21-C22	-2.19	119.04	123.52
7	P	102	BCL	CMB-C2B-C3B	2.19	132.57	125.67
7	T	102	BCL	CHC-C1C-NC	2.18	127.55	124.40
7	V	101	BCL	CHD-C1D-C2D	2.18	130.03	125.49
7	Q	105	BCL	C2A-C1A-CHA	-2.18	120.08	123.87
7	Q	105	BCL	C1D-CHD-C4C	-2.18	121.36	126.62
15	F	104	SPO	C24-C23-C25	2.18	121.42	118.09
15	S	105	SPO	C34-C33-C35	2.18	119.01	115.23
7	R	102	BCL	CAC-C3C-C4C	-2.17	107.76	112.58
15	I	104	SPO	C18-C17-C16	2.17	121.41	118.09
7	R	102	BCL	CHC-C1C-NC	2.17	127.53	124.40
15	P	101	SPO	C24-C23-C25	2.17	121.40	118.09
7	Z	101	BCL	C1D-ND-C4D	-2.16	104.79	106.31
15	G	102	SPO	C20-C21-C22	-2.16	119.10	123.52
7	V	101	BCL	C4A-NA-C1A	2.16	107.66	106.68
13	A	102	LMT	O2B-C2B-C1B	2.16	115.21	110.08
7	Q	105	BCL	CAC-C3C-C4C	-2.15	107.80	112.58
7	I	102	BCL	CMD-C2D-C3D	-2.15	122.75	127.69
13	X	101	LMT	O5B-C1B-C2B	2.15	114.79	110.37
15	P	101	SPO	C26-C27-C28	-2.15	124.66	127.69
7	P	102	BCL	O2A-CGA-O1A	-2.15	118.25	123.63
13	M	411	LMT	C1-O1'-C1'	-2.15	110.01	113.68
9	M	407	U10	C7-C6-C1	-2.15	121.21	124.89
7	Y	102	BCL	C3C-C4C-CHD	-2.15	118.87	123.39
15	E	101	SPO	C10-C11-C12	2.15	132.25	126.36
7	I	102	BCL	CHB-C1B-C2B	-2.15	121.20	127.43
15	R	101	SPO	C9-C10-C11	-2.14	116.99	123.20
15	N	101	SPO	C13-C12-C14	-2.14	119.34	122.82
7	B	101	BCL	CED-O2D-CGD	2.14	120.77	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	102	BCL	CMB-C2B-C3B	2.14	132.42	125.67
15	O	104	SPO	C26-C25-C23	-2.14	120.50	126.36
7	G	101	BCL	C1-C2-C3	-2.13	122.71	126.20
7	F	101	BCL	C6-C5-C3	-2.13	108.28	113.47
15	D	105	SPO	C15-C14-C12	-2.13	124.30	127.28
7	B	101	BCL	O2A-CGA-CBA	2.13	118.31	111.83
10	H	303	PGV	O03-C19-O04	-2.12	118.31	123.63
15	D	105	SPO	C13-C12-C11	2.12	121.33	118.09
7	A	101	BCL	O1D-CGD-CBD	-2.12	120.34	124.52
15	I	103	SPO	C40-C38-C39	2.12	119.47	114.59
7	A	101	BCL	CBA-CAA-C2A	-2.12	107.49	113.79
7	O	102	BCL	CMD-C2D-C3D	-2.11	122.84	127.69
7	R	102	BCL	CHB-C1B-NB	-2.11	120.88	124.05
8	M	405	BPH	CBA-CAA-C2A	-2.11	107.56	113.78
7	K	102	BCL	C2A-C1A-CHA	-2.11	120.21	123.87
7	M	403	BCL	CHB-C1B-NB	-2.11	120.89	124.05
15	P	101	SPO	C9-C10-C11	-2.11	117.09	123.20
15	R	101	SPO	C13-C12-C11	2.11	121.31	118.09
15	D	103	SPO	C40-C38-C39	2.11	119.44	114.59
7	B	101	BCL	CHB-C1B-NB	-2.10	120.89	124.05
7	L	301	BCL	CHB-C1B-C2B	-2.10	121.33	127.43
13	S	101	LMT	O5'-C5'-C6'	2.10	111.64	106.44
7	M	403	BCL	O1D-CGD-CBD	-2.10	120.38	124.52
7	P	102	BCL	CHB-C1B-NB	-2.10	120.90	124.05
7	Q	105	BCL	C1C-NC-C4C	-2.10	105.72	106.68
15	F	104	SPO	C40-C38-C39	2.10	119.41	114.59
15	F	104	SPO	C26-C27-C28	-2.09	124.75	127.69
15	T	101	SPO	C13-C12-C11	2.09	121.28	118.09
13	M	410	LMT	C1B-O1B-C4'	-2.09	113.02	117.98
7	S	103	BCL	CAC-C3C-C4C	-2.09	107.95	112.58
13	I	101	LMT	O5'-C1'-C2'	-2.09	106.09	110.37
7	J	101	BCL	O2A-CGA-O1A	-2.08	118.42	123.63
15	O	103	SPO	C20-C21-C22	-2.08	119.26	123.52
15	S	105	SPO	C27-C26-C25	-2.08	117.17	123.20
15	I	103	SPO	C18-C17-C16	2.08	121.27	118.09
7	A	101	BCL	CED-O2D-CGD	2.08	120.63	115.92
7	L	301	BCL	C2A-C1A-CHA	-2.08	120.26	123.87
15	D	101	SPO	C13-C12-C11	2.08	121.26	118.09
7	Y	102	BCL	C2A-C1A-CHA	-2.08	120.26	123.87
7	W	102	BCL	CMD-C2D-C3D	-2.07	122.94	127.69
9	M	407	U10	O4-C4-C5	-2.07	109.66	116.64
7	N	102	BCL	CHB-C1B-C2B	-2.06	121.43	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	G	102	SPO	C14-C15-C16	-2.06	117.22	123.20
7	W	102	BCL	O2D-CGD-O1D	-2.06	119.85	123.85
7	W	102	BCL	CED-O2D-CGD	2.05	120.57	115.92
15	N	101	SPO	C4-C5-C6	2.05	127.80	124.91
7	J	101	BCL	C4D-CHA-C1A	-2.05	118.80	121.24
15	G	102	SPO	C24-C23-C25	2.05	121.22	118.09
15	O	103	SPO	C15-C14-C12	-2.05	124.41	127.28
15	S	104	SPO	C21-C20-C19	-2.05	119.33	123.52
15	O	103	SPO	C40-C38-C39	2.05	119.30	114.59
7	J	101	BCL	CHB-C1B-C2B	-2.05	121.48	127.43
7	E	102	BCL	CHB-C1B-C2B	-2.04	121.49	127.43
15	D	103	SPO	C27-C26-C25	-2.04	117.29	123.20
15	R	101	SPO	C27-C26-C25	-2.04	117.30	123.20
7	M	404	BCL	CHB-C1B-C2B	-2.03	121.52	127.43
15	S	104	SPO	C15-C14-C12	-2.03	124.43	127.28
7	Z	101	BCL	C1D-CHD-C4C	-2.03	121.72	126.62
15	S	104	SPO	C36-C37-C38	-2.03	120.87	127.64
15	D	101	SPO	C21-C20-C19	-2.02	119.38	123.52
7	R	102	BCL	O2A-CGA-O1A	-2.02	118.57	123.63
7	Q	105	BCL	C6-C5-C3	-2.02	108.54	113.47
7	F	101	BCL	CMB-C2B-C3B	2.02	132.04	125.67
7	V	101	BCL	C1C-NC-C4C	-2.02	105.76	106.68
15	O	104	SPO	C5-C6-C7	-2.02	122.84	125.89
10	H	304	PGV	O03-C19-O04	-2.01	118.59	123.63
15	I	103	SPO	C15-C14-C12	-2.01	124.46	127.28
7	S	103	BCL	CHD-C1D-C2D	2.01	129.66	125.49
10	H	303	PGV	O01-C1-O02	-2.01	119.02	123.70
7	P	102	BCL	CED-O2D-CGD	2.01	120.47	115.92
15	T	101	SPO	C10-C9-C7	-2.00	124.47	127.28
7	O	102	BCL	CAC-C3C-C4C	-2.00	108.14	112.58

There are no chirality outliers.

All (653) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L	310	BCL	CHA-CBD-CGD-O1D
7	L	310	BCL	CHA-CBD-CGD-O2D
7	M	403	BCL	C1A-C2A-CAA-CBA
7	M	403	BCL	C3A-C2A-CAA-CBA
7	A	101	BCL	C2C-C3C-CAC-CBC
7	A	101	BCL	C4C-C3C-CAC-CBC
7	D	102	BCL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
7	E	102	BCL	C1A-C2A-CAA-CBA
7	E	102	BCL	C3A-C2A-CAA-CBA
7	F	101	BCL	C1A-C2A-CAA-CBA
7	F	103	BCL	C11-C10-C8-C9
7	N	102	BCL	C1A-C2A-CAA-CBA
7	N	102	BCL	C3A-C2A-CAA-CBA
7	P	102	BCL	C1A-C2A-CAA-CBA
7	P	102	BCL	C3A-C2A-CAA-CBA
7	R	102	BCL	C1A-C2A-CAA-CBA
7	R	102	BCL	C3A-C2A-CAA-CBA
7	S	103	BCL	C4C-C3C-CAC-CBC
7	V	101	BCL	C4C-C3C-CAC-CBC
7	W	102	BCL	C1A-C2A-CAA-CBA
7	W	102	BCL	C4C-C3C-CAC-CBC
7	Z	101	BCL	C3A-C2A-CAA-CBA
10	M	402	PGV	C03-O11-P-O12
10	M	402	PGV	C03-O11-P-O13
10	M	402	PGV	C03-O11-P-O14
10	M	402	PGV	C04-O12-P-O11
10	M	402	PGV	C04-O12-P-O13
10	M	402	PGV	O12-C04-C05-O05
10	M	413	PGV	C03-O11-P-O12
10	M	413	PGV	C03-O11-P-O14
10	M	413	PGV	C04-O12-P-O11
10	M	413	PGV	C04-O12-P-O14
10	M	413	PGV	C2-C1-O01-C02
10	M	415	PGV	C03-O11-P-O12
10	M	415	PGV	C03-O11-P-O13
10	M	415	PGV	C03-O11-P-O14
10	H	304	PGV	C03-O11-P-O12
10	H	304	PGV	C03-O11-P-O13
10	H	304	PGV	C03-O11-P-O14
10	H	304	PGV	C04-O12-P-O11
10	H	304	PGV	C2-C1-O01-C02
10	Q	103	PGV	C03-O11-P-O12
10	Q	103	PGV	C03-O11-P-O14
10	Q	103	PGV	C04-O12-P-O11
10	Q	103	PGV	C04-O12-P-O14
11	L	306	PEE	C2-C1-O3P-P
12	L	307	LDA	N1-C1-C2-C3
12	H	301	LDA	C2-C1-N1-CM2
12	H	301	LDA	N1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
12	H	302	LDA	N1-C1-C2-C3
12	D	104	LDA	C2-C1-N1-CM2
13	A	102	LMT	C2B-C1B-O1B-C4'
13	Q	101	LMT	O5'-C1'-O1'-C1
13	X	101	LMT	O5'-C1'-O1'-C1
15	D	103	SPO	C10-C11-C12-C14
15	D	103	SPO	C28-C30-C31-C32
15	D	103	SPO	C32-C33-C35-C36
15	D	103	SPO	C34-C33-C35-C36
15	E	101	SPO	C10-C11-C12-C13
15	E	101	SPO	C10-C11-C12-C14
15	E	101	SPO	C15-C16-C17-C18
15	E	101	SPO	C15-C16-C17-C19
15	F	104	SPO	O1-C1-C4-C5
15	F	104	SPO	C2-C1-C4-C5
15	F	104	SPO	C3-C1-C4-C5
15	F	104	SPO	C5-C6-C7-C8
15	F	104	SPO	C5-C6-C7-C9
15	F	104	SPO	C27-C28-C30-C31
15	F	104	SPO	C29-C28-C30-C31
15	G	102	SPO	C5-C6-C7-C8
15	G	102	SPO	C5-C6-C7-C9
15	I	103	SPO	C32-C33-C35-C36
15	I	103	SPO	C34-C33-C35-C36
15	I	104	SPO	C34-C33-C35-C36
15	N	101	SPO	C5-C6-C7-C9
15	N	101	SPO	C10-C11-C12-C13
15	N	101	SPO	C10-C11-C12-C14
15	O	104	SPO	C32-C33-C35-C36
15	O	104	SPO	C34-C33-C35-C36
15	P	101	SPO	C27-C28-C30-C31
15	P	101	SPO	C29-C28-C30-C31
15	R	101	SPO	C2-C1-O1-CM1
13	Q	101	LMT	C3'-C4'-O1B-C1B
7	F	101	BCL	CBD-CGD-O2D-CED
7	Z	101	BCL	CBD-CGD-O2D-CED
13	S	101	LMT	O5B-C1B-O1B-C4'
13	L	311	LMT	O5B-C1B-O1B-C4'
13	I	101	LMT	O5B-C1B-O1B-C4'
13	Y	103	LMT	O5B-C1B-O1B-C4'
10	M	413	PGV	O02-C1-O01-C02
10	H	304	PGV	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
7	K	102	BCL	C4-C3-C5-C6
7	O	102	BCL	C4-C3-C5-C6
9	L	304	U10	C40-C39-C41-C42
9	L	304	U10	C50-C49-C51-C52
9	M	407	U10	C30-C29-C31-C32
15	E	101	SPO	C29-C28-C30-C31
15	E	101	SPO	C34-C33-C35-C36
15	F	104	SPO	C34-C33-C35-C36
15	G	102	SPO	C29-C28-C30-C31
15	G	102	SPO	C34-C33-C35-C36
15	P	101	SPO	C34-C33-C35-C36
15	R	101	SPO	C29-C28-C30-C31
15	S	104	SPO	C34-C33-C35-C36
7	K	102	BCL	C2-C3-C5-C6
7	O	102	BCL	C2-C3-C5-C6
15	E	101	SPO	C27-C28-C30-C31
15	E	101	SPO	C32-C33-C35-C36
15	F	104	SPO	C32-C33-C35-C36
15	I	104	SPO	C32-C33-C35-C36
15	R	101	SPO	C27-C28-C30-C31
15	S	104	SPO	C32-C33-C35-C36
9	M	407	U10	C27-C28-C29-C30
9	M	407	U10	C27-C28-C29-C31
7	Q	105	BCL	C3-C5-C6-C7
7	A	101	BCL	CBD-CGD-O2D-CED
7	Z	101	BCL	O1D-CGD-O2D-CED
7	M	403	BCL	CBA-CGA-O2A-C1
7	B	101	BCL	CBA-CGA-O2A-C1
7	F	101	BCL	O1D-CGD-O2D-CED
7	Q	105	BCL	C4-C3-C5-C6
9	L	303	U10	C15-C14-C16-C17
9	L	304	U10	C35-C34-C36-C37
15	T	101	SPO	C29-C28-C30-C31
9	L	303	U10	C13-C14-C16-C17
9	L	304	U10	C33-C34-C36-C37
9	L	304	U10	C38-C39-C41-C42
9	M	407	U10	C28-C29-C31-C32
15	G	102	SPO	C27-C28-C30-C31
15	G	102	SPO	C32-C33-C35-C36
7	B	101	BCL	O1A-CGA-O2A-C1
15	D	101	SPO	C28-C30-C31-C32
15	D	103	SPO	C33-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
15	D	105	SPO	C28-C30-C31-C32
15	E	101	SPO	C28-C30-C31-C32
15	I	103	SPO	C28-C30-C31-C32
15	I	103	SPO	C33-C35-C36-C37
15	I	104	SPO	C28-C30-C31-C32
15	I	104	SPO	C33-C35-C36-C37
15	N	101	SPO	C28-C30-C31-C32
15	N	101	SPO	C33-C35-C36-C37
15	O	103	SPO	C28-C30-C31-C32
15	O	104	SPO	C28-C30-C31-C32
15	O	104	SPO	C33-C35-C36-C37
15	R	101	SPO	C33-C35-C36-C37
15	S	104	SPO	C28-C30-C31-C32
15	S	104	SPO	C33-C35-C36-C37
15	T	101	SPO	C33-C35-C36-C37
7	M	404	BCL	CBD-CGD-O2D-CED
13	X	102	LMT	O5'-C5'-C6'-O6'
7	M	403	BCL	O1A-CGA-O2A-C1
13	M	411	LMT	O5'-C5'-C6'-O6'
10	M	402	PGV	O12-C04-C05-C06
15	R	101	SPO	C34-C33-C35-C36
9	L	304	U10	C48-C49-C51-C52
15	P	101	SPO	C32-C33-C35-C36
15	R	101	SPO	C32-C33-C35-C36
15	T	101	SPO	C27-C28-C30-C31
7	L	310	BCL	C6-C7-C8-C9
7	B	101	BCL	C6-C7-C8-C9
7	D	102	BCL	C14-C13-C15-C16
7	G	101	BCL	C6-C7-C8-C9
7	G	101	BCL	C14-C13-C15-C16
7	J	101	BCL	C6-C7-C8-C9
7	N	102	BCL	C6-C7-C8-C9
7	P	102	BCL	C6-C7-C8-C9
7	Q	105	BCL	C11-C12-C13-C14
7	R	102	BCL	C6-C7-C8-C9
7	S	103	BCL	C11-C10-C8-C9
7	T	102	BCL	C6-C7-C8-C9
7	Y	102	BCL	C11-C10-C8-C9
7	Z	101	BCL	C11-C10-C8-C9
13	Q	101	LMT	C2'-C1'-O1'-C1
10	H	304	PGV	O12-C04-C05-O05
15	D	103	SPO	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
15	G	102	SPO	C10-C11-C12-C13
15	N	101	SPO	C5-C6-C7-C8
15	G	102	SPO	C10-C11-C12-C14
13	X	102	LMT	C4'-C5'-C6'-O6'
7	D	102	BCL	C3-C5-C6-C7
13	K	101	LMT	C3'-C4'-O1B-C1B
7	S	103	BCL	C15-C16-C17-C18
11	L	306	PEE	C37-C38-C39-C40
7	R	102	BCL	C10-C11-C12-C13
13	L	311	LMT	C5'-C4'-O1B-C1B
7	F	103	BCL	C6-C7-C8-C10
7	Q	105	BCL	C6-C7-C8-C10
7	S	103	BCL	C6-C7-C8-C10
7	W	102	BCL	C11-C10-C8-C7
7	Y	102	BCL	C6-C7-C8-C10
15	D	101	SPO	C29-C28-C30-C31
15	D	101	SPO	C33-C35-C36-C37
15	D	105	SPO	C33-C35-C36-C37
15	S	105	SPO	C33-C35-C36-C37
15	W	101	SPO	C33-C35-C36-C37
7	Q	105	BCL	C13-C15-C16-C17
7	D	102	BCL	C5-C6-C7-C8
7	G	101	BCL	C10-C11-C12-C13
7	J	101	BCL	C15-C16-C17-C18
7	O	102	BCL	C10-C11-C12-C13
7	V	101	BCL	C8-C10-C11-C12
7	M	403	BCL	C15-C16-C17-C18
7	Z	101	BCL	C5-C6-C7-C8
13	Y	103	LMT	C5'-C4'-O1B-C1B
7	F	101	BCL	C10-C11-C12-C13
7	G	101	BCL	C8-C10-C11-C12
7	J	101	BCL	C13-C15-C16-C17
7	E	102	BCL	C10-C11-C12-C13
7	K	102	BCL	C8-C10-C11-C12
7	L	301	BCL	CBD-CGD-O2D-CED
7	O	102	BCL	C5-C6-C7-C8
10	L	305	PGV	C2-C1-O01-C02
7	A	101	BCL	O1D-CGD-O2D-CED
7	I	102	BCL	C3-C5-C6-C7
10	L	305	PGV	O02-C1-O01-C02
7	B	101	BCL	C15-C16-C17-C18
7	N	102	BCL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
7	Y	102	BCL	C8-C10-C11-C12
7	M	404	BCL	C10-C11-C12-C13
7	F	103	BCL	C15-C16-C17-C18
7	B	101	BCL	C8-C10-C11-C12
7	W	102	BCL	C4-C3-C5-C6
15	W	101	SPO	C29-C28-C30-C31
7	V	101	BCL	C15-C16-C17-C18
13	L	311	LMT	C3'-C4'-O1B-C1B
9	L	303	U10	C24-C26-C27-C28
13	Y	103	LMT	C3'-C4'-O1B-C1B
7	R	102	BCL	C16-C17-C18-C19
13	M	410	LMT	O1'-C1-C2-C3
7	M	404	BCL	O1D-CGD-O2D-CED
15	E	101	SPO	C5-C6-C7-C8
15	S	105	SPO	C10-C11-C12-C13
15	E	101	SPO	C5-C6-C7-C9
7	N	102	BCL	C2A-CAA-CBA-CGA
7	I	102	BCL	C15-C16-C17-C18
7	W	102	BCL	C3-C5-C6-C7
7	F	101	BCL	C15-C16-C17-C18
13	S	102	LMT	O5'-C1'-O1'-C1
7	Q	105	BCL	C2-C3-C5-C6
12	D	104	LDA	C5-C6-C7-C8
12	D	104	LDA	C7-C8-C9-C10
13	M	417	LMT	C5-C6-C7-C8
10	L	305	PGV	C5-C6-C7-C8
13	A	102	LMT	C3-C4-C5-C6
9	L	303	U10	C32-C33-C34-C36
7	D	102	BCL	C11-C12-C13-C15
7	E	102	BCL	C6-C7-C8-C10
7	J	101	BCL	C3-C5-C6-C7
7	D	102	BCL	C3A-C2A-CAA-CBA
7	G	101	BCL	C3A-C2A-CAA-CBA
7	J	101	BCL	C3A-C2A-CAA-CBA
7	T	102	BCL	C3A-C2A-CAA-CBA
7	W	102	BCL	C3A-C2A-CAA-CBA
7	Q	105	BCL	C10-C11-C12-C13
7	T	102	BCL	C15-C16-C17-C18
7	E	102	BCL	C16-C17-C18-C19
7	G	101	BCL	CBA-CGA-O2A-C1
12	M	419	LDA	C11-C10-C9-C8
10	H	304	PGV	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
12	L	307	LDA	C2-C3-C4-C5
13	M	417	LMT	C4-C5-C6-C7
7	E	102	BCL	C2A-CAA-CBA-CGA
10	L	305	PGV	C24-C25-C26-C27
13	M	410	LMT	C2-C3-C4-C5
13	I	101	LMT	C5'-C4'-O1B-C1B
7	W	102	BCL	C2-C3-C5-C6
15	D	101	SPO	C27-C28-C30-C31
15	W	101	SPO	C27-C28-C30-C31
10	M	402	PGV	C22-C23-C24-C25
10	Q	103	PGV	C22-C23-C24-C25
13	M	412	LMT	O5'-C1'-O1'-C1
13	A	102	LMT	C5'-C4'-O1B-C1B
7	R	102	BCL	C16-C17-C18-C20
10	M	414	PGV	C2-C1-O01-C02
10	M	415	PGV	C2-C1-O01-C02
7	G	101	BCL	O1A-CGA-O2A-C1
10	M	415	PGV	O02-C1-O01-C02
13	A	102	LMT	C3'-C4'-O1B-C1B
13	I	101	LMT	C3'-C4'-O1B-C1B
12	H	301	LDA	C7-C8-C9-C10
7	E	102	BCL	C16-C17-C18-C20
7	V	101	BCL	C16-C17-C18-C19
7	V	101	BCL	C16-C17-C18-C20
7	A	101	BCL	C4-C3-C5-C6
10	M	414	PGV	C23-C24-C25-C26
12	H	301	LDA	C1-C2-C3-C4
13	Q	101	LMT	O1'-C1-C2-C3
13	Q	101	LMT	O5'-C5'-C6'-O6'
7	L	301	BCL	C15-C16-C17-C18
7	F	101	BCL	CBA-CGA-O2A-C1
13	Q	101	LMT	C3-C4-C5-C6
10	M	414	PGV	O02-C1-O01-C02
13	S	102	LMT	O5'-C5'-C6'-O6'
13	K	101	LMT	C5'-C4'-O1B-C1B
7	M	404	BCL	C5-C6-C7-C8
10	M	402	PGV	C23-C24-C25-C26
13	M	417	LMT	O5B-C5B-C6B-O6B
12	H	302	LDA	C5-C6-C7-C8
13	M	411	LMT	C4'-C5'-C6'-O6'
12	D	104	LDA	C1-C2-C3-C4
10	L	305	PGV	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
7	W	102	BCL	C2A-CAA-CBA-CGA
10	Q	103	PGV	C2-C1-O01-C02
16	F	102	MYR	C6-C7-C8-C9
13	S	101	LMT	C4'-C5'-C6'-O6'
7	L	310	BCL	C1A-C2A-CAA-CBA
7	J	101	BCL	C1A-C2A-CAA-CBA
7	T	102	BCL	C1A-C2A-CAA-CBA
7	Z	101	BCL	C1A-C2A-CAA-CBA
10	H	303	PGV	C11-C10-C9-C8
13	Q	101	LMT	C2-C3-C4-C5
13	Y	101	LMT	O5B-C5B-C6B-O6B
7	M	403	BCL	C11-C10-C8-C7
7	A	101	BCL	C11-C10-C8-C7
7	E	102	BCL	C11-C10-C8-C7
7	K	102	BCL	C11-C10-C8-C7
7	P	102	BCL	C6-C7-C8-C10
7	Q	105	BCL	C11-C12-C13-C15
7	R	102	BCL	C6-C7-C8-C10
7	Y	102	BCL	C11-C10-C8-C7
7	S	103	BCL	C2C-C3C-CAC-CBC
7	V	101	BCL	C2C-C3C-CAC-CBC
7	W	102	BCL	C2C-C3C-CAC-CBC
15	G	102	SPO	C3-C1-C4-C5
7	P	102	BCL	C5-C6-C7-C8
7	P	102	BCL	C2A-CAA-CBA-CGA
7	M	403	BCL	C11-C10-C8-C9
7	O	102	BCL	C6-C7-C8-C9
7	O	102	BCL	C11-C10-C8-C9
7	Q	105	BCL	C11-C10-C8-C9
13	L	309	LMT	C2-C3-C4-C5
7	Q	105	BCL	C15-C16-C17-C18
13	M	409	LMT	O5'-C5'-C6'-O6'
13	I	101	LMT	C2-C3-C4-C5
13	Y	101	LMT	O5'-C5'-C6'-O6'
13	Y	103	LMT	O5B-C5B-C6B-O6B
13	L	309	LMT	O1'-C1-C2-C3
12	M	420	LDA	C4-C5-C6-C7
7	D	102	BCL	C13-C15-C16-C17
13	Y	103	LMT	C1-C2-C3-C4
10	H	303	PGV	C1-C2-C3-C4
7	F	101	BCL	O1A-CGA-O2A-C1
7	V	101	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
7	O	102	BCL	C15-C16-C17-C18
13	M	417	LMT	O5'-C5'-C6'-O6'
12	O	101	LDA	C4-C5-C6-C7
7	L	310	BCL	C15-C16-C17-C18
7	I	102	BCL	C13-C15-C16-C17
8	L	302	BPH	O2A-C1-C2-C3
10	M	402	PGV	O01-C02-C03-O11
12	D	104	LDA	C4-C5-C6-C7
12	D	104	LDA	C3-C4-C5-C6
13	M	417	LMT	O1'-C1-C2-C3
7	L	301	BCL	O1D-CGD-O2D-CED
15	R	101	SPO	C3-C1-O1-CM1
7	M	403	BCL	C4-C3-C5-C6
7	V	101	BCL	C4-C3-C5-C6
13	X	102	LMT	O1'-C1-C2-C3
13	K	101	LMT	C2-C1-O1'-C1'
13	S	102	LMT	C2-C1-O1'-C1'
7	A	101	BCL	C11-C10-C8-C9
7	E	102	BCL	C11-C10-C8-C9
7	W	102	BCL	C6-C7-C8-C9
7	M	403	BCL	C2A-CAA-CBA-CGA
10	M	402	PGV	C01-C02-C03-O11
7	D	102	BCL	C11-C10-C8-C7
7	O	102	BCL	C6-C7-C8-C10
7	O	102	BCL	C11-C10-C8-C7
7	Q	105	BCL	C11-C10-C8-C7
7	W	102	BCL	C6-C7-C8-C10
10	M	413	PGV	C19-C20-C21-C22
7	F	101	BCL	C3A-C2A-CAA-CBA
7	T	102	BCL	C4-C3-C5-C6
7	Z	101	BCL	C4-C3-C5-C6
13	L	309	LMT	O5'-C1'-O1'-C1
13	L	309	LMT	C5'-C4'-O1B-C1B
13	L	311	LMT	C7-C8-C9-C10
7	K	102	BCL	C3-C5-C6-C7
7	E	102	BCL	C15-C16-C17-C18
7	D	102	BCL	C2A-CAA-CBA-CGA
15	S	105	SPO	C34-C33-C35-C36
13	L	309	LMT	C3'-C4'-O1B-C1B
7	M	403	BCL	C2-C3-C5-C6
7	T	102	BCL	C2-C3-C5-C6
7	Z	101	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	I	101	LMT	C1-C2-C3-C4
10	M	413	PGV	O01-C02-C03-O11
10	H	303	PGV	O01-C02-C03-O11
7	R	102	BCL	C2A-CAA-CBA-CGA
7	M	403	BCL	C8-C10-C11-C12
15	S	105	SPO	C32-C33-C35-C36
10	L	305	PGV	C23-C24-C25-C26
7	F	101	BCL	C6-C7-C8-C9
7	K	102	BCL	C11-C10-C8-C9
12	M	418	LDA	C4-C5-C6-C7
15	E	101	SPO	C33-C35-C36-C37
7	K	102	BCL	C5-C6-C7-C8
7	I	102	BCL	C10-C11-C12-C13
7	W	102	BCL	C5-C6-C7-C8
10	H	303	PGV	C01-C02-C03-O11
10	H	304	PGV	C01-C02-C03-O11
7	F	101	BCL	C6-C7-C8-C10
15	N	101	SPO	C1-C4-C5-C6
9	L	303	U10	C32-C33-C34-C35
15	S	105	SPO	C10-C11-C12-C14
13	S	101	LMT	C3'-C4'-O1B-C1B
10	Q	103	PGV	O02-C1-O01-C02
13	S	101	LMT	C5'-C4'-O1B-C1B
7	N	102	BCL	C15-C16-C17-C18
12	M	418	LDA	C7-C8-C9-C10
10	H	304	PGV	O01-C02-C03-O11
9	L	304	U10	C9-C11-C12-C13
15	T	101	SPO	C28-C30-C31-C32
7	V	101	BCL	C5-C6-C7-C8
9	L	304	U10	C12-C11-C9-C10
7	A	101	BCL	C2-C3-C5-C6
10	L	305	PGV	O03-C01-C02-O01
7	D	102	BCL	C11-C10-C8-C9
7	N	102	BCL	C14-C13-C15-C16
7	Q	105	BCL	C6-C7-C8-C9
7	W	102	BCL	C11-C10-C8-C9
10	M	402	PGV	C21-C22-C23-C24
7	E	102	BCL	C5-C6-C7-C8
12	H	301	LDA	C2-C1-N1-CM1
12	D	104	LDA	C2-C1-N1-CM1
9	L	304	U10	C45-C44-C46-C47
9	M	401	U10	C12-C11-C9-C10

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Mol	Chain	Res	Type	Atoms
7	F	101	BCL	C16-C17-C18-C20
7	J	101	BCL	CBA-CGA-O2A-C1
10	M	413	PGV	C20-C21-C22-C23
15	P	101	SPO	C28-C30-C31-C32
7	G	101	BCL	C1A-C2A-CAA-CBA
7	P	102	BCL	C4-C3-C5-C6
15	M	408	SPO	C34-C33-C35-C36
9	L	304	U10	C12-C11-C9-C8
15	F	104	SPO	C11-C10-C9-C7
7	J	101	BCL	C2A-CAA-CBA-CGA
7	N	102	BCL	C8-C10-C11-C12
10	L	305	PGV	C01-C02-C03-O11
10	Q	103	PGV	C01-C02-C03-O11
7	V	101	BCL	C6-C7-C8-C10
7	M	404	BCL	C16-C17-C18-C19
15	G	102	SPO	C2-C1-C4-C5
11	L	306	PEE	C18-C19-C20-C21
13	K	101	LMT	C6-C7-C8-C9
7	B	101	BCL	C16-C17-C18-C19
7	J	101	BCL	O1A-CGA-O2A-C1
10	L	305	PGV	O01-C02-C03-O11
10	Q	103	PGV	O01-C02-C03-O11
12	H	301	LDA	C2-C1-N1-O1
12	D	104	LDA	C2-C1-N1-O1
7	A	101	BCL	O1A-CGA-O2A-C1
7	L	310	BCL	C13-C15-C16-C17
13	M	410	LMT	C3-C4-C5-C6
9	M	401	U10	C12-C11-C9-C8
7	L	310	BCL	C8-C10-C11-C12
7	M	404	BCL	CHA-CBD-CGD-O1D
7	M	404	BCL	CHA-CBD-CGD-O2D
10	M	414	PGV	C04-O12-P-O13
10	H	304	PGV	C04-O12-P-O13
11	L	306	PEE	C1-O3P-P-O2P
10	L	305	PGV	C22-C23-C24-C25
7	G	101	BCL	C2-C3-C5-C6
9	L	304	U10	C43-C44-C46-C47
10	M	415	PGV	C5-C6-C7-C8
10	M	413	PGV	C4-C5-C6-C7
13	A	102	LMT	O5B-C5B-C6B-O6B
13	M	417	LMT	C3-C4-C5-C6
15	E	101	SPO	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
10	M	413	PGV	C01-C02-C03-O11
7	A	101	BCL	CBA-CGA-O2A-C1
7	Y	102	BCL	C6-C7-C8-C9
7	L	310	BCL	C6-C7-C8-C10
7	I	102	BCL	C6-C7-C8-C10
11	L	306	PEE	C16-C17-C18-C19
10	H	304	PGV	O12-C04-C05-C06
7	N	102	BCL	C16-C17-C18-C20
7	G	101	BCL	C4-C3-C5-C6
9	L	303	U10	C30-C29-C31-C32
7	F	101	BCL	C16-C17-C18-C19
7	P	102	BCL	C16-C17-C18-C19
12	Q	104	LDA	N1-C1-C2-C3
10	M	413	PGV	O03-C01-C02-O01
8	M	405	BPH	C13-C15-C16-C17
7	N	102	BCL	C16-C17-C18-C19
9	L	304	U10	C6-C7-C8-C9
7	G	101	BCL	C13-C15-C16-C17
7	Q	105	BCL	C5-C6-C7-C8
13	Y	103	LMT	O1'-C1-C2-C3
8	L	302	BPH	C16-C17-C18-C20
15	R	101	SPO	C1-C4-C5-C6
13	I	101	LMT	C7-C8-C9-C10
11	L	306	PEE	C38-C39-C40-C41
15	E	101	SPO	C11-C10-C9-C7
9	L	303	U10	C28-C29-C31-C32
10	M	402	PGV	C3-C4-C5-C6
13	X	101	LMT	C7-C8-C9-C10
13	L	311	LMT	C2-C3-C4-C5
7	D	102	BCL	C11-C12-C13-C14
7	P	102	BCL	C2-C3-C5-C6
7	F	101	BCL	C5-C6-C7-C8
15	N	101	SPO	C25-C26-C27-C28
7	K	102	BCL	C13-C15-C16-C17
7	D	102	BCL	C6-C7-C8-C10
7	B	101	BCL	C16-C17-C18-C20
7	E	102	BCL	C3-C5-C6-C7
15	D	105	SPO	C34-C33-C35-C36
13	M	417	LMT	C2-C3-C4-C5
12	D	104	LDA	C2-C3-C4-C5
13	S	101	LMT	O5'-C5'-C6'-O6'
12	M	419	LDA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
13	X	101	LMT	C6-C7-C8-C9
7	D	102	BCL	C10-C11-C12-C13
7	Z	101	BCL	C2-C1-O2A-CGA
10	H	303	PGV	C4-C5-C6-C7
13	S	102	LMT	C4-C5-C6-C7
7	N	102	BCL	C4-C3-C5-C6
7	R	102	BCL	C4-C3-C5-C6
9	L	304	U10	C25-C24-C26-C27
7	L	301	BCL	C2A-CAA-CBA-CGA
10	H	304	PGV	O03-C01-C02-C03
15	R	101	SPO	C28-C30-C31-C32
7	E	102	BCL	C6-C7-C8-C9
7	T	102	BCL	C14-C13-C15-C16
7	V	101	BCL	C6-C7-C8-C9
15	M	408	SPO	C29-C28-C30-C31
7	N	102	BCL	C2-C3-C5-C6
7	R	102	BCL	C2-C3-C5-C6
9	L	304	U10	C13-C14-C16-C17
15	M	408	SPO	C27-C28-C30-C31
7	I	102	BCL	C1A-C2A-CAA-CBA
11	L	306	PEE	O3P-C1-C2-O2
12	O	101	LDA	C11-C10-C9-C8
10	H	304	PGV	C2-C3-C4-C5
16	F	102	MYR	C3-C4-C5-C6
16	F	102	MYR	O2-C1-C2-C3
7	F	103	BCL	C4-C3-C5-C6
7	J	101	BCL	C6-C7-C8-C10
7	T	102	BCL	C2A-CAA-CBA-CGA
10	H	303	PGV	C19-C20-C21-C22
15	D	101	SPO	C10-C11-C12-C13
9	L	304	U10	C23-C24-C26-C27
13	L	309	LMT	C5-C6-C7-C8
16	F	102	MYR	O1-C1-C2-C3
7	W	102	BCL	C16-C17-C18-C19
7	N	102	BCL	C11-C10-C8-C9
10	Q	103	PGV	C21-C22-C23-C24
15	G	102	SPO	C11-C10-C9-C7
7	Z	101	BCL	C16-C17-C18-C19
16	F	102	MYR	C11-C10-C9-C8
9	L	303	U10	C35-C34-C36-C37
9	L	303	U10	C33-C34-C36-C37
15	M	408	SPO	C32-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
15	D	105	SPO	C32-C33-C35-C36
7	P	102	BCL	C16-C17-C18-C20
10	L	305	PGV	O03-C01-C02-C03
13	Y	101	LMT	C5'-C4'-O1B-C1B
8	M	405	BPH	C4-C3-C5-C6
9	L	304	U10	C15-C14-C16-C17
9	L	303	U10	C5-C4-O4-C4M
7	G	101	BCL	CAA-CBA-CGA-O2A
7	K	102	BCL	C16-C17-C18-C19
10	M	415	PGV	O12-C04-C05-C06
7	D	102	BCL	C8-C10-C11-C12
11	L	306	PEE	C36-C37-C38-C39
7	Y	102	BCL	C15-C16-C17-C18
7	R	102	BCL	C11-C10-C8-C9
8	L	302	BPH	C14-C13-C15-C16
13	L	311	LMT	C1-C2-C3-C4
7	L	301	BCL	C2-C1-O2A-CGA
7	O	102	BCL	C2-C1-O2A-CGA
7	S	103	BCL	C2-C1-O2A-CGA
10	M	413	PGV	C7-C8-C9-C10
13	X	101	LMT	C2'-C1'-O1'-C1
7	M	403	BCL	C16-C17-C18-C19
7	O	102	BCL	C16-C17-C18-C19
9	M	407	U10	C5-C4-O4-C4M
7	R	102	BCL	C8-C10-C11-C12
12	Q	104	LDA	C1-C2-C3-C4
8	M	405	BPH	C10-C11-C12-C13
10	M	413	PGV	O03-C01-C02-C03
13	S	101	LMT	O5B-C5B-C6B-O6B
11	L	306	PEE	O2-C2-C3-O3
11	L	306	PEE	O3P-C1-C2-C3
7	F	103	BCL	C13-C15-C16-C17
9	M	401	U10	C3-C4-O4-C4M
15	G	102	SPO	O1-C1-C4-C5
10	Q	103	PGV	C25-C26-C27-C28
7	B	101	BCL	C6-C7-C8-C10
7	G	101	BCL	C6-C7-C8-C10
7	I	102	BCL	C11-C12-C13-C15
7	N	102	BCL	C6-C7-C8-C10
7	N	102	BCL	C11-C10-C8-C7
7	R	102	BCL	C11-C10-C8-C7
7	T	102	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
8	L	302	BPH	C11-C12-C13-C15
10	M	413	PGV	C6-C7-C8-C9
13	X	101	LMT	C5-C6-C7-C8
7	M	403	BCL	C2-C1-O2A-CGA
7	F	103	BCL	C2-C1-O2A-CGA
7	K	102	BCL	C2-C1-O2A-CGA
10	L	305	PGV	C3-C4-C5-C6
10	H	303	PGV	C3-C4-C5-C6
13	A	102	LMT	C6-C7-C8-C9
12	M	420	LDA	C2-C1-N1-CM1
10	M	415	PGV	C21-C22-C23-C24
10	H	304	PGV	C3-C4-C5-C6
7	Y	102	BCL	C2A-CAA-CBA-CGA
7	F	103	BCL	C2-C3-C5-C6
13	L	309	LMT	C6-C7-C8-C9
13	X	101	LMT	C4-C5-C6-C7
12	H	301	LDA	C4-C5-C6-C7
7	A	101	BCL	C1A-C2A-CAA-CBA
9	L	304	U10	C2-C3-O3-C3M
7	F	101	BCL	C4-C3-C5-C6
7	S	103	BCL	C4-C3-C5-C6
10	M	402	PGV	O03-C01-C02-O01
12	M	420	LDA	C1-C2-C3-C4
13	L	309	LMT	C4-C5-C6-C7
13	L	308	LMT	C11-C10-C9-C8
13	Y	101	LMT	C3'-C4'-O1B-C1B
7	J	101	BCL	C4-C3-C5-C6
10	H	304	PGV	O03-C19-C20-C21
7	L	301	BCL	C11-C10-C8-C7
7	F	103	BCL	C11-C10-C8-C7
7	Z	101	BCL	C11-C10-C8-C7
10	M	414	PGV	C22-C23-C24-C25
10	H	303	PGV	C11-C12-C13-C14
7	G	101	BCL	C2C-C3C-CAC-CBC
10	M	402	PGV	C20-C19-O03-C01
10	H	304	PGV	C23-C24-C25-C26
15	N	101	SPO	C30-C31-C32-C33
7	I	102	BCL	C3A-C2A-CAA-CBA
13	M	410	LMT	C4'-C5'-C6'-O6'
13	M	411	LMT	C5'-C4'-O1B-C1B
9	M	401	U10	C5-C4-O4-C4M
7	L	301	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
7	I	102	BCL	C11-C12-C13-C14
7	Q	105	BCL	C8-C10-C11-C12
7	M	403	BCL	C3-C5-C6-C7
10	L	305	PGV	O01-C1-C2-C3
10	H	304	PGV	O04-C19-C20-C21
7	F	103	BCL	O1A-CGA-O2A-C1
7	M	404	BCL	CAD-CBD-CGD-O2D
7	E	102	BCL	CAD-CBD-CGD-O2D
13	K	101	LMT	C3-C4-C5-C6
10	M	402	PGV	O04-C19-O03-C01
7	Q	105	BCL	C2-C1-O2A-CGA
13	X	102	LMT	C2-C3-C4-C5
9	L	303	U10	C26-C27-C28-C29
7	R	102	BCL	CAA-CBA-CGA-O2A
7	B	101	BCL	CAA-CBA-CGA-O2A
12	M	416	LDA	C2-C3-C4-C5

There are no ring outliers.

82 monomers are involved in 286 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	E	101	SPO	6	0
15	P	101	SPO	5	0
10	H	303	PGV	2	0
12	O	101	LDA	1	0
15	S	105	SPO	6	0
7	R	102	BCL	4	0
10	M	402	PGV	3	0
9	L	304	U10	7	0
7	G	101	BCL	8	0
7	L	310	BCL	2	0
8	M	405	BPH	8	0
13	M	410	LMT	3	0
10	L	305	PGV	5	0
8	L	302	BPH	3	0
13	I	101	LMT	3	0
7	E	102	BCL	3	0
13	S	102	LMT	6	0
7	K	102	BCL	7	0
15	R	101	SPO	6	0
7	V	101	BCL	6	0
13	Q	101	LMT	2	0

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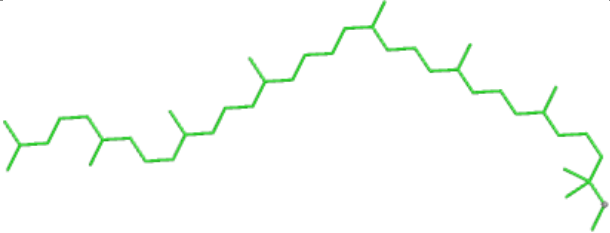
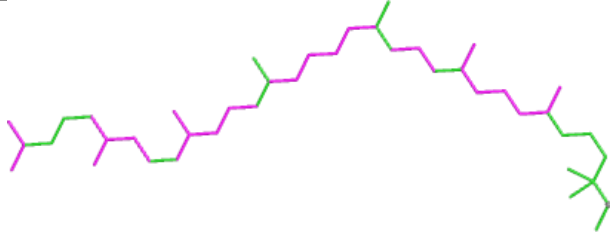
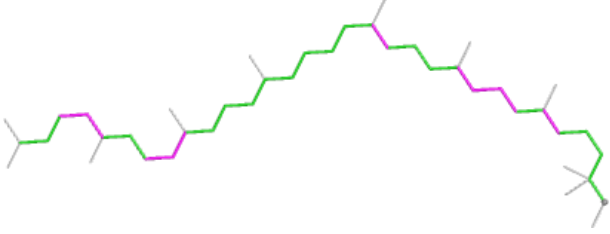
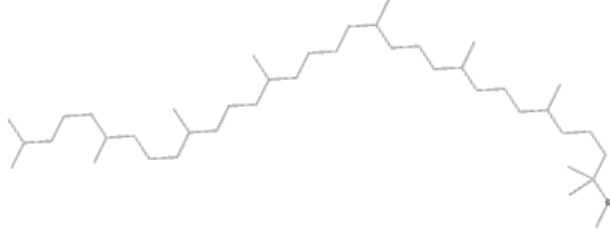
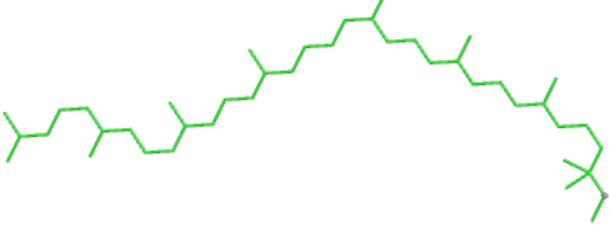
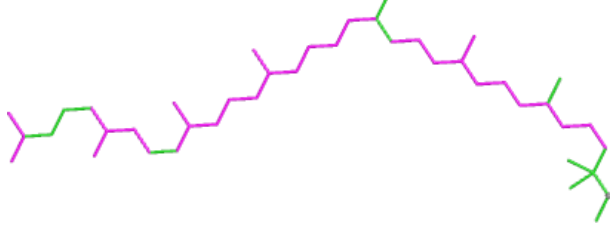
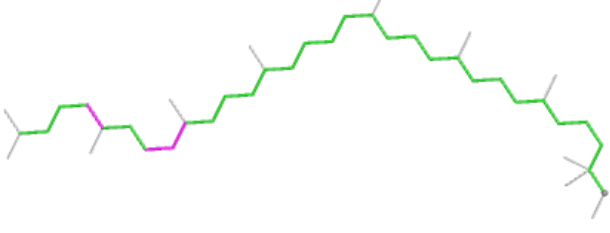
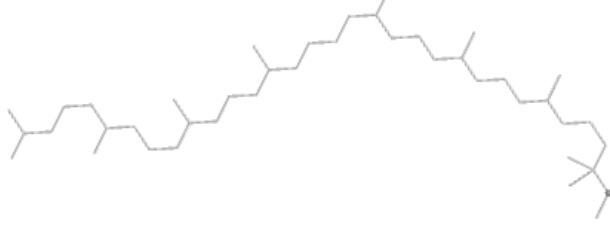
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	104	LDA	3	0
7	S	103	BCL	5	0
13	Y	101	LMT	1	0
16	F	102	MYR	2	0
15	I	103	SPO	4	0
15	M	408	SPO	6	0
13	M	412	LMT	6	0
13	M	409	LMT	3	0
15	D	105	SPO	7	0
13	L	311	LMT	4	0
12	M	419	LDA	2	0
7	F	101	BCL	7	0
7	M	403	BCL	6	0
10	M	414	PGV	2	0
7	J	101	BCL	6	0
13	K	101	LMT	2	0
15	S	104	SPO	8	0
10	H	304	PGV	3	0
13	S	101	LMT	3	0
7	P	102	BCL	8	0
12	M	418	LDA	1	0
10	M	415	PGV	5	0
15	D	101	SPO	6	0
12	Q	104	LDA	2	0
9	L	303	U10	3	0
7	I	102	BCL	6	0
7	B	101	BCL	4	0
7	N	102	BCL	7	0
15	N	101	SPO	6	0
13	M	411	LMT	1	0
12	H	301	LDA	3	0
10	Q	103	PGV	5	0
11	L	306	PEE	3	0
12	L	307	LDA	2	0
7	A	101	BCL	3	0
9	M	401	U10	3	0
12	M	420	LDA	3	0
15	T	101	SPO	3	0
7	F	103	BCL	1	0
15	D	103	SPO	4	0
15	O	104	SPO	10	0
15	O	103	SPO	5	0

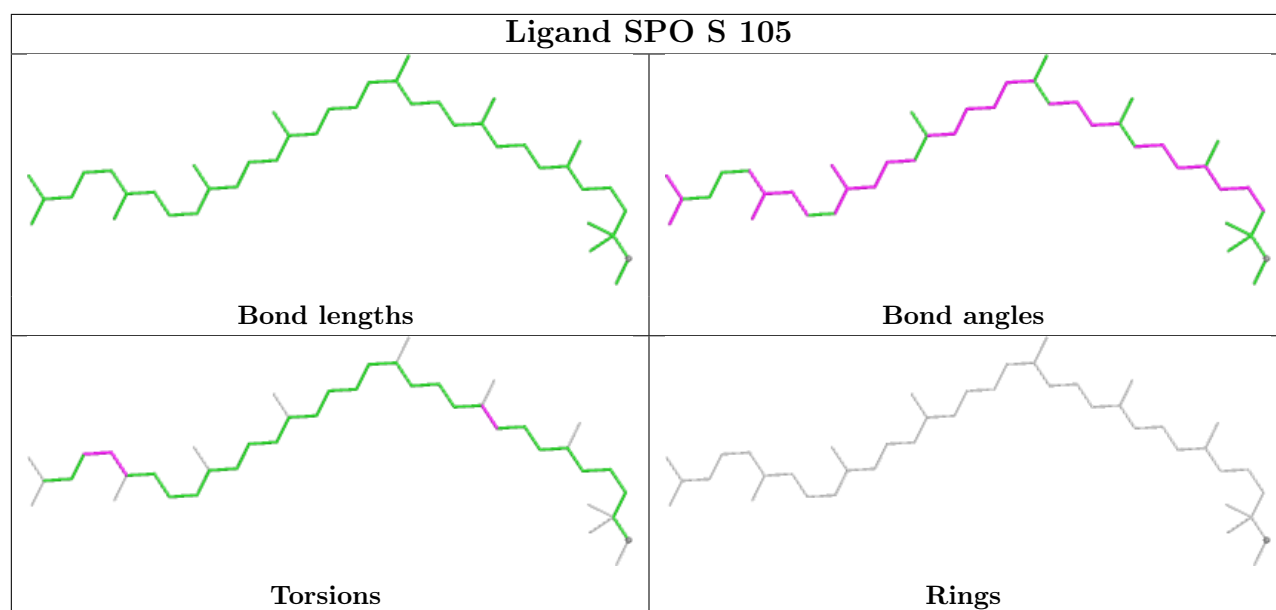
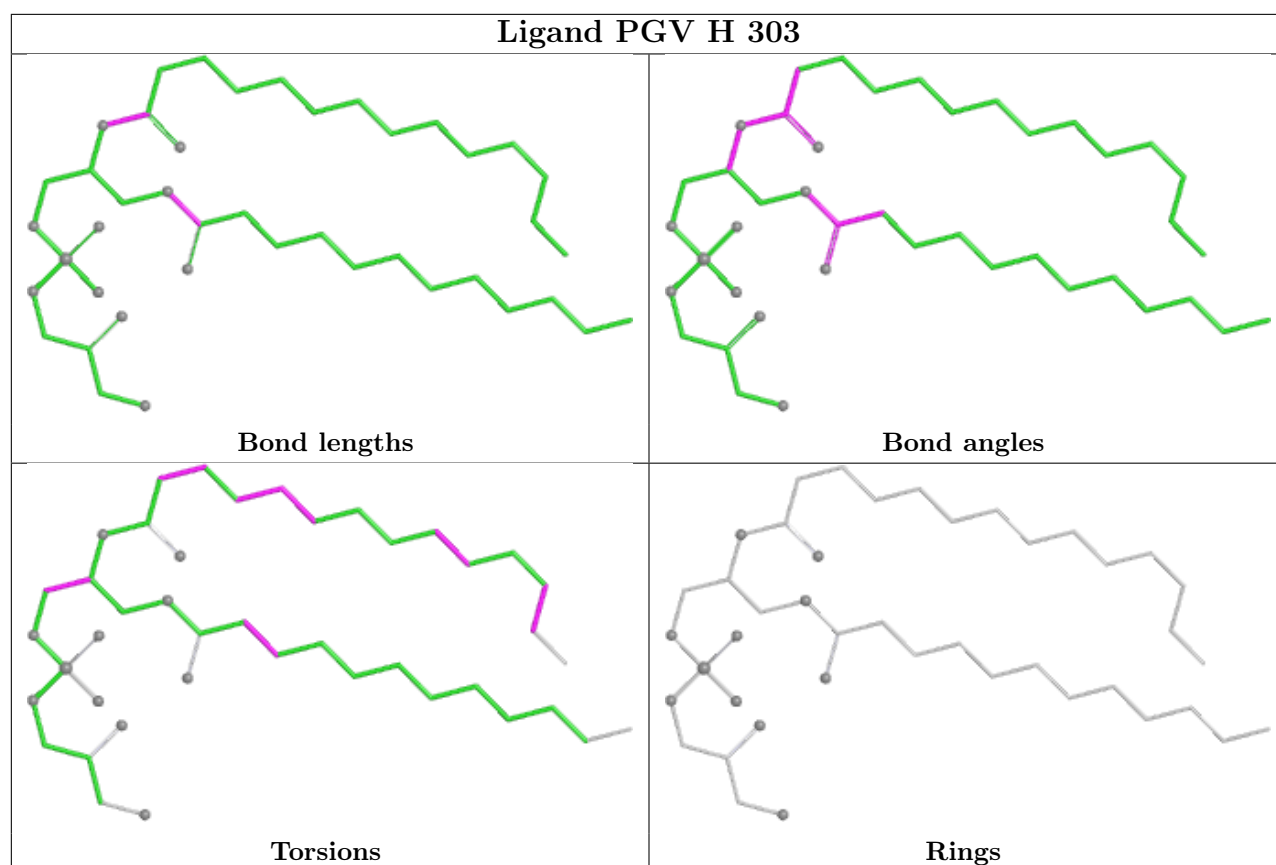
Continued on next page...

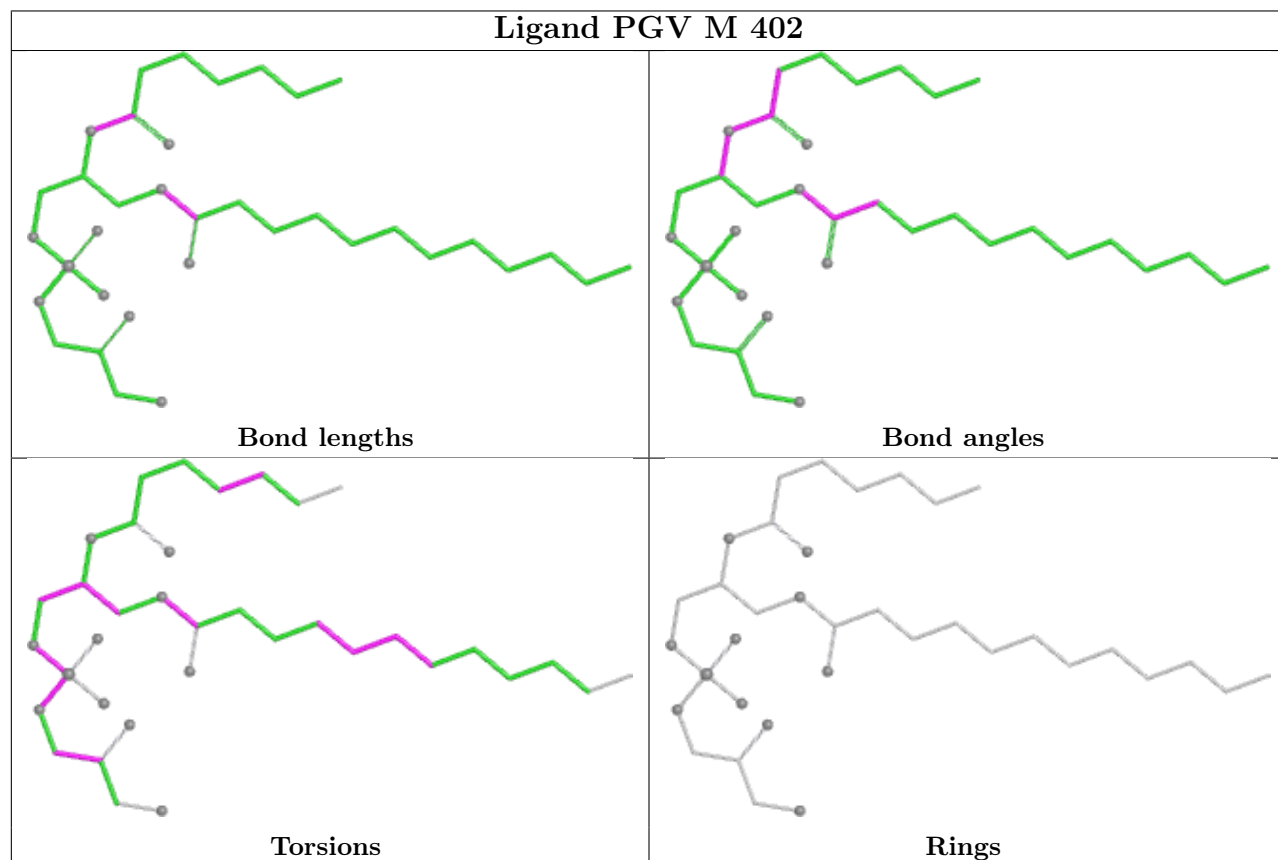
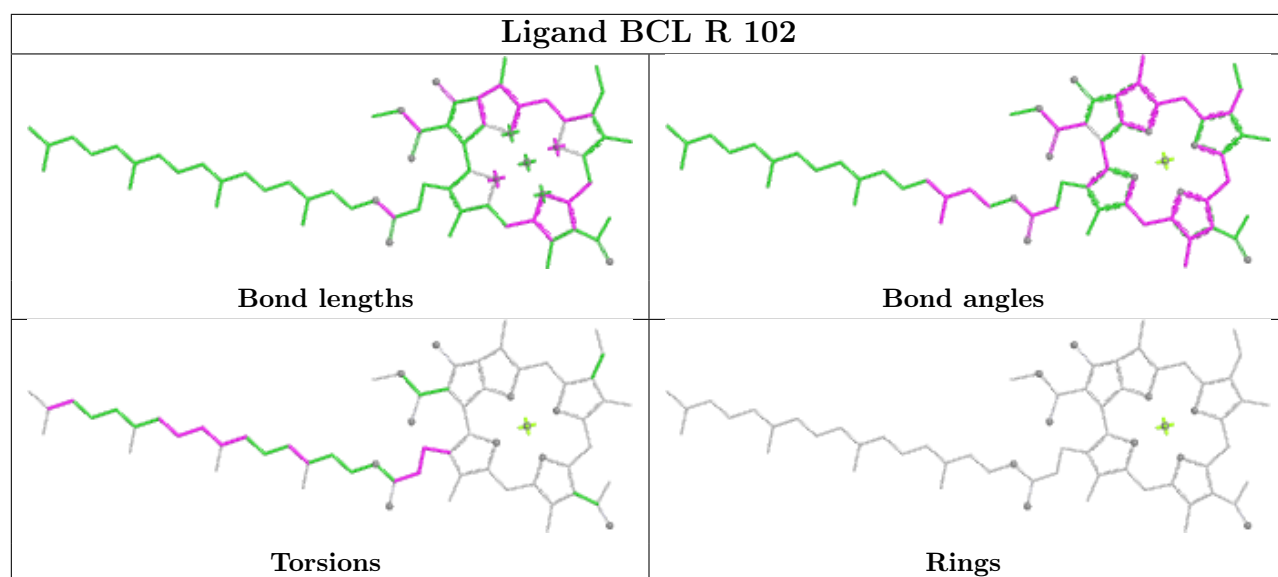
Continued from previous page...

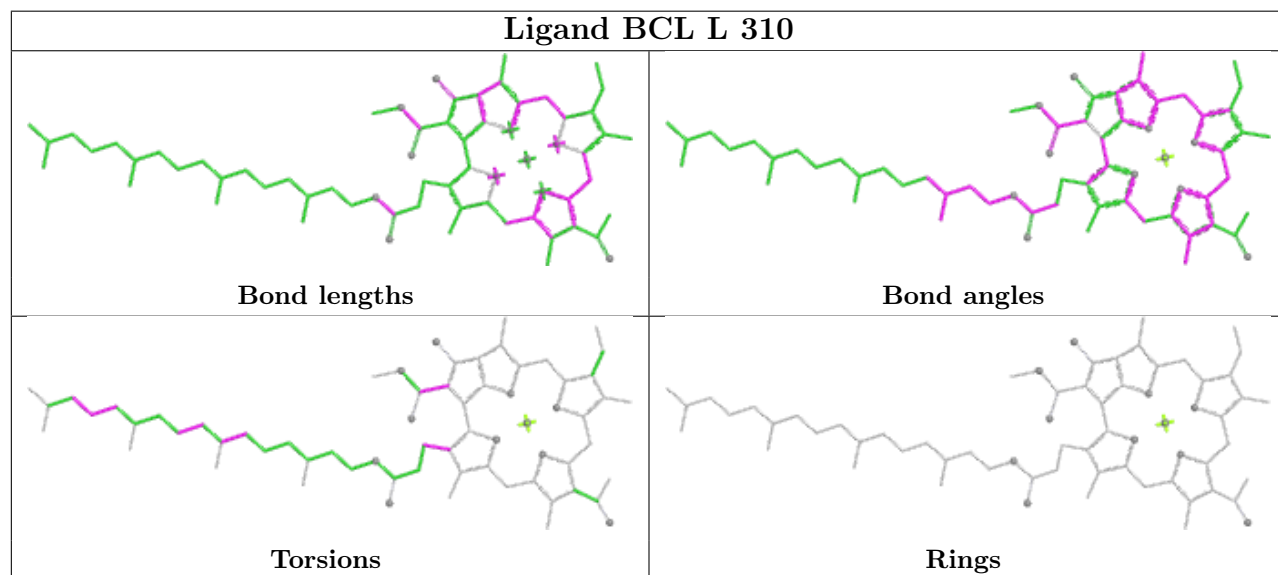
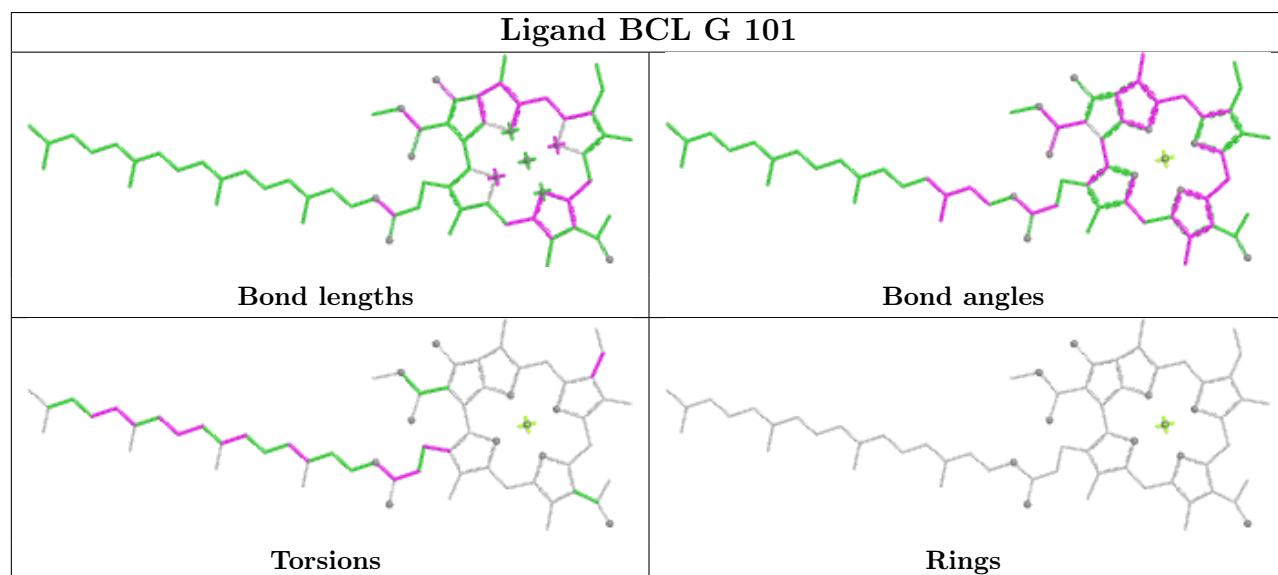
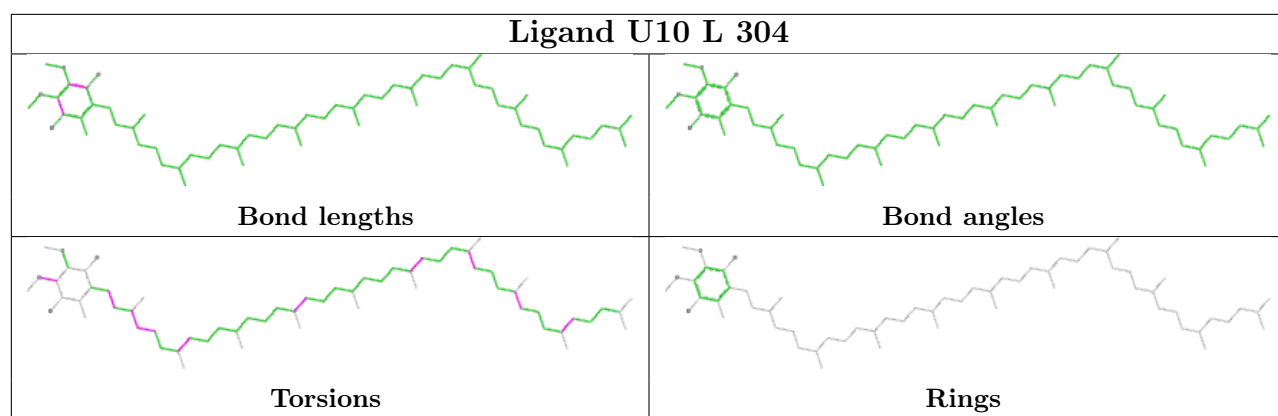
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	G	102	SPO	3	0
12	Q	102	LDA	1	0
15	F	104	SPO	5	0
15	W	101	SPO	8	0
7	Z	101	BCL	3	0
13	L	308	LMT	2	0
7	M	404	BCL	3	0
7	W	102	BCL	6	0
7	T	102	BCL	5	0
10	M	413	PGV	5	0
9	M	407	U10	3	0
7	Y	102	BCL	3	0
13	A	102	LMT	3	0
13	Y	103	LMT	1	0
7	O	102	BCL	4	0
7	D	102	BCL	8	0
13	M	417	LMT	2	0
13	X	101	LMT	1	0
15	I	104	SPO	9	0

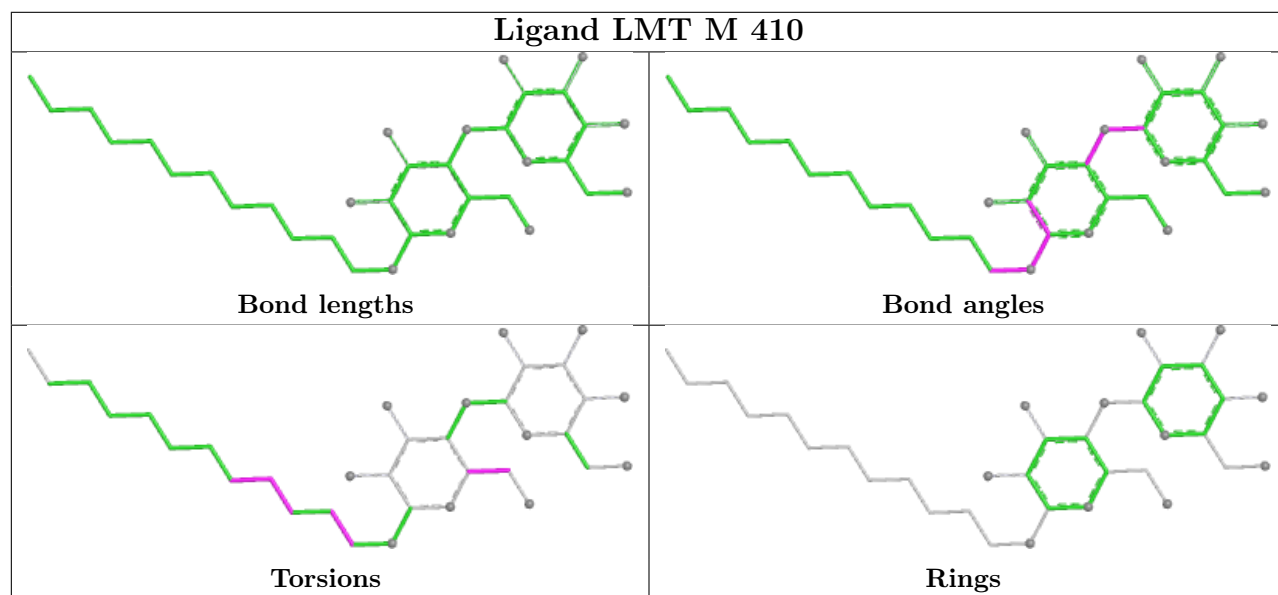
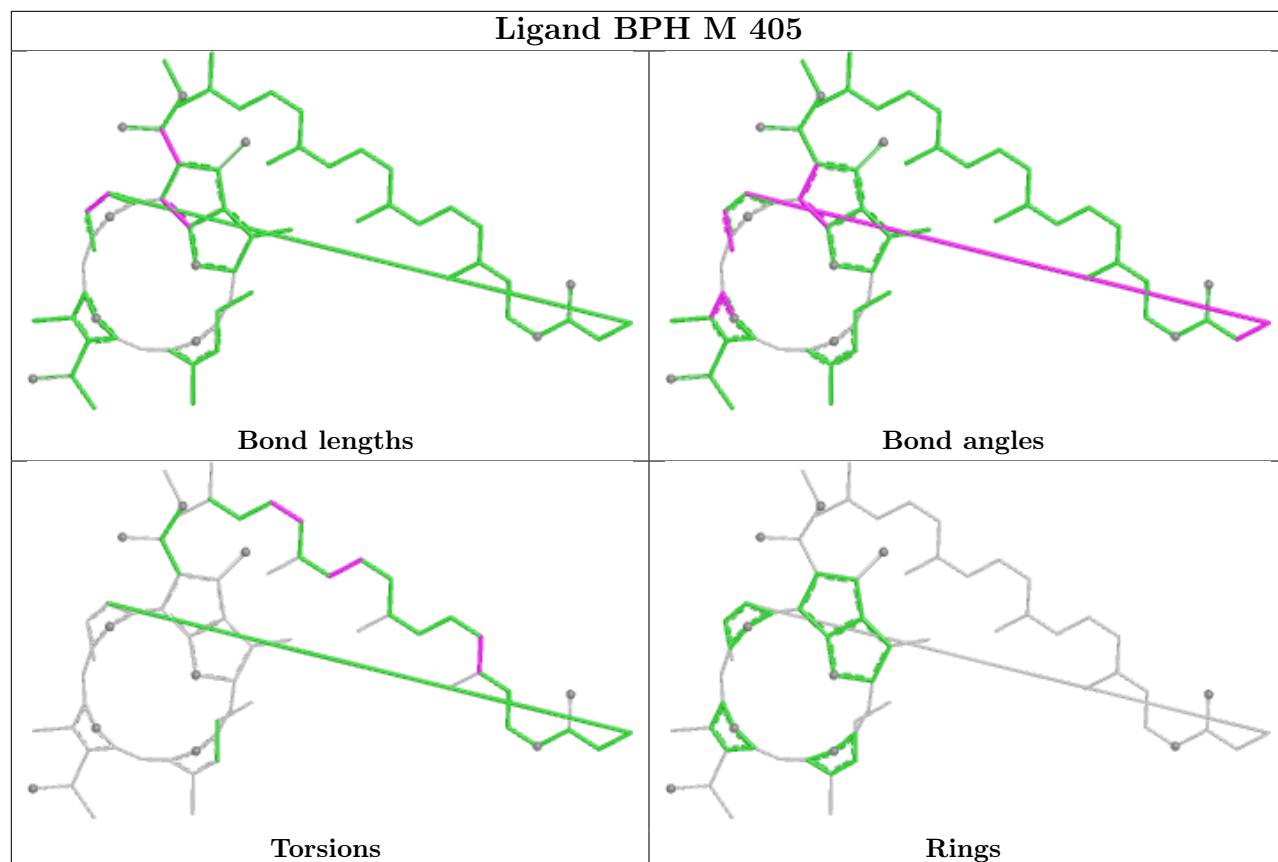
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

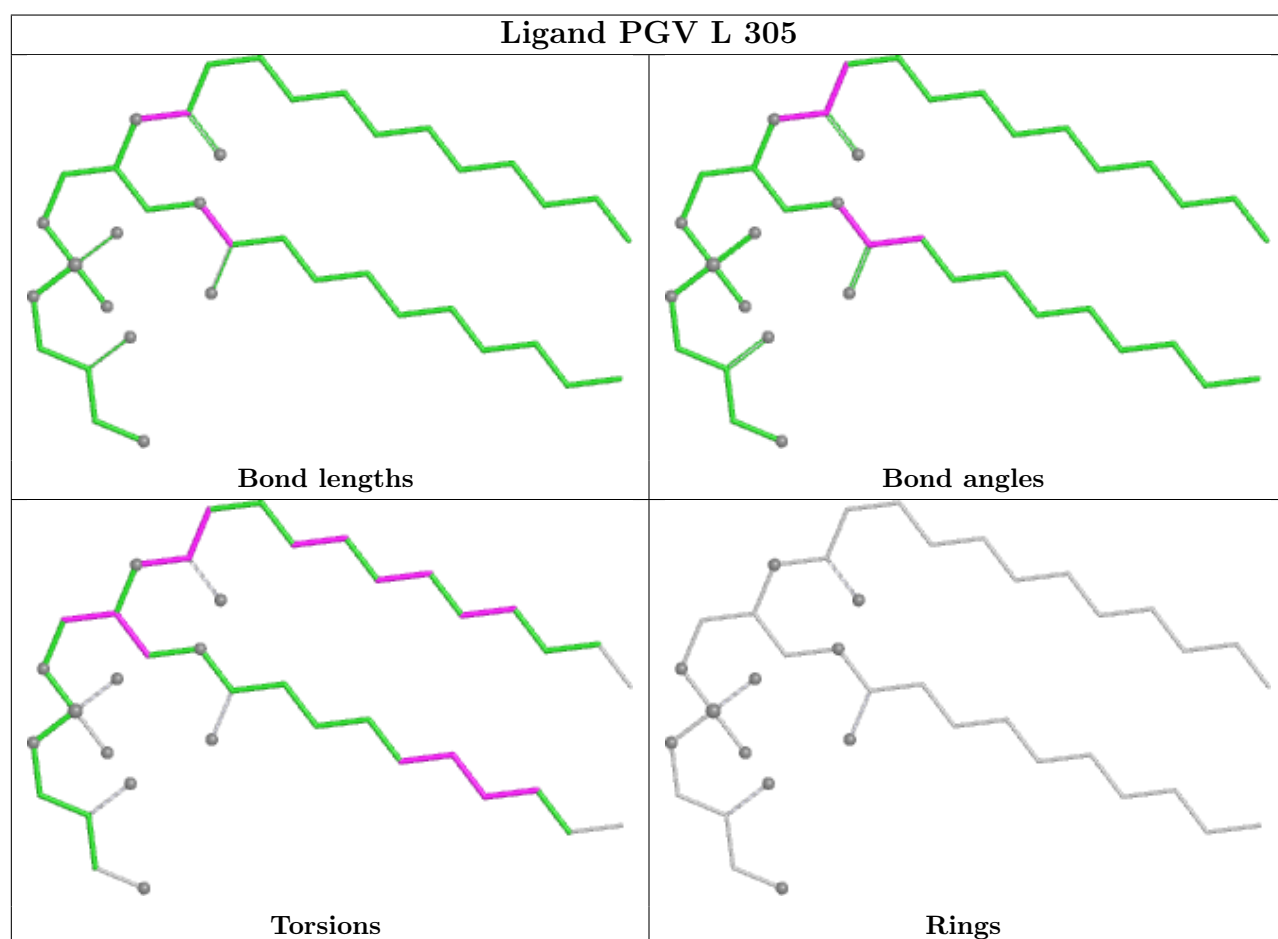
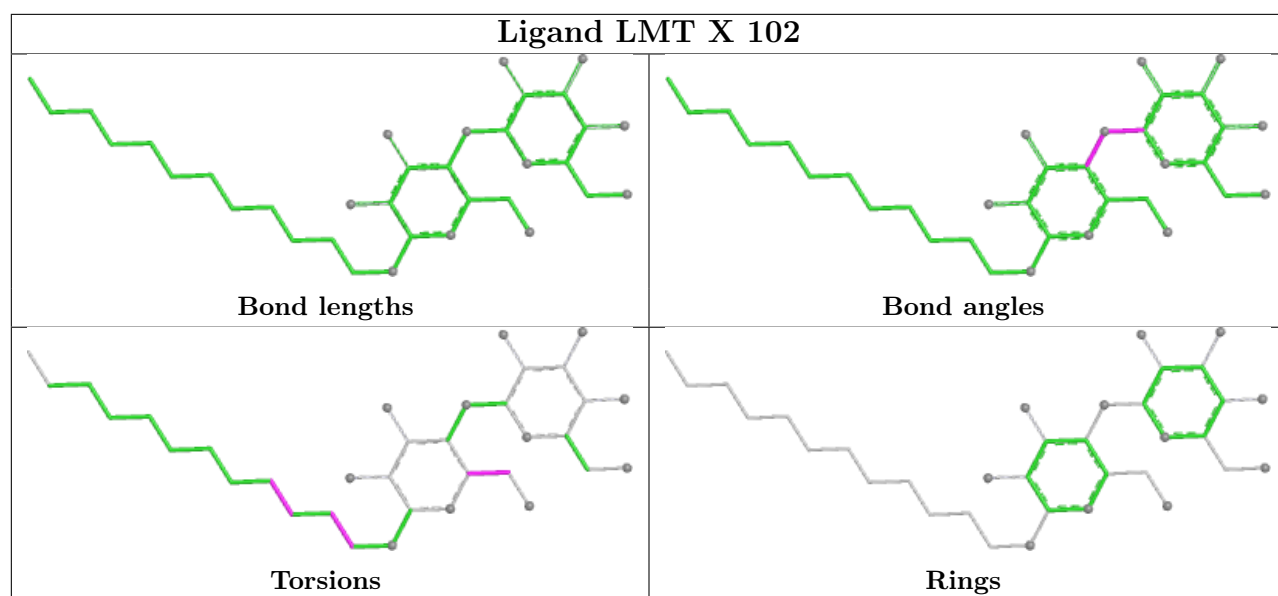
Ligand SPO E 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO P 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

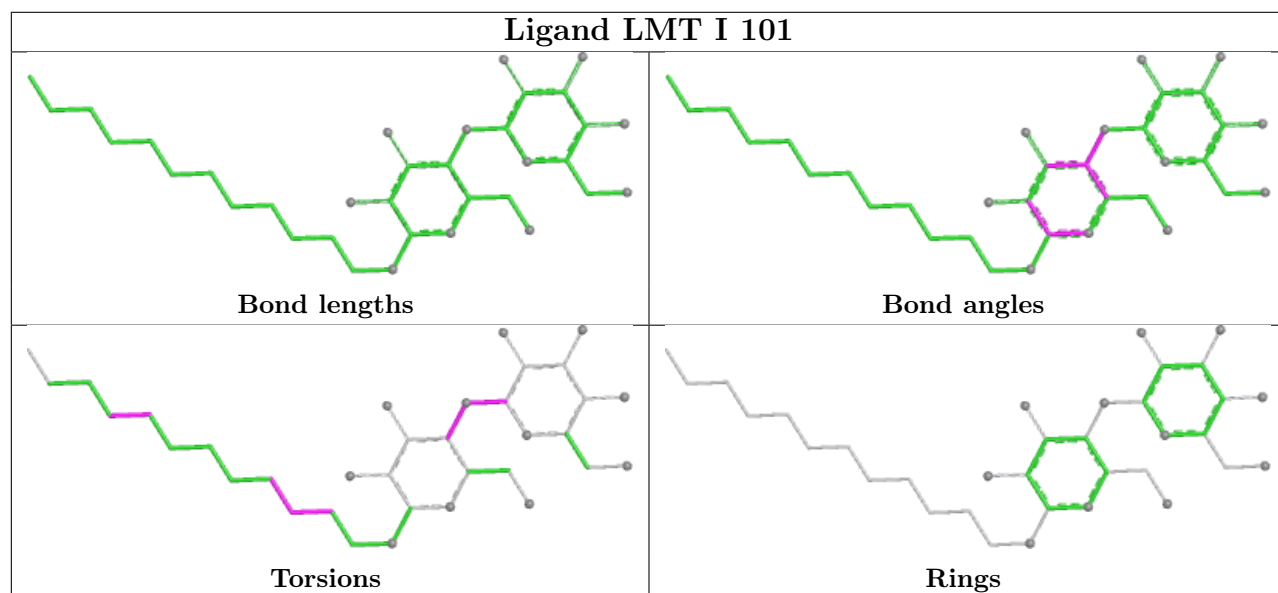
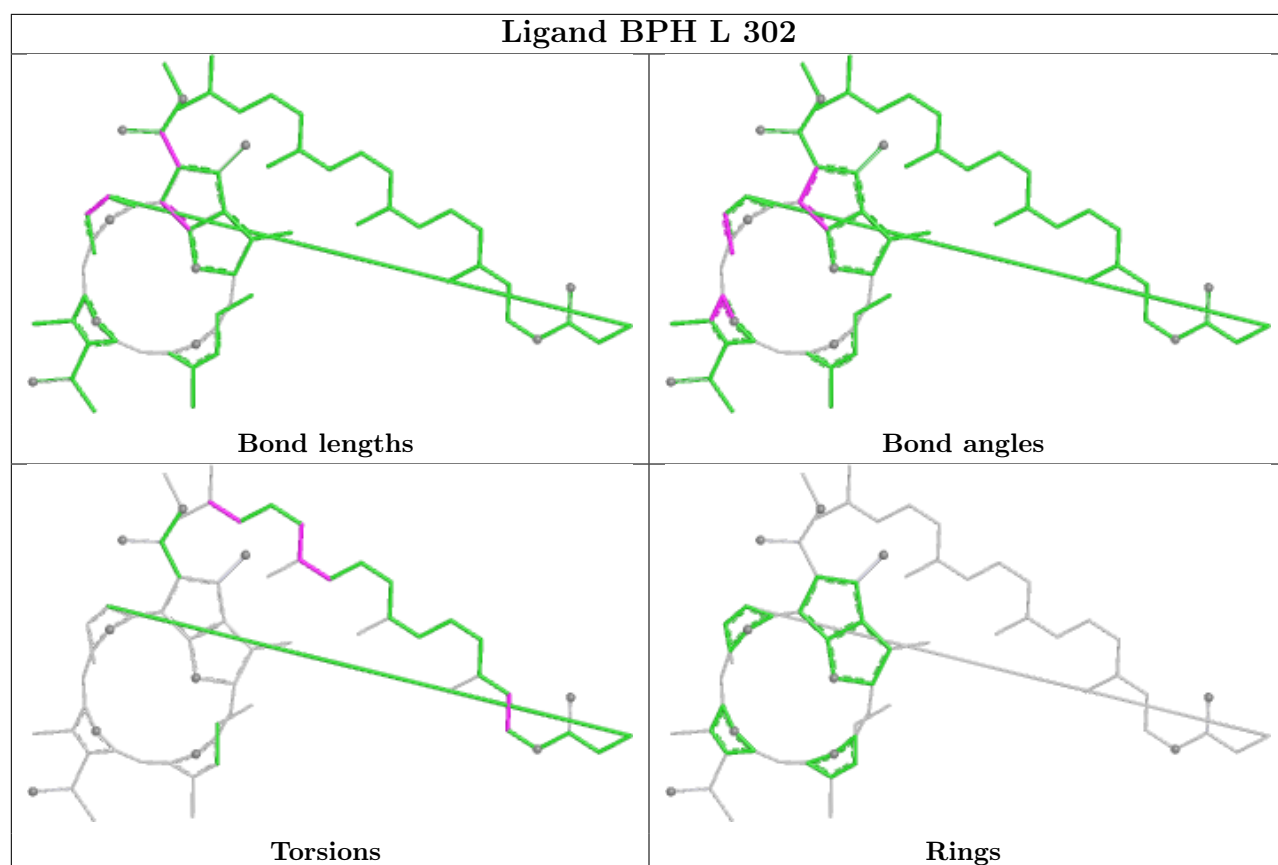


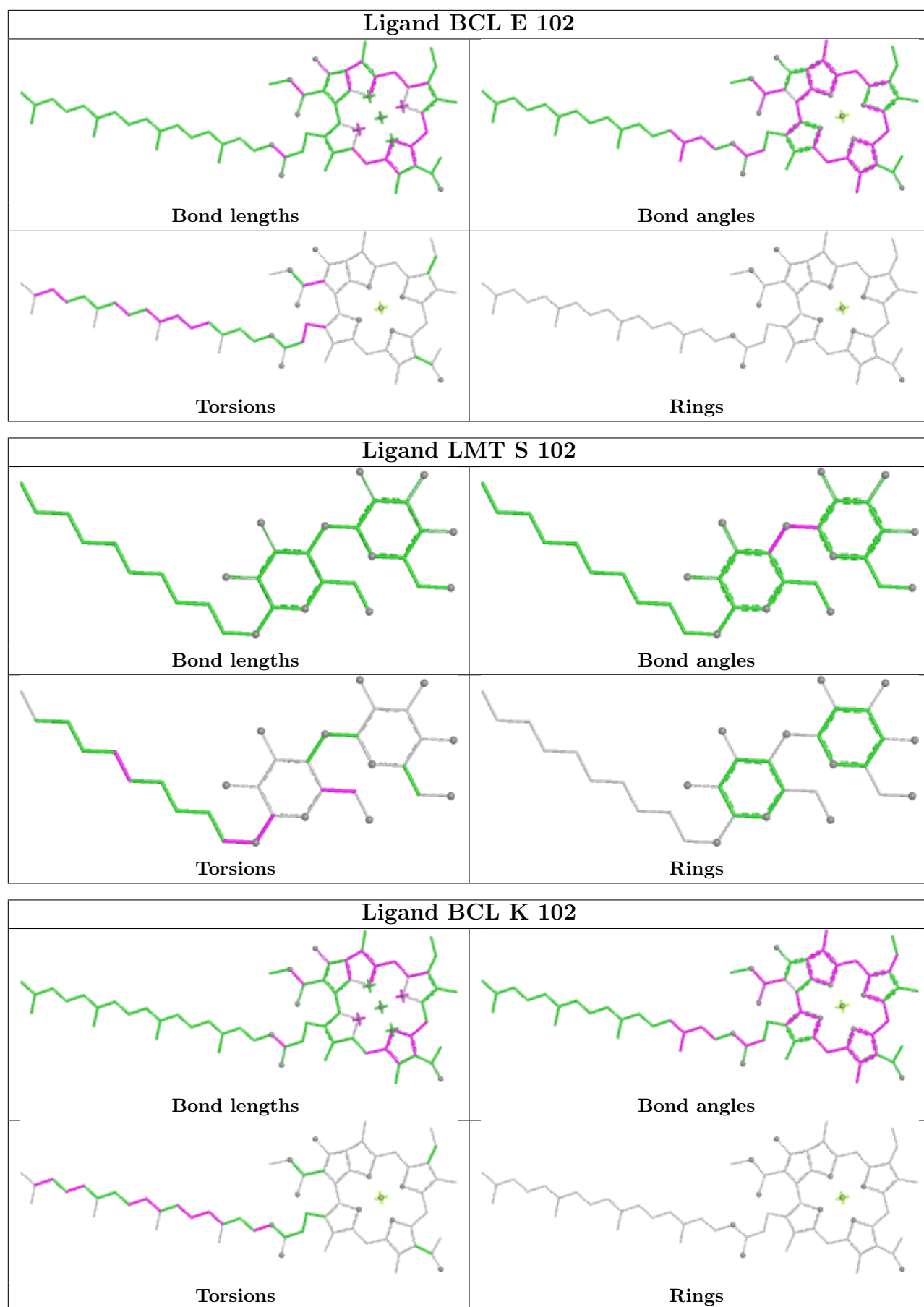


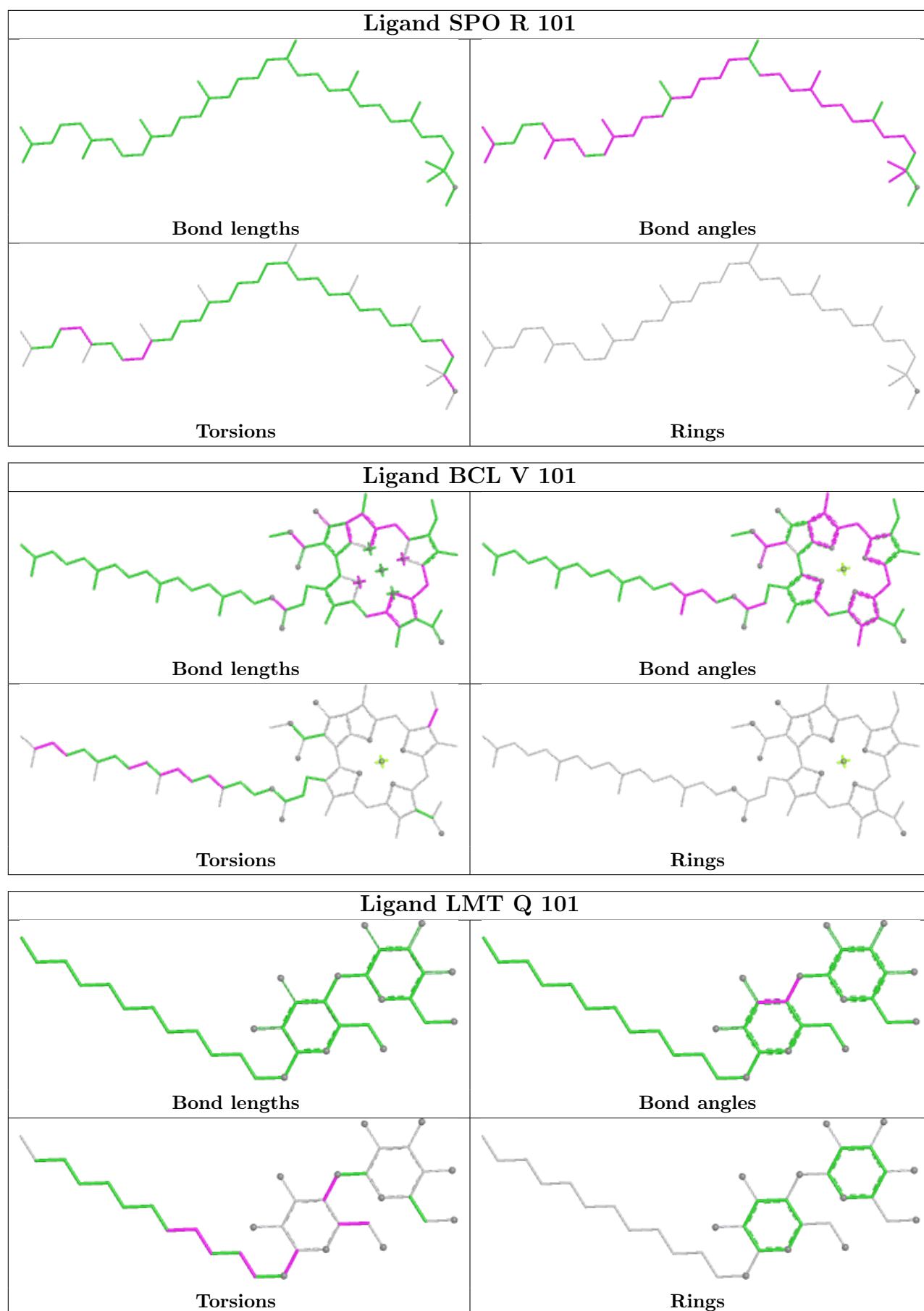


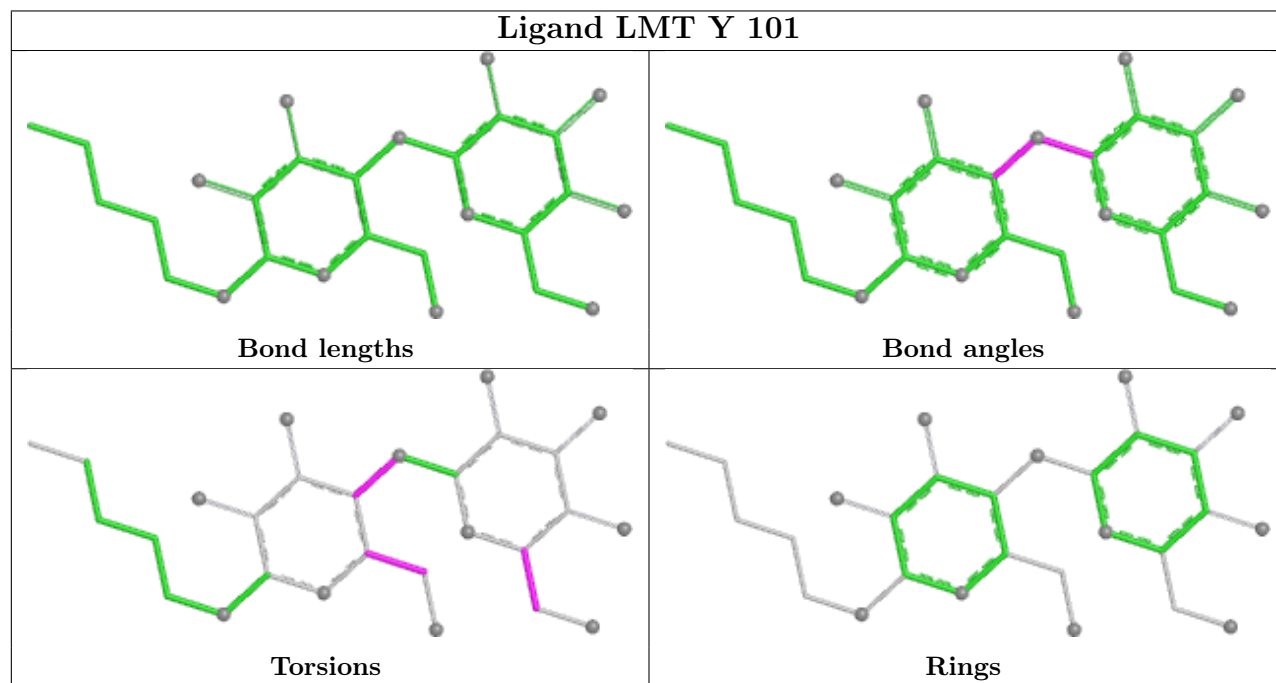
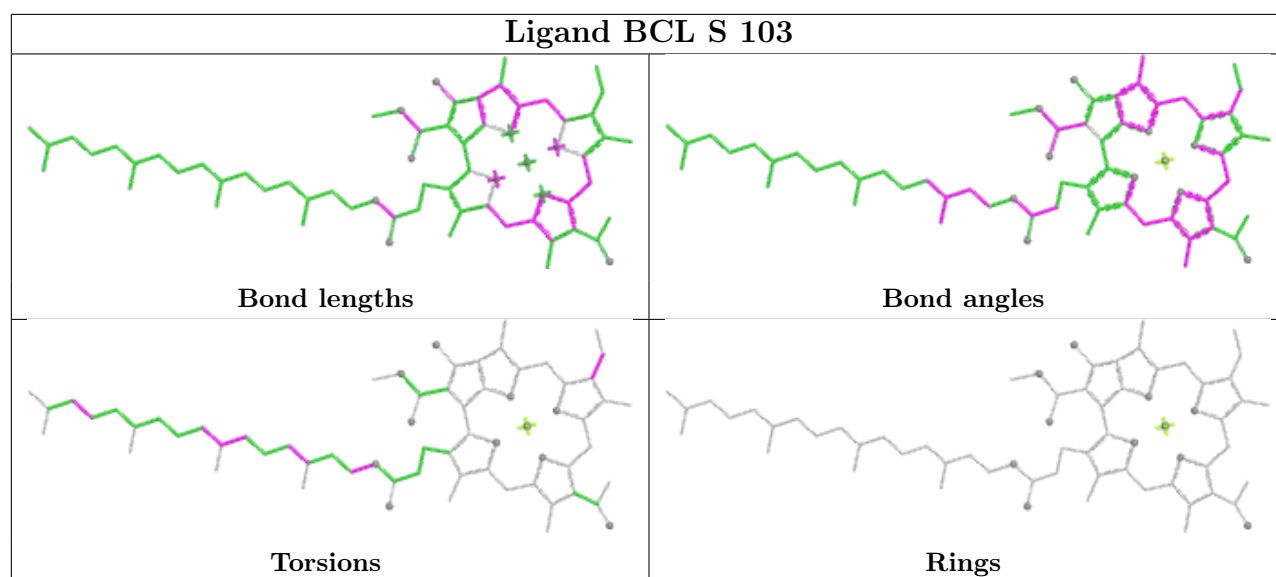


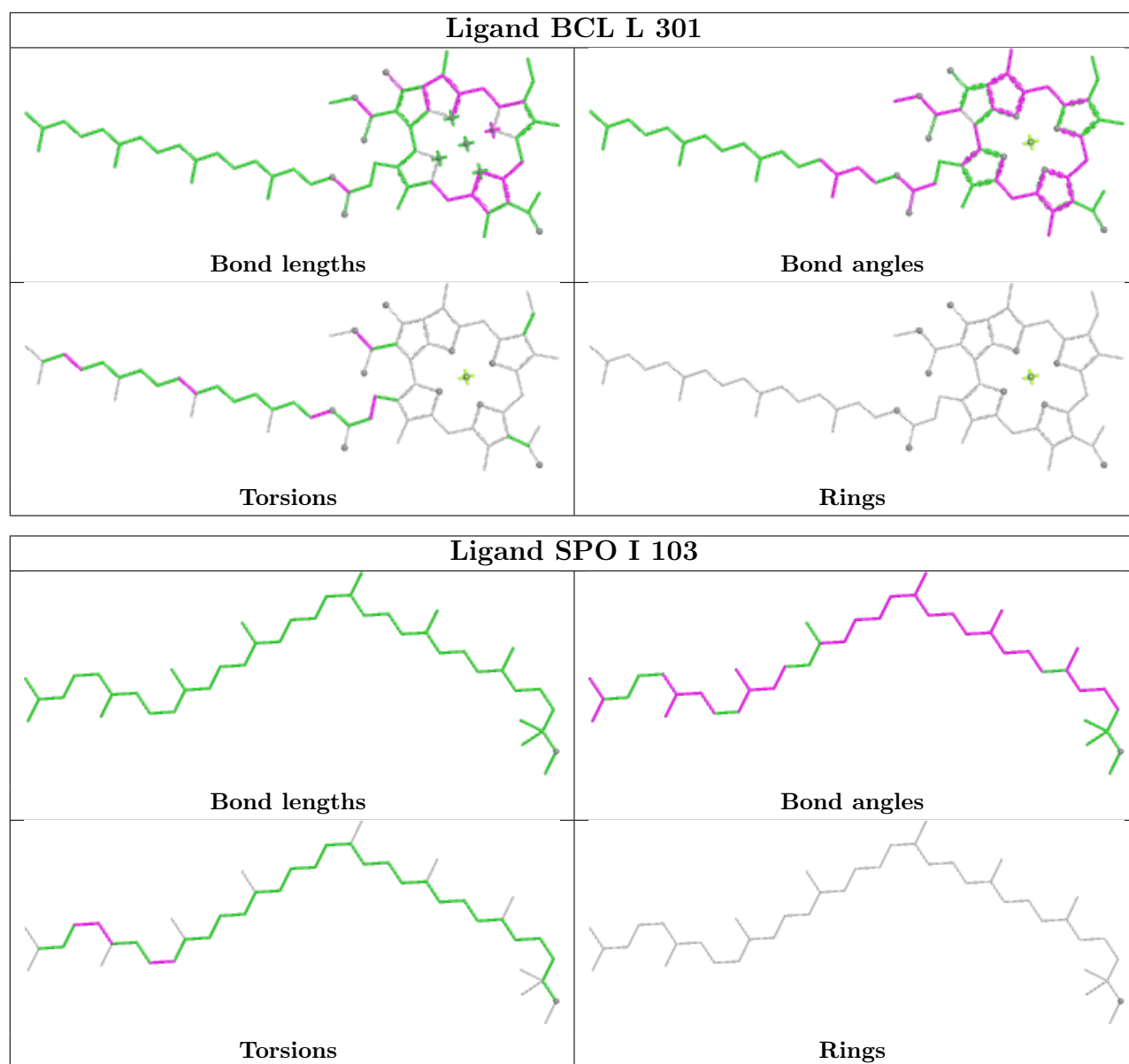


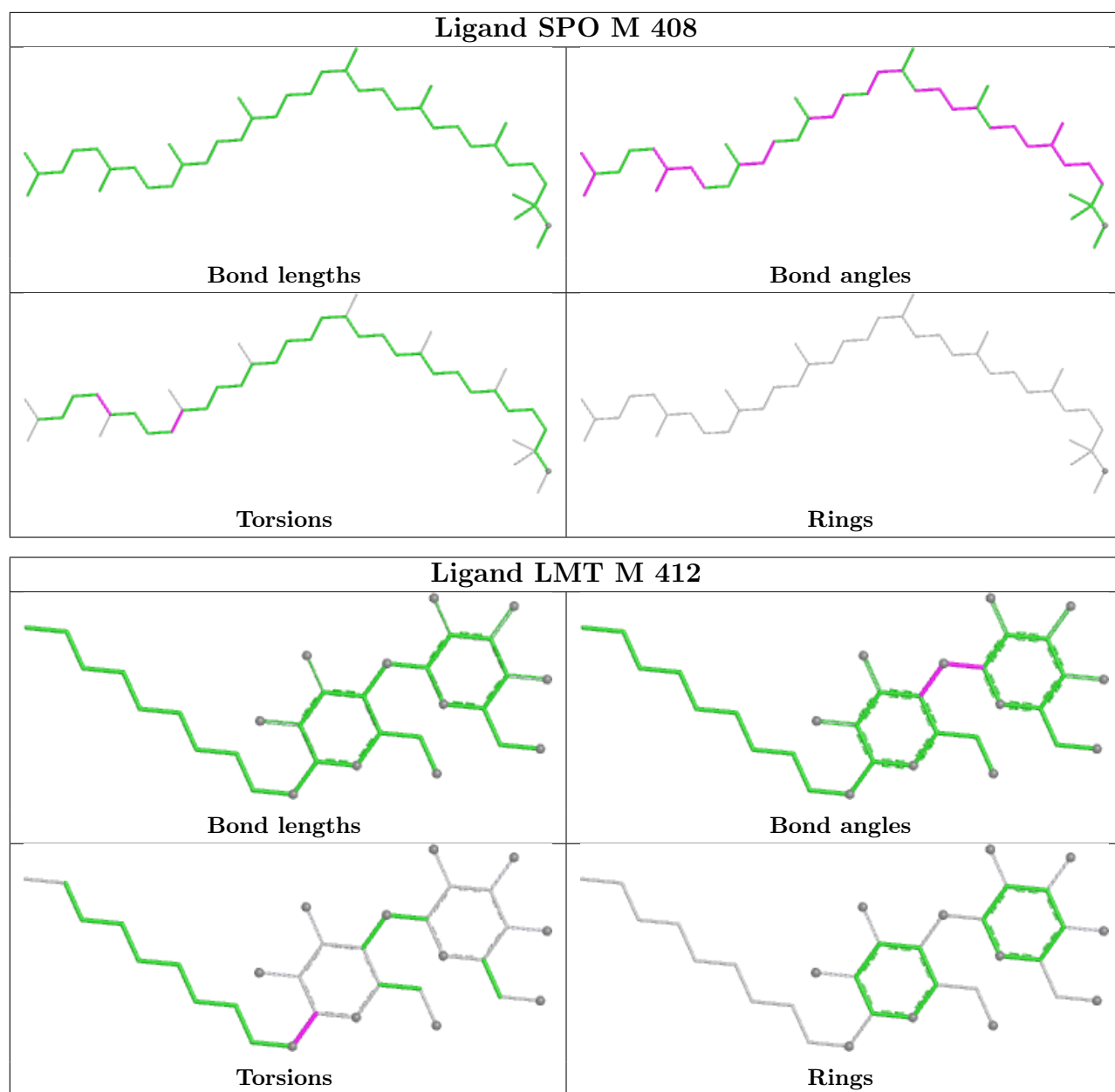


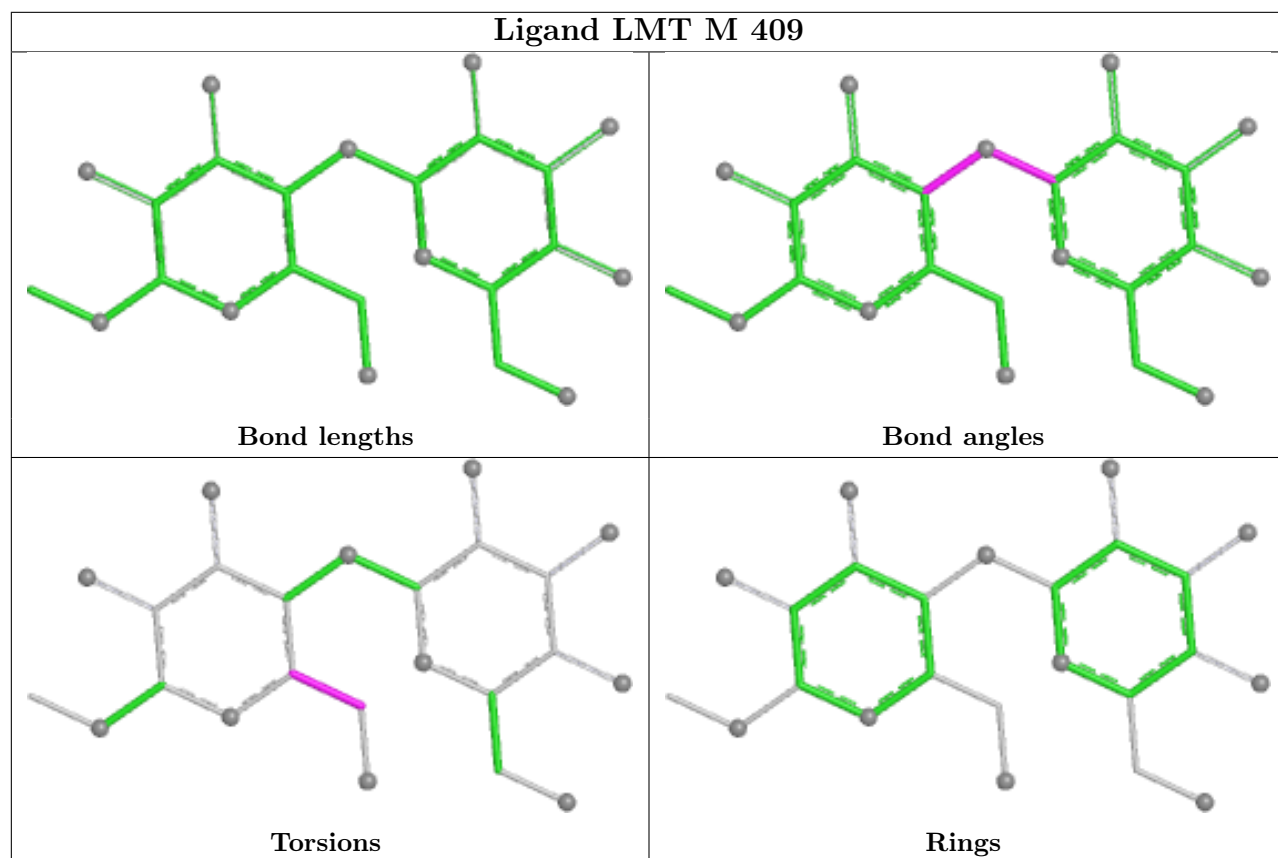
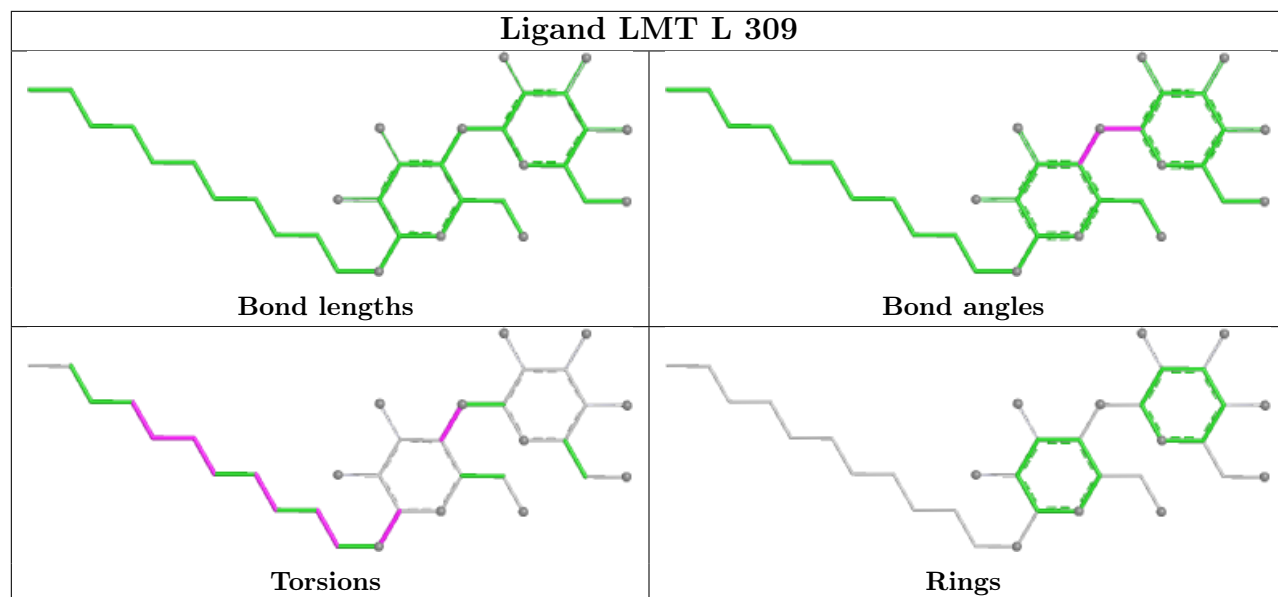


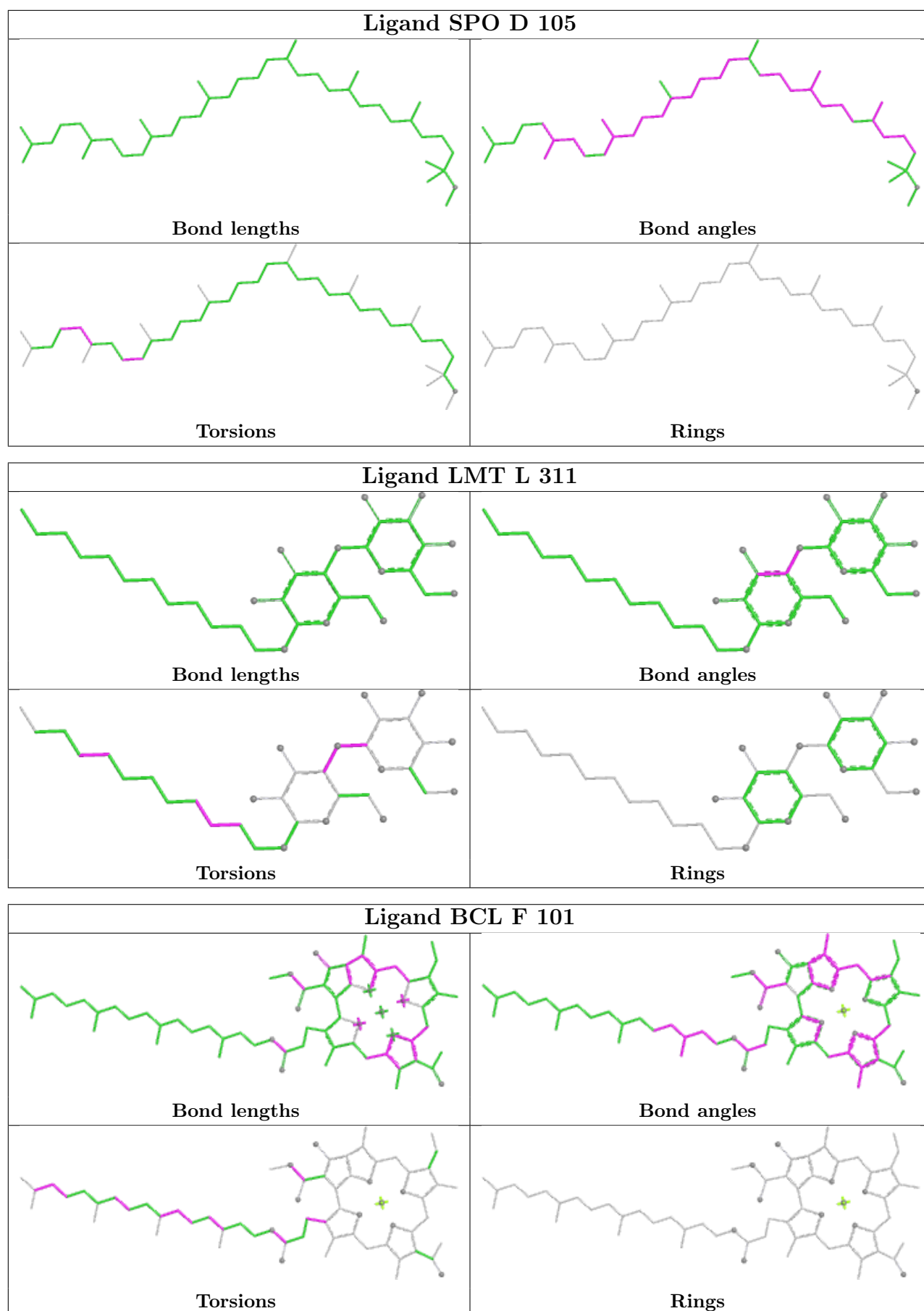


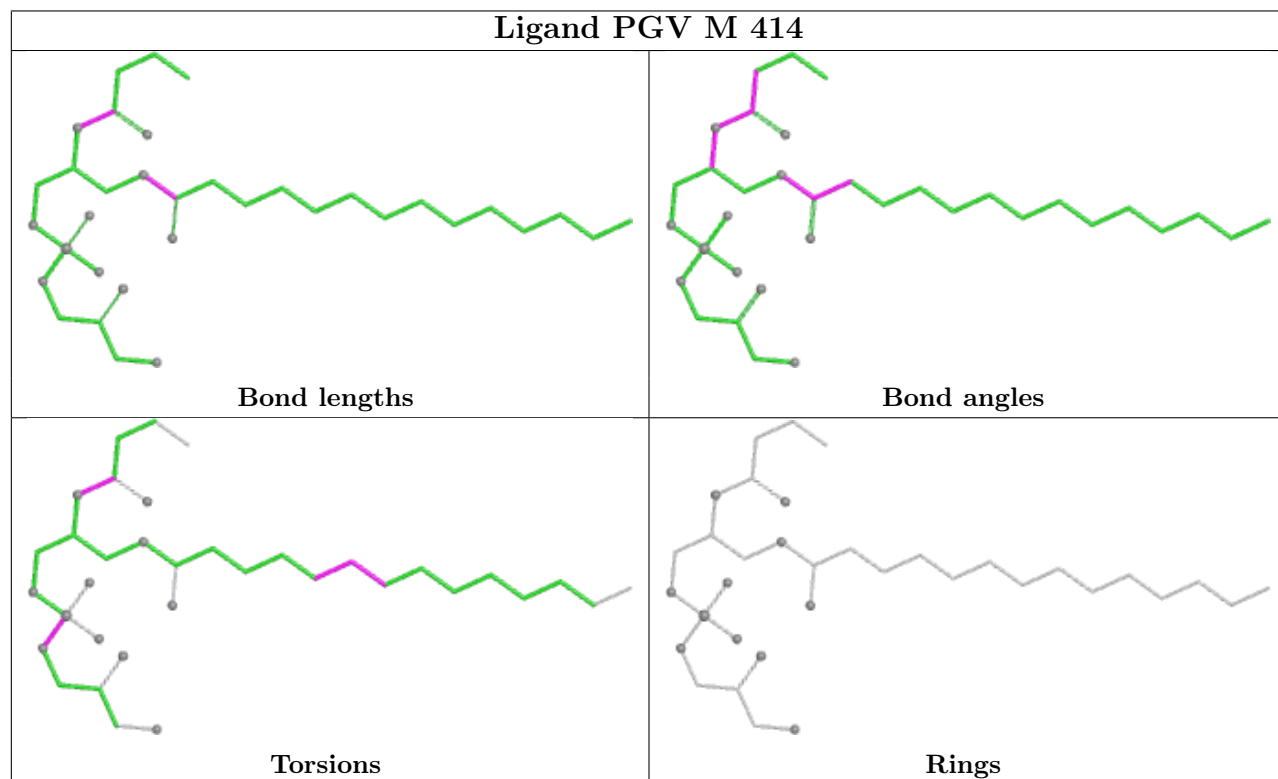
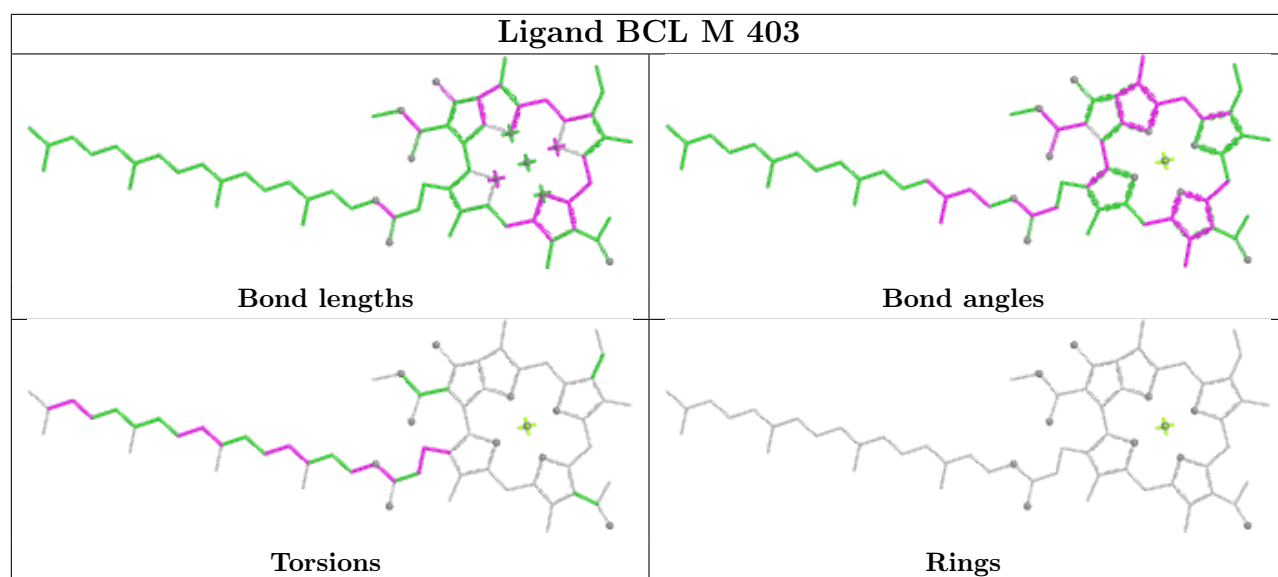


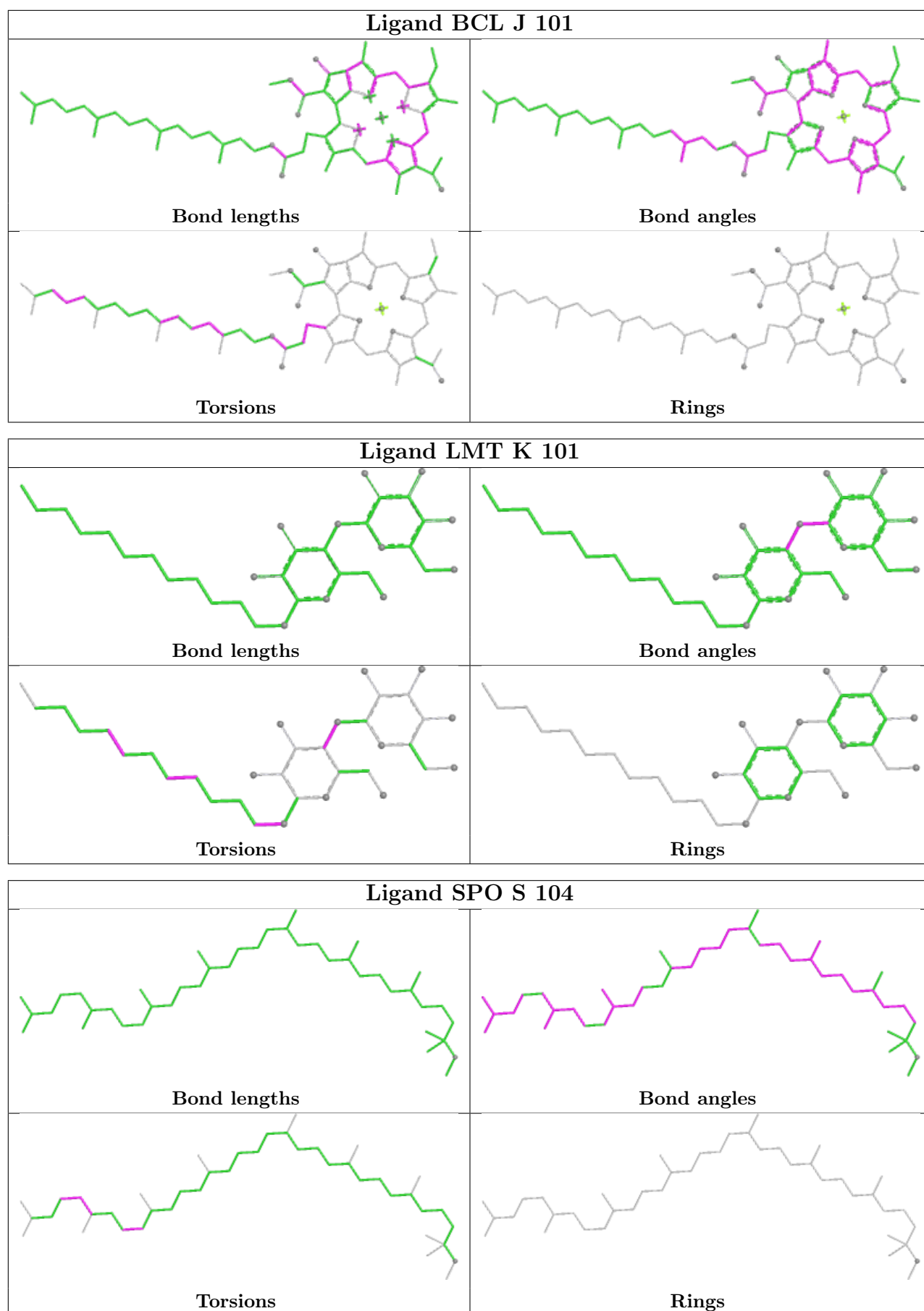


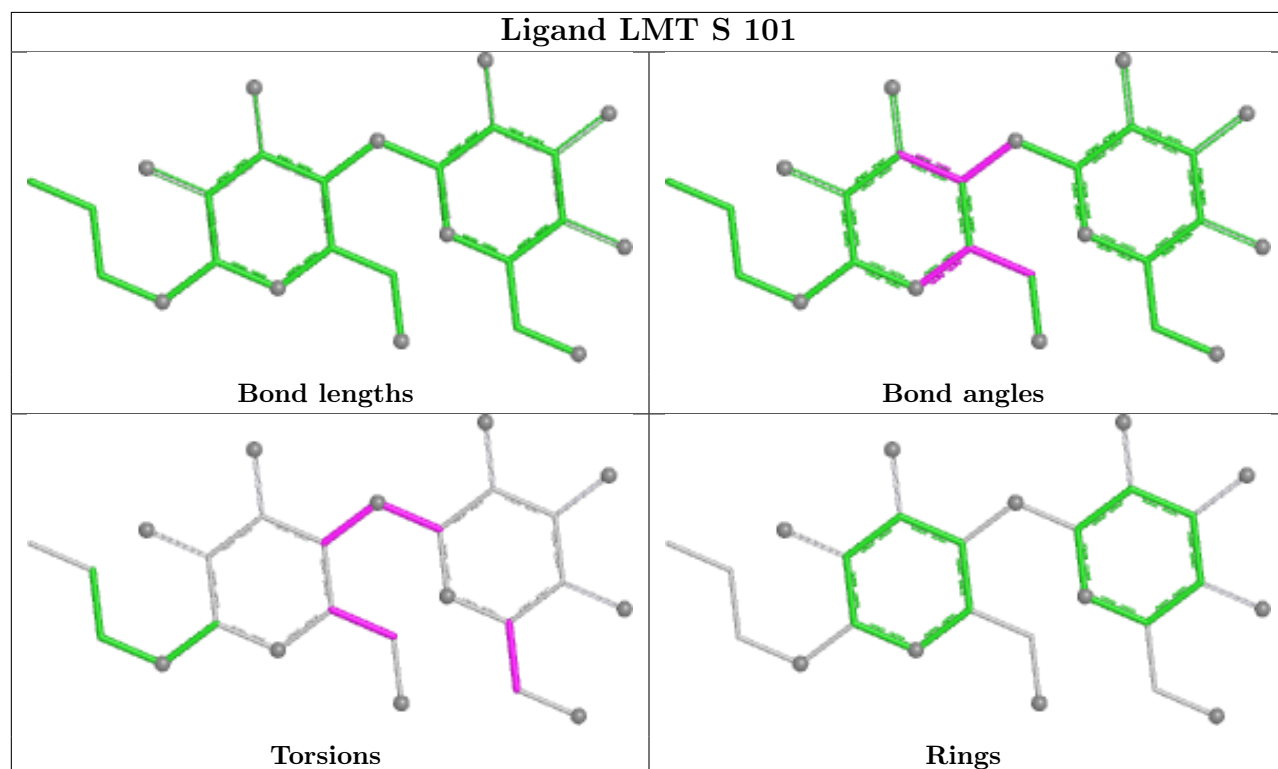
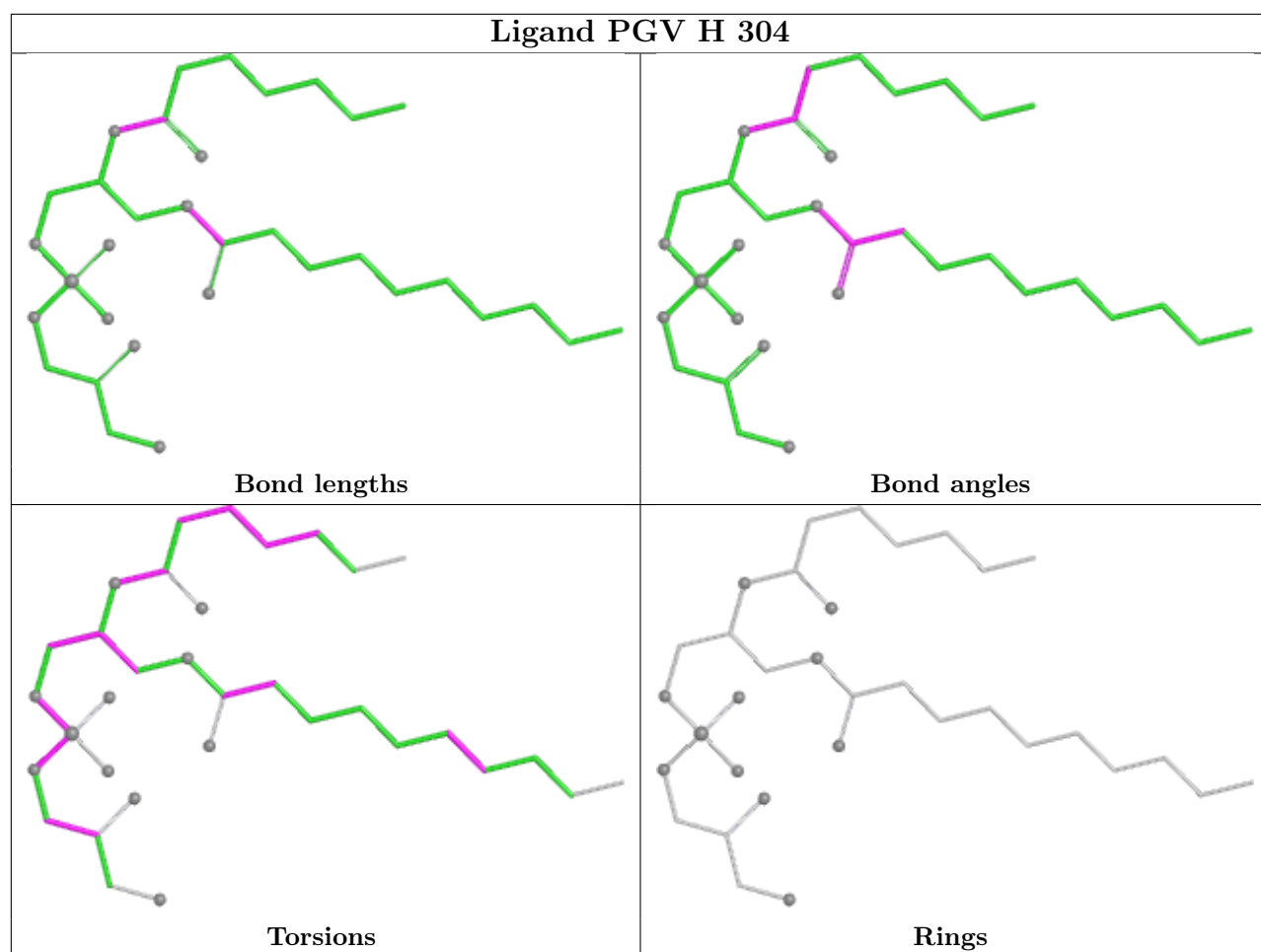


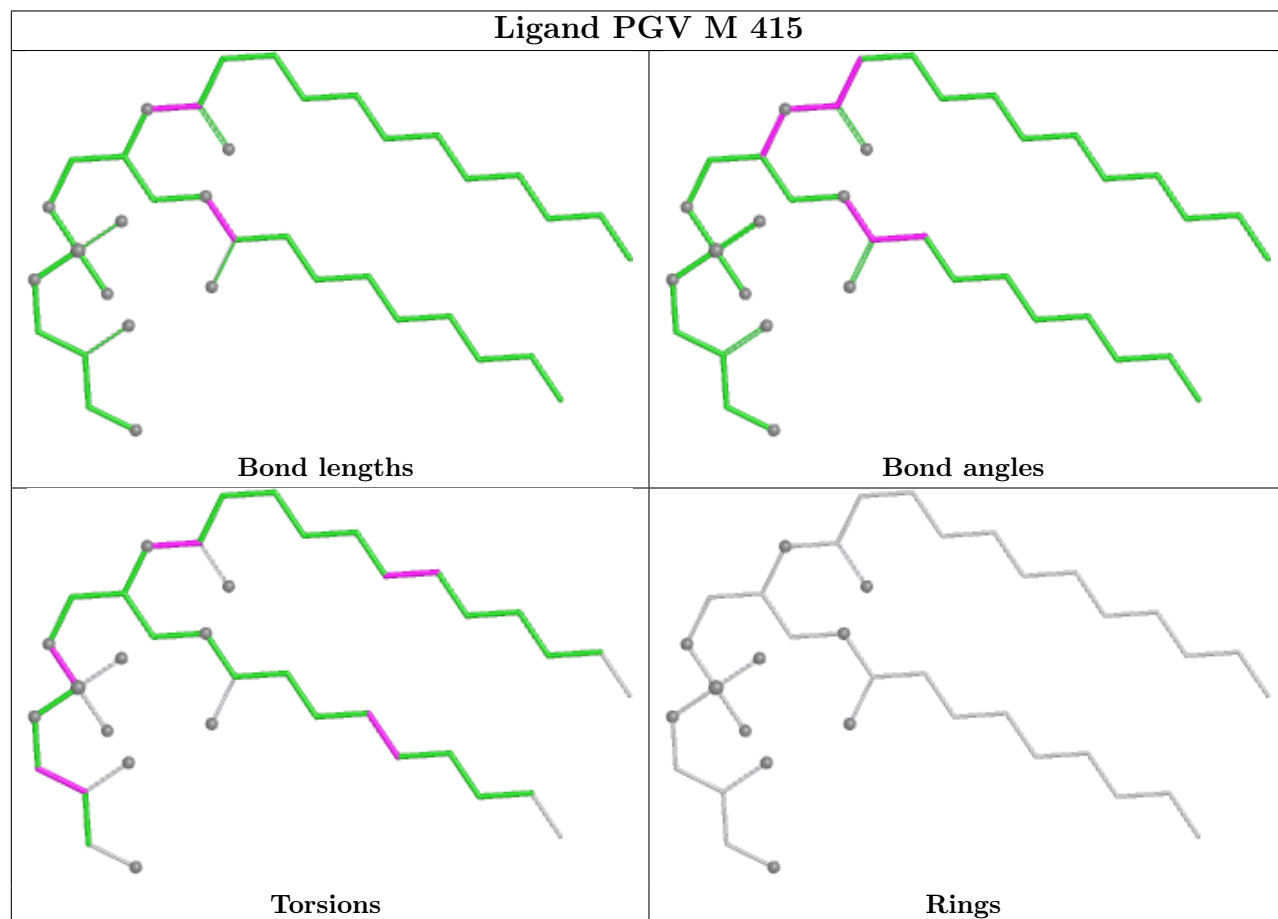
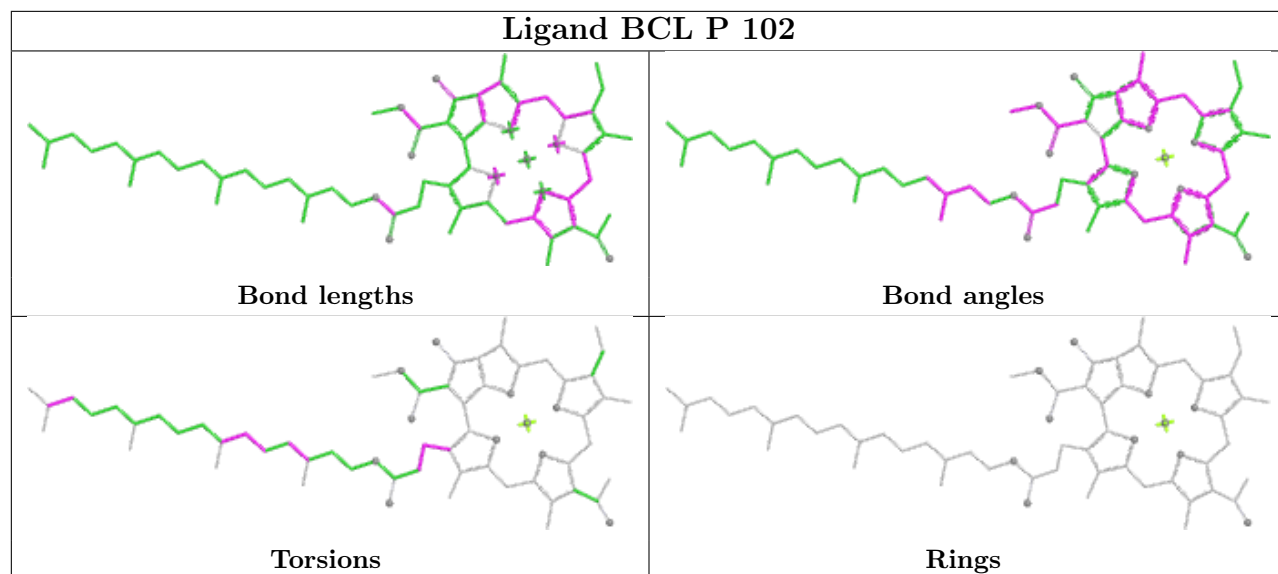


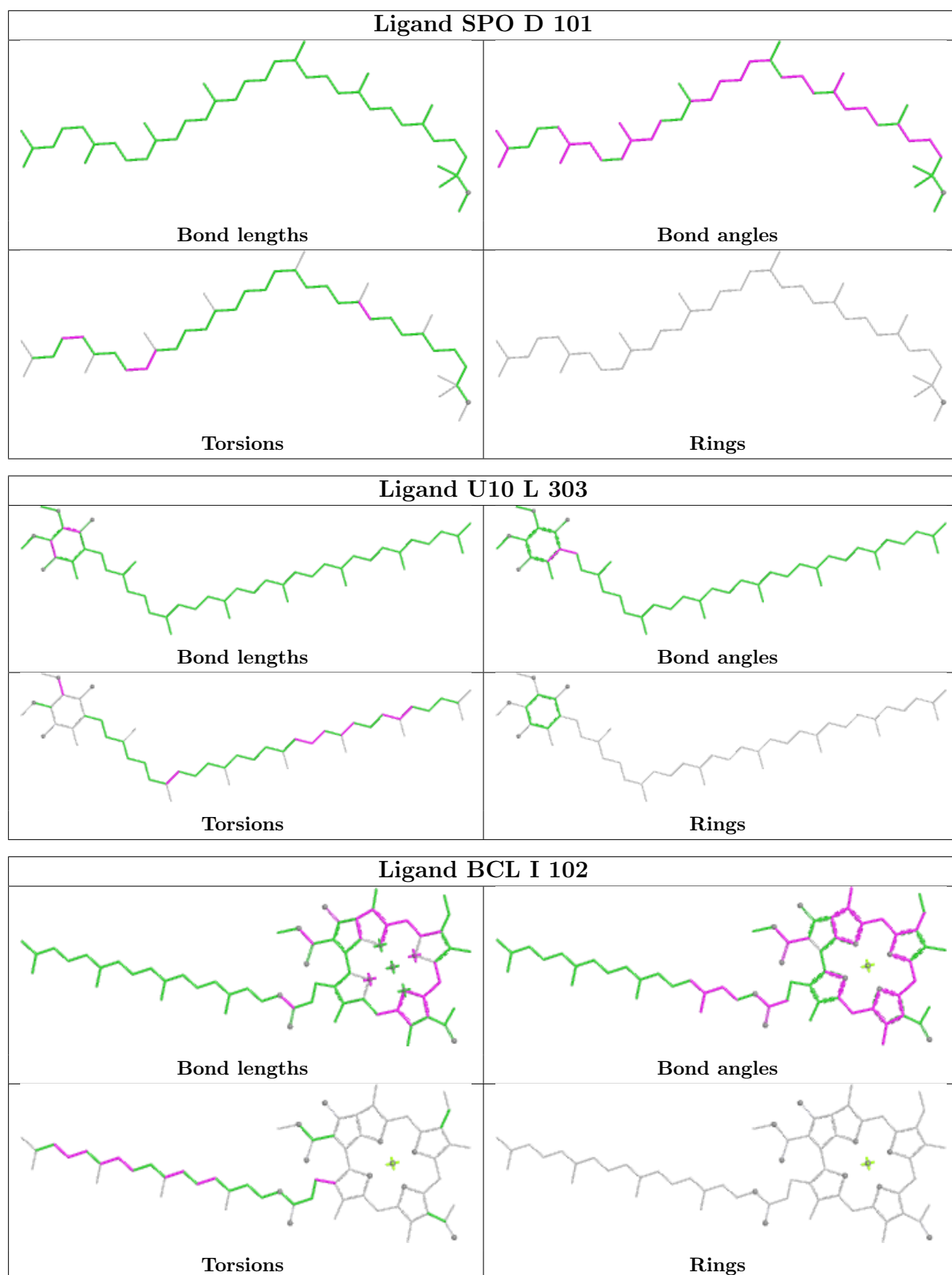


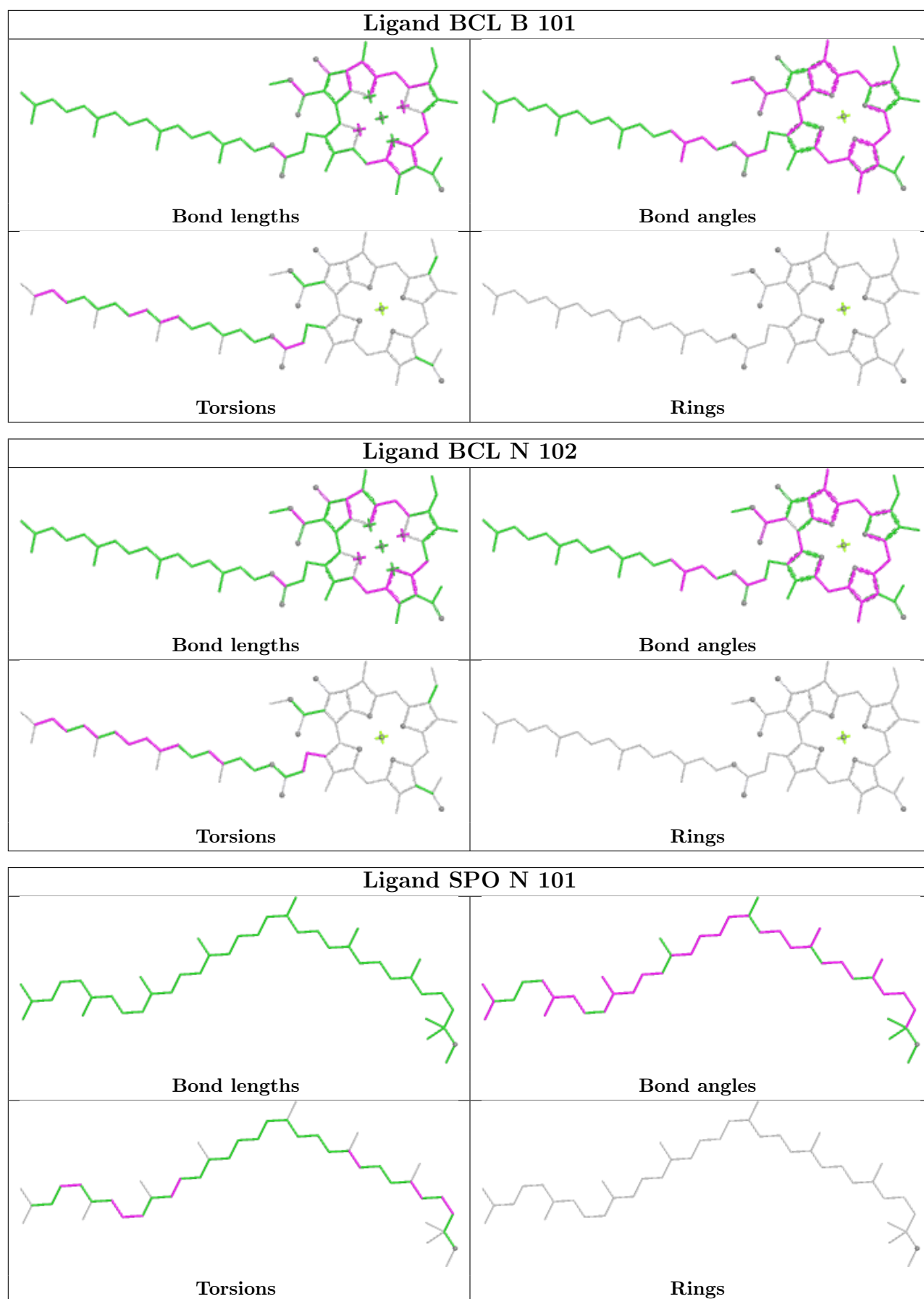


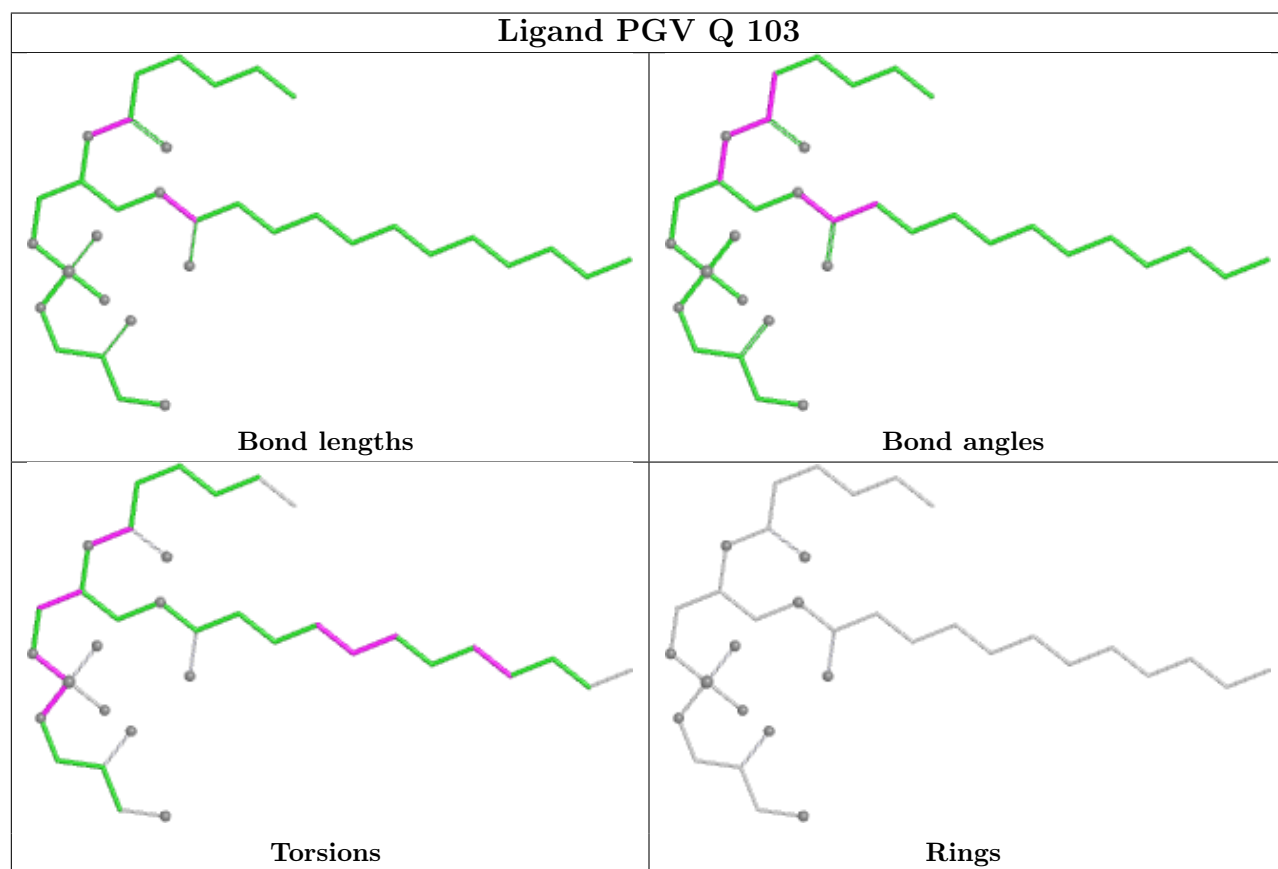
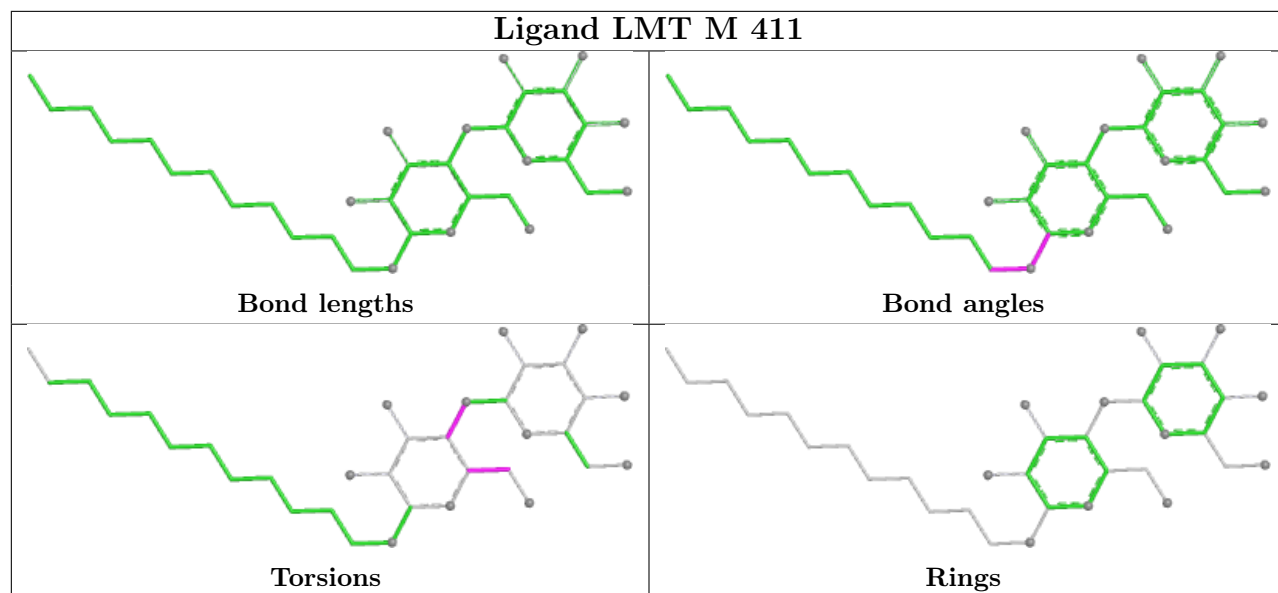


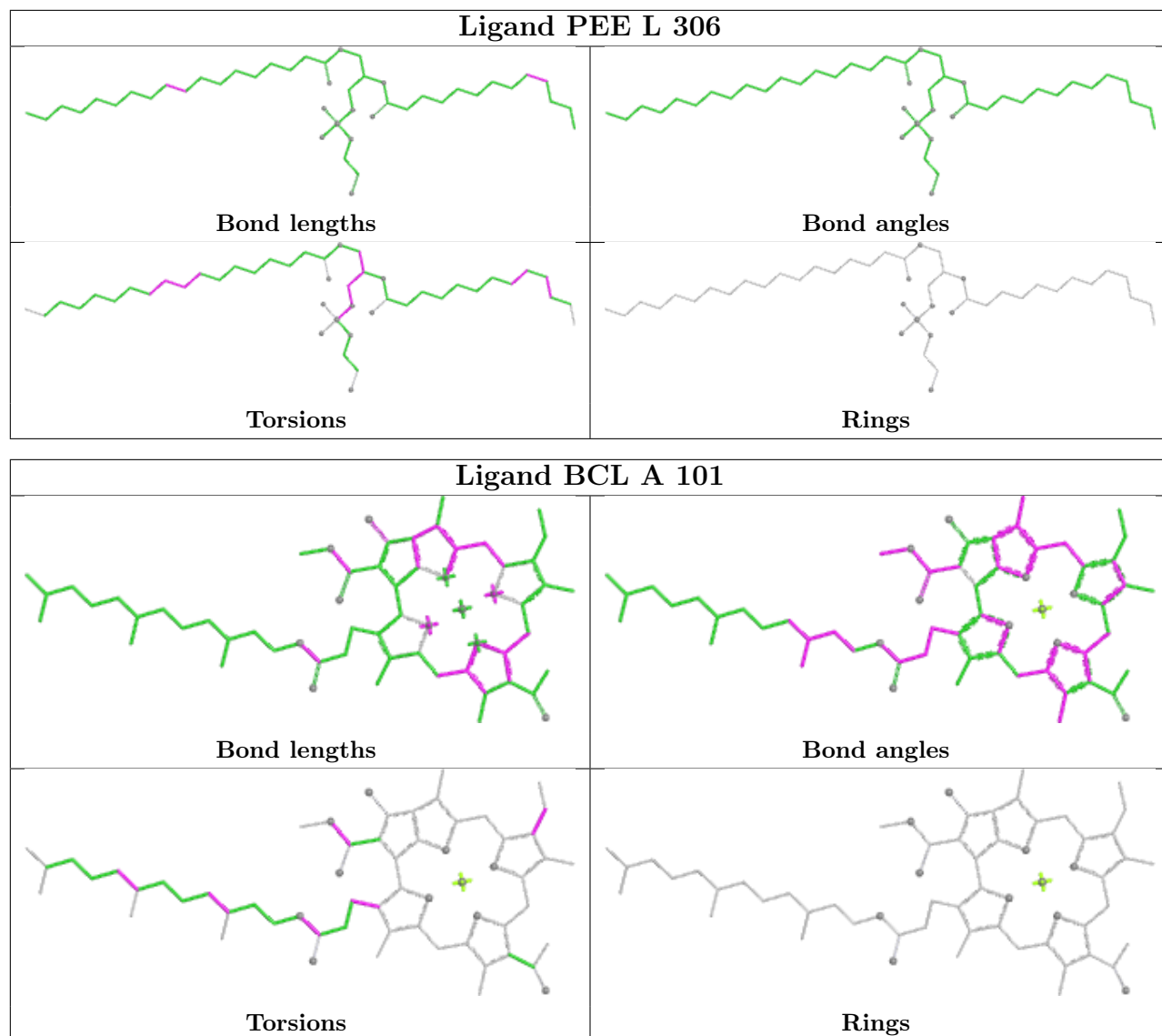


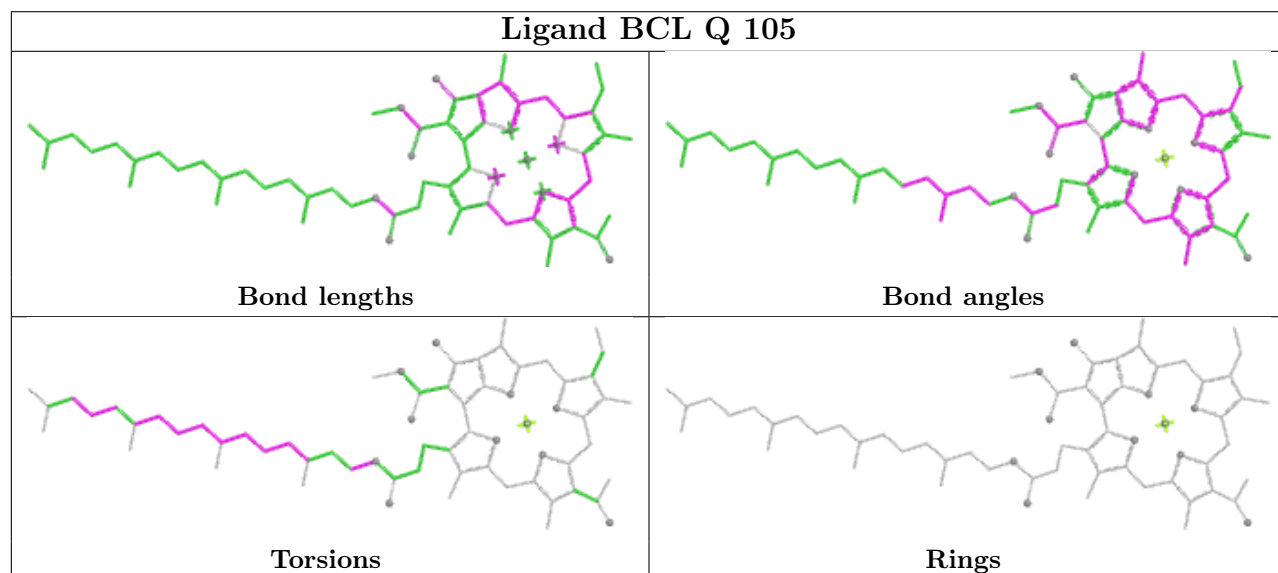
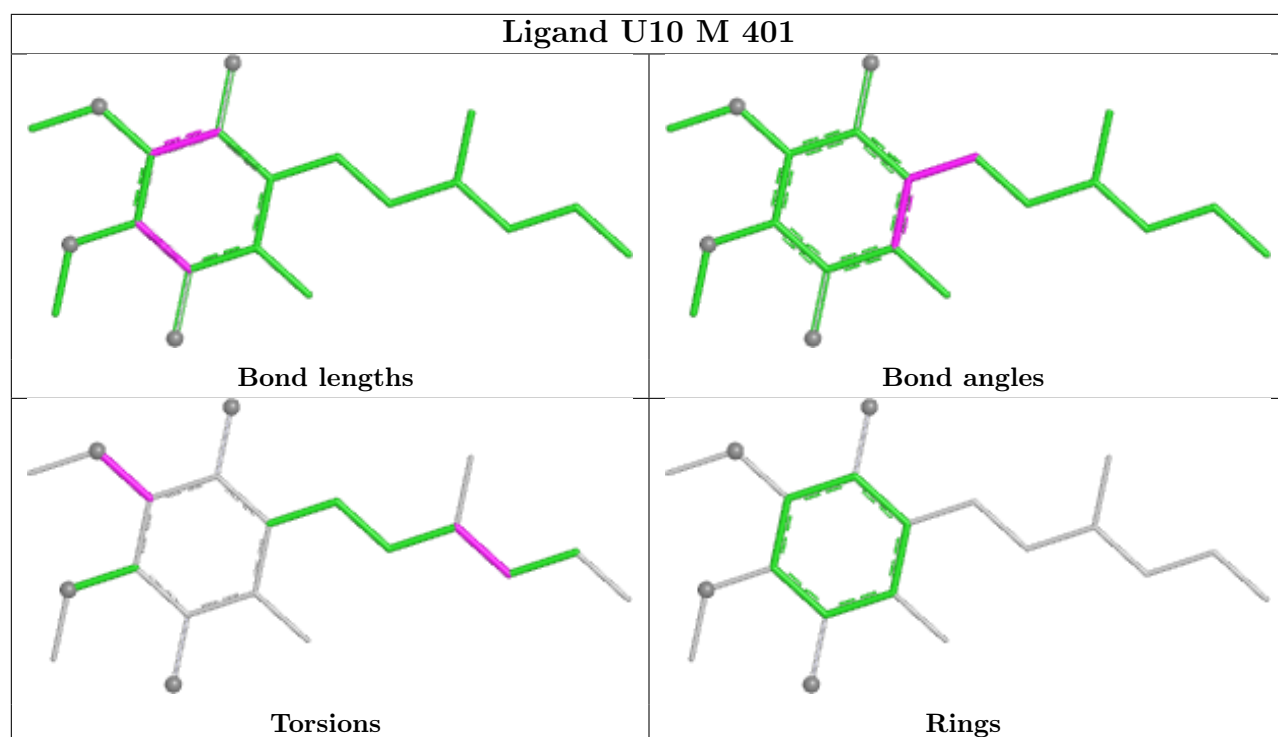


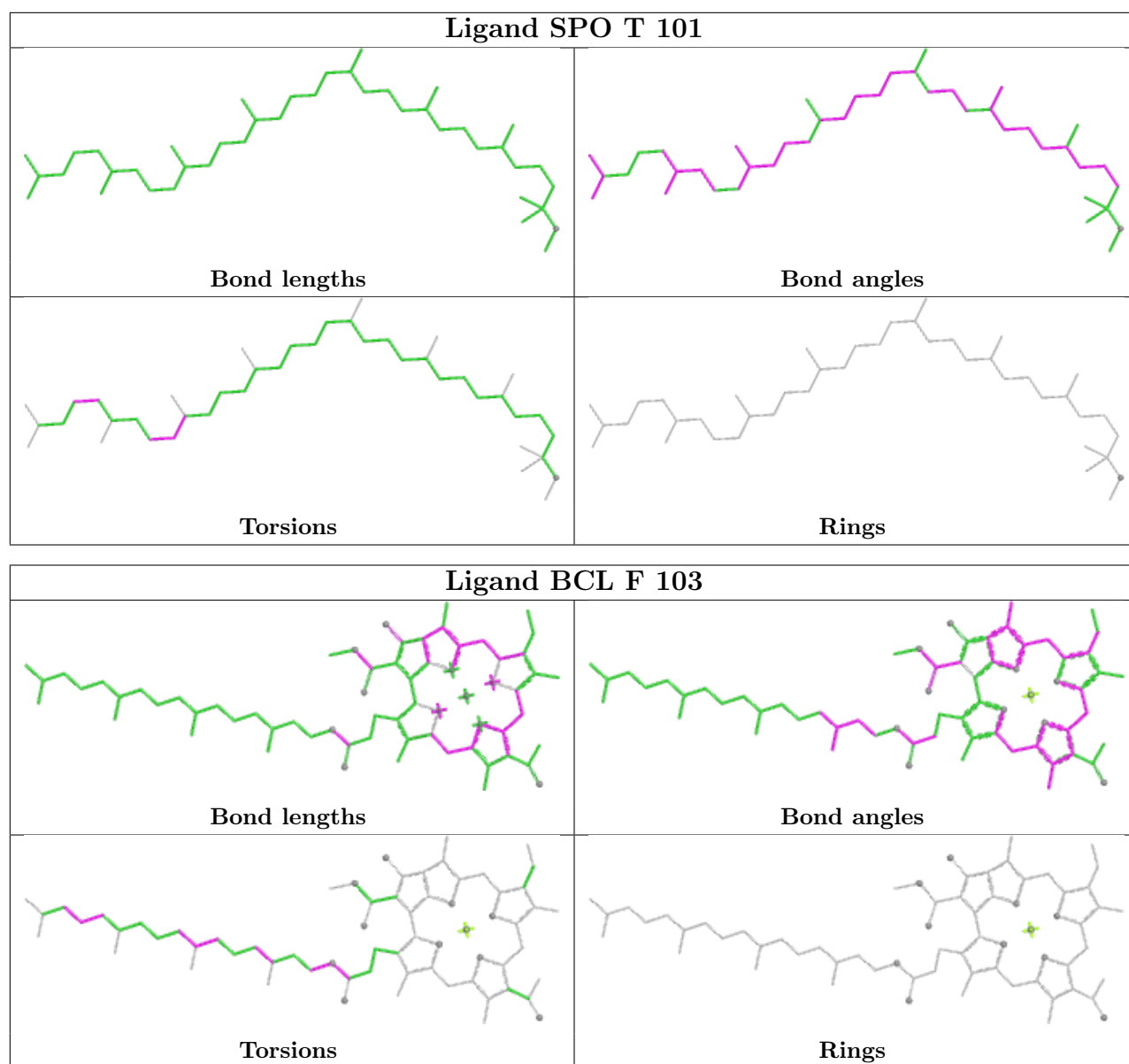


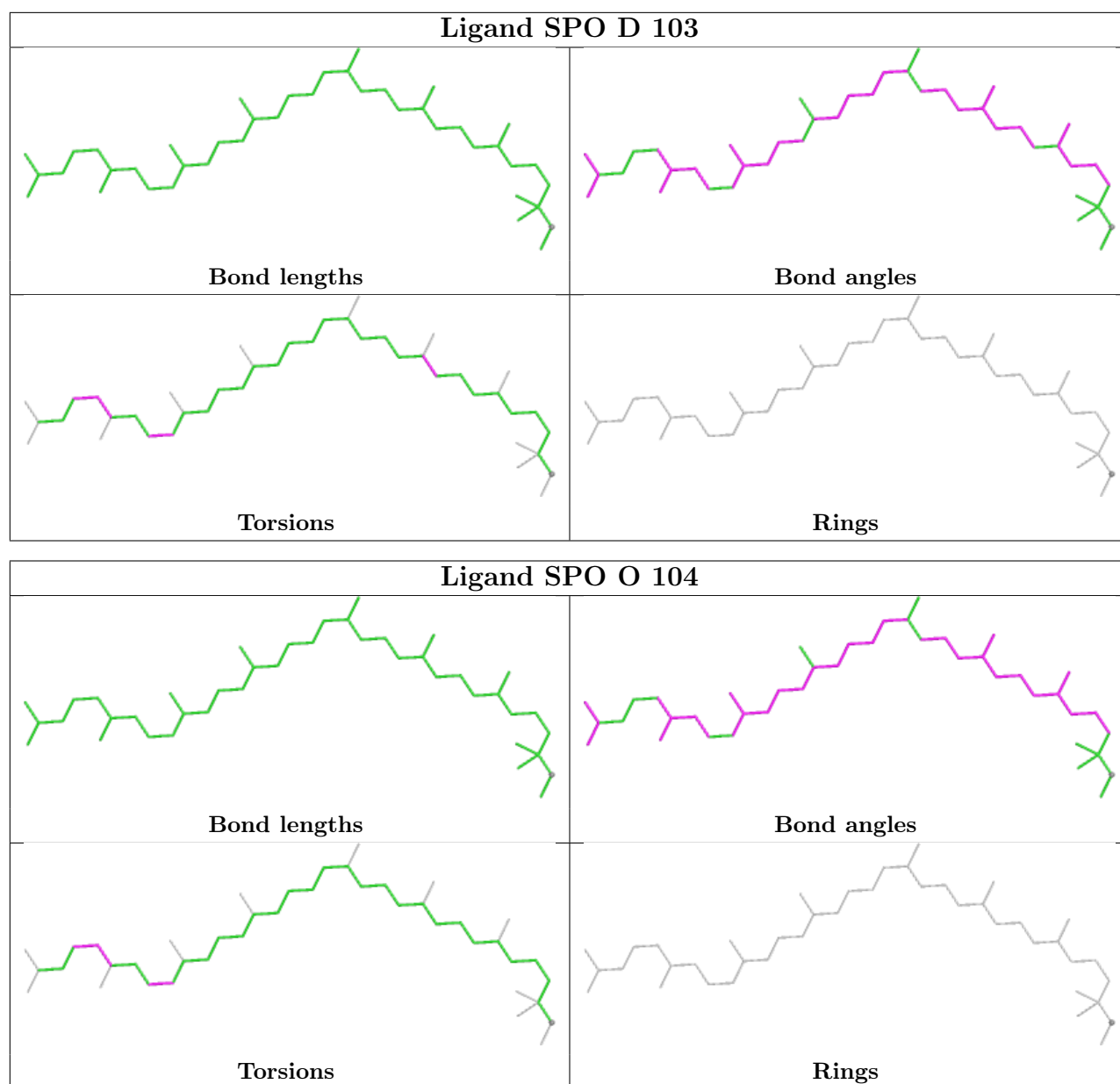


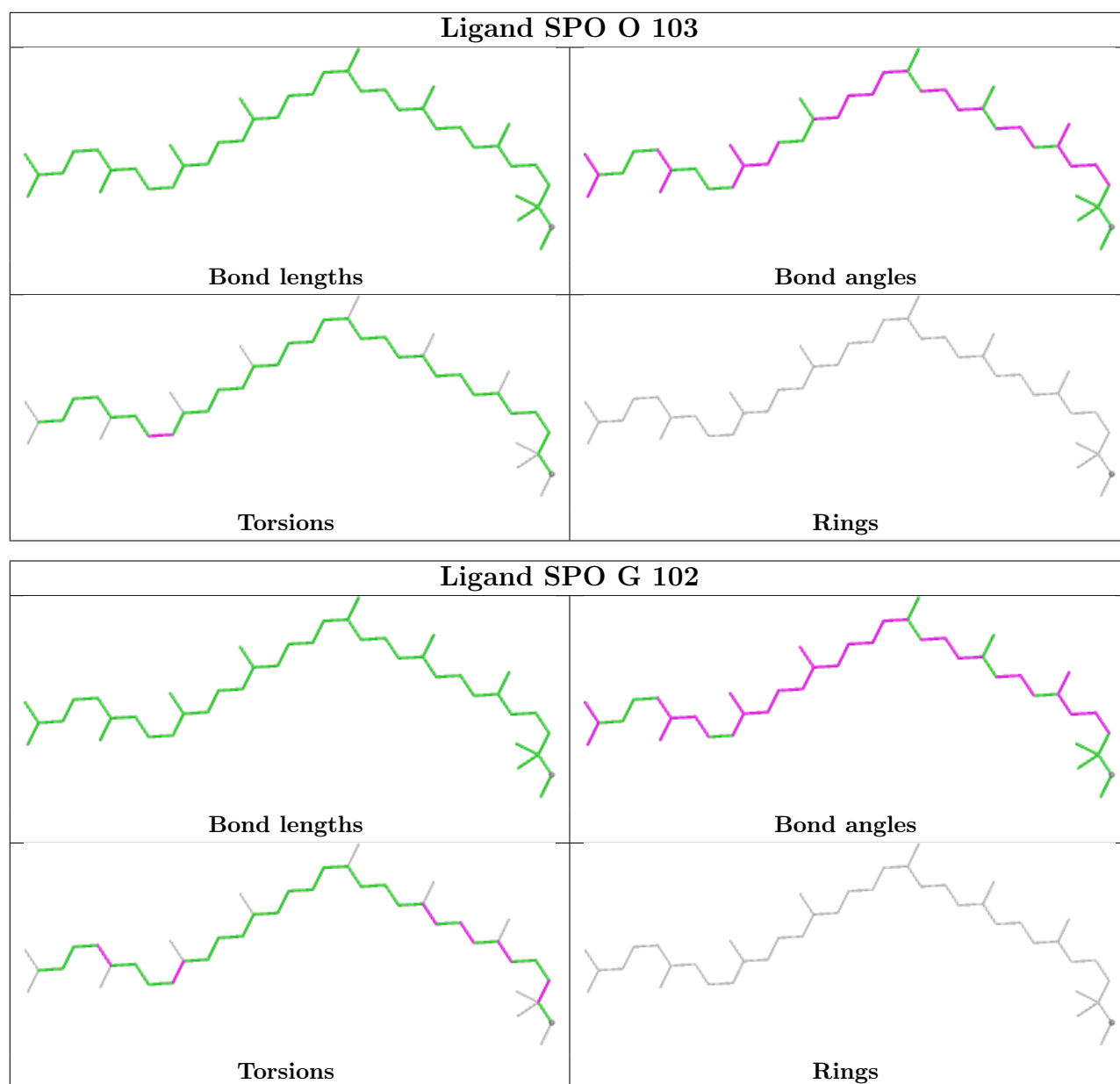


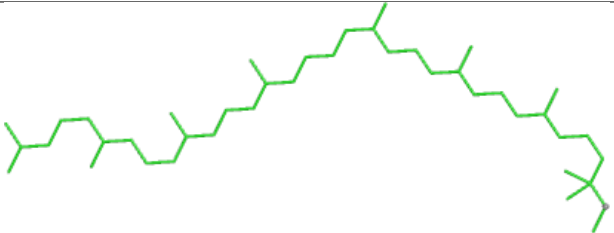
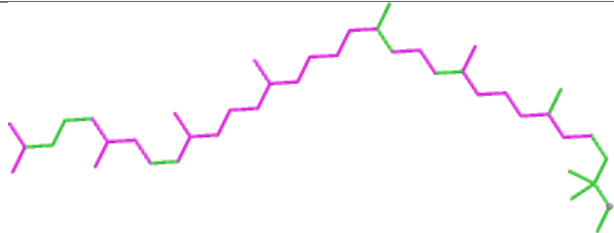
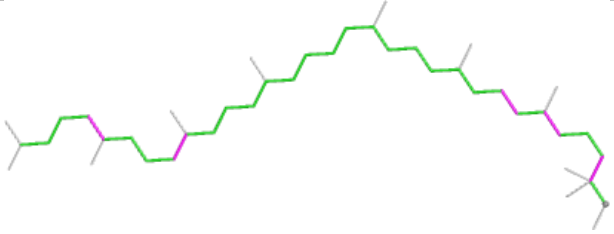
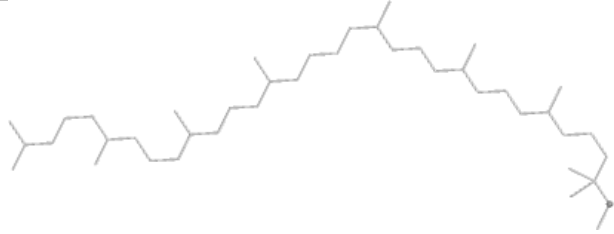
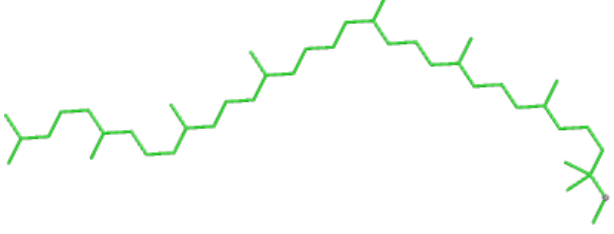
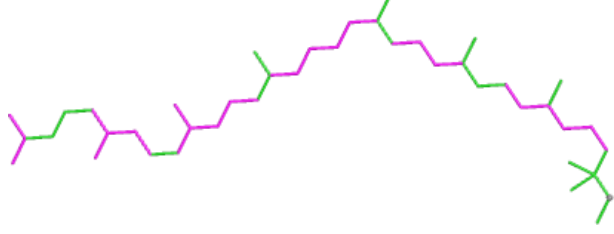
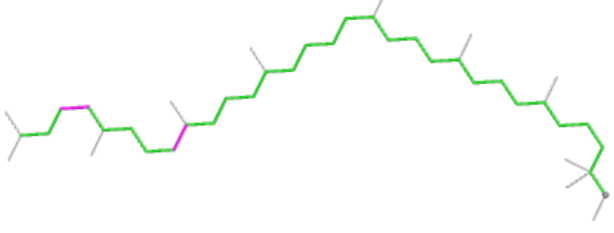


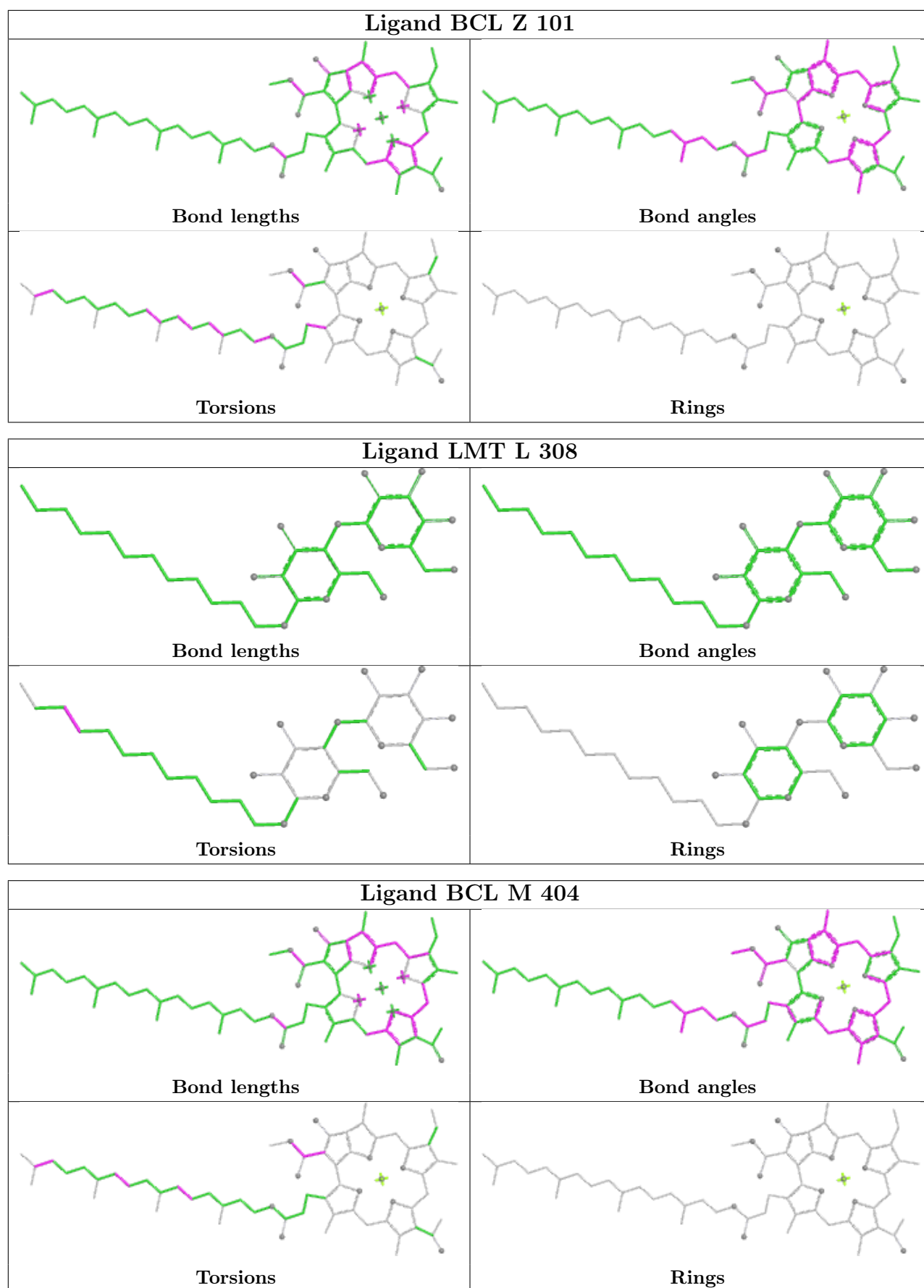


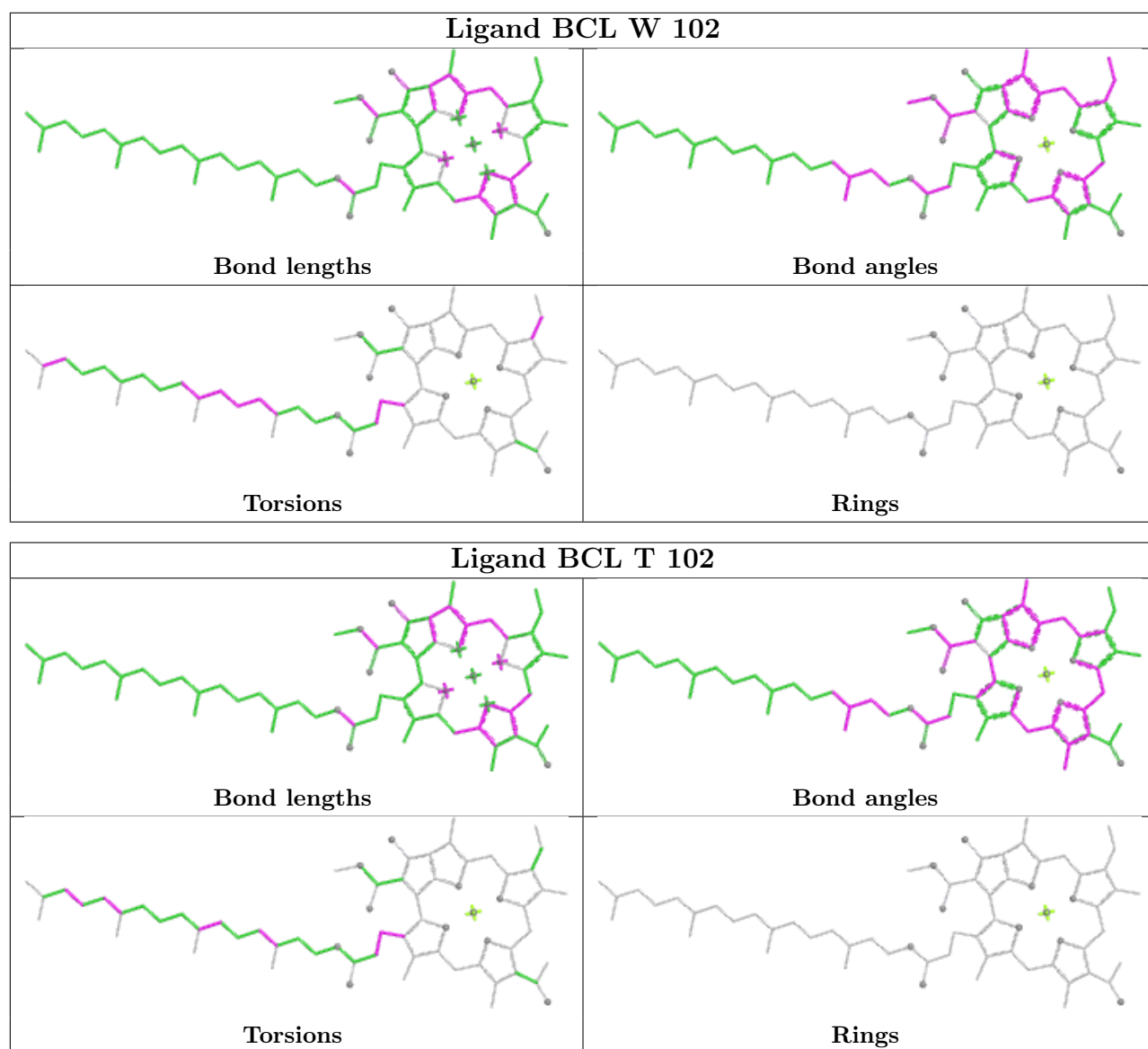


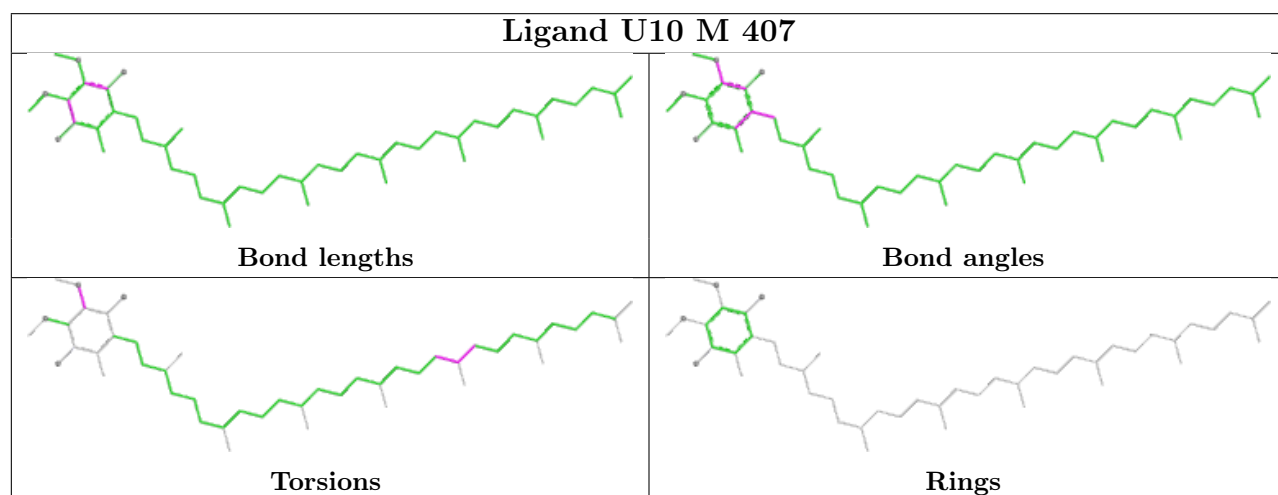
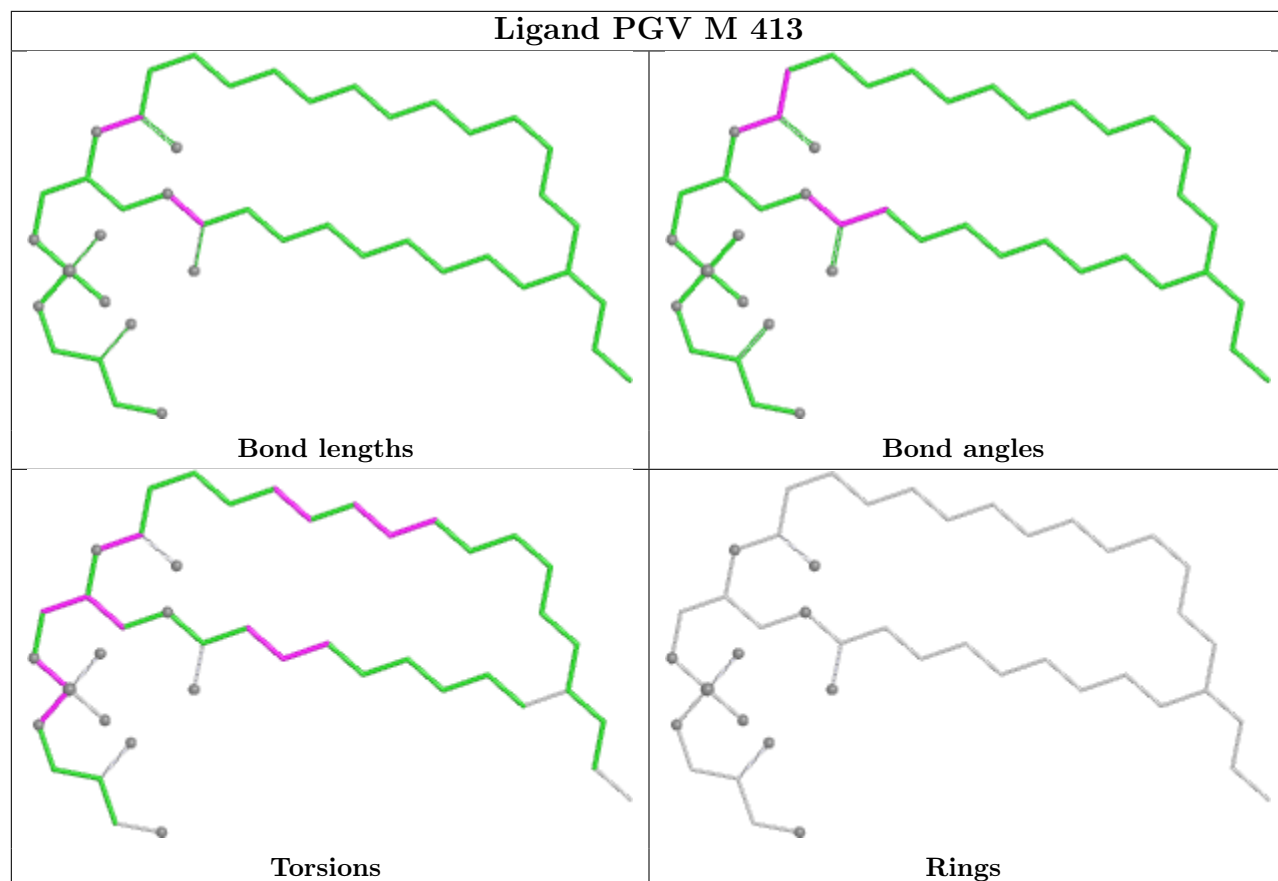


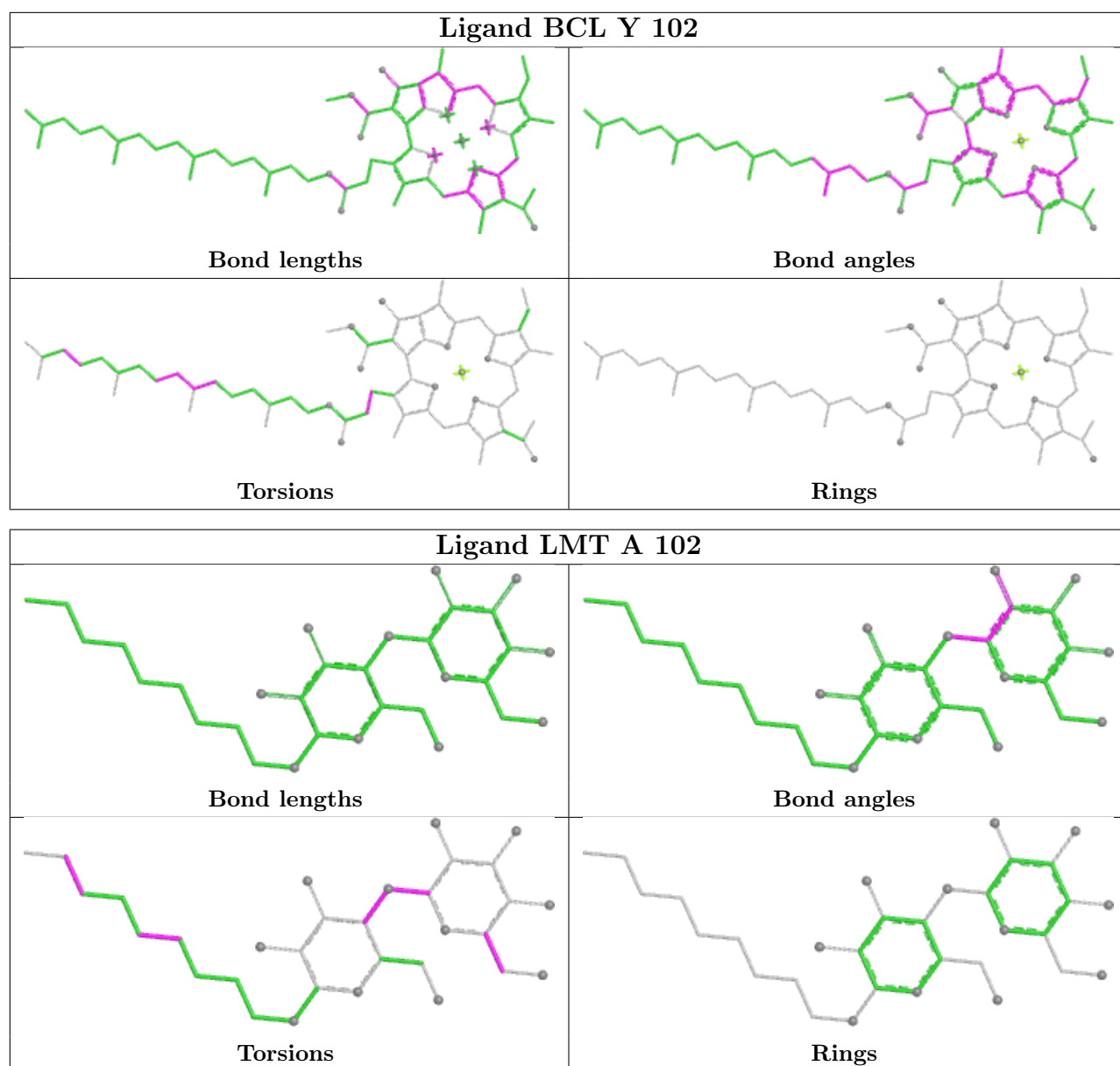


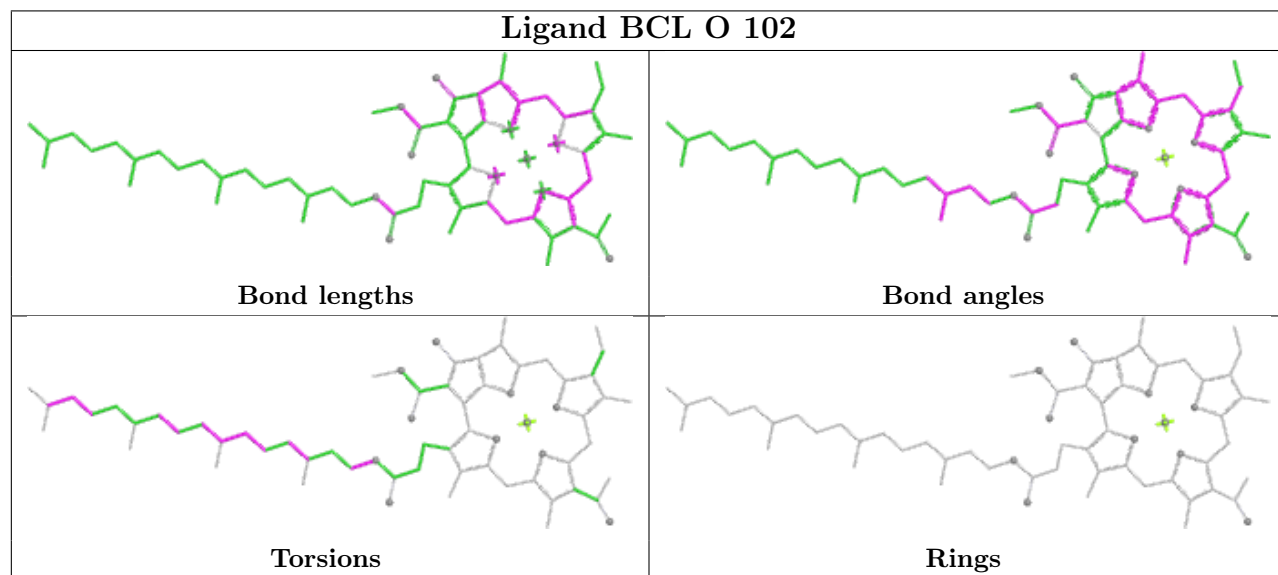
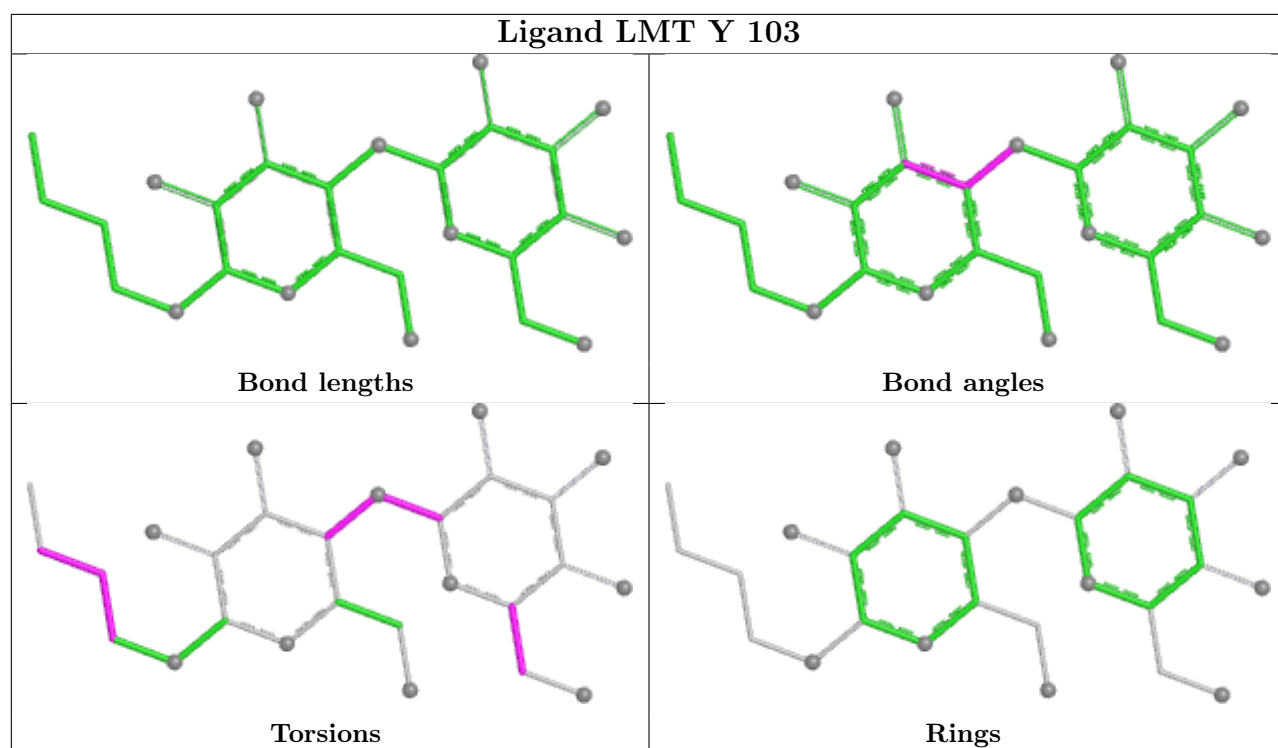
Ligand SPO F 104	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO W 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

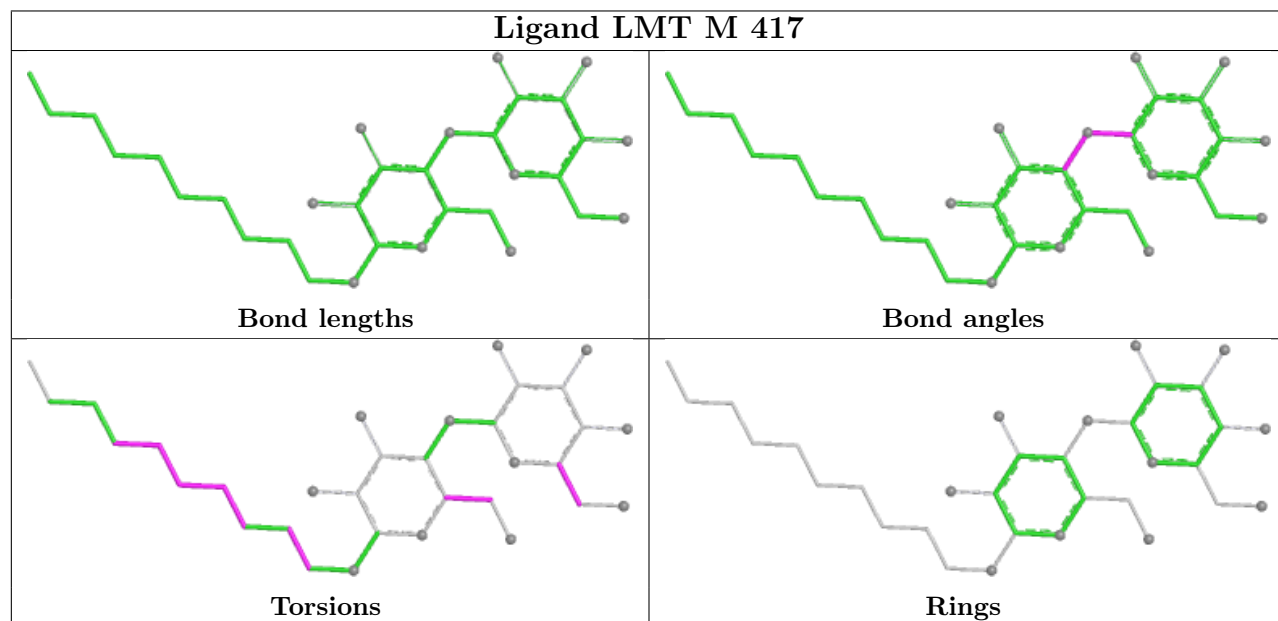
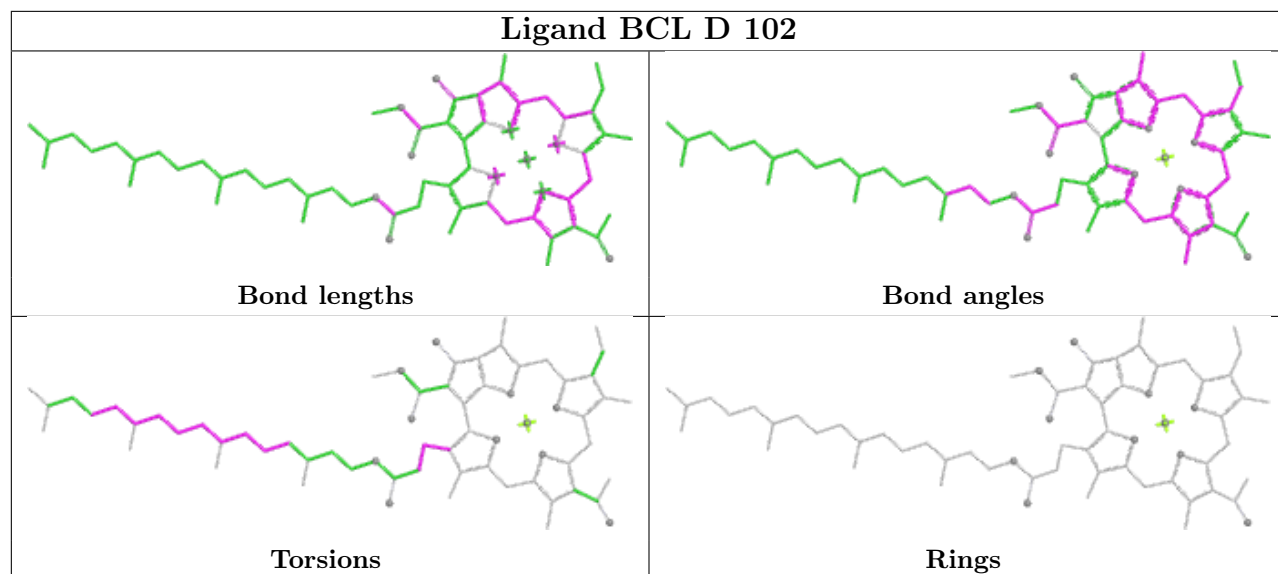


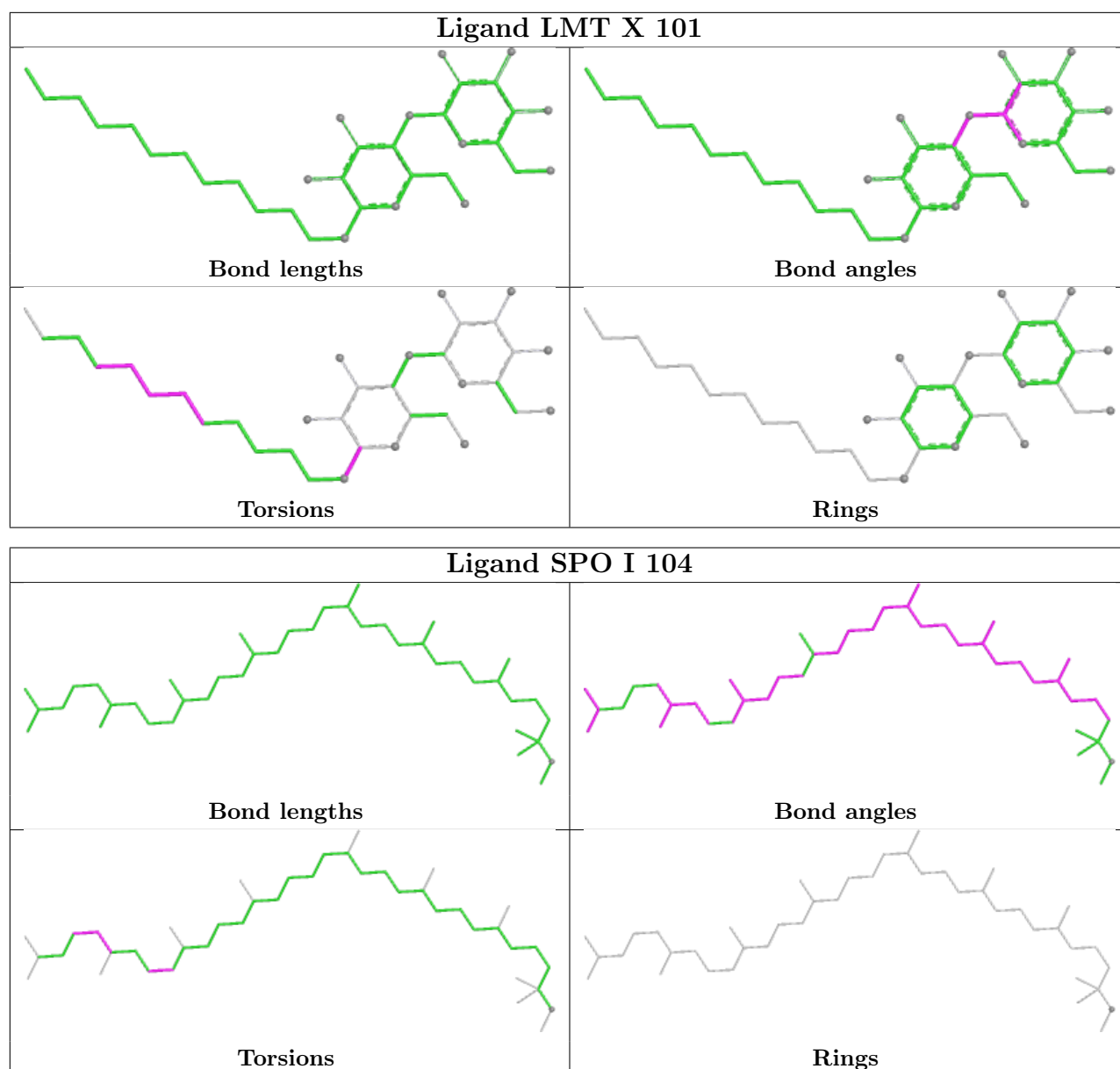












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

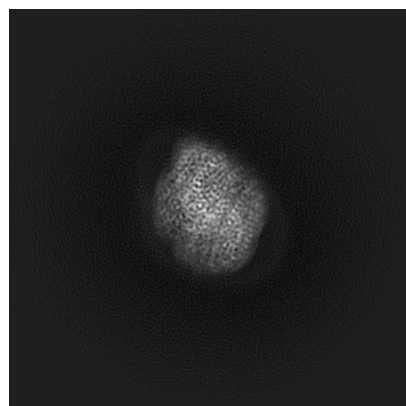
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33931. These allow visual inspection of the internal detail of the map and identification of artifacts.

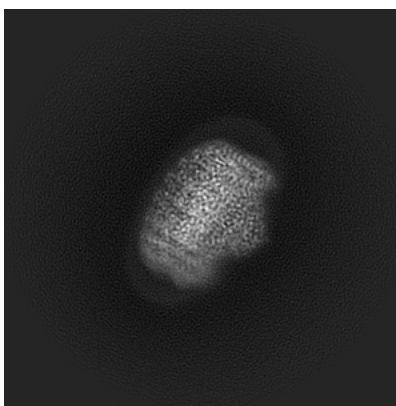
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

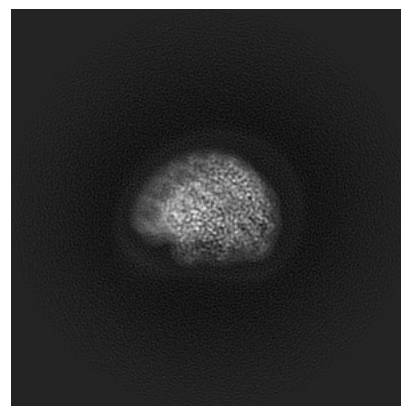
6.1.1 Primary map



X

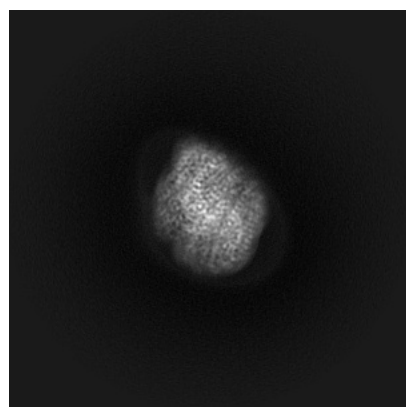


Y

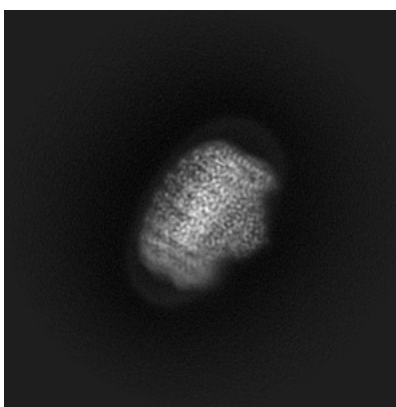


Z

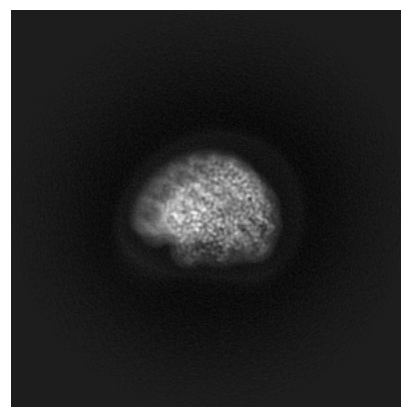
6.1.2 Raw map



X



Y

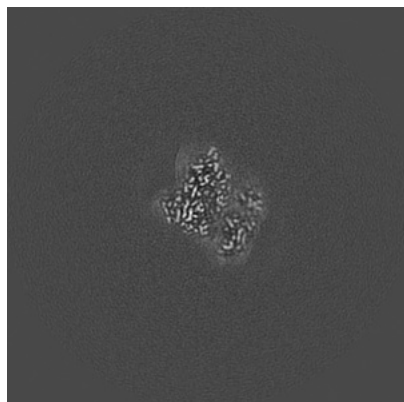


Z

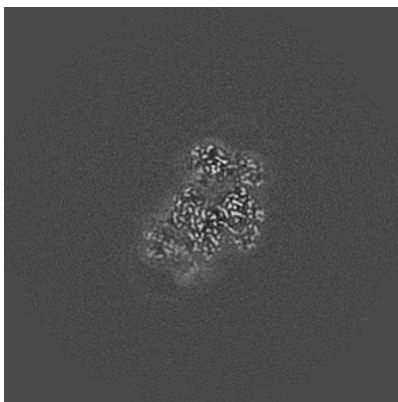
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

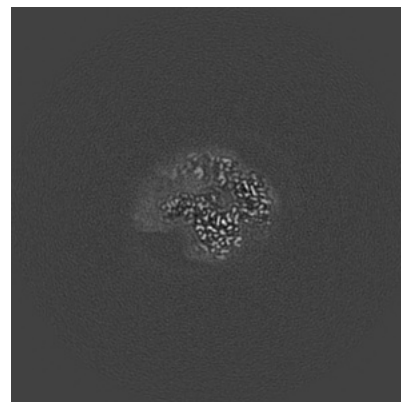
6.2.1 Primary map



X Index: 200

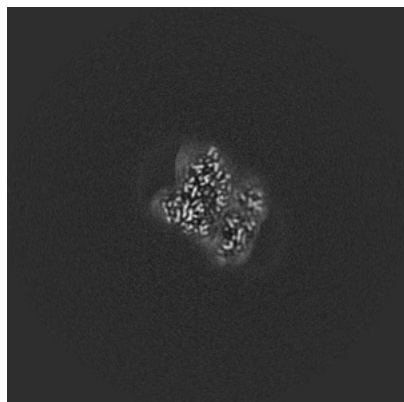


Y Index: 200

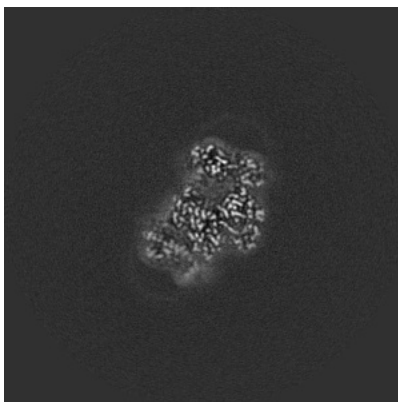


Z Index: 200

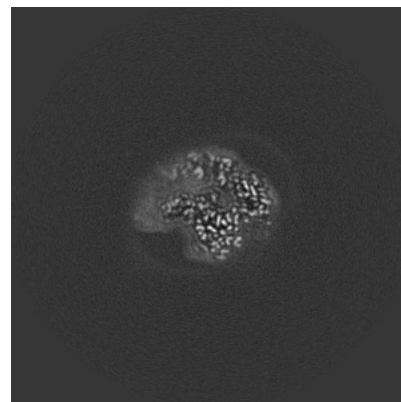
6.2.2 Raw map



X Index: 200



Y Index: 200

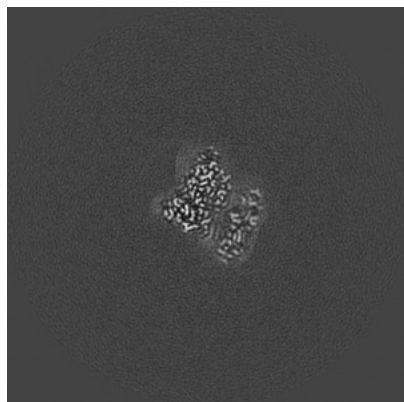


Z Index: 200

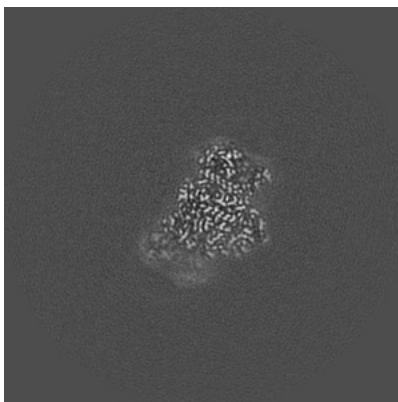
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

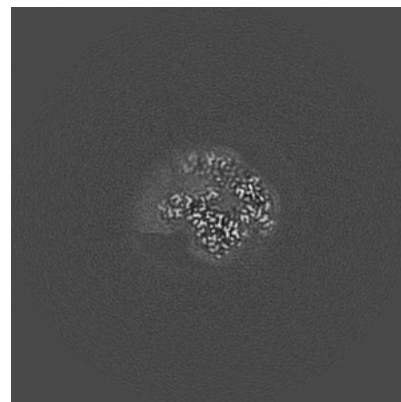
6.3.1 Primary map



X Index: 198

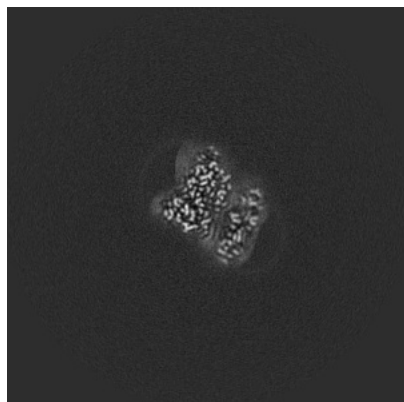


Y Index: 190

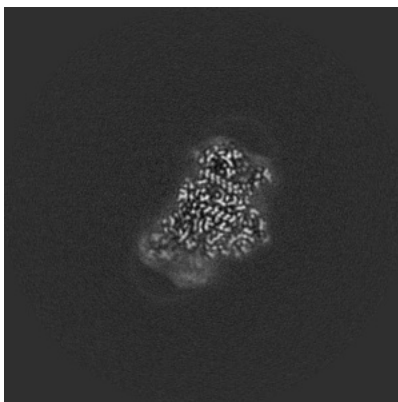


Z Index: 203

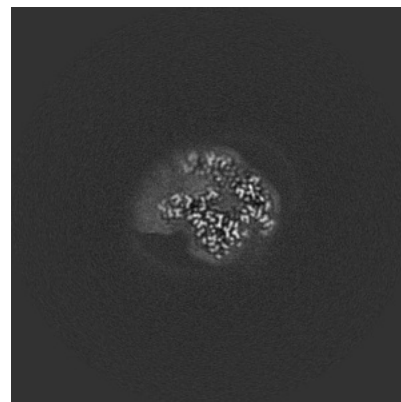
6.3.2 Raw map



X Index: 198



Y Index: 190

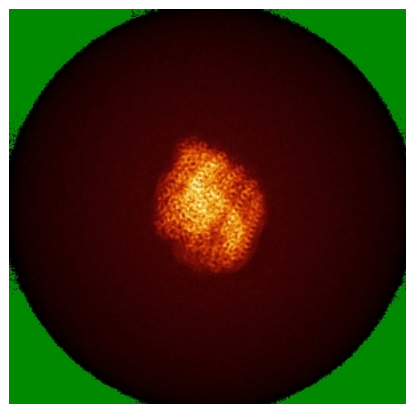


Z Index: 203

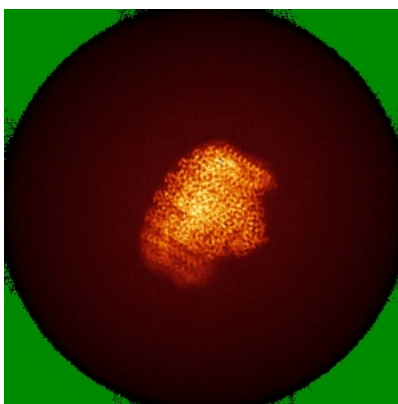
The images above show the largest variance slices of the map in three orthogonal directions.

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

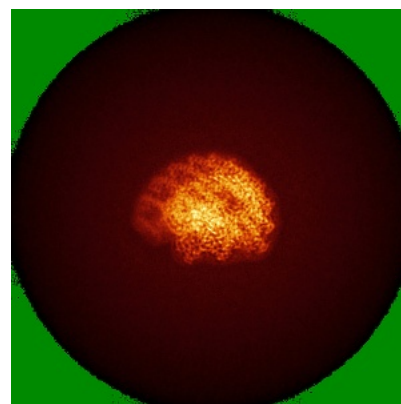
6.4.1 Primary map



X

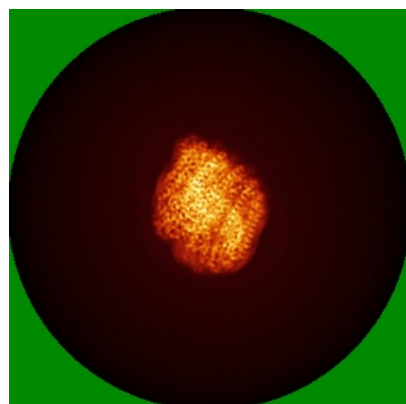


Y

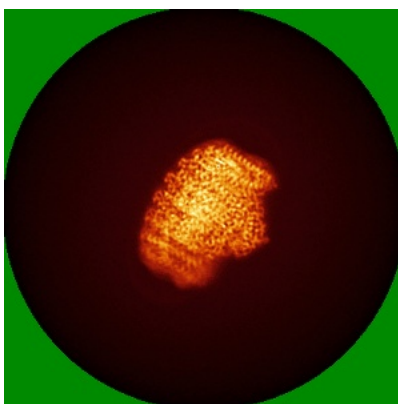


Z

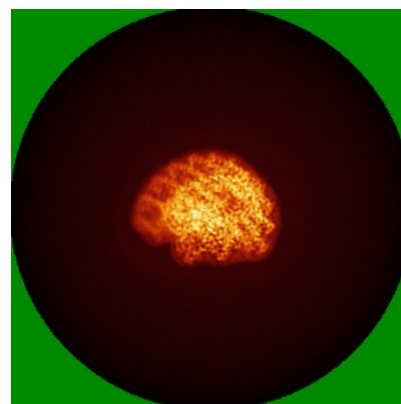
6.4.2 Raw map



X



Y

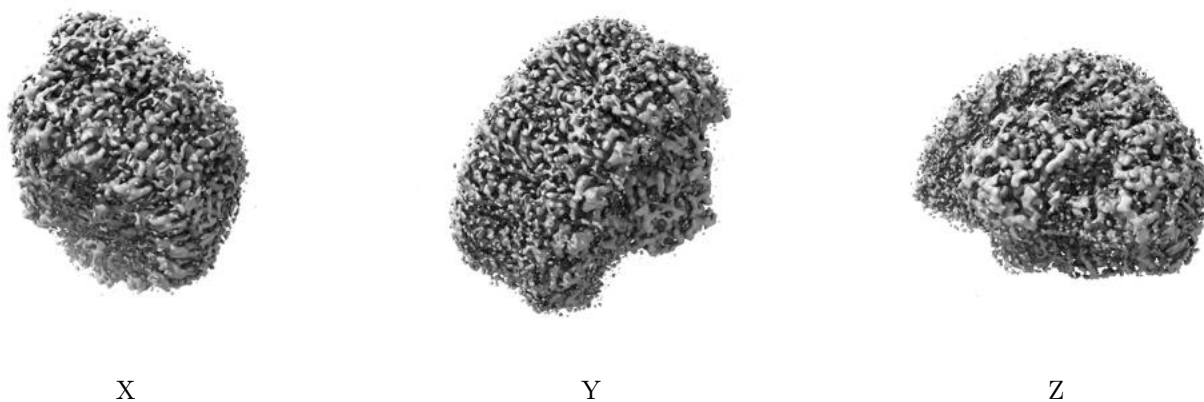


Z

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.

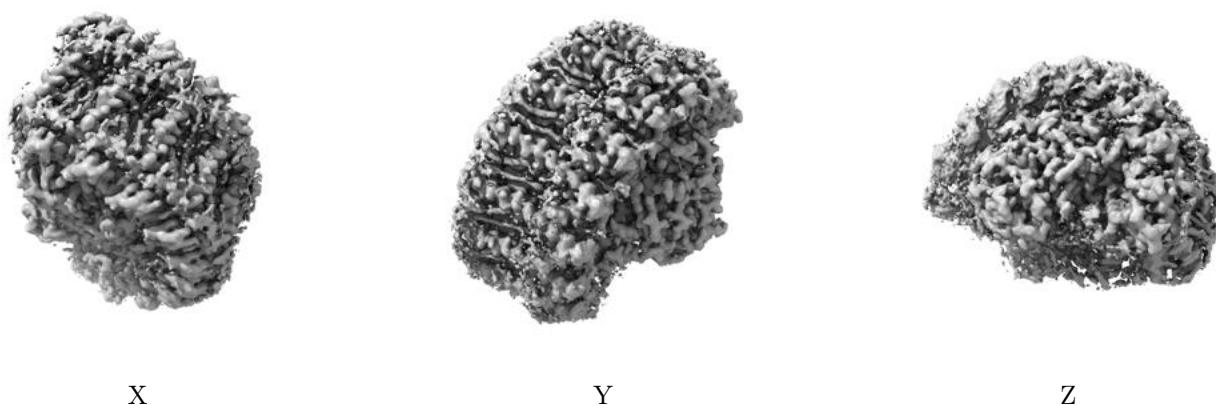
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.019. 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.

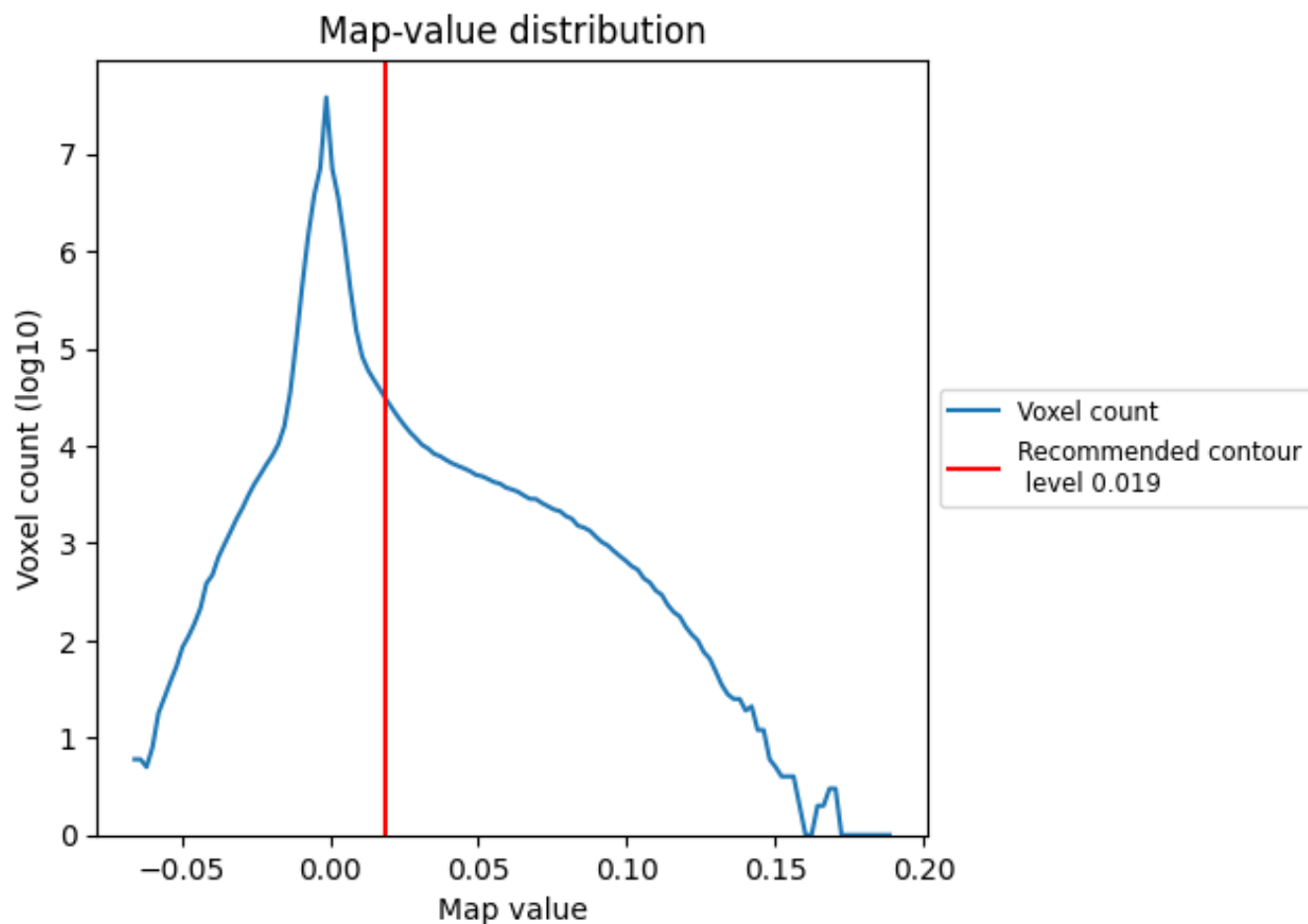
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

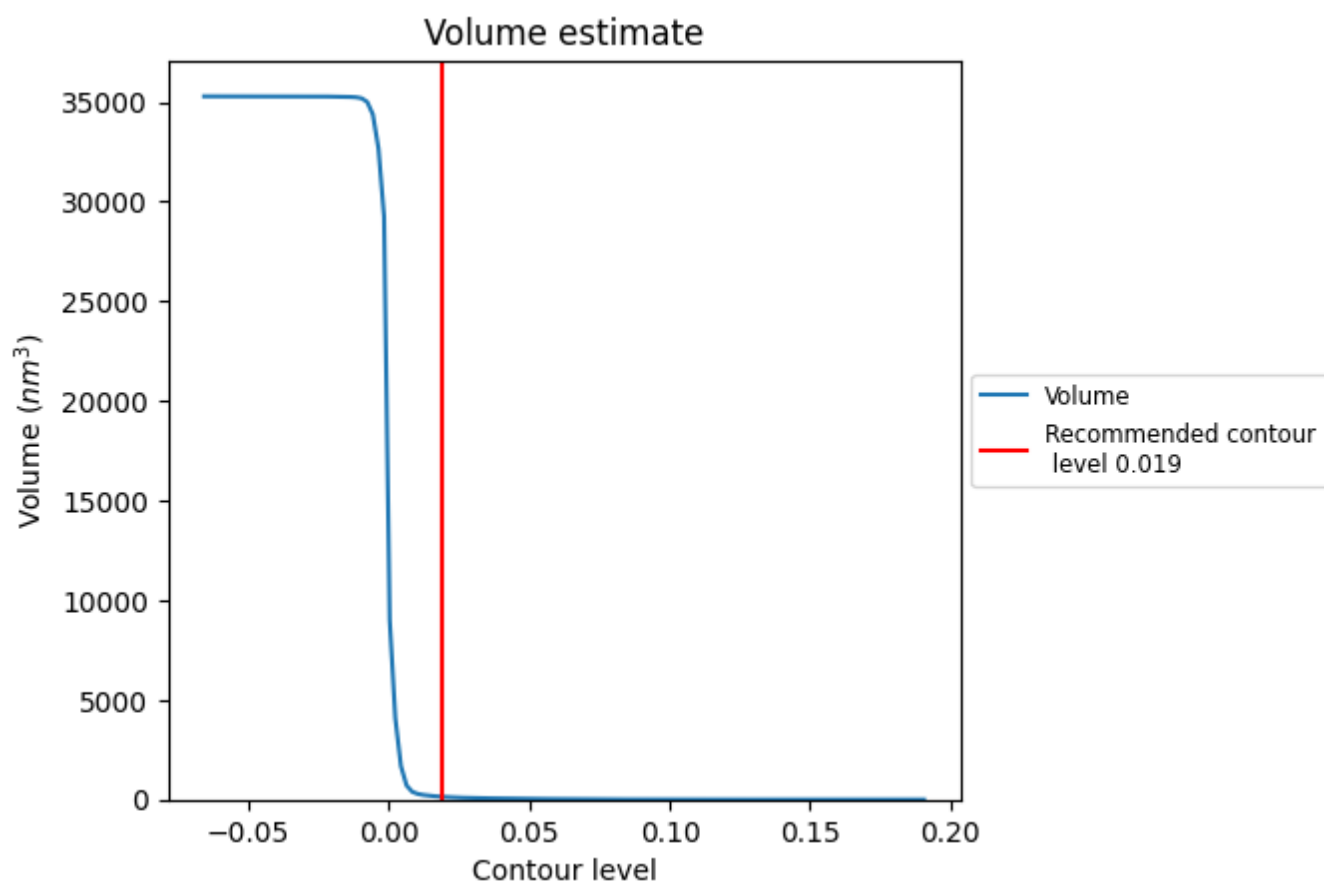
This section contains the results of statistical analysis of the map.

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.

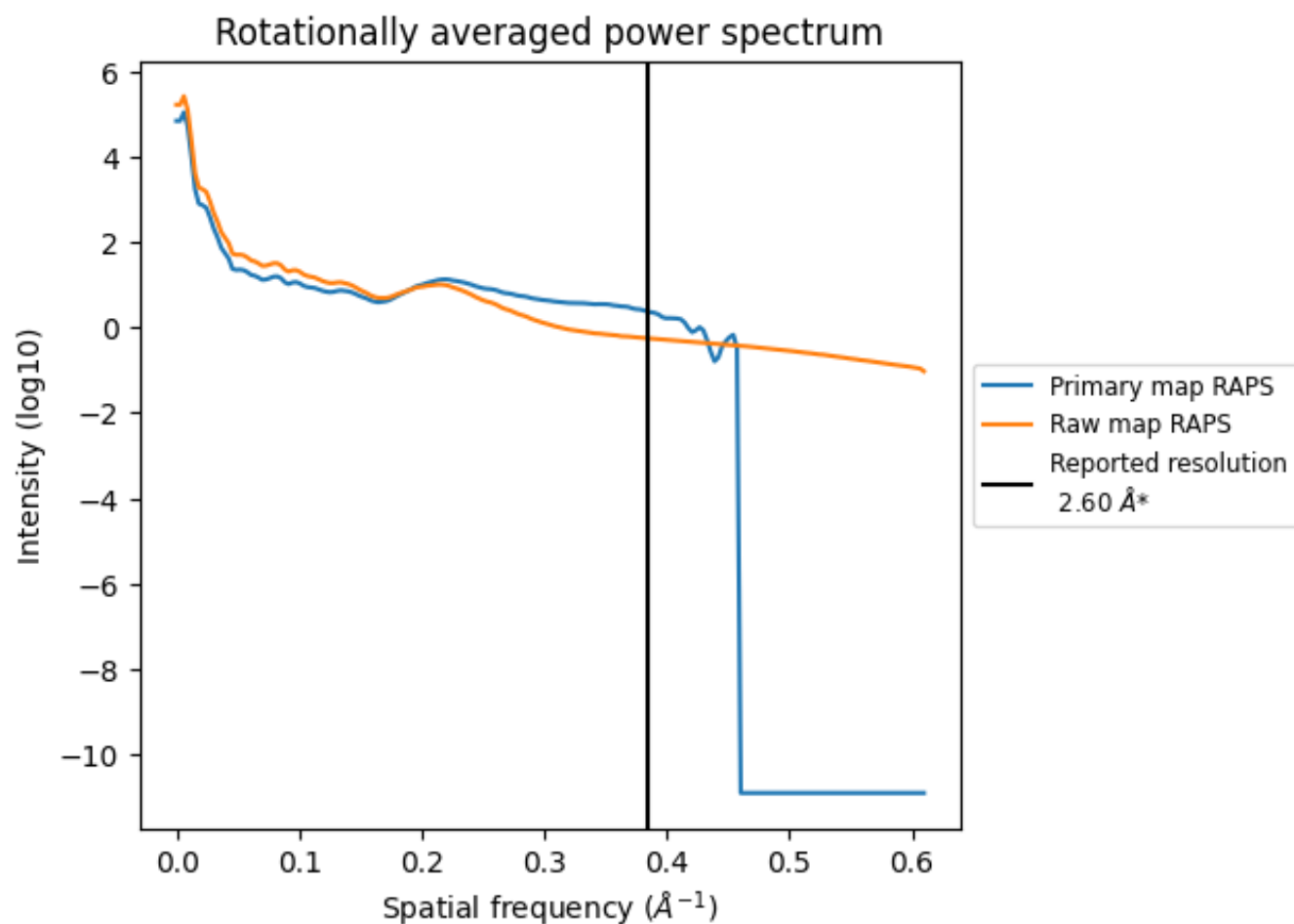
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 139 nm³; this corresponds to an approximate mass of 125 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

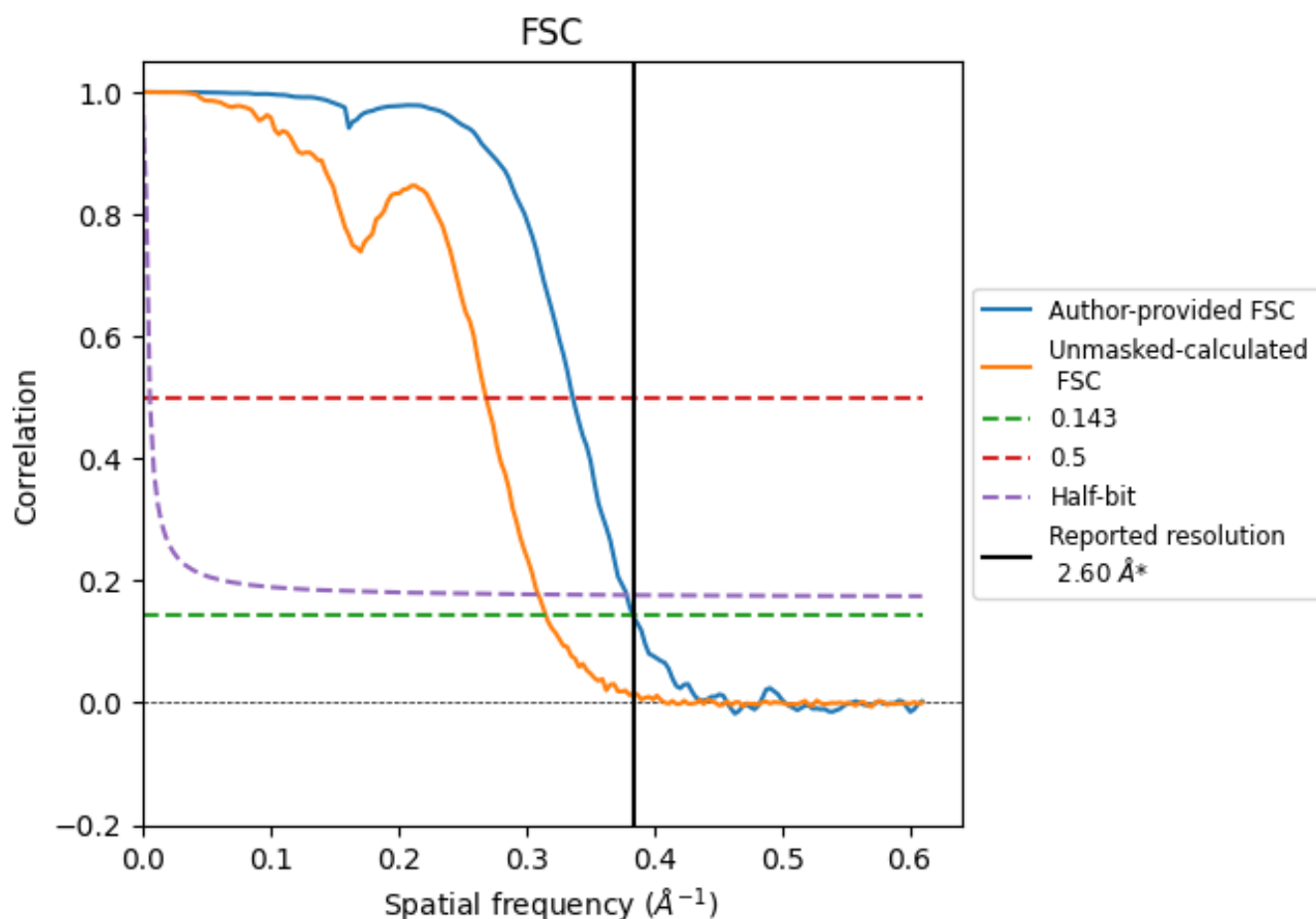


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.385 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

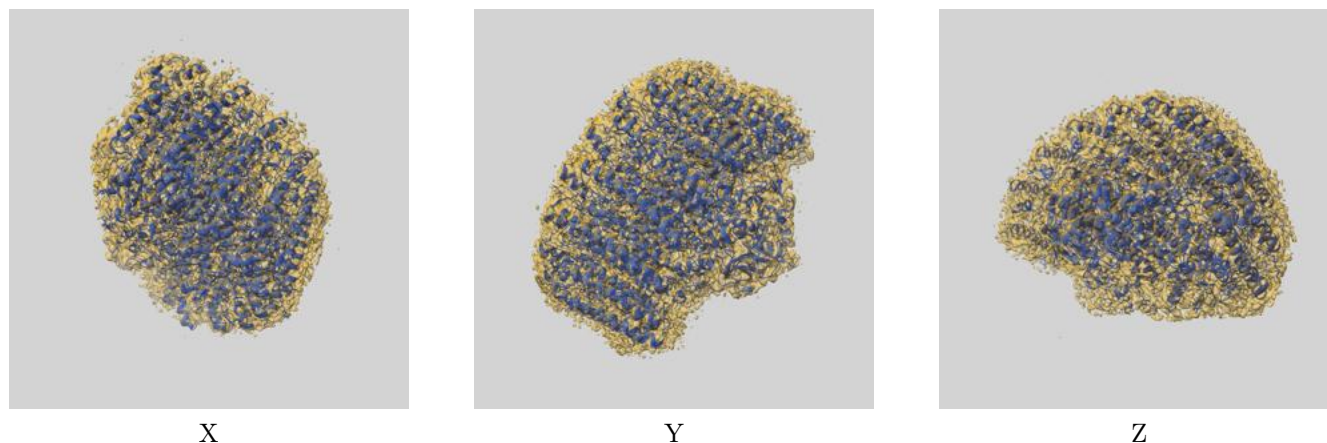
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.61	2.97	2.64
Unmasked-calculated*	3.17	3.72	3.23

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.17 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

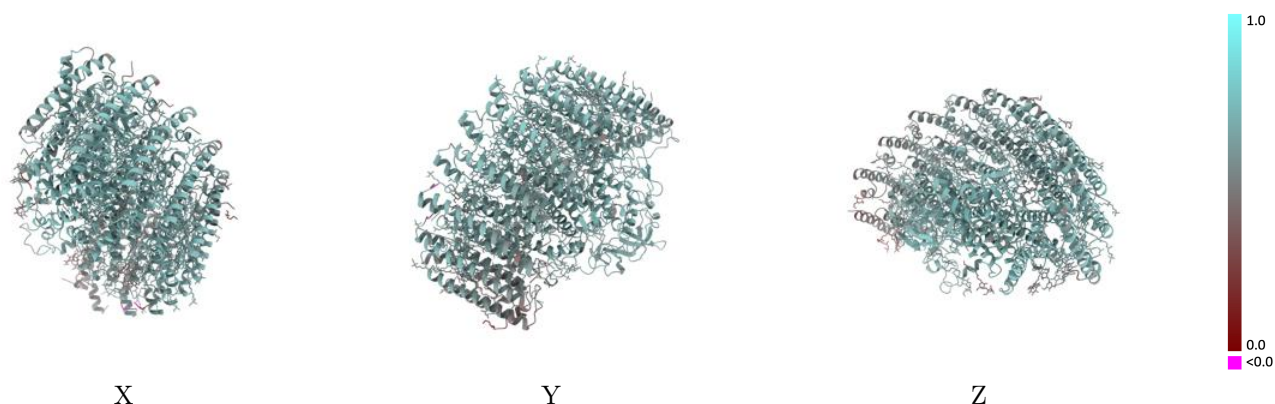
This section contains information regarding the fit between EMDB map EMD-33931 and PDB model 7YML. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



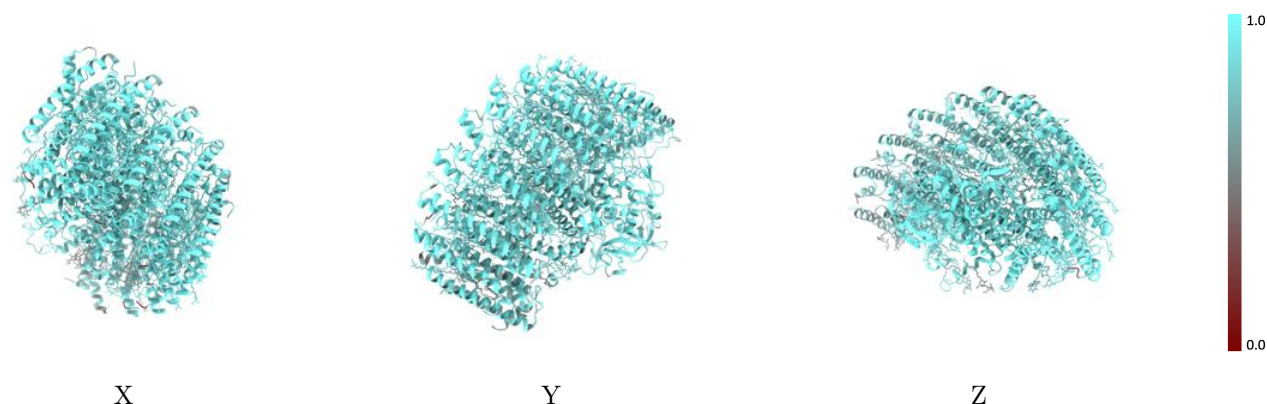
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



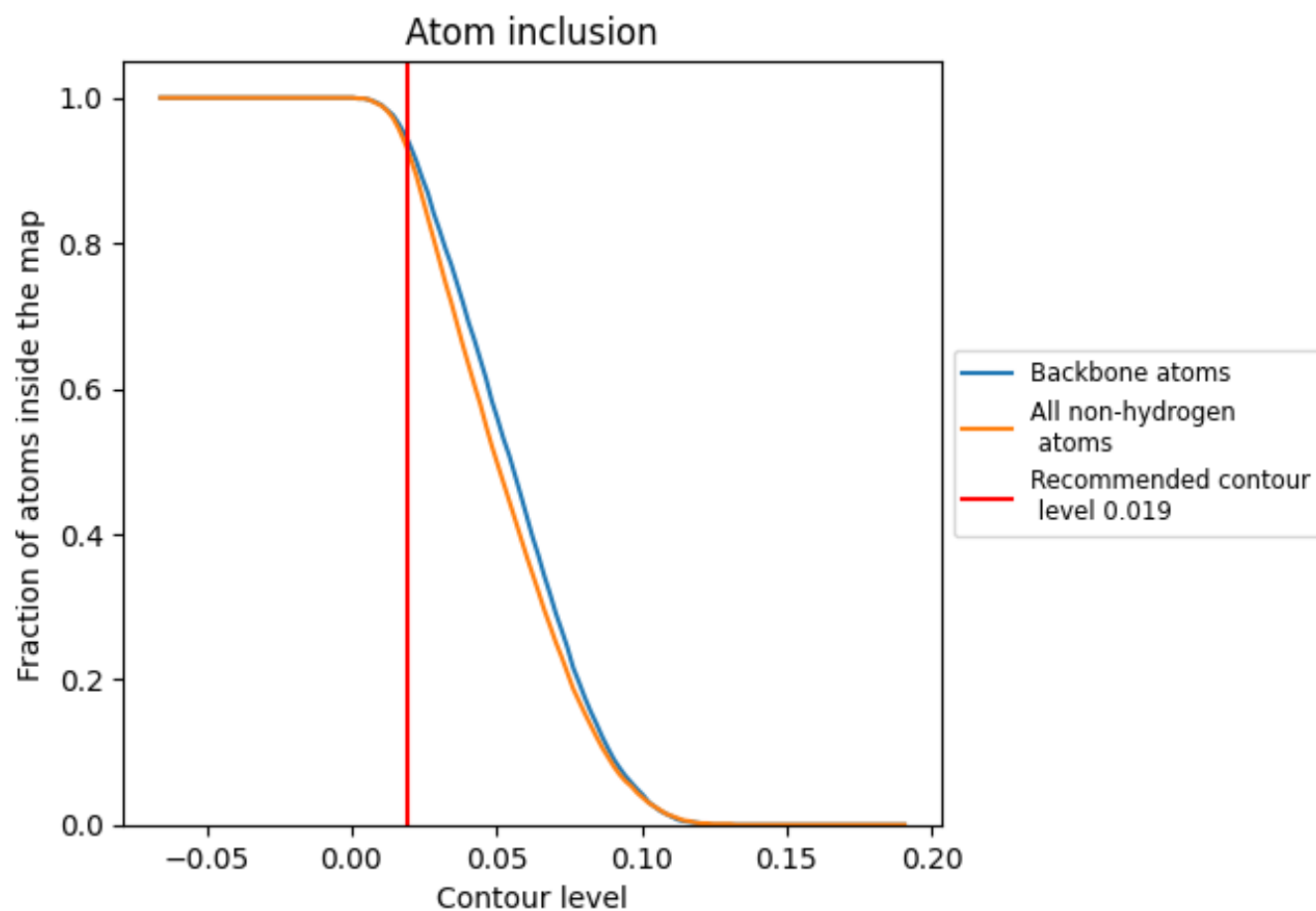
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.9320	 0.6130
A	 0.9610	 0.6030
B	 0.9350	 0.5990
D	 0.9530	 0.6350
E	 0.9480	 0.6210
F	 0.9730	 0.6430
G	 0.9660	 0.6390
H	 0.9480	 0.6270
I	 0.9380	 0.6340
J	 0.9550	 0.6250
K	 0.9650	 0.6230
L	 0.9630	 0.6550
M	 0.9590	 0.6470
N	 0.9310	 0.6180
O	 0.9360	 0.6260
P	 0.9310	 0.6000
Q	 0.8920	 0.5800
R	 0.9190	 0.5840
S	 0.8880	 0.5580
T	 0.9040	 0.5780
V	 0.8530	 0.5280
W	 0.8600	 0.5320
X	 0.9320	 0.6100
Y	 0.7180	 0.4540
Z	 0.6650	 0.3590

