



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 11:35 AM UTC

PDB ID : 7F0L / pdb_00007f0l
EMDB ID : EMD-31400
Title : STRUCTURE OF PHOTOSYNTHETIC LH1-RC SUPER-COMPLEX OF RHODOBACTER SPHAEROIDES MONOMER
Authors : Tani, K.; Nagashima, V.P.; Kanno, R.; Kawamura, S.; Kikuchi, R.; Ji, X.-C.; Hall, M.; Yu, L.-J.; Kimura, Y.; Madigan, M.T.; Mizoguchi, A.; Humbel, B.M.; Wang-Otomo, Z.-Y.
Deposited on : 2021-06-05
Resolution : 2.94 Å(reported)
Based on initial model : 5Y5S

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)

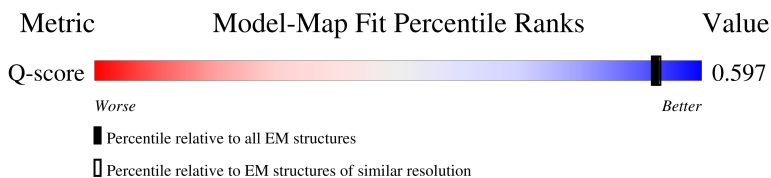
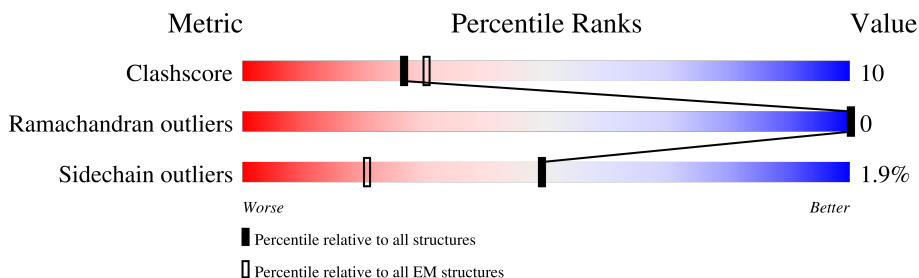
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.94 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	13068 (2.44 - 3.44)

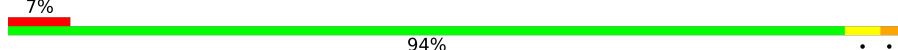
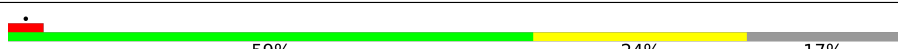
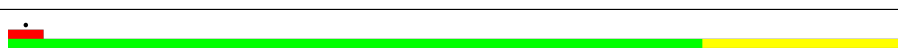
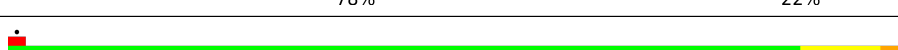
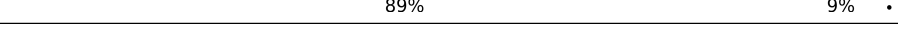
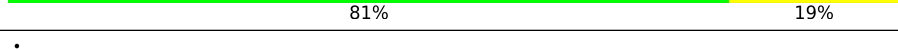
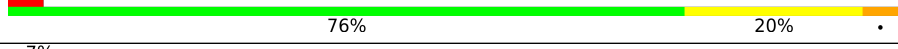
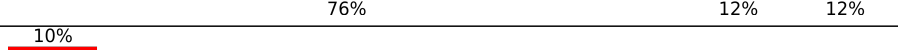
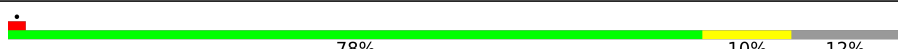
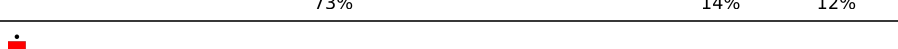
The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment 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	308	
3	H	260	

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Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
4	1	54	
4	3	54	
4	A	54	
4	D	54	
4	F	54	
4	I	54	
4	K	54	
4	O	54	
4	Q	54	
4	S	54	
4	V	54	
4	Y	54	
5	2	49	
5	4	49	
5	6	49	
5	8	49	
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	

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Mol	Chain	Length	Quality of chain
5	Z	49	12% 78% 8% • 12%
6	5	54	6% 80% 19% •
6	7	54	26% 80% 15% 6%
7	X	82	• 51% 13% 35%
8	U	53	9% 83% 11% 6%

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 23458 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 Photosynthetic reaction center L subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	281	Total	C	N	O	S	0	0
			2233	1508	355	362	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	306	Total	C	N	O	S	0	0
			2437	1627	398	401	11		

- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	246	Total	C	N	O	S	0	0
			1864	1197	314	343	10		

- Molecule 4 is a protein called Light-harvesting protein B-875 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	45	Total	C	N	O	S	0	0
			386	266	59	58	3		
4	D	54	Total	C	N	O	S	0	0
			455	309	73	70	3		
4	F	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	I	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	K	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	O	54	Total	C	N	O	S	0	0
			453	308	72	70	3		
4	Q	54	Total	C	N	O	S	0	0
			457	311	73	70	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	54	Total	C	N	O	S	0	0
			454	309	73	70	2		
4	V	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	Y	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	1	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	3	54	Total	C	N	O	S	0	0
			457	311	73	70	3		

- Molecule 5 is a protein called Antenna pigment protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	E	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	G	45	Total	C	N	O	S	0	0
			365	243	57	64	1		
5	J	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	N	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	P	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	R	43	Total	C	N	O	S	0	0
			347	234	55	57	1		
5	T	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	W	43	Total	C	N	O	S	0	0
			347	234	55	57	1		
5	Z	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	2	42	Total	C	N	O	S	0	0
			343	230	54	58	1		
5	4	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	6	42	Total	C	N	O	S	0	0
			332	222	54	55	1		
5	8	38	Total	C	N	O	S	0	0
			296	202	49	44	1		

- Molecule 6 is a protein called Light-harvesting protein B-875 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	53	Total	C	N	O	S	0	0
			447	305	72	68	2		
6	7	51	Total	C	N	O	S	0	0
			415	281	68	64	2		

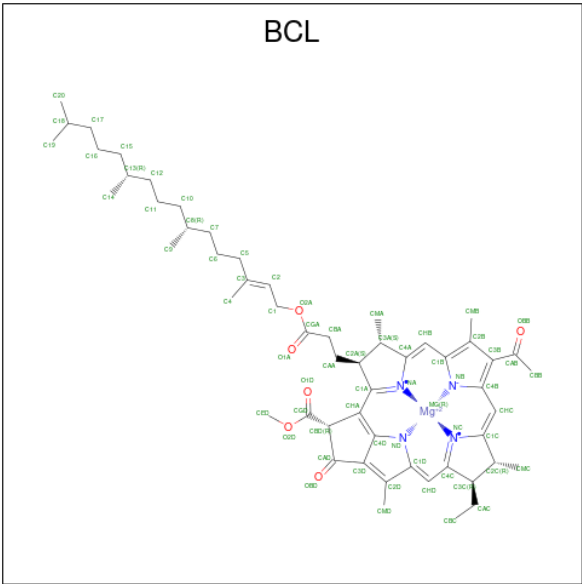
- Molecule 7 is a protein called PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	X	53	Total	C	N	O	S	0	0
			405	269	69	64	3		

- Molecule 8 is a protein called protein-U.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	50	Total	C	N	O	S	0	0
			369	252	57	57	3		

- Molecule 9 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



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

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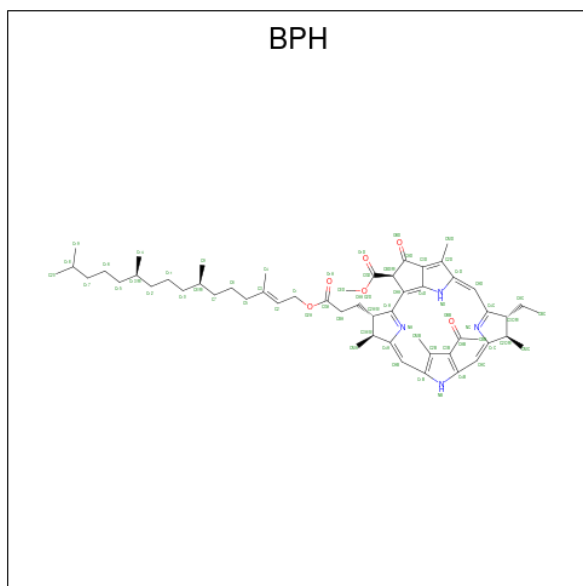
Mol	Chain	Residues	Atoms					AltConf
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	A	1	Total 61	C 50	Mg 1	N 4	O 6	0
9	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0

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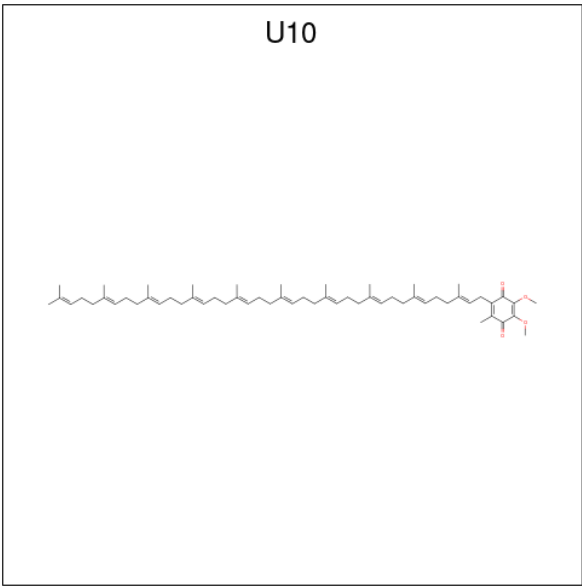
Mol	Chain	Residues	Atoms					AltConf
9	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	8	1	Total	C	Mg	N	O	0
			60	49	1	4	6	

- Molecule 10 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



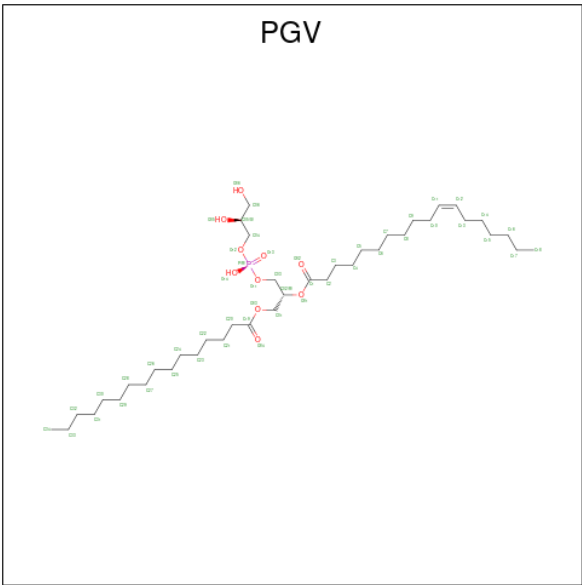
Mol	Chain	Residues	Atoms				AltConf
10	L	1	Total	C	N	O	0
			65	55	4	6	
10	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 11 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).



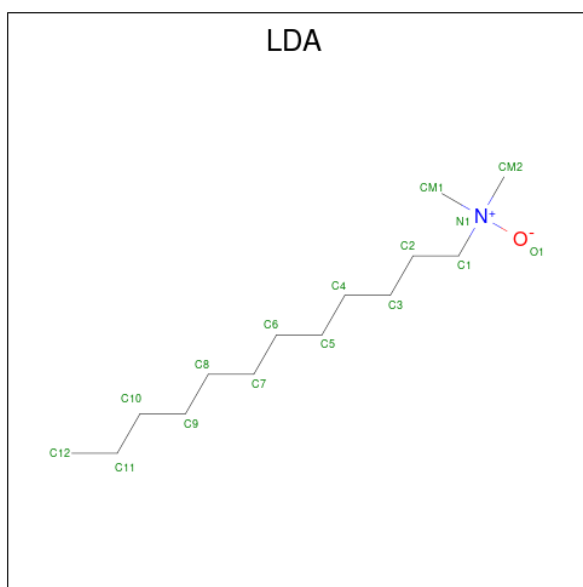
Mol	Chain	Residues	Atoms			AltConf
11	L	1	Total	C	O	0
			35	31	4	
11	L	1	Total	C	O	0
			35	31	4	
11	M	1	Total	C	O	0
			48	44	4	

- Molecule 12 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
12	L	1	Total	C	O	P	0
			39	28	10	1	
12	L	1	Total	C	O	P	0
			33	22	10	1	
12	L	1	Total	C	O	P	0
			45	36	8	1	
12	M	1	Total	C	O	P	0
			47	36	10	1	
12	M	1	Total	C	O	P	0
			38	27	10	1	
12	H	1	Total	C	O	P	0
			34	25	8	1	
12	H	1	Total	C	O	P	0
			40	29	10	1	
12	H	1	Total	C	O	P	0
			47	36	10	1	
12	K	1	Total	C	O	P	0
			41	34	6	1	
12	Q	1	Total	C	O	P	0
			39	28	10	1	
12	Y	1	Total	C	O	P	0
			43	32	10	1	
12	3	1	Total	C	O	P	0
			51	40	10	1	
12	X	1	Total	C	O	P	0
			39	28	10	1	

- Molecule 13 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).

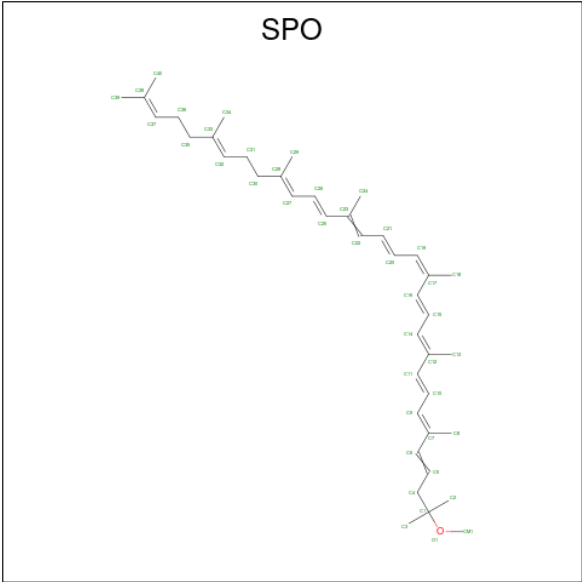


Mol	Chain	Residues	Atoms				AltConf
13	L	1	Total	C	N	O	0
			16	14	1	1	
13	L	1	Total	C	N	O	0
			16	14	1	1	
13	M	1	Total	C	N	O	0
			16	14	1	1	
13	Y	1	Total	C	N	O	0
			12	10	1	1	
13	X	1	Total	C	N	O	0
			13	11	1	1	
13	X	1	Total	C	N	O	0
			16	14	1	1	

- 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) (labeled as "Ligand of Interest" by depositor).



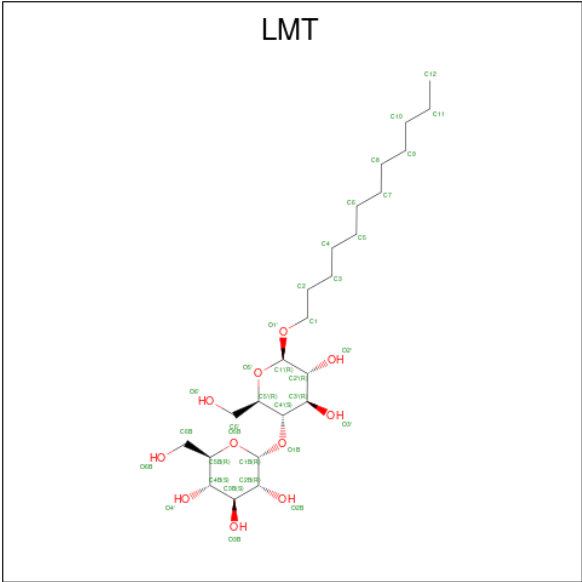
Mol	Chain	Residues	Atoms			AltConf
15	M	1	Total	C	O	0
			42	41	1	
15	D	1	Total	C	O	0
			42	41	1	
15	E	1	Total	C	O	0
			42	41	1	
15	F	1	Total	C	O	0
			42	41	1	
15	F	1	Total	C	O	0
			42	41	1	
15	G	1	Total	C	O	0
			42	41	1	
15	G	1	Total	C	O	0
			42	41	1	
15	K	1	Total	C	O	0
			42	41	1	
15	N	1	Total	C	O	0
			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	
15	S	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	T	1	Total	C	O	0
			42	41	1	
15	V	1	Total	C	O	0
			42	41	1	
15	V	1	Total	C	O	0
			42	41	1	
15	W	1	Total	C	O	0
			42	41	1	
15	1	1	Total	C	O	0
			42	41	1	
15	1	1	Total	C	O	0
			42	41	1	
15	1	1	Total	C	O	0
			42	41	1	
15	3	1	Total	C	O	0
			42	41	1	
15	5	1	Total	C	O	0
			42	41	1	
15	5	1	Total	C	O	0
			42	41	1	
15	8	1	Total	C	O	0
			42	41	1	
15	X	1	Total	C	O	0
			42	41	1	

- Molecule 16 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



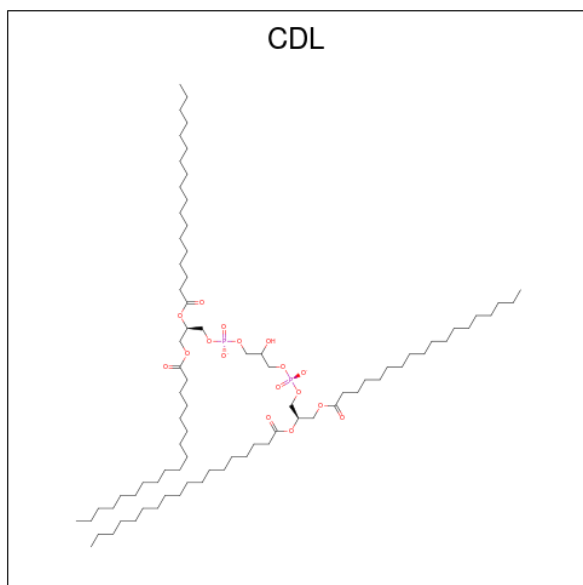
Mol	Chain	Residues	Atoms			AltConf
16	M	1	Total	C	O	0
			27	20	7	
16	M	1	Total	C	O	0
			35	24	11	
16	M	1	Total	C	O	0
			33	22	11	
16	H	1	Total	C	O	0
			35	24	11	
16	H	1	Total	C	O	0
			30	19	11	
16	A	1	Total	C	O	0
			35	24	11	
16	A	1	Total	C	O	0
			35	24	11	
16	A	1	Total	C	O	0
			27	16	11	
16	D	1	Total	C	O	0
			27	16	11	
16	F	1	Total	C	O	0
			26	16	10	
16	F	1	Total	C	O	0
			17	11	6	
16	I	1	Total	C	O	0
			27	16	11	
16	K	1	Total	C	O	0
			35	24	11	
16	Q	1	Total	C	O	0
			24	18	6	

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Mol	Chain	Residues	Atoms			AltConf
16	Q	1	Total	C	O	0
			19	13	6	
16	S	1	Total	C	O	0
			25	19	6	
16	S	1	Total	C	O	0
			30	19	11	
16	1	1	Total	C	O	0
			24	15	9	
16	3	1	Total	C	O	0
			35	24	11	
16	4	1	Total	C	O	0
			27	16	11	
16	5	1	Total	C	O	0
			33	22	11	
16	X	1	Total	C	O	0
			31	20	11	
16	U	1	Total	C	O	0
			32	21	11	
16	U	1	Total	C	O	0
			35	24	11	

- Molecule 17 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
17	M	1	Total	C	O	P	0
			79	60	17	2	

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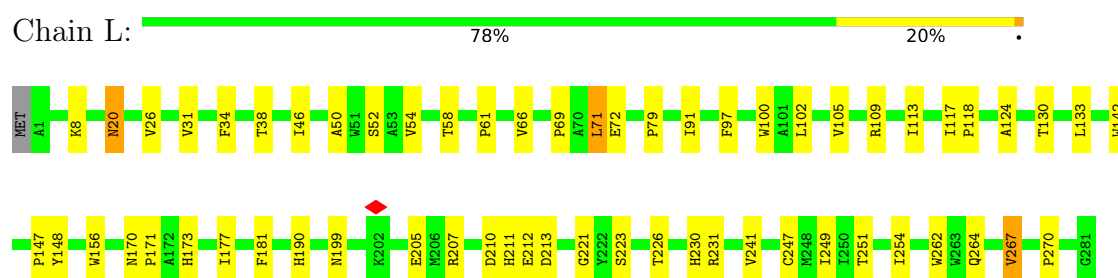
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Mol	Chain	Residues	Atoms				AltConf
17	H	1	Total	C	O	P	0
			61	42	17	2	
17	H	1	Total	C	O	P	0
			37	20	15	2	
17	Y	1	Total	C	O	P	0
			48	30	16	2	

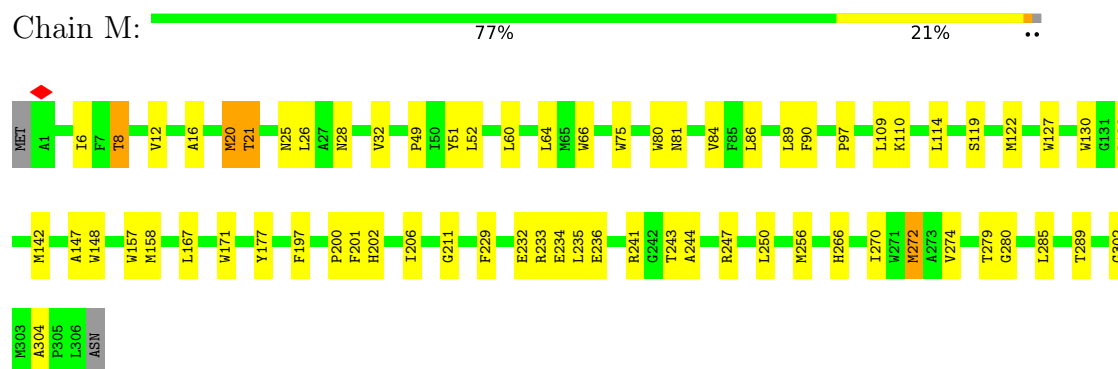
3 Residue-property plots [i](#)

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

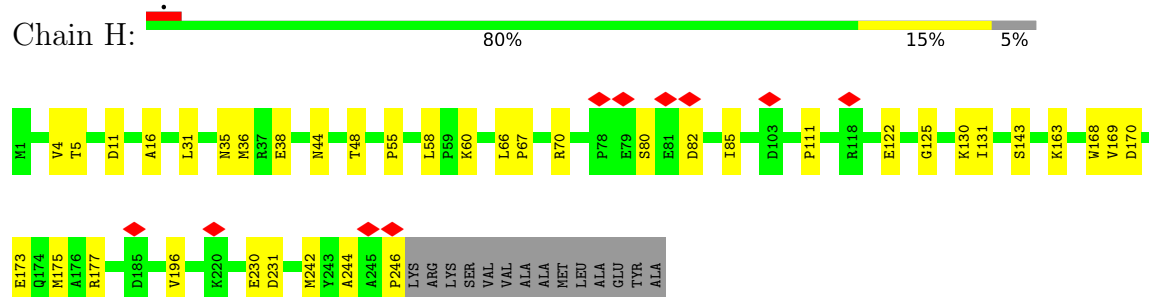
- Molecule 1: Photosynthetic reaction center L subunit



- Molecule 2: Reaction center protein M chain



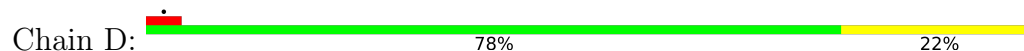
- Molecule 3: Reaction center protein H chain



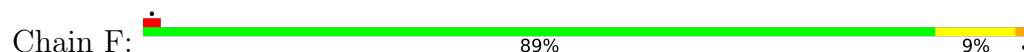
- Molecule 4: Light-harvesting protein B-875 alpha chain



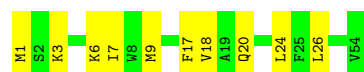
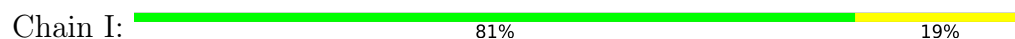
- Molecule 4: Light-harvesting protein B-875 alpha chain



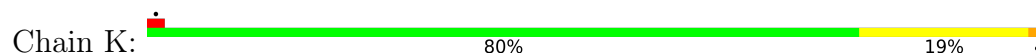
- Molecule 4: Light-harvesting protein B-875 alpha chain



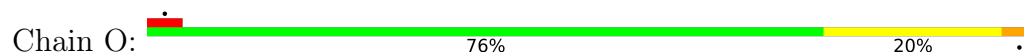
- Molecule 4: Light-harvesting protein B-875 alpha chain



- Molecule 4: Light-harvesting protein B-875 alpha chain



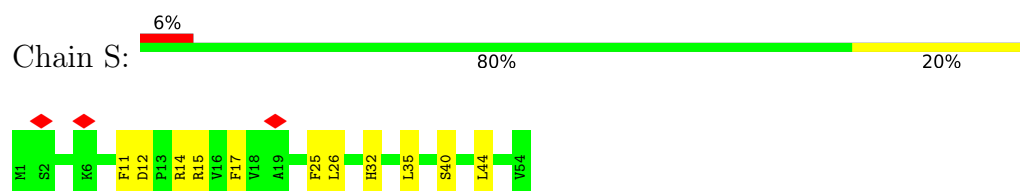
- Molecule 4: Light-harvesting protein B-875 alpha chain



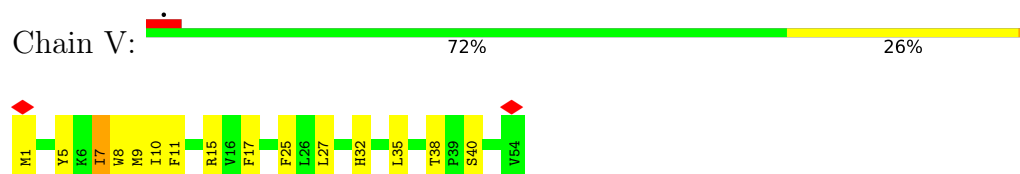
- Molecule 4: Light-harvesting protein B-875 alpha chain



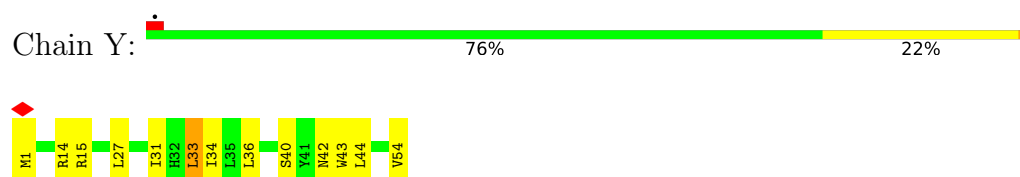
- Molecule 4: Light-harvesting protein B-875 alpha chain



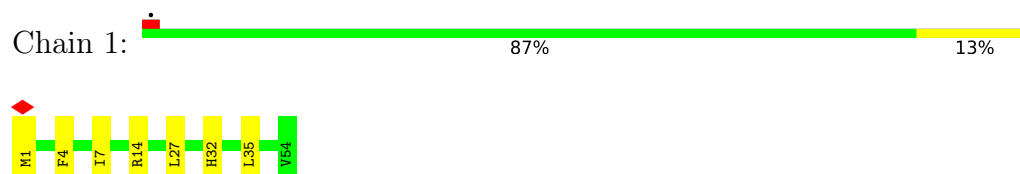
- Molecule 4: Light-harvesting protein B-875 alpha chain



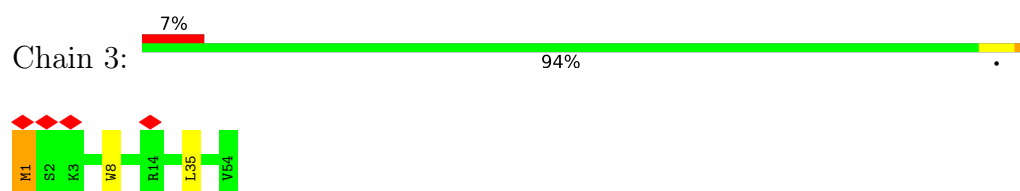
- Molecule 4: Light-harvesting protein B-875 alpha chain



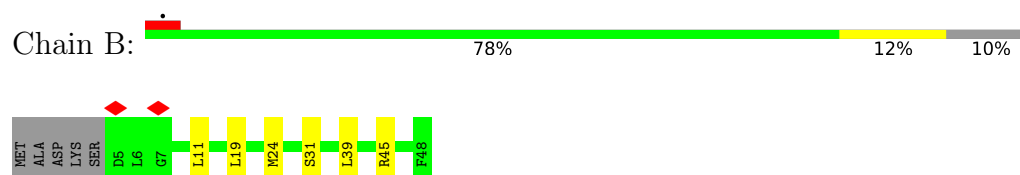
- Molecule 4: Light-harvesting protein B-875 alpha chain



- Molecule 4: Light-harvesting protein B-875 alpha chain

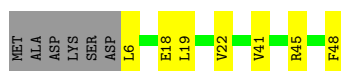


- Molecule 5: Antenna pigment protein beta chain

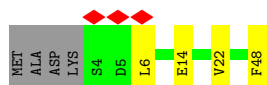
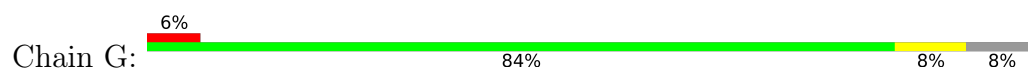


- Molecule 5: Antenna pigment protein beta chain

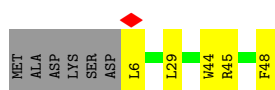
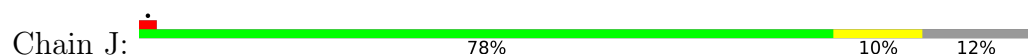




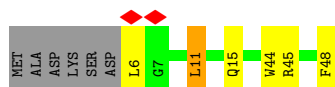
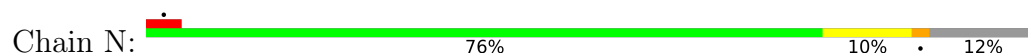
- Molecule 5: Antenna pigment protein beta chain



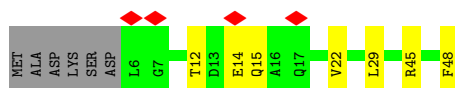
- Molecule 5: Antenna pigment protein beta chain



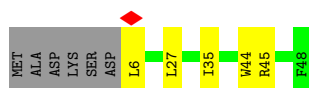
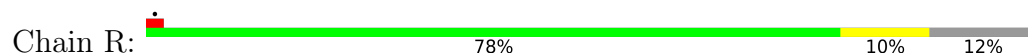
- Molecule 5: Antenna pigment protein beta chain



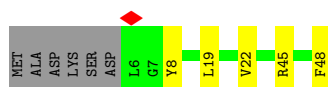
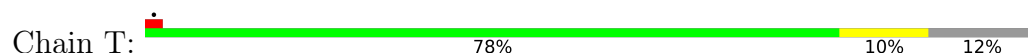
- Molecule 5: Antenna pigment protein beta chain



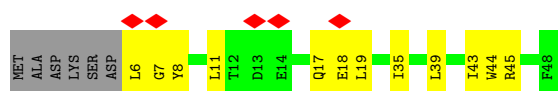
- Molecule 5: Antenna pigment protein beta chain



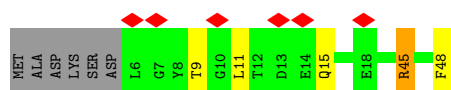
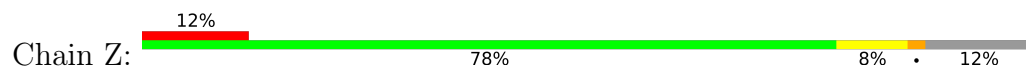
- Molecule 5: Antenna pigment protein beta chain



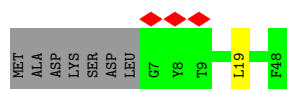
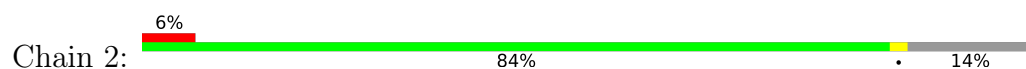
- Molecule 5: Antenna pigment protein beta chain



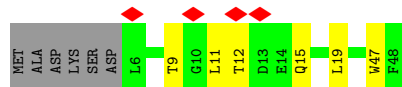
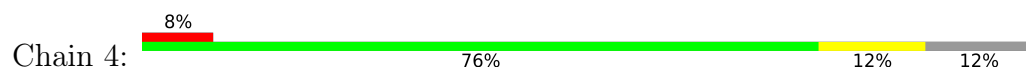
- Molecule 5: Antenna pigment protein beta chain



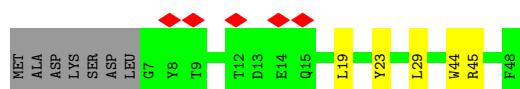
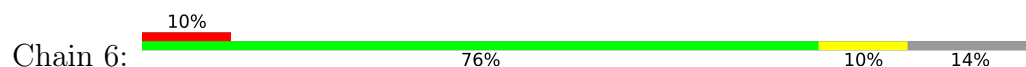
- Molecule 5: Antenna pigment protein beta chain



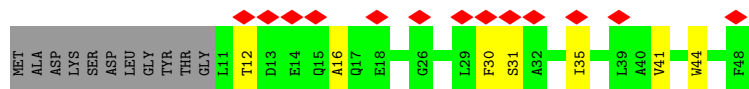
- Molecule 5: Antenna pigment protein beta chain



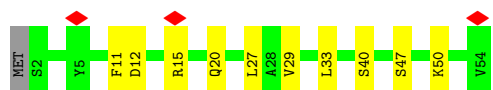
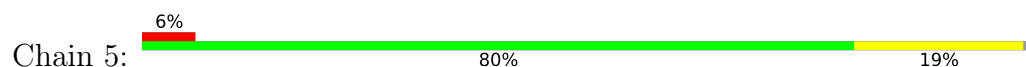
- Molecule 5: Antenna pigment protein beta chain



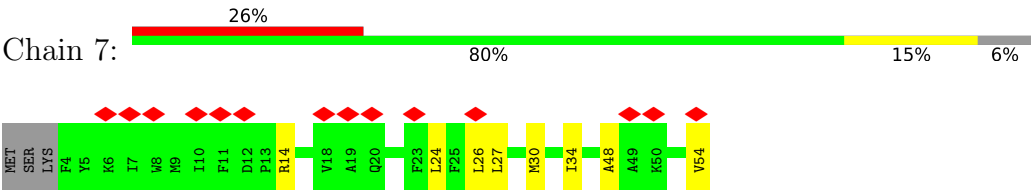
- Molecule 5: Antenna pigment protein beta chain



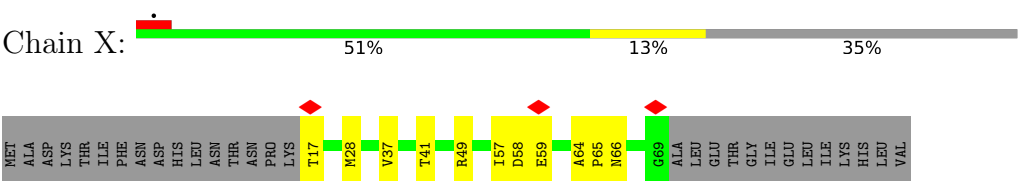
- Molecule 6: Light-harvesting protein B-875 alpha chain



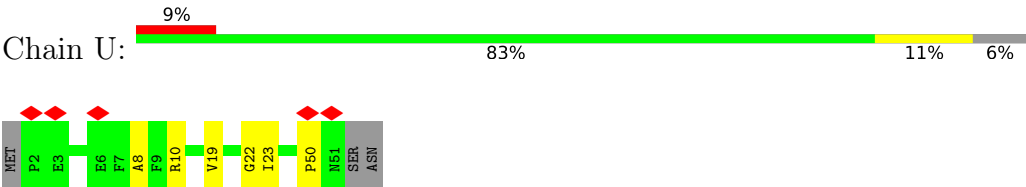
• Molecule 6: Light-harvesting protein B-875 alpha chain



• Molecule 7: PufX



• Molecule 8: protein-U



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	160448	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.466	Depositor
Minimum map value	-0.288	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.064	Depositor
Map size ($\text{\AA}$)	306.32, 306.32, 306.32	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.094, 1.094, 1.094	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.24	0/2321	0.29	0/3177
2	M	0.24	0/2530	0.31	0/3455
3	H	0.19	0/1914	0.29	0/2607
4	1	0.19	0/461	0.26	0/625
4	3	0.17	0/461	0.23	0/625
4	A	0.19	0/389	0.24	0/528
4	D	0.19	0/459	0.27	0/622
4	F	0.21	0/461	0.25	0/625
4	I	0.21	0/461	0.26	0/625
4	K	0.20	0/461	0.25	0/625
4	O	0.21	0/457	0.26	0/621
4	Q	0.20	0/461	0.27	0/625
4	S	0.19	0/461	0.25	0/625
4	V	0.20	0/461	0.25	0/625
4	Y	0.20	0/461	0.25	0/625
5	2	0.16	0/356	0.23	0/488
5	4	0.16	0/364	0.30	0/499
5	6	0.12	0/344	0.22	0/472
5	8	0.11	0/308	0.21	0/424
5	B	0.18	0/372	0.26	0/510
5	E	0.20	0/364	0.23	0/499
5	G	0.18	0/378	0.24	0/518
5	J	0.17	0/364	0.24	0/499
5	N	0.17	0/364	0.21	0/499
5	P	0.17	0/364	0.27	0/499
5	R	0.18	0/360	0.25	0/494
5	T	0.17	0/364	0.22	0/499
5	W	0.17	0/360	0.22	0/494
5	Z	0.16	0/364	0.21	0/499
6	5	0.16	0/461	0.24	0/625
6	7	0.12	0/427	0.24	0/582
7	X	0.16	0/417	0.27	0/566

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	U	0.14	0/381	0.25	0/516
All	All	0.20	0/18931	0.26	0/25817

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2233	0	2189	47	0
2	M	2437	0	2355	56	0
3	H	1864	0	1862	26	0
4	1	457	0	476	7	0
4	3	457	0	476	3	0
4	A	386	0	400	15	0
4	D	455	0	469	10	0
4	F	457	0	476	6	0
4	I	457	0	476	10	0
4	K	457	0	476	9	0
4	O	453	0	465	14	0
4	Q	457	0	476	16	0
4	S	454	0	469	12	0
4	V	457	0	476	16	0
4	Y	457	0	476	13	0
5	2	343	0	325	1	0
5	4	351	0	336	5	0
5	6	332	0	314	5	0
5	8	296	0	273	6	0
5	B	359	0	340	5	0
5	E	351	0	336	8	0
5	G	365	0	345	4	0
5	J	351	0	336	9	0
5	N	351	0	336	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	351	0	336	7	0
5	R	347	0	332	5	0
5	T	351	0	336	5	0
5	W	347	0	332	11	0
5	Z	351	0	336	5	0
6	5	447	0	465	11	0
6	7	415	0	422	6	0
7	X	405	0	412	8	0
8	U	369	0	366	7	0
9	1	66	0	74	4	0
9	2	66	0	74	4	0
9	3	66	0	74	3	0
9	4	66	0	74	3	0
9	5	66	0	74	6	0
9	6	66	0	74	3	0
9	7	66	0	74	6	0
9	8	60	0	58	6	0
9	A	61	0	61	2	0
9	B	66	0	74	8	0
9	D	66	0	74	4	0
9	E	66	0	74	6	0
9	F	66	0	74	2	0
9	G	66	0	74	2	0
9	I	66	0	74	6	0
9	J	66	0	74	3	0
9	K	66	0	74	5	0
9	L	198	0	222	14	0
9	M	66	0	74	3	0
9	N	66	0	74	1	0
9	O	66	0	74	4	0
9	P	66	0	74	2	0
9	Q	66	0	74	1	0
9	R	66	0	74	3	0
9	S	66	0	74	4	0
9	T	66	0	74	5	0
9	V	66	0	74	7	0
9	W	66	0	74	6	0
9	Y	66	0	74	6	0
9	Z	66	0	74	2	0
10	L	65	0	76	5	0
10	M	65	0	76	6	0
11	L	70	0	86	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	M	48	0	63	2	0
12	3	51	0	76	1	0
12	H	121	0	149	6	0
12	K	41	0	60	3	0
12	L	117	0	147	8	0
12	M	85	0	110	6	0
12	Q	39	0	48	1	0
12	X	39	0	48	3	0
12	Y	43	0	54	7	0
13	L	32	0	62	2	0
13	M	16	0	31	0	0
13	X	29	0	53	3	0
13	Y	12	0	20	5	0
14	M	1	0	0	0	0
15	1	126	0	180	14	0
15	3	42	0	60	2	0
15	5	84	0	120	11	0
15	8	42	0	60	5	0
15	D	42	0	60	3	0
15	E	42	0	60	3	0
15	F	84	0	120	6	0
15	G	84	0	120	15	0
15	K	42	0	60	6	0
15	M	42	0	60	4	0
15	N	42	0	60	8	0
15	O	84	0	120	12	0
15	P	42	0	60	2	0
15	R	42	0	60	6	0
15	S	84	0	120	11	0
15	T	42	0	60	10	0
15	V	84	0	120	8	0
15	W	42	0	60	4	0
15	X	42	0	60	4	0
16	1	24	0	21	0	0
16	3	35	0	46	4	0
16	4	27	0	27	0	0
16	5	33	0	39	2	0
16	A	97	0	119	7	0
16	D	27	0	27	0	0
16	F	43	0	40	0	0
16	H	65	0	79	5	0
16	I	27	0	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	K	35	0	46	2	0
16	M	95	0	121	6	0
16	Q	43	0	55	4	0
16	S	55	0	68	2	0
16	U	67	0	83	2	0
16	X	31	0	35	0	0
17	H	98	0	92	6	0
17	M	79	0	105	6	0
17	Y	48	0	46	2	0
All	All	23458	0	24489	480	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 10.

All (480) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:231:ARG:HH12	2:M:8:THR:HG22	1.49	0.77
16:H:302:LMT:H5'	4:O:38:THR:HG22	1.65	0.76
2:M:75:TRP:HE1	15:M:807:SPO:HM12	1.50	0.76
2:M:247:ARG:NH2	3:H:111:PRO:O	2.20	0.74
4:A:40:SER:O	5:B:45:ARG:NH1	2.21	0.74
5:R:35:ILE:HG12	9:R:102:BCL:H92	1.69	0.73
4:Q:7:ILE:HB	15:S:103:SPO:H343	1.69	0.73
5:N:6:LEU:HD13	5:P:15:GLN:HB3	1.71	0.73
3:H:31:LEU:O	3:H:35:ASN:ND2	2.23	0.71
1:L:38:THR:HG21	1:L:100:TRP:HE3	1.56	0.69
1:L:31:VAL:HG22	11:M:806:U10:H362	1.74	0.69
5:G:48:PHE:HB3	15:G:103:SPO:H82	1.73	0.69
4:A:18:VAL:HG11	13:X:103:LDA:HM12	1.74	0.68
5:T:48:PHE:HB3	15:T:102:SPO:H82	1.75	0.68
1:L:26:VAL:HG13	12:H:307:PGV:H011	1.75	0.68
1:L:199:ASN:HB3	17:M:811:CDL:HA22	1.76	0.68
4:3:1:FME:HE1	5:6:29:LEU:HD22	1.74	0.68
12:H:307:PGV:H02	4:F:18:VAL:HG21	1.77	0.66
5:P:48:PHE:HB3	15:R:101:SPO:H82	1.76	0.66
6:5:15:ARG:HH12	8:U:10:ARG:HH21	1.41	0.66
1:L:264:GLN:HB2	12:L:306:PGV:H061	1.76	0.66
12:K:104:PGV:H251	4:O:21:GLY:HA3	1.77	0.66
15:W:102:SPO:H25	9:Y:103:BCL:HED3	1.78	0.66
6:5:40:SER:O	5:6:45:ARG:NH1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:38:THR:HG21	4:Y:44:LEU:HD13	1.79	0.65
2:M:6:ILE:HD12	16:M:810:LMT:H11	1.79	0.65
15:1:105:SPO:H392	5:4:19:LEU:HA	1.78	0.65
2:M:20:MET:HE1	3:H:125:GLY:HA3	1.78	0.65
3:H:173:GLU:HB3	3:H:175:MET:HE3	1.79	0.64
4:O:40:SER:O	5:P:45:ARG:NH1	2.29	0.64
2:M:110:LYS:HG3	13:Y:101:LDA:H12	1.80	0.64
9:L:301:BCL:H2	10:L:302:BPH:HBB3	1.78	0.64
15:1:105:SPO:H6	9:5:102:BCL:HMB1	1.80	0.64
4:O:1:FME:SD	4:O:1:FME:N	2.70	0.63
9:K:102:BCL:HED3	15:N:101:SPO:H25	1.81	0.63
15:5:103:SPO:H32A	9:7:101:BCL:HBB2	1.81	0.63
2:M:21:THR:HB	2:M:26:LEU:HD21	1.79	0.62
8:U:10:ARG:HG3	8:U:50:PRO:HB3	1.82	0.62
3:H:130:LYS:NZ	3:H:170:ASP:OD2	2.25	0.62
2:M:32:VAL:HG22	2:M:49:PRO:HD3	1.81	0.62
10:M:804:BPH:HHC	10:M:804:BPH:HBB3	1.82	0.62
16:H:301:LMT:O6'	16:H:301:LMT:O1B	2.17	0.62
4:1:7:ILE:HB	15:1:105:SPO:H343	1.80	0.62
5:N:44:TRP:CD1	15:N:101:SPO:H83	2.35	0.61
4:V:11:PHE:HE1	4:Y:14:ARG:HA	1.66	0.61
9:8:102:BCL:HBA2	9:8:102:BCL:HBD	1.83	0.61
2:M:12:VAL:HG11	3:H:169:VAL:HG11	1.81	0.61
1:L:170:ASN:HB3	1:L:173:HIS:HB2	1.83	0.60
4:Y:36:LEU:O	4:Y:42:ASN:ND2	2.34	0.60
4:F:1:FME:HE1	5:J:29:LEU:HD22	1.83	0.60
5:J:48:PHE:HB3	15:N:101:SPO:H82	1.83	0.60
5:E:48:PHE:HB3	15:F:104:SPO:H82	1.83	0.60
2:M:256:MET:HE1	11:M:806:U10:H102	1.84	0.60
4:V:40:SER:O	5:W:45:ARG:NH1	2.34	0.60
4:Q:10:ILE:HG23	4:S:14:ARG:HG2	1.84	0.59
12:L:306:PGV:H222	16:U:102:LMT:H101	1.83	0.59
10:M:804:BPH:HBC3	10:M:804:BPH:HHD	1.83	0.59
9:L:301:BCL:H111	9:L:308:BCL:HBB2	1.84	0.59
13:L:311:LDA:H12	13:X:103:LDA:HM22	1.84	0.59
2:M:119:SER:HB3	15:M:807:SPO:H311	1.85	0.59
15:G:103:SPO:H83	5:J:44:TRP:CD1	2.37	0.59
11:L:304:U10:H1M3	2:M:89:LEU:HD23	1.84	0.59
7:X:49:ARG:HH11	7:X:49:ARG:HA	1.69	0.58
9:D:101:BCL:HBB2	15:X:102:SPO:H31	1.85	0.58
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:7:ILE:HB	15:K:103:SPO:H343	1.85	0.58
9:J:101:BCL:H61	15:N:101:SPO:H243	1.85	0.58
15:D:102:SPO:H182	9:F:102:BCL:H91	1.86	0.57
1:L:247:CYS:O	1:L:251:THR:OG1	2.22	0.57
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.86	0.57
2:M:233:ARG:NH2	3:H:230:GLU:OE1	2.37	0.57
3:H:5:THR:HG22	3:H:11:ASP:HB3	1.87	0.57
5:R:44:TRP:CD1	15:R:101:SPO:H83	2.39	0.57
6:7:27:LEU:HD23	9:8:102:BCL:HED2	1.86	0.57
16:H:302:LMT:H21	4:O:34:ILE:HG12	1.86	0.57
4:D:3:LYS:HD3	5:G:22:VAL:HG22	1.86	0.57
5:W:6:LEU:N	5:Z:15:GLN:OE1	2.38	0.57
4:S:35:LEU:HD11	9:T:101:BCL:HHD	1.87	0.57
4:K:40:SER:O	5:N:45:ARG:NH1	2.37	0.56
2:M:201:PHE:HD2	2:M:279:THR:HG23	1.70	0.56
2:M:52:LEU:O	4:V:15:ARG:NH2	2.33	0.56
4:K:37:SER:HA	16:K:101:LMT:H6'1	1.88	0.56
9:1:101:BCL:HED3	15:1:103:SPO:H25	1.88	0.55
15:T:102:SPO:H351	9:V:101:BCL:H122	1.87	0.55
2:M:60:LEU:HD12	10:M:804:BPH:H121	1.88	0.55
4:K:1:FME:HE3	5:P:29:LEU:HD22	1.89	0.55
5:Z:9:THR:HG23	5:Z:11:LEU:H	1.71	0.55
15:5:104:SPO:H83	5:6:44:TRP:CD1	2.42	0.54
1:L:147:PRO:HD3	7:X:66:ASN:HD22	1.73	0.54
3:H:36:MET:HE2	3:H:58:LEU:HD23	1.89	0.54
5:8:31:SER:HB3	9:8:102:BCL:H51	1.90	0.54
4:I:6:LYS:HB3	15:K:103:SPO:H392	1.89	0.54
15:F:103:SPO:H293	15:F:104:SPO:H402	1.88	0.54
15:5:103:SPO:H6	9:7:101:BCL:HMB2	1.89	0.54
5:Z:48:PHE:HB3	15:1:103:SPO:H82	1.90	0.54
1:L:58:THR:HA	12:L:305:PGV:H062	1.90	0.53
4:A:32:HIS:CE1	9:B:101:BCL:HMD1	2.43	0.53
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.89	0.53
16:M:808:LMT:H122	3:H:16:ALA:HB2	1.89	0.53
5:G:48:PHE:HD2	9:G:101:BCL:H202	1.73	0.53
9:S:102:BCL:HED3	15:S:104:SPO:H25	1.90	0.53
12:Y:104:PGV:H72	9:1:101:BCL:H102	1.89	0.53
9:B:101:BCL:H193	15:E:101:SPO:H14	1.89	0.53
5:8:44:TRP:CG	15:8:101:SPO:H133	2.44	0.53
2:M:81:ASN:HB3	2:M:84:VAL:HB	1.90	0.53
9:B:101:BCL:H193	15:E:101:SPO:H11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:47:SER:OG	4:Q:53:ARG:NH1	2.42	0.53
16:3:101:LMT:H2'	16:5:101:LMT:H5'	1.90	0.53
2:M:243:THR:OG1	2:M:247:ARG:NH1	2.40	0.52
2:M:211:GLY:HA3	2:M:272:MET:HE2	1.91	0.52
1:L:156:TRP:CD1	7:X:65:PRO:HB2	2.45	0.52
7:X:28:MET:HE1	13:X:104:LDA:H82	1.91	0.52
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.45	0.52
8:U:22:GLY:HA3	16:U:102:LMT:H112	1.91	0.52
1:L:133:LEU:HD13	16:A:701:LMT:H112	1.90	0.52
17:H:304:CDL:H1	4:K:14:ARG:HB3	1.90	0.52
10:L:302:BPH:HBB3	10:L:302:BPH:HHC	1.91	0.52
5:J:6:LEU:HD12	5:N:15:GLN:HE22	1.75	0.52
9:Q:104:BCL:HMA1	15:R:101:SPO:H25	1.92	0.52
4:Y:15:ARG:HG2	17:Y:102:CDL:H711	1.92	0.52
15:T:102:SPO:H83	5:W:44:TRP:CD1	2.45	0.51
4:Y:40:SER:O	5:Z:45:ARG:NH1	2.43	0.51
1:L:205:GLU:O	1:L:207:ARG:NH1	2.43	0.51
4:A:30:MET:HG3	16:A:702:LMT:H102	1.92	0.51
4:Y:42:ASN:HD21	13:Y:101:LDA:H22	1.74	0.51
12:K:104:PGV:H72	4:O:15:ARG:HG2	1.93	0.51
16:S:105:LMT:H5B	16:S:105:LMT:H6D	1.92	0.51
4:V:25:PHE:HB2	9:V:101:BCL:H52	1.93	0.51
6:5:15:ARG:HH12	8:U:10:ARG:NH2	2.08	0.51
5:W:8:TYR:OH	5:Z:9:THR:OG1	2.26	0.51
8:U:19:VAL:O	8:U:23:ILE:HG12	2.11	0.51
15:T:102:SPO:H351	9:V:101:BCL:H8	1.93	0.51
4:S:12:ASP:HB3	4:S:15:ARG:HG3	1.92	0.51
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.93	0.50
5:J:48:PHE:HD2	9:J:101:BCL:H202	1.75	0.50
15:1:105:SPO:HM11	6:5:29:VAL:HG13	1.93	0.50
4:I:3:LYS:HB3	4:I:6:LYS:HE2	1.92	0.50
5:8:35:ILE:HD13	9:8:102:BCL:H93	1.92	0.50
17:M:811:CDL:H212	17:H:304:CDL:H151	1.92	0.50
4:A:27:LEU:HD23	9:B:101:BCL:HED3	1.92	0.50
4:D:13:PRO:HG3	5:E:19:LEU:HD21	1.93	0.50
4:I:26:LEU:HD22	16:K:101:LMT:H101	1.93	0.50
1:L:8:LYS:HB3	3:H:85:ILE:HD12	1.93	0.50
2:M:130:TRP:NE1	2:M:147:ALA:O	2.43	0.50
2:M:232:GLU:OE2	3:H:177:ARG:NH1	2.45	0.50
2:M:280:GLY:HA2	9:M:803:BCL:HED2	1.93	0.50
4:F:11:PHE:HZ	4:I:17:PHE:HB2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:103:SPO:H31	9:S:102:BCL:HBB2	1.94	0.50
4:V:35:LEU:HD11	9:W:101:BCL:HHD	1.93	0.50
5:W:35:ILE:HG12	9:W:101:BCL:H71	1.93	0.50
4:3:35:LEU:HD11	9:4:101:BCL:HHD	1.94	0.50
5:J:6:LEU:HD12	5:N:15:GLN:NE2	2.27	0.50
4:A:37:SER:HG	16:A:702:LMT:H2O2	1.47	0.50
1:L:91:ILE:HD13	16:A:702:LMT:H112	1.94	0.49
3:H:55:PRO:HB2	17:H:304:CDL:H541	1.94	0.49
2:M:285:LEU:O	2:M:289:THR:OG1	2.27	0.49
4:A:37:SER:OG	16:A:702:LMT:O2'	2.20	0.49
15:G:103:SPO:H25	9:I:101:BCL:H2A	1.94	0.49
15:O:102:SPO:H352	5:P:22:VAL:HB	1.95	0.49
9:T:101:BCL:H42	15:T:102:SPO:H293	1.95	0.49
6:7:30:MET:HE1	8:U:23:ILE:HB	1.93	0.49
1:L:213:ASP:OD1	1:L:223:SER:OG	2.20	0.49
16:M:809:LMT:H6D	16:M:809:LMT:H51	1.94	0.49
1:L:181:PHE:HB3	10:M:804:BPH:HBB2	1.94	0.49
4:A:6:LYS:HD3	15:D:102:SPO:H393	1.94	0.49
5:8:41:VAL:HG11	9:8:102:BCL:HBC1	1.95	0.49
4:O:7:ILE:HB	15:O:103:SPO:H343	1.95	0.49
2:M:233:ARG:NH1	3:H:122:GLU:OE1	2.46	0.49
9:A:703:BCL:H101	15:X:102:SPO:H292	1.94	0.49
15:T:102:SPO:H25	9:V:101:BCL:HED3	1.95	0.49
5:J:6:LEU:HB2	5:N:11:LEU:HD11	1.95	0.49
15:S:103:SPO:H41	4:V:32:HIS:CG	2.47	0.49
9:8:102:BCL:HAA1	9:8:102:BCL:H72	1.95	0.49
4:Q:27:LEU:HD23	9:R:102:BCL:HED3	1.95	0.48
15:5:103:SPO:H402	5:6:19:LEU:HA	1.95	0.48
15:O:102:SPO:H32	5:P:22:VAL:HG12	1.96	0.48
4:Q:33:LEU:HB3	16:Q:101:LMT:H42	1.94	0.48
4:1:4:PHE:CE1	15:1:105:SPO:H302	2.48	0.48
15:G:102:SPO:H6	9:K:102:BCL:HHB	1.95	0.48
1:L:79:PRO:HG3	16:A:702:LMT:H1B	1.95	0.48
10:L:302:BPH:HHC	10:L:302:BPH:CBB	2.43	0.48
2:M:64:LEU:HD13	10:M:804:BPH:H111	1.95	0.48
4:O:10:ILE:HG23	4:Q:14:ARG:HG2	1.95	0.48
15:W:102:SPO:H22	9:Y:103:BCL:O1D	2.12	0.48
6:5:20:GLN:NE2	5:6:23:TYR:OH	2.43	0.48
4:A:38:THR:HG21	4:D:44:LEU:HD13	1.94	0.48
15:V:102:SPO:HM11	4:Y:33:LEU:HD13	1.95	0.48
15:K:103:SPO:C13	9:O:101:BCL:H2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:20:ASN:N	1:L:20:ASN:OD1	2.47	0.47
1:L:262:TRP:HE1	12:L:306:PGV:H22	1.78	0.47
12:L:305:PGV:H012	12:M:801:PGV:H061	1.94	0.47
4:I:20:GLN:HG3	9:K:102:BCL:H91	1.96	0.47
5:N:6:LEU:HD21	15:O:102:SPO:H401	1.95	0.47
15:S:103:SPO:H361	15:S:103:SPO:H341	1.37	0.47
4:Y:33:LEU:HG	13:Y:101:LDA:H71	1.95	0.47
4:D:41:TYR:OH	5:E:45:ARG:O	2.19	0.47
9:7:101:BCL:H18	9:7:101:BCL:H152	1.52	0.47
1:L:46:ILE:HD11	9:L:308:BCL:H201	1.97	0.47
4:A:35:LEU:HD21	9:B:101:BCL:HHD	1.97	0.47
2:M:148:TRP:HD1	17:M:811:CDL:HB32	1.79	0.47
15:O:102:SPO:H41	4:Q:32:HIS:CG	2.50	0.47
4:3:8:TRP:HB3	5:4:19:LEU:HD23	1.96	0.47
9:7:101:BCL:H41	9:7:101:BCL:H61	1.59	0.47
4:K:11:PHE:HZ	4:O:17:PHE:HB2	1.77	0.47
15:W:102:SPO:H392	9:Y:103:BCL:H41	1.95	0.47
1:L:171:PRO:HG2	12:X:101:PGV:H91	1.96	0.47
2:M:167:LEU:HD21	16:Q:101:LMT:H71	1.96	0.47
9:O:101:BCL:H2A	15:P:101:SPO:H25	1.96	0.47
6:5:33:LEU:HD11	16:5:101:LMT:H51	1.97	0.47
9:5:102:BCL:H62	9:5:102:BCL:H41	1.68	0.47
9:7:101:BCL:H2A	15:8:101:SPO:H25	1.96	0.47
1:L:50:ALA:HA	12:L:305:PGV:H101	1.96	0.47
1:L:105:VAL:O	1:L:109:ARG:HG3	2.15	0.47
4:A:40:SER:HB2	4:D:53:ARG:HD2	1.97	0.47
9:E:102:BCL:H42	15:F:104:SPO:H293	1.96	0.47
5:W:39:LEU:O	5:W:43:ILE:HG12	2.15	0.47
4:D:8:TRP:HB3	5:E:19:LEU:HD23	1.97	0.47
15:D:102:SPO:H342	5:E:22:VAL:HG11	1.97	0.47
12:Y:104:PGV:H042	4:1:14:ARG:HD2	1.96	0.47
15:5:103:SPO:H293	15:5:104:SPO:H352	1.97	0.47
6:7:30:MET:O	6:7:34:ILE:HG12	2.15	0.47
4:O:11:PHE:HZ	4:Q:17:PHE:HB2	1.80	0.47
4:O:24:LEU:HG	9:P:102:BCL:HED1	1.98	0.46
9:5:102:BCL:H141	9:5:102:BCL:H171	1.97	0.46
15:8:101:SPO:H20	15:8:101:SPO:H181	1.84	0.46
1:L:124:ALA:HB1	9:L:301:BCL:H71	1.95	0.46
1:L:205:GLU:HB3	3:H:67:PRO:HA	1.97	0.46
10:M:804:BPH:H201	12:Y:104:PGV:H211	1.96	0.46
3:H:175:MET:SD	3:H:177:ARG:NH1	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:25:PHE:HD1	9:D:101:BCL:H2	1.80	0.46
9:T:101:BCL:H203	9:T:101:BCL:H162	1.73	0.46
16:3:101:LMT:H52	16:3:101:LMT:H81	1.70	0.46
5:8:30:PHE:CE2	15:8:101:SPO:H302	2.51	0.46
1:L:130:THR:HG23	1:L:249:ILE:HD13	1.97	0.46
4:A:35:LEU:HD21	9:B:101:BCL:HAC1	1.96	0.46
15:O:102:SPO:H20	15:O:102:SPO:H181	1.72	0.46
12:Y:104:PGV:H41	9:1:101:BCL:H111	1.96	0.46
2:M:109:LEU:HB2	13:Y:101:LDA:H32	1.98	0.46
9:N:102:BCL:H93	9:N:102:BCL:H61	1.75	0.46
4:V:27:LEU:HD23	9:W:101:BCL:HED3	1.98	0.46
15:V:103:SPO:H292	15:W:102:SPO:H351	1.97	0.46
5:N:48:PHE:HB3	15:P:101:SPO:H82	1.96	0.46
15:N:101:SPO:H10	15:N:101:SPO:H81	1.64	0.46
6:5:12:ASP:HB3	6:5:15:ARG:HD2	1.97	0.46
1:L:264:GLN:HA	1:L:267:VAL:HG12	1.98	0.46
2:M:177:TYR:HE1	15:M:807:SPO:H22	1.79	0.46
4:A:13:PRO:HB3	5:B:19:LEU:HD21	1.96	0.46
1:L:97:PHE:CZ	9:L:301:BCL:H112	2.49	0.46
4:Q:11:PHE:HZ	4:S:17:PHE:HB2	1.81	0.46
1:L:254:ILE:HG23	12:X:101:PGV:H011	1.98	0.46
1:L:270:PRO:HB2	16:3:101:LMT:H3'	1.97	0.46
2:M:302:GLY:O	2:M:304:ALA:N	2.49	0.46
4:A:14:ARG:HA	4:A:14:ARG:HD3	1.77	0.46
5:J:45:ARG:NH1	4:K:53:ARG:HD2	2.31	0.46
9:W:101:BCL:H112	9:W:101:BCL:H72	1.42	0.46
9:L:301:BCL:H192	9:L:301:BCL:H162	1.69	0.46
5:E:6:LEU:HD12	15:F:103:SPO:H401	1.97	0.46
9:I:101:BCL:H192	9:I:101:BCL:H162	1.73	0.46
15:N:101:SPO:H361	15:N:101:SPO:H341	1.65	0.46
9:1:101:BCL:H141	9:1:101:BCL:H161	1.73	0.46
4:I:24:LEU:HB2	9:I:101:BCL:H42	1.98	0.45
15:O:103:SPO:H22	5:R:27:LEU:HD12	1.98	0.45
12:3:102:PGV:H102	12:3:102:PGV:H131	1.71	0.45
1:L:71:LEU:HD22	7:X:64:ALA:HB2	1.98	0.45
2:M:289:THR:HB	16:M:808:LMT:H41	1.97	0.45
12:M:812:PGV:H222	4:S:26:LEU:HD11	1.98	0.45
4:D:35:LEU:HD11	9:E:102:BCL:HHD	1.97	0.45
5:J:48:PHE:CD2	9:J:101:BCL:H202	2.50	0.45
15:V:102:SPO:H361	15:V:102:SPO:H341	1.46	0.45
9:W:101:BCL:H62	9:W:101:BCL:H41	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:104:PGV:H52	12:Y:104:PGV:H21	1.66	0.45
9:L:309:BCL:H61	9:L:309:BCL:H41	1.65	0.45
2:M:97:PRO:HG2	2:M:171:TRP:HB2	1.99	0.45
16:M:809:LMT:H12	16:M:809:LMT:H42	1.70	0.45
16:M:810:LMT:H4B	8:U:8:ALA:HB2	1.98	0.45
3:H:60:LYS:HA	3:H:60:LYS:HD3	1.67	0.45
15:1:105:SPO:H20	15:1:105:SPO:H181	1.75	0.45
5:4:9:THR:HG23	5:4:11:LEU:H	1.81	0.45
5:R:6:LEU:HD21	5:T:19:LEU:HD12	1.98	0.45
9:Y:103:BCL:H142	9:Y:103:BCL:H111	1.74	0.45
2:M:28:ASN:HA	4:V:15:ARG:HH21	1.82	0.45
17:M:811:CDL:HB62	17:M:811:CDL:HA61	1.98	0.45
5:T:8:TYR:HE1	5:W:11:LEU:HD11	1.82	0.45
15:5:104:SPO:H20	15:5:104:SPO:H181	1.75	0.45
10:L:302:BPH:H112	9:L:308:BCL:H202	1.99	0.45
2:M:20:MET:HE2	2:M:20:MET:HB3	1.69	0.45
4:A:24:LEU:HB2	9:A:703:BCL:H43	1.98	0.45
9:Y:103:BCL:H141	9:Y:103:BCL:H161	1.75	0.45
5:8:12:THR:O	5:8:16:ALA:N	2.43	0.45
2:M:25:ASN:HB3	2:M:28:ASN:HD22	1.82	0.45
2:M:80:TRP:CH2	4:Y:34:ILE:HG12	2.51	0.45
12:M:812:PGV:H91	12:M:812:PGV:H201	1.99	0.45
12:M:812:PGV:O14	12:Q:103:PGV:H222	2.17	0.45
4:F:6:LYS:HB3	15:G:102:SPO:H402	1.98	0.45
9:5:102:BCL:H192	9:5:102:BCL:H162	1.72	0.45
15:1:102:SPO:H20	15:1:102:SPO:H181	1.73	0.45
1:L:117:ILE:HB	1:L:118:PRO:HD3	1.99	0.44
15:1:105:SPO:H6	9:5:102:BCL:CMB	2.45	0.44
15:5:104:SPO:H311	15:5:104:SPO:H291	1.42	0.44
16:3:101:LMT:O1B	16:3:101:LMT:O6'	2.34	0.44
1:L:34:PHE:O	1:L:38:THR:OG1	2.23	0.44
1:L:221:GLY:HA3	17:Y:102:CDL:H342	1.98	0.44
9:D:101:BCL:HHH	5:E:41:VAL:HG21	1.98	0.44
9:F:102:BCL:H193	9:F:102:BCL:H162	1.86	0.44
4:Q:27:LEU:O	4:Q:31:ILE:HG13	2.18	0.44
15:T:102:SPO:H25	9:V:101:BCL:H2A	1.99	0.44
15:1:102:SPO:H392	5:2:19:LEU:HA	1.99	0.44
4:1:32:HIS:CE1	9:2:101:BCL:HMD1	2.52	0.44
15:1:102:SPO:H6	9:3:103:BCL:HMB2	1.99	0.44
9:L:309:BCL:H161	9:L:309:BCL:H122	1.69	0.44
2:M:200:PRO:HB3	12:M:801:PGV:O04	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:103:SPO:H181	15:K:103:SPO:H20	1.81	0.44
4:O:23:PHE:HE1	4:Q:25:PHE:CE1	2.36	0.44
12:H:306:PGV:O13	4:F:15:ARG:NH1	2.51	0.44
4:Q:38:THR:HG21	4:S:44:LEU:HD13	2.00	0.44
4:S:32:HIS:CE1	9:T:101:BCL:HMD1	2.52	0.44
9:T:101:BCL:H52	15:T:102:SPO:H243	1.99	0.44
15:V:102:SPO:H26	15:V:102:SPO:H241	1.84	0.44
9:5:102:BCL:H111	9:5:102:BCL:H143	1.73	0.44
17:H:304:CDL:H352	4:K:26:LEU:HD12	2.00	0.44
5:E:48:PHE:HE2	9:E:102:BCL:H161	1.83	0.44
3:H:131:ILE:HG22	3:H:168:TRP:HE3	1.83	0.44
4:K:6:LYS:HB3	15:O:102:SPO:H392	2.00	0.43
1:L:61:PRO:HG3	12:L:305:PGV:H62	2.01	0.43
15:S:103:SPO:H37	5:T:22:VAL:HG21	2.00	0.43
4:Y:27:LEU:O	4:Y:31:ILE:HG13	2.19	0.43
15:X:102:SPO:H26	15:X:102:SPO:H241	1.80	0.43
3:H:44:ASN:N	3:H:48:THR:O	2.41	0.43
9:Z:101:BCL:H93	9:Z:101:BCL:H112	1.75	0.43
1:L:241:VAL:HG21	10:L:302:BPH:HBC3	2.01	0.43
15:G:102:SPO:H291	9:I:101:BCL:H193	1.99	0.43
9:P:102:BCL:H102	9:P:102:BCL:H61	1.52	0.43
15:S:103:SPO:H20	15:S:103:SPO:H181	1.68	0.43
15:T:102:SPO:C25	9:V:101:BCL:HED3	2.47	0.43
9:W:101:BCL:H141	9:W:101:BCL:H162	1.78	0.43
12:H:307:PGV:H292	4:F:22:VAL:HG22	2.00	0.43
15:G:103:SPO:H10	15:G:103:SPO:H81	1.59	0.43
5:W:6:LEU:HB3	5:W:7:GLY:H	1.62	0.43
9:3:103:BCL:HHD	9:3:103:BCL:HAC1	1.88	0.43
9:6:101:BCL:H202	9:6:101:BCL:H162	1.82	0.43
6:7:26:LEU:O	6:7:30:MET:HG2	2.18	0.43
9:L:308:BCL:H18	9:L:308:BCL:H151	1.59	0.43
2:M:157:TRP:CE3	2:M:158:MET:HG2	2.54	0.43
9:E:102:BCL:H91	9:E:102:BCL:H112	1.68	0.43
15:V:103:SPO:H361	15:V:103:SPO:H341	1.77	0.43
9:Z:101:BCL:H141	9:Z:101:BCL:H162	1.77	0.43
1:L:66:VAL:HB	1:L:148:TYR:HB2	2.01	0.43
9:L:309:BCL:HHC	9:M:803:BCL:H42	2.00	0.43
16:H:302:LMT:H22	16:Q:102:LMT:H31	2.00	0.43
5:P:12:THR:C	5:P:14:GLU:H	2.26	0.43
15:5:104:SPO:H10	15:5:104:SPO:H81	1.79	0.43
9:M:803:BCL:HAA2	9:M:803:BCL:HBD	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:F:103:SPO:H15	15:F:103:SPO:H131	1.93	0.43
4:O:34:ILE:O	4:O:38:THR:HG23	2.19	0.43
12:Y:104:PGV:H042	4:1:14:ARG:HH11	1.84	0.43
12:Y:104:PGV:H241	12:Y:104:PGV:H212	1.92	0.43
6:5:27:LEU:HD23	9:6:101:BCL:HED2	1.99	0.43
16:A:704:LMT:H4'	5:B:24:MET:HE2	2.01	0.43
15:O:102:SPO:H26	15:O:102:SPO:H241	1.82	0.43
1:L:207:ARG:HD2	1:L:211:HIS:CD2	2.53	0.43
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.53	0.43
2:M:148:TRP:CD1	17:M:811:CDL:HB32	2.53	0.43
15:G:103:SPO:H20	15:G:103:SPO:H181	1.85	0.43
5:N:6:LEU:HD11	15:O:102:SPO:H401	2.01	0.43
7:X:57:ILE:O	7:X:58:ASP:HB2	2.19	0.43
12:H:306:PGV:H62	12:H:306:PGV:H31	1.81	0.42
15:R:101:SPO:H15	15:R:101:SPO:H131	1.91	0.42
15:S:104:SPO:H15	15:S:104:SPO:H131	1.90	0.42
2:M:241:ARG:NH1	3:H:38:GLU:OE1	2.53	0.42
9:G:101:BCL:H42	15:G:103:SPO:H293	2.01	0.42
4:V:7:ILE:HA	4:V:7:ILE:HD12	1.73	0.42
9:3:103:BCL:H141	9:3:103:BCL:H162	1.89	0.42
5:4:12:THR:H	5:4:15:GLN:HB2	1.84	0.42
7:X:37:VAL:O	7:X:41:THR:HG23	2.18	0.42
9:L:301:BCL:H13	9:L:308:BCL:HMB2	2.01	0.42
2:M:114:LEU:HD23	2:M:114:LEU:HA	1.87	0.42
17:H:304:CDL:H351	4:K:23:PHE:HA	2.01	0.42
9:O:101:BCL:HHD	9:O:101:BCL:HAC1	1.88	0.42
15:R:101:SPO:H10	15:R:101:SPO:H81	1.60	0.42
4:S:17:PHE:HD2	15:S:104:SPO:H401	1.83	0.42
15:S:104:SPO:H82	15:S:104:SPO:H42	2.00	0.42
6:5:11:PHE:HE1	6:7:14:ARG:HG3	1.85	0.42
6:5:50:LYS:NZ	15:5:104:SPO:HM12	2.34	0.42
15:8:101:SPO:H81	15:8:101:SPO:H10	1.76	0.42
1:L:113:ILE:HG22	2:M:229:PHE:HE2	1.85	0.42
1:L:207:ARG:HG3	2:M:142:MET:HG2	2.00	0.42
1:L:212:GLU:HB3	11:L:303:U10:H4M3	2.01	0.42
12:H:306:PGV:H042	4:I:18:VAL:HG21	2.02	0.42
15:G:102:SPO:H20	15:G:102:SPO:H181	1.81	0.42
15:O:103:SPO:H341	15:O:103:SPO:H361	1.41	0.42
17:M:811:CDL:HB62	17:M:811:CDL:OA9	2.19	0.42
4:V:7:ILE:HB	15:V:103:SPO:H343	2.01	0.42
15:5:103:SPO:H6	9:7:101:BCL:CMB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5:104:SPO:H15	15:5:104:SPO:H131	1.83	0.42
9:E:102:BCL:H61	9:E:102:BCL:H101	1.71	0.42
9:S:102:BCL:HHH	9:S:102:BCL:HAC1	1.79	0.42
11:L:304:U10:H13	2:M:90:PHE:HZ	1.84	0.42
2:M:127:TRP:CB	12:M:812:PGV:H212	2.50	0.42
3:H:163:LYS:HB2	3:H:163:LYS:HE3	1.81	0.42
5:B:31:SER:HB3	9:B:101:BCL:H72	2.01	0.42
4:1:27:LEU:HD23	9:2:101:BCL:HED3	2.02	0.42
15:G:102:SPO:H26	15:G:102:SPO:H241	1.87	0.42
9:K:102:BCL:H61	9:K:102:BCL:H41	1.84	0.42
12:K:104:PGV:H301	12:K:104:PGV:H272	1.86	0.42
4:S:11:PHE:HZ	4:V:17:PHE:HB2	1.85	0.42
15:V:102:SPO:H20	15:V:102:SPO:H181	1.81	0.42
4:O:38:THR:HG21	4:Q:44:LEU:HD13	2.01	0.42
9:S:102:BCL:O1D	15:S:104:SPO:H22	2.19	0.42
5:4:47:TRP:O	6:5:47:SER:OG	2.35	0.42
9:6:101:BCL:H162	9:6:101:BCL:H141	1.83	0.42
1:L:226:THR:HA	11:L:303:U10:H3M2	2.02	0.42
15:M:807:SPO:H15	15:M:807:SPO:H131	1.88	0.42
4:D:10:ILE:HD11	15:F:103:SPO:H37	2.02	0.42
15:K:103:SPO:H361	15:K:103:SPO:H341	1.55	0.42
15:3:104:SPO:H20	15:3:104:SPO:H181	1.89	0.42
1:L:230:HIS:CE1	2:M:234:GLU:OE1	2.73	0.41
11:L:304:U10:H121	11:L:304:U10:H101	1.64	0.41
9:B:101:BCL:H141	9:B:101:BCL:H162	1.77	0.41
5:G:14:GLU:H	5:G:14:GLU:CD	2.28	0.41
9:V:101:BCL:H62	9:V:101:BCL:H41	1.71	0.41
12:X:101:PGV:H252	12:X:101:PGV:H281	1.86	0.41
4:Q:41:TYR:OH	5:R:45:ARG:O	2.26	0.41
4:V:8:TRP:HB3	5:W:19:LEU:HD23	2.01	0.41
9:O:101:BCL:H141	9:O:101:BCL:H161	1.74	0.41
9:2:101:BCL:H192	9:2:101:BCL:H162	1.82	0.41
2:M:51:TYR:O	2:M:132:ARG:NH1	2.42	0.41
3:H:111:PRO:HG3	3:H:242:MET:SD	2.61	0.41
15:K:103:SPO:H293	15:N:101:SPO:H37	2.02	0.41
4:Q:32:HIS:CE1	9:R:102:BCL:HMD1	2.55	0.41
4:S:40:SER:O	5:T:45:ARG:NH1	2.54	0.41
15:3:104:SPO:H10	15:3:104:SPO:H81	1.74	0.41
3:H:66:LEU:HB3	3:H:70:ARG:HB2	2.02	0.41
9:D:101:BCL:H102	15:E:101:SPO:H343	2.03	0.41
9:K:102:BCL:H151	9:K:102:BCL:H111	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:36:LEU:HD13	4:Y:43:TRP:CH2	2.56	0.41
2:M:270:ILE:O	2:M:274:VAL:HG13	2.19	0.41
3:H:80:SER:OG	3:H:82:ASP:OD1	2.26	0.41
15:G:102:SPO:H361	15:G:102:SPO:H341	1.58	0.41
15:T:102:SPO:H15	15:T:102:SPO:H131	1.86	0.41
4:V:9:MET:HE3	4:V:9:MET:HB2	1.79	0.41
4:1:35:LEU:HD11	9:2:101:BCL:HHD	2.03	0.41
15:N:101:SPO:H20	15:N:101:SPO:H181	1.82	0.41
4:Y:42:ASN:ND2	13:Y:101:LDA:H22	2.35	0.41
15:1:103:SPO:H10	15:1:103:SPO:H81	1.74	0.41
6:7:48:ALA:HB1	6:7:54:VAL:HB	2.03	0.41
15:G:103:SPO:H27	9:I:101:BCL:HBA1	2.02	0.41
15:R:101:SPO:H20	15:R:101:SPO:H181	1.81	0.41
9:4:101:BCL:HBB2	9:4:101:BCL:H122	2.03	0.41
1:L:190:HIS:HA	11:L:303:U10:O2	2.20	0.41
2:M:234:GLU:OE2	2:M:266:HIS:CE1	2.74	0.41
2:M:250:LEU:HD23	2:M:250:LEU:HA	1.84	0.41
5:B:39:LEU:HD12	5:B:39:LEU:HA	1.91	0.41
9:I:101:BCL:H141	9:I:101:BCL:H161	1.83	0.41
9:4:101:BCL:H162	9:4:101:BCL:H141	1.78	0.41
15:X:102:SPO:H15	15:X:102:SPO:H131	1.95	0.41
13:L:311:LDA:H21	13:L:311:LDA:HM23	1.79	0.41
15:G:103:SPO:H393	4:I:20:GLN:HE21	1.84	0.41
16:S:101:LMT:H62	16:S:101:LMT:H32	1.93	0.41
15:V:103:SPO:H391	5:W:6:LEU:HD21	2.03	0.41
12:L:310:PGV:H291	12:L:310:PGV:H322	1.79	0.40
2:M:202:HIS:O	2:M:206:ILE:HG13	2.21	0.40
3:H:244:ALA:C	3:H:246:PRO:HD3	2.46	0.40
4:I:6:LYS:HG2	4:I:9:MET:SD	2.61	0.40
15:1:103:SPO:H15	15:1:103:SPO:H131	1.83	0.40
7:X:57:ILE:C	7:X:59:GLU:H	2.29	0.40
17:H:304:CDL:H172	17:H:304:CDL:H141	1.76	0.40
15:G:102:SPO:H10	15:G:102:SPO:H81	1.97	0.40
16:Q:101:LMT:H82	16:Q:101:LMT:H111	1.92	0.40
4:V:5:TYR:CD2	5:W:17:GLN:HG2	2.56	0.40
9:Y:103:BCL:H192	9:Y:103:BCL:H162	1.74	0.40
3:H:4:VAL:HG11	16:H:302:LMT:O2'	2.22	0.40
4:V:7:ILE:HG13	4:V:11:PHE:CD2	2.56	0.40
4:Y:33:LEU:HD12	4:Y:33:LEU:HA	1.88	0.40
11:L:304:U10:H13	2:M:90:PHE:CZ	2.57	0.40
9:L:308:BCL:H121	9:L:308:BCL:H162	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:27:LEU:O	4:D:31:ILE:HG13	2.21	0.40
9:E:102:BCL:H162	9:E:102:BCL:H141	1.74	0.40
4:S:17:PHE:CZ	15:S:103:SPO:H32	2.57	0.40
9:L:301:BCL:H143	9:L:301:BCL:H161	1.79	0.40
4:Q:23:PHE:HE1	4:S:25:PHE:CE1	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	279/282 (99%)	267 (96%)	12 (4%)	0	100	100
2	M	304/308 (99%)	293 (96%)	11 (4%)	0	100	100
3	H	244/260 (94%)	231 (95%)	13 (5%)	0	100	100
4	1	52/54 (96%)	48 (92%)	4 (8%)	0	100	100
4	3	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	A	43/54 (80%)	43 (100%)	0	0	100	100
4	D	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	F	52/54 (96%)	52 (100%)	0	0	100	100
4	I	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	K	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	O	52/54 (96%)	52 (100%)	0	0	100	100
4	Q	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	S	52/54 (96%)	52 (100%)	0	0	100	100
4	V	52/54 (96%)	47 (90%)	5 (10%)	0	100	100
4	Y	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
5	2	40/49 (82%)	39 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	4	41/49 (84%)	39 (95%)	2 (5%)	0	100	100
5	6	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
5	8	36/49 (74%)	36 (100%)	0	0	100	100
5	B	42/49 (86%)	42 (100%)	0	0	100	100
5	E	41/49 (84%)	41 (100%)	0	0	100	100
5	G	43/49 (88%)	42 (98%)	1 (2%)	0	100	100
5	J	41/49 (84%)	41 (100%)	0	0	100	100
5	N	41/49 (84%)	41 (100%)	0	0	100	100
5	P	41/49 (84%)	37 (90%)	4 (10%)	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	41/49 (84%)	41 (100%)	0	0	100	100
5	Z	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
6	5	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
6	7	49/54 (91%)	49 (100%)	0	0	100	100
7	X	51/82 (62%)	48 (94%)	3 (6%)	0	100	100
8	U	48/53 (91%)	47 (98%)	1 (2%)	0	100	100
All	All	2211/2427 (91%)	2144 (97%)	67 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	220/221 (100%)	212 (96%)	8 (4%)	31	56
2	M	239/241 (99%)	231 (97%)	8 (3%)	33	58
3	H	197/208 (95%)	194 (98%)	3 (2%)	57	75
4	1	48/48 (100%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	3	48/48 (100%)	48 (100%)	0	100	100
4	A	41/48 (85%)	41 (100%)	0	100	100
4	D	47/48 (98%)	47 (100%)	0	100	100
4	F	48/48 (100%)	48 (100%)	0	100	100
4	I	48/48 (100%)	48 (100%)	0	100	100
4	K	48/48 (100%)	46 (96%)	2 (4%)	26	52
4	O	47/48 (98%)	45 (96%)	2 (4%)	26	51
4	Q	48/48 (100%)	47 (98%)	1 (2%)	47	70
4	S	48/48 (100%)	48 (100%)	0	100	100
4	V	48/48 (100%)	46 (96%)	2 (4%)	26	52
4	Y	48/48 (100%)	46 (96%)	2 (4%)	26	52
5	2	34/40 (85%)	34 (100%)	0	100	100
5	4	35/40 (88%)	35 (100%)	0	100	100
5	6	32/40 (80%)	32 (100%)	0	100	100
5	8	26/40 (65%)	26 (100%)	0	100	100
5	B	36/40 (90%)	35 (97%)	1 (3%)	38	63
5	E	35/40 (88%)	34 (97%)	1 (3%)	37	62
5	G	37/40 (92%)	36 (97%)	1 (3%)	39	64
5	J	35/40 (88%)	35 (100%)	0	100	100
5	N	35/40 (88%)	34 (97%)	1 (3%)	37	62
5	P	35/40 (88%)	35 (100%)	0	100	100
5	R	34/40 (85%)	34 (100%)	0	100	100
5	T	35/40 (88%)	35 (100%)	0	100	100
5	W	34/40 (85%)	33 (97%)	1 (3%)	37	62
5	Z	35/40 (88%)	34 (97%)	1 (3%)	37	62
6	5	48/49 (98%)	48 (100%)	0	100	100
6	7	43/49 (88%)	42 (98%)	1 (2%)	44	68
7	X	40/66 (61%)	39 (98%)	1 (2%)	42	66
8	U	34/37 (92%)	34 (100%)	0	100	100
All	All	1866/2007 (93%)	1830 (98%)	36 (2%)	49	71

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	20	ASN
1	L	52	SER
1	L	54	VAL
1	L	71	LEU
1	L	72	GLU
1	L	102	LEU
1	L	210	ASP
1	L	267	VAL
2	M	8	THR
2	M	20	MET
2	M	21	THR
2	M	86	LEU
2	M	197	PHE
2	M	235	LEU
2	M	236	GLU
2	M	272	MET
3	H	143	SER
3	H	196	VAL
3	H	231	ASP
5	B	11	LEU
5	E	18	GLU
5	G	6	LEU
4	K	12	ASP
4	K	20	GLN
5	N	11	LEU
4	O	14	ARG
4	O	24	LEU
4	Q	54	VAL
4	V	7	ILE
4	V	10	ILE
5	W	18	GLU
4	Y	33	LEU
4	Y	54	VAL
5	Z	45	ARG
6	7	24	LEU
7	X	17	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	62	GLN
2	M	187	ASN
2	M	301	HIS

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Mol	Chain	Res	Type
3	H	44	ASN
3	H	199	GLN
5	G	17	GLN
4	S	42	ASN
4	Y	42	ASN
7	X	26	GLN
7	X	60	ASN
7	X	66	ASN
8	U	51	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	K	1	4	8,9,10	0.54	0	8,9,11	0.94	1 (12%)
4	FME	A	1	4	8,9,10	0.54	0	8,9,11	0.83	1 (12%)
4	FME	1	1	4	8,9,10	0.54	0	8,9,11	0.95	1 (12%)
4	FME	3	1	4	8,9,10	0.53	0	8,9,11	0.91	1 (12%)
4	FME	S	1	4	5,6,10	0.79	0	4,6,11	1.05	0
4	FME	Y	1	4	8,9,10	0.54	0	8,9,11	0.94	1 (12%)
4	FME	Q	1	4	8,9,10	0.54	0	8,9,11	0.93	1 (12%)
4	FME	V	1	4	8,9,10	0.55	0	8,9,11	0.98	1 (12%)
4	FME	D	1	4	8,9,10	0.52	0	8,9,11	1.00	1 (12%)
4	FME	O	1	4	8,9,10	0.55	0	8,9,11	1.00	1 (12%)
4	FME	F	1	4	8,9,10	0.56	0	8,9,11	0.88	1 (12%)
4	FME	I	1	4	8,9,10	0.55	0	8,9,11	0.92	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	K	1	4	-	1/7/9/11	-
4	FME	A	1	4	-	3/7/9/11	-
4	FME	1	1	4	-	0/7/9/11	-
4	FME	3	1	4	-	0/7/9/11	-
4	FME	S	1	4	-	2/3/5/11	-
4	FME	Y	1	4	-	1/7/9/11	-
4	FME	Q	1	4	-	0/7/9/11	-
4	FME	V	1	4	-	1/7/9/11	-
4	FME	D	1	4	-	0/7/9/11	-
4	FME	O	1	4	-	1/7/9/11	-
4	FME	F	1	4	-	1/7/9/11	-
4	FME	I	1	4	-	1/7/9/11	-

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	1	FME	O-C-CA	-2.58	118.14	124.77
4	D	1	FME	O-C-CA	-2.58	118.14	124.77
4	I	1	FME	O-C-CA	-2.53	118.26	124.77
4	Y	1	FME	O-C-CA	-2.52	118.28	124.77
4	1	1	FME	O-C-CA	-2.51	118.31	124.77
4	K	1	FME	O-C-CA	-2.49	118.36	124.77
4	V	1	FME	O-C-CA	-2.46	118.45	124.77
4	3	1	FME	O-C-CA	-2.45	118.47	124.77
4	Q	1	FME	O-C-CA	-2.43	118.51	124.77
4	F	1	FME	O-C-CA	-2.37	118.67	124.77
4	A	1	FME	O-C-CA	-2.31	118.83	124.77

There are no chirality outliers.

All (11) 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
4	K	1	FME	O1-CN-N-CA
4	O	1	FME	O1-CN-N-CA

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

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1	FME	1	0
4	3	1	FME	1	0
4	O	1	FME	1	0
4	F	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 112 ligands modelled in this entry, 1 is monoatomic - leaving 111 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	5	104	-	41,41,41	0.58	0	47,50,50	2.11	14 (29%)
16	LMT	I	102	-	28,28,36	0.44	0	39,39,47	0.72	1 (2%)
9	BCL	K	102	-	69,74,74	1.79	18 (26%)	79,115,115	2.24	22 (27%)
15	SPO	V	103	-	41,41,41	0.59	0	47,50,50	2.10	16 (34%)
13	LDA	X	104	-	13,15,15	2.28	2 (15%)	14,17,17	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	4	101	-	69,74,74	1.81	17 (24%)	79,115,115	2.17	22 (27%)
16	LMT	5	101	-	34,34,36	0.40	0	45,45,47	0.74	1 (2%)
13	LDA	Y	101	-	9,11,15	2.64	2 (22%)	10,13,17	0.45	0
12	PGV	L	310	-	44,44,50	1.00	2 (4%)	47,49,56	1.14	4 (8%)
16	LMT	4	102	-	28,28,36	0.46	0	39,39,47	0.78	1 (2%)
16	LMT	X	105	-	32,32,36	0.40	0	43,43,47	0.81	1 (2%)
16	LMT	D	103	-	28,28,36	0.43	0	39,39,47	0.69	1 (2%)
12	PGV	M	801	-	46,46,50	0.94	2 (4%)	49,52,56	1.19	4 (8%)
9	BCL	V	101	-	69,74,74	1.77	17 (24%)	79,115,115	2.20	21 (26%)
16	LMT	K	101	-	36,36,36	0.41	0	47,47,47	0.97	3 (6%)
9	BCL	M	803	-	69,74,74	1.81	18 (26%)	79,115,115	2.30	23 (29%)
12	PGV	3	102	-	50,50,50	0.90	2 (4%)	53,56,56	1.06	4 (7%)
12	PGV	M	812	-	37,37,50	1.06	2 (5%)	40,43,56	1.19	4 (10%)
16	LMT	A	701	-	36,36,36	0.34	0	47,47,47	0.72	1 (2%)
16	LMT	A	704	-	28,28,36	0.45	0	39,39,47	0.76	1 (2%)
15	SPO	W	102	-	41,41,41	0.60	0	47,50,50	2.12	15 (31%)
13	LDA	L	311	-	13,15,15	2.23	2 (15%)	14,17,17	0.53	0
9	BCL	6	101	-	69,74,74	1.81	17 (24%)	79,115,115	2.10	20 (25%)
15	SPO	O	103	-	41,41,41	0.57	0	47,50,50	2.26	16 (34%)
9	BCL	L	308	-	69,74,74	1.77	18 (26%)	79,115,115	2.27	25 (31%)
9	BCL	W	101	-	69,74,74	1.78	19 (27%)	79,115,115	2.21	23 (29%)
16	LMT	U	102	-	36,36,36	0.36	0	47,47,47	0.73	1 (2%)
9	BCL	S	102	-	69,74,74	1.78	17 (24%)	79,115,115	2.39	24 (30%)
11	U10	L	304	-	35,35,63	0.78	2 (5%)	43,45,79	0.79	1 (2%)
10	BPH	L	302	-	59,70,70	0.83	3 (5%)	59,101,101	0.90	3 (5%)
16	LMT	A	702	-	36,36,36	0.39	0	47,47,47	0.76	1 (2%)
17	CDL	M	811	-	78,78,99	1.03	4 (5%)	84,90,111	1.21	6 (7%)
13	LDA	L	307	-	13,15,15	2.23	2 (15%)	14,17,17	0.50	0
9	BCL	Y	103	-	69,74,74	1.76	17 (24%)	79,115,115	2.30	24 (30%)
15	SPO	5	103	-	41,41,41	0.58	0	47,50,50	2.29	16 (34%)
11	U10	L	303	-	35,35,63	0.82	2 (5%)	43,45,79	0.78	1 (2%)
16	LMT	1	104	-	25,25,36	0.66	0	33,34,47	0.84	1 (3%)
15	SPO	F	103	-	41,41,41	0.58	0	47,50,50	1.90	14 (29%)
15	SPO	D	102	-	41,41,41	0.56	0	47,50,50	2.03	17 (36%)
9	BCL	J	101	-	69,74,74	1.81	19 (27%)	79,115,115	2.20	21 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	LMT	Q	101	-	24,24,36	0.44	0	29,29,47	0.97	1 (3%)
11	U10	M	806	-	48,48,63	0.72	2 (4%)	60,61,79	0.66	1 (1%)
16	LMT	M	810	-	34,34,36	0.42	0	45,45,47	1.15	4 (8%)
9	BCL	T	101	-	69,74,74	1.80	18 (26%)	79,115,115	2.15	21 (26%)
17	CDL	Y	102	-	47,47,99	1.17	3 (6%)	52,58,111	1.09	3 (5%)
9	BCL	3	103	-	69,74,74	1.79	17 (24%)	79,115,115	2.26	21 (26%)
16	LMT	M	809	-	36,36,36	0.37	0	47,47,47	0.70	1 (2%)
16	LMT	3	101	-	36,36,36	0.43	0	47,47,47	0.92	3 (6%)
17	CDL	H	305	-	35,35,99	1.39	3 (8%)	40,44,111	1.32	6 (15%)
9	BCL	B	101	-	69,74,74	1.79	17 (24%)	79,115,115	2.14	23 (29%)
15	SPO	S	104	-	41,41,41	0.63	0	47,50,50	1.67	15 (31%)
12	PGV	Q	103	-	38,38,50	1.05	2 (5%)	41,44,56	1.06	3 (7%)
16	LMT	F	101	-	27,27,36	0.48	0	38,38,47	0.90	2 (5%)
9	BCL	G	101	-	69,74,74	1.79	17 (24%)	79,115,115	2.09	21 (26%)
12	PGV	L	306	-	32,32,50	1.11	2 (6%)	35,38,56	1.20	4 (11%)
15	SPO	G	102	-	41,41,41	0.57	0	47,50,50	2.14	14 (29%)
15	SPO	3	104	-	41,41,41	0.59	0	47,50,50	2.09	17 (36%)
9	BCL	N	102	-	69,74,74	1.79	18 (26%)	79,115,115	2.24	22 (27%)
10	BPH	M	804	-	59,70,70	0.78	3 (5%)	59,101,101	0.92	5 (8%)
15	SPO	1	103	-	41,41,41	0.62	0	47,50,50	2.04	18 (38%)
16	LMT	U	101	-	33,33,36	0.39	0	44,44,47	0.80	1 (2%)
15	SPO	S	103	-	41,41,41	0.56	0	47,50,50	2.31	16 (34%)
9	BCL	F	102	-	69,74,74	1.77	18 (26%)	79,115,115	2.25	25 (31%)
9	BCL	R	102	-	69,74,74	1.78	17 (24%)	79,115,115	2.20	24 (30%)
15	SPO	K	103	-	41,41,41	0.59	0	47,50,50	2.09	13 (27%)
9	BCL	5	102	-	69,74,74	1.78	19 (27%)	79,115,115	2.28	24 (30%)
12	PGV	H	303	-	33,33,50	1.15	2 (6%)	36,38,56	1.16	4 (11%)
15	SPO	T	102	-	41,41,41	0.65	0	47,50,50	1.96	15 (31%)
16	LMT	M	808	-	27,27,36	0.47	0	32,33,47	0.66	1 (3%)
9	BCL	L	301	-	69,74,74	1.79	17 (24%)	79,115,115	2.27	26 (32%)
15	SPO	E	101	-	41,41,41	0.59	0	47,50,50	1.85	15 (31%)
12	PGV	H	307	-	46,46,50	0.96	2 (4%)	49,52,56	1.03	3 (6%)
9	BCL	8	102	-	63,68,74	1.94	17 (26%)	71,107,115	2.22	18 (25%)
15	SPO	V	102	-	41,41,41	0.59	0	47,50,50	2.08	15 (31%)
17	CDL	H	304	-	60,60,99	1.18	4 (6%)	66,72,111	1.18	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	SPO	F	104	-	41,41,41	0.58	0	47,50,50	1.98	14 (29%)
16	LMT	F	105	-	17,17,36	0.45	0	22,22,47	0.58	0
9	BCL	1	101	-	69,74,74	1.77	18 (26%)	79,115,115	2.39	26 (32%)
9	BCL	D	101	-	69,74,74	1.77	17 (24%)	79,115,115	2.29	25 (31%)
9	BCL	Z	101	-	69,74,74	1.78	19 (27%)	79,115,115	2.18	22 (27%)
9	BCL	P	102	-	69,74,74	1.76	17 (24%)	79,115,115	2.22	22 (27%)
16	LMT	H	301	-	36,36,36	0.37	0	47,47,47	0.93	2 (4%)
16	LMT	S	105	-	31,31,36	0.45	0	42,42,47	0.69	1 (2%)
15	SPO	1	102	-	41,41,41	0.56	0	47,50,50	2.18	14 (29%)
15	SPO	R	101	-	41,41,41	0.59	0	47,50,50	2.58	15 (31%)
15	SPO	N	101	-	41,41,41	0.57	0	47,50,50	2.18	18 (38%)
12	PGV	K	104	-	37,40,50	1.03	2 (5%)	39,42,56	1.18	3 (7%)
16	LMT	Q	102	-	19,19,36	0.49	0	24,24,47	0.55	0
13	LDA	X	103	-	10,12,15	2.53	2 (20%)	11,14,17	0.49	0
9	BCL	E	102	-	69,74,74	1.82	18 (26%)	79,115,115	2.17	26 (32%)
9	BCL	L	309	-	69,74,74	1.79	17 (24%)	79,115,115	2.16	23 (29%)
15	SPO	1	105	-	41,41,41	0.59	0	47,50,50	2.07	15 (31%)
15	SPO	X	102	-	41,41,41	0.58	0	47,50,50	2.07	14 (29%)
12	PGV	Y	104	-	42,42,50	0.99	2 (4%)	45,48,56	1.10	3 (6%)
9	BCL	Q	104	-	69,74,74	1.75	18 (26%)	79,115,115	2.26	22 (27%)
9	BCL	2	101	-	69,74,74	1.77	18 (26%)	79,115,115	2.22	21 (26%)
15	SPO	8	101	-	41,41,41	0.59	0	47,50,50	2.23	17 (36%)
15	SPO	O	102	-	41,41,41	0.59	0	47,50,50	2.08	15 (31%)
16	LMT	H	302	-	31,31,36	0.45	0	42,42,47	1.11	3 (7%)
9	BCL	O	101	-	69,74,74	1.76	18 (26%)	79,115,115	2.23	21 (26%)
13	LDA	M	802	-	13,15,15	2.23	2 (15%)	14,17,17	0.56	0
9	BCL	A	703	-	64,69,74	1.85	18 (28%)	73,109,115	2.28	22 (30%)
12	PGV	L	305	-	38,38,50	1.05	2 (5%)	41,44,56	1.08	3 (7%)
15	SPO	M	807	-	41,41,41	0.59	0	47,50,50	1.90	11 (23%)
15	SPO	G	103	-	41,41,41	0.60	0	47,50,50	2.19	15 (31%)
9	BCL	I	101	-	69,74,74	1.78	19 (27%)	79,115,115	2.31	23 (29%)
9	BCL	7	101	-	69,74,74	1.78	18 (26%)	79,115,115	2.29	23 (29%)
16	LMT	S	101	-	25,25,36	0.46	0	30,30,47	0.81	0
15	SPO	P	101	-	41,41,41	0.60	0	47,50,50	1.91	14 (29%)
12	PGV	X	101	-	38,38,50	1.04	2 (5%)	41,44,56	1.12	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	PGV	H	306	-	39,39,50	1.07	2 (5%)	42,45,56	1.24	3 (7%)

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	5	104	-	-	9/47/47/47	-
16	LMT	I	102	-	-	3/13/53/61	0/2/2/2
9	BCL	K	102	-	-	11/41/137/137	-
15	SPO	V	103	-	-	5/47/47/47	-
13	LDA	X	104	-	-	0/13/13/13	-
9	BCL	4	101	-	-	9/41/137/137	-
16	LMT	5	101	-	-	5/19/59/61	0/2/2/2
13	LDA	Y	101	-	-	1/9/9/13	-
12	PGV	L	310	-	-	6/46/46/55	-
16	LMT	4	102	-	-	2/13/53/61	0/2/2/2
16	LMT	X	105	-	-	4/17/57/61	0/2/2/2
16	LMT	D	103	-	-	2/13/53/61	0/2/2/2
12	PGV	M	801	-	-	15/51/51/55	-
9	BCL	V	101	-	-	15/41/137/137	-
16	LMT	K	101	-	-	2/21/61/61	0/2/2/2
9	BCL	M	803	-	-	10/41/137/137	-
12	PGV	3	102	-	-	8/55/55/55	-
12	PGV	M	812	-	-	18/42/42/55	-
16	LMT	A	701	-	-	4/21/61/61	0/2/2/2
16	LMT	A	704	-	-	0/13/53/61	0/2/2/2
15	SPO	W	102	-	-	10/47/47/47	-
13	LDA	L	311	-	-	2/13/13/13	-
9	BCL	6	101	-	-	16/41/137/137	-
15	SPO	O	103	-	-	10/47/47/47	-
9	BCL	L	308	-	-	7/41/137/137	-
9	BCL	W	101	-	-	19/41/137/137	-
16	LMT	U	102	-	-	3/21/61/61	0/2/2/2
9	BCL	S	102	-	-	15/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	U10	L	304	-	-	4/30/54/87	0/1/1/1
10	BPH	L	302	-	-	3/37/105/105	0/5/6/6
16	LMT	A	702	-	-	6/21/61/61	0/2/2/2
17	CDL	M	811	-	-	30/89/89/110	-
13	LDA	L	307	-	-	4/13/13/13	-
9	BCL	Y	103	-	-	15/41/137/137	-
15	SPO	5	103	-	-	5/47/47/47	-
11	U10	L	303	-	-	9/30/54/87	0/1/1/1
16	LMT	1	104	-	-	2/11/44/61	0/2/2/2
15	SPO	F	103	-	-	4/47/47/47	-
15	SPO	D	102	-	-	3/47/47/47	-
9	BCL	J	101	-	-	12/41/137/137	-
16	LMT	Q	101	-	-	2/15/35/61	0/1/1/2
11	U10	M	806	-	-	1/45/69/87	0/1/1/1
16	LMT	M	810	-	-	7/19/59/61	0/2/2/2
9	BCL	T	101	-	-	13/41/137/137	-
17	CDL	Y	102	-	-	12/56/56/110	-
9	BCL	3	103	-	-	10/41/137/137	-
16	LMT	M	809	-	-	8/21/61/61	0/2/2/2
16	LMT	3	101	-	-	7/21/61/61	0/2/2/2
17	CDL	H	305	-	-	8/37/37/110	-
9	BCL	B	101	-	-	7/41/137/137	-
15	SPO	S	104	-	-	9/47/47/47	-
12	PGV	Q	103	-	-	7/43/43/55	-
16	LMT	F	101	-	-	5/11/51/61	0/2/2/2
9	BCL	G	101	-	-	15/41/137/137	-
12	PGV	L	306	-	-	13/37/37/55	-
15	SPO	G	102	-	-	7/47/47/47	-
15	SPO	3	104	-	-	4/47/47/47	-
9	BCL	N	102	-	-	11/41/137/137	-
10	BPH	M	804	-	-	4/37/105/105	0/5/6/6
15	SPO	1	103	-	-	4/47/47/47	-
16	LMT	U	101	-	-	1/18/58/61	0/2/2/2
15	SPO	S	103	-	-	6/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	F	102	-	-	9/41/137/137	-
9	BCL	R	102	-	-	13/41/137/137	-
15	SPO	K	103	-	-	4/47/47/47	-
9	BCL	5	102	-	-	12/41/137/137	-
12	PGV	H	303	-	-	3/35/35/55	-
15	SPO	T	102	-	-	8/47/47/47	-
16	LMT	M	808	-	-	2/19/39/61	0/1/1/2
9	BCL	L	301	-	-	19/41/137/137	-
15	SPO	E	101	-	-	6/47/47/47	-
12	PGV	H	307	-	-	12/51/51/55	-
9	BCL	8	102	-	-	14/33/129/137	-
15	SPO	V	102	-	-	3/47/47/47	-
17	CDL	H	304	-	-	22/71/71/110	-
15	SPO	F	104	-	-	1/47/47/47	-
16	LMT	F	105	-	-	1/9/29/61	0/1/1/2
9	BCL	1	101	-	-	12/41/137/137	-
9	BCL	D	101	-	-	9/41/137/137	-
9	BCL	Z	101	-	-	12/41/137/137	-
9	BCL	P	102	-	-	15/41/137/137	-
16	LMT	H	301	-	-	4/21/61/61	0/2/2/2
16	LMT	S	105	-	-	5/16/56/61	0/2/2/2
15	SPO	1	102	-	-	5/47/47/47	-
15	SPO	R	101	-	-	7/47/47/47	-
15	SPO	N	101	-	-	9/47/47/47	-
12	PGV	K	104	-	-	14/40/42/55	-
16	LMT	Q	102	-	-	2/11/31/61	0/1/1/2
13	LDA	X	103	-	-	1/10/10/13	-
9	BCL	E	102	-	-	12/41/137/137	-
9	BCL	L	309	-	-	14/41/137/137	-
15	SPO	1	105	-	-	6/47/47/47	-
15	SPO	X	102	-	-	4/47/47/47	-
12	PGV	Y	104	-	-	11/47/47/55	-
9	BCL	Q	104	-	-	17/41/137/137	-
9	BCL	2	101	-	-	15/41/137/137	-
15	SPO	8	101	-	-	2/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	SPO	O	102	-	-	5/47/47/47	-
16	LMT	H	302	-	-	6/16/56/61	0/2/2/2
9	BCL	O	101	-	-	11/41/137/137	-
13	LDA	M	802	-	-	2/13/13/13	-
9	BCL	A	703	-	-	13/35/131/137	-
12	PGV	L	305	-	-	12/43/43/55	-
15	SPO	M	807	-	-	8/47/47/47	-
15	SPO	G	103	-	-	6/47/47/47	-
9	BCL	I	101	-	-	10/41/137/137	-
9	BCL	7	101	-	-	13/41/137/137	-
16	LMT	S	101	-	-	4/17/37/61	0/1/1/2
15	SPO	P	101	-	-	9/47/47/47	-
12	PGV	X	101	-	-	6/43/43/55	-
12	PGV	H	306	-	-	12/44/44/55	-

All (631) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	X	104	LDA	O1-N1	-6.99	1.25	1.42
13	X	103	LDA	O1-N1	-6.94	1.25	1.42
13	L	311	LDA	O1-N1	-6.86	1.25	1.42
13	L	307	LDA	O1-N1	-6.86	1.25	1.42
13	Y	101	LDA	O1-N1	-6.85	1.25	1.42
13	M	802	LDA	O1-N1	-6.84	1.25	1.42
9	F	102	BCL	O2D-CGD	5.08	1.45	1.33
9	6	101	BCL	O2D-CGD	5.05	1.45	1.33
9	8	102	BCL	O2D-CGD	5.03	1.45	1.33
9	5	102	BCL	O2D-CGD	5.01	1.45	1.33
9	A	703	BCL	O2D-CGD	5.00	1.45	1.33
9	3	103	BCL	O2D-CGD	4.97	1.45	1.33
9	I	101	BCL	O2D-CGD	4.97	1.45	1.33
9	P	102	BCL	O2D-CGD	4.97	1.45	1.33
9	T	101	BCL	O2D-CGD	4.96	1.45	1.33
9	N	102	BCL	O2D-CGD	4.95	1.45	1.33
9	W	101	BCL	O2D-CGD	4.94	1.45	1.33
9	E	102	BCL	O2D-CGD	4.94	1.45	1.33
9	6	101	BCL	C3D-C4D	-4.94	1.33	1.44
9	J	101	BCL	O2D-CGD	4.94	1.45	1.33
9	4	101	BCL	O2D-CGD	4.94	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	O	101	BCL	O2D-CGD	4.93	1.45	1.33
9	G	101	BCL	O2D-CGD	4.93	1.45	1.33
9	D	101	BCL	O2D-CGD	4.92	1.45	1.33
9	V	101	BCL	O2D-CGD	4.92	1.45	1.33
9	B	101	BCL	O2D-CGD	4.91	1.45	1.33
9	2	101	BCL	O2D-CGD	4.91	1.45	1.33
9	8	102	BCL	C3D-C4D	-4.90	1.33	1.44
9	K	102	BCL	O2D-CGD	4.90	1.45	1.33
9	Q	104	BCL	O2D-CGD	4.89	1.45	1.33
9	L	308	BCL	C3D-C4D	-4.88	1.33	1.44
9	Z	101	BCL	O2D-CGD	4.88	1.45	1.33
9	7	101	BCL	O2D-CGD	4.88	1.45	1.33
9	Y	103	BCL	O2D-CGD	4.87	1.45	1.33
9	N	102	BCL	C3D-C4D	-4.85	1.33	1.44
9	M	803	BCL	O2D-CGD	4.84	1.45	1.33
9	1	101	BCL	O2D-CGD	4.83	1.45	1.33
9	L	301	BCL	O2D-CGD	4.83	1.45	1.33
9	L	301	BCL	C3D-C4D	-4.83	1.33	1.44
9	M	803	BCL	C3D-C4D	-4.83	1.33	1.44
9	L	309	BCL	O2D-CGD	4.82	1.45	1.33
9	L	309	BCL	C3D-C4D	-4.82	1.33	1.44
9	R	102	BCL	C3D-C4D	-4.81	1.33	1.44
9	E	102	BCL	C3D-C4D	-4.81	1.33	1.44
9	S	102	BCL	O2D-CGD	4.81	1.45	1.33
9	J	101	BCL	C3D-C4D	-4.78	1.33	1.44
9	T	101	BCL	C3D-C4D	-4.78	1.33	1.44
9	4	101	BCL	C3D-C4D	-4.76	1.33	1.44
9	W	101	BCL	C3D-C4D	-4.75	1.33	1.44
9	R	102	BCL	O2D-CGD	4.74	1.44	1.33
9	K	102	BCL	C3D-C4D	-4.74	1.33	1.44
9	Y	103	BCL	C3D-C4D	-4.73	1.33	1.44
9	O	101	BCL	C3D-C4D	-4.71	1.33	1.44
9	2	101	BCL	C3D-C4D	-4.70	1.33	1.44
9	7	101	BCL	C3D-C4D	-4.70	1.33	1.44
9	B	101	BCL	C3D-C4D	-4.69	1.33	1.44
9	P	102	BCL	C3D-C4D	-4.69	1.33	1.44
9	Z	101	BCL	C3D-C4D	-4.67	1.33	1.44
9	S	102	BCL	C3D-C4D	-4.66	1.33	1.44
9	L	308	BCL	O2D-CGD	4.65	1.44	1.33
9	Q	104	BCL	C3D-C4D	-4.64	1.33	1.44
9	D	101	BCL	C3D-C4D	-4.63	1.33	1.44
9	1	101	BCL	C3D-C4D	-4.62	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	703	BCL	C3D-C4D	-4.61	1.33	1.44
9	5	102	BCL	C3D-C4D	-4.61	1.33	1.44
9	V	101	BCL	C3D-C4D	-4.60	1.33	1.44
9	I	101	BCL	C3D-C4D	-4.59	1.33	1.44
9	G	101	BCL	C3D-C4D	-4.56	1.33	1.44
9	3	103	BCL	C3D-C4D	-4.50	1.34	1.44
9	F	102	BCL	C3D-C4D	-4.48	1.34	1.44
9	E	102	BCL	O2A-CGA	4.42	1.46	1.33
12	H	306	PGV	O03-C19	4.41	1.46	1.33
9	A	703	BCL	O2A-CGA	4.36	1.46	1.33
9	3	103	BCL	O2A-CGA	4.31	1.45	1.33
9	K	102	BCL	O2A-CGA	4.31	1.45	1.33
17	Y	102	CDL	OB8-CB7	4.31	1.45	1.33
17	H	304	CDL	OA8-CA7	4.30	1.45	1.33
17	H	305	CDL	OA6-CA5	4.30	1.46	1.34
12	H	307	PGV	O03-C19	4.29	1.45	1.33
9	7	101	BCL	O2A-CGA	4.28	1.45	1.33
17	H	305	CDL	OA8-CA7	4.28	1.45	1.33
9	O	101	BCL	O2A-CGA	4.27	1.45	1.33
12	Q	103	PGV	O03-C19	4.27	1.45	1.33
9	5	102	BCL	O2A-CGA	4.27	1.45	1.33
13	X	104	LDA	C1-N1	-4.27	1.47	1.51
9	L	301	BCL	O2A-CGA	4.27	1.45	1.33
17	H	304	CDL	OB8-CB7	4.26	1.45	1.33
12	X	101	PGV	O03-C19	4.26	1.45	1.33
9	6	101	BCL	O2A-CGA	4.24	1.45	1.33
17	Y	102	CDL	OA8-CA7	4.24	1.45	1.33
12	L	306	PGV	O03-C19	4.24	1.45	1.33
17	M	811	CDL	OA8-CA7	4.23	1.45	1.33
12	L	310	PGV	O03-C19	4.22	1.45	1.33
9	L	308	BCL	O2A-CGA	4.21	1.45	1.33
9	8	102	BCL	O2A-CGA	4.20	1.45	1.33
12	H	303	PGV	O03-C19	4.20	1.45	1.33
9	B	101	BCL	O2A-CGA	4.19	1.45	1.33
12	K	104	PGV	O03-C19	4.19	1.45	1.33
13	M	802	LDA	C1-N1	-4.19	1.47	1.51
17	M	811	CDL	OB8-CB7	4.18	1.45	1.33
9	M	803	BCL	O2A-CGA	4.18	1.45	1.33
9	G	101	BCL	O2A-CGA	4.18	1.45	1.33
9	T	101	BCL	O2A-CGA	4.18	1.45	1.33
9	L	309	BCL	O2A-CGA	4.17	1.45	1.33
12	H	306	PGV	O01-C1	4.17	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	102	CDL	OB6-CB5	4.17	1.46	1.34
17	M	811	CDL	OB6-CB5	4.17	1.46	1.34
9	S	102	BCL	O2A-CGA	4.17	1.45	1.33
12	L	305	PGV	O03-C19	4.16	1.45	1.33
12	L	305	PGV	O01-C1	4.16	1.46	1.34
9	4	101	BCL	O2A-CGA	4.15	1.45	1.33
9	8	102	BCL	CHD-C1D	4.15	1.46	1.38
9	F	102	BCL	O2A-CGA	4.15	1.45	1.33
17	H	304	CDL	OB6-CB5	4.15	1.46	1.34
13	L	307	LDA	C1-N1	-4.14	1.47	1.51
9	Q	104	BCL	O2A-CGA	4.14	1.45	1.33
9	P	102	BCL	O2A-CGA	4.13	1.45	1.33
12	Y	104	PGV	O03-C19	4.13	1.45	1.33
9	D	101	BCL	O2A-CGA	4.12	1.45	1.33
12	K	104	PGV	O01-C1	4.11	1.45	1.34
9	J	101	BCL	O2A-CGA	4.11	1.45	1.33
12	3	102	PGV	O01-C1	4.11	1.45	1.34
9	I	101	BCL	O2A-CGA	4.11	1.45	1.33
13	L	311	LDA	C1-N1	-4.11	1.47	1.51
12	3	102	PGV	O03-C19	4.11	1.45	1.33
12	M	812	PGV	O01-C1	4.10	1.45	1.34
17	H	305	CDL	OB8-CB7	4.10	1.45	1.33
12	Q	103	PGV	O01-C1	4.09	1.45	1.34
9	L	301	BCL	C3B-C4B	4.09	1.49	1.41
17	H	304	CDL	OA6-CA5	4.09	1.45	1.34
9	Z	101	BCL	O2A-CGA	4.09	1.45	1.33
9	V	101	BCL	O2A-CGA	4.08	1.45	1.33
9	2	101	BCL	O2A-CGA	4.08	1.45	1.33
9	W	101	BCL	O2A-CGA	4.08	1.45	1.33
12	M	801	PGV	O03-C19	4.07	1.45	1.33
12	M	812	PGV	O03-C19	4.06	1.45	1.33
12	X	101	PGV	O01-C1	4.06	1.45	1.34
9	R	102	BCL	O2A-CGA	4.05	1.45	1.33
12	H	307	PGV	O01-C1	4.05	1.45	1.34
9	D	101	BCL	C3B-C4B	4.03	1.49	1.41
12	L	310	PGV	O01-C1	4.03	1.45	1.34
12	M	801	PGV	O01-C1	4.03	1.45	1.34
9	O	101	BCL	C3B-C4B	4.03	1.49	1.41
9	F	102	BCL	C3B-C4B	4.01	1.49	1.41
9	7	101	BCL	C3B-C4B	4.00	1.49	1.41
9	N	102	BCL	O2A-CGA	3.99	1.45	1.33
12	H	303	PGV	O01-C1	3.99	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	M	811	CDL	OA6-CA5	3.99	1.45	1.34
9	S	102	BCL	C3B-C4B	3.98	1.49	1.41
9	E	102	BCL	C3B-C4B	3.97	1.49	1.41
9	I	101	BCL	C3B-C4B	3.97	1.49	1.41
12	Y	104	PGV	O01-C1	3.96	1.45	1.34
13	X	103	LDA	C1-N1	-3.96	1.47	1.51
9	3	103	BCL	C3B-C4B	3.95	1.48	1.41
13	Y	101	LDA	C1-N1	-3.95	1.47	1.51
9	1	101	BCL	O2A-CGA	3.95	1.44	1.33
9	A	703	BCL	CHD-C1D	3.95	1.46	1.38
9	Y	103	BCL	O2A-CGA	3.94	1.44	1.33
9	M	803	BCL	C3B-C4B	3.93	1.48	1.41
9	N	102	BCL	C3B-C4B	3.92	1.48	1.41
9	5	102	BCL	C3B-C4B	3.89	1.48	1.41
9	8	102	BCL	C3B-C4B	3.85	1.48	1.41
9	K	102	BCL	C3B-C4B	3.80	1.48	1.41
9	6	101	BCL	C3B-C4B	3.80	1.48	1.41
9	1	101	BCL	C3B-C4B	3.79	1.48	1.41
9	L	308	BCL	C3B-C4B	3.76	1.48	1.41
12	L	306	PGV	O01-C1	3.76	1.44	1.34
9	R	102	BCL	C3B-C4B	3.76	1.48	1.41
9	P	102	BCL	C3B-C4B	3.73	1.48	1.41
9	4	101	BCL	C3B-C4B	3.72	1.48	1.41
9	T	101	BCL	C3B-C4B	3.70	1.48	1.41
9	B	101	BCL	C3B-C4B	3.70	1.48	1.41
9	W	101	BCL	C3B-C4B	3.70	1.48	1.41
9	7	101	BCL	CHD-C1D	3.69	1.45	1.38
9	6	101	BCL	CHD-C1D	3.67	1.45	1.38
9	V	101	BCL	C3B-C4B	3.67	1.48	1.41
9	Y	103	BCL	C3B-C4B	3.67	1.48	1.41
9	L	309	BCL	CHD-C1D	3.66	1.45	1.38
9	8	102	BCL	OBD-CAD	3.63	1.28	1.22
9	J	101	BCL	CHB-C1B	3.62	1.47	1.39
9	A	703	BCL	C3B-C4B	3.62	1.48	1.41
9	J	101	BCL	OBD-CAD	3.61	1.28	1.22
9	V	101	BCL	CHD-C1D	3.61	1.45	1.38
9	8	102	BCL	CHB-C1B	3.60	1.47	1.39
9	4	101	BCL	CHD-C1D	3.59	1.45	1.38
9	J	101	BCL	C3B-C4B	3.59	1.48	1.41
9	5	102	BCL	CHD-C1D	3.57	1.45	1.38
9	G	101	BCL	CHD-C1D	3.57	1.45	1.38
9	L	309	BCL	C3B-C4B	3.57	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	4	101	BCL	OBD-CAD	3.56	1.28	1.22
9	G	101	BCL	C3B-C4B	3.56	1.48	1.41
9	F	102	BCL	OBD-CAD	3.54	1.28	1.22
9	8	102	BCL	CHC-C4B	3.54	1.47	1.39
9	J	101	BCL	CHD-C1D	3.54	1.45	1.38
9	3	103	BCL	OBD-CAD	3.53	1.28	1.22
9	Z	101	BCL	CHD-C1D	3.53	1.45	1.38
9	L	301	BCL	CHD-C1D	3.53	1.45	1.38
9	I	101	BCL	CHD-C1D	3.52	1.45	1.38
9	Q	104	BCL	C3B-C4B	3.52	1.48	1.41
9	L	301	BCL	OBD-CAD	3.52	1.28	1.22
9	Z	101	BCL	C3B-C4B	3.51	1.48	1.41
9	L	301	BCL	CHC-C4B	3.51	1.47	1.39
9	B	101	BCL	CHD-C1D	3.50	1.45	1.38
9	B	101	BCL	OBD-CAD	3.50	1.28	1.22
9	7	101	BCL	OBD-CAD	3.49	1.28	1.22
9	3	103	BCL	CHD-C1D	3.49	1.45	1.38
9	K	102	BCL	CHD-C1D	3.49	1.45	1.38
9	E	102	BCL	OBD-CAD	3.48	1.28	1.22
9	F	102	BCL	CHD-C1D	3.48	1.45	1.38
9	2	101	BCL	CHD-C1D	3.47	1.45	1.38
9	L	308	BCL	CHD-C1D	3.47	1.45	1.38
9	Q	104	BCL	OBD-CAD	3.47	1.28	1.22
9	R	102	BCL	OBD-CAD	3.47	1.28	1.22
9	5	102	BCL	OBD-CAD	3.47	1.28	1.22
9	Z	101	BCL	CHB-C1B	3.47	1.47	1.39
9	E	102	BCL	CHC-C4B	3.46	1.47	1.39
9	G	101	BCL	OBD-CAD	3.46	1.28	1.22
9	L	308	BCL	CHB-C1B	3.46	1.47	1.39
9	R	102	BCL	CHD-C1D	3.46	1.45	1.38
9	E	102	BCL	CHD-C1D	3.45	1.45	1.38
9	W	101	BCL	OBD-CAD	3.45	1.28	1.22
9	I	101	BCL	OBD-CAD	3.45	1.28	1.22
9	Z	101	BCL	OBD-CAD	3.44	1.28	1.22
9	A	703	BCL	CHB-C1B	3.44	1.47	1.39
9	M	803	BCL	CHD-C1D	3.44	1.45	1.38
9	4	101	BCL	CHC-C4B	3.44	1.47	1.39
9	D	101	BCL	OBD-CAD	3.44	1.28	1.22
9	A	703	BCL	OBD-CAD	3.43	1.28	1.22
9	V	101	BCL	OBD-CAD	3.43	1.28	1.22
9	M	803	BCL	CHB-C1B	3.43	1.47	1.39
9	2	101	BCL	C3B-C4B	3.43	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	S	102	BCL	OBD-CAD	3.42	1.28	1.22
9	6	101	BCL	OBD-CAD	3.42	1.28	1.22
9	T	101	BCL	OBD-CAD	3.42	1.28	1.22
9	6	101	BCL	CHC-C4B	3.41	1.47	1.39
9	Q	104	BCL	CHD-C1D	3.41	1.45	1.38
9	K	102	BCL	OBD-CAD	3.41	1.28	1.22
9	T	101	BCL	CHD-C1D	3.41	1.45	1.38
9	P	102	BCL	OBD-CAD	3.41	1.28	1.22
9	S	102	BCL	CHB-C1B	3.40	1.47	1.39
9	B	101	BCL	CHB-C1B	3.40	1.47	1.39
9	M	803	BCL	OBD-CAD	3.40	1.28	1.22
9	N	102	BCL	CHD-C1D	3.40	1.45	1.38
9	N	102	BCL	OBD-CAD	3.39	1.28	1.22
9	W	101	BCL	CHD-C1D	3.39	1.45	1.38
9	B	101	BCL	CHC-C4B	3.39	1.47	1.39
9	2	101	BCL	OBD-CAD	3.39	1.28	1.22
9	4	101	BCL	CHB-C1B	3.39	1.47	1.39
9	1	101	BCL	OBD-CAD	3.38	1.28	1.22
9	D	101	BCL	CHB-C1B	3.37	1.47	1.39
9	6	101	BCL	CHB-C1B	3.36	1.46	1.39
9	Y	103	BCL	OBD-CAD	3.35	1.28	1.22
9	L	309	BCL	OBD-CAD	3.35	1.28	1.22
9	O	101	BCL	OBD-CAD	3.34	1.28	1.22
9	2	101	BCL	CHB-C1B	3.34	1.46	1.39
9	P	102	BCL	CHD-C1D	3.34	1.44	1.38
9	Y	103	BCL	CHB-C1B	3.33	1.46	1.39
9	Q	104	BCL	CHB-C1B	3.33	1.46	1.39
9	W	101	BCL	CHB-C1B	3.33	1.46	1.39
9	D	101	BCL	CHD-C1D	3.31	1.44	1.38
9	N	102	BCL	CHC-C4B	3.31	1.46	1.39
9	T	101	BCL	CHB-C1B	3.30	1.46	1.39
9	T	101	BCL	CHC-C4B	3.30	1.46	1.39
9	1	101	BCL	CHB-C1B	3.29	1.46	1.39
9	O	101	BCL	CHD-C1D	3.29	1.44	1.38
9	N	102	BCL	CHB-C1B	3.28	1.46	1.39
9	G	101	BCL	CHB-C1B	3.28	1.46	1.39
9	1	101	BCL	CHD-C1D	3.27	1.44	1.38
9	G	101	BCL	CHC-C4B	3.27	1.46	1.39
9	R	102	BCL	CHC-C4B	3.27	1.46	1.39
9	P	102	BCL	CHB-C1B	3.27	1.46	1.39
9	L	309	BCL	CHB-C1B	3.26	1.46	1.39
9	3	103	BCL	CHB-C1B	3.25	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	101	BCL	CHC-C4B	3.24	1.46	1.39
9	Y	103	BCL	CHD-C1D	3.24	1.44	1.38
9	S	102	BCL	CHD-C1D	3.23	1.44	1.38
9	E	102	BCL	CHB-C1B	3.23	1.46	1.39
9	M	803	BCL	CHC-C4B	3.22	1.46	1.39
9	R	102	BCL	CHB-C1B	3.22	1.46	1.39
9	O	101	BCL	CHC-C4B	3.22	1.46	1.39
9	D	101	BCL	CHC-C4B	3.21	1.46	1.39
9	L	309	BCL	CHC-C4B	3.20	1.46	1.39
9	L	301	BCL	CHB-C1B	3.19	1.46	1.39
9	P	102	BCL	CHC-C4B	3.19	1.46	1.39
9	F	102	BCL	CHC-C4B	3.19	1.46	1.39
9	I	101	BCL	CHC-C4B	3.18	1.46	1.39
9	1	101	BCL	C4B-NB	-3.18	1.33	1.37
9	K	102	BCL	CHB-C1B	3.17	1.46	1.39
9	L	309	BCL	C4B-NB	-3.16	1.33	1.37
9	L	308	BCL	OBD-CAD	3.16	1.27	1.22
9	V	101	BCL	CHC-C4B	3.15	1.46	1.39
9	J	101	BCL	CHC-C4B	3.15	1.46	1.39
9	L	308	BCL	CHC-C4B	3.15	1.46	1.39
9	Z	101	BCL	CHC-C4B	3.13	1.46	1.39
9	F	102	BCL	CHB-C1B	3.13	1.46	1.39
10	L	302	BPH	C4D-CHA	3.12	1.44	1.39
9	8	102	BCL	CHD-C4C	3.12	1.48	1.39
9	V	101	BCL	CHB-C1B	3.11	1.46	1.39
9	7	101	BCL	CHC-C4B	3.11	1.46	1.39
9	7	101	BCL	CHB-C1B	3.10	1.46	1.39
9	T	101	BCL	C1D-ND	-3.09	1.33	1.37
9	I	101	BCL	CHB-C1B	3.08	1.46	1.39
9	Y	103	BCL	CHC-C4B	3.08	1.46	1.39
9	B	101	BCL	C3D-C2D	3.08	1.47	1.39
9	2	101	BCL	CHC-C4B	3.07	1.46	1.39
9	3	103	BCL	CHC-C4B	3.07	1.46	1.39
9	K	102	BCL	CHC-C4B	3.06	1.46	1.39
9	L	309	BCL	C3D-C2D	3.06	1.47	1.39
10	M	804	BPH	C4D-CHA	3.06	1.44	1.39
9	5	102	BCL	CHB-C1B	3.05	1.46	1.39
9	G	101	BCL	C3D-C2D	3.04	1.47	1.39
9	E	102	BCL	C1D-ND	-3.04	1.33	1.37
9	K	102	BCL	C3D-C2D	3.04	1.47	1.39
9	T	101	BCL	C4B-NB	-3.03	1.33	1.37
9	P	102	BCL	C3D-C2D	3.03	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	5	102	BCL	CHC-C4B	3.03	1.46	1.39
9	A	703	BCL	CHC-C4B	3.01	1.46	1.39
9	4	101	BCL	C3D-C2D	3.00	1.47	1.39
9	B	101	BCL	C1D-ND	-3.00	1.33	1.37
9	S	102	BCL	C4B-NB	-2.99	1.33	1.37
9	S	102	BCL	CHC-C4B	2.99	1.46	1.39
9	8	102	BCL	C3D-C2D	2.99	1.47	1.39
9	Z	101	BCL	C1D-ND	-2.99	1.33	1.37
9	A	703	BCL	C3D-C2D	2.99	1.47	1.39
9	Z	101	BCL	C3D-C2D	2.99	1.47	1.39
9	2	101	BCL	C3D-C2D	2.98	1.47	1.39
9	O	101	BCL	CHB-C1B	2.98	1.46	1.39
9	5	102	BCL	C4B-NB	-2.98	1.34	1.37
9	Y	103	BCL	C1D-ND	-2.98	1.34	1.37
9	Q	104	BCL	C3D-C2D	2.97	1.47	1.39
9	5	102	BCL	C3D-C2D	2.96	1.47	1.39
9	6	101	BCL	C3D-C2D	2.94	1.47	1.39
9	1	101	BCL	C3D-C2D	2.94	1.47	1.39
9	2	101	BCL	C1D-ND	-2.93	1.34	1.37
9	3	103	BCL	C3D-C2D	2.93	1.47	1.39
9	G	101	BCL	C4B-NB	-2.93	1.34	1.37
9	Q	104	BCL	CHC-C4B	2.92	1.46	1.39
9	J	101	BCL	C3D-C2D	2.92	1.47	1.39
9	T	101	BCL	C3D-C2D	2.92	1.46	1.39
9	Q	104	BCL	C4B-NB	-2.91	1.34	1.37
9	I	101	BCL	C3D-C2D	2.91	1.46	1.39
9	O	101	BCL	C3D-C2D	2.91	1.46	1.39
9	R	102	BCL	C4B-NB	-2.91	1.34	1.37
9	K	102	BCL	C4B-NB	-2.90	1.34	1.37
9	N	102	BCL	C3D-C2D	2.90	1.46	1.39
9	N	102	BCL	C1D-ND	-2.90	1.34	1.37
9	1	101	BCL	CHC-C4B	2.89	1.45	1.39
9	L	308	BCL	C3D-C2D	2.89	1.46	1.39
9	S	102	BCL	C3D-C2D	2.89	1.46	1.39
9	7	101	BCL	C3D-C2D	2.89	1.46	1.39
9	E	102	BCL	C4B-NB	-2.89	1.34	1.37
9	F	102	BCL	C3D-C2D	2.88	1.46	1.39
9	R	102	BCL	C3D-C2D	2.88	1.46	1.39
9	A	703	BCL	CHD-C4C	2.88	1.47	1.39
9	Y	103	BCL	C4B-NB	-2.88	1.34	1.37
9	M	803	BCL	C3D-C2D	2.87	1.46	1.39
9	R	102	BCL	C1D-ND	-2.87	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	703	BCL	C4B-NB	-2.86	1.34	1.37
9	Y	103	BCL	C3D-C2D	2.86	1.46	1.39
9	W	101	BCL	C3D-C2D	2.85	1.46	1.39
9	D	101	BCL	C3D-C2D	2.85	1.46	1.39
9	1	101	BCL	MG-NA	-2.85	1.99	2.06
9	8	102	BCL	C4B-NB	-2.85	1.34	1.37
9	1	101	BCL	C1D-ND	-2.84	1.34	1.37
9	6	101	BCL	C4B-NB	-2.84	1.34	1.37
9	V	101	BCL	C3D-C2D	2.84	1.46	1.39
9	L	308	BCL	C4B-NB	-2.84	1.34	1.37
9	V	101	BCL	C4B-NB	-2.84	1.34	1.37
9	L	309	BCL	C1D-ND	-2.84	1.34	1.37
9	4	101	BCL	C4B-NB	-2.84	1.34	1.37
9	4	101	BCL	C1D-ND	-2.83	1.34	1.37
9	8	102	BCL	C1B-C2B	2.82	1.49	1.43
9	O	101	BCL	C4B-NB	-2.82	1.34	1.37
9	L	301	BCL	C3D-C2D	2.81	1.46	1.39
9	M	803	BCL	C4B-NB	-2.81	1.34	1.37
9	S	102	BCL	C1D-ND	-2.81	1.34	1.37
9	7	101	BCL	CHD-C4C	2.80	1.47	1.39
9	2	101	BCL	C4B-NB	-2.80	1.34	1.37
9	L	308	BCL	C1D-ND	-2.80	1.34	1.37
9	P	102	BCL	C1D-ND	-2.80	1.34	1.37
9	D	101	BCL	C4B-NB	-2.80	1.34	1.37
9	E	102	BCL	C3D-C2D	2.79	1.46	1.39
9	Z	101	BCL	C4B-NB	-2.79	1.34	1.37
9	G	101	BCL	C1D-ND	-2.79	1.34	1.37
9	J	101	BCL	C1D-ND	-2.78	1.34	1.37
9	8	102	BCL	MG-NC	-2.78	1.99	2.06
9	W	101	BCL	C1D-ND	-2.78	1.34	1.37
9	J	101	BCL	C4B-NB	-2.77	1.34	1.37
9	N	102	BCL	C4B-NB	-2.76	1.34	1.37
9	V	101	BCL	CHD-C4C	2.75	1.46	1.39
9	F	102	BCL	C1D-ND	-2.75	1.34	1.37
9	Q	104	BCL	C1D-ND	-2.75	1.34	1.37
9	3	103	BCL	C4B-NB	-2.75	1.34	1.37
9	3	103	BCL	CHD-C4C	2.75	1.46	1.39
9	L	309	BCL	CHD-C4C	2.74	1.46	1.39
9	I	101	BCL	CHD-C4C	2.74	1.46	1.39
11	L	304	U10	C3-C2	-2.73	1.41	1.48
9	8	102	BCL	C1D-C2D	2.73	1.50	1.45
9	5	102	BCL	CHD-C4C	2.73	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	101	BCL	C1D-ND	-2.72	1.34	1.37
9	6	101	BCL	CHD-C4C	2.72	1.46	1.39
9	W	101	BCL	C4B-NB	-2.71	1.34	1.37
9	M	803	BCL	C1D-ND	-2.71	1.34	1.37
10	L	302	BPH	C3A-C2A	-2.71	1.52	1.54
9	B	101	BCL	C4B-NB	-2.71	1.34	1.37
11	L	303	U10	C3-C2	-2.71	1.41	1.48
9	8	102	BCL	MG-NA	-2.70	1.99	2.06
9	G	101	BCL	C1B-NB	-2.70	1.34	1.37
9	5	102	BCL	C1D-ND	-2.69	1.34	1.37
9	6	101	BCL	C1D-ND	-2.69	1.34	1.37
9	7	101	BCL	C4B-NB	-2.68	1.34	1.37
9	J	101	BCL	C1B-C2B	2.68	1.49	1.43
9	I	101	BCL	C4B-NB	-2.68	1.34	1.37
9	M	803	BCL	C1B-NB	-2.67	1.34	1.37
9	4	101	BCL	CHD-C4C	2.67	1.46	1.39
9	7	101	BCL	C1D-C2D	2.67	1.50	1.45
9	K	102	BCL	C1B-NB	-2.66	1.34	1.37
9	L	301	BCL	C1D-ND	-2.65	1.34	1.37
9	J	101	BCL	C1B-NB	-2.65	1.34	1.37
9	S	102	BCL	MG-NA	-2.64	2.00	2.06
9	L	301	BCL	CHD-C4C	2.63	1.46	1.39
9	1	101	BCL	CHD-C4C	2.62	1.46	1.39
9	A	703	BCL	C1B-C2B	2.62	1.49	1.43
9	3	103	BCL	C1D-C2D	2.62	1.50	1.45
9	G	101	BCL	CHD-C4C	2.62	1.46	1.39
9	A	703	BCL	C1D-C2D	2.62	1.50	1.45
9	R	102	BCL	CHD-C4C	2.61	1.46	1.39
9	3	103	BCL	C1D-ND	-2.61	1.34	1.37
9	B	101	BCL	CHD-C4C	2.60	1.46	1.39
9	K	102	BCL	CHD-C4C	2.60	1.46	1.39
9	L	308	BCL	CHD-C4C	2.60	1.46	1.39
9	F	102	BCL	CHD-C4C	2.60	1.46	1.39
9	W	101	BCL	CHD-C4C	2.60	1.46	1.39
9	Y	103	BCL	C1B-C2B	2.59	1.49	1.43
9	Q	104	BCL	CHD-C4C	2.59	1.46	1.39
9	M	803	BCL	CHD-C4C	2.58	1.46	1.39
9	V	101	BCL	C1D-ND	-2.58	1.34	1.37
9	D	101	BCL	CHD-C4C	2.57	1.46	1.39
10	M	804	BPH	C3A-C2A	-2.57	1.52	1.54
11	M	806	U10	C4-C5	-2.56	1.41	1.48
9	Z	101	BCL	CHD-C4C	2.56	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	101	BCL	C1D-C2D	2.56	1.50	1.45
9	E	102	BCL	CHD-C4C	2.56	1.46	1.39
9	N	102	BCL	CHD-C4C	2.56	1.46	1.39
9	F	102	BCL	C4B-NB	-2.55	1.34	1.37
9	J	101	BCL	CHD-C4C	2.55	1.46	1.39
9	S	102	BCL	CHD-C4C	2.55	1.46	1.39
9	P	102	BCL	C4B-NB	-2.55	1.34	1.37
9	M	803	BCL	C1D-C2D	2.55	1.50	1.45
9	E	102	BCL	C1B-NB	-2.55	1.34	1.37
9	8	102	BCL	C1D-ND	-2.53	1.34	1.37
9	F	102	BCL	C1B-NB	-2.53	1.34	1.37
9	2	101	BCL	C1B-C2B	2.53	1.49	1.43
11	M	806	U10	C3-C2	-2.53	1.41	1.48
9	L	301	BCL	C4B-NB	-2.52	1.34	1.37
9	V	101	BCL	C1B-NB	-2.52	1.34	1.37
9	L	309	BCL	C1B-NB	-2.52	1.34	1.37
9	2	101	BCL	CHD-C4C	2.52	1.46	1.39
9	L	301	BCL	C1D-C2D	2.52	1.50	1.45
9	B	101	BCL	C1B-C2B	2.52	1.49	1.43
9	4	101	BCL	C1B-C2B	2.52	1.49	1.43
9	3	103	BCL	MG-NA	-2.52	2.00	2.06
9	O	101	BCL	CHD-C4C	2.51	1.46	1.39
9	L	309	BCL	C1D-C2D	2.51	1.50	1.45
9	P	102	BCL	CHD-C4C	2.51	1.46	1.39
9	Z	101	BCL	C1B-C2B	2.51	1.49	1.43
9	T	101	BCL	C1B-NB	-2.51	1.34	1.37
9	5	102	BCL	C1D-C2D	2.50	1.50	1.45
9	O	101	BCL	C1D-ND	-2.50	1.34	1.37
9	7	101	BCL	C1B-NB	-2.49	1.34	1.37
9	4	101	BCL	C1B-NB	-2.49	1.34	1.37
9	I	101	BCL	C1B-NB	-2.49	1.34	1.37
9	Y	103	BCL	CHD-C4C	2.48	1.46	1.39
9	4	101	BCL	MG-NC	-2.48	2.00	2.06
9	K	102	BCL	C1D-ND	-2.47	1.34	1.37
9	O	101	BCL	C1B-NB	-2.47	1.34	1.37
9	L	309	BCL	MG-NC	-2.47	2.00	2.06
9	6	101	BCL	C1B-C2B	2.46	1.48	1.43
11	L	303	U10	C4-C5	-2.46	1.41	1.48
9	6	101	BCL	C1B-NB	-2.46	1.34	1.37
9	T	101	BCL	CHD-C4C	2.45	1.46	1.39
9	V	101	BCL	C1D-C2D	2.44	1.50	1.45
9	T	101	BCL	C1B-C2B	2.44	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	101	BCL	C1D-ND	-2.44	1.34	1.37
9	4	101	BCL	C1D-C2D	2.43	1.50	1.45
9	E	102	BCL	MG-NC	-2.43	2.00	2.06
9	R	102	BCL	C1B-C2B	2.43	1.48	1.43
9	2	101	BCL	MG-NA	-2.43	2.00	2.06
9	L	308	BCL	C1B-NB	-2.42	1.34	1.37
9	N	102	BCL	C1B-NB	-2.42	1.34	1.37
9	A	703	BCL	MG-NC	-2.42	2.00	2.06
9	1	101	BCL	C1D-C2D	2.41	1.50	1.45
9	S	102	BCL	C1D-C2D	2.41	1.50	1.45
9	7	101	BCL	C1D-ND	-2.40	1.34	1.37
9	L	309	BCL	MG-NA	-2.40	2.00	2.06
9	6	101	BCL	MG-NC	-2.40	2.00	2.06
9	W	101	BCL	C1B-C2B	2.40	1.48	1.43
9	P	102	BCL	C1B-NB	-2.40	1.34	1.37
9	Q	104	BCL	C1B-C2B	2.39	1.48	1.43
9	G	101	BCL	C1B-C2B	2.39	1.48	1.43
9	J	101	BCL	MG-NA	-2.39	2.00	2.06
9	N	102	BCL	C1B-C2B	2.38	1.48	1.43
9	R	102	BCL	C1B-NB	-2.38	1.34	1.37
9	3	103	BCL	C1B-NB	-2.38	1.34	1.37
9	2	101	BCL	MG-NC	-2.37	2.00	2.06
9	L	308	BCL	MG-NA	-2.37	2.00	2.06
9	J	101	BCL	MG-NC	-2.37	2.00	2.06
9	B	101	BCL	C1B-NB	-2.37	1.34	1.37
9	D	101	BCL	C1B-NB	-2.36	1.34	1.37
9	P	102	BCL	C1B-C2B	2.36	1.48	1.43
9	5	102	BCL	C1B-NB	-2.36	1.34	1.37
9	G	101	BCL	MG-NC	-2.36	2.00	2.06
9	W	101	BCL	C1B-NB	-2.36	1.34	1.37
9	K	102	BCL	MG-NA	-2.36	2.00	2.06
9	R	102	BCL	MG-NA	-2.35	2.00	2.06
9	Y	103	BCL	C1B-NB	-2.35	1.34	1.37
9	4	101	BCL	MG-NA	-2.35	2.00	2.06
9	L	301	BCL	C1B-C2B	2.34	1.48	1.43
9	K	102	BCL	C1D-C2D	2.34	1.50	1.45
9	1	101	BCL	C1B-C2B	2.34	1.48	1.43
9	R	102	BCL	MG-NC	-2.34	2.00	2.06
9	W	101	BCL	MG-NC	-2.33	2.00	2.06
9	D	101	BCL	C1D-C2D	2.33	1.49	1.45
9	N	102	BCL	MG-NC	-2.33	2.00	2.06
9	S	102	BCL	C1B-NB	-2.32	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	301	BCL	C1B-NB	-2.32	1.34	1.37
9	Q	104	BCL	C1D-C2D	2.32	1.49	1.45
9	M	803	BCL	MG-NA	-2.32	2.00	2.06
9	A	703	BCL	C1D-ND	-2.32	1.34	1.37
9	2	101	BCL	C1B-NB	-2.32	1.34	1.37
9	F	102	BCL	C1D-C2D	2.31	1.49	1.45
9	3	103	BCL	C1B-C2B	2.31	1.48	1.43
9	Y	103	BCL	MG-NA	-2.31	2.00	2.06
9	L	308	BCL	C1D-C2D	2.31	1.49	1.45
9	E	102	BCL	MG-NA	-2.31	2.00	2.06
9	K	102	BCL	C1B-C2B	2.30	1.48	1.43
9	M	803	BCL	MG-NC	-2.30	2.00	2.06
9	O	101	BCL	C1D-C2D	2.30	1.49	1.45
9	D	101	BCL	C1B-C2B	2.30	1.48	1.43
9	7	101	BCL	MG-NC	-2.29	2.00	2.06
9	E	102	BCL	C1B-C2B	2.29	1.48	1.43
9	T	101	BCL	MG-NC	-2.29	2.00	2.06
9	3	103	BCL	MG-NC	-2.29	2.00	2.06
9	6	101	BCL	MG-NA	-2.29	2.00	2.06
9	D	101	BCL	MG-NA	-2.29	2.00	2.06
9	Q	104	BCL	C1B-NB	-2.29	1.34	1.37
9	R	102	BCL	C1D-C2D	2.28	1.49	1.45
9	T	101	BCL	MG-NA	-2.28	2.00	2.06
9	J	101	BCL	C1D-C2D	2.28	1.49	1.45
9	S	102	BCL	C1B-C2B	2.28	1.48	1.43
9	5	102	BCL	C1B-C2B	2.28	1.48	1.43
9	L	308	BCL	C1B-C2B	2.28	1.48	1.43
9	M	803	BCL	C1B-C2B	2.28	1.48	1.43
9	Q	104	BCL	MG-NA	-2.27	2.00	2.06
9	V	101	BCL	MG-NC	-2.27	2.00	2.06
9	Z	101	BCL	C1B-NB	-2.27	1.34	1.37
9	I	101	BCL	MG-NA	-2.27	2.00	2.06
9	P	102	BCL	C1D-C2D	2.27	1.49	1.45
9	N	102	BCL	MG-NA	-2.26	2.00	2.06
9	A	703	BCL	MG-NA	-2.26	2.00	2.06
9	F	102	BCL	MG-NC	-2.26	2.00	2.06
9	Y	103	BCL	C1D-C2D	2.25	1.49	1.45
9	Z	101	BCL	C1D-C2D	2.25	1.49	1.45
9	8	102	BCL	C1B-NB	-2.24	1.34	1.37
9	7	101	BCL	C1B-C2B	2.24	1.48	1.43
9	W	101	BCL	MG-NA	-2.24	2.00	2.06
9	5	102	BCL	MG-NC	-2.24	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	1	101	BCL	C1B-NB	-2.24	1.34	1.37
9	Z	101	BCL	MG-NC	-2.23	2.01	2.06
9	G	101	BCL	MG-NA	-2.23	2.01	2.06
9	L	309	BCL	C1B-C2B	2.23	1.48	1.43
9	5	102	BCL	MG-NA	-2.22	2.01	2.06
9	B	101	BCL	MG-NC	-2.21	2.01	2.06
9	B	101	BCL	MG-NA	-2.21	2.01	2.06
9	K	102	BCL	MG-NC	-2.21	2.01	2.06
9	L	301	BCL	MG-NC	-2.21	2.01	2.06
9	V	101	BCL	C1B-C2B	2.21	1.48	1.43
9	Z	101	BCL	MG-NA	-2.21	2.01	2.06
10	L	302	BPH	CBD-CGD	-2.20	1.49	1.52
9	I	101	BCL	MG-NC	-2.20	2.01	2.06
9	E	102	BCL	C1D-C2D	2.20	1.49	1.45
9	W	101	BCL	C1D-C2D	2.20	1.49	1.45
9	F	102	BCL	C1B-C2B	2.20	1.48	1.43
9	V	101	BCL	MG-NA	-2.19	2.01	2.06
9	L	308	BCL	MG-NC	-2.19	2.01	2.06
9	2	101	BCL	C1D-C2D	2.18	1.49	1.45
9	B	101	BCL	C1D-C2D	2.18	1.49	1.45
9	A	703	BCL	C1B-NB	-2.18	1.35	1.37
9	F	102	BCL	MG-NA	-2.18	2.01	2.06
9	O	101	BCL	CHB-C4A	-2.17	1.32	1.37
9	N	102	BCL	C1D-C2D	2.17	1.49	1.45
9	7	101	BCL	MG-NA	-2.16	2.01	2.06
9	I	101	BCL	C1B-C2B	2.16	1.48	1.43
9	6	101	BCL	C1D-C2D	2.16	1.49	1.45
9	P	102	BCL	MG-NA	-2.16	2.01	2.06
9	P	102	BCL	MG-NC	-2.16	2.01	2.06
9	J	101	BCL	C3C-C4C	-2.15	1.48	1.51
9	Q	104	BCL	CHC-C1C	-2.14	1.32	1.37
9	T	101	BCL	C1D-C2D	2.14	1.49	1.45
9	G	101	BCL	C1D-C2D	2.14	1.49	1.45
9	I	101	BCL	C3C-C4C	-2.14	1.48	1.51
9	7	101	BCL	CHB-C4A	-2.13	1.32	1.37
9	O	101	BCL	MG-NA	-2.12	2.01	2.06
9	5	102	BCL	CHC-C1C	-2.11	1.32	1.37
10	M	804	BPH	CBD-CGD	-2.11	1.49	1.52
9	J	101	BCL	CHC-C1C	-2.10	1.32	1.37
9	2	101	BCL	C3C-C4C	-2.10	1.49	1.51
9	Y	103	BCL	MG-NC	-2.10	2.01	2.06
11	L	304	U10	C4-C5	-2.08	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	101	BCL	CHB-C4A	-2.08	1.32	1.37
9	L	301	BCL	MG-NA	-2.08	2.01	2.06
9	1	101	BCL	C4D-CHA	2.08	1.45	1.38
9	T	101	BCL	CHC-C1C	-2.07	1.32	1.37
9	Z	101	BCL	C3C-C4C	-2.07	1.49	1.51
9	O	101	BCL	C1B-C2B	2.07	1.48	1.43
9	Z	101	BCL	CHC-C1C	-2.07	1.32	1.37
9	1	101	BCL	CHC-C1C	-2.07	1.32	1.37
9	K	102	BCL	CHC-C1C	-2.06	1.32	1.37
9	Q	104	BCL	C4D-CHA	2.06	1.45	1.38
9	W	101	BCL	C3C-C4C	-2.06	1.49	1.51
9	A	703	BCL	C4D-CHA	2.05	1.45	1.38
9	W	101	BCL	CHC-C1C	-2.05	1.32	1.37
9	M	803	BCL	C3C-C4C	-2.05	1.49	1.51
9	D	101	BCL	MG-NC	-2.04	2.01	2.06
9	N	102	BCL	C3C-C4C	-2.04	1.49	1.51
9	L	308	BCL	CHC-C1C	-2.03	1.32	1.37
9	E	102	BCL	C3C-C4C	-2.03	1.49	1.51
9	S	102	BCL	MG-NC	-2.02	2.01	2.06
9	O	101	BCL	C4D-CHA	2.02	1.45	1.38
9	F	102	BCL	CHB-C4A	-2.02	1.32	1.37
9	5	102	BCL	CHB-C4A	-2.00	1.32	1.37

All (1241) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	301	BCL	CMD-C2D-C1D	8.27	139.28	124.73
9	8	102	BCL	CMD-C2D-C1D	8.14	139.06	124.73
9	M	803	BCL	CMD-C2D-C1D	8.13	139.05	124.73
9	A	703	BCL	CMD-C2D-C1D	8.09	138.97	124.73
9	7	101	BCL	CMD-C2D-C1D	8.09	138.97	124.73
9	I	101	BCL	CMD-C2D-C1D	7.98	138.78	124.73
9	S	102	BCL	CMD-C2D-C1D	7.89	138.62	124.73
9	V	101	BCL	CMD-C2D-C1D	7.84	138.53	124.73
9	3	103	BCL	CMD-C2D-C1D	7.81	138.48	124.73
9	1	101	BCL	CMD-C2D-C1D	7.80	138.47	124.73
9	D	101	BCL	CMD-C2D-C1D	7.76	138.40	124.73
9	5	102	BCL	CMD-C2D-C1D	7.74	138.37	124.73
9	K	102	BCL	CMD-C2D-C1D	7.65	138.20	124.73
15	R	101	SPO	C26-C27-C28	-7.63	116.97	127.69
9	F	102	BCL	CMD-C2D-C1D	7.60	138.11	124.73
9	L	308	BCL	CMD-C2D-C1D	7.60	138.11	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Q	104	BCL	CMD-C2D-C1D	7.57	138.05	124.73
9	4	101	BCL	CMD-C2D-C1D	7.56	138.04	124.73
9	O	101	BCL	CMD-C2D-C1D	7.54	138.01	124.73
15	W	102	SPO	C26-C27-C28	-7.52	117.11	127.69
9	W	101	BCL	CMD-C2D-C1D	7.52	137.98	124.73
9	Y	103	BCL	CMD-C2D-C1D	7.50	137.94	124.73
9	E	102	BCL	CMD-C2D-C1D	7.42	137.79	124.73
9	L	309	BCL	CMD-C2D-C1D	7.41	137.77	124.73
9	J	101	BCL	CMD-C2D-C1D	7.34	137.65	124.73
9	R	102	BCL	CMD-C2D-C1D	7.33	137.64	124.73
9	6	101	BCL	CMD-C2D-C1D	7.28	137.55	124.73
9	N	102	BCL	CMD-C2D-C1D	7.27	137.53	124.73
9	P	102	BCL	CMD-C2D-C1D	7.05	137.14	124.73
9	7	101	BCL	C2B-C1B-NB	7.03	117.62	110.33
9	Z	101	BCL	CMD-C2D-C1D	7.01	137.08	124.73
9	5	102	BCL	C2B-C1B-NB	7.01	117.60	110.33
9	T	101	BCL	CMD-C2D-C1D	6.96	136.99	124.73
9	O	101	BCL	C2B-C1B-NB	6.87	117.45	110.33
9	B	101	BCL	CMD-C2D-C1D	6.85	136.79	124.73
9	I	101	BCL	C2B-C1B-NB	6.85	117.43	110.33
9	2	101	BCL	CMD-C2D-C1D	6.84	136.77	124.73
9	3	103	BCL	C2B-C1B-NB	6.75	117.32	110.33
15	G	103	SPO	C10-C9-C7	-6.74	117.83	127.28
9	K	102	BCL	C2B-C1B-NB	6.72	117.30	110.33
9	F	102	BCL	C2B-C1B-NB	6.69	117.26	110.33
9	V	101	BCL	C2B-C1B-NB	6.69	117.26	110.33
9	L	301	BCL	C2B-C1B-NB	6.66	117.23	110.33
9	S	102	BCL	C2B-C1B-NB	6.66	117.23	110.33
9	D	101	BCL	C2B-C1B-NB	6.64	117.21	110.33
15	O	103	SPO	C4-C5-C6	-6.63	115.60	124.91
15	S	103	SPO	C4-C5-C6	-6.62	115.62	124.91
9	G	101	BCL	CMD-C2D-C1D	6.62	136.38	124.73
9	P	102	BCL	C2B-C1B-NB	6.51	117.08	110.33
9	N	102	BCL	C2B-C1B-NB	6.50	117.06	110.33
9	1	101	BCL	C2B-C1B-NB	6.50	117.06	110.33
9	R	102	BCL	C2B-C1B-NB	6.44	117.01	110.33
15	R	101	SPO	C10-C9-C7	-6.44	118.25	127.28
9	L	308	BCL	O2D-CGD-CBD	6.43	122.47	111.23
9	E	102	BCL	C2B-C1B-NB	6.43	116.99	110.33
9	L	309	BCL	C2B-C1B-NB	6.41	116.97	110.33
9	M	803	BCL	C2B-C1B-NB	6.41	116.97	110.33
15	G	102	SPO	C4-C5-C6	-6.40	115.92	124.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Q	104	BCL	C2B-C1B-NB	6.35	116.91	110.33
9	Y	103	BCL	C2B-C1B-NB	6.33	116.89	110.33
15	5	103	SPO	C4-C5-C6	-6.31	116.05	124.91
15	N	101	SPO	C10-C9-C7	-6.26	118.49	127.28
9	T	101	BCL	C2B-C1B-NB	6.26	116.82	110.33
15	R	101	SPO	C21-C22-C23	-6.24	118.53	127.28
15	G	103	SPO	C5-C6-C7	-6.23	116.47	125.89
15	3	104	SPO	C5-C6-C7	-6.22	116.49	125.89
9	W	101	BCL	C2B-C1B-NB	6.22	116.77	110.33
9	4	101	BCL	C2B-C1B-NB	6.13	116.69	110.33
9	L	308	BCL	C2B-C1B-NB	6.13	116.68	110.33
9	2	101	BCL	C2B-C1B-NB	6.12	116.67	110.33
9	B	101	BCL	C2B-C1B-NB	6.04	116.59	110.33
15	N	101	SPO	C5-C6-C7	-6.03	116.78	125.89
9	6	101	BCL	C2B-C1B-NB	6.03	116.58	110.33
9	S	102	BCL	CHD-C1D-ND	-6.00	116.36	124.80
9	L	301	BCL	CHD-C1D-ND	-6.00	116.36	124.80
15	X	102	SPO	C4-C5-C6	-5.99	116.51	124.91
15	8	101	SPO	C21-C22-C23	-5.98	118.89	127.28
15	O	103	SPO	C26-C27-C28	-5.96	119.30	127.69
9	A	703	BCL	C2B-C1B-NB	5.96	116.50	110.33
9	1	101	BCL	CHD-C1D-ND	-5.95	116.43	124.80
15	T	102	SPO	C10-C9-C7	-5.95	118.94	127.28
15	V	102	SPO	C4-C5-C6	-5.93	116.59	124.91
15	3	104	SPO	C10-C9-C7	-5.92	118.97	127.28
15	R	101	SPO	C5-C6-C7	-5.91	116.96	125.89
9	3	103	BCL	CHD-C1D-ND	-5.88	116.53	124.80
9	G	101	BCL	C2B-C1B-NB	5.88	116.42	110.33
15	V	103	SPO	C4-C5-C6	-5.88	116.66	124.91
9	8	102	BCL	CHD-C1D-ND	-5.86	116.55	124.80
9	M	803	BCL	CHD-C1D-ND	-5.86	116.56	124.80
9	Z	101	BCL	C2B-C1B-NB	5.81	116.35	110.33
15	K	103	SPO	C4-C5-C6	-5.81	116.76	124.91
9	I	101	BCL	CHD-C1D-ND	-5.80	116.64	124.80
9	A	703	BCL	CHD-C1D-ND	-5.80	116.64	124.80
9	D	101	BCL	CHD-C1D-ND	-5.77	116.68	124.80
15	F	103	SPO	C4-C5-C6	-5.69	116.92	124.91
9	7	101	BCL	CHD-C1D-ND	-5.66	116.84	124.80
9	J	101	BCL	C2B-C1B-NB	5.64	116.18	110.33
9	5	102	BCL	CHD-C1D-ND	-5.63	116.88	124.80
9	L	309	BCL	CHD-C1D-ND	-5.63	116.88	124.80
15	1	102	SPO	C20-C19-C17	-5.63	119.39	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	1	102	SPO	C4-C5-C6	-5.62	117.02	124.91
9	Q	104	BCL	CHD-C1D-ND	-5.60	116.92	124.80
9	L	309	BCL	O2D-CGD-CBD	5.60	121.02	111.23
15	S	103	SPO	C20-C19-C17	-5.59	119.44	127.28
15	1	103	SPO	C5-C6-C7	-5.58	117.45	125.89
9	4	101	BCL	CHD-C1D-ND	-5.56	116.97	124.80
15	D	102	SPO	C4-C5-C6	-5.56	117.11	124.91
9	K	102	BCL	CHD-C1D-ND	-5.55	116.99	124.80
9	R	102	BCL	CHD-C1D-ND	-5.52	117.04	124.80
9	V	101	BCL	CHD-C1D-ND	-5.49	117.08	124.80
15	1	102	SPO	C21-C22-C23	-5.47	119.61	127.28
9	J	101	BCL	CHD-C1D-ND	-5.46	117.12	124.80
9	E	102	BCL	CHD-C1D-ND	-5.45	117.13	124.80
9	2	101	BCL	CHD-C1D-ND	-5.41	117.18	124.80
15	5	103	SPO	C21-C22-C23	-5.41	119.69	127.28
9	O	101	BCL	CHD-C1D-ND	-5.39	117.22	124.80
15	G	102	SPO	C21-C22-C23	-5.39	119.72	127.28
9	F	102	BCL	CHD-C1D-ND	-5.38	117.23	124.80
9	7	101	BCL	O2D-CGD-CBD	5.38	120.63	111.23
9	L	308	BCL	CHD-C1D-ND	-5.38	117.23	124.80
9	Y	103	BCL	CHD-C1D-ND	-5.37	117.24	124.80
15	O	102	SPO	C21-C22-C23	-5.36	119.76	127.28
9	W	101	BCL	CHD-C1D-ND	-5.33	117.30	124.80
15	V	102	SPO	C26-C27-C28	-5.33	120.20	127.69
9	P	102	BCL	CHD-C1D-ND	-5.33	117.31	124.80
15	1	105	SPO	C4-C5-C6	-5.31	117.46	124.91
9	N	102	BCL	CHD-C1D-ND	-5.30	117.34	124.80
9	Z	101	BCL	CHD-C1D-ND	-5.29	117.36	124.80
15	1	103	SPO	C10-C9-C7	-5.29	119.86	127.28
9	8	102	BCL	C2B-C1B-NB	5.27	115.79	110.33
9	5	102	BCL	O2D-CGD-CBD	5.24	120.38	111.23
9	T	101	BCL	CHD-C1D-ND	-5.22	117.46	124.80
15	O	102	SPO	C20-C19-C17	-5.15	120.06	127.28
15	O	102	SPO	C4-C5-C6	-5.14	117.69	124.91
9	O	101	BCL	O2D-CGD-CBD	5.13	120.20	111.23
9	S	102	BCL	C3D-C2D-C1D	-5.13	98.84	105.83
15	S	103	SPO	C21-C22-C23	-5.12	120.09	127.28
9	6	101	BCL	CHD-C1D-ND	-5.12	117.60	124.80
9	O	101	BCL	C3D-C2D-C1D	-5.11	98.85	105.83
9	K	102	BCL	O2D-CGD-CBD	5.11	120.17	111.23
9	B	101	BCL	CHD-C1D-ND	-5.10	117.62	124.80
9	S	102	BCL	O2D-CGD-CBD	5.07	120.10	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	101	BCL	CHD-C1D-ND	-5.04	117.70	124.80
9	L	301	BCL	C3D-C2D-C1D	-5.04	98.95	105.83
15	1	105	SPO	C26-C27-C28	-5.04	120.60	127.69
9	M	803	BCL	C3D-C2D-C1D	-5.03	98.96	105.83
9	8	102	BCL	O2D-CGD-CBD	5.03	120.02	111.23
9	Q	104	BCL	C3D-C2D-C1D	-5.02	98.97	105.83
9	I	101	BCL	C3D-C2D-C1D	-5.02	98.98	105.83
17	M	811	CDL	OB6-CB5-C51	5.00	122.29	111.48
9	D	101	BCL	C3D-C2D-C1D	-4.96	99.06	105.83
9	5	102	BCL	C3D-C2D-C1D	-4.96	99.06	105.83
15	M	807	SPO	C26-C27-C28	-4.96	120.72	127.69
15	K	103	SPO	C21-C22-C23	-4.94	120.34	127.28
15	5	103	SPO	C26-C27-C28	-4.93	120.76	127.69
9	1	101	BCL	C3C-C4C-CHD	-4.92	113.02	123.39
9	1	101	BCL	C3D-C2D-C1D	-4.91	99.13	105.83
9	3	103	BCL	C3D-C2D-C1D	-4.88	99.17	105.83
15	F	104	SPO	C10-C9-C7	-4.88	120.44	127.28
9	K	102	BCL	C3D-C2D-C1D	-4.86	99.20	105.83
9	N	102	BCL	O2D-CGD-CBD	4.86	119.72	111.23
9	Y	103	BCL	C3D-C2D-C1D	-4.86	99.20	105.83
9	1	101	BCL	O2D-CGD-CBD	4.86	119.72	111.23
9	M	803	BCL	O2D-CGD-CBD	4.85	119.71	111.23
9	A	703	BCL	C3D-C2D-C1D	-4.85	99.21	105.83
9	7	101	BCL	C3D-C2D-C1D	-4.85	99.22	105.83
15	G	102	SPO	C26-C27-C28	-4.84	120.88	127.69
9	F	102	BCL	C3D-C2D-C1D	-4.83	99.23	105.83
9	2	101	BCL	O2D-CGD-CBD	4.83	119.67	111.23
9	O	101	BCL	C3C-C4C-CHD	-4.82	113.23	123.39
9	V	101	BCL	C3D-C2D-C1D	-4.82	99.26	105.83
9	P	102	BCL	C3D-C2D-C1D	-4.81	99.27	105.83
9	Y	103	BCL	C3C-C4C-CHD	-4.81	113.25	123.39
15	O	102	SPO	C26-C27-C28	-4.80	120.94	127.69
9	S	102	BCL	C3C-C4C-CHD	-4.79	113.30	123.39
9	D	101	BCL	C3C-C4C-CHD	-4.78	113.30	123.39
15	X	102	SPO	C21-C22-C23	-4.78	120.58	127.28
9	I	101	BCL	O2D-CGD-CBD	4.78	119.58	111.23
9	Q	104	BCL	O2D-CGD-CBD	4.77	119.58	111.23
15	P	101	SPO	C4-C5-C6	-4.77	118.21	124.91
15	5	104	SPO	C20-C19-C17	-4.77	120.58	127.28
15	5	103	SPO	C20-C19-C17	-4.77	120.59	127.28
9	D	101	BCL	O2D-CGD-CBD	4.76	119.55	111.23
9	N	102	BCL	C3D-C2D-C1D	-4.75	99.35	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	101	BCL	O2D-CGD-CBD	4.75	119.54	111.23
9	T	101	BCL	C3D-C2D-C1D	-4.74	99.36	105.83
9	Z	101	BCL	C3D-C2D-C1D	-4.74	99.36	105.83
9	2	101	BCL	C3D-C2D-C1D	-4.73	99.37	105.83
9	R	102	BCL	O2D-CGD-CBD	4.73	119.50	111.23
9	Y	103	BCL	O2D-CGD-CBD	4.73	119.50	111.23
9	J	101	BCL	C3D-C2D-C1D	-4.72	99.39	105.83
15	8	101	SPO	C10-C9-C7	-4.70	120.68	127.28
9	W	101	BCL	C3D-C2D-C1D	-4.70	99.42	105.83
9	L	308	BCL	C3D-C2D-C1D	-4.69	99.43	105.83
9	6	101	BCL	O2D-CGD-CBD	4.69	119.42	111.23
9	4	101	BCL	C3D-C2D-C1D	-4.68	99.44	105.83
9	N	102	BCL	C3C-C4C-CHD	-4.68	113.52	123.39
9	E	102	BCL	C3D-C2D-C1D	-4.67	99.46	105.83
15	S	103	SPO	C26-C27-C28	-4.65	121.15	127.69
9	B	101	BCL	C3D-C2D-C1D	-4.65	99.49	105.83
9	R	102	BCL	C3D-C2D-C1D	-4.64	99.50	105.83
15	V	103	SPO	C21-C22-C23	-4.64	120.78	127.28
9	Q	104	BCL	C3C-C4C-CHD	-4.63	113.64	123.39
9	2	101	BCL	C3C-C4C-CHD	-4.63	113.64	123.39
15	X	102	SPO	C29-C28-C30	4.62	123.25	115.23
9	J	101	BCL	O2D-CGD-CBD	4.60	119.27	111.23
15	1	105	SPO	C20-C19-C17	-4.60	120.83	127.28
9	P	102	BCL	O2D-CGD-CBD	4.59	119.25	111.23
9	L	309	BCL	C3D-C2D-C1D	-4.59	99.57	105.83
9	Z	101	BCL	C3C-C4C-CHD	-4.59	113.72	123.39
9	M	803	BCL	C3C-C4C-CHD	-4.58	113.74	123.39
15	P	101	SPO	C10-C9-C7	-4.57	120.87	127.28
9	P	102	BCL	C3C-C4C-CHD	-4.56	113.78	123.39
9	G	101	BCL	C3D-C2D-C1D	-4.55	99.62	105.83
9	6	101	BCL	C3D-C2D-C1D	-4.54	99.63	105.83
9	B	101	BCL	O2D-CGD-CBD	4.54	119.17	111.23
9	T	101	BCL	C3C-C4C-CHD	-4.53	113.83	123.39
9	3	103	BCL	C3C-C4C-CHD	-4.53	113.84	123.39
15	8	101	SPO	C15-C14-C12	-4.53	120.93	127.28
15	O	103	SPO	C31-C32-C33	-4.50	117.31	127.62
9	A	703	BCL	O2D-CGD-CBD	4.50	119.10	111.23
15	F	104	SPO	C5-C6-C7	-4.48	119.12	125.89
15	5	104	SPO	C26-C27-C28	-4.47	121.40	127.69
9	I	101	BCL	C3C-C4C-CHD	-4.46	113.99	123.39
9	R	102	BCL	C3C-C4C-CHD	-4.44	114.03	123.39
9	E	102	BCL	C3C-C4C-CHD	-4.44	114.03	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	102	BCL	C3C-C4C-CHD	-4.42	114.07	123.39
9	W	101	BCL	C3C-C4C-CHD	-4.42	114.08	123.39
9	B	101	BCL	C3C-C4C-CHD	-4.40	114.11	123.39
9	W	101	BCL	O2D-CGD-CBD	4.38	118.89	111.23
9	P	102	BCL	C1D-ND-C4D	-4.38	103.24	106.31
9	M	803	BCL	C1D-ND-C4D	-4.36	103.25	106.31
15	E	101	SPO	C4-C5-C6	-4.36	118.79	124.91
9	3	103	BCL	O2D-CGD-CBD	4.34	118.82	111.23
12	M	801	PGV	O01-C1-C2	4.32	120.82	111.48
9	Z	101	BCL	O2D-CGD-CBD	4.32	118.78	111.23
9	2	101	BCL	C1D-ND-C4D	-4.32	103.28	106.31
9	K	102	BCL	C3C-C4C-CHD	-4.31	114.30	123.39
15	W	102	SPO	C4-C5-C6	-4.31	118.86	124.91
9	J	101	BCL	C3C-C4C-CHD	-4.30	114.32	123.39
15	8	101	SPO	C5-C6-C7	-4.30	119.39	125.89
9	1	101	BCL	C4A-NA-C1A	4.30	108.64	106.68
9	E	102	BCL	O2D-CGD-CBD	4.30	118.75	111.23
15	M	807	SPO	C31-C32-C33	-4.29	117.80	127.62
9	B	101	BCL	C1-C2-C3	-4.29	119.17	126.20
9	T	101	BCL	O2D-CGD-CBD	4.28	118.71	111.23
9	N	102	BCL	C1D-ND-C4D	-4.27	103.31	106.31
15	K	103	SPO	C20-C19-C17	-4.27	121.28	127.28
9	8	102	BCL	C3D-C2D-C1D	-4.27	100.00	105.83
15	5	104	SPO	C5-C6-C7	-4.27	119.44	125.89
15	K	103	SPO	C26-C27-C28	-4.26	121.69	127.69
12	3	102	PGV	O01-C1-C2	4.25	120.68	111.48
9	F	102	BCL	O2D-CGD-CBD	4.25	118.66	111.23
9	S	102	BCL	C1D-ND-C4D	-4.25	103.33	106.31
9	Y	103	BCL	C1D-ND-C4D	-4.24	103.33	106.31
9	L	308	BCL	C3C-C4C-CHD	-4.24	114.45	123.39
12	H	306	PGV	O01-C1-C2	4.23	120.64	111.48
9	5	102	BCL	C3C-C4C-CHD	-4.22	114.49	123.39
9	W	101	BCL	C1D-ND-C4D	-4.21	103.36	106.31
9	V	101	BCL	O2D-CGD-CBD	4.21	118.59	111.23
15	M	807	SPO	C21-C22-C23	-4.19	121.39	127.28
9	4	101	BCL	O2D-CGD-CBD	4.19	118.56	111.23
15	T	102	SPO	C5-C6-C7	-4.19	119.56	125.89
15	1	105	SPO	C21-C22-C23	-4.18	121.42	127.28
12	M	812	PGV	O01-C1-C2	4.17	120.51	111.48
9	N	102	BCL	C1-C2-C3	-4.17	119.37	126.20
9	4	101	BCL	C3C-C4C-CHD	-4.16	114.62	123.39
15	V	102	SPO	C21-C22-C23	-4.16	121.44	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	301	BCL	C1D-ND-C4D	-4.16	103.39	106.31
9	Y	103	BCL	C3B-C4B-NB	4.15	115.24	109.76
15	V	103	SPO	C20-C19-C17	-4.15	121.45	127.28
9	G	101	BCL	C3C-C4C-CHD	-4.15	114.65	123.39
9	D	101	BCL	C1D-ND-C4D	-4.15	103.40	106.31
9	1	101	BCL	C1C-NC-C4C	-4.14	104.79	106.68
9	Z	101	BCL	C1D-ND-C4D	-4.14	103.41	106.31
15	R	101	SPO	C20-C19-C17	-4.14	121.48	127.28
9	S	102	BCL	C2D-C1D-ND	4.13	114.22	110.13
15	5	104	SPO	C10-C9-C7	-4.13	121.48	127.28
9	3	103	BCL	C1D-ND-C4D	-4.13	103.42	106.31
9	Y	103	BCL	C1-C2-C3	-4.13	119.43	126.20
9	2	101	BCL	C1-C2-C3	-4.12	119.44	126.20
9	L	308	BCL	C1-C2-C3	-4.12	119.44	126.20
9	I	101	BCL	C1D-ND-C4D	-4.12	103.42	106.31
12	K	104	PGV	O01-C1-C2	4.10	120.34	111.48
9	J	101	BCL	C1D-ND-C4D	-4.08	103.45	106.31
9	W	101	BCL	C1-C2-C3	-4.08	119.52	126.20
9	E	102	BCL	C1D-ND-C4D	-4.07	103.45	106.31
9	6	101	BCL	C3C-C4C-CHD	-4.07	114.81	123.39
9	1	101	BCL	C1D-ND-C4D	-4.07	103.45	106.31
9	K	102	BCL	C3B-C4B-NB	4.07	115.13	109.76
9	L	301	BCL	O2D-CGD-CBD	4.07	118.34	111.23
9	S	102	BCL	C4A-NA-C1A	4.06	108.53	106.68
9	F	102	BCL	C1D-ND-C4D	-4.05	103.47	106.31
9	J	101	BCL	C3B-C4B-NB	4.05	115.11	109.76
9	L	301	BCL	C3C-C4C-CHD	-4.05	114.85	123.39
9	1	101	BCL	C3B-C4B-NB	4.05	115.10	109.76
9	7	101	BCL	C1D-ND-C4D	-4.04	103.47	106.31
12	L	310	PGV	O01-C1-C2	4.03	120.20	111.48
17	H	304	CDL	OB6-CB5-C51	4.03	120.20	111.48
15	V	102	SPO	C20-C19-C17	-4.03	121.63	127.28
15	O	103	SPO	C21-C22-C23	-4.02	121.63	127.28
15	G	102	SPO	C20-C19-C17	-4.02	121.64	127.28
9	F	102	BCL	C3B-C4B-NB	4.02	115.06	109.76
9	R	102	BCL	C1D-ND-C4D	-4.01	103.50	106.31
9	3	103	BCL	C3B-C4B-NB	4.00	115.04	109.76
9	P	102	BCL	C2D-C1D-ND	3.98	114.07	110.13
9	M	803	BCL	C3B-C4B-NB	3.98	115.01	109.76
9	1	101	BCL	C2D-C1D-ND	3.97	114.06	110.13
15	D	102	SPO	C21-C22-C23	-3.97	121.70	127.28
9	T	101	BCL	C1D-ND-C4D	-3.97	103.52	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	M	811	CDL	OA6-CA5-C11	3.97	120.06	111.48
15	W	102	SPO	C21-C22-C23	-3.97	121.72	127.28
15	5	104	SPO	C4-C5-C6	-3.96	119.35	124.91
15	5	103	SPO	C31-C32-C33	-3.96	118.56	127.62
15	D	102	SPO	C20-C19-C17	-3.96	121.73	127.28
9	D	101	BCL	C2D-C1D-ND	3.96	114.04	110.13
15	W	102	SPO	C20-C19-C17	-3.95	121.73	127.28
9	Y	103	BCL	C2D-C1D-ND	3.95	114.04	110.13
15	M	807	SPO	C4-C5-C6	-3.95	119.37	124.91
9	5	102	BCL	C3B-C4B-NB	3.93	114.95	109.76
9	7	101	BCL	C3B-C4B-NB	3.93	114.94	109.76
15	V	103	SPO	C26-C27-C28	-3.92	122.18	127.69
9	F	102	BCL	C2D-C1D-ND	3.92	114.00	110.13
9	Q	104	BCL	C2D-C1D-ND	3.91	114.00	110.13
15	X	102	SPO	C20-C19-C17	-3.90	121.80	127.28
17	H	304	CDL	OA6-CA5-C11	3.90	119.92	111.48
9	7	101	BCL	C3C-C4C-CHD	-3.90	115.17	123.39
9	Q	104	BCL	C3B-C4B-NB	3.89	114.90	109.76
12	X	101	PGV	O01-C1-C2	3.89	119.90	111.48
9	2	101	BCL	C2D-C1D-ND	3.89	113.98	110.13
9	5	102	BCL	C1D-ND-C4D	-3.88	103.59	106.31
9	V	101	BCL	C3C-C4C-CHD	-3.88	115.21	123.39
9	L	308	BCL	C3B-C4B-NB	3.88	114.87	109.76
12	Y	104	PGV	O01-C1-C2	3.87	119.86	111.48
9	4	101	BCL	C1D-ND-C4D	-3.87	103.60	106.31
9	O	101	BCL	C2D-C1D-ND	3.87	113.95	110.13
16	H	301	LMT	O1B-C4'-C3'	3.86	117.05	107.23
15	8	101	SPO	C4-C5-C6	-3.86	119.49	124.91
9	Z	101	BCL	C2D-C1D-ND	3.86	113.95	110.13
9	L	308	BCL	C1D-ND-C4D	-3.86	103.60	106.31
15	1	102	SPO	C27-C26-C25	-3.86	112.03	123.20
9	S	102	BCL	C3B-C4B-NB	3.86	114.85	109.76
9	I	101	BCL	C2D-C1D-ND	3.85	113.94	110.13
9	N	102	BCL	C3B-C4B-NB	3.85	114.84	109.76
9	Q	104	BCL	C1D-ND-C4D	-3.85	103.61	106.31
12	Q	103	PGV	O01-C1-C2	3.83	119.78	111.48
9	Z	101	BCL	C3B-C4B-NB	3.83	114.82	109.76
9	M	803	BCL	C2D-C1D-ND	3.83	113.92	110.13
9	L	301	BCL	C3B-C4B-NB	3.83	114.81	109.76
9	P	102	BCL	C3B-C4B-NB	3.82	114.81	109.76
9	O	101	BCL	C1D-ND-C4D	-3.82	103.63	106.31
9	3	103	BCL	C2D-C1D-ND	3.81	113.90	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	1	101	BCL	C1-C2-C3	-3.81	119.96	126.20
9	2	101	BCL	C3B-C4B-NB	3.80	114.78	109.76
15	P	101	SPO	C5-C6-C7	-3.80	120.15	125.89
9	N	102	BCL	C2D-C1D-ND	3.80	113.88	110.13
9	5	102	BCL	C2D-C1D-ND	3.79	113.88	110.13
9	D	101	BCL	C3B-C4B-NB	3.78	114.74	109.76
15	E	101	SPO	C10-C9-C7	-3.77	121.98	127.28
9	T	101	BCL	C3B-C4B-NB	3.77	114.73	109.76
9	L	301	BCL	C2D-C1D-ND	3.77	113.86	110.13
15	M	807	SPO	C20-C19-C17	-3.76	122.00	127.28
9	T	101	BCL	C2D-C1D-ND	3.76	113.85	110.13
9	I	101	BCL	C3B-C4B-NB	3.76	114.72	109.76
9	W	101	BCL	C3B-C4B-NB	3.76	114.72	109.76
15	N	101	SPO	C20-C19-C17	-3.75	122.01	127.28
12	H	303	PGV	O01-C1-C2	3.75	119.60	111.48
17	Y	102	CDL	OB6-CB5-C51	3.75	119.60	111.48
15	X	102	SPO	C26-C27-C28	-3.75	122.42	127.69
9	S	102	BCL	C1-C2-C3	-3.73	120.09	126.20
9	W	101	BCL	C2D-C1D-ND	3.73	113.81	110.13
9	I	101	BCL	C1-C2-C3	-3.71	120.12	126.20
12	H	307	PGV	O01-C1-C2	3.69	119.47	111.48
15	5	104	SPO	C15-C14-C12	-3.69	122.11	127.28
9	E	102	BCL	C2D-C1D-ND	3.67	113.76	110.13
9	L	309	BCL	C3D-C4D-ND	3.67	115.95	109.99
9	P	102	BCL	C1-C2-C3	-3.67	120.19	126.20
9	J	101	BCL	C2D-C1D-ND	3.67	113.75	110.13
15	R	101	SPO	C26-C25-C23	-3.67	116.31	126.36
9	J	101	BCL	C1-C2-C3	-3.67	120.19	126.20
9	B	101	BCL	C1D-ND-C4D	-3.66	103.74	106.31
15	8	101	SPO	C21-C20-C19	-3.66	116.03	123.52
9	V	101	BCL	C3B-C4B-NB	3.65	114.58	109.76
9	K	102	BCL	C1D-ND-C4D	-3.65	103.75	106.31
15	R	101	SPO	C34-C33-C35	3.65	121.56	115.23
9	2	101	BCL	C3D-C4D-ND	3.63	115.89	109.99
15	T	102	SPO	C4-C5-C6	-3.63	119.81	124.91
15	F	103	SPO	C21-C22-C23	-3.63	122.19	127.28
15	1	102	SPO	C29-C28-C30	3.63	121.52	115.23
9	B	101	BCL	C2D-C1D-ND	3.62	113.71	110.13
9	L	309	BCL	C1D-ND-C4D	-3.62	103.77	106.31
12	L	305	PGV	O01-C1-C2	3.61	119.30	111.48
12	L	306	PGV	O01-C1-C2	3.60	119.27	111.48
9	G	101	BCL	C3B-C4B-NB	3.60	114.51	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	F	103	SPO	C20-C19-C17	-3.60	122.23	127.28
15	W	102	SPO	C5-C6-C7	-3.59	120.47	125.89
9	M	803	BCL	C3D-C4D-ND	3.59	115.82	109.99
9	L	309	BCL	C3B-C4B-NB	3.58	114.49	109.76
9	V	101	BCL	C1D-ND-C4D	-3.58	103.80	106.31
15	3	104	SPO	C26-C27-C28	-3.57	122.67	127.69
9	P	102	BCL	C3D-C4D-ND	3.57	115.79	109.99
15	T	102	SPO	C26-C27-C28	-3.57	122.67	127.69
9	8	102	BCL	C3D-C4D-ND	3.57	115.79	109.99
9	R	102	BCL	C3D-C4D-ND	3.57	115.79	109.99
17	H	305	CDL	OA6-CA5-C11	3.56	119.17	111.48
9	8	102	BCL	CHB-C1B-NB	-3.55	118.72	124.05
9	N	102	BCL	C3D-C4D-ND	3.55	115.76	109.99
15	8	101	SPO	C20-C19-C17	-3.55	122.30	127.28
9	R	102	BCL	C3B-C4B-NB	3.54	114.43	109.76
10	L	302	BPH	C4D-CHA-CBD	-3.54	106.76	108.45
9	6	101	BCL	C3B-C4B-NB	3.54	114.43	109.76
9	K	102	BCL	C2D-C1D-ND	3.54	113.62	110.13
9	7	101	BCL	C2D-C1D-ND	3.53	113.62	110.13
9	Q	104	BCL	C1-C2-C3	-3.52	120.42	126.20
9	Z	101	BCL	C3D-C4D-ND	3.52	115.70	109.99
9	4	101	BCL	C2D-C1D-ND	3.51	113.60	110.13
9	W	101	BCL	C3D-C4D-ND	3.51	115.69	109.99
9	R	102	BCL	C2D-C1D-ND	3.51	113.60	110.13
9	V	101	BCL	C2D-C1D-ND	3.51	113.59	110.13
9	4	101	BCL	C3D-C4D-ND	3.50	115.68	109.99
9	4	101	BCL	C3B-C4B-NB	3.50	114.38	109.76
15	V	103	SPO	C31-C32-C33	-3.50	119.62	127.62
9	O	101	BCL	C3B-C4B-NB	3.50	114.37	109.76
9	A	703	BCL	CHB-C1B-NB	-3.49	118.81	124.05
15	F	104	SPO	C4-C5-C6	-3.49	120.01	124.91
15	K	103	SPO	C15-C14-C12	-3.49	122.38	127.28
9	J	101	BCL	C3D-C4D-ND	3.48	115.65	109.99
15	8	101	SPO	C29-C28-C30	3.48	121.28	115.23
15	1	103	SPO	C26-C27-C28	-3.48	122.80	127.69
9	L	308	BCL	C3D-C4D-ND	3.48	115.64	109.99
9	G	101	BCL	C2D-C1D-ND	3.48	113.57	110.13
9	L	301	BCL	O2A-CGA-CBA	3.47	122.42	111.83
15	D	102	SPO	C31-C32-C33	-3.47	119.68	127.62
9	B	101	BCL	C3B-C4B-NB	3.47	114.33	109.76
9	T	101	BCL	C3D-C4D-ND	3.46	115.61	109.99
9	A	703	BCL	O2A-CGA-CBA	3.46	122.37	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	801	PGV	O03-C19-C20	3.46	122.37	111.83
9	7	101	BCL	C3D-C4D-ND	3.45	115.60	109.99
9	G	101	BCL	C1D-ND-C4D	-3.45	103.89	106.31
9	E	102	BCL	C3D-C4D-ND	3.45	115.60	109.99
15	O	103	SPO	C15-C14-C12	-3.44	122.45	127.28
9	L	308	BCL	C2D-C1D-ND	3.44	113.53	110.13
9	Z	101	BCL	C1-C2-C3	-3.44	120.56	126.20
9	E	102	BCL	C3B-C4B-NB	3.44	114.30	109.76
15	5	104	SPO	C20-C21-C22	-3.43	116.51	123.52
15	E	101	SPO	C20-C19-C17	-3.43	122.47	127.28
9	A	703	BCL	C4A-NA-C1A	3.42	108.24	106.68
9	6	101	BCL	C1D-ND-C4D	-3.42	103.92	106.31
15	G	103	SPO	C26-C27-C28	-3.41	122.89	127.69
9	3	103	BCL	C3D-C4D-ND	3.41	115.53	109.99
10	M	804	BPH	C4D-CHA-CBD	-3.41	106.82	108.45
9	L	301	BCL	C3D-C4D-ND	3.41	115.53	109.99
15	1	105	SPO	C31-C32-C33	-3.41	119.82	127.62
15	D	102	SPO	C9-C10-C11	-3.41	113.33	123.20
9	G	101	BCL	C4-C3-C5	3.41	121.14	115.23
9	Y	103	BCL	C3D-C4D-ND	3.40	115.52	109.99
9	A	703	BCL	C3B-C4B-NB	3.40	114.24	109.76
15	V	102	SPO	C31-C32-C33	-3.40	119.85	127.62
9	L	309	BCL	C3C-C4C-CHD	-3.38	116.26	123.39
9	A	703	BCL	C3C-C4C-CHD	-3.38	116.26	123.39
9	8	102	BCL	C3C-C4C-CHD	-3.38	116.26	123.39
15	1	103	SPO	C31-C32-C33	-3.38	119.89	127.62
9	F	102	BCL	C1-C2-C3	-3.38	120.66	126.20
15	G	103	SPO	C20-C19-C17	-3.37	122.55	127.28
15	5	104	SPO	C31-C32-C33	-3.37	119.91	127.62
9	B	101	BCL	C3D-C4D-ND	3.37	115.46	109.99
15	5	103	SPO	C10-C9-C7	-3.36	122.57	127.28
15	S	104	SPO	C34-C33-C35	3.36	121.06	115.23
9	6	101	BCL	C3D-C4D-ND	3.34	115.42	109.99
15	S	104	SPO	C29-C28-C30	3.31	120.97	115.23
15	E	101	SPO	C5-C6-C7	-3.31	120.90	125.89
9	F	102	BCL	C3D-C4D-ND	3.30	115.36	109.99
9	Z	101	BCL	O2A-CGA-CBA	3.30	121.90	111.83
9	I	101	BCL	C3D-C4D-ND	3.30	115.34	109.99
9	S	102	BCL	C3D-C4D-ND	3.29	115.34	109.99
9	5	102	BCL	C3D-C4D-ND	3.29	115.34	109.99
9	8	102	BCL	C3B-C4B-NB	3.29	114.10	109.76
9	D	101	BCL	C3D-C4D-ND	3.28	115.33	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	8	102	BCL	CHC-C4B-NB	-3.28	119.12	124.05
9	G	101	BCL	C3D-C4D-ND	3.28	115.31	109.99
9	L	308	BCL	O2D-CGD-O1D	-3.28	117.47	123.85
15	8	101	SPO	C26-C27-C28	-3.27	123.09	127.69
9	6	101	BCL	C1-C2-C3	-3.27	120.84	126.20
9	S	102	BCL	C1C-NC-C4C	-3.27	105.19	106.68
9	1	101	BCL	C3D-C4D-ND	3.27	115.30	109.99
9	J	101	BCL	O2A-CGA-CBA	3.26	121.77	111.83
9	8	102	BCL	C1D-ND-C4D	-3.26	104.03	106.31
15	G	103	SPO	C15-C14-C12	-3.26	122.71	127.28
9	K	102	BCL	C3D-C4D-ND	3.25	115.27	109.99
15	O	103	SPO	C9-C10-C11	-3.25	113.80	123.20
15	R	101	SPO	C21-C20-C19	-3.24	116.89	123.52
15	N	101	SPO	C29-C28-C30	3.24	120.85	115.23
9	P	102	BCL	O2A-CGA-CBA	3.22	121.65	111.83
9	L	309	BCL	C2D-C1D-ND	3.22	113.31	110.13
9	V	101	BCL	C4-C3-C5	3.22	120.81	115.23
15	P	101	SPO	C29-C28-C30	3.21	120.81	115.23
15	K	103	SPO	C9-C10-C11	-3.20	113.92	123.20
15	1	105	SPO	C9-C10-C11	-3.19	113.95	123.20
9	A	703	BCL	C2D-C1D-ND	3.19	113.28	110.13
15	E	101	SPO	C29-C28-C30	3.18	120.75	115.23
15	5	104	SPO	C29-C28-C30	3.18	120.75	115.23
15	S	104	SPO	C27-C26-C25	-3.18	113.98	123.20
9	Q	104	BCL	C3D-C4D-ND	3.18	115.15	109.99
15	D	102	SPO	C29-C28-C30	3.17	120.74	115.23
15	S	103	SPO	C15-C14-C12	-3.17	122.83	127.28
15	V	102	SPO	C9-C10-C11	-3.16	114.04	123.20
16	F	101	LMT	O1B-C4'-C3'	3.16	115.26	107.23
9	6	101	BCL	C2D-C1D-ND	3.15	113.25	110.13
9	T	101	BCL	C1-C2-C3	-3.15	121.03	126.20
9	V	101	BCL	C3D-C4D-ND	3.14	115.09	109.99
9	1	101	BCL	CHC-C1C-NC	3.14	128.93	124.40
15	F	104	SPO	C26-C27-C28	-3.14	123.28	127.69
15	M	807	SPO	C5-C6-C7	-3.14	121.15	125.89
12	L	306	PGV	O03-C19-C20	3.14	121.39	111.83
15	P	101	SPO	C21-C20-C19	-3.12	117.13	123.52
9	L	309	BCL	C1-C2-C3	-3.12	121.09	126.20
9	4	101	BCL	C1-C2-C3	-3.12	121.09	126.20
15	F	104	SPO	C21-C22-C23	-3.11	122.91	127.28
17	H	305	CDL	OB8-CB7-C71	3.11	120.59	111.15
15	G	103	SPO	C21-C22-C23	-3.11	122.92	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	3	103	BCL	O2A-CGA-CBA	3.10	121.30	111.83
15	V	103	SPO	C9-C10-C11	-3.10	114.21	123.20
9	7	101	BCL	C4-C3-C5	3.10	120.61	115.23
15	O	103	SPO	C21-C20-C19	-3.10	117.18	123.52
9	Z	101	BCL	C4-C3-C5	3.10	120.60	115.23
15	S	103	SPO	C31-C32-C33	-3.09	120.54	127.62
9	A	703	BCL	C1D-ND-C4D	-3.09	104.14	106.31
9	O	101	BCL	O2A-CGA-CBA	3.09	121.26	111.83
15	N	101	SPO	C34-C33-C35	3.09	120.59	115.23
9	Q	104	BCL	C1C-NC-C4C	-3.09	105.27	106.68
9	F	102	BCL	C4-C3-C5	3.08	120.58	115.23
9	P	102	BCL	C4-C3-C5	3.08	120.57	115.23
16	U	101	LMT	C1B-O1B-C4'	-3.08	110.69	117.98
9	T	101	BCL	O2A-CGA-CBA	3.07	121.21	111.83
12	H	306	PGV	O03-C19-C20	3.07	121.21	111.83
15	F	103	SPO	C34-C33-C35	3.07	120.56	115.23
9	S	102	BCL	CHC-C1C-NC	3.07	128.83	124.40
15	E	101	SPO	C31-C32-C33	-3.07	120.60	127.62
9	A	703	BCL	C3D-C4D-ND	3.07	114.97	109.99
9	V	101	BCL	C1-C2-C3	-3.07	121.17	126.20
15	5	103	SPO	C29-C28-C30	3.06	120.55	115.23
9	G	101	BCL	O2A-CGA-CBA	3.06	121.17	111.83
9	F	102	BCL	O2A-CGA-CBA	3.06	121.15	111.83
15	F	104	SPO	C20-C19-C17	-3.05	123.00	127.28
15	P	101	SPO	C34-C33-C35	3.05	120.52	115.23
9	6	101	BCL	CHC-C4B-NB	-3.05	119.48	124.05
9	5	102	BCL	C4-C3-C5	3.04	120.51	115.23
9	2	101	BCL	C4-C3-C5	3.04	120.50	115.23
12	H	306	PGV	C02-O01-C1	-3.03	110.54	117.80
15	G	103	SPO	C31-C32-C33	-3.03	120.68	127.62
9	3	103	BCL	C4-C3-C5	3.03	120.49	115.23
15	K	103	SPO	C29-C28-C30	3.03	120.48	115.23
9	3	103	BCL	CHC-C4B-NB	-3.02	119.51	124.05
9	I	101	BCL	CHB-C4A-NA	3.02	128.76	124.40
15	F	104	SPO	C29-C28-C30	3.02	120.46	115.23
15	1	103	SPO	C15-C14-C12	-3.02	123.05	127.28
9	Y	103	BCL	O2A-CGA-CBA	3.02	121.03	111.83
9	O	101	BCL	C3D-C4D-ND	3.01	114.89	109.99
9	D	101	BCL	C1-C2-C3	-3.01	121.26	126.20
15	F	103	SPO	C31-C32-C33	-3.01	120.73	127.62
9	7	101	BCL	O2A-CGA-CBA	3.01	121.00	111.83
9	B	101	BCL	C4-C3-C5	3.01	120.45	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	101	BCL	O2A-CGA-CBA	3.01	121.00	111.83
9	I	101	BCL	O2A-CGA-CBA	3.00	120.99	111.83
12	M	812	PGV	O03-C19-C20	2.99	120.96	111.83
9	L	309	BCL	O2D-CGD-O1D	-2.99	118.03	123.85
9	5	102	BCL	O2A-CGA-CBA	2.99	120.95	111.83
12	Y	104	PGV	C02-O01-C1	-2.99	110.64	117.80
15	P	101	SPO	C27-C26-C25	-2.98	114.55	123.20
15	G	102	SPO	C31-C32-C33	-2.98	120.80	127.62
15	F	103	SPO	C26-C27-C28	-2.98	123.50	127.69
9	K	102	BCL	O2A-CGA-CBA	2.98	120.92	111.83
9	3	103	BCL	CHC-C1C-NC	2.97	128.69	124.40
15	5	103	SPO	C9-C10-C11	-2.97	114.58	123.20
9	R	102	BCL	C1-C2-C3	-2.97	121.33	126.20
9	R	102	BCL	O2A-CGA-CBA	2.97	120.90	111.83
15	G	102	SPO	C15-C14-C12	-2.97	123.11	127.28
9	4	101	BCL	C4-C3-C5	2.96	120.36	115.23
15	G	103	SPO	C29-C28-C30	2.95	120.35	115.23
9	V	101	BCL	O2A-CGA-CBA	2.95	120.83	111.83
9	5	102	BCL	CHB-C4A-NA	2.95	128.66	124.40
15	N	101	SPO	C14-C15-C16	-2.95	114.66	123.20
9	8	102	BCL	O2A-CGA-CBA	2.95	120.82	111.83
9	8	102	BCL	CMD-C2D-C3D	-2.94	120.94	127.69
9	D	101	BCL	O2A-CGA-CBA	2.94	120.80	111.83
16	3	101	LMT	O1B-C4'-C3'	2.94	114.70	107.23
9	J	101	BCL	C4-C3-C5	2.94	120.33	115.23
9	T	101	BCL	C4-C3-C5	2.93	120.32	115.23
9	A	703	BCL	CHC-C4B-NB	-2.93	119.65	124.05
15	1	105	SPO	C14-C15-C16	-2.93	114.71	123.20
9	4	101	BCL	O2A-CGA-CBA	2.93	120.75	111.83
9	Q	104	BCL	O2A-CGA-CBA	2.92	120.75	111.83
15	X	102	SPO	C9-C10-C11	-2.92	114.73	123.20
15	3	104	SPO	C29-C28-C30	2.92	120.30	115.23
9	S	102	BCL	C4-C3-C5	2.92	120.29	115.23
15	V	103	SPO	C14-C15-C16	-2.92	114.75	123.20
12	K	104	PGV	O03-C19-C20	2.91	120.70	111.83
9	R	102	BCL	C4-C3-C5	2.90	120.27	115.23
9	L	309	BCL	O2A-CGA-CBA	2.90	120.67	111.83
15	3	104	SPO	C31-C32-C33	-2.90	120.99	127.62
15	O	103	SPO	C14-C15-C16	-2.90	114.81	123.20
15	N	101	SPO	C27-C26-C25	-2.89	114.81	123.20
9	M	803	BCL	CHC-C4B-NB	-2.89	119.71	124.05
9	K	102	BCL	C4-C3-C5	2.89	120.25	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	101	SPO	C26-C27-C28	-2.89	123.62	127.69
15	K	103	SPO	C31-C32-C33	-2.89	121.01	127.62
9	6	101	BCL	O2A-CGA-CBA	2.89	120.64	111.83
15	F	103	SPO	C9-C10-C11	-2.89	114.84	123.20
9	S	102	BCL	CHC-C4B-NB	-2.88	119.72	124.05
15	S	103	SPO	C34-C33-C35	2.88	120.23	115.23
16	I	102	LMT	O1B-C4'-C3'	2.88	114.55	107.23
15	V	103	SPO	C34-C33-C35	2.88	120.23	115.23
16	4	102	LMT	C1B-O1B-C4'	-2.88	111.15	117.98
15	T	102	SPO	C31-C32-C33	-2.88	121.04	127.62
15	N	101	SPO	C31-C32-C33	-2.87	121.05	127.62
16	M	810	LMT	O1'-C1'-C2'	2.87	112.63	108.27
15	F	103	SPO	C29-C28-C30	2.87	120.21	115.23
9	Q	104	BCL	CHC-C1C-NC	2.87	128.54	124.40
15	8	101	SPO	C34-C33-C35	2.87	120.20	115.23
15	G	103	SPO	C6-C7-C9	2.87	123.52	119.01
9	1	101	BCL	CHC-C4B-NB	-2.86	119.75	124.05
9	Y	103	BCL	C4-C3-C5	2.86	120.20	115.23
15	S	103	SPO	C29-C28-C30	2.86	120.20	115.23
15	T	102	SPO	C29-C28-C30	2.86	120.19	115.23
15	1	103	SPO	C20-C19-C17	-2.86	123.27	127.28
15	X	102	SPO	C34-C33-C35	2.85	120.18	115.23
16	D	103	LMT	C1B-O1B-C4'	-2.85	111.22	117.98
15	O	103	SPO	C20-C19-C17	-2.85	123.28	127.28
15	O	102	SPO	C15-C14-C12	-2.85	123.28	127.28
9	W	101	BCL	C4-C3-C5	2.85	120.17	115.23
9	6	101	BCL	CHB-C1B-NB	-2.84	119.78	124.05
9	F	102	BCL	CHC-C1C-NC	2.84	128.50	124.40
15	D	102	SPO	C27-C26-C25	-2.84	114.97	123.20
15	E	101	SPO	C34-C33-C35	2.84	120.15	115.23
9	E	102	BCL	C4-C3-C5	2.84	120.15	115.23
9	8	102	BCL	C1C-NC-C4C	2.83	107.97	106.68
9	M	803	BCL	C4-C3-C5	2.83	120.14	115.23
9	D	101	BCL	C4-C3-C5	2.83	120.14	115.23
15	G	102	SPO	C34-C33-C35	2.83	120.13	115.23
15	3	104	SPO	C34-C33-C35	2.82	120.13	115.23
9	A	703	BCL	C1-C2-C3	-2.82	121.57	126.20
15	3	104	SPO	C20-C19-C17	-2.82	123.32	127.28
16	X	105	LMT	O1B-C4'-C3'	2.82	114.41	107.23
17	M	811	CDL	OB8-CB7-C71	2.82	120.44	111.83
17	M	811	CDL	OA8-CA7-C31	2.82	120.43	111.83
12	L	306	PGV	C02-O01-C1	-2.82	111.06	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	R	101	SPO	C14-C15-C16	-2.81	115.06	123.20
15	T	102	SPO	C15-C14-C12	-2.81	123.34	127.28
15	1	102	SPO	C34-C33-C35	2.81	120.10	115.23
9	1	101	BCL	O2A-CGA-CBA	2.81	120.39	111.83
15	P	101	SPO	C26-C27-C28	-2.80	123.75	127.69
9	D	101	BCL	CHC-C4B-NB	-2.80	119.84	124.05
15	M	807	SPO	C9-C10-C11	-2.80	115.08	123.20
15	V	102	SPO	C14-C15-C16	-2.80	115.09	123.20
9	4	101	BCL	CHC-C4B-NB	-2.80	119.85	124.05
9	A	703	BCL	CMB-C2B-C1B	2.80	129.68	125.42
15	5	104	SPO	C34-C33-C35	2.80	120.08	115.23
15	G	103	SPO	C34-C33-C35	2.80	120.08	115.23
15	5	103	SPO	C14-C15-C16	-2.79	115.11	123.20
15	F	104	SPO	C34-C33-C35	2.79	120.07	115.23
9	W	101	BCL	O2A-CGA-CBA	2.79	120.34	111.83
9	J	101	BCL	CHC-C4B-NB	-2.78	119.88	124.05
9	V	101	BCL	CHB-C4A-NA	2.78	128.41	124.40
15	1	105	SPO	C13-C12-C11	2.78	122.33	118.09
9	R	102	BCL	CHB-C4A-NA	2.78	128.41	124.40
9	L	309	BCL	CHC-C4B-NB	-2.77	119.89	124.05
9	J	101	BCL	CHB-C1B-NB	-2.77	119.90	124.05
15	1	102	SPO	C9-C10-C11	-2.77	115.18	123.20
15	E	101	SPO	C27-C26-C25	-2.77	115.18	123.20
15	O	102	SPO	C29-C28-C30	2.77	120.03	115.23
15	O	103	SPO	C29-C28-C30	2.77	120.03	115.23
9	F	102	BCL	CHC-C4B-NB	-2.76	119.90	124.05
12	3	102	PGV	C02-O01-C1	-2.76	111.19	117.80
15	P	101	SPO	C21-C22-C23	-2.76	123.41	127.28
9	Q	104	BCL	CHB-C4A-NA	2.76	128.38	124.40
9	N	102	BCL	C4-C3-C5	2.75	120.00	115.23
15	M	807	SPO	C15-C14-C12	-2.75	123.42	127.28
9	D	101	BCL	C1C-NC-C4C	-2.75	105.43	106.68
9	M	803	BCL	O2D-CGD-O1D	-2.75	118.50	123.85
9	6	101	BCL	C4-C3-C5	2.74	119.99	115.23
9	2	101	BCL	CHB-C4A-NA	2.74	128.36	124.40
15	W	102	SPO	C15-C14-C12	-2.74	123.43	127.28
16	A	702	LMT	C1B-O1B-C4'	-2.74	111.48	117.98
9	Y	103	BCL	CHB-C4A-NA	2.74	128.35	124.40
15	F	104	SPO	C14-C15-C16	-2.74	115.26	123.20
16	Q	101	LMT	O5'-C5'-C4'	2.74	114.63	109.70
15	D	102	SPO	C14-C15-C16	-2.74	115.27	123.20
9	7	101	BCL	CHC-C1C-NC	2.73	128.34	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	D	102	SPO	C20-C21-C22	-2.73	117.93	123.52
12	H	303	PGV	O03-C19-C20	2.73	120.16	111.83
9	M	803	BCL	O2A-CGA-CBA	2.73	120.15	111.83
9	S	102	BCL	O2A-CGA-CBA	2.72	120.14	111.83
9	T	101	BCL	CHB-C4A-NA	2.72	128.33	124.40
12	M	801	PGV	C02-O01-C1	-2.72	111.28	117.80
9	P	102	BCL	CHB-C4A-NA	2.72	128.32	124.40
15	F	104	SPO	C27-C26-C25	-2.72	115.32	123.20
9	P	102	BCL	CHC-C1C-NC	2.72	128.32	124.40
15	5	103	SPO	C8-C7-C6	2.72	122.24	118.09
9	K	102	BCL	CHC-C1C-NC	2.71	128.32	124.40
9	2	101	BCL	O2A-CGA-CBA	2.71	120.11	111.83
15	G	102	SPO	C9-C10-C11	-2.71	115.34	123.20
16	A	704	LMT	C1B-O1B-C4'	-2.71	111.55	117.98
9	D	101	BCL	CHC-C1C-NC	2.71	128.31	124.40
9	L	308	BCL	O2A-CGA-CBA	2.71	120.10	111.83
9	I	101	BCL	CHC-C1C-NC	2.70	128.30	124.40
15	W	102	SPO	C31-C32-C33	-2.70	121.45	127.62
9	L	301	BCL	C1D-CHD-C4C	-2.70	120.11	126.62
12	H	307	PGV	O03-C19-C20	2.70	120.06	111.83
9	G	101	BCL	C1-C2-C3	-2.69	121.78	126.20
15	W	102	SPO	C14-C15-C16	-2.69	115.40	123.20
9	M	803	BCL	CAA-C2A-C3A	-2.69	105.72	113.00
15	F	104	SPO	C31-C32-C33	-2.69	121.47	127.62
9	8	102	BCL	O2D-CGD-O1D	-2.69	118.61	123.85
9	F	102	BCL	CHB-C4A-NA	2.69	128.28	124.40
15	S	103	SPO	C8-C7-C6	2.69	122.19	118.09
15	3	104	SPO	C14-C15-C16	-2.69	115.41	123.20
15	V	103	SPO	C13-C12-C11	2.69	122.19	118.09
15	X	102	SPO	C14-C15-C16	-2.69	115.42	123.20
15	W	102	SPO	C10-C9-C7	-2.68	123.51	127.28
16	1	104	LMT	C1B-O1B-C4'	-2.68	111.62	117.98
15	K	103	SPO	C13-C12-C11	2.68	122.19	118.09
9	K	102	BCL	O2D-CGD-O1D	-2.68	118.63	123.85
17	Y	102	CDL	OA8-CA7-C31	2.68	120.00	111.83
17	Y	102	CDL	OB8-CB7-C71	2.68	120.00	111.83
9	E	102	BCL	O2A-CGA-CBA	2.68	120.00	111.83
15	E	101	SPO	C14-C15-C16	-2.68	115.45	123.20
15	V	103	SPO	C29-C28-C30	2.67	119.86	115.23
15	G	103	SPO	C8-C7-C9	-2.66	118.50	122.82
9	M	803	BCL	CHC-C1C-NC	2.66	128.24	124.40
15	8	101	SPO	C31-C32-C33	-2.66	121.54	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	101	BCL	CHC-C4B-NB	-2.65	120.07	124.05
15	1	102	SPO	C31-C32-C33	-2.65	121.55	127.62
15	D	102	SPO	C15-C14-C12	-2.65	123.56	127.28
9	K	102	BCL	CHC-C4B-NB	-2.65	120.08	124.05
9	4	101	BCL	CHB-C1B-NB	-2.65	120.08	124.05
9	Z	101	BCL	O2D-CGD-O1D	-2.64	118.71	123.85
12	Q	103	PGV	O03-C19-C20	2.64	119.88	111.83
17	H	304	CDL	OB8-CB7-C71	2.64	119.88	111.83
9	Y	103	BCL	C1C-NC-C4C	-2.64	105.48	106.68
15	X	102	SPO	C10-C9-C7	-2.64	123.58	127.28
15	G	102	SPO	C29-C28-C30	2.63	119.80	115.23
9	D	101	BCL	CHB-C4A-NA	2.63	128.19	124.40
9	D	101	BCL	C4A-NA-C1A	2.63	107.88	106.68
9	K	102	BCL	C1-C2-C3	-2.63	121.90	126.20
9	S	102	BCL	CHB-C4A-NA	2.62	128.19	124.40
15	R	101	SPO	C15-C14-C12	-2.62	123.60	127.28
9	O	101	BCL	CHB-C4A-NA	2.62	128.18	124.40
16	M	810	LMT	C1'-C2'-C3'	2.62	115.52	110.01
12	X	101	PGV	O03-C19-C20	2.62	119.82	111.83
9	O	101	BCL	C4-C3-C5	2.62	119.77	115.23
15	1	105	SPO	C29-C28-C30	2.61	119.77	115.23
15	T	102	SPO	C21-C20-C19	-2.61	118.17	123.52
15	N	101	SPO	C4-C5-C6	-2.61	121.25	124.91
9	8	102	BCL	C2D-C1D-ND	2.60	112.70	110.13
9	I	101	BCL	CAC-C3C-C4C	-2.60	106.81	112.58
15	1	103	SPO	C29-C28-C30	2.60	119.75	115.23
15	O	102	SPO	C9-C10-C11	-2.60	115.67	123.20
9	5	102	BCL	CHC-C1C-NC	2.60	128.15	124.40
15	P	101	SPO	C20-C19-C17	-2.59	123.64	127.28
15	S	103	SPO	C40-C38-C39	2.59	120.55	114.59
12	L	310	PGV	O03-C19-C20	2.59	119.73	111.83
10	M	804	BPH	C2B-C1B-NB	-2.59	107.56	109.43
15	S	103	SPO	C36-C37-C38	-2.58	119.03	127.64
12	L	305	PGV	O03-C19-C20	2.58	119.71	111.83
9	E	102	BCL	CHC-C4B-NB	-2.58	120.17	124.05
9	N	102	BCL	CHC-C4B-NB	-2.58	120.17	124.05
9	O	101	BCL	CHC-C4B-NB	-2.58	120.17	124.05
9	L	301	BCL	CMD-C2D-C3D	-2.58	121.77	127.69
10	L	302	BPH	C2B-C1B-NB	-2.58	107.56	109.43
9	5	102	BCL	CHC-C4B-NB	-2.58	120.17	124.05
15	1	102	SPO	C13-C12-C11	2.58	122.03	118.09
9	8	102	BCL	C4D-CHA-C1A	-2.58	118.17	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	1	101	BCL	C1D-CHD-C4C	-2.58	120.41	126.62
9	Y	103	BCL	CHC-C1C-NC	2.57	128.11	124.40
9	L	308	BCL	CHC-C4B-NB	-2.57	120.20	124.05
17	H	305	CDL	OB4-PB2-OB3	2.57	120.83	110.83
15	K	103	SPO	C21-C20-C19	-2.57	118.27	123.52
15	S	104	SPO	C21-C20-C19	-2.57	118.27	123.52
15	V	102	SPO	C29-C28-C30	2.56	119.68	115.23
9	A	703	BCL	CMD-C2D-C3D	-2.56	121.81	127.69
9	G	101	BCL	CHC-C4B-NB	-2.56	120.21	124.05
9	N	102	BCL	CHB-C4A-NA	2.56	128.10	124.40
9	7	101	BCL	CMD-C2D-C3D	-2.56	121.82	127.69
15	1	103	SPO	C40-C38-C39	2.56	120.48	114.59
9	2	101	BCL	CHC-C1C-NC	2.56	128.09	124.40
15	S	104	SPO	C14-C15-C16	-2.56	115.79	123.20
9	7	101	BCL	CHB-C4A-NA	2.55	128.09	124.40
9	L	308	BCL	C4-C3-C5	2.55	119.66	115.23
9	I	101	BCL	C4-C3-C5	2.55	119.66	115.23
10	L	302	BPH	CMA-C3A-C4A	-2.55	109.12	114.61
9	L	301	BCL	CHC-C4B-NB	-2.55	120.23	124.05
15	1	103	SPO	C13-C12-C11	2.55	121.98	118.09
15	S	103	SPO	C9-C10-C11	-2.54	115.83	123.20
9	W	101	BCL	CHB-C4A-NA	2.54	128.07	124.40
16	H	302	LMT	O1B-C1B-C2B	2.54	114.34	108.09
9	B	101	BCL	CHB-C4A-NA	2.54	128.06	124.40
15	N	101	SPO	C21-C20-C19	-2.53	118.33	123.52
15	T	102	SPO	C20-C19-C17	-2.53	123.73	127.28
9	Z	101	BCL	CHB-C4A-NA	2.53	128.05	124.40
11	L	304	U10	C7-C6-C1	-2.53	120.55	124.89
9	7	101	BCL	O2D-CGD-O1D	-2.53	118.92	123.85
9	1	101	BCL	CHB-C4A-NA	2.53	128.05	124.40
9	8	102	BCL	CHD-C1D-C2D	2.53	130.74	125.49
9	O	101	BCL	O2D-CGD-O1D	-2.53	118.93	123.85
9	1	101	BCL	O2D-CGD-O1D	-2.52	118.94	123.85
15	S	103	SPO	C20-C21-C22	-2.52	118.36	123.52
9	2	101	BCL	C2A-C1A-CHA	-2.52	119.49	123.87
9	W	101	BCL	CHC-C1C-NC	2.52	128.04	124.40
12	X	101	PGV	C02-O01-C1	-2.52	111.78	117.80
9	Q	104	BCL	O2D-CGD-O1D	-2.51	118.95	123.85
15	F	104	SPO	C21-C20-C19	-2.51	118.39	123.52
9	N	102	BCL	CHC-C1C-NC	2.51	128.02	124.40
9	1	101	BCL	C4-C3-C5	2.51	119.58	115.23
9	O	101	BCL	C1C-NC-C4C	-2.51	105.53	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	V	102	SPO	C13-C12-C11	2.51	121.92	118.09
15	1	103	SPO	C34-C33-C35	2.50	119.57	115.23
15	D	102	SPO	C13-C12-C11	2.50	121.91	118.09
9	Y	103	BCL	O2D-CGD-O1D	-2.50	118.99	123.85
9	T	101	BCL	CHC-C4B-NB	-2.50	120.30	124.05
9	7	101	BCL	CHC-C4B-NB	-2.50	120.31	124.05
15	F	103	SPO	C14-C15-C16	-2.49	115.97	123.20
9	B	101	BCL	CHB-C1B-NB	-2.49	120.31	124.05
9	G	101	BCL	O2D-CGD-O1D	-2.49	119.00	123.85
9	M	803	BCL	CMD-C2D-C3D	-2.49	121.99	127.69
9	S	102	BCL	O2D-CGD-O1D	-2.48	119.01	123.85
9	S	102	BCL	C1D-CHD-C4C	-2.48	120.63	126.62
15	W	102	SPO	C9-C10-C11	-2.48	116.02	123.20
15	G	102	SPO	C40-C38-C39	2.47	120.28	114.59
9	L	308	BCL	CMB-C2B-C3B	2.46	133.44	125.67
15	D	102	SPO	C34-C33-C35	2.46	119.51	115.23
12	Y	104	PGV	O03-C19-C20	2.46	119.34	111.83
15	5	103	SPO	C13-C12-C11	2.46	121.85	118.09
15	T	102	SPO	C21-C22-C23	-2.46	123.83	127.28
9	R	102	BCL	CHC-C4B-NB	-2.46	120.36	124.05
15	S	104	SPO	C8-C7-C6	2.46	121.84	118.09
9	O	101	BCL	CMB-C2B-C3B	2.46	133.43	125.67
9	L	308	BCL	C1D-CHD-C4C	-2.45	120.70	126.62
9	M	803	BCL	C1-C2-C3	-2.45	122.19	126.20
16	K	101	LMT	O1'-C1'-C2'	2.45	111.99	108.27
16	H	301	LMT	C1-O1'-C1'	-2.44	109.51	113.68
15	K	103	SPO	C34-C33-C35	2.44	119.47	115.23
15	X	102	SPO	C40-C38-C39	2.44	120.21	114.59
9	V	101	BCL	CHC-C1C-NC	2.44	127.92	124.40
15	S	104	SPO	C13-C12-C11	2.44	121.82	118.09
9	L	301	BCL	C4-C3-C5	2.44	119.46	115.23
9	N	102	BCL	C2A-C1A-CHA	-2.44	119.63	123.87
9	O	101	BCL	CHC-C1C-NC	2.44	127.92	124.40
15	G	102	SPO	C21-C20-C19	-2.43	118.55	123.52
15	V	103	SPO	C21-C20-C19	-2.43	118.55	123.52
9	7	101	BCL	CMB-C2B-C3B	2.43	133.33	125.67
9	O	101	BCL	C1D-CHD-C4C	-2.43	120.76	126.62
15	S	103	SPO	C10-C9-C7	-2.43	123.88	127.28
15	S	104	SPO	C20-C19-C17	-2.43	123.88	127.28
15	R	101	SPO	C8-C7-C9	-2.43	118.89	122.82
15	O	103	SPO	C8-C7-C6	2.42	121.79	118.09
15	1	105	SPO	C34-C33-C35	2.42	119.44	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	308	BCL	C2A-C1A-CHA	-2.42	119.66	123.87
9	G	101	BCL	CHB-C1B-NB	-2.42	120.42	124.05
9	Z	101	BCL	C2A-C1A-CHA	-2.42	119.67	123.87
15	O	102	SPO	C10-C9-C7	-2.42	123.89	127.28
15	N	101	SPO	C40-C38-C39	2.42	120.16	114.59
9	D	101	BCL	O2D-CGD-O1D	-2.41	119.15	123.85
15	F	104	SPO	C40-C38-C39	2.41	120.14	114.59
9	V	101	BCL	CHC-C4B-NB	-2.41	120.43	124.05
9	5	102	BCL	O2D-CGD-O1D	-2.41	119.16	123.85
9	L	301	BCL	CHC-C1C-NC	2.41	127.88	124.40
9	Y	103	BCL	CHC-C4B-NB	-2.41	120.44	124.05
15	R	101	SPO	C4-C5-C6	-2.41	121.53	124.91
15	F	103	SPO	C27-C26-C25	-2.41	116.23	123.20
12	K	104	PGV	C02-O01-C1	-2.41	112.04	117.80
15	T	102	SPO	C8-C7-C9	-2.41	118.92	122.82
9	P	102	BCL	O2D-CGD-O1D	-2.40	119.17	123.85
15	5	104	SPO	C27-C26-C25	-2.40	116.23	123.20
9	M	803	BCL	CMB-C2B-C3B	2.40	133.25	125.67
9	P	102	BCL	C2A-C1A-CHA	-2.40	119.69	123.87
15	1	102	SPO	C21-C20-C19	-2.40	118.60	123.52
9	B	101	BCL	O2D-CGD-O1D	-2.40	119.17	123.85
15	1	102	SPO	C15-C16-C17	-2.40	119.78	126.36
9	6	101	BCL	C1D-CHD-C4C	-2.40	120.83	126.62
15	3	104	SPO	C40-C38-C39	2.40	120.11	114.59
9	5	102	BCL	C1-C2-C3	-2.40	122.27	126.20
12	M	812	PGV	C02-O01-C1	-2.40	112.06	117.80
15	P	101	SPO	C15-C14-C12	-2.39	123.92	127.28
9	Y	103	BCL	C2A-C1A-CHA	-2.39	119.72	123.87
15	T	102	SPO	C14-C15-C16	-2.39	116.27	123.20
15	R	101	SPO	C40-C38-C39	2.39	120.09	114.59
15	1	102	SPO	C15-C14-C12	-2.39	123.93	127.28
9	L	309	BCL	C2A-C1A-CHA	-2.39	119.73	123.87
9	V	101	BCL	CMD-C2D-C3D	-2.39	122.22	127.69
16	M	810	LMT	C1-O1'-C1'	-2.38	109.61	113.68
9	F	102	BCL	CMB-C2B-C3B	2.38	133.19	125.67
9	L	301	BCL	O2A-CGA-O1A	-2.38	117.67	123.63
9	S	102	BCL	CMB-C2B-C3B	2.38	133.18	125.67
17	H	305	CDL	OA4-PA1-OA3	2.38	120.11	110.83
9	3	103	BCL	CMB-C2B-C3B	2.38	133.17	125.67
9	I	101	BCL	CMD-C2D-C3D	-2.38	122.24	127.69
9	6	101	BCL	O2D-CGD-O1D	-2.38	119.22	123.85
12	L	310	PGV	C02-O01-C1	-2.38	112.11	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	S	104	SPO	C40-C38-C39	2.38	120.06	114.59
15	1	103	SPO	C6-C7-C9	2.38	122.75	119.01
9	K	102	BCL	C1D-CHD-C4C	-2.37	120.89	126.62
15	1	103	SPO	C21-C22-C23	-2.37	123.95	127.28
9	G	101	BCL	CHB-C4A-NA	2.37	127.82	124.40
9	J	101	BCL	O2A-CGA-O1A	-2.37	117.70	123.63
15	K	103	SPO	C14-C15-C16	-2.37	116.34	123.20
15	F	103	SPO	C40-C38-C39	2.37	120.03	114.59
9	A	703	BCL	C1D-CHD-C4C	-2.37	120.91	126.62
15	G	102	SPO	C14-C15-C16	-2.37	116.35	123.20
9	5	102	BCL	CMB-C2B-C3B	2.36	133.13	125.67
9	R	102	BCL	O2D-CGD-O1D	-2.36	119.25	123.85
17	H	305	CDL	OA8-CA7-C31	2.36	119.03	111.83
15	D	102	SPO	C8-C7-C6	2.36	121.69	118.09
9	Z	101	BCL	CHC-C1C-NC	2.36	127.80	124.40
9	K	102	BCL	CMB-C2B-C3B	2.36	133.10	125.67
9	Q	104	BCL	C4-C3-C5	2.36	119.32	115.23
9	L	308	BCL	C1C-NC-C4C	-2.35	105.61	106.68
15	1	103	SPO	C14-C15-C16	-2.35	116.38	123.20
15	3	104	SPO	C1-C4-C5	-2.35	106.89	112.98
15	N	101	SPO	C1-C4-C5	-2.35	106.89	112.98
15	D	102	SPO	C40-C38-C39	2.35	119.99	114.59
9	N	102	BCL	C1D-CHD-C4C	-2.35	120.96	126.62
16	M	809	LMT	C1B-O1B-C4'	-2.34	112.43	117.98
15	R	101	SPO	C31-C32-C33	-2.34	122.27	127.62
12	M	801	PGV	O03-C19-O04	-2.34	117.78	123.63
17	M	811	CDL	CA4-OA6-CA5	-2.34	112.20	117.80
15	1	102	SPO	C40-C38-C39	2.33	119.96	114.59
15	E	101	SPO	C24-C23-C25	2.33	121.65	118.09
9	N	102	BCL	O2A-CGA-CBA	2.33	118.94	111.83
15	S	104	SPO	C9-C10-C11	-2.33	116.45	123.20
9	3	103	BCL	CMD-C2D-C3D	-2.33	122.35	127.69
9	Y	103	BCL	C1D-CHD-C4C	-2.32	121.02	126.62
9	M	803	BCL	CED-O2D-CGD	2.32	121.18	115.92
15	1	102	SPO	C8-C7-C6	2.32	121.64	118.09
15	V	103	SPO	C8-C7-C6	2.32	121.63	118.09
17	H	304	CDL	OA8-CA7-C31	2.32	118.90	111.83
9	W	101	BCL	C2A-C1A-CHA	-2.32	119.84	123.87
9	E	102	BCL	CMB-C2B-C3B	2.32	132.98	125.67
9	T	101	BCL	CMB-C2B-C3B	2.32	132.98	125.67
9	2	101	BCL	O2D-CGD-O1D	-2.32	119.34	123.85
9	F	102	BCL	CED-O2D-CGD	2.32	121.17	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Q	104	BCL	C4A-NA-C1A	2.31	107.73	106.68
9	E	102	BCL	CHB-C1B-NB	-2.31	120.58	124.05
9	D	101	BCL	CMB-C2B-C3B	2.31	132.97	125.67
15	P	101	SPO	C14-C15-C16	-2.31	116.50	123.20
12	3	102	PGV	O03-C19-C20	2.31	118.88	111.83
15	X	102	SPO	C13-C12-C11	2.31	121.62	118.09
9	K	102	BCL	CHB-C4A-NA	2.31	127.73	124.40
9	V	101	BCL	CMB-C2B-C3B	2.31	132.95	125.67
15	E	101	SPO	C40-C38-C39	2.31	119.90	114.59
9	4	101	BCL	O2D-CGD-O1D	-2.31	119.35	123.85
15	E	101	SPO	C26-C27-C28	-2.31	124.44	127.69
9	1	101	BCL	CMD-C2D-C3D	-2.31	122.40	127.69
15	F	103	SPO	C13-C12-C11	2.30	121.61	118.09
9	A	703	BCL	O2D-CGD-O1D	-2.30	119.36	123.85
15	V	103	SPO	C36-C37-C38	-2.30	119.96	127.64
9	R	102	BCL	C11-C12-C13	-2.30	108.31	115.97
15	O	102	SPO	C34-C33-C35	2.30	119.22	115.23
15	G	103	SPO	C27-C26-C25	-2.30	116.53	123.20
16	K	101	LMT	C1-O1'-C1'	-2.30	109.75	113.68
9	N	102	BCL	O2D-CGD-O1D	-2.30	119.37	123.85
9	P	102	BCL	CHC-C4B-NB	-2.30	120.60	124.05
9	J	101	BCL	C1D-CHD-C4C	-2.30	121.08	126.62
9	R	102	BCL	C1D-CHD-C4C	-2.30	121.08	126.62
9	L	301	BCL	CMB-C2B-C3B	2.30	132.91	125.67
15	5	103	SPO	C20-C21-C22	-2.30	118.82	123.52
15	N	101	SPO	C24-C23-C25	2.30	121.59	118.09
9	2	101	BCL	CHB-C1B-NB	-2.29	120.61	124.05
9	R	102	BCL	C2A-C1A-CHA	-2.29	119.89	123.87
9	S	102	BCL	CAC-C3C-C4C	-2.29	107.50	112.58
9	M	803	BCL	C1D-CHD-C4C	-2.29	121.09	126.62
15	O	103	SPO	C34-C33-C35	2.29	119.20	115.23
9	W	101	BCL	C1D-CHD-C4C	-2.29	121.10	126.62
9	E	102	BCL	C1-O2A-CGA	2.29	122.19	116.65
9	N	102	BCL	CMB-C2B-C3B	2.28	132.87	125.67
9	L	308	BCL	CMD-C2D-C3D	-2.28	122.45	127.69
15	5	103	SPO	C40-C38-C39	2.28	119.84	114.59
9	I	101	BCL	C1D-CHD-C4C	-2.28	121.12	126.62
12	L	305	PGV	C02-O01-C1	-2.28	112.34	117.80
15	5	104	SPO	C40-C38-C39	2.28	119.83	114.59
9	E	102	BCL	C4D-CHA-C1A	-2.28	118.53	121.24
9	E	102	BCL	CHB-C4A-NA	2.28	127.69	124.40
9	L	309	BCL	CMB-C2B-C3B	2.28	132.85	125.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	3	103	BCL	C1D-CHD-C4C	-2.28	121.13	126.62
15	3	104	SPO	C15-C14-C12	-2.27	124.09	127.28
9	L	309	BCL	CHB-C1B-NB	-2.27	120.64	124.05
9	Z	101	BCL	C1D-CHD-C4C	-2.27	121.14	126.62
15	S	103	SPO	C26-C25-C23	-2.27	120.13	126.36
9	3	103	BCL	CHB-C4A-NA	2.27	127.67	124.40
15	D	102	SPO	C24-C23-C25	2.27	121.55	118.09
9	V	101	BCL	C1D-CHD-C4C	-2.27	121.15	126.62
15	R	101	SPO	C13-C12-C11	2.27	121.55	118.09
9	P	102	BCL	O2A-CGA-O1A	-2.27	117.96	123.63
9	2	101	BCL	C1D-CHD-C4C	-2.27	121.15	126.62
15	3	104	SPO	C20-C21-C22	-2.27	118.88	123.52
9	L	308	BCL	O1D-CGD-CBD	-2.26	120.05	124.52
9	M	803	BCL	CHB-C1B-NB	-2.26	120.65	124.05
12	H	307	PGV	C02-O01-C1	-2.26	112.38	117.80
9	D	101	BCL	CAC-C3C-C4C	-2.26	107.57	112.58
9	Z	101	BCL	O2A-CGA-O1A	-2.26	117.98	123.63
15	O	103	SPO	C13-C12-C11	2.26	121.53	118.09
9	4	101	BCL	CMD-C2D-C3D	-2.25	122.52	127.69
9	J	101	BCL	CHB-C4A-NA	2.25	127.65	124.40
9	L	308	BCL	CHC-C1C-NC	2.25	127.65	124.40
15	8	101	SPO	C40-C38-C39	2.25	119.77	114.59
9	I	101	BCL	O2D-CGD-O1D	-2.25	119.47	123.85
9	G	101	BCL	C1D-CHD-C4C	-2.25	121.19	126.62
15	V	102	SPO	C34-C33-C35	2.25	119.14	115.23
9	L	301	BCL	C1-C2-C3	-2.25	122.51	126.20
9	3	103	BCL	C1-C2-C3	-2.25	122.51	126.20
15	W	102	SPO	C34-C33-C35	2.25	119.13	115.23
15	O	102	SPO	C5-C6-C7	-2.25	122.50	125.89
9	S	102	BCL	CMD-C2D-C3D	-2.25	122.54	127.69
9	D	101	BCL	CMD-C2D-C3D	-2.24	122.55	127.69
12	L	310	PGV	O14-P-O13	2.24	119.57	110.83
15	8	101	SPO	C10-C11-C12	-2.24	120.22	126.36
9	Q	104	BCL	C1D-CHD-C4C	-2.24	121.22	126.62
15	P	101	SPO	C40-C38-C39	2.24	119.74	114.59
9	M	803	BCL	CHB-C4A-NA	2.24	127.63	124.40
15	3	104	SPO	C36-C37-C38	-2.23	120.19	127.64
9	J	101	BCL	O2D-CGD-O1D	-2.23	119.50	123.85
15	S	104	SPO	C31-C32-C33	-2.23	122.51	127.62
16	M	810	LMT	O5'-C1'-C2'	2.23	114.96	110.37
16	F	101	LMT	O3'-C3'-C2'	-2.23	105.11	110.38
15	1	105	SPO	C8-C7-C6	2.23	121.50	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	1	105	SPO	C40-C38-C39	2.23	119.72	114.59
9	5	102	BCL	CMD-C2D-C3D	-2.23	122.58	127.69
9	1	101	BCL	CMB-C2B-C3B	2.23	132.70	125.67
15	S	103	SPO	C14-C15-C16	-2.23	116.74	123.20
11	M	806	U10	C7-C6-C1	-2.23	121.07	124.89
9	T	101	BCL	CHB-C1B-NB	-2.23	120.71	124.05
9	D	101	BCL	C1D-CHD-C4C	-2.23	121.25	126.62
9	7	101	BCL	C1-C2-C3	-2.23	122.55	126.20
9	I	101	BCL	CMB-C2B-C3B	2.22	132.69	125.67
9	F	102	BCL	O2D-CGD-O1D	-2.22	119.52	123.85
9	T	101	BCL	O2A-CGA-O1A	-2.22	118.07	123.63
9	W	101	BCL	CMD-C2D-C3D	-2.22	122.59	127.69
9	K	102	BCL	CMD-C2D-C3D	-2.22	122.60	127.69
9	L	308	BCL	CHB-C4A-NA	2.22	127.60	124.40
15	O	103	SPO	C36-C35-C33	-2.22	105.83	113.19
9	G	101	BCL	CMB-C2B-C3B	2.22	132.67	125.67
15	O	102	SPO	C31-C32-C33	-2.22	122.55	127.62
15	E	101	SPO	C20-C21-C22	-2.22	118.98	123.52
9	B	101	BCL	CHC-C4B-NB	-2.22	120.72	124.05
15	N	101	SPO	C36-C37-C38	-2.21	120.26	127.64
9	E	102	BCL	C1-C2-C3	-2.21	122.57	126.20
15	W	102	SPO	C21-C20-C19	-2.21	118.99	123.52
9	P	102	BCL	C1D-CHD-C4C	-2.21	121.28	126.62
16	H	302	LMT	O5'-C5'-C4'	2.21	114.30	109.72
15	D	102	SPO	C36-C37-C38	-2.21	120.27	127.64
9	T	101	BCL	C1D-CHD-C4C	-2.21	121.28	126.62
15	M	807	SPO	C13-C12-C11	2.21	121.47	118.09
9	K	102	BCL	CHB-C1B-NB	-2.21	120.73	124.05
15	G	103	SPO	C14-C15-C16	-2.21	116.80	123.20
16	M	808	LMT	C1B-O1B-C4'	-2.21	112.74	117.98
9	4	101	BCL	C1D-CHD-C4C	-2.21	121.30	126.62
9	A	703	BCL	C4-C3-C5	2.21	119.06	115.23
9	B	101	BCL	CHC-C1C-NC	2.21	127.58	124.40
17	M	811	CDL	OB6-CB5-OB7	-2.21	118.55	123.70
15	G	103	SPO	C40-C38-C39	2.21	119.67	114.59
15	V	102	SPO	C15-C14-C12	-2.21	124.19	127.28
15	3	104	SPO	C27-C26-C25	-2.20	116.81	123.20
9	A	703	BCL	CHD-C1D-C2D	2.20	130.07	125.49
16	U	102	LMT	C1B-O1B-C4'	-2.20	112.76	117.98
9	F	102	BCL	C1D-CHD-C4C	-2.20	121.32	126.62
16	H	302	LMT	O5'-C1'-C2'	-2.20	105.86	110.37
9	F	102	BCL	CMD-C2D-C3D	-2.20	122.65	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	309	BCL	CMD-C2D-C3D	-2.19	122.66	127.69
9	B	101	BCL	C1D-CHD-C4C	-2.19	121.33	126.62
15	1	105	SPO	C20-C21-C22	-2.19	119.03	123.52
12	H	303	PGV	O14-P-O13	2.19	119.38	110.83
9	6	101	BCL	C4D-CHA-C1A	-2.19	118.63	121.24
15	V	103	SPO	C18-C17-C16	2.18	121.42	118.09
15	1	103	SPO	C20-C21-C22	-2.18	119.06	123.52
9	Y	103	BCL	CHB-C1B-NB	-2.18	120.78	124.05
15	P	101	SPO	C31-C32-C33	-2.18	122.63	127.62
15	S	104	SPO	C24-C23-C25	2.18	121.41	118.09
9	A	703	BCL	O2A-CGA-O1A	-2.17	118.19	123.63
9	5	102	BCL	CAC-C3C-C4C	-2.17	107.76	112.58
15	V	103	SPO	C10-C9-C7	-2.17	124.24	127.28
9	R	102	BCL	CHC-C1C-NC	2.17	127.53	124.40
15	E	101	SPO	C9-C10-C11	-2.17	116.92	123.20
9	O	101	BCL	CHB-C1B-C2B	-2.17	121.14	127.43
15	G	103	SPO	C21-C20-C19	-2.17	119.09	123.52
15	W	102	SPO	C20-C21-C22	-2.16	119.09	123.52
9	T	101	BCL	O2D-CGD-O1D	-2.16	119.64	123.85
9	5	102	BCL	C1D-CHD-C4C	-2.16	121.41	126.62
15	1	103	SPO	C27-C26-C25	-2.16	116.94	123.20
12	H	303	PGV	C02-O01-C1	-2.16	112.63	117.80
9	L	301	BCL	C2A-C1A-CHA	-2.16	120.12	123.87
9	S	102	BCL	CHB-C1B-C2B	-2.16	121.16	127.43
15	1	105	SPO	C36-C37-C38	-2.16	120.45	127.64
9	W	101	BCL	O2D-CGD-O1D	-2.16	119.65	123.85
15	G	102	SPO	C13-C12-C11	2.16	121.38	118.09
15	3	104	SPO	C8-C7-C9	-2.15	119.33	122.82
15	O	103	SPO	C40-C38-C39	2.15	119.54	114.59
9	E	102	BCL	CMD-C2D-C3D	-2.15	122.75	127.69
9	I	101	BCL	CHB-C1B-C2B	-2.15	121.18	127.43
15	N	101	SPO	C8-C7-C9	-2.15	119.33	122.82
15	5	103	SPO	C34-C33-C35	2.15	118.96	115.23
9	L	309	BCL	CHC-C1C-NC	2.15	127.50	124.40
15	S	104	SPO	C10-C9-C7	-2.14	124.27	127.28
9	R	102	BCL	O2A-CGA-O1A	-2.14	118.27	123.63
9	E	102	BCL	CHC-C1C-NC	2.14	127.49	124.40
9	E	102	BCL	CBA-CAA-C2A	-2.14	107.42	113.79
9	6	101	BCL	CMB-C2B-C3B	2.14	132.42	125.67
9	L	301	BCL	CHB-C4A-NA	2.14	127.49	124.40
15	T	102	SPO	C34-C33-C35	2.14	118.94	115.23
15	F	103	SPO	C20-C21-C22	-2.14	119.14	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	R	102	BCL	CHB-C1B-NB	-2.14	120.84	124.05
9	Z	101	BCL	C4D-CHA-C1A	-2.14	118.69	121.24
9	W	101	BCL	C4D-CHA-C1A	-2.14	118.70	121.24
11	L	303	U10	C7-C6-C1	-2.14	121.23	124.89
9	R	102	BCL	CMB-C2B-C3B	2.14	132.41	125.67
9	7	101	BCL	C1D-CHD-C4C	-2.13	121.47	126.62
9	W	101	BCL	CHB-C1B-NB	-2.13	120.85	124.05
15	V	102	SPO	C8-C7-C6	2.13	121.34	118.09
9	3	103	BCL	O2D-CGD-O1D	-2.13	119.70	123.85
9	4	101	BCL	CHB-C4A-NA	2.13	127.48	124.40
15	1	103	SPO	C8-C7-C9	-2.13	119.36	122.82
9	E	102	BCL	C1D-CHD-C4C	-2.13	121.49	126.62
9	Y	103	BCL	O2A-CGA-O1A	-2.13	118.30	123.63
15	3	104	SPO	C6-C7-C9	2.13	122.36	119.01
15	G	102	SPO	C8-C7-C6	2.13	121.34	118.09
9	E	102	BCL	O2D-CGD-O1D	-2.13	119.71	123.85
9	4	101	BCL	CMB-C2B-C3B	2.13	132.38	125.67
9	7	101	BCL	CHB-C1B-C2B	-2.13	121.25	127.43
9	J	101	BCL	CAC-C3C-C4C	-2.13	107.87	112.58
9	N	102	BCL	CHB-C1B-NB	-2.13	120.86	124.05
9	6	101	BCL	CMD-C2D-C3D	-2.12	122.82	127.69
9	3	103	BCL	CHB-C1B-NB	-2.12	120.87	124.05
9	B	101	BCL	C4D-CHA-C1A	-2.12	118.72	121.24
15	S	104	SPO	C15-C14-C12	-2.12	124.31	127.28
15	X	102	SPO	C15-C14-C12	-2.12	124.31	127.28
15	M	807	SPO	C40-C38-C39	2.12	119.46	114.59
9	5	102	BCL	CHB-C1B-C2B	-2.12	121.28	127.43
9	T	101	BCL	C2A-C1A-CHA	-2.12	120.19	123.87
15	8	101	SPO	C27-C26-C25	-2.11	117.07	123.20
9	5	102	BCL	C1C-NC-C4C	-2.11	105.72	106.68
9	Y	103	BCL	CMD-C2D-C3D	-2.11	122.85	127.69
9	R	102	BCL	CMD-C2D-C3D	-2.11	122.86	127.69
9	F	102	BCL	CHB-C1B-C2B	-2.11	121.31	127.43
9	V	101	BCL	CHB-C1B-C2B	-2.11	121.31	127.43
9	F	102	BCL	CAC-C3C-C4C	-2.10	107.91	112.58
9	1	101	BCL	CHB-C1B-C2B	-2.10	121.32	127.43
9	L	301	BCL	CHB-C1B-C2B	-2.10	121.32	127.43
9	4	101	BCL	C4D-CHA-C1A	-2.10	118.74	121.24
15	1	105	SPO	C26-C25-C23	-2.10	120.60	126.36
9	E	102	BCL	C2A-C1A-CHA	-2.10	120.22	123.87
15	T	102	SPO	C40-C38-C39	2.10	119.42	114.59
15	O	102	SPO	C26-C25-C23	-2.10	120.61	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	1	103	SPO	C4-C5-C6	-2.10	121.97	124.91
9	F	102	BCL	O2A-CGA-O1A	-2.10	118.39	123.63
9	F	102	BCL	C2A-C1A-CHA	-2.10	120.23	123.87
9	Z	101	BCL	C6-C5-C3	-2.09	108.36	113.47
9	L	308	BCL	C6-C5-C3	-2.09	108.38	113.47
9	L	301	BCL	CED-O2D-CGD	2.09	120.65	115.92
9	E	102	BCL	CAC-C3C-C4C	-2.09	107.95	112.58
17	H	305	CDL	OB8-CB7-OB9	-2.09	118.41	123.63
10	M	804	BPH	CMA-C3A-C4A	-2.09	110.12	114.61
9	L	309	BCL	C1D-CHD-C4C	-2.08	121.59	126.62
15	V	103	SPO	C40-C38-C39	2.08	119.39	114.59
9	P	102	BCL	CMB-C2B-C3B	2.08	132.24	125.67
9	G	101	BCL	O2A-CGA-O1A	-2.08	118.42	123.63
15	T	102	SPO	C6-C7-C9	2.08	122.28	119.01
15	V	102	SPO	C36-C37-C38	-2.08	120.70	127.64
15	W	102	SPO	C24-C23-C25	2.08	121.27	118.09
9	7	101	BCL	O1D-CGD-CBD	-2.08	120.41	124.52
9	O	101	BCL	C1-C2-C3	-2.08	122.79	126.20
9	L	309	BCL	C6-C5-C3	-2.08	108.41	113.47
9	Q	104	BCL	CHC-C4B-NB	-2.08	120.93	124.05
9	N	102	BCL	C11-C12-C13	-2.08	109.06	115.97
12	M	812	PGV	O03-C19-O04	-2.08	118.43	123.63
9	L	308	BCL	C1-O2A-CGA	2.08	121.68	116.65
15	O	102	SPO	C14-C15-C16	-2.07	117.19	123.20
9	L	309	BCL	CHD-C1D-C2D	2.07	129.80	125.49
15	F	103	SPO	C15-C14-C12	-2.07	124.37	127.28
9	W	101	BCL	CHC-C4B-NB	-2.07	120.94	124.05
9	L	301	BCL	C4A-NA-C1A	-2.07	105.73	106.68
15	W	102	SPO	C40-C38-C39	2.07	119.35	114.59
9	B	101	BCL	O2A-CGA-O1A	-2.07	118.46	123.63
9	1	101	BCL	CAC-C3C-C4C	-2.07	108.00	112.58
16	5	101	LMT	O1B-C4'-C3'	2.06	112.47	107.23
9	L	301	BCL	CHD-C1D-C2D	2.06	129.77	125.49
9	5	102	BCL	O1D-CGD-CBD	-2.06	120.45	124.52
9	D	101	BCL	CHB-C1B-C2B	-2.06	121.45	127.43
9	J	101	BCL	CMD-C2D-C3D	-2.06	122.97	127.69
9	I	101	BCL	O2A-CGA-O1A	-2.06	118.48	123.63
15	V	102	SPO	C40-C38-C39	2.06	119.33	114.59
15	3	104	SPO	C21-C22-C23	-2.06	124.39	127.28
9	Q	104	BCL	CHB-C1B-NB	-2.06	120.96	124.05
9	Q	104	BCL	CMD-C2D-C3D	-2.06	122.97	127.69
9	7	101	BCL	C2A-C1A-CHA	-2.06	120.30	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	8	101	SPO	C14-C15-C16	-2.06	117.25	123.20
15	5	104	SPO	C15-C16-C17	-2.06	120.73	126.36
15	X	102	SPO	C26-C25-C23	-2.06	120.73	126.36
15	O	103	SPO	C18-C17-C16	2.05	121.23	118.09
15	N	101	SPO	C15-C14-C12	-2.05	124.40	127.28
15	O	102	SPO	C40-C38-C39	2.05	119.31	114.59
9	Z	101	BCL	CMB-C2B-C3B	2.05	132.15	125.67
16	3	101	LMT	C1'-O5'-C5'	-2.05	109.72	113.72
15	N	101	SPO	C20-C21-C22	-2.05	119.33	123.52
9	1	101	BCL	O2A-CGA-O1A	-2.05	118.50	123.63
9	D	101	BCL	O2A-CGA-O1A	-2.05	118.51	123.63
15	S	104	SPO	C21-C22-C23	-2.05	124.41	127.28
12	Q	103	PGV	C02-O01-C1	-2.04	112.90	117.80
15	K	103	SPO	C8-C7-C6	2.04	121.21	118.09
15	M	807	SPO	C34-C33-C35	2.04	118.78	115.23
15	5	103	SPO	C26-C25-C23	-2.04	120.76	126.36
9	B	101	BCL	C6-C5-C3	-2.04	108.50	113.47
15	5	103	SPO	C21-C20-C19	-2.04	119.36	123.52
15	1	103	SPO	C36-C37-C38	-2.03	120.86	127.64
15	O	102	SPO	C8-C7-C6	2.03	121.19	118.09
9	W	101	BCL	CMB-C2B-C3B	2.03	132.08	125.67
16	A	701	LMT	C1B-O1B-C4'	-2.03	113.17	117.98
12	L	306	PGV	O03-C19-O04	-2.03	118.55	123.63
9	V	101	BCL	CED-O2D-CGD	2.03	120.52	115.92
9	2	101	BCL	CHC-C4B-NB	-2.03	121.01	124.05
15	F	104	SPO	C20-C21-C22	-2.02	119.38	123.52
9	P	102	BCL	C4D-CHA-C1A	-2.02	118.83	121.24
15	8	101	SPO	C36-C37-C38	-2.02	120.90	127.64
9	B	101	BCL	CAC-C3C-C4C	-2.02	108.10	112.58
16	S	105	LMT	C1B-O1B-C4'	-2.02	113.19	117.98
9	1	101	BCL	CBA-CAA-C2A	-2.02	107.79	113.79
9	K	102	BCL	O2A-CGA-O1A	-2.02	118.58	123.63
15	X	102	SPO	C31-C32-C33	-2.02	123.01	127.62
15	V	102	SPO	C20-C21-C22	-2.02	119.40	123.52
16	3	101	LMT	O3'-C3'-C2'	-2.01	105.63	110.38
10	M	804	BPH	CBA-CAA-C2A	-2.01	107.85	113.78
15	E	101	SPO	C13-C12-C11	2.01	121.16	118.09
9	2	101	BCL	C6-C5-C3	-2.01	108.57	113.47
15	5	104	SPO	C24-C23-C25	2.01	121.16	118.09
9	L	301	BCL	C11-C12-C13	-2.01	109.29	115.97
15	D	102	SPO	C21-C20-C19	-2.01	119.41	123.52
9	4	101	BCL	C2A-C1A-CHA	-2.01	120.38	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	804	BPH	C1-C2-C3	-2.01	122.91	126.20
9	L	309	BCL	CHB-C4A-NA	2.01	127.29	124.40
9	Y	103	BCL	CMB-C2B-C3B	2.01	132.00	125.67
15	8	101	SPO	C18-C17-C16	2.00	121.15	118.09
12	3	102	PGV	O01-C1-O02	-2.00	119.03	123.70
9	G	101	BCL	C4D-CHA-C1A	-2.00	118.86	121.24
16	K	101	LMT	O5'-C1'-C2'	-2.00	106.26	110.37

There are no chirality outliers.

All (891) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	L	301	BCL	C2C-C3C-CAC-CBC
9	L	301	BCL	C4C-C3C-CAC-CBC
9	L	308	BCL	CHA-CBD-CGD-O1D
9	L	308	BCL	CHA-CBD-CGD-O2D
9	M	803	BCL	CHA-CBD-CGD-O1D
9	M	803	BCL	CHA-CBD-CGD-O2D
9	B	101	BCL	C1A-C2A-CAA-CBA
9	B	101	BCL	C3A-C2A-CAA-CBA
9	E	102	BCL	C6-C7-C8-C10
9	J	101	BCL	C1A-C2A-CAA-CBA
9	J	101	BCL	C3A-C2A-CAA-CBA
9	K	102	BCL	C2C-C3C-CAC-CBC
9	K	102	BCL	C4C-C3C-CAC-CBC
9	N	102	BCL	C1A-C2A-CAA-CBA
9	N	102	BCL	C3A-C2A-CAA-CBA
9	P	102	BCL	C1A-C2A-CAA-CBA
9	P	102	BCL	C3A-C2A-CAA-CBA
9	V	101	BCL	C2C-C3C-CAC-CBC
9	V	101	BCL	C4C-C3C-CAC-CBC
9	W	101	BCL	C1A-C2A-CAA-CBA
9	W	101	BCL	C3A-C2A-CAA-CBA
9	Z	101	BCL	C1A-C2A-CAA-CBA
9	2	101	BCL	C1A-C2A-CAA-CBA
9	2	101	BCL	C3A-C2A-CAA-CBA
9	2	101	BCL	C6-C7-C8-C9
9	4	101	BCL	C1A-C2A-CAA-CBA
9	6	101	BCL	C1A-C2A-CAA-CBA
9	8	102	BCL	C1A-C2A-CAA-CBA
12	L	305	PGV	C03-O11-P-O12
12	L	305	PGV	C04-O12-P-O13

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Mol	Chain	Res	Type	Atoms
12	L	306	PGV	C03-O11-P-O13
12	L	306	PGV	C04-O12-P-O11
12	L	306	PGV	C04-O12-P-O14
12	L	306	PGV	C05-C04-O12-P
12	M	801	PGV	C03-O11-P-O12
12	M	801	PGV	C03-O11-P-O13
12	M	801	PGV	C03-O11-P-O14
12	M	812	PGV	C03-O11-P-O12
12	M	812	PGV	C03-O11-P-O13
12	M	812	PGV	C03-O11-P-O14
12	M	812	PGV	O01-C02-C03-O11
12	M	812	PGV	O02-C1-O01-C02
12	M	812	PGV	C2-C1-O01-C02
12	H	307	PGV	C03-O11-P-O12
12	H	307	PGV	C03-O11-P-O14
12	H	307	PGV	C04-O12-P-O13
12	H	307	PGV	O01-C02-C03-O11
12	K	104	PGV	O02-C1-O01-C02
12	K	104	PGV	C2-C1-O01-C02
12	3	102	PGV	C03-O11-P-O13
12	3	102	PGV	C04-O12-P-O11
12	3	102	PGV	C04-O12-P-O14
15	E	101	SPO	O1-C1-C4-C5
15	E	101	SPO	C2-C1-C4-C5
15	E	101	SPO	C3-C1-C4-C5
15	F	103	SPO	C28-C30-C31-C32
15	G	103	SPO	C3-C1-C4-C5
15	N	101	SPO	C5-C6-C7-C8
15	N	101	SPO	C5-C6-C7-C9
15	O	102	SPO	C10-C11-C12-C14
15	O	103	SPO	C34-C33-C35-C36
15	P	101	SPO	O1-C1-C4-C5
15	P	101	SPO	C2-C1-C4-C5
15	P	101	SPO	C3-C1-C4-C5
15	R	101	SPO	C22-C23-C25-C26
15	S	103	SPO	C10-C11-C12-C14
15	T	102	SPO	O1-C1-C4-C5
15	T	102	SPO	C2-C1-C4-C5
15	W	102	SPO	O1-C1-C4-C5
15	W	102	SPO	C2-C1-C4-C5
15	W	102	SPO	C3-C1-C4-C5
15	W	102	SPO	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	W	102	SPO	C5-C6-C7-C9
15	3	104	SPO	C5-C6-C7-C9
15	5	103	SPO	O1-C1-C4-C5
15	5	103	SPO	C2-C1-C4-C5
15	5	103	SPO	C3-C1-C4-C5
16	H	301	LMT	C3'-C4'-O1B-C1B
16	F	101	LMT	O5'-C1'-O1'-C1
16	I	102	LMT	C3'-C4'-O1B-C1B
16	U	101	LMT	O5'-C1'-O1'-C1
17	M	811	CDL	CA2-OA2-PA1-OA4
17	M	811	CDL	CA3-OA5-PA1-OA2
17	M	811	CDL	CA3-OA5-PA1-OA3
17	M	811	CDL	CA3-OA5-PA1-OA4
17	M	811	CDL	CB2-OB2-PB2-OB5
17	M	811	CDL	CB3-OB5-PB2-OB2
17	M	811	CDL	CB3-OB5-PB2-OB3
17	M	811	CDL	CB3-OB5-PB2-OB4
17	M	811	CDL	OB7-CB5-OB6-CB4
17	M	811	CDL	C51-CB5-OB6-CB4
17	H	304	CDL	CA3-OA5-PA1-OA3
17	H	304	CDL	C11-CA5-OA6-CA4
17	H	304	CDL	CB2-OB2-PB2-OB4
17	H	304	CDL	CB2-OB2-PB2-OB5
17	H	304	CDL	CB3-OB5-PB2-OB2
17	H	304	CDL	CB3-OB5-PB2-OB4
17	H	305	CDL	CA3-OA5-PA1-OA2
17	H	305	CDL	CA3-OA5-PA1-OA4
17	H	305	CDL	CB3-OB5-PB2-OB2
17	H	305	CDL	CB3-OB5-PB2-OB4
17	Y	102	CDL	CA2-OA2-PA1-OA3
17	Y	102	CDL	CA3-CA4-CA6-OA8
17	Y	102	CDL	OA6-CA4-CA6-OA8
17	Y	102	CDL	CB2-OB2-PB2-OB3
17	Y	102	CDL	CB3-OB5-PB2-OB3
16	H	302	LMT	C2B-C1B-O1B-C4'
16	3	101	LMT	C3'-C4'-O1B-C1B
16	X	105	LMT	C3'-C4'-O1B-C1B
9	L	301	BCL	CBD-CGD-O2D-CED
9	M	803	BCL	CBD-CGD-O2D-CED
16	K	101	LMT	C3'-C4'-O1B-C1B
16	F	101	LMT	O5B-C1B-O1B-C4'
17	H	304	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
9	A	703	BCL	C3-C5-C6-C7
9	D	101	BCL	C3-C5-C6-C7
9	G	101	BCL	C3-C5-C6-C7
9	6	101	BCL	CBD-CGD-O2D-CED
9	F	102	BCL	C4-C3-C5-C6
9	K	102	BCL	C4-C3-C5-C6
9	S	102	BCL	C4-C3-C5-C6
9	W	101	BCL	C4-C3-C5-C6
9	7	101	BCL	C4-C3-C5-C6
15	E	101	SPO	C29-C28-C30-C31
15	R	101	SPO	C34-C33-C35-C36
15	S	104	SPO	C34-C33-C35-C36
15	V	102	SPO	C34-C33-C35-C36
15	1	103	SPO	C29-C28-C30-C31
9	F	102	BCL	C2-C3-C5-C6
9	K	102	BCL	C2-C3-C5-C6
9	7	101	BCL	C2-C3-C5-C6
15	O	103	SPO	C32-C33-C35-C36
15	R	101	SPO	C32-C33-C35-C36
15	S	104	SPO	C32-C33-C35-C36
15	V	102	SPO	C32-C33-C35-C36
9	L	301	BCL	C3-C5-C6-C7
16	5	101	LMT	C3'-C4'-O1B-C1B
9	J	101	BCL	C3-C5-C6-C7
12	L	306	PGV	O12-C04-C05-O05
9	L	301	BCL	O1D-CGD-O2D-CED
16	H	301	LMT	O5'-C5'-C6'-O6'
16	M	809	LMT	O5'-C5'-C6'-O6'
12	L	305	PGV	C2-C1-O01-C02
9	M	803	BCL	O1D-CGD-O2D-CED
9	V	101	BCL	C4-C3-C5-C6
9	5	102	BCL	C4-C3-C5-C6
11	L	304	U10	C12-C11-C9-C10
15	K	103	SPO	C34-C33-C35-C36
15	5	104	SPO	C29-C28-C30-C31
9	S	102	BCL	C2-C3-C5-C6
9	V	101	BCL	C2-C3-C5-C6
9	W	101	BCL	C2-C3-C5-C6
9	5	102	BCL	C2-C3-C5-C6
11	L	304	U10	C12-C11-C9-C8
15	E	101	SPO	C27-C28-C30-C31
15	S	103	SPO	C32-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
15	5	104	SPO	C27-C28-C30-C31
16	S	105	LMT	O5B-C5B-C6B-O6B
11	M	806	U10	C24-C26-C27-C28
15	E	101	SPO	C33-C35-C36-C37
15	F	103	SPO	C33-C35-C36-C37
15	K	103	SPO	C28-C30-C31-C32
15	N	101	SPO	C33-C35-C36-C37
15	O	102	SPO	C28-C30-C31-C32
15	O	103	SPO	C33-C35-C36-C37
15	S	103	SPO	C28-C30-C31-C32
15	T	102	SPO	C33-C35-C36-C37
15	V	102	SPO	C33-C35-C36-C37
15	V	103	SPO	C28-C30-C31-C32
15	1	103	SPO	C28-C30-C31-C32
15	1	105	SPO	C28-C30-C31-C32
15	1	105	SPO	C33-C35-C36-C37
15	5	103	SPO	C28-C30-C31-C32
15	5	103	SPO	C33-C35-C36-C37
15	5	104	SPO	C28-C30-C31-C32
9	G	101	BCL	CBD-CGD-O2D-CED
9	A	703	BCL	C2A-CAA-CBA-CGA
16	M	808	LMT	O5'-C1'-O1'-C1
9	N	102	BCL	CBD-CGD-O2D-CED
12	H	307	PGV	C2-C1-O01-C02
16	F	101	LMT	C3'-C4'-O1B-C1B
12	L	305	PGV	O02-C1-O01-C02
15	G	102	SPO	C34-C33-C35-C36
15	N	101	SPO	C34-C33-C35-C36
15	S	103	SPO	C34-C33-C35-C36
15	V	103	SPO	C34-C33-C35-C36
15	8	101	SPO	C29-C28-C30-C31
15	G	102	SPO	C32-C33-C35-C36
15	K	103	SPO	C32-C33-C35-C36
15	N	101	SPO	C32-C33-C35-C36
15	V	103	SPO	C32-C33-C35-C36
15	1	103	SPO	C27-C28-C30-C31
15	8	101	SPO	C27-C28-C30-C31
9	3	103	BCL	C3-C5-C6-C7
9	L	301	BCL	C14-C13-C15-C16
9	L	308	BCL	C11-C10-C8-C9
9	B	101	BCL	C6-C7-C8-C9
9	D	101	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
9	G	101	BCL	C11-C10-C8-C9
9	J	101	BCL	C11-C10-C8-C9
9	R	102	BCL	C6-C7-C8-C9
9	T	101	BCL	C6-C7-C8-C9
9	W	101	BCL	C11-C12-C13-C14
9	Y	103	BCL	C11-C10-C8-C9
9	Z	101	BCL	C11-C10-C8-C9
9	6	101	BCL	C6-C7-C8-C9
9	8	102	BCL	C6-C7-C8-C9
16	M	808	LMT	C2'-C1'-O1'-C1
12	M	812	PGV	O12-C04-C05-O05
15	O	102	SPO	C10-C11-C12-C13
15	R	101	SPO	C24-C23-C25-C26
15	S	103	SPO	C10-C11-C12-C13
15	S	104	SPO	C5-C6-C7-C8
15	3	104	SPO	C5-C6-C7-C8
15	X	102	SPO	C5-C6-C7-C8
15	S	104	SPO	C5-C6-C7-C9
9	R	102	BCL	C2A-CAA-CBA-CGA
9	G	101	BCL	C8-C10-C11-C12
17	M	811	CDL	OA6-CA4-CA6-OA8
9	P	102	BCL	CBD-CGD-O2D-CED
9	F	102	BCL	C15-C16-C17-C18
9	K	102	BCL	C8-C10-C11-C12
9	K	102	BCL	C15-C16-C17-C18
9	R	102	BCL	C8-C10-C11-C12
9	6	101	BCL	O1D-CGD-O2D-CED
9	K	102	BCL	C5-C6-C7-C8
9	P	102	BCL	C6-C7-C8-C10
9	W	101	BCL	C11-C10-C8-C7
9	3	103	BCL	C6-C7-C8-C10
9	6	101	BCL	C11-C10-C8-C7
15	D	102	SPO	C28-C30-C31-C32
15	G	102	SPO	C33-C35-C36-C37
15	S	103	SPO	C33-C35-C36-C37
15	1	103	SPO	C33-C35-C36-C37
9	L	308	BCL	C13-C15-C16-C17
9	S	102	BCL	C15-C16-C17-C18
9	2	101	BCL	C10-C11-C12-C13
12	L	306	PGV	C1-C2-C3-C4
9	O	101	BCL	C15-C16-C17-C18
9	Y	103	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
9	1	101	BCL	C8-C10-C11-C12
9	6	101	BCL	C10-C11-C12-C13
9	E	102	BCL	C2A-CAA-CBA-CGA
16	F	101	LMT	C5'-C4'-O1B-C1B
9	A	703	BCL	C5-C6-C7-C8
9	T	101	BCL	C10-C11-C12-C13
12	L	305	PGV	C19-C20-C21-C22
12	M	812	PGV	C1-C2-C3-C4
9	J	101	BCL	C10-C11-C12-C13
9	J	101	BCL	C13-C15-C16-C17
9	S	102	BCL	C5-C6-C7-C8
9	5	102	BCL	C5-C6-C7-C8
12	L	305	PGV	O12-C04-C05-O05
16	M	809	LMT	C4'-C5'-C6'-O6'
12	H	306	PGV	C1-C2-C3-C4
9	R	102	BCL	C15-C16-C17-C18
9	Z	101	BCL	C8-C10-C11-C12
12	H	307	PGV	O02-C1-O01-C02
17	H	304	CDL	CB5-C51-C52-C53
9	J	101	BCL	C5-C6-C7-C8
9	7	101	BCL	C5-C6-C7-C8
15	W	102	SPO	C25-C26-C27-C28
9	F	102	BCL	C5-C6-C7-C8
12	L	305	PGV	O12-C04-C05-C06
9	P	102	BCL	C2A-CAA-CBA-CGA
9	V	101	BCL	C15-C16-C17-C18
9	K	102	BCL	C10-C11-C12-C13
9	N	102	BCL	C13-C15-C16-C17
9	R	102	BCL	C13-C15-C16-C17
9	Y	103	BCL	C10-C11-C12-C13
16	H	301	LMT	C4'-C5'-C6'-O6'
9	B	101	BCL	C8-C10-C11-C12
9	I	101	BCL	C10-C11-C12-C13
9	R	102	BCL	C5-C6-C7-C8
9	1	101	BCL	C10-C11-C12-C13
15	O	103	SPO	C28-C30-C31-C32
9	W	101	BCL	CBA-CGA-O2A-C1
9	2	101	BCL	CBA-CGA-O2A-C1
9	3	103	BCL	C16-C17-C18-C19
15	G	102	SPO	C10-C11-C12-C13
15	V	103	SPO	C10-C11-C12-C13
15	1	105	SPO	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
15	X	102	SPO	C10-C11-C12-C13
9	T	101	BCL	C2A-CAA-CBA-CGA
9	6	101	BCL	C8-C10-C11-C12
17	M	811	CDL	C17-C18-C19-C20
9	4	101	BCL	C16-C17-C18-C19
9	G	101	BCL	O1D-CGD-O2D-CED
9	E	102	BCL	C2-C1-O2A-CGA
9	T	101	BCL	C16-C17-C18-C19
9	V	101	BCL	C16-C17-C18-C19
16	S	105	LMT	C1-C2-C3-C4
9	L	301	BCL	C15-C16-C17-C18
12	Q	103	PGV	C24-C25-C26-C27
16	H	301	LMT	C6-C7-C8-C9
16	M	809	LMT	C2-C1-O1'-C1'
16	Q	101	LMT	C2-C1-O1'-C1'
12	L	305	PGV	C21-C22-C23-C24
9	E	102	BCL	C16-C17-C18-C19
9	V	101	BCL	C5-C6-C7-C8
12	Q	103	PGV	C01-C02-C03-O11
9	K	102	BCL	C11-C12-C13-C15
9	R	102	BCL	C6-C7-C8-C10
9	D	101	BCL	C8-C10-C11-C12
9	Z	101	BCL	C5-C6-C7-C8
13	L	307	LDA	C3-C4-C5-C6
9	W	101	BCL	C3-C5-C6-C7
9	G	101	BCL	C3A-C2A-CAA-CBA
9	R	102	BCL	C3A-C2A-CAA-CBA
9	T	101	BCL	C3A-C2A-CAA-CBA
9	Y	103	BCL	C3A-C2A-CAA-CBA
9	Z	101	BCL	C3A-C2A-CAA-CBA
9	4	101	BCL	C3A-C2A-CAA-CBA
9	6	101	BCL	C3A-C2A-CAA-CBA
9	O	101	BCL	C13-C15-C16-C17
9	T	101	BCL	C15-C16-C17-C18
9	8	102	BCL	C8-C10-C11-C12
9	L	309	BCL	C16-C17-C18-C19
12	Y	104	PGV	C4-C5-C6-C7
12	K	104	PGV	C22-C23-C24-C25
16	5	101	LMT	O5'-C5'-C6'-O6'
9	8	102	BCL	CBA-CGA-O2A-C1
9	2	101	BCL	C15-C16-C17-C18
12	Y	104	PGV	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
13	L	307	LDA	C2-C3-C4-C5
9	W	101	BCL	O1A-CGA-O2A-C1
16	S	105	LMT	C4B-C5B-C6B-O6B
9	N	102	BCL	O1D-CGD-O2D-CED
12	Q	103	PGV	C22-C23-C24-C25
9	4	101	BCL	C16-C17-C18-C20
9	2	101	BCL	O1A-CGA-O2A-C1
9	Y	103	BCL	C3-C5-C6-C7
9	G	101	BCL	C2A-CAA-CBA-CGA
9	4	101	BCL	C2A-CAA-CBA-CGA
15	S	104	SPO	C29-C28-C30-C31
15	T	102	SPO	C29-C28-C30-C31
12	3	102	PGV	C4-C5-C6-C7
9	T	101	BCL	C8-C10-C11-C12
13	X	103	LDA	C2-C3-C4-C5
16	M	809	LMT	C5-C6-C7-C8
12	H	307	PGV	C5-C6-C7-C8
12	K	104	PGV	C25-C26-C27-C28
16	D	103	LMT	O5B-C5B-C6B-O6B
16	Q	101	LMT	C1-C2-C3-C4
16	U	102	LMT	O5'-C5'-C6'-O6'
16	F	105	LMT	O1'-C1-C2-C3
9	Y	103	BCL	CBA-CGA-O2A-C1
12	L	306	PGV	C2-C1-O01-C02
13	M	802	LDA	C11-C10-C9-C8
9	M	803	BCL	C5-C6-C7-C8
9	N	102	BCL	C8-C10-C11-C12
15	O	103	SPO	C5-C6-C7-C8
15	S	104	SPO	C10-C11-C12-C13
15	1	102	SPO	C10-C11-C12-C13
15	5	104	SPO	C1-C4-C5-C6
9	Q	104	BCL	C16-C17-C18-C19
9	Q	104	BCL	C16-C17-C18-C20
9	3	103	BCL	C16-C17-C18-C20
12	K	104	PGV	C23-C24-C25-C26
15	S	104	SPO	C27-C28-C30-C31
15	T	102	SPO	C27-C28-C30-C31
9	L	309	BCL	C15-C16-C17-C18
9	Y	103	BCL	C8-C10-C11-C12
9	8	102	BCL	O1A-CGA-O2A-C1
16	I	102	LMT	O5'-C5'-C6'-O6'
17	H	304	CDL	OA5-CA3-CA4-OA6

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Mol	Chain	Res	Type	Atoms
16	K	101	LMT	O5'-C5'-C6'-O6'
15	G	103	SPO	C33-C35-C36-C37
12	Y	104	PGV	C2-C1-O01-C02
9	Q	104	BCL	C5-C6-C7-C8
16	A	701	LMT	O5B-C5B-C6B-O6B
12	L	305	PGV	C11-C10-C9-C8
12	M	801	PGV	C13-C14-C15-C16
16	H	302	LMT	O5B-C5B-C6B-O6B
16	Q	102	LMT	O5'-C5'-C6'-O6'
12	L	310	PGV	C4-C5-C6-C7
16	M	810	LMT	O5B-C1B-O1B-C4'
9	V	101	BCL	C16-C17-C18-C20
9	1	101	BCL	C16-C17-C18-C19
12	L	306	PGV	O02-C1-O01-C02
12	L	306	PGV	O12-C04-C05-C06
9	J	101	BCL	C2A-CAA-CBA-CGA
9	Z	101	BCL	C2A-CAA-CBA-CGA
16	3	101	LMT	C2-C3-C4-C5
9	P	102	BCL	O1D-CGD-O2D-CED
9	5	102	BCL	C15-C16-C17-C18
16	3	101	LMT	O5'-C5'-C6'-O6'
16	4	102	LMT	O5B-C5B-C6B-O6B
16	H	302	LMT	C3'-C4'-O1B-C1B
12	Y	104	PGV	C3-C4-C5-C6
9	L	309	BCL	C1A-C2A-CAA-CBA
9	G	101	BCL	C1A-C2A-CAA-CBA
9	R	102	BCL	C1A-C2A-CAA-CBA
9	T	101	BCL	C1A-C2A-CAA-CBA
9	Y	103	BCL	C1A-C2A-CAA-CBA
16	5	101	LMT	C1-C2-C3-C4
9	Y	103	BCL	O1A-CGA-O2A-C1
12	M	812	PGV	C01-C02-C03-O11
9	B	101	BCL	C6-C7-C8-C10
9	D	101	BCL	C6-C7-C8-C10
9	J	101	BCL	C11-C10-C8-C7
9	O	101	BCL	C6-C7-C8-C10
9	Q	104	BCL	C6-C7-C8-C10
9	Y	103	BCL	C11-C10-C8-C7
9	Z	101	BCL	C11-C10-C8-C7
9	6	101	BCL	C6-C7-C8-C10
9	8	102	BCL	C6-C7-C8-C10
15	M	807	SPO	C3-C1-C4-C5

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Mol	Chain	Res	Type	Atoms
15	G	103	SPO	C2-C1-C4-C5
15	T	102	SPO	C3-C1-C4-C5
9	1	101	BCL	C5-C6-C7-C8
9	6	101	BCL	C4-C3-C5-C6
15	1	102	SPO	C34-C33-C35-C36
15	W	102	SPO	C27-C28-C30-C31
9	4	101	BCL	C15-C16-C17-C18
9	7	101	BCL	C15-C16-C17-C18
9	6	101	BCL	C2A-CAA-CBA-CGA
9	A	703	BCL	C11-C10-C8-C9
9	P	102	BCL	C6-C7-C8-C9
9	Q	104	BCL	C11-C12-C13-C14
9	W	101	BCL	C6-C7-C8-C9
9	6	101	BCL	C11-C10-C8-C9
17	H	304	CDL	C31-CA7-OA8-CA6
16	A	701	LMT	O5'-C5'-C6'-O6'
16	1	104	LMT	O5'-C5'-C6'-O6'
16	D	103	LMT	O5'-C5'-C6'-O6'
12	H	306	PGV	O03-C01-C02-C03
15	D	102	SPO	C33-C35-C36-C37
15	S	104	SPO	C33-C35-C36-C37
17	M	811	CDL	CA3-CA4-CA6-OA8
16	A	702	LMT	O5'-C5'-C6'-O6'
16	3	101	LMT	C3-C4-C5-C6
16	A	702	LMT	O5B-C5B-C6B-O6B
9	W	101	BCL	C16-C17-C18-C19
12	M	812	PGV	C2-C3-C4-C5
16	3	101	LMT	C4-C5-C6-C7
9	Z	101	BCL	C15-C16-C17-C18
9	L	309	BCL	C4-C3-C5-C6
15	W	102	SPO	C29-C28-C30-C31
9	6	101	BCL	C2-C3-C5-C6
15	1	102	SPO	C32-C33-C35-C36
9	L	308	BCL	C15-C16-C17-C18
9	1	101	BCL	C16-C17-C18-C20
15	X	102	SPO	C5-C6-C7-C9
17	H	304	CDL	OA9-CA7-OA8-CA6
9	G	101	BCL	C15-C16-C17-C18
12	L	310	PGV	C03-O11-P-O13
16	4	102	LMT	O5'-C5'-C6'-O6'
16	M	810	LMT	C2-C3-C4-C5
9	N	102	BCL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
10	M	804	BPH	C4-C3-C5-C6
15	P	101	SPO	C34-C33-C35-C36
17	H	304	CDL	C51-C52-C53-C54
12	Q	103	PGV	O03-C01-C02-O01
9	V	101	BCL	C13-C15-C16-C17
9	S	102	BCL	CBA-CGA-O2A-C1
9	S	102	BCL	C8-C10-C11-C12
12	M	812	PGV	C6-C7-C8-C9
9	Y	103	BCL	C13-C15-C16-C17
9	2	101	BCL	C8-C10-C11-C12
9	G	101	BCL	C4-C3-C5-C6
9	Q	104	BCL	C4-C3-C5-C6
9	R	102	BCL	C4-C3-C5-C6
9	T	101	BCL	C4-C3-C5-C6
15	M	807	SPO	C29-C28-C30-C31
16	M	810	LMT	C2-C1-O1'-C1'
9	L	301	BCL	C11-C10-C8-C9
9	D	101	BCL	C6-C7-C8-C9
9	O	101	BCL	C6-C7-C8-C9
9	P	102	BCL	C11-C10-C8-C9
9	Q	104	BCL	C6-C7-C8-C9
9	3	103	BCL	C11-C10-C8-C9
9	E	102	BCL	C13-C15-C16-C17
9	O	101	BCL	C5-C6-C7-C8
9	P	102	BCL	C5-C6-C7-C8
12	L	305	PGV	C2-C3-C4-C5
17	M	811	CDL	C14-C15-C16-C17
17	H	304	CDL	OA5-CA3-CA4-CA6
16	I	102	LMT	O1'-C1-C2-C3
9	L	309	BCL	C6-C7-C8-C10
9	A	703	BCL	C11-C10-C8-C7
9	G	101	BCL	C11-C10-C8-C7
9	P	102	BCL	C11-C10-C8-C7
9	W	101	BCL	C6-C7-C8-C10
9	3	103	BCL	C11-C10-C8-C7
9	5	102	BCL	C6-C7-C8-C10
9	L	301	BCL	C13-C15-C16-C17
9	D	101	BCL	C15-C16-C17-C18
9	V	101	BCL	C8-C10-C11-C12
17	Y	102	CDL	O1-C1-CA2-OA2
16	A	701	LMT	C4-C5-C6-C7
9	8	102	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
10	L	302	BPH	C4-C3-C5-C6
15	M	807	SPO	C34-C33-C35-C36
16	S	105	LMT	C2-C3-C4-C5
16	X	105	LMT	O5'-C1'-O1'-C1
9	G	101	BCL	C5-C6-C7-C8
15	N	101	SPO	C24-C23-C25-C26
16	H	302	LMT	C5'-C4'-O1B-C1B
9	J	101	BCL	C15-C16-C17-C18
17	H	305	CDL	CA3-CA4-CA6-OA8
9	W	101	BCL	C16-C17-C18-C20
9	I	101	BCL	C5-C6-C7-C8
16	S	101	LMT	C3-C4-C5-C6
16	5	101	LMT	C5'-C4'-O1B-C1B
9	L	301	BCL	C4-C3-C5-C6
9	G	101	BCL	C2-C3-C5-C6
9	R	102	BCL	C2-C3-C5-C6
9	T	101	BCL	C2-C3-C5-C6
15	M	807	SPO	C32-C33-C35-C36
12	K	104	PGV	C14-C15-C16-C17
9	6	101	BCL	C16-C17-C18-C19
12	M	801	PGV	O01-C02-C03-O11
12	Q	103	PGV	O01-C02-C03-O11
12	Y	104	PGV	C5-C6-C7-C8
12	L	306	PGV	C2-C3-C4-C5
16	S	101	LMT	C2-C3-C4-C5
9	L	309	BCL	C16-C17-C18-C20
9	T	101	BCL	C16-C17-C18-C20
9	1	101	BCL	C13-C15-C16-C17
9	7	101	BCL	C8-C10-C11-C12
12	M	801	PGV	O03-C01-C02-O01
12	H	306	PGV	O03-C01-C02-O01
12	Y	104	PGV	O02-C1-O01-C02
10	L	302	BPH	C2-C3-C5-C6
10	M	804	BPH	C2-C3-C5-C6
15	M	807	SPO	C27-C28-C30-C31
12	K	104	PGV	C7-C8-C9-C10
10	M	804	BPH	C1-C2-C3-C5
9	A	703	BCL	C4B-C3B-CAB-OBB
17	Y	102	CDL	C71-C72-C73-C74
9	N	102	BCL	O1A-CGA-O2A-C1
9	E	102	BCL	C16-C17-C18-C20
12	M	812	PGV	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
15	F	104	SPO	C33-C35-C36-C37
15	K	103	SPO	C33-C35-C36-C37
15	N	101	SPO	C28-C30-C31-C32
12	H	306	PGV	C19-C20-C21-C22
12	K	104	PGV	C15-C16-C17-C18
9	Q	104	BCL	C2-C3-C5-C6
12	K	104	PGV	C26-C27-C28-C29
12	H	307	PGV	C01-C02-C03-O11
15	5	104	SPO	C10-C11-C12-C13
9	L	301	BCL	C11-C10-C8-C7
9	F	102	BCL	C6-C7-C8-C10
9	J	101	BCL	C6-C7-C8-C10
9	Q	104	BCL	C11-C10-C8-C7
9	S	102	BCL	C11-C12-C13-C15
9	1	101	BCL	C6-C7-C8-C10
9	5	102	BCL	C12-C13-C15-C16
9	7	101	BCL	C6-C7-C8-C10
15	M	807	SPO	C1-C4-C5-C6
15	V	103	SPO	C10-C11-C12-C14
15	1	102	SPO	C10-C11-C12-C14
15	1	105	SPO	C15-C16-C17-C19
12	M	812	PGV	C23-C24-C25-C26
12	H	306	PGV	C2-C1-O01-C02
9	S	102	BCL	O1A-CGA-O2A-C1
9	I	101	BCL	C15-C16-C17-C18
9	7	101	BCL	C3-C5-C6-C7
17	M	811	CDL	OB5-CB3-CB4-OB6
12	M	801	PGV	O03-C01-C02-C03
12	K	104	PGV	C1-C2-C3-C4
17	M	811	CDL	C13-C14-C15-C16
9	N	102	BCL	C4-C3-C5-C6
15	W	102	SPO	C34-C33-C35-C36
17	H	305	CDL	OA6-CA4-CA6-OA8
9	F	102	BCL	C6-C7-C8-C9
9	W	101	BCL	C11-C10-C8-C9
12	H	303	PGV	C20-C21-C22-C23
15	G	103	SPO	O1-C1-C4-C5
16	A	702	LMT	C3-C4-C5-C6
9	L	301	BCL	C10-C11-C12-C13
9	6	101	BCL	C16-C17-C18-C20
11	L	303	U10	C12-C11-C9-C10
15	1	105	SPO	C34-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
9	L	301	BCL	C2-C3-C5-C6
15	W	102	SPO	C32-C33-C35-C36
12	Y	104	PGV	O12-C04-C05-O05
9	2	101	BCL	C5-C6-C7-C8
16	A	702	LMT	O1'-C1-C2-C3
9	8	102	BCL	O2A-C1-C2-C3
15	G	103	SPO	C10-C11-C12-C13
12	H	303	PGV	C22-C23-C24-C25
17	H	304	CDL	C16-C17-C18-C19
9	L	308	BCL	C1A-C2A-CAA-CBA
9	E	102	BCL	C1A-C2A-CAA-CBA
9	F	102	BCL	C1A-C2A-CAA-CBA
9	Q	104	BCL	C1A-C2A-CAA-CBA
11	L	303	U10	C15-C14-C16-C17
9	8	102	BCL	CAA-CBA-CGA-O2A
15	G	102	SPO	C10-C11-C12-C14
15	X	102	SPO	C10-C11-C12-C14
9	R	102	BCL	C16-C17-C18-C19
17	M	811	CDL	C60-C61-C62-C63
12	M	801	PGV	C01-C02-C03-O11
12	X	101	PGV	C01-C02-C03-O11
17	M	811	CDL	OB5-CB3-CB4-CB6
9	L	308	BCL	C11-C10-C8-C7
9	M	803	BCL	C11-C10-C8-C7
9	I	101	BCL	C11-C12-C13-C15
9	S	102	BCL	C11-C10-C8-C7
9	V	101	BCL	C6-C7-C8-C10
9	8	102	BCL	C11-C10-C8-C7
9	L	301	BCL	C16-C17-C18-C19
9	M	803	BCL	C16-C17-C18-C19
9	5	102	BCL	C16-C17-C18-C19
15	M	807	SPO	C2-C1-C4-C5
9	8	102	BCL	CBD-CGD-O2D-CED
9	W	101	BCL	C15-C16-C17-C18
12	H	306	PGV	O02-C1-O01-C02
12	X	101	PGV	O01-C02-C03-O11
9	3	103	BCL	C13-C15-C16-C17
9	A	703	BCL	C4B-C3B-CAB-CBB
12	H	306	PGV	C21-C22-C23-C24
9	L	309	BCL	C6-C7-C8-C9
9	Q	104	BCL	C11-C10-C8-C9
9	S	102	BCL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
9	1	101	BCL	C6-C7-C8-C9
9	5	102	BCL	C14-C13-C15-C16
9	7	101	BCL	C6-C7-C8-C9
15	P	101	SPO	C25-C26-C27-C28
9	L	309	BCL	C5-C6-C7-C8
9	Y	103	BCL	C15-C16-C17-C18
9	7	101	BCL	C13-C15-C16-C17
17	Y	102	CDL	O1-C1-CB2-OB2
9	E	102	BCL	C8-C10-C11-C12
9	S	102	BCL	C10-C11-C12-C13
12	X	101	PGV	C22-C23-C24-C25
9	L	309	BCL	CHA-CBD-CGD-O1D
9	L	309	BCL	CHA-CBD-CGD-O2D
12	L	305	PGV	C03-O11-P-O13
12	L	306	PGV	C03-O11-P-O12
12	M	812	PGV	C04-O12-P-O13
12	Q	103	PGV	C04-O12-P-O13
12	X	101	PGV	C04-O12-P-O13
17	M	811	CDL	CA2-OA2-PA1-OA5
17	M	811	CDL	CB2-OB2-PB2-OB3
17	H	304	CDL	CA2-OA2-PA1-OA4
17	H	304	CDL	CA2-OA2-PA1-OA5
17	H	304	CDL	CB3-OB5-PB2-OB3
9	2	101	BCL	C4-C3-C5-C6
9	N	102	BCL	C2-C3-C5-C6
15	P	101	SPO	C32-C33-C35-C36
12	M	812	PGV	C02-C03-O11-P
15	1	102	SPO	C24-C23-C25-C26
13	Y	101	LDA	C3-C4-C5-C6
16	M	809	LMT	C3-C4-C5-C6
17	M	811	CDL	C38-C39-C40-C41
13	L	311	LDA	C6-C7-C8-C9
12	H	306	PGV	O12-C04-C05-O05
13	L	311	LDA	C11-C10-C9-C8
16	5	101	LMT	C6-C7-C8-C9
9	M	803	BCL	C6-C7-C8-C9
9	E	102	BCL	C11-C10-C8-C9
9	J	101	BCL	C6-C7-C8-C9
9	V	101	BCL	C6-C7-C8-C9
9	5	102	BCL	C6-C7-C8-C9
16	H	302	LMT	O5'-C5'-C6'-O6'
9	M	803	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
9	D	101	BCL	C11-C10-C8-C7
9	W	101	BCL	C11-C12-C13-C15
9	4	101	BCL	C6-C7-C8-C10
12	M	812	PGV	O12-C04-C05-C06
17	M	811	CDL	C71-CB7-OB8-CB6
12	X	101	PGV	C1-C2-C3-C4
9	P	102	BCL	C15-C16-C17-C18
9	L	309	BCL	C2-C3-C5-C6
12	3	102	PGV	C13-C14-C15-C16
12	Y	104	PGV	C20-C21-C22-C23
16	U	102	LMT	C7-C8-C9-C10
9	7	101	BCL	C10-C11-C12-C13
11	L	303	U10	C25-C24-C26-C27
9	3	103	BCL	C8-C10-C11-C12
12	Q	103	PGV	O03-C01-C02-C03
9	T	101	BCL	C3-C5-C6-C7
15	O	103	SPO	C3-C1-O1-CM1
15	R	101	SPO	C1-C4-C5-C6
12	3	102	PGV	C21-C22-C23-C24
9	W	101	BCL	C10-C11-C12-C13
9	L	301	BCL	C2A-CAA-CBA-CGA
11	L	303	U10	C13-C14-C16-C17
17	M	811	CDL	C73-C74-C75-C76
12	M	801	PGV	C2-C3-C4-C5
9	I	101	BCL	C11-C12-C13-C14
9	S	102	BCL	C11-C10-C8-C9
9	A	703	BCL	C10-C11-C12-C13
17	H	304	CDL	CA4-CA3-OA5-PA1
17	M	811	CDL	OB9-CB7-OB8-CB6
9	Z	101	BCL	C16-C17-C18-C19
9	I	101	BCL	C4-C3-C5-C6
9	Y	103	BCL	C4-C3-C5-C6
11	L	303	U10	C23-C24-C26-C27
9	F	102	BCL	C11-C12-C13-C15
9	S	102	BCL	C6-C7-C8-C10
9	1	101	BCL	C11-C10-C8-C7
17	M	811	CDL	C31-CA7-OA8-CA6
9	R	102	BCL	C16-C17-C18-C20
12	H	307	PGV	O03-C01-C02-O01
9	F	102	BCL	C3A-C2A-CAA-CBA
9	Q	104	BCL	C3A-C2A-CAA-CBA
9	2	101	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
15	O	103	SPO	C12-C14-C15-C16
9	Q	104	BCL	C13-C15-C16-C17
15	N	101	SPO	C22-C23-C25-C26
15	S	104	SPO	C10-C11-C12-C14
9	A	703	BCL	C4-C3-C5-C6
11	L	303	U10	C12-C11-C9-C8
9	7	101	BCL	C16-C17-C18-C19
15	R	101	SPO	C28-C30-C31-C32
9	K	102	BCL	C13-C15-C16-C17
9	P	102	BCL	C14-C13-C15-C16
9	V	101	BCL	C14-C13-C15-C16
9	1	101	BCL	C11-C10-C8-C9
9	2	101	BCL	C11-C10-C8-C9
9	4	101	BCL	C11-C10-C8-C9
17	Y	102	CDL	C34-C35-C36-C37
17	H	304	CDL	C52-C53-C54-C55
15	O	103	SPO	C25-C26-C27-C28
9	N	102	BCL	CAA-CBA-CGA-O2A
16	F	101	LMT	C1-C2-C3-C4
17	M	811	CDL	OA9-CA7-OA8-CA6
9	3	103	BCL	C1A-C2A-CAA-CBA
16	M	809	LMT	C7-C8-C9-C10
16	M	810	LMT	C3-C4-C5-C6
9	L	309	BCL	C3-C5-C6-C7
9	B	101	BCL	C15-C16-C17-C18
16	1	104	LMT	C1-C2-C3-C4
9	A	703	BCL	C2-C3-C5-C6
9	G	101	BCL	C6-C7-C8-C10
9	T	101	BCL	C6-C7-C8-C10
15	O	102	SPO	C2-C1-C4-C5
12	Y	104	PGV	O12-C04-C05-C06
12	H	306	PGV	C7-C8-C9-C10
9	Z	101	BCL	C4-C3-C5-C6
9	1	101	BCL	C4-C3-C5-C6
9	I	101	BCL	C2-C3-C5-C6
9	Y	103	BCL	C2-C3-C5-C6
9	L	301	BCL	C2-C1-O2A-CGA
17	H	304	CDL	C14-C15-C16-C17
9	S	102	BCL	C6-C7-C8-C9
9	P	102	BCL	C16-C17-C18-C19
11	L	303	U10	C21-C22-C23-C24
12	Y	104	PGV	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
15	F	103	SPO	C34-C33-C35-C36
15	G	102	SPO	C29-C28-C30-C31
15	P	101	SPO	C29-C28-C30-C31
15	T	102	SPO	C34-C33-C35-C36
15	1	105	SPO	C32-C33-C35-C36
9	8	102	BCL	O1D-CGD-O2D-CED
12	L	310	PGV	C22-C23-C24-C25
9	Q	104	BCL	O1A-CGA-O2A-C1
11	L	303	U10	C11-C12-C13-C14
12	L	310	PGV	C29-C30-C31-C32
12	3	102	PGV	O03-C19-C20-C21
9	5	102	BCL	C10-C11-C12-C13
12	M	801	PGV	C22-C23-C24-C25
12	K	104	PGV	C9-C10-C11-C12
9	E	102	BCL	O1D-CGD-O2D-CED
12	H	307	PGV	C1-C2-C3-C4
17	H	304	CDL	CA5-C11-C12-C13
9	Z	101	BCL	C2-C3-C5-C6
15	G	102	SPO	C27-C28-C30-C31
17	M	811	CDL	C61-C62-C63-C64
16	A	702	LMT	C7-C8-C9-C10
9	2	101	BCL	C11-C10-C8-C7
16	M	809	LMT	C1-C2-C3-C4
9	E	102	BCL	C6-C7-C8-C9
9	I	101	BCL	C6-C7-C8-C9
9	8	102	BCL	C11-C10-C8-C9
9	V	101	BCL	C2-C1-O2A-CGA
9	Z	101	BCL	C16-C17-C18-C20
9	E	102	BCL	C3A-C2A-CAA-CBA
9	3	103	BCL	C3A-C2A-CAA-CBA
16	3	101	LMT	C5'-C4'-O1B-C1B
9	1	101	BCL	C2-C3-C5-C6
12	Y	104	PGV	C2-C3-C4-C5
9	5	102	BCL	C3-C5-C6-C7
12	H	303	PGV	C7-C8-C9-C10
9	A	703	BCL	C2B-C3B-CAB-OBB
17	H	304	CDL	C17-C18-C19-C20
16	X	105	LMT	C4-C5-C6-C7
16	M	810	LMT	C2B-C1B-O1B-C4'
17	M	811	CDL	O1-C1-CB2-OB2
16	M	809	LMT	C6-C7-C8-C9
9	Q	104	BCL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	M	801	PGV	C9-C10-C11-C12
16	3	101	LMT	C5-C6-C7-C8
17	Y	102	CDL	OB5-CB3-CB4-OB6
16	M	810	LMT	C5'-C4'-O1B-C1B
12	H	307	PGV	O03-C01-C02-C03
12	H	306	PGV	C23-C24-C25-C26
16	H	302	LMT	O1'-C1-C2-C3
16	S	105	LMT	C4'-C5'-C6'-O6'
15	F	103	SPO	C17-C19-C20-C21
15	N	101	SPO	C25-C26-C27-C28
17	M	811	CDL	C11-C12-C13-C14
9	O	101	BCL	C3-C5-C6-C7
12	M	812	PGV	O03-C01-C02-O01
9	M	803	BCL	C11-C10-C8-C9
9	O	101	BCL	C11-C10-C8-C9
12	H	306	PGV	C9-C10-C11-C12
15	G	103	SPO	C10-C11-C12-C14
15	O	103	SPO	C5-C6-C7-C9
17	M	811	CDL	C63-C64-C65-C66
15	M	807	SPO	O1-C1-C4-C5
15	O	102	SPO	C29-C28-C30-C31
17	H	305	CDL	OA9-CA7-OA8-CA6
12	H	307	PGV	C22-C23-C24-C25
9	Y	103	BCL	C2A-CAA-CBA-CGA
9	L	301	BCL	C12-C13-C15-C16
9	I	101	BCL	C6-C7-C8-C10
9	2	101	BCL	C6-C7-C8-C10
10	M	804	BPH	C6-C7-C8-C10
9	O	101	BCL	C8-C10-C11-C12
12	M	801	PGV	O02-C1-O01-C02
12	L	306	PGV	C6-C7-C8-C9
16	A	702	LMT	C5-C6-C7-C8
11	L	304	U10	C9-C11-C12-C13
9	W	101	BCL	CAA-CBA-CGA-O2A
13	L	307	LDA	C2-C1-N1-CM1
13	L	307	LDA	C2-C1-N1-CM2
15	O	103	SPO	C2-C1-O1-CM1
15	P	101	SPO	C3-C1-O1-CM1
15	T	102	SPO	C3-C1-O1-CM1
9	P	102	BCL	C10-C11-C12-C13
12	M	801	PGV	O01-C1-C2-C3
12	L	305	PGV	O01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
17	Y	102	CDL	C73-C74-C75-C76
9	Q	104	BCL	C14-C13-C15-C16
9	4	101	BCL	C11-C12-C13-C14
9	7	101	BCL	C11-C10-C8-C9
12	X	101	PGV	C25-C26-C27-C28
15	5	104	SPO	C5-C6-C7-C8
9	D	101	BCL	O1D-CGD-O2D-CED
9	O	101	BCL	C1A-C2A-CAA-CBA
9	O	101	BCL	C4-C3-C5-C6
15	5	104	SPO	C10-C11-C12-C14
15	3	104	SPO	C11-C10-C9-C7
12	K	104	PGV	O03-C19-C20-C21
9	I	101	BCL	C13-C15-C16-C17
9	A	703	BCL	C2-C1-O2A-CGA
9	D	101	BCL	C2-C1-O2A-CGA
9	Q	104	BCL	C2-C1-O2A-CGA
9	S	102	BCL	C2-C1-O2A-CGA
9	L	301	BCL	C6-C7-C8-C10
9	A	703	BCL	C2B-C3B-CAB-CBB
10	L	302	BPH	O2A-C1-C2-C3
13	M	802	LDA	C6-C7-C8-C9
15	3	104	SPO	C3-C1-C4-C5
9	7	101	BCL	C16-C17-C18-C20
12	M	812	PGV	O01-C1-C2-C3
16	S	101	LMT	O1'-C1-C2-C3
9	O	101	BCL	C3A-C2A-CAA-CBA
12	3	102	PGV	C22-C23-C24-C25
17	Y	102	CDL	C72-C73-C74-C75
12	L	306	PGV	O01-C1-C2-C3
9	5	102	BCL	C13-C15-C16-C17
12	M	801	PGV	O02-C1-C2-C3
17	H	305	CDL	C31-CA7-OA8-CA6
9	L	301	BCL	C6-C7-C8-C9
9	G	101	BCL	C6-C7-C8-C9
9	K	102	BCL	C11-C12-C13-C14
15	P	101	SPO	C27-C28-C30-C31
16	S	101	LMT	C1-C2-C3-C4
12	K	104	PGV	O04-C19-C20-C21
9	W	101	BCL	C5-C6-C7-C8
12	L	310	PGV	C13-C14-C15-C16
12	H	306	PGV	O03-C19-C20-C21
15	R	101	SPO	C10-C11-C12-C14

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Mol	Chain	Res	Type	Atoms
15	5	104	SPO	C5-C6-C7-C9
12	K	104	PGV	C24-C25-C26-C27
9	V	101	BCL	O1A-CGA-O2A-C1
9	2	101	BCL	CAA-CBA-CGA-O2A
9	P	102	BCL	C16-C17-C18-C20
16	Q	102	LMT	C1-C2-C3-C4
15	D	102	SPO	C29-C28-C30-C31
15	5	104	SPO	C34-C33-C35-C36
11	L	303	U10	C16-C17-C18-C19
9	8	102	BCL	CAA-CBA-CGA-O1A
9	L	309	BCL	CAD-CBD-CGD-O2D
9	6	101	BCL	CAD-CBD-CGD-O2D
16	M	810	LMT	O5'-C1'-O1'-C1
9	B	101	BCL	C2-C1-O2A-CGA
16	U	102	LMT	C9-C10-C11-C12
9	L	309	BCL	CAA-CBA-CGA-O2A
12	L	310	PGV	O03-C19-C20-C21
11	L	304	U10	C2-C3-O3-C3M
12	M	801	PGV	C2-C1-O01-C02
16	X	105	LMT	C3-C4-C5-C6
16	A	701	LMT	C5-C6-C7-C8

There are no ring outliers.

99 monomers are involved in 325 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	5	104	SPO	7	0
9	K	102	BCL	5	0
15	V	103	SPO	4	0
13	X	104	LDA	1	0
9	4	101	BCL	3	0
16	5	101	LMT	2	0
13	Y	101	LDA	5	0
12	L	310	PGV	1	0
12	M	801	PGV	2	0
9	V	101	BCL	7	0
16	K	101	LMT	2	0
9	M	803	BCL	3	0
12	3	102	PGV	1	0
12	M	812	PGV	4	0
16	A	701	LMT	1	0
16	A	704	LMT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	W	102	SPO	4	0
13	L	311	LDA	2	0
9	6	101	BCL	3	0
15	O	103	SPO	4	0
9	L	308	BCL	6	0
9	W	101	BCL	6	0
16	U	102	LMT	2	0
9	S	102	BCL	4	0
11	L	304	U10	4	0
10	L	302	BPH	5	0
16	A	702	LMT	5	0
17	M	811	CDL	6	0
9	Y	103	BCL	6	0
15	5	103	SPO	5	0
11	L	303	U10	3	0
15	F	103	SPO	4	0
15	D	102	SPO	3	0
9	J	101	BCL	3	0
16	Q	101	LMT	3	0
11	M	806	U10	2	0
16	M	810	LMT	2	0
9	T	101	BCL	5	0
17	Y	102	CDL	2	0
9	3	103	BCL	3	0
16	M	809	LMT	2	0
16	3	101	LMT	4	0
9	B	101	BCL	8	0
15	S	104	SPO	5	0
12	Q	103	PGV	1	0
9	G	101	BCL	2	0
12	L	306	PGV	3	0
15	G	102	SPO	7	0
15	3	104	SPO	2	0
9	N	102	BCL	1	0
10	M	804	BPH	6	0
15	1	103	SPO	4	0
15	S	103	SPO	6	0
9	F	102	BCL	2	0
9	R	102	BCL	3	0
15	K	103	SPO	6	0
9	5	102	BCL	6	0
15	T	102	SPO	10	0

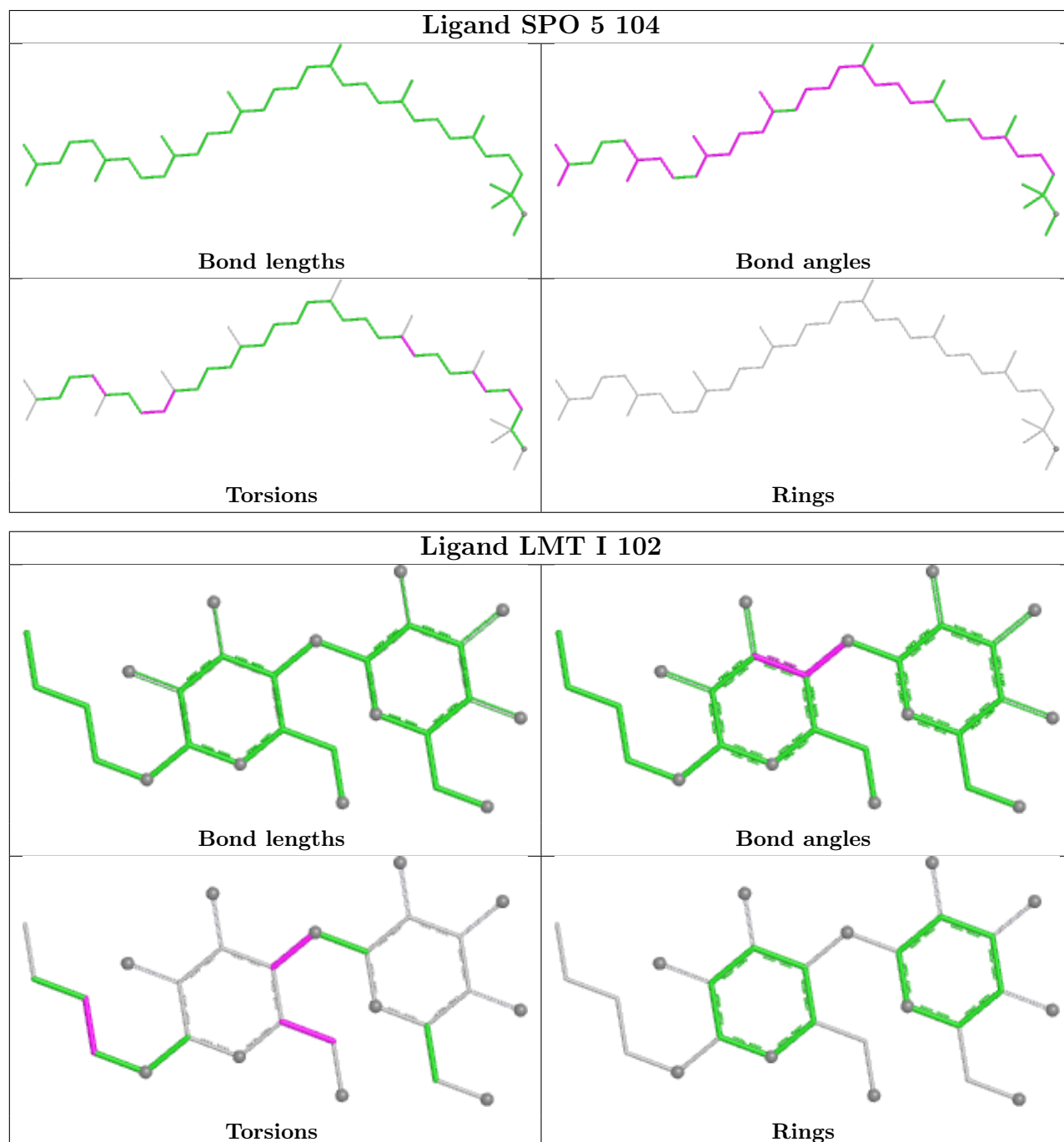
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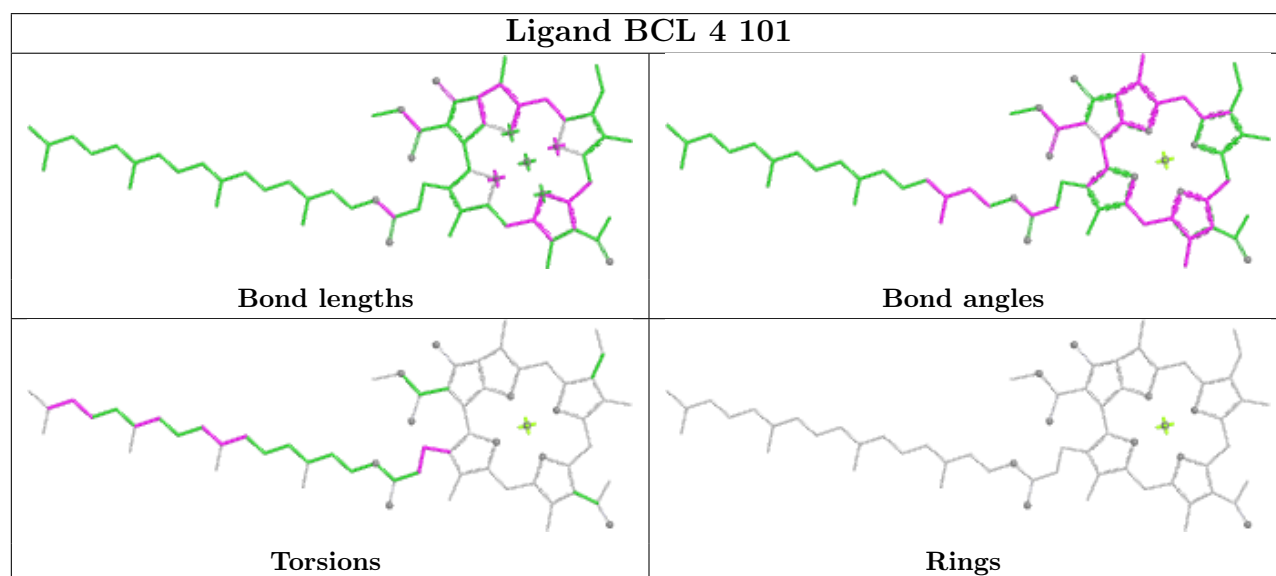
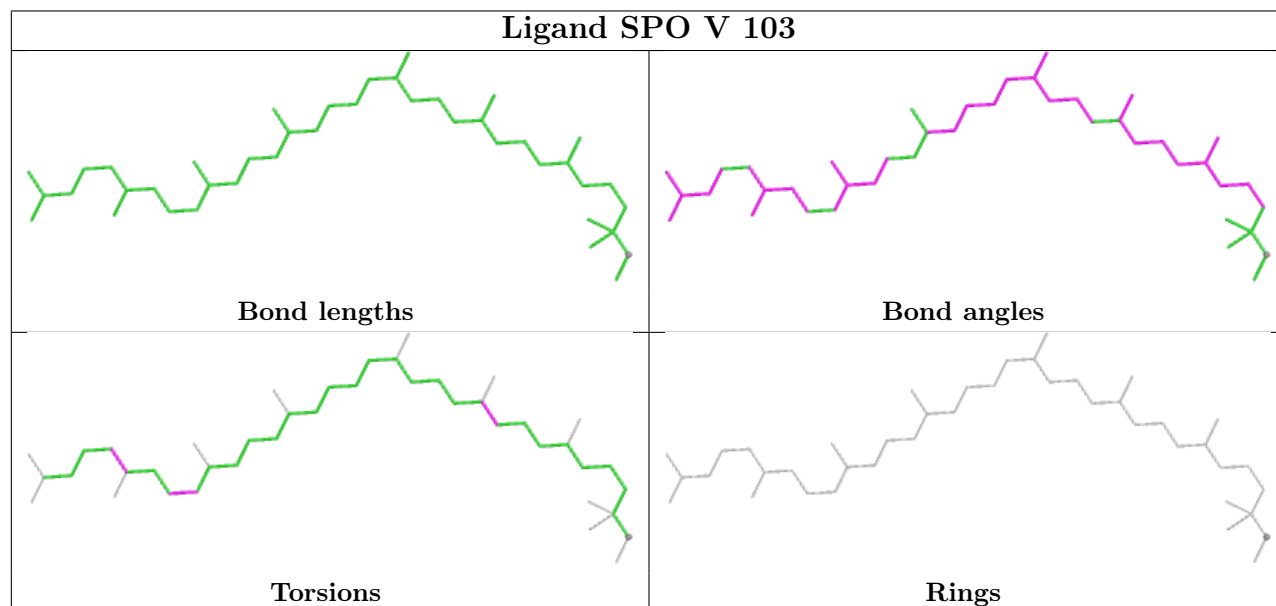
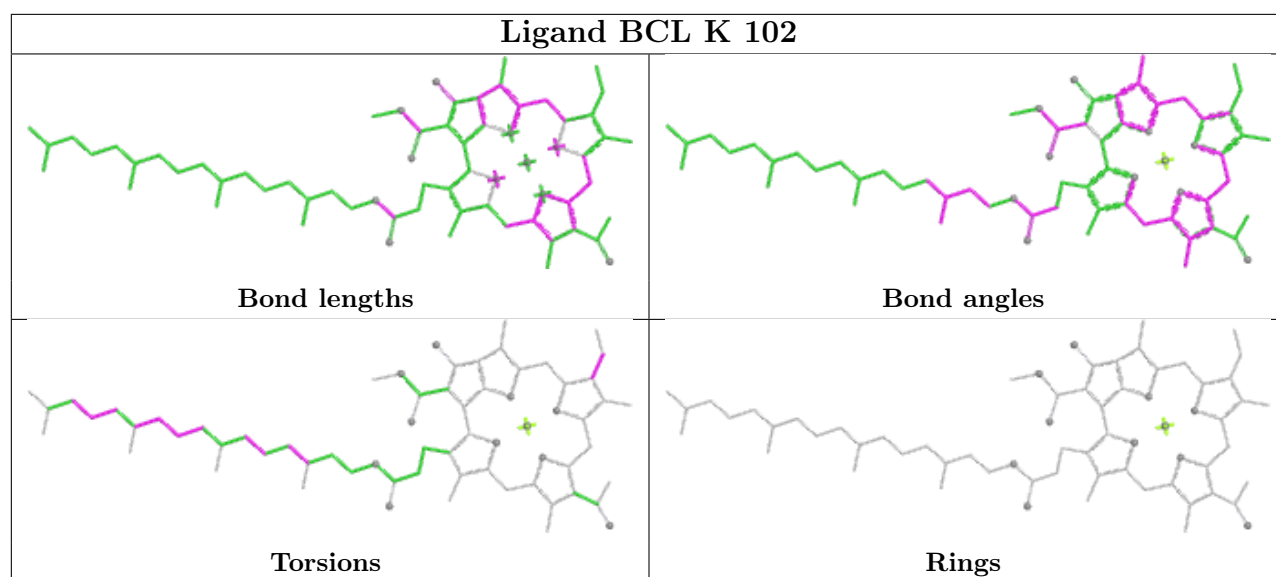
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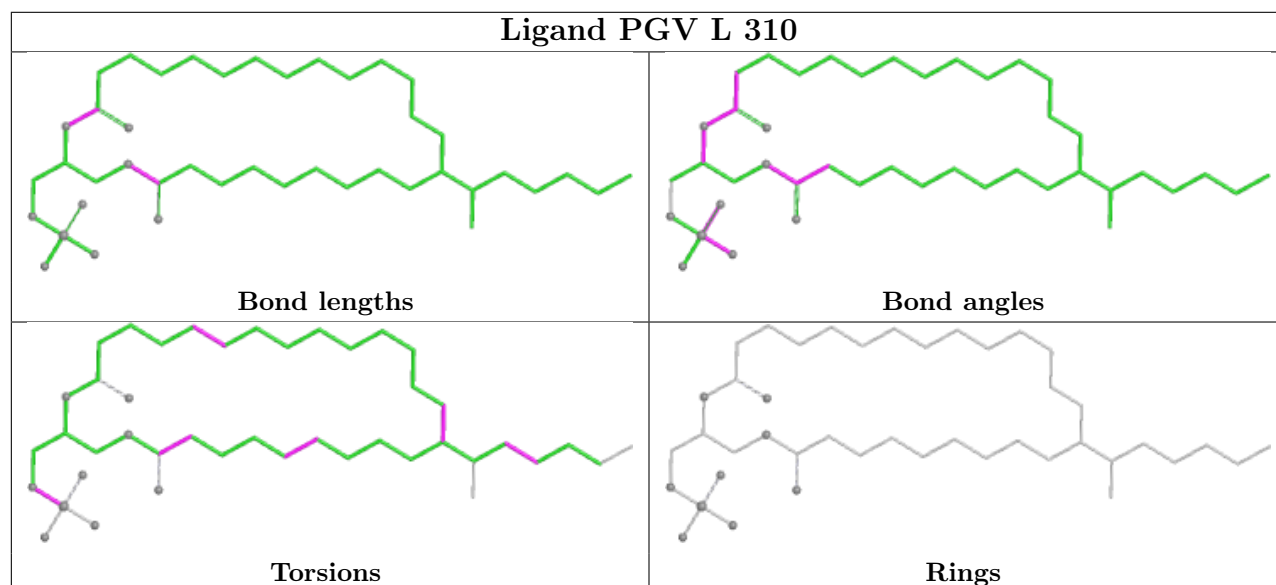
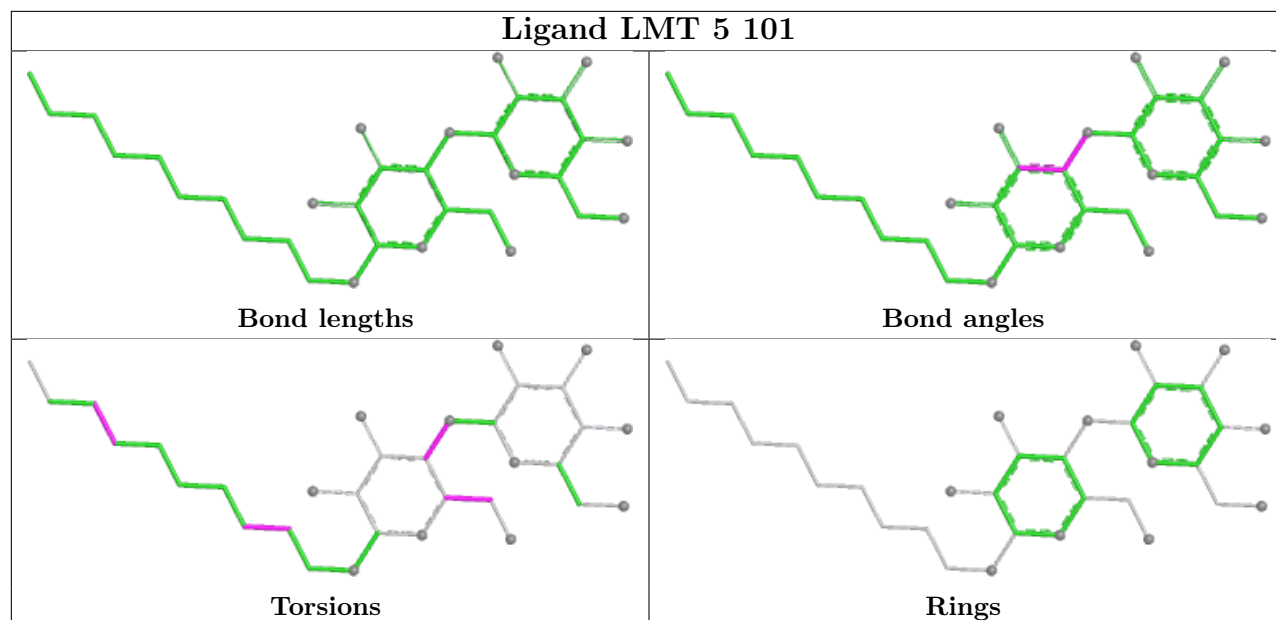
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	M	808	LMT	2	0
9	L	301	BCL	7	0
15	E	101	SPO	3	0
12	H	307	PGV	3	0
9	8	102	BCL	6	0
15	V	102	SPO	4	0
17	H	304	CDL	6	0
15	F	104	SPO	3	0
9	1	101	BCL	4	0
9	D	101	BCL	4	0
9	Z	101	BCL	2	0
9	P	102	BCL	2	0
16	H	301	LMT	1	0
16	S	105	LMT	1	0
15	1	102	SPO	3	0
15	R	101	SPO	6	0
15	N	101	SPO	8	0
12	K	104	PGV	3	0
16	Q	102	LMT	1	0
13	X	103	LDA	2	0
9	E	102	BCL	6	0
9	L	309	BCL	3	0
15	1	105	SPO	7	0
15	X	102	SPO	4	0
12	Y	104	PGV	7	0
9	Q	104	BCL	1	0
9	2	101	BCL	4	0
15	8	101	SPO	5	0
15	O	102	SPO	8	0
16	H	302	LMT	4	0
9	O	101	BCL	4	0
9	A	703	BCL	2	0
12	L	305	PGV	4	0
15	M	807	SPO	4	0
15	G	103	SPO	8	0
9	I	101	BCL	6	0
9	7	101	BCL	6	0
16	S	101	LMT	1	0
15	P	101	SPO	2	0
12	X	101	PGV	3	0
12	H	306	PGV	3	0

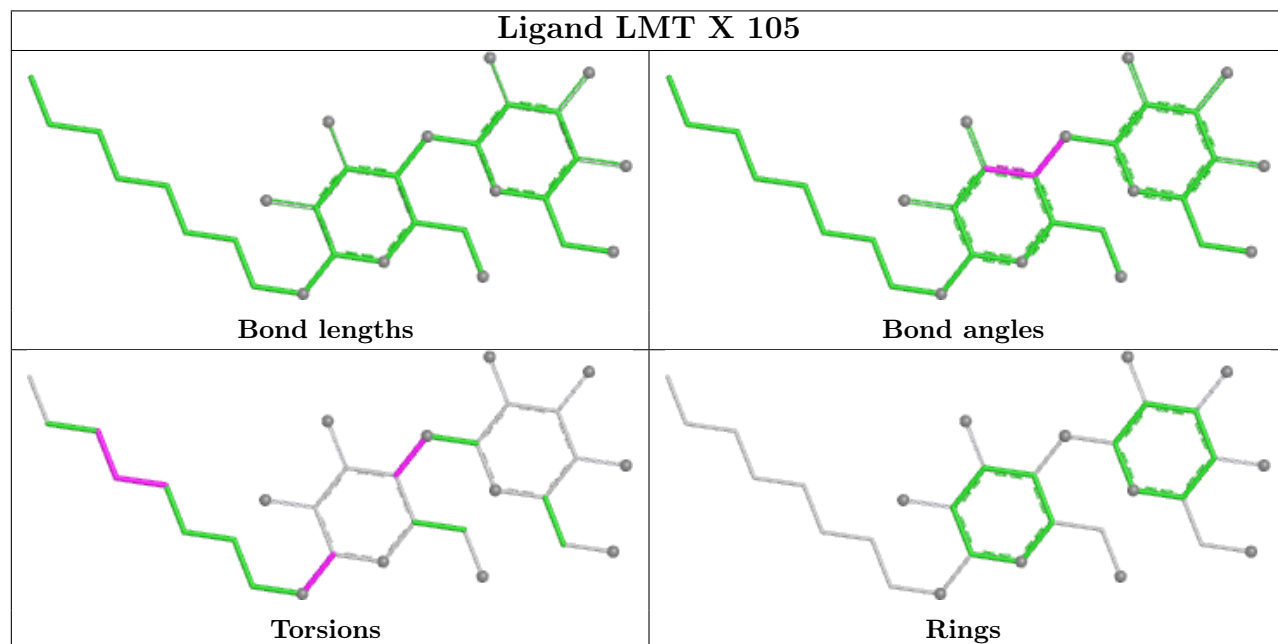
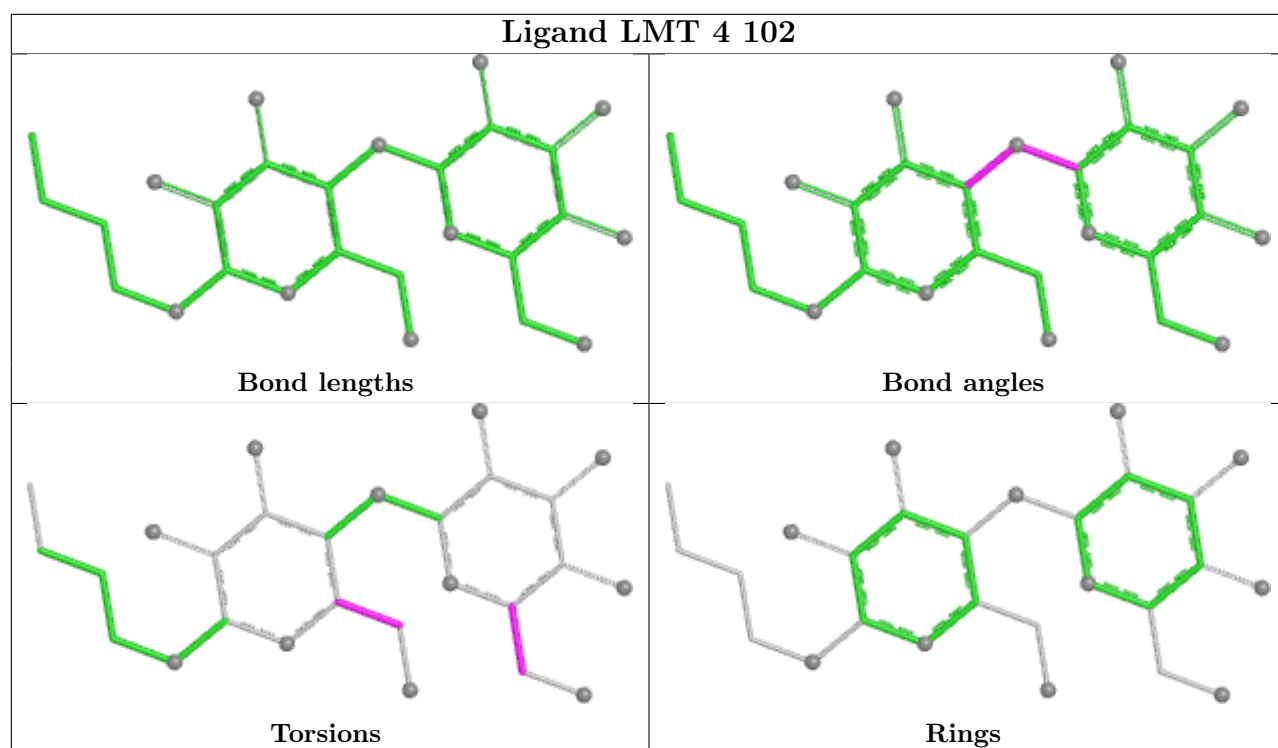
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

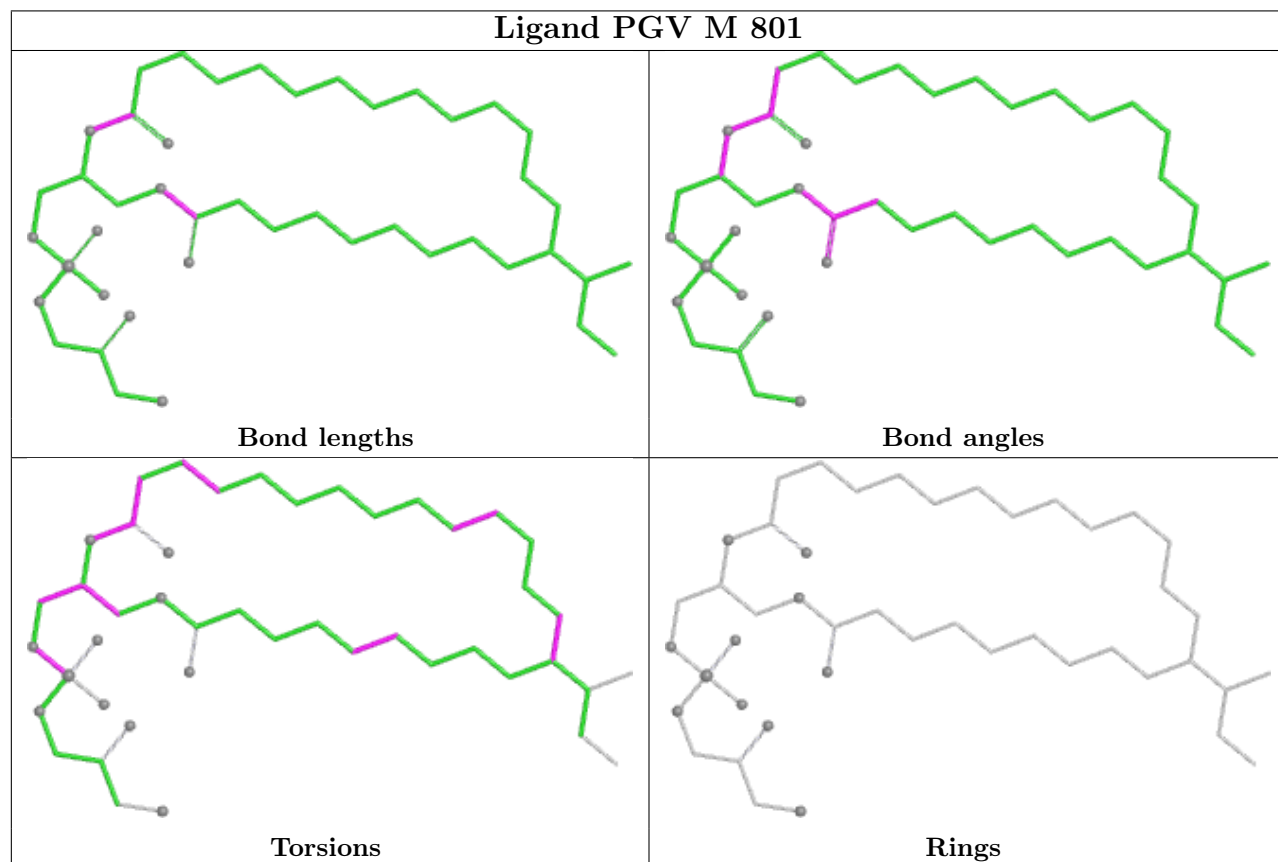
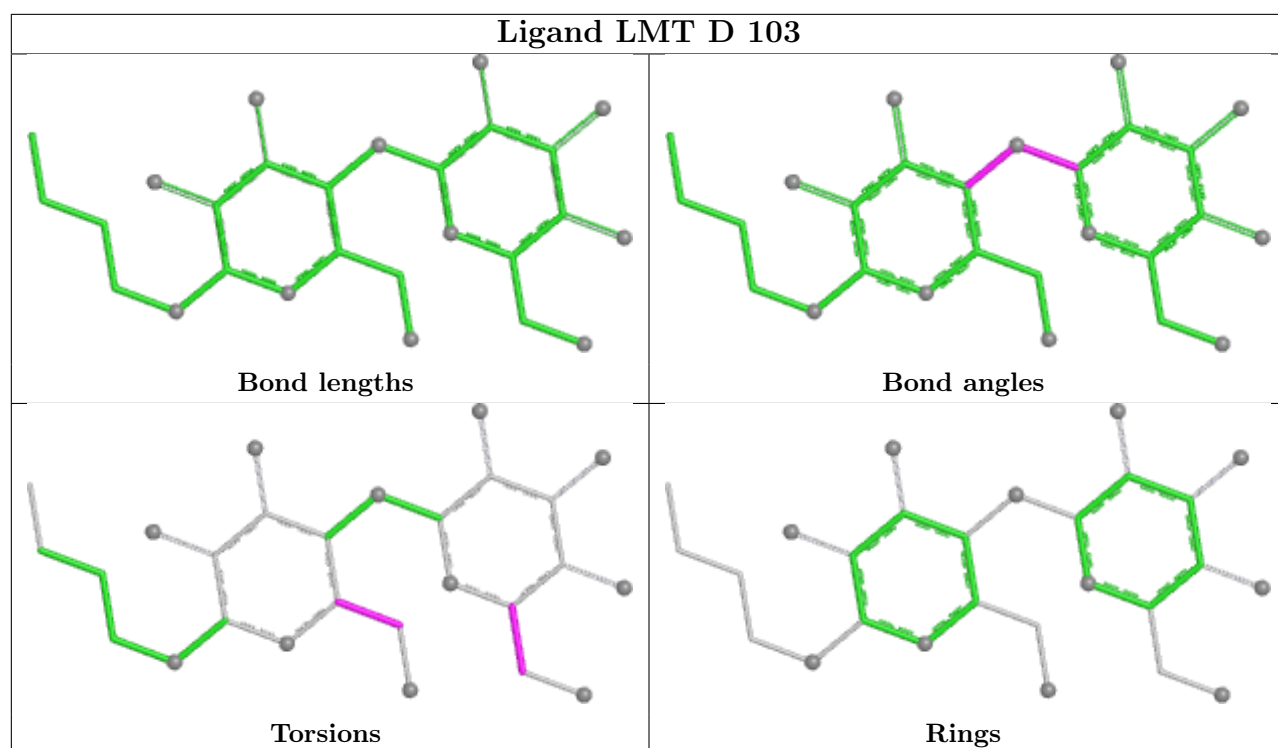
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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

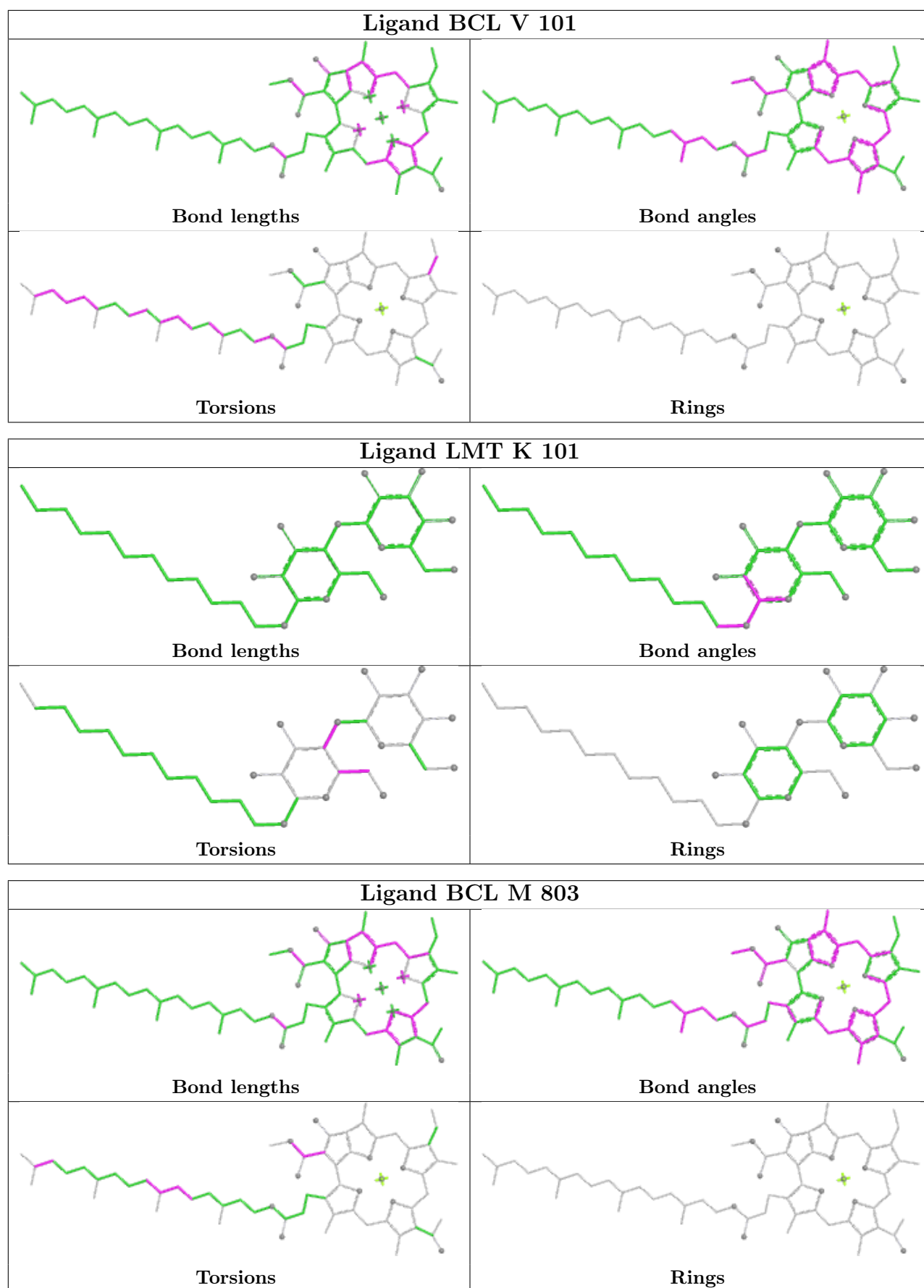


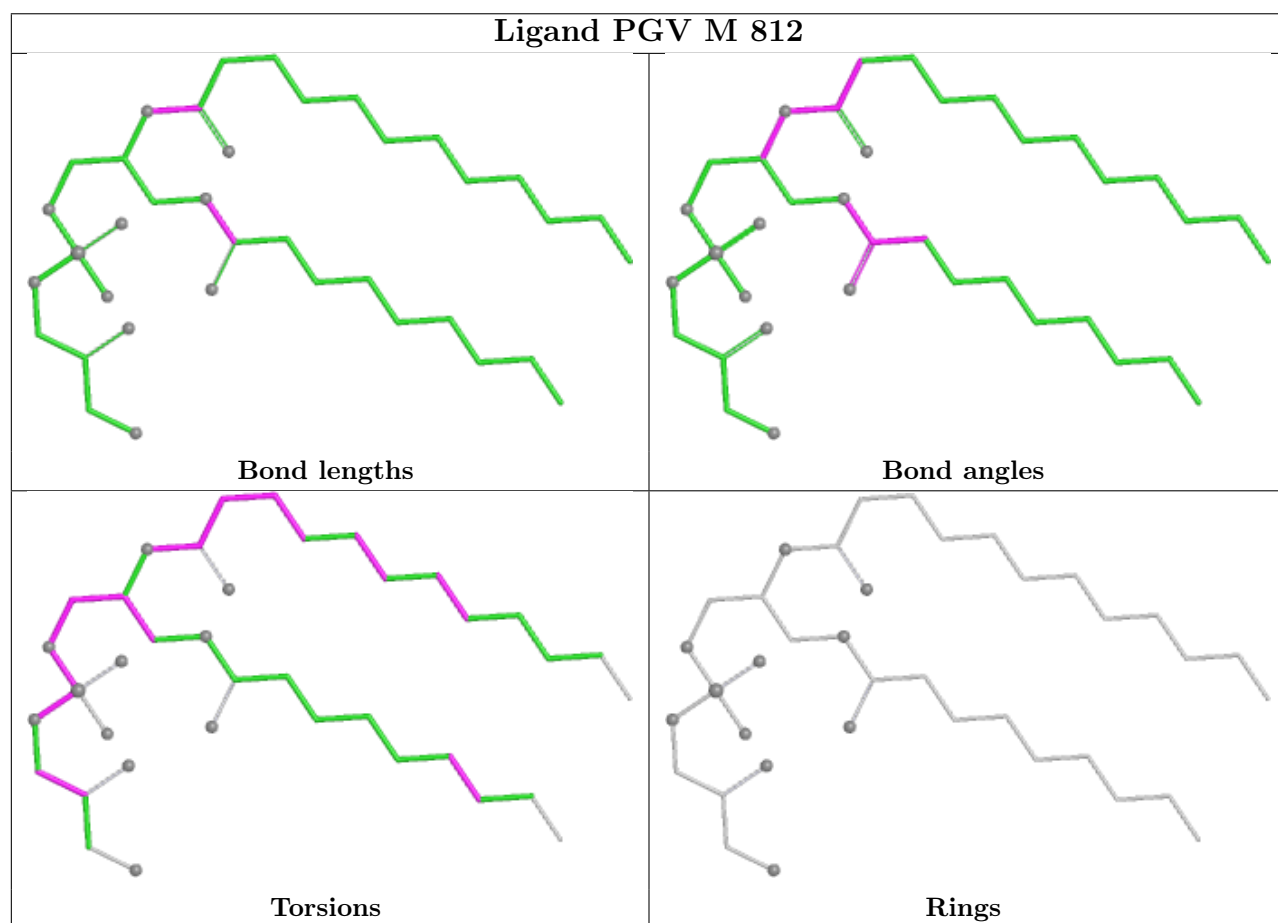
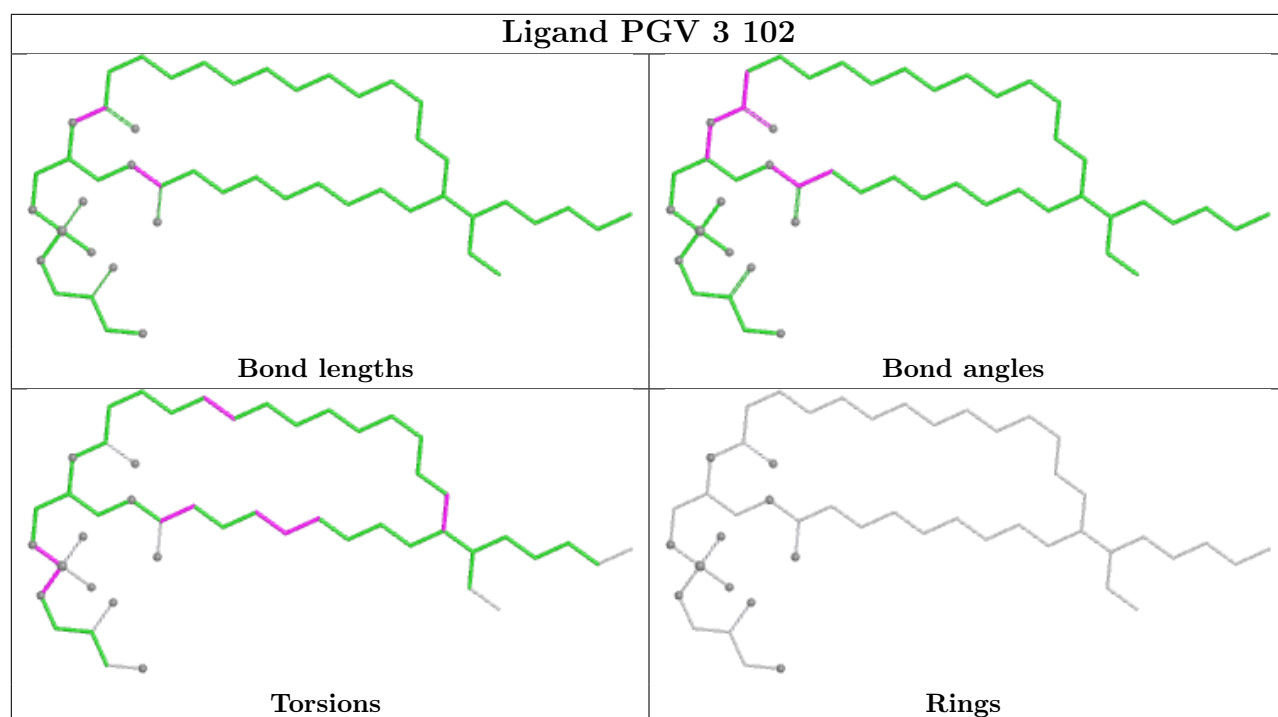


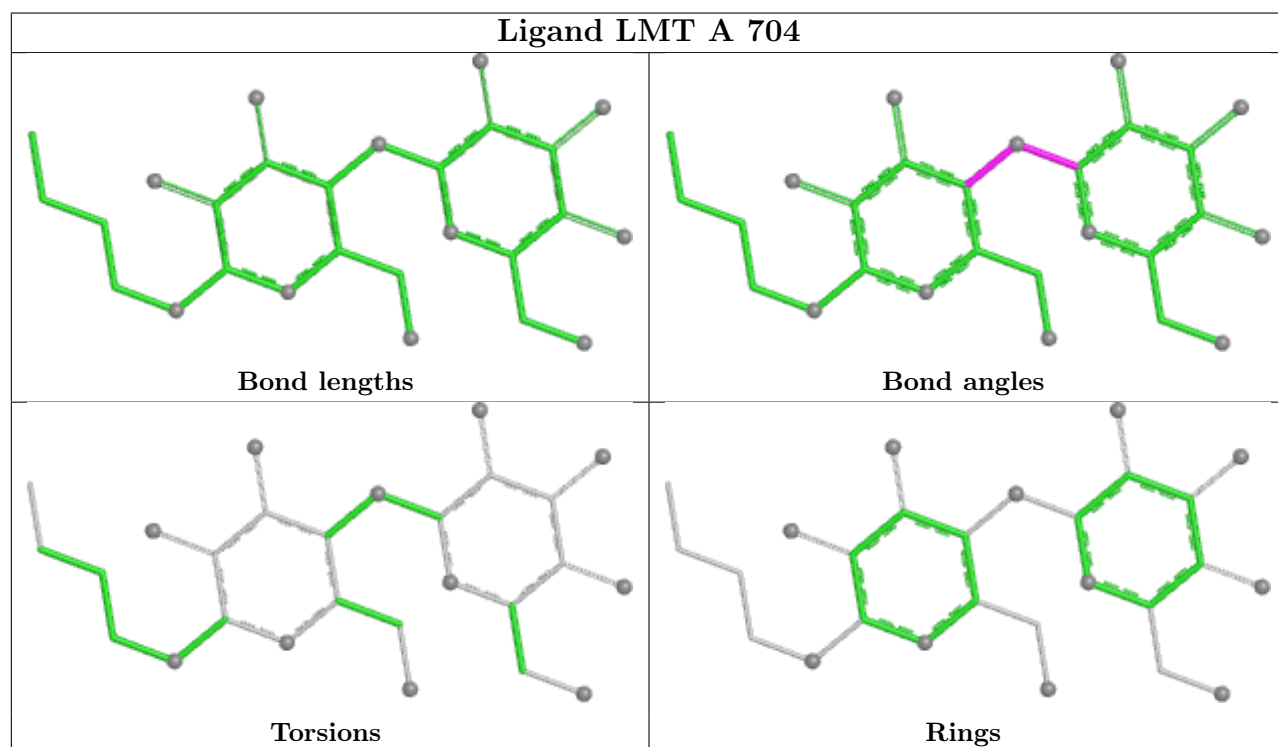
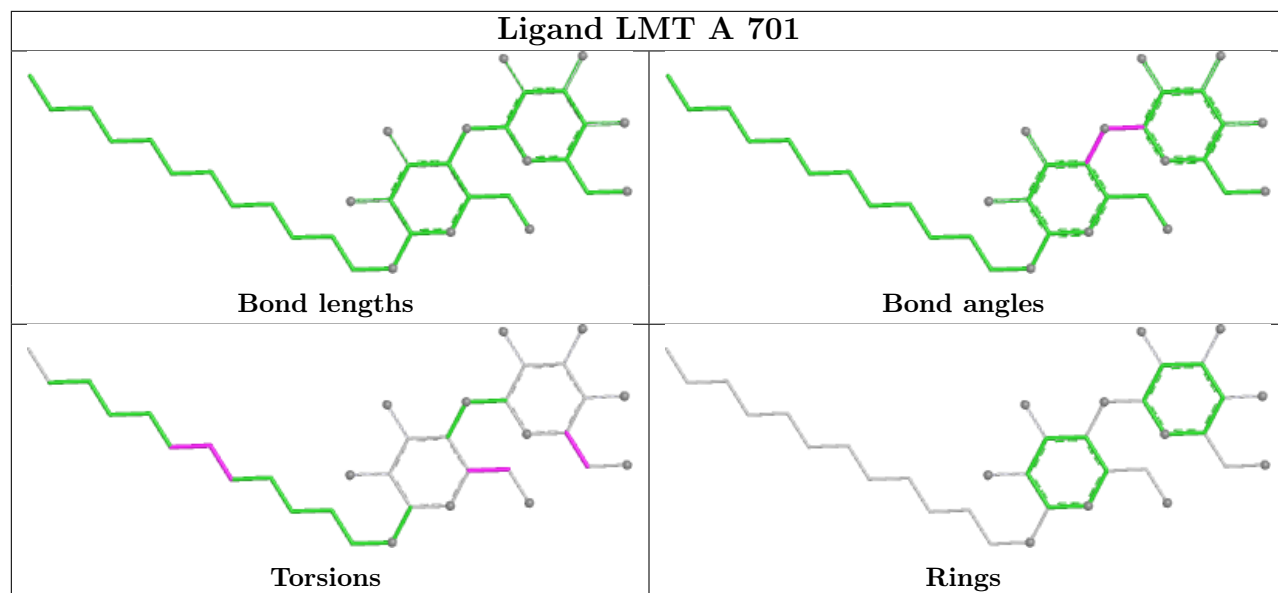


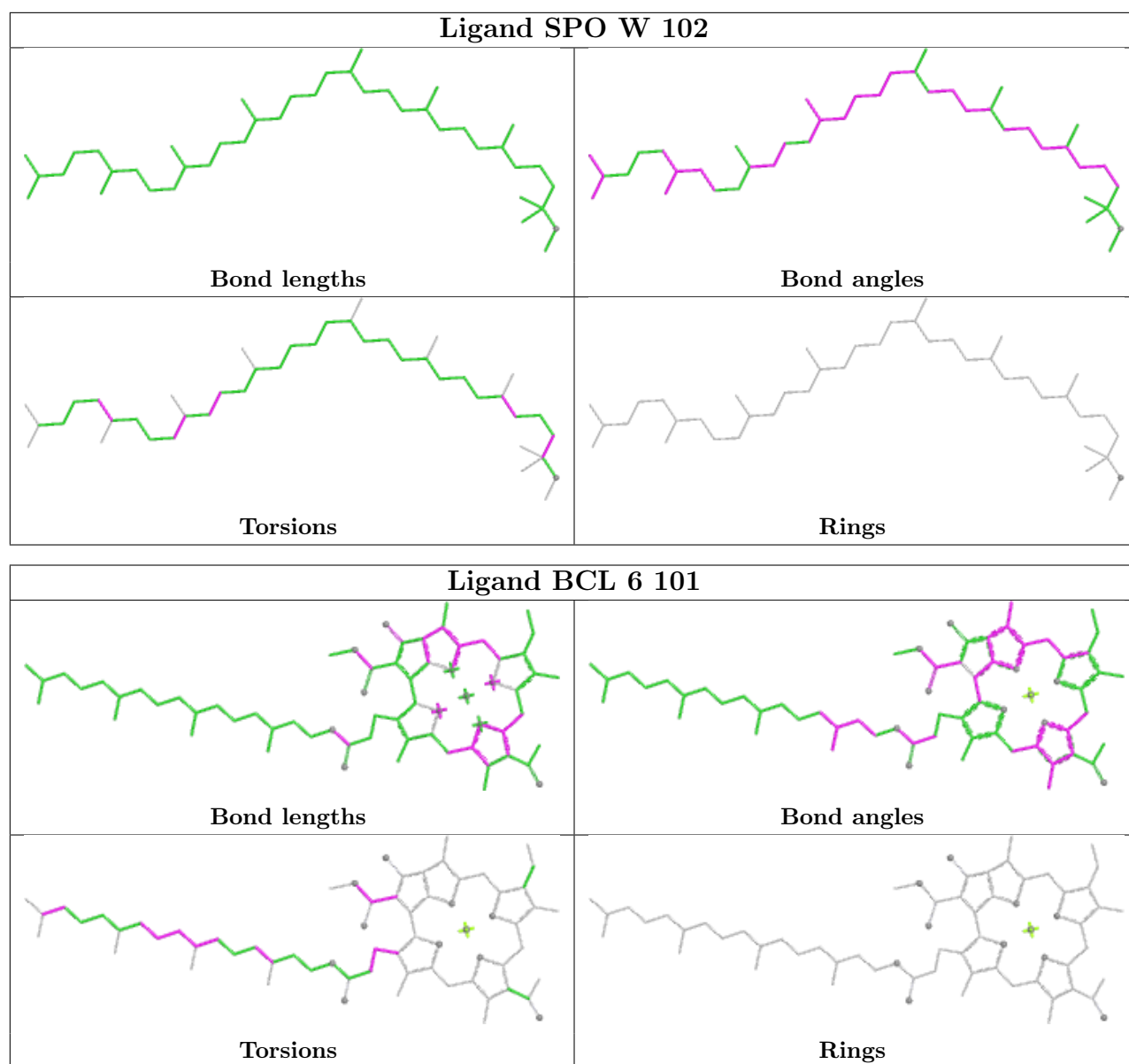


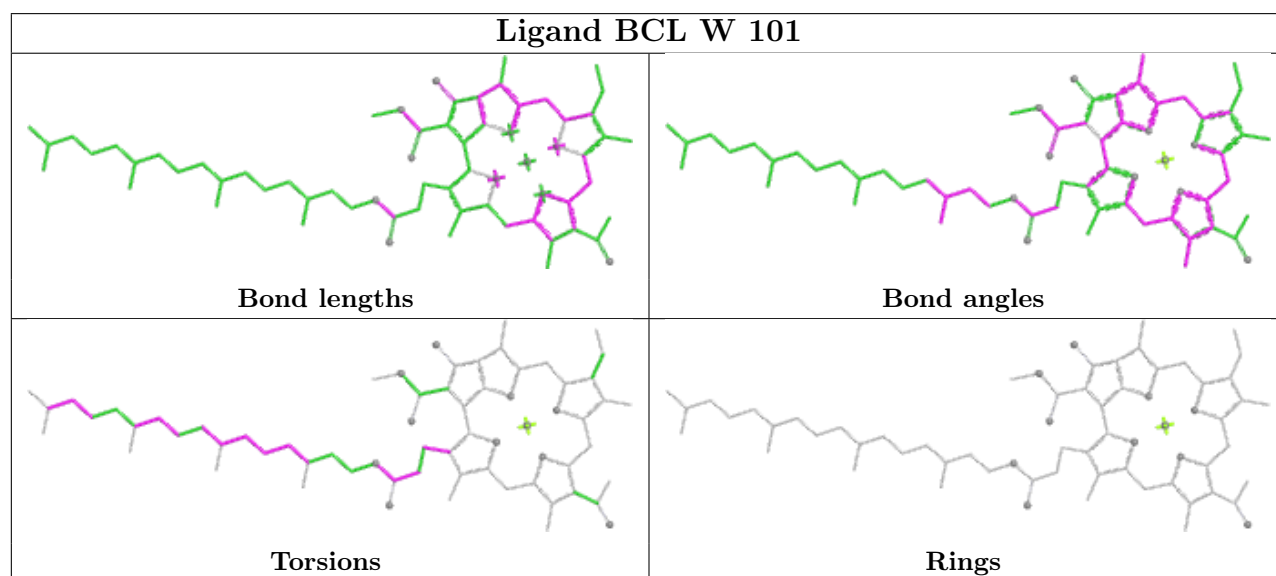
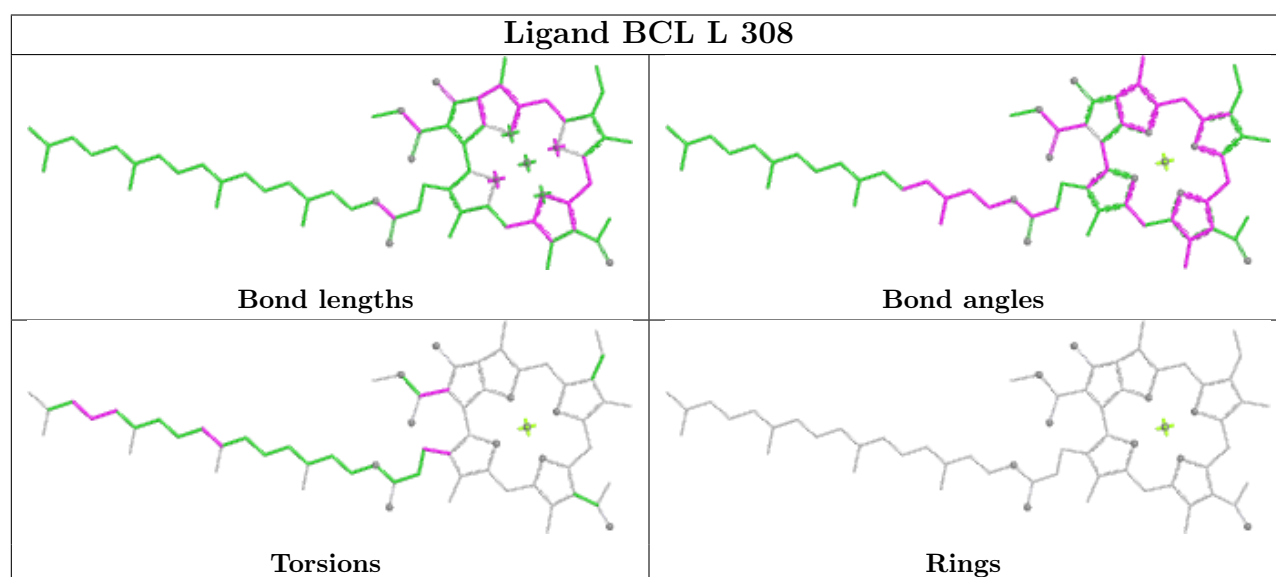
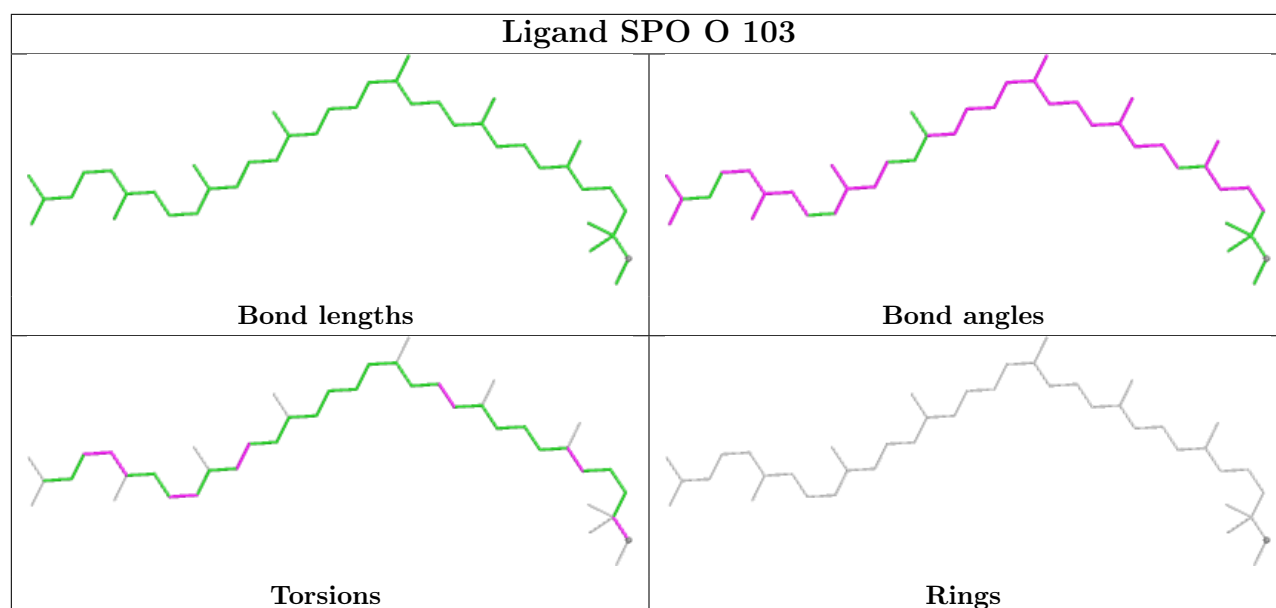


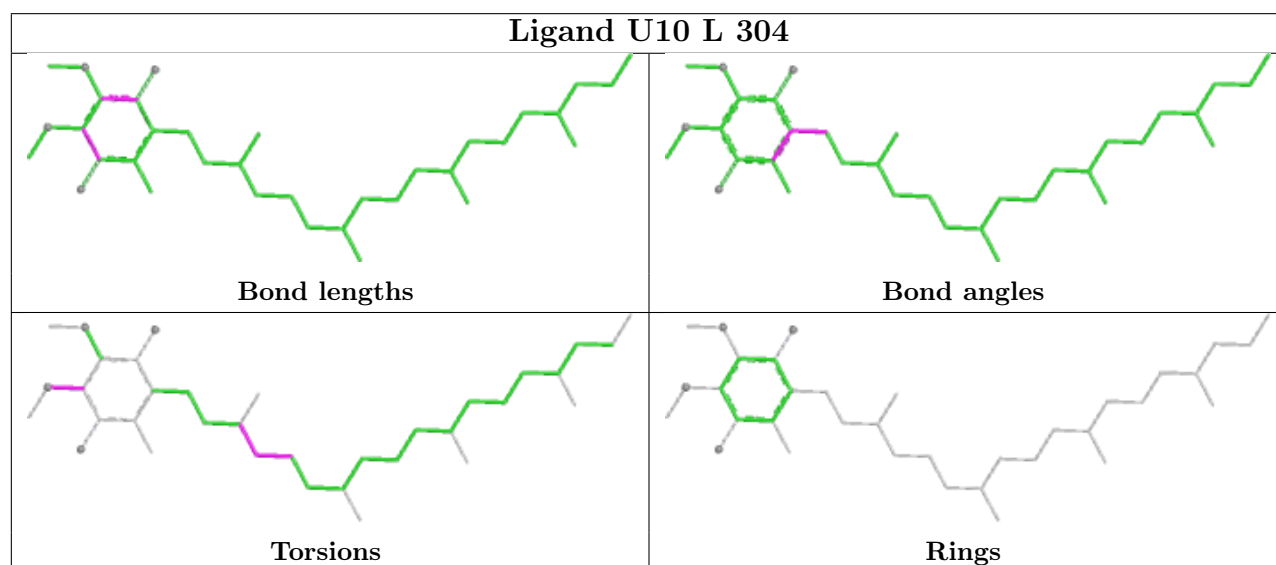
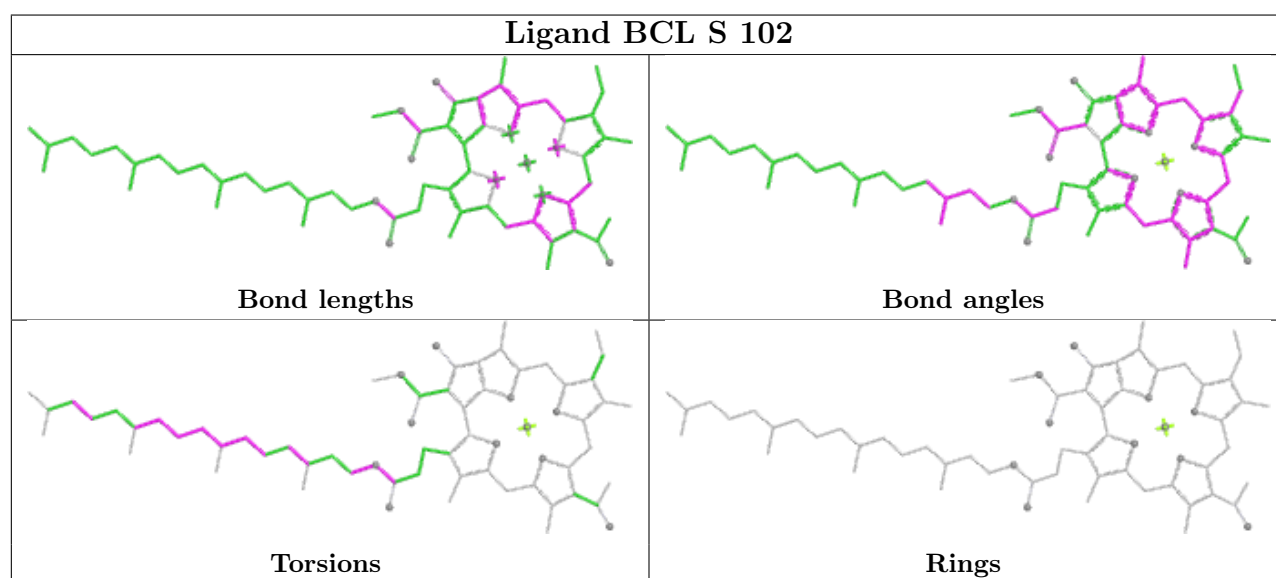
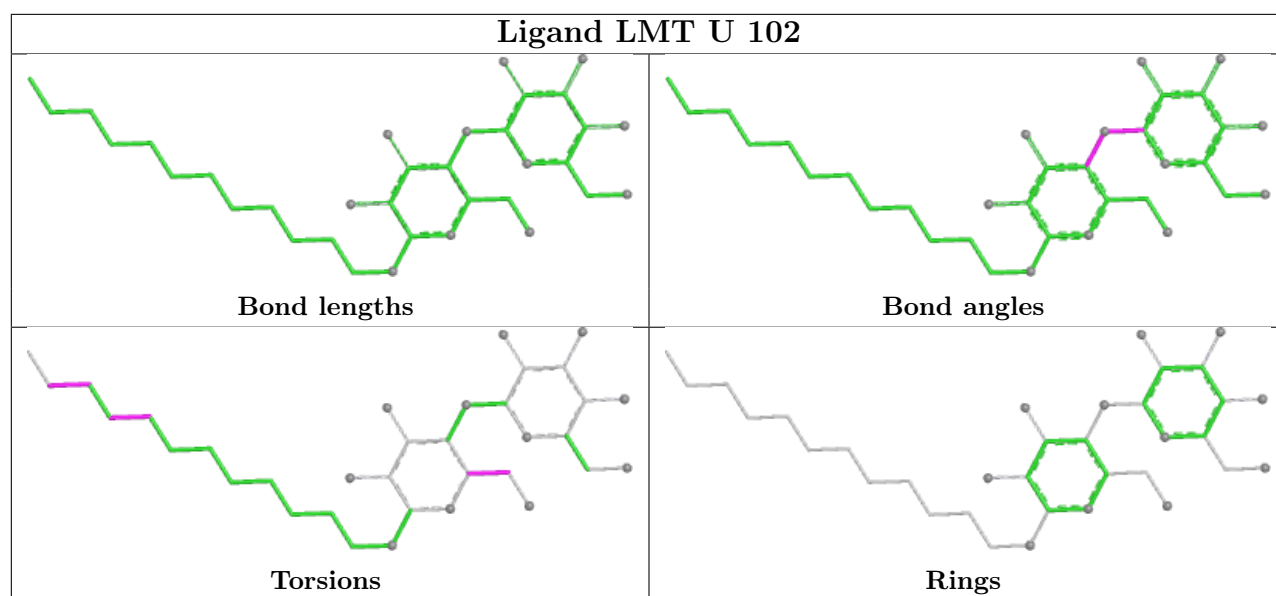


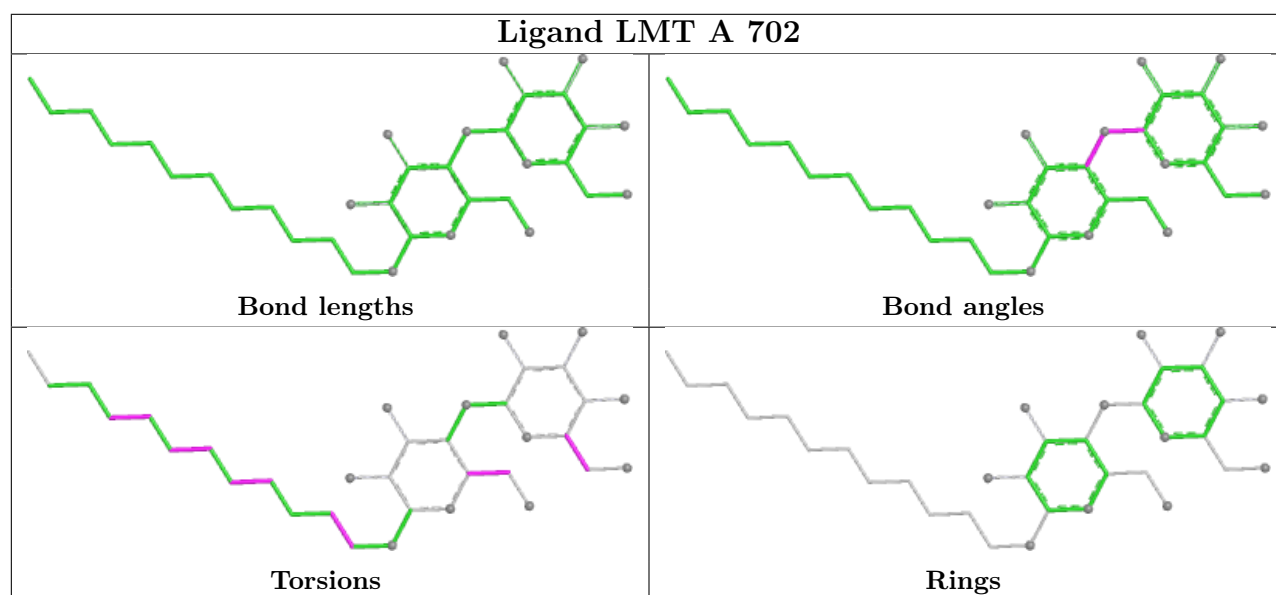
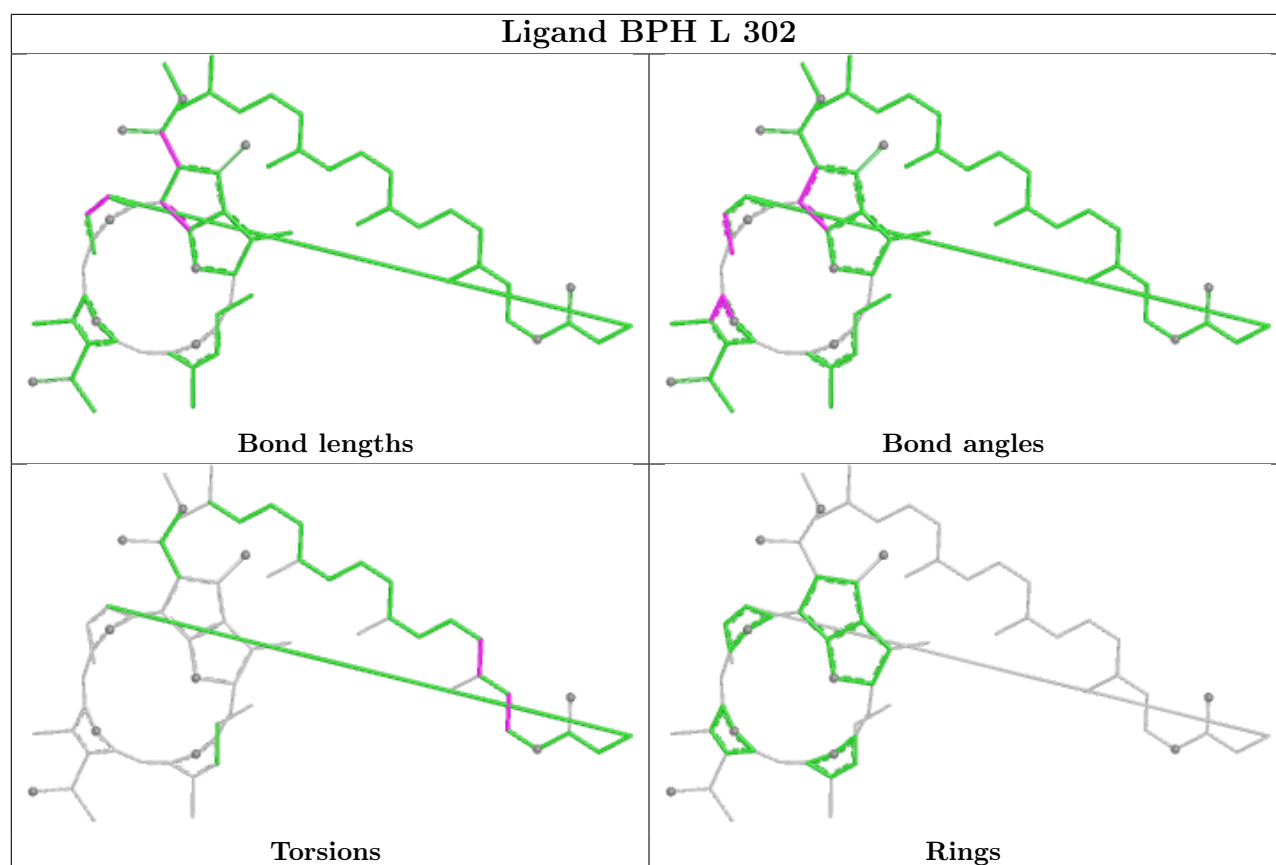


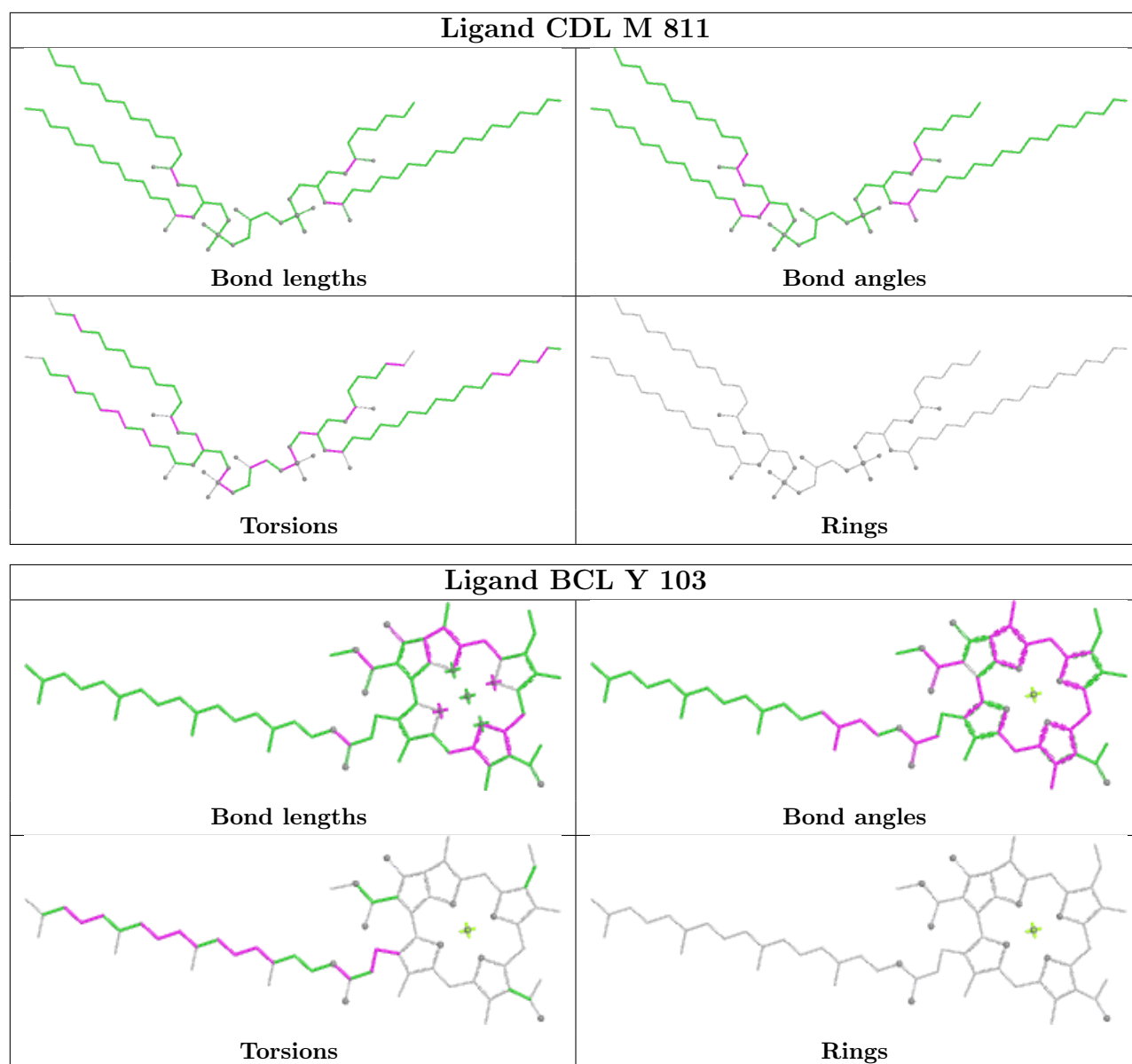


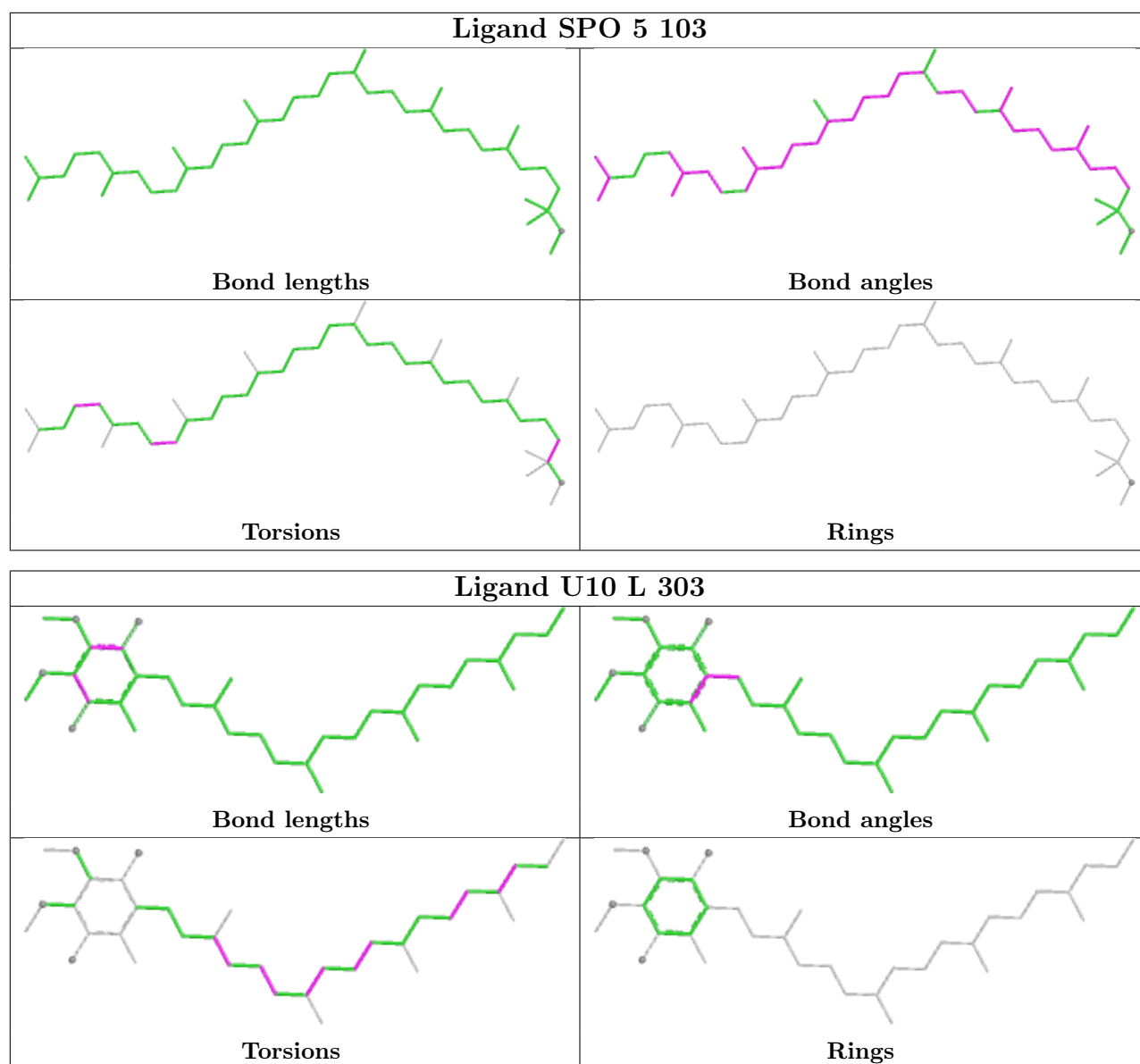


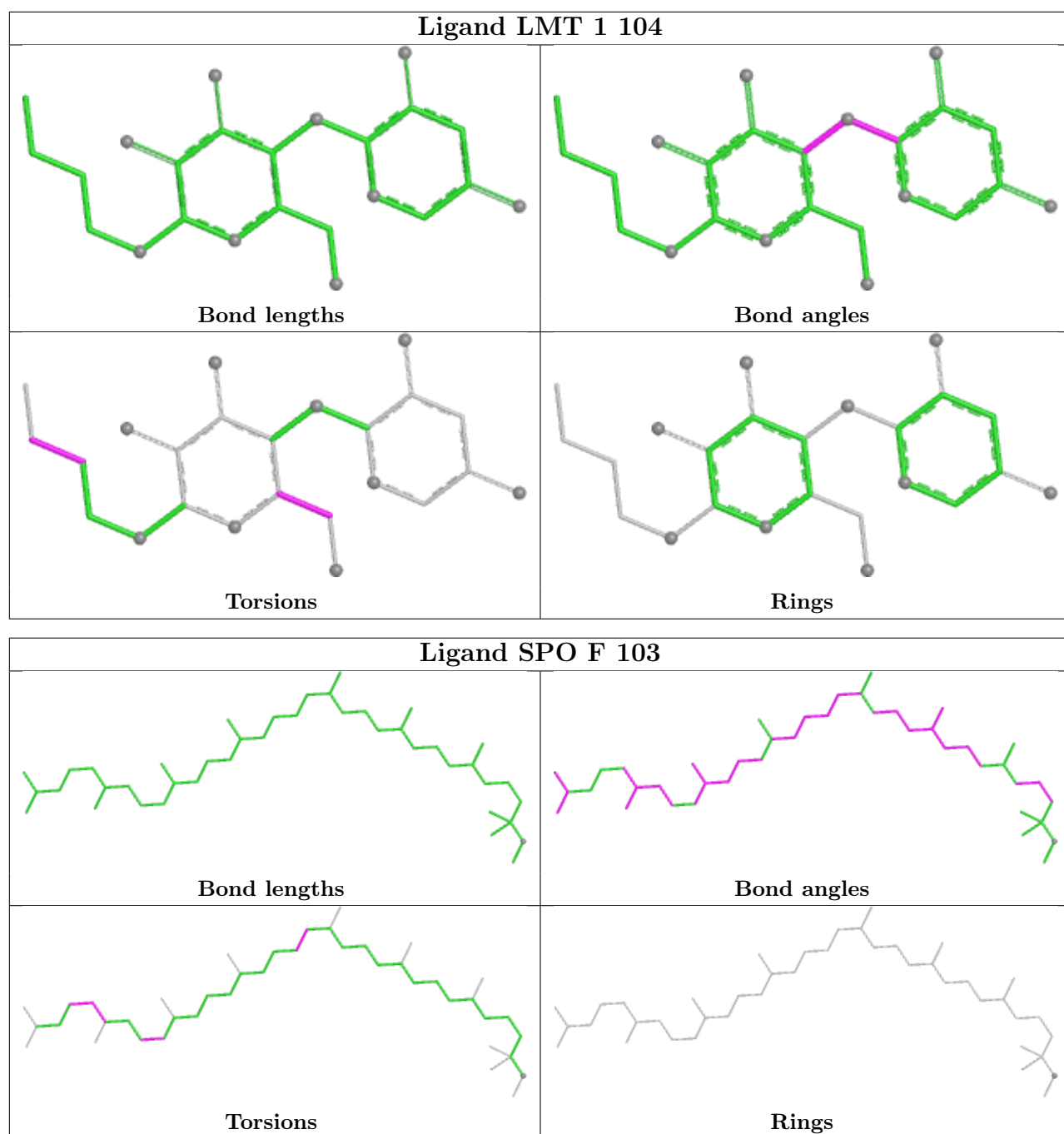


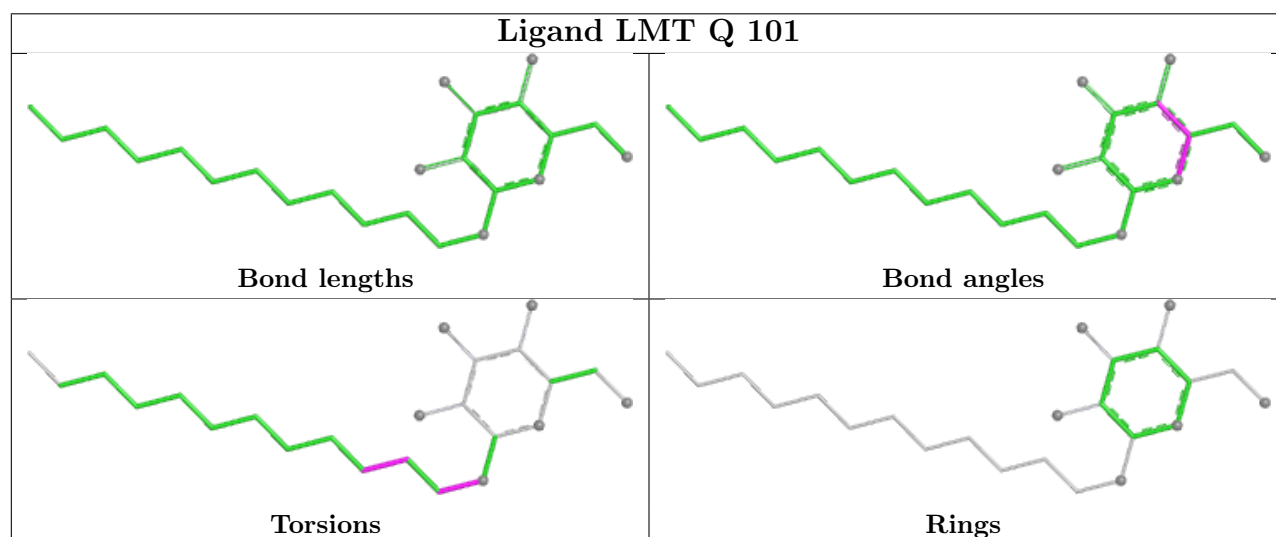
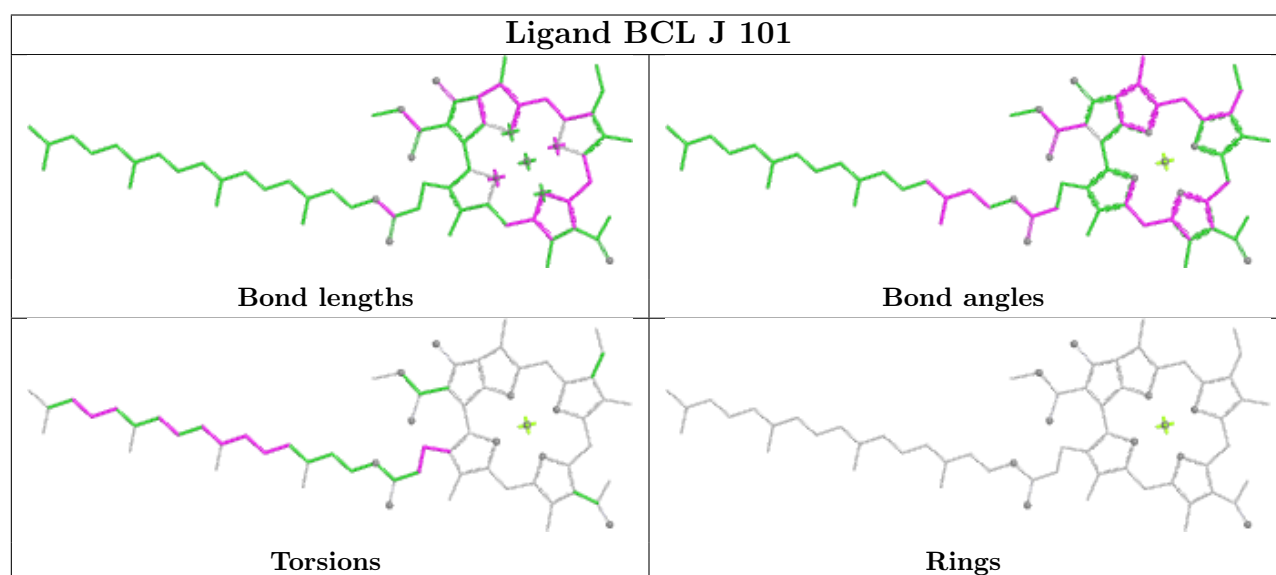
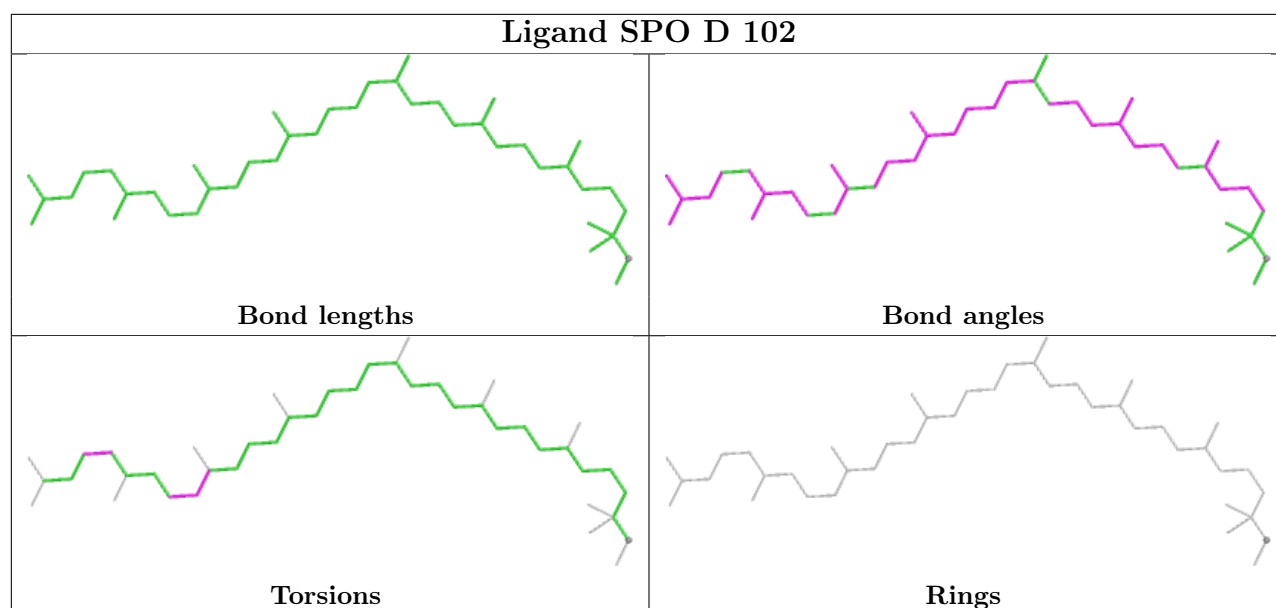


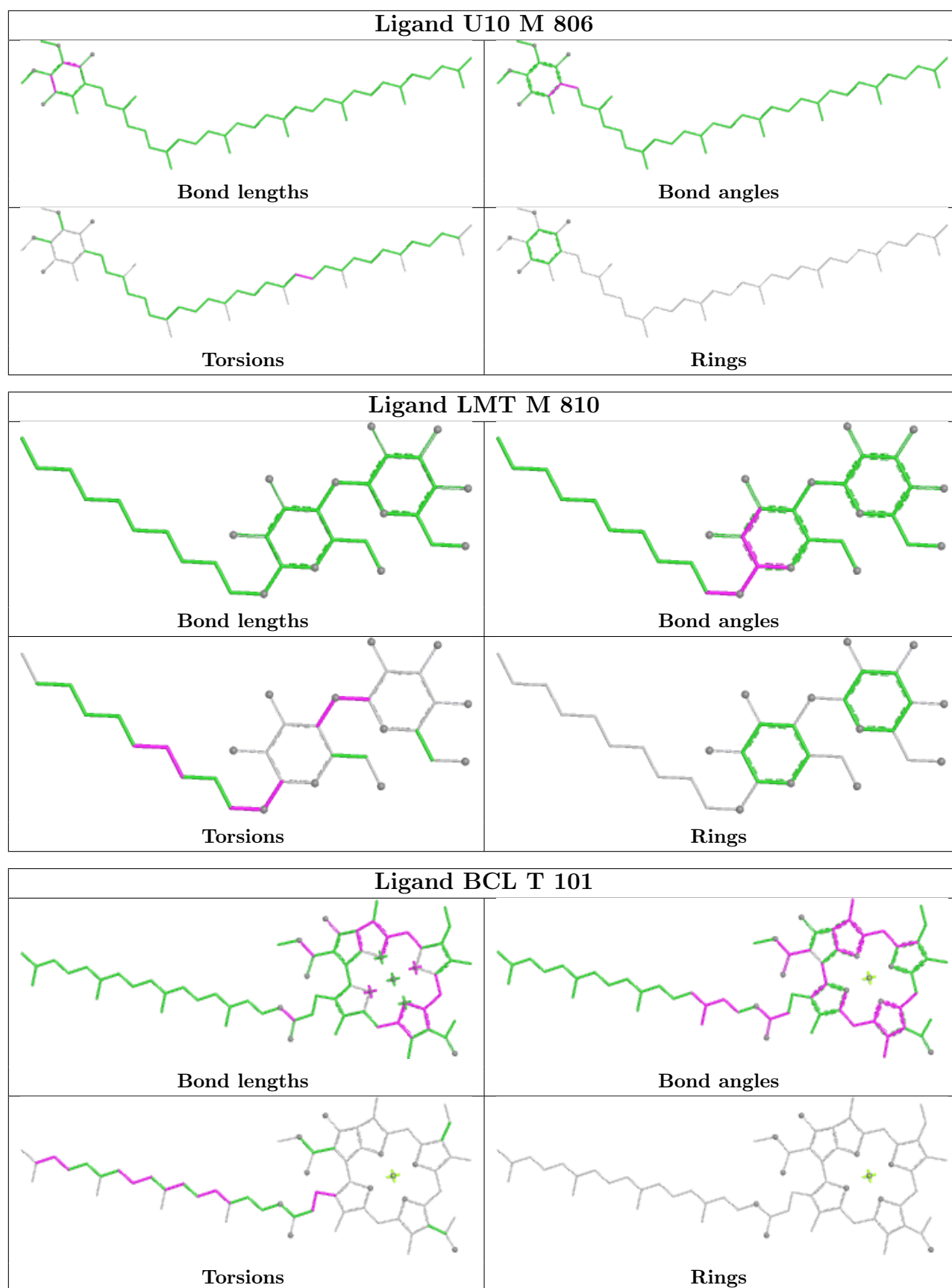


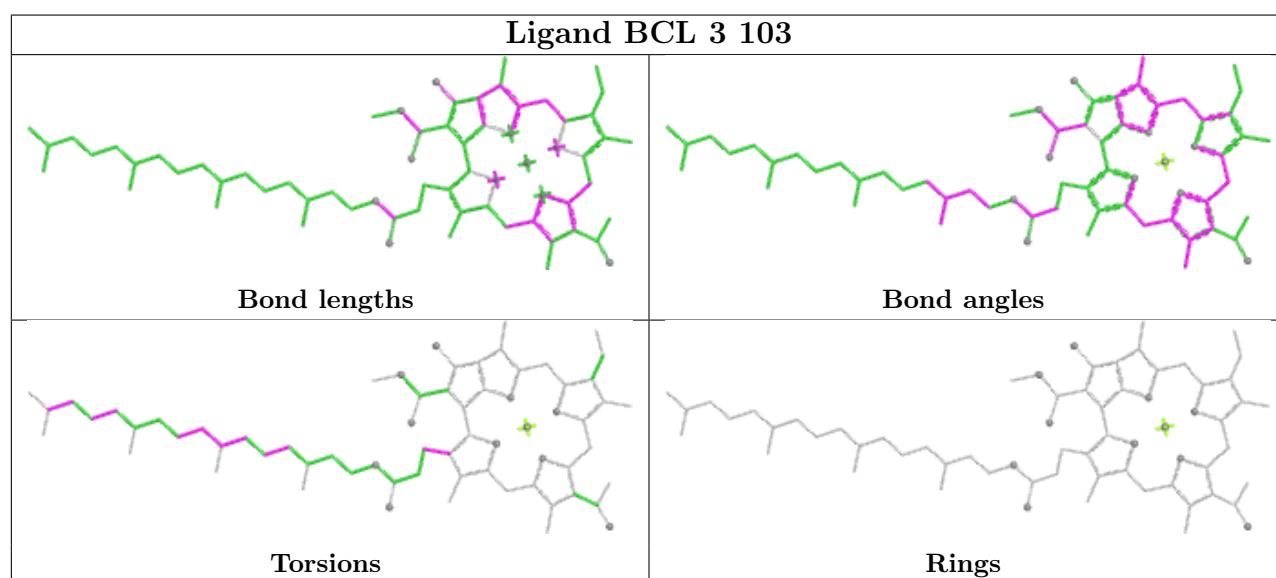
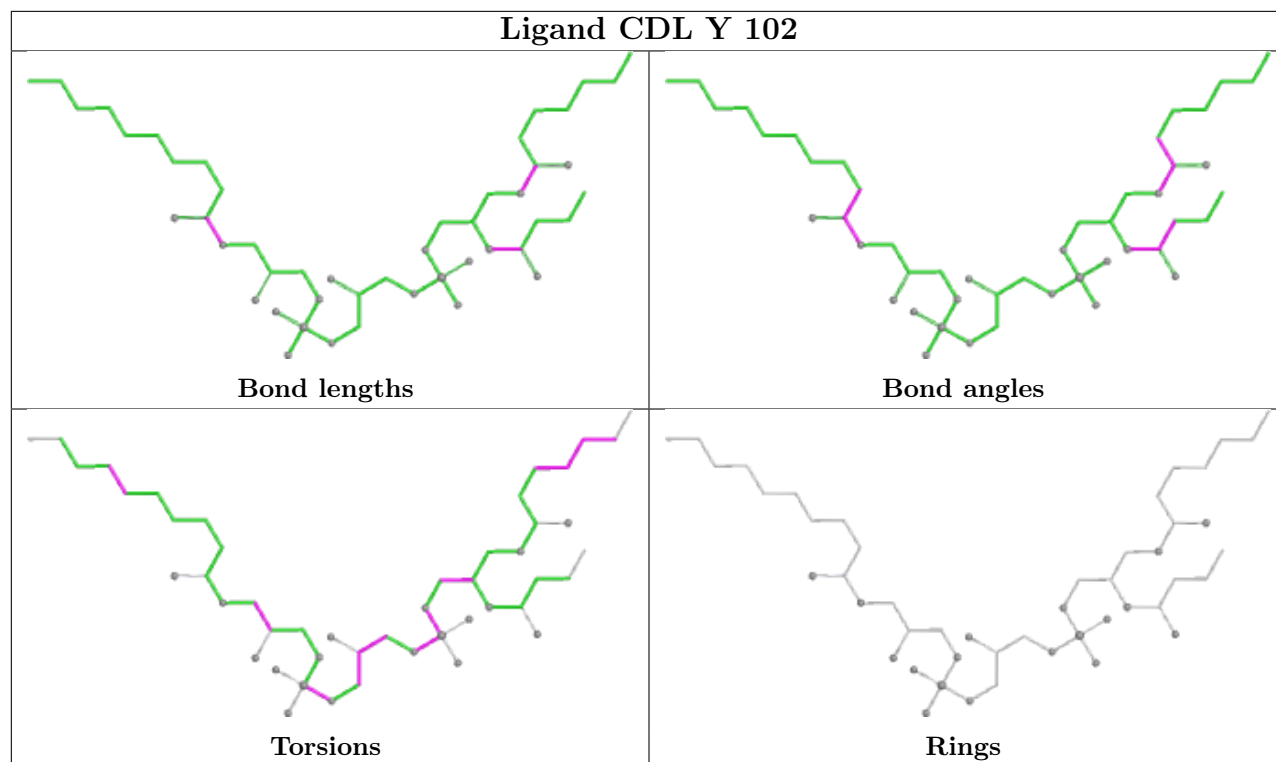


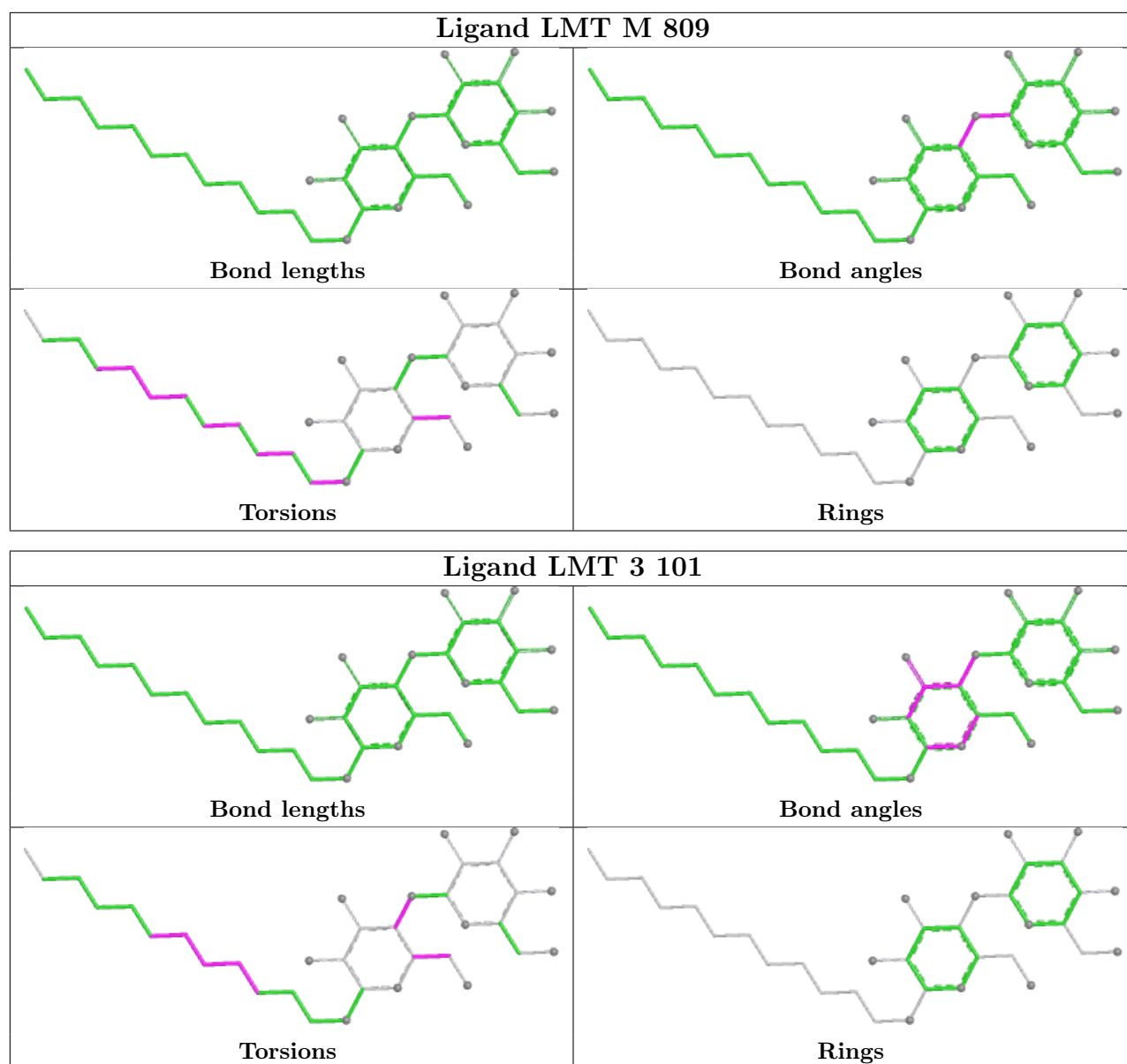


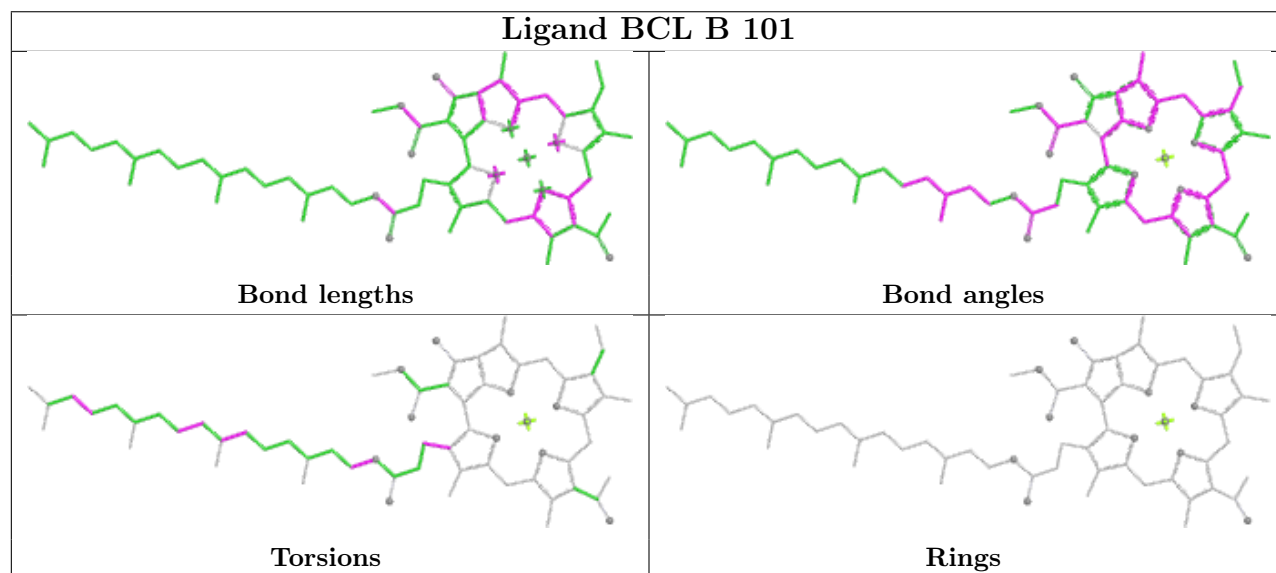
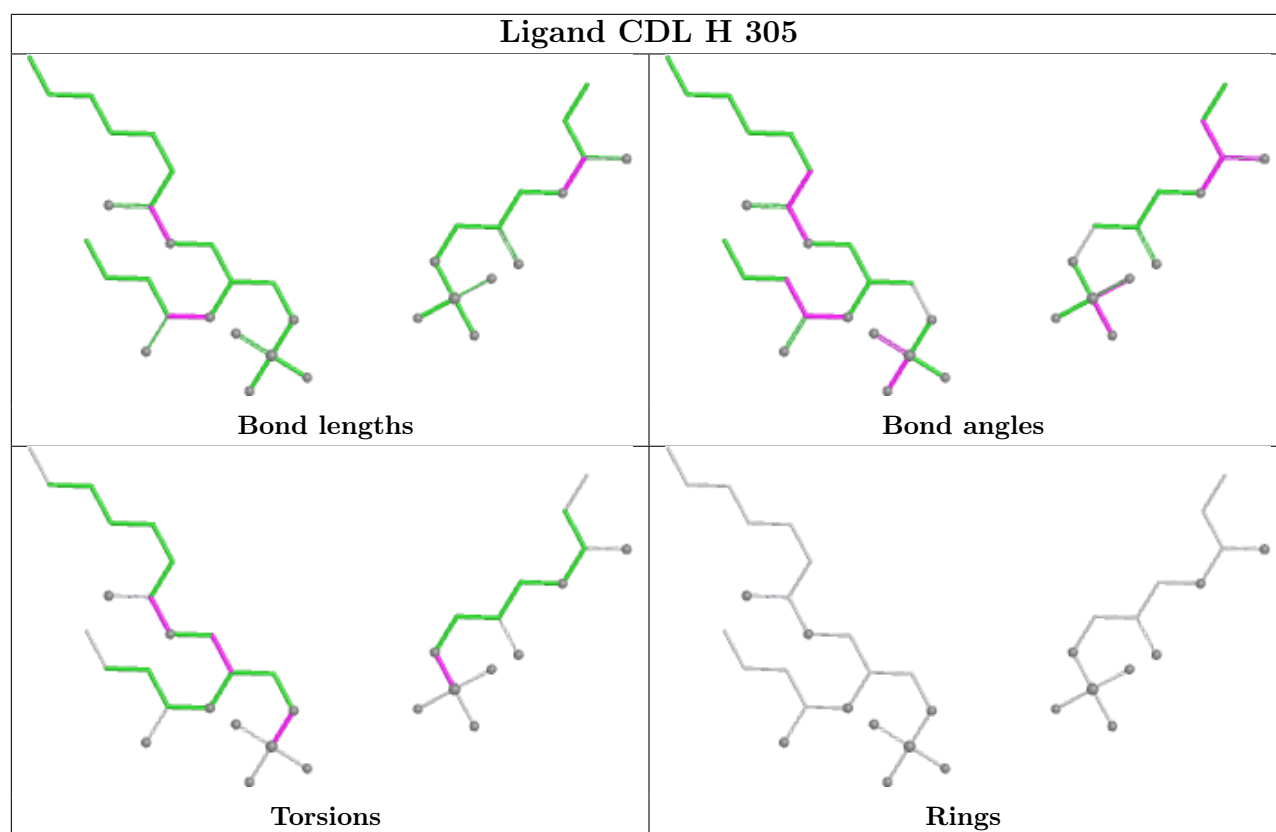


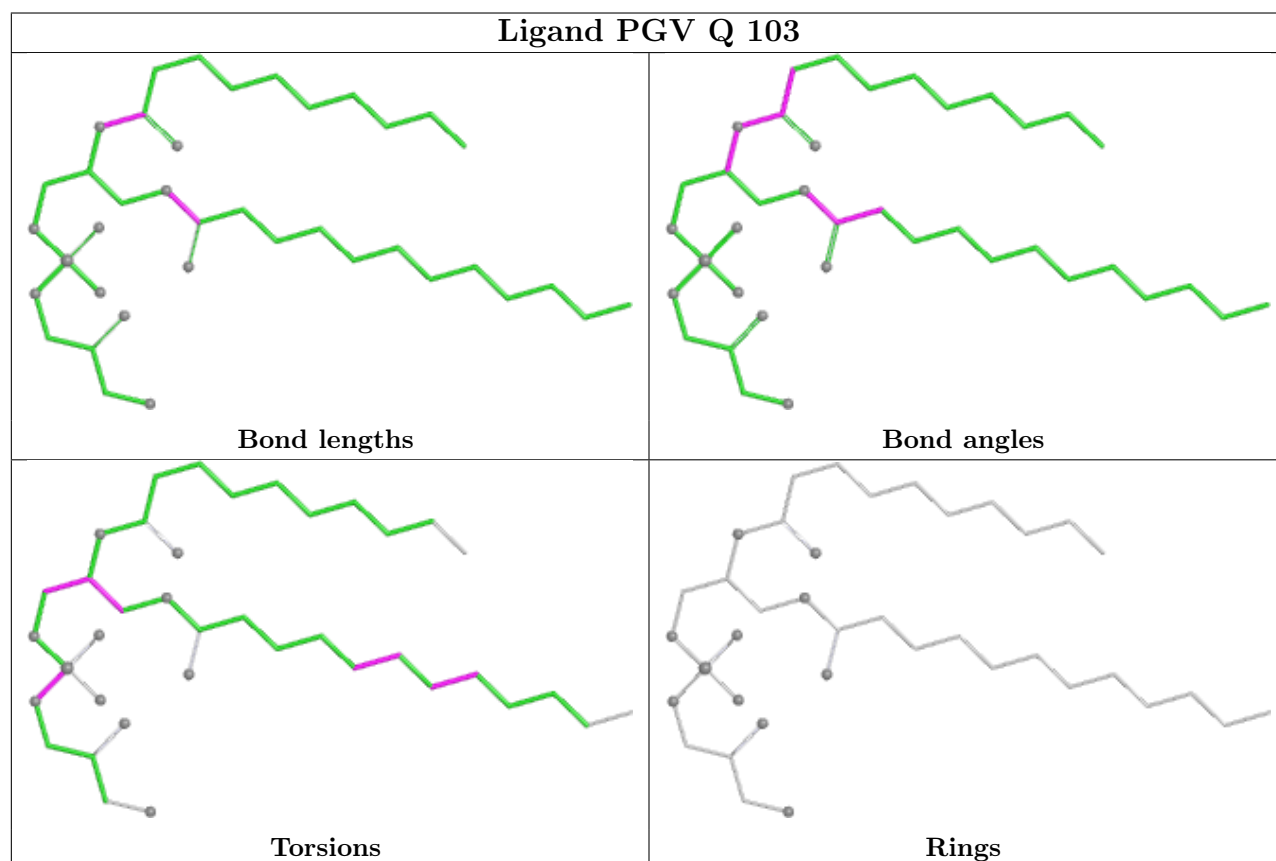
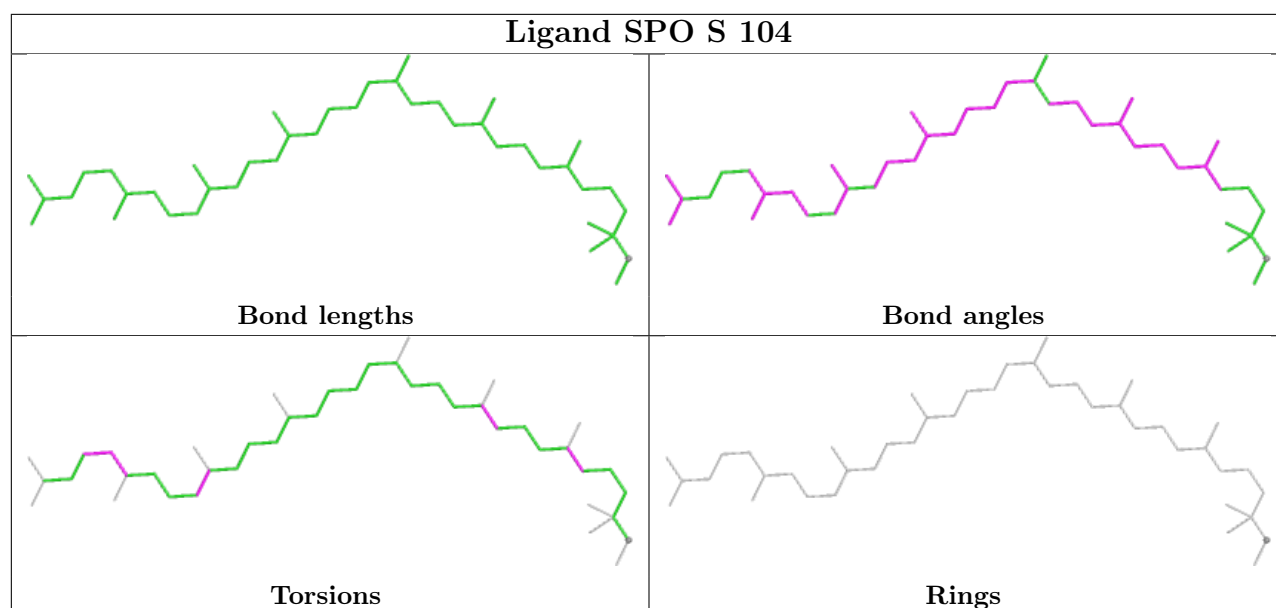


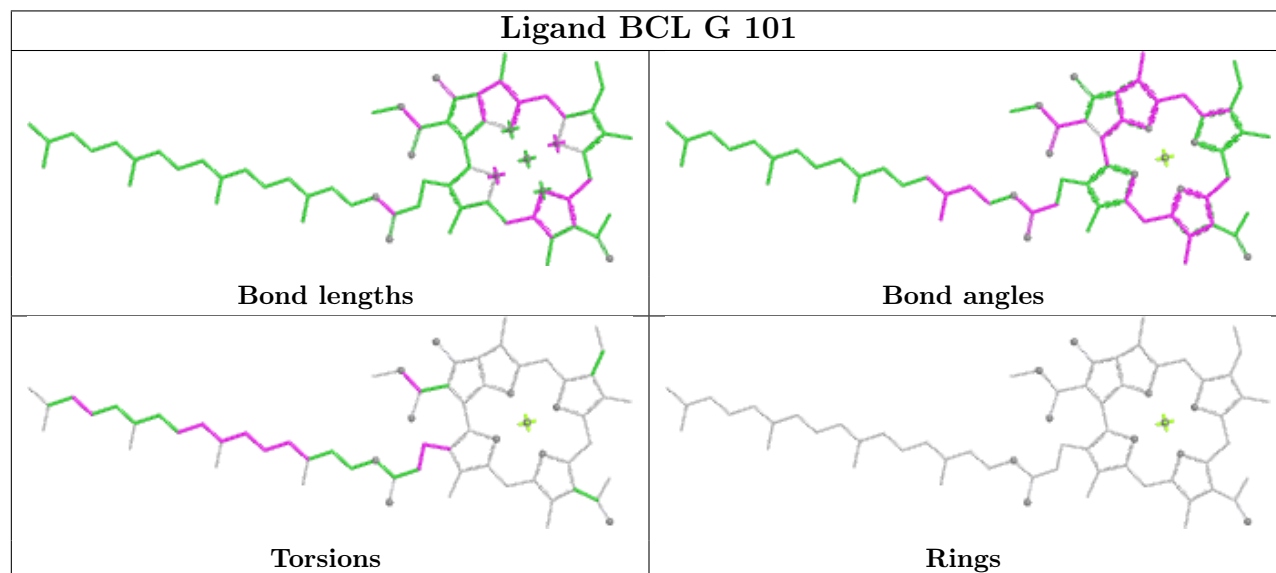
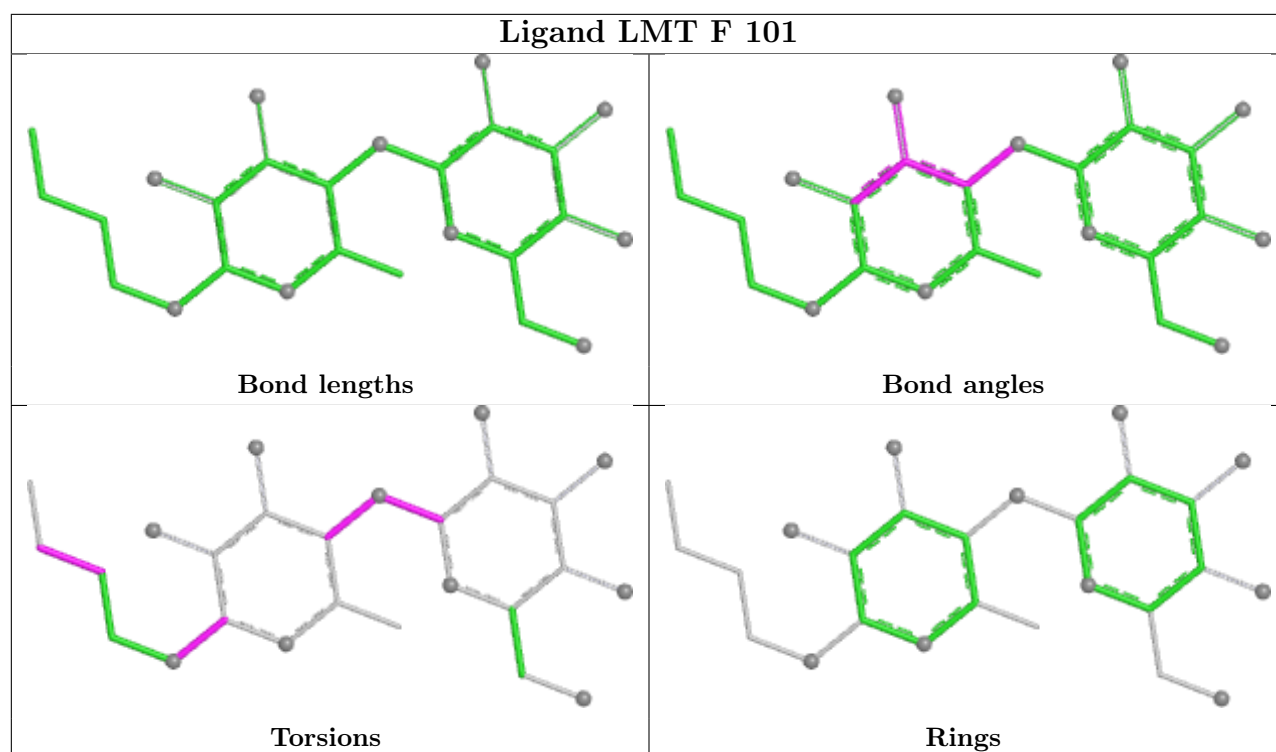


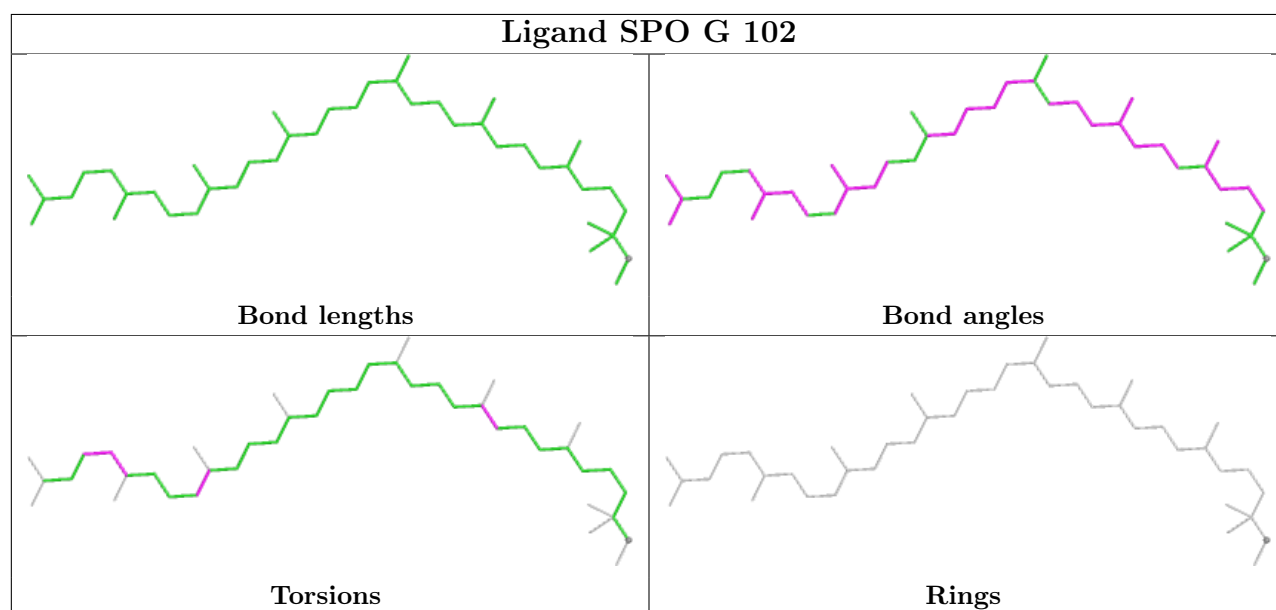
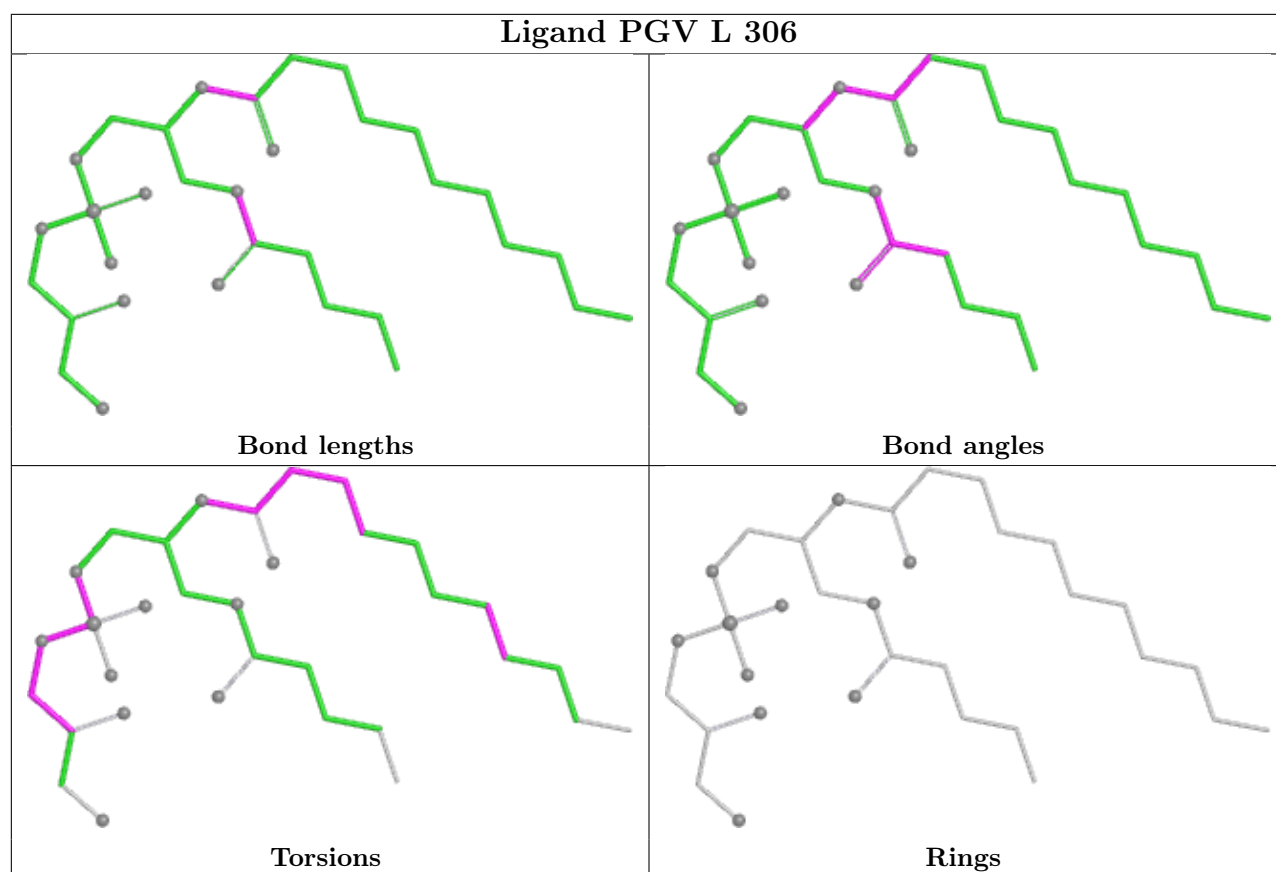


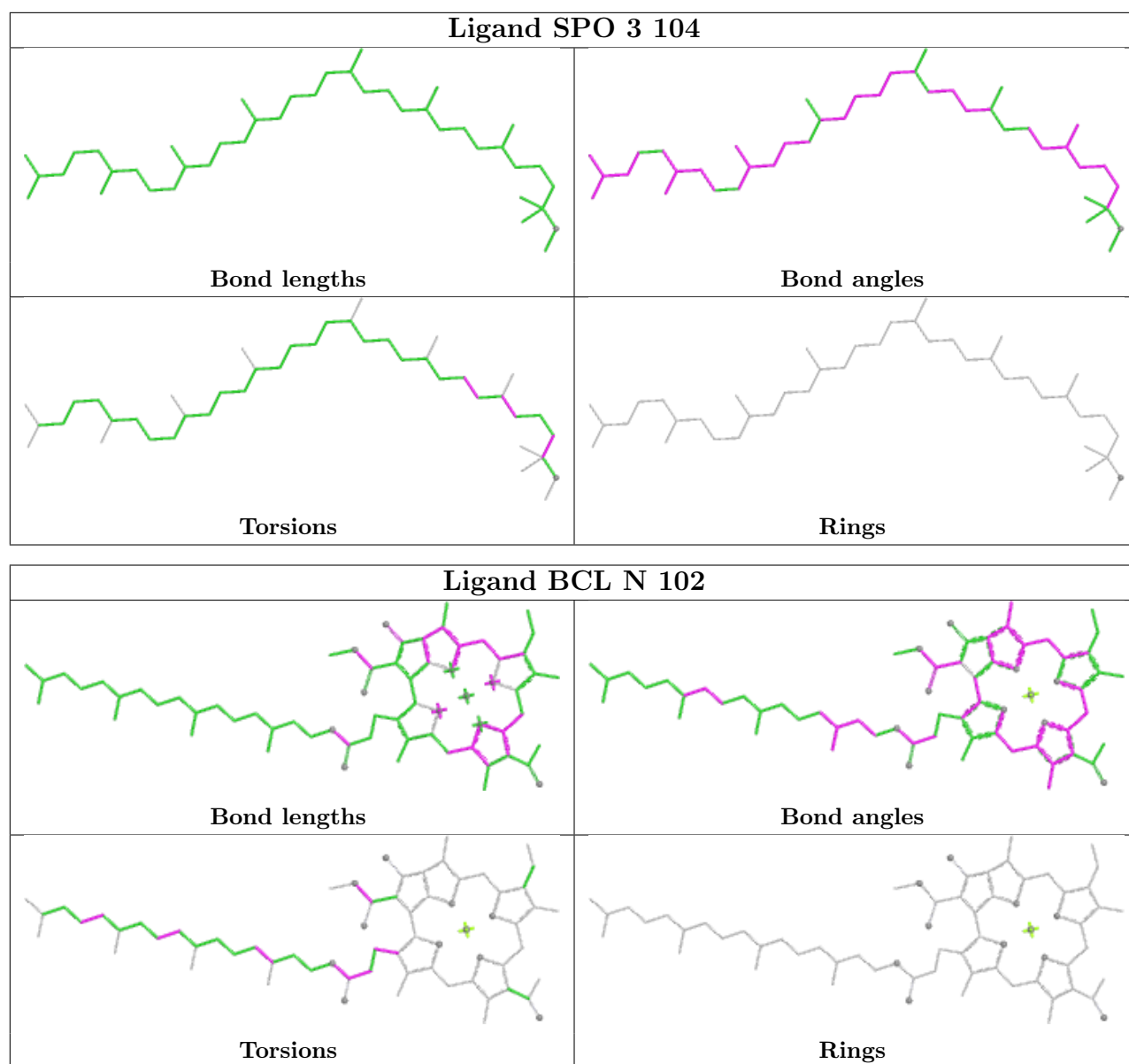


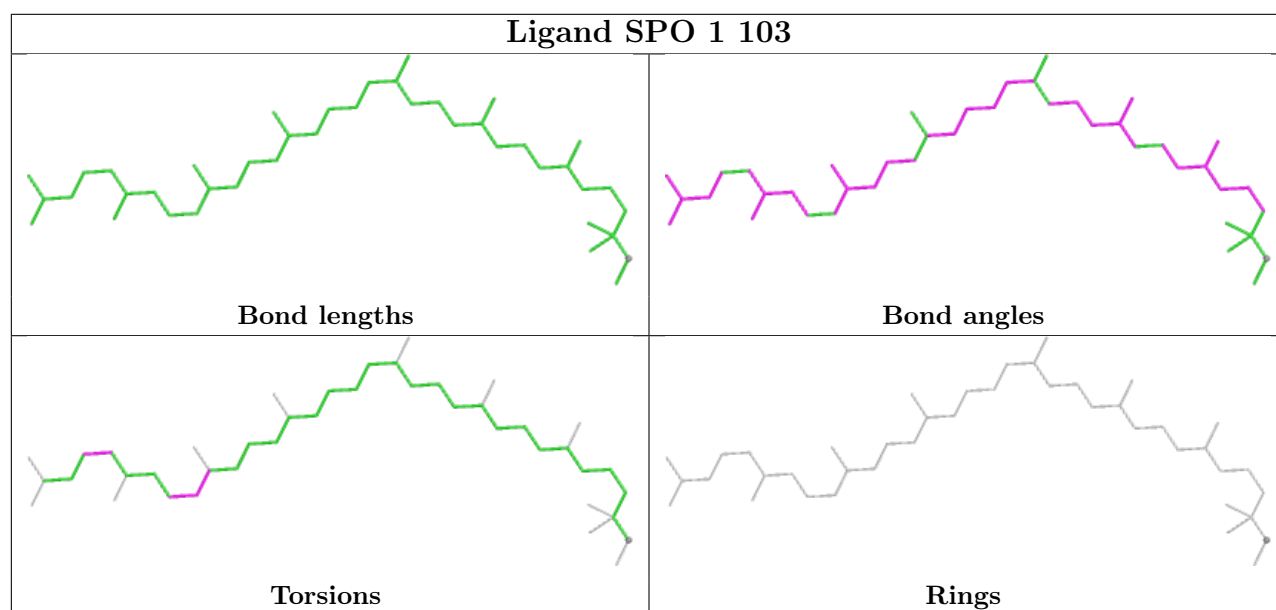
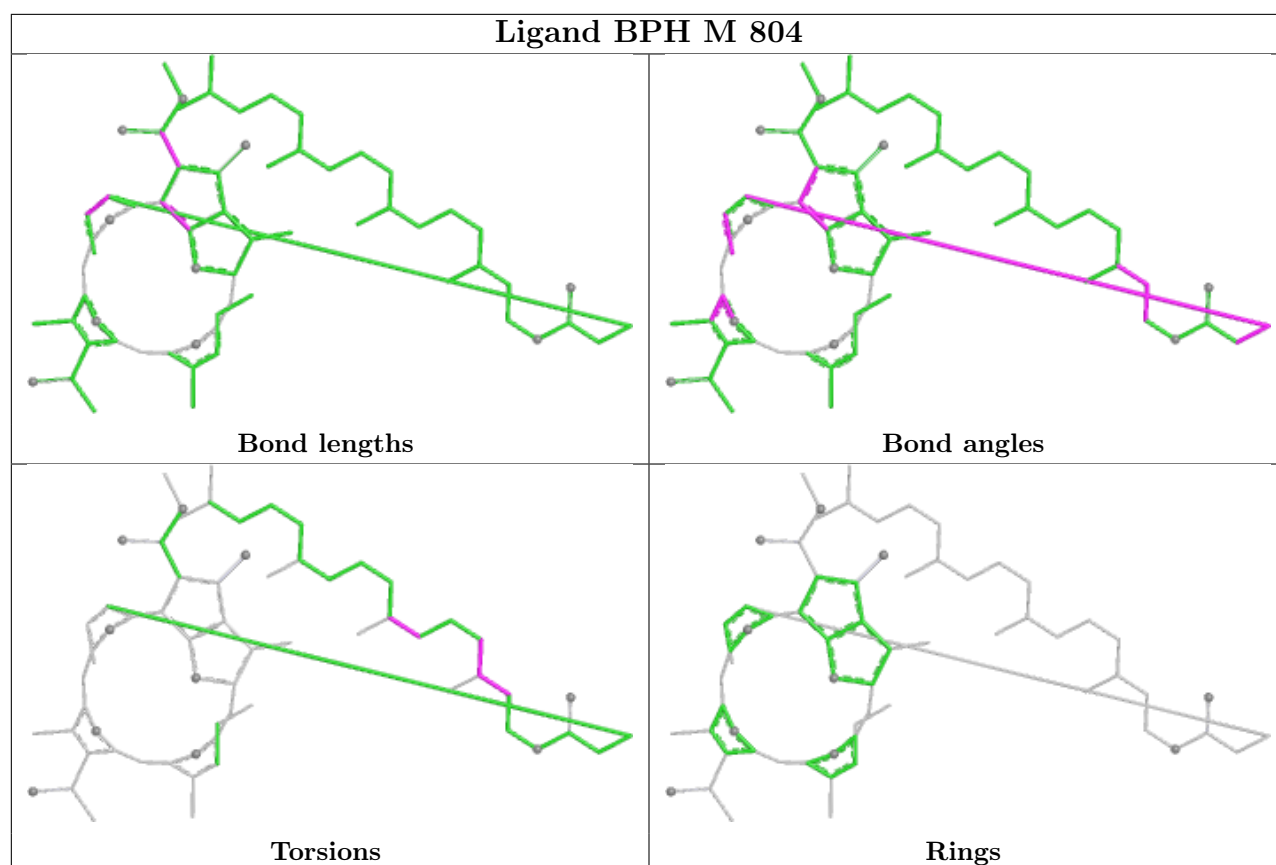


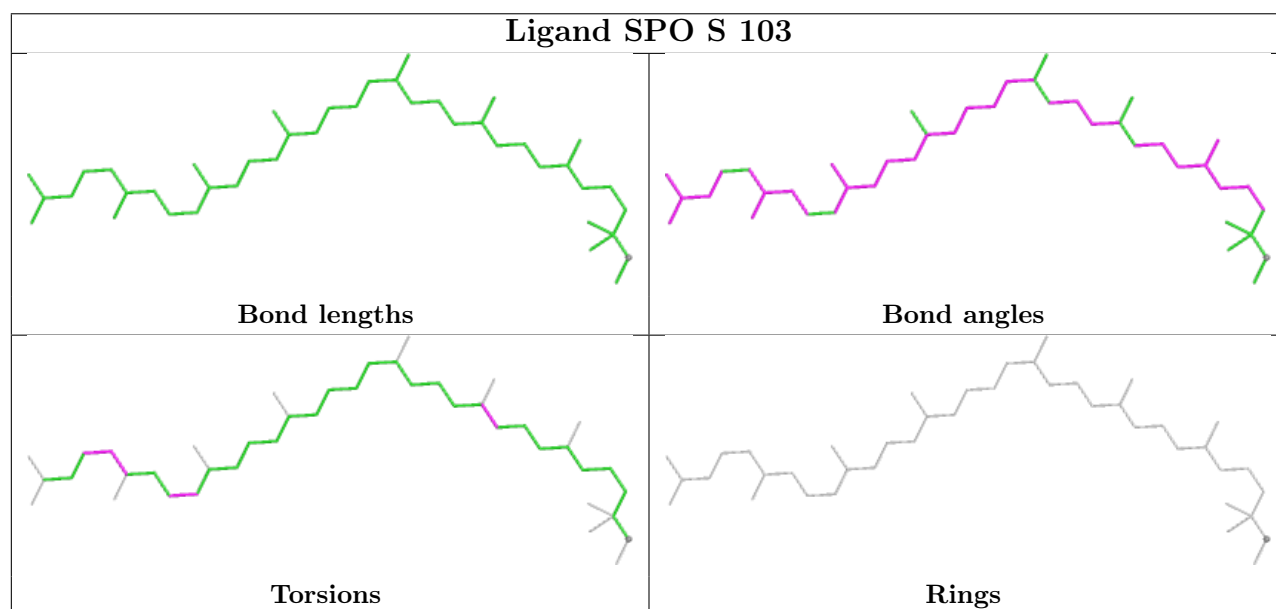
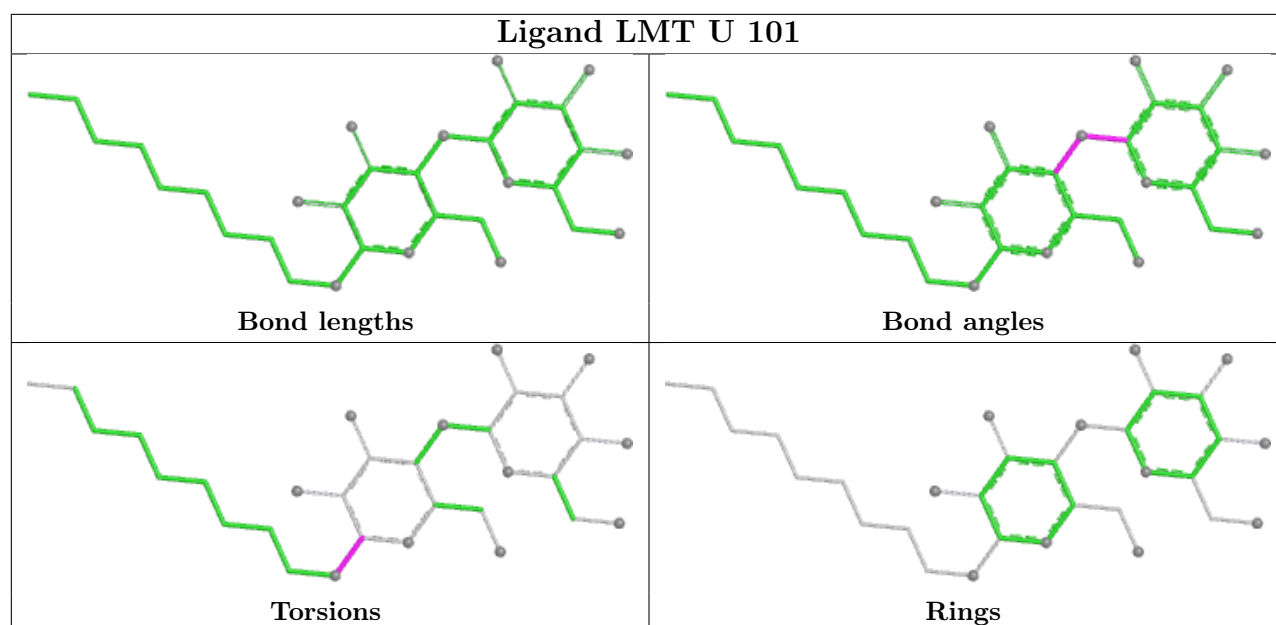


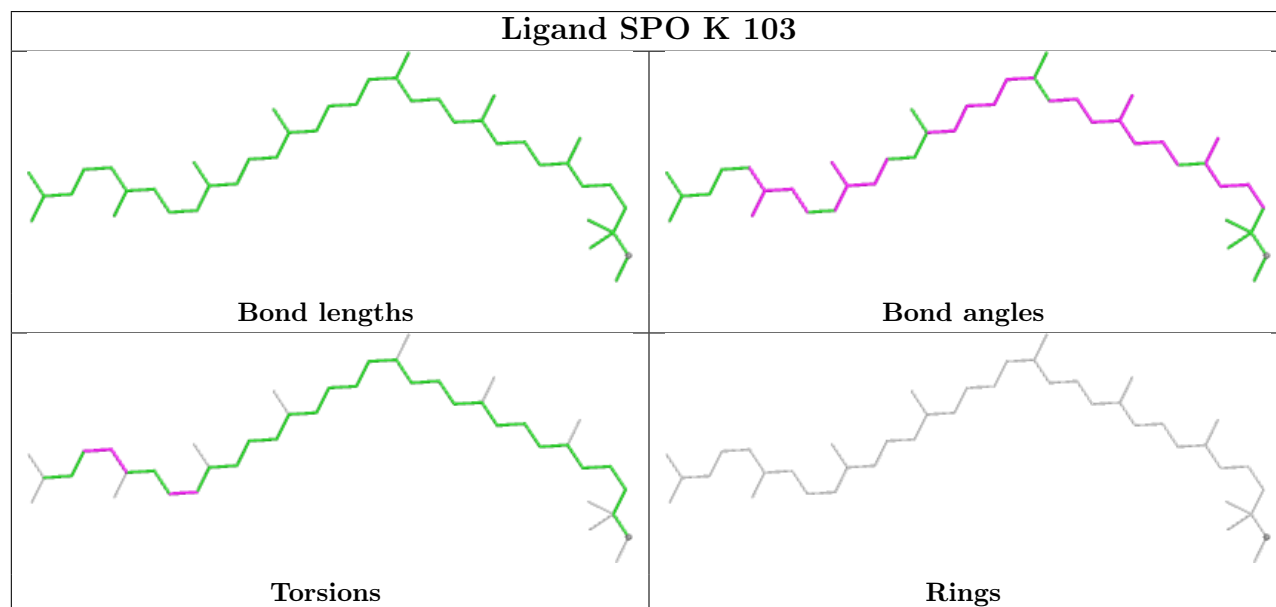
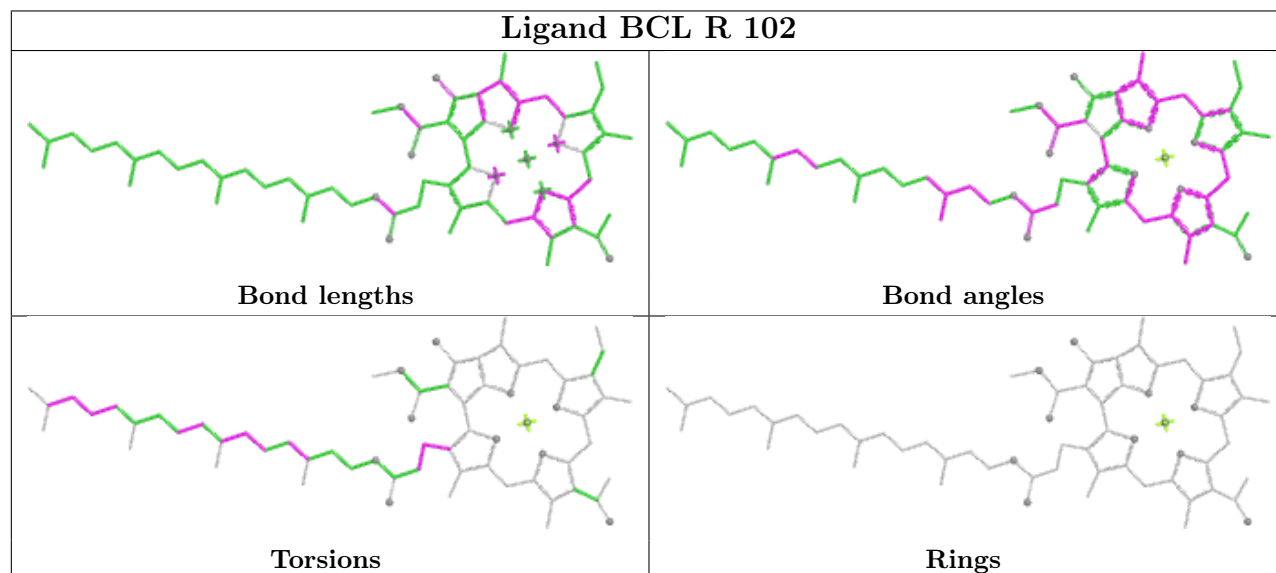
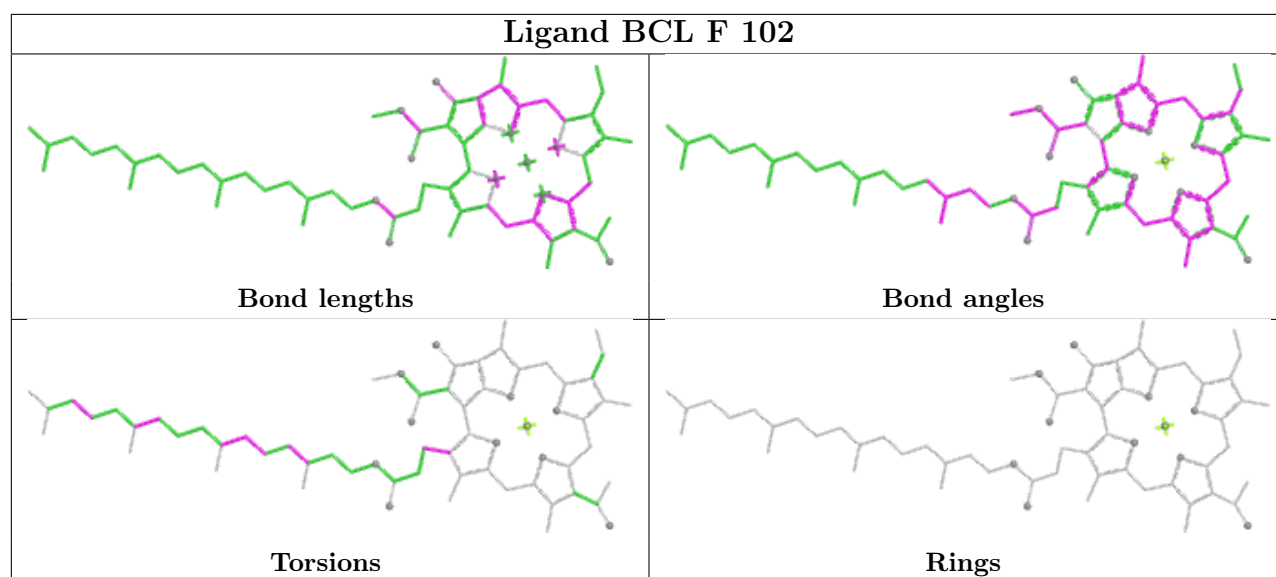


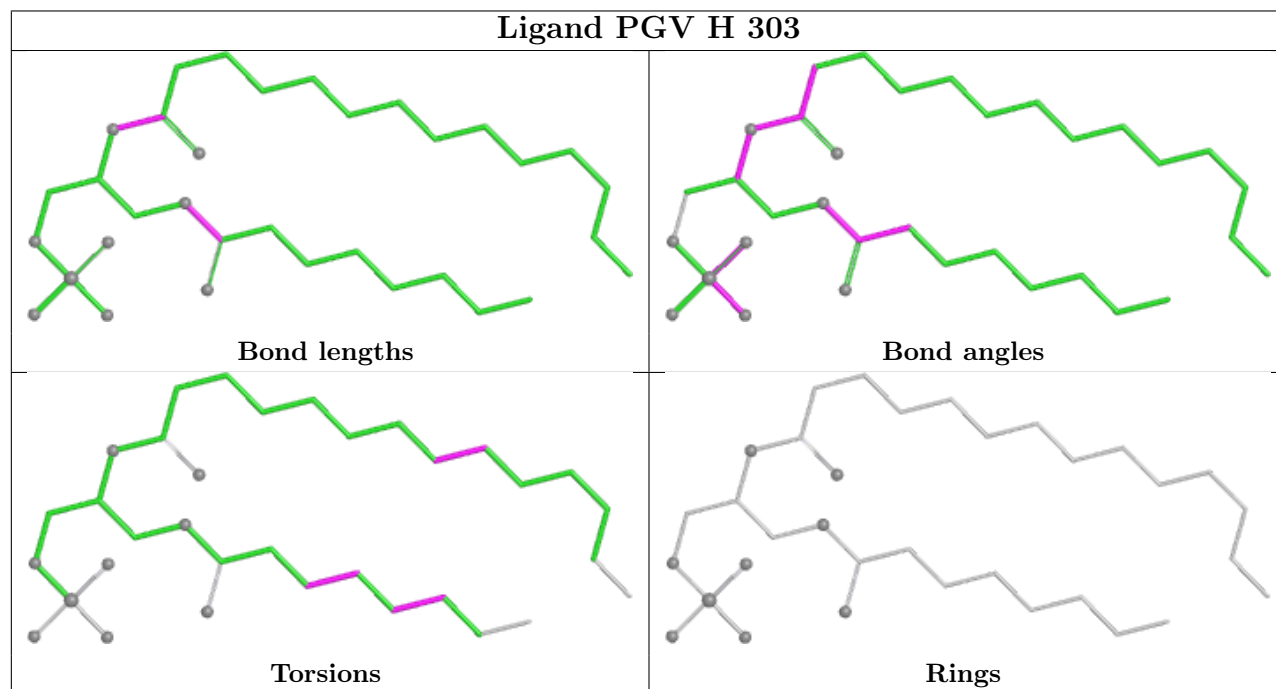
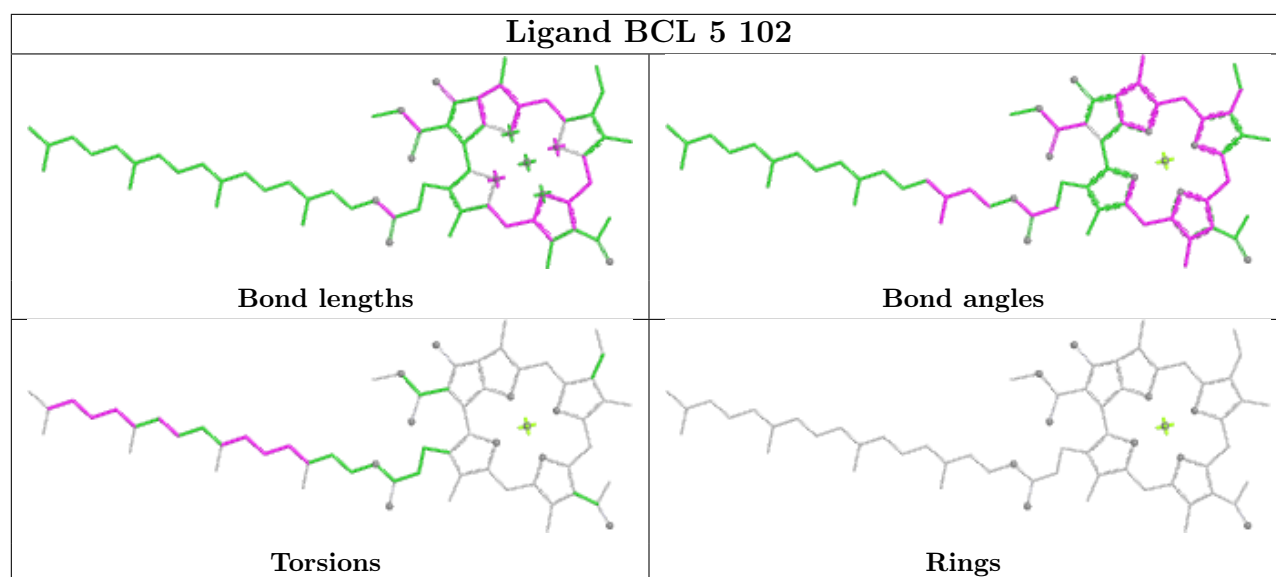


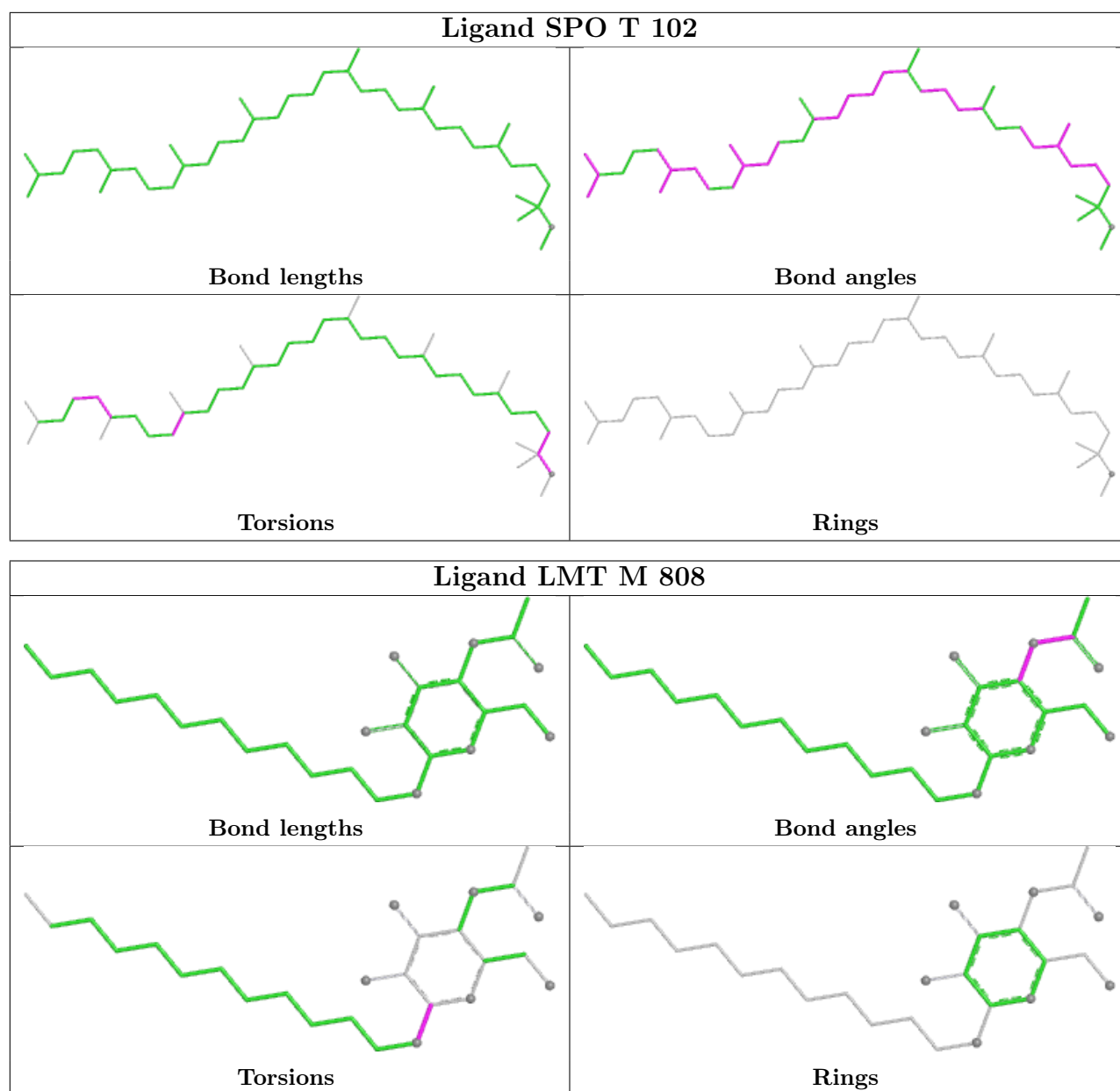


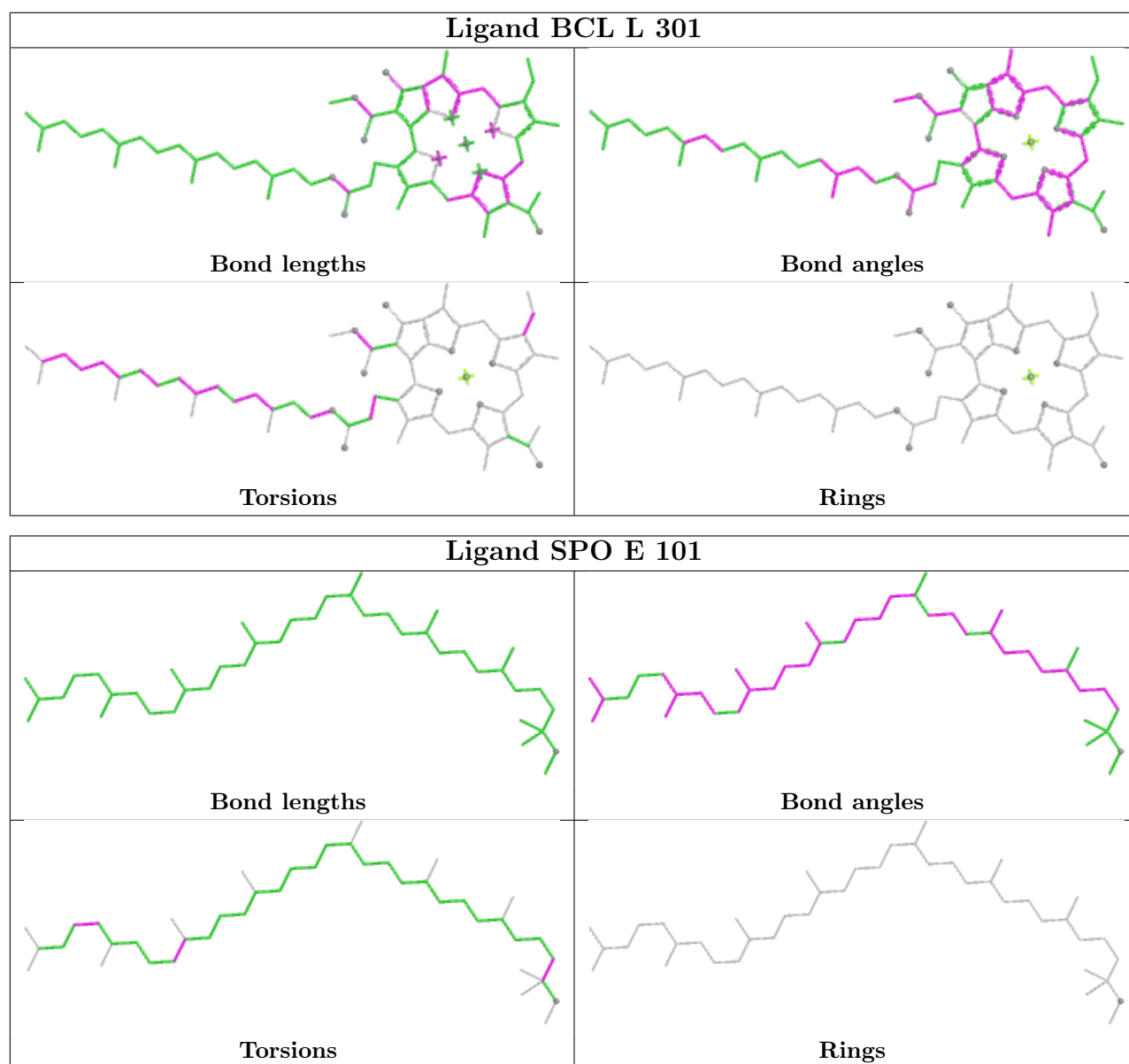


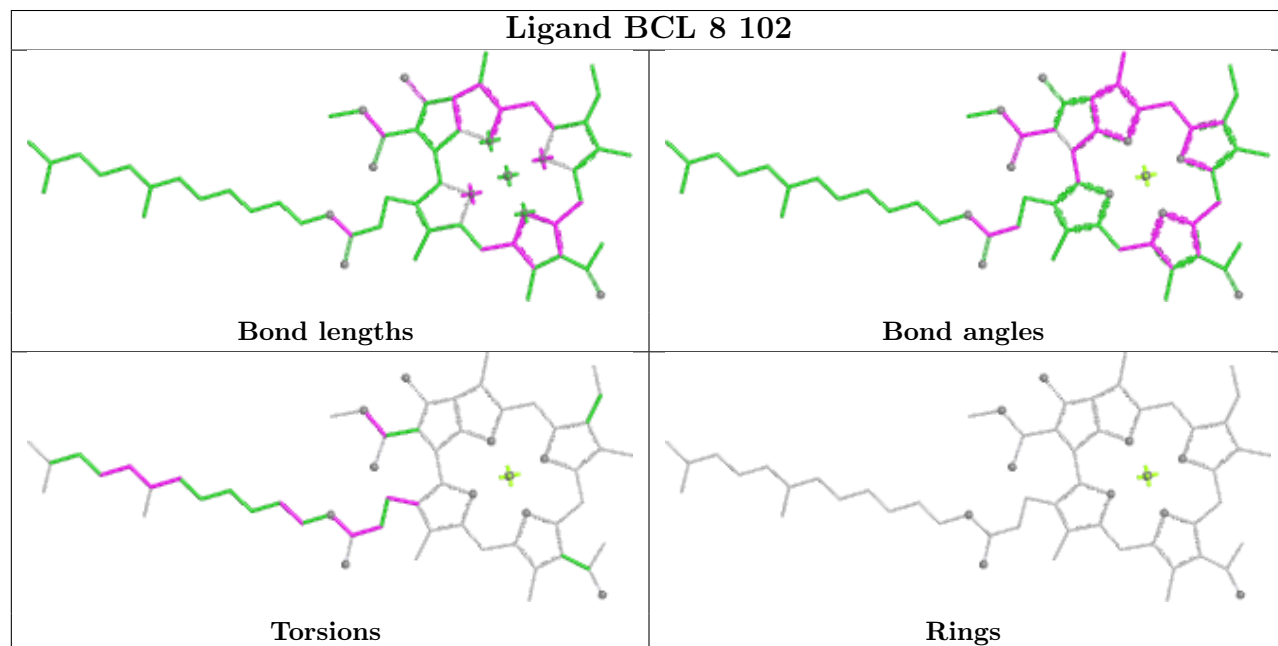
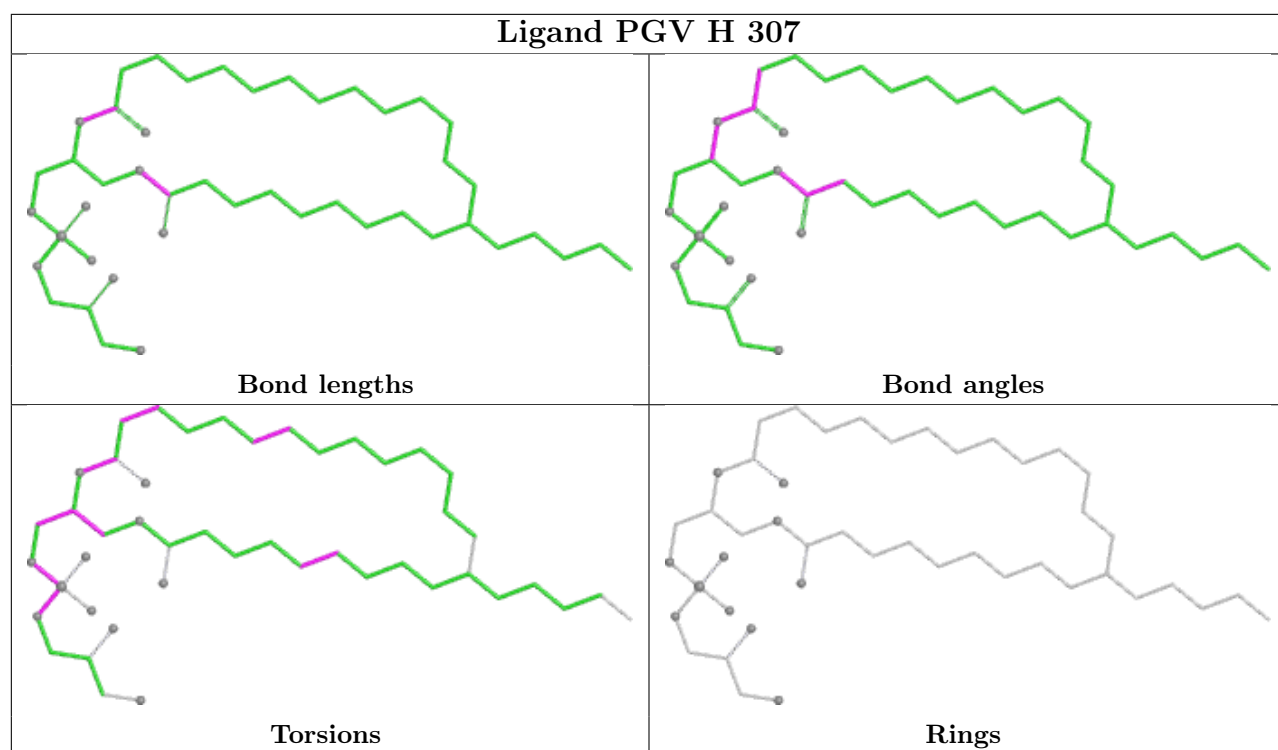


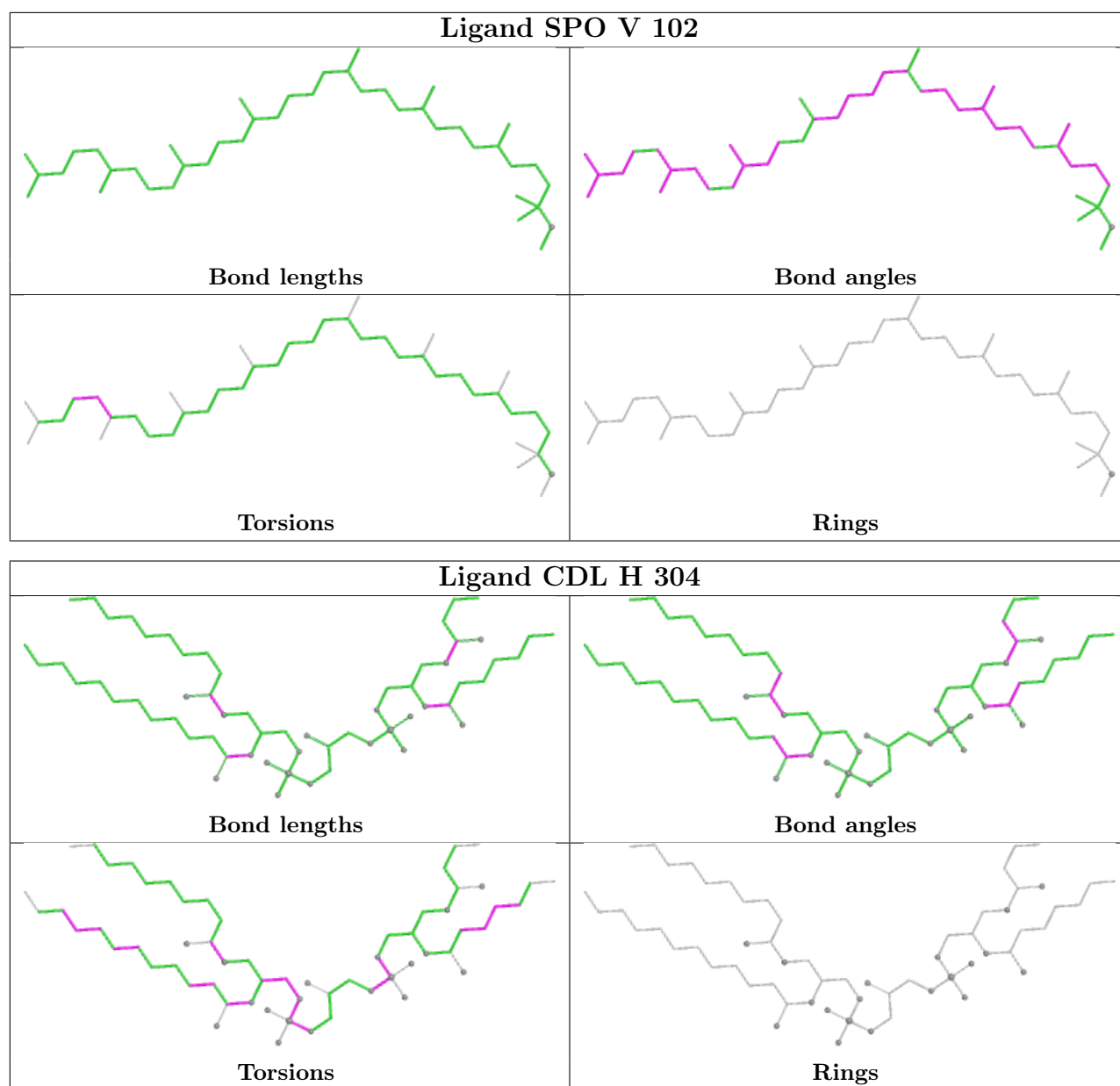


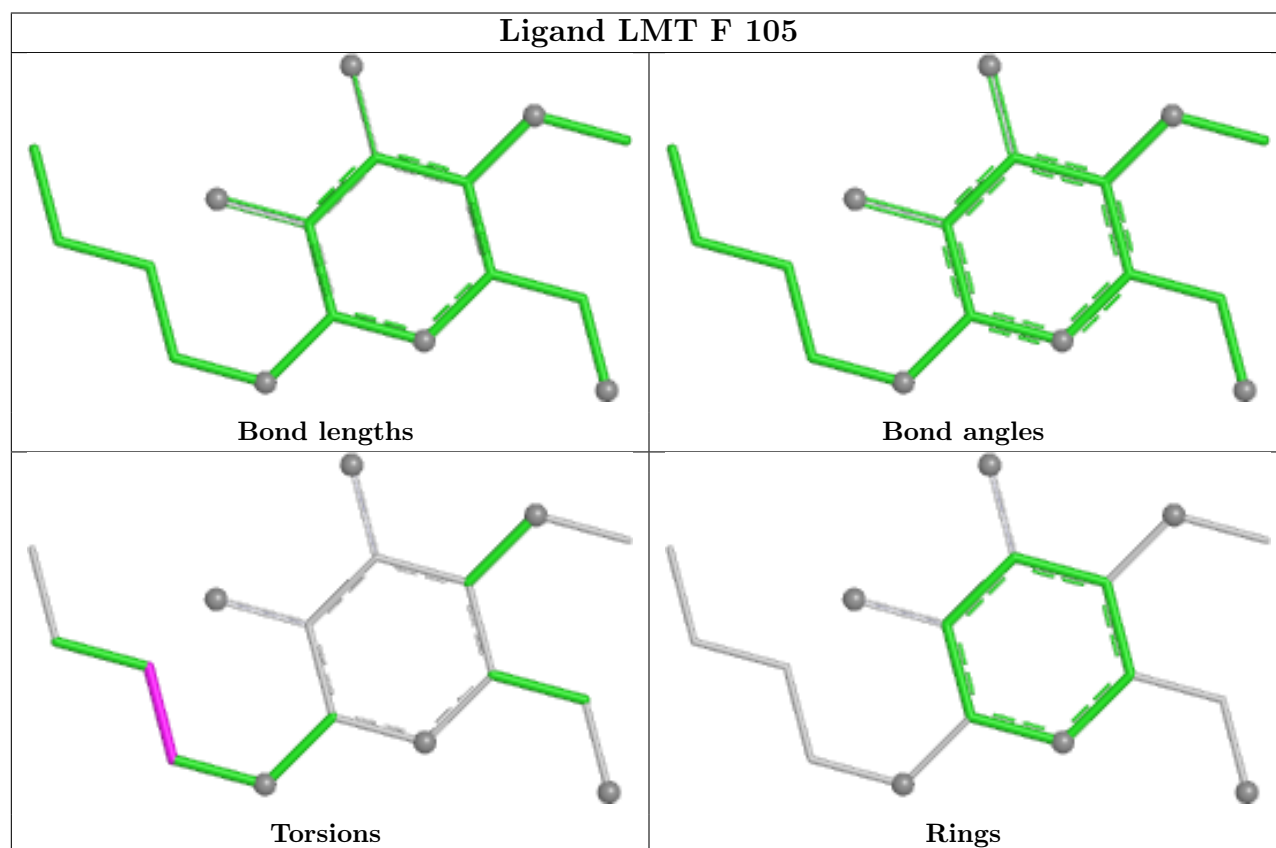
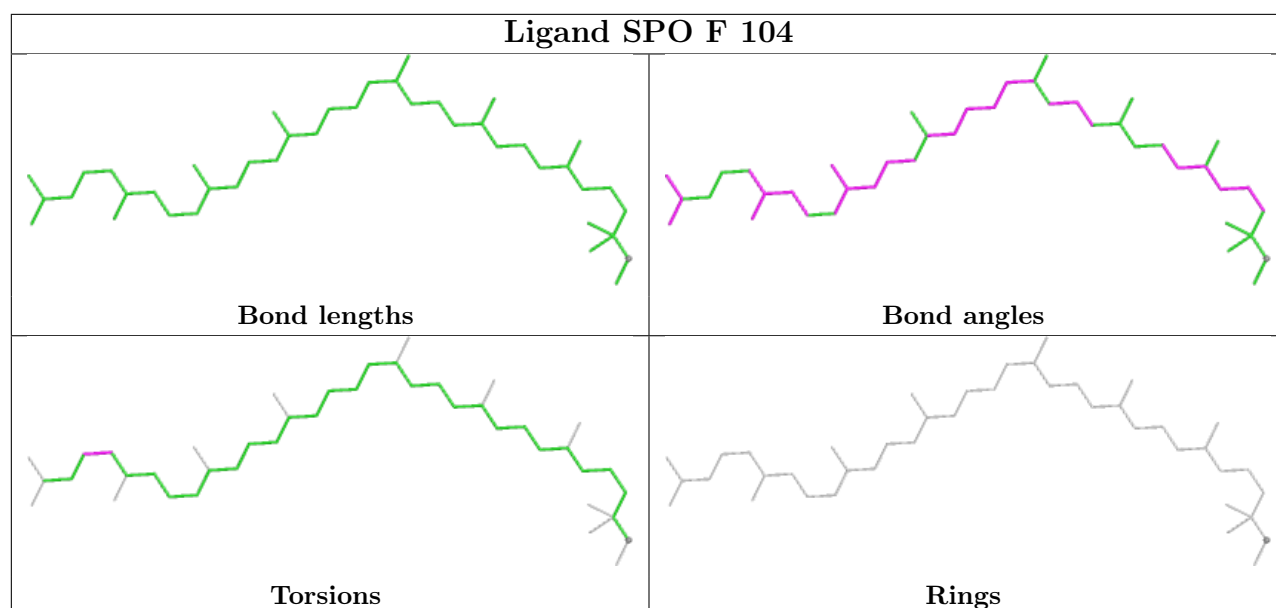


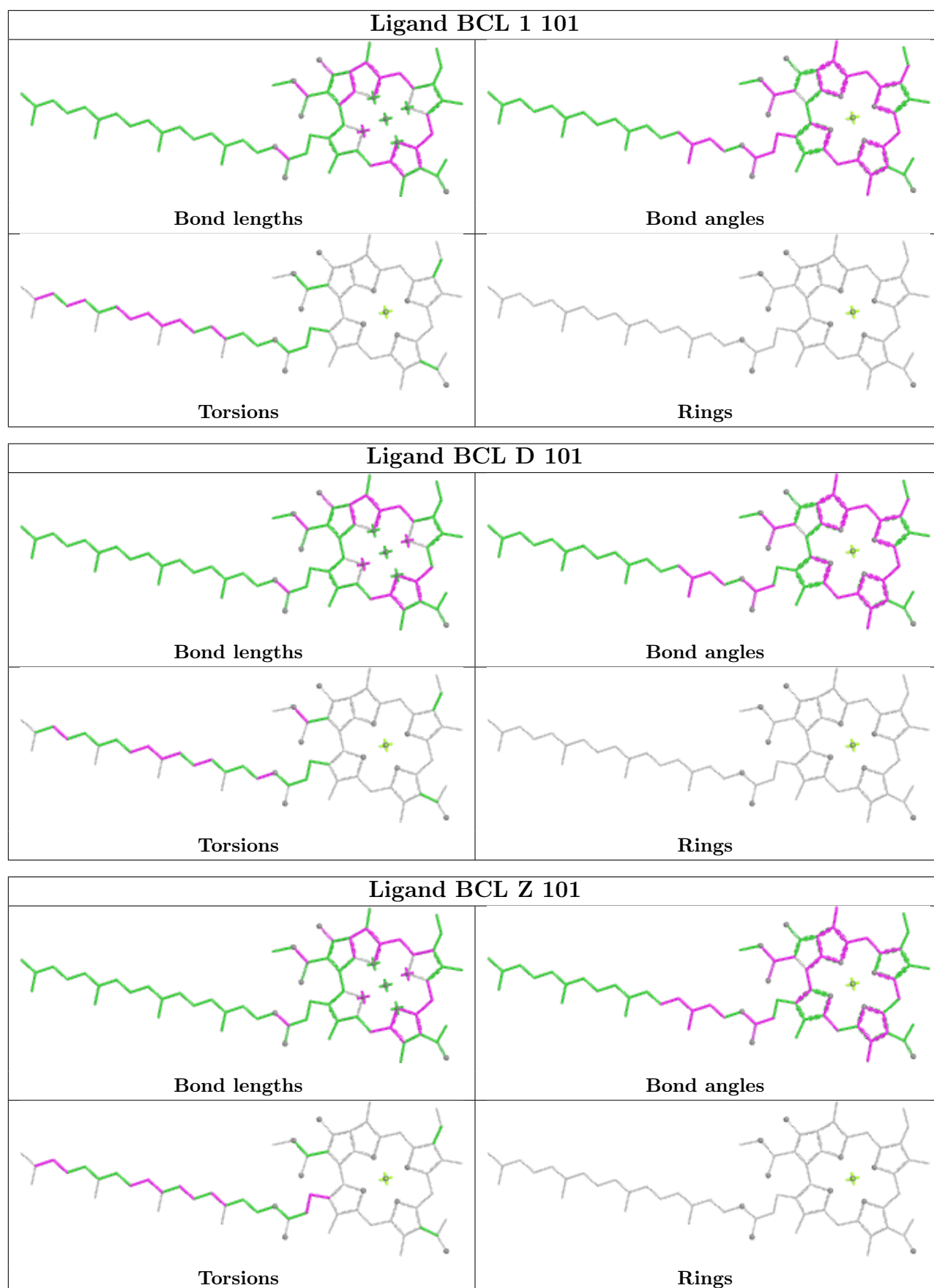


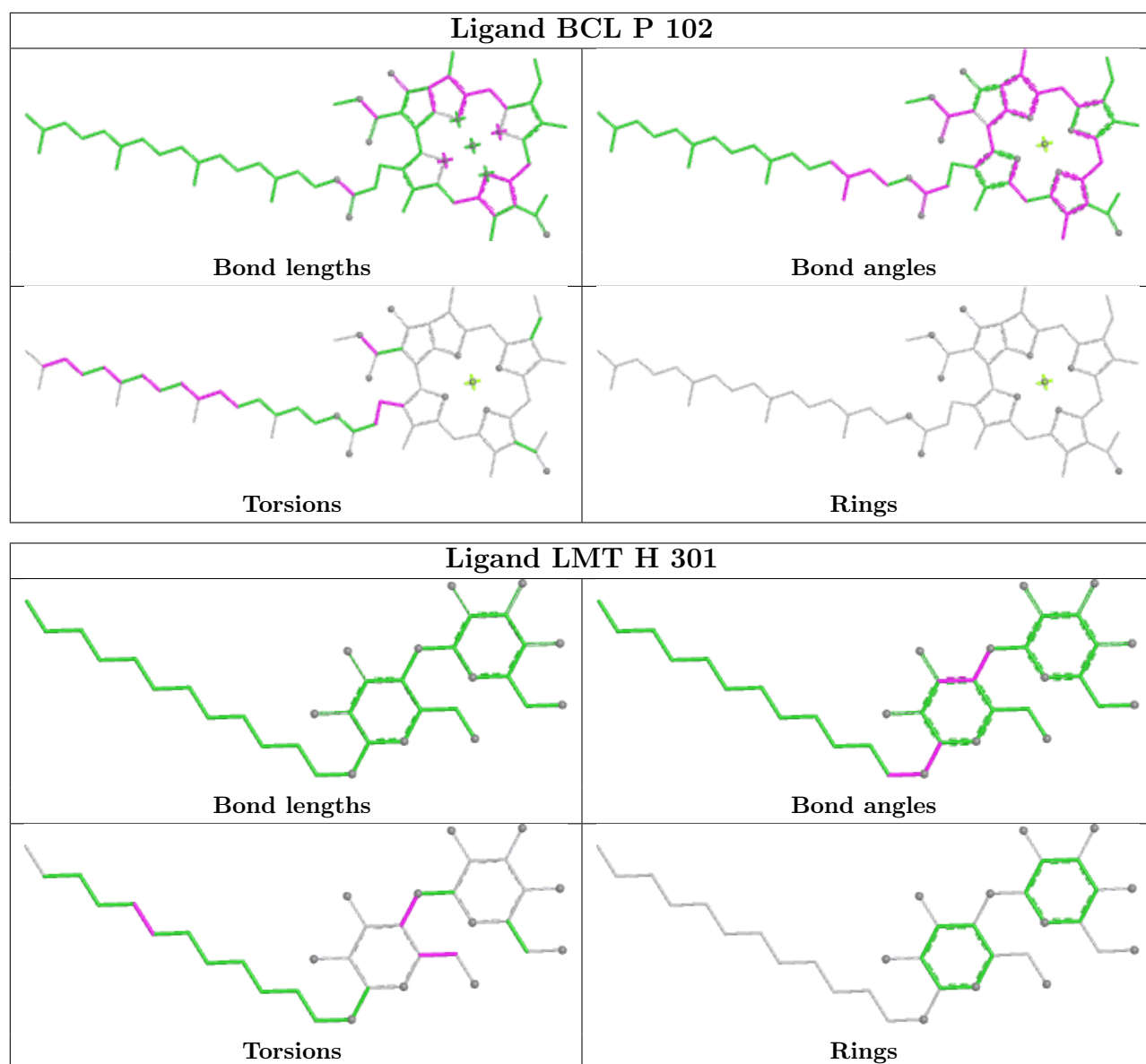


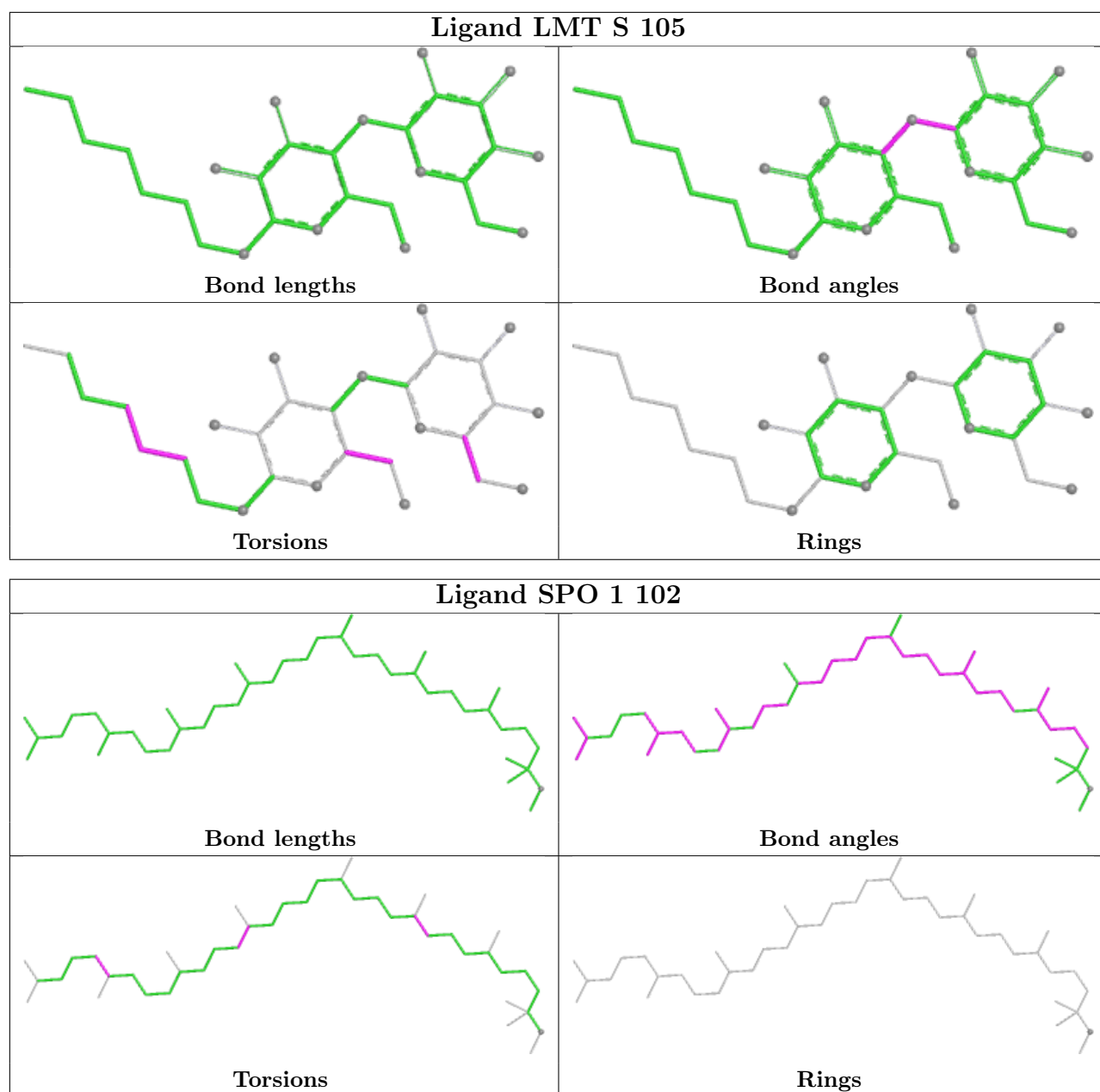


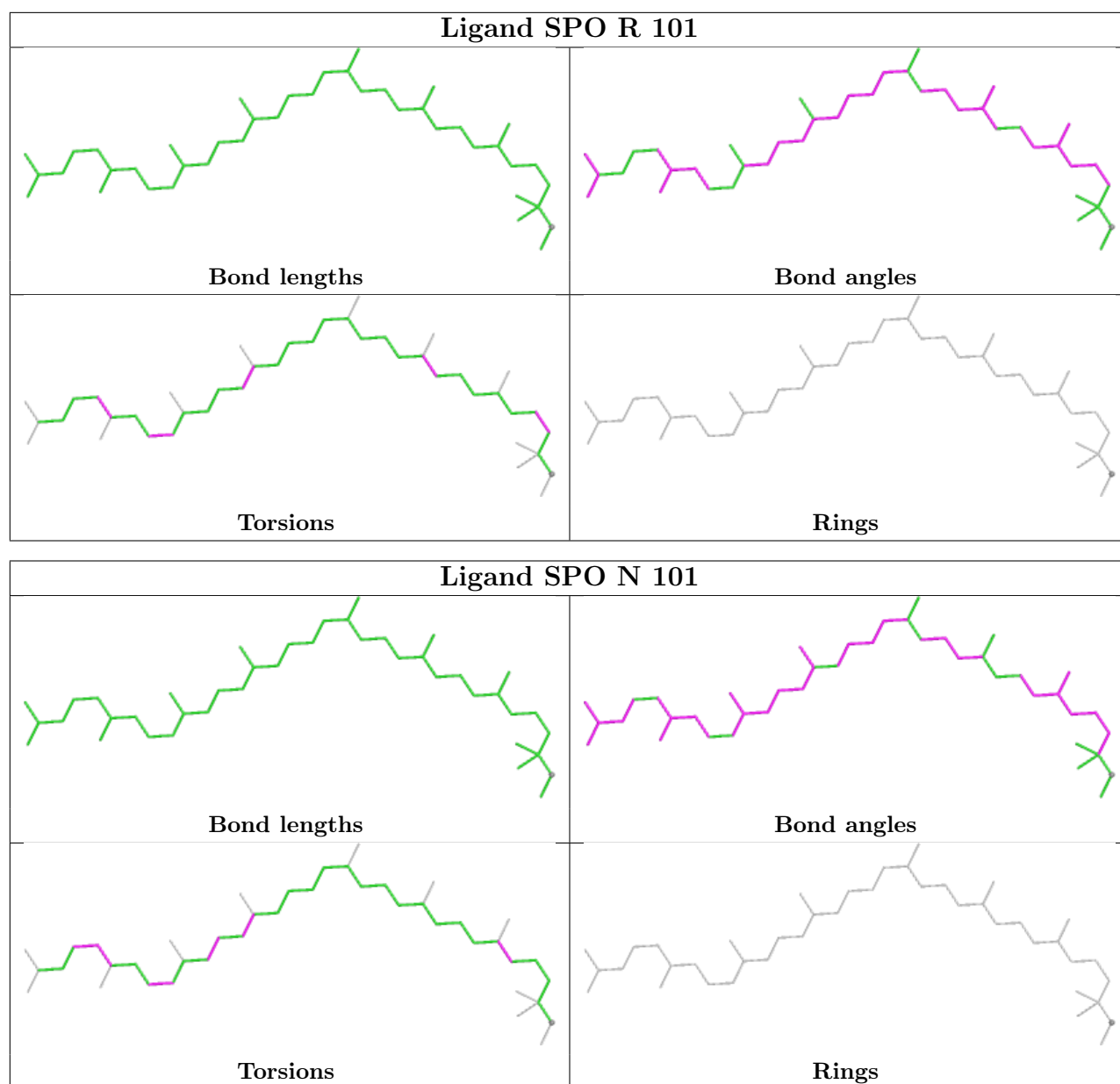


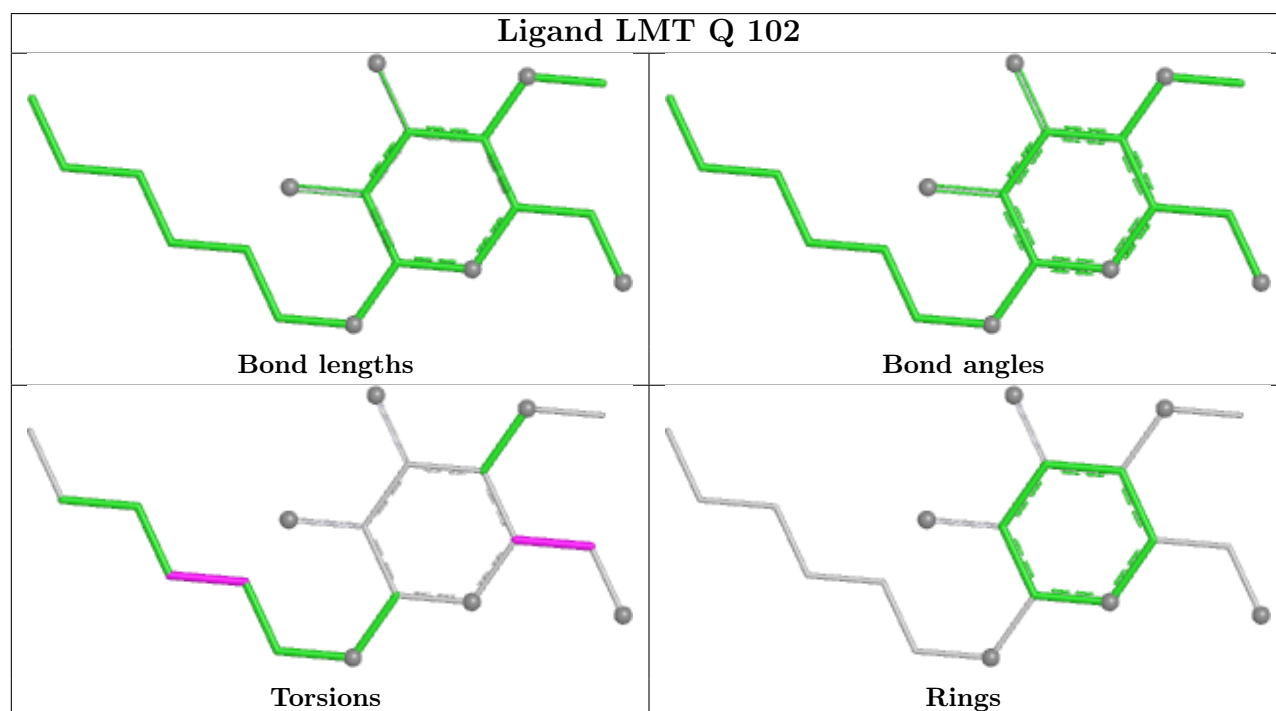
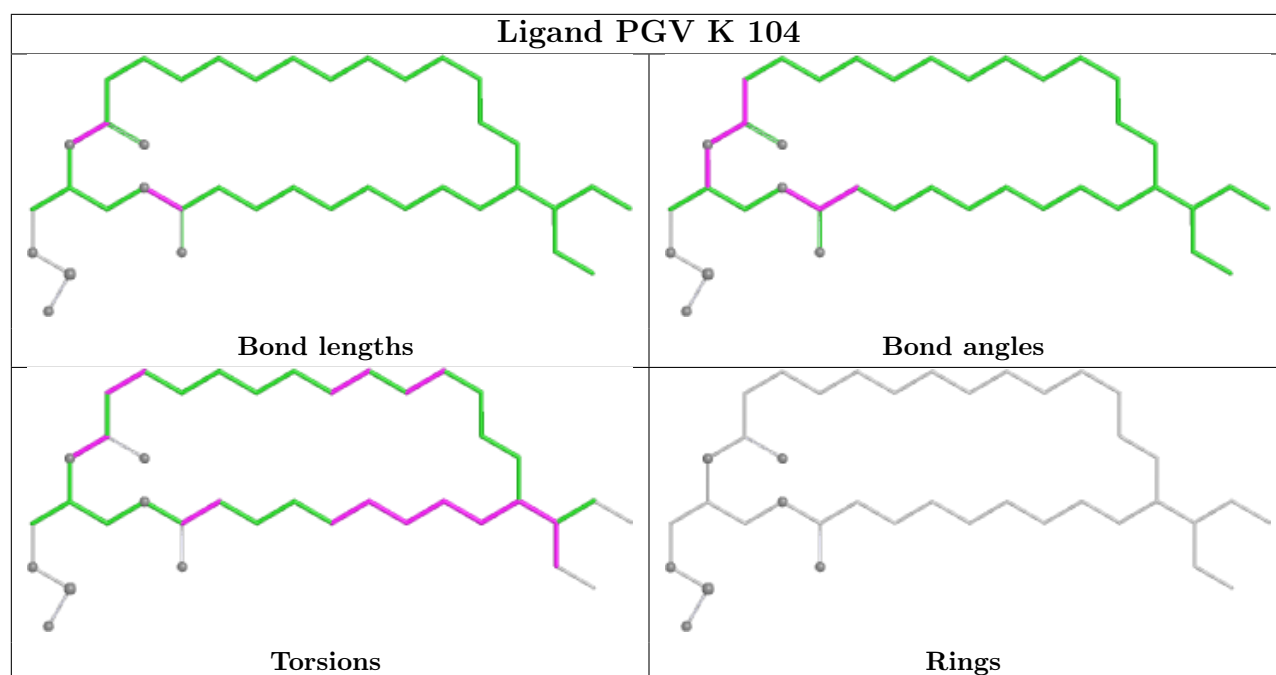


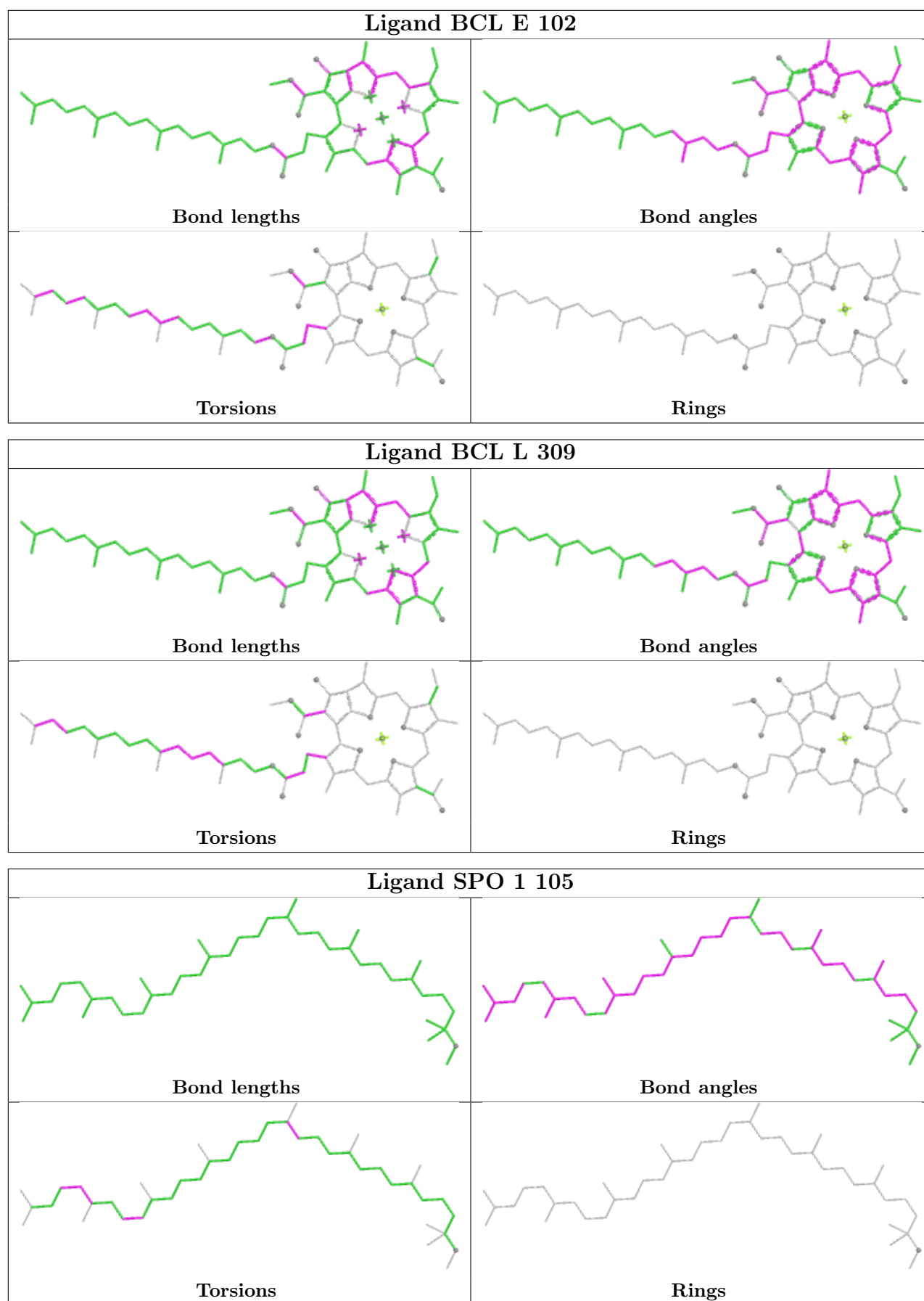


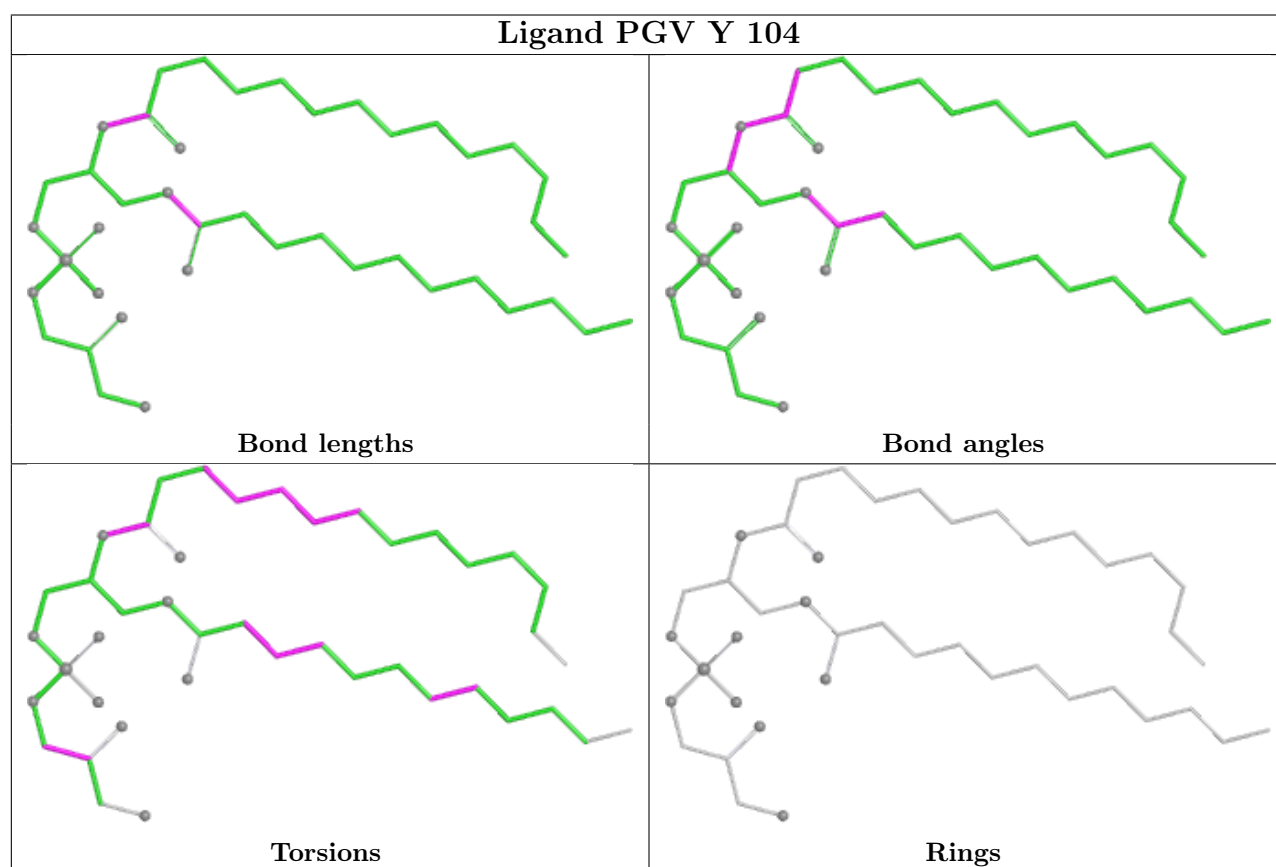
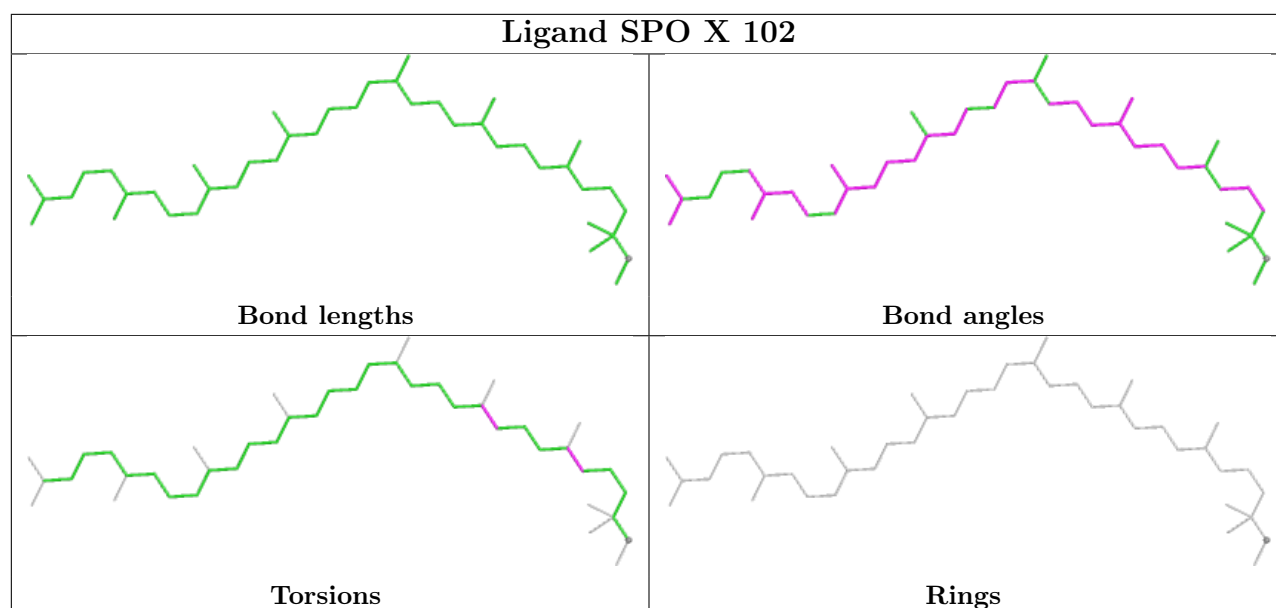


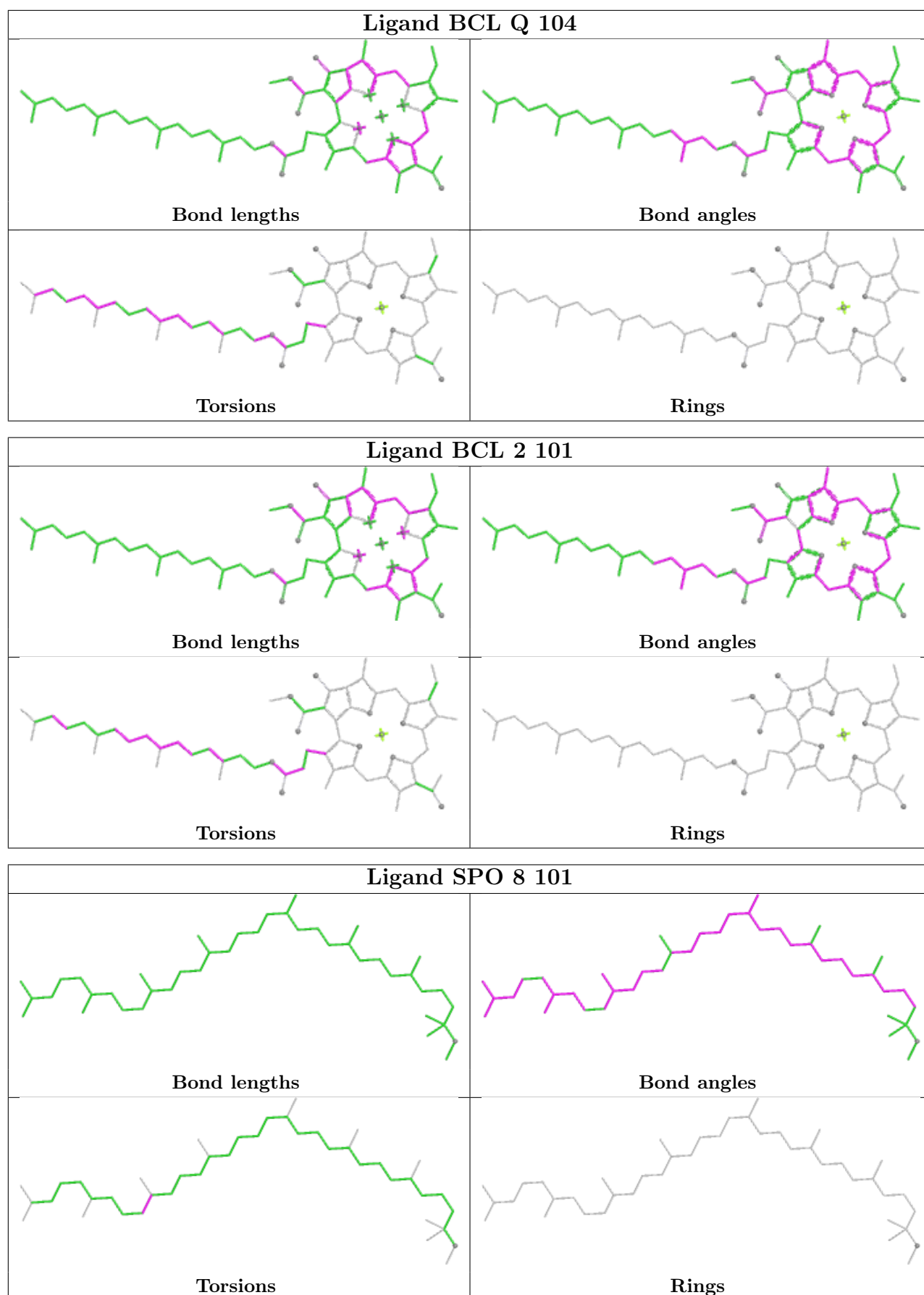


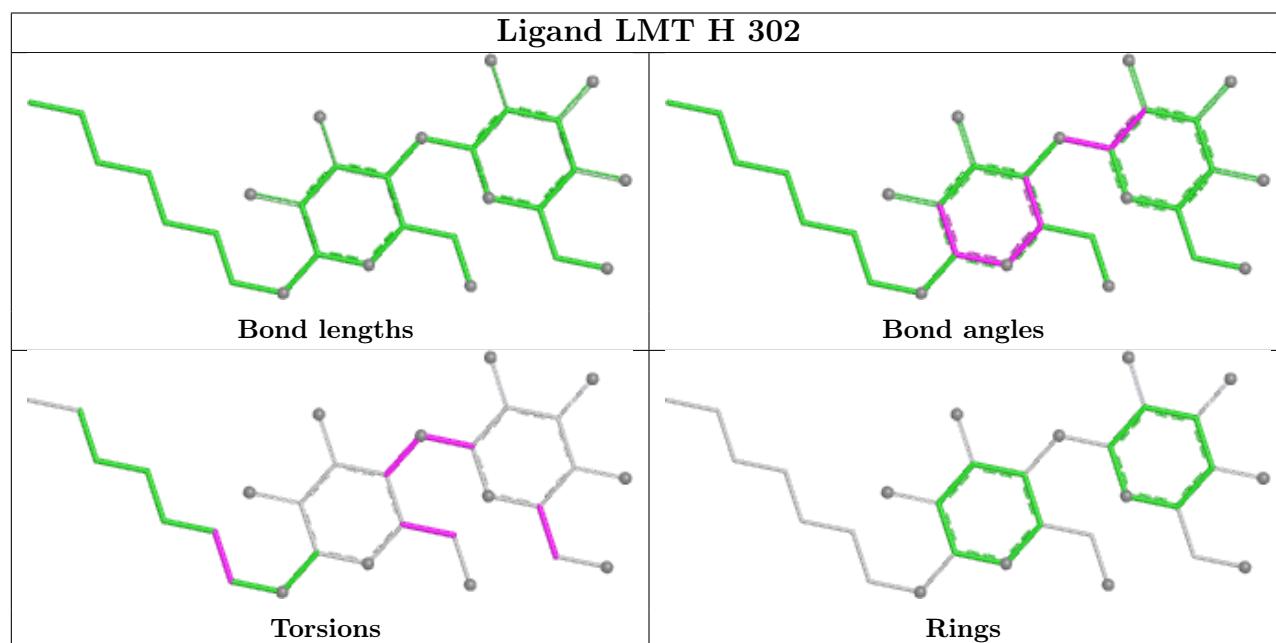
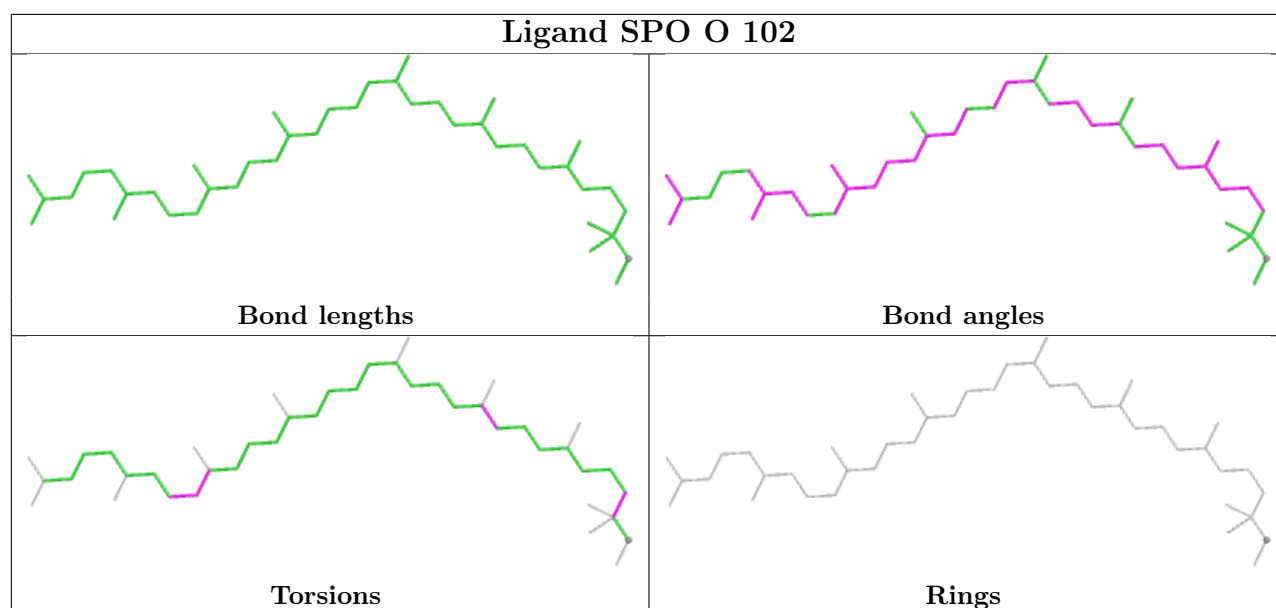


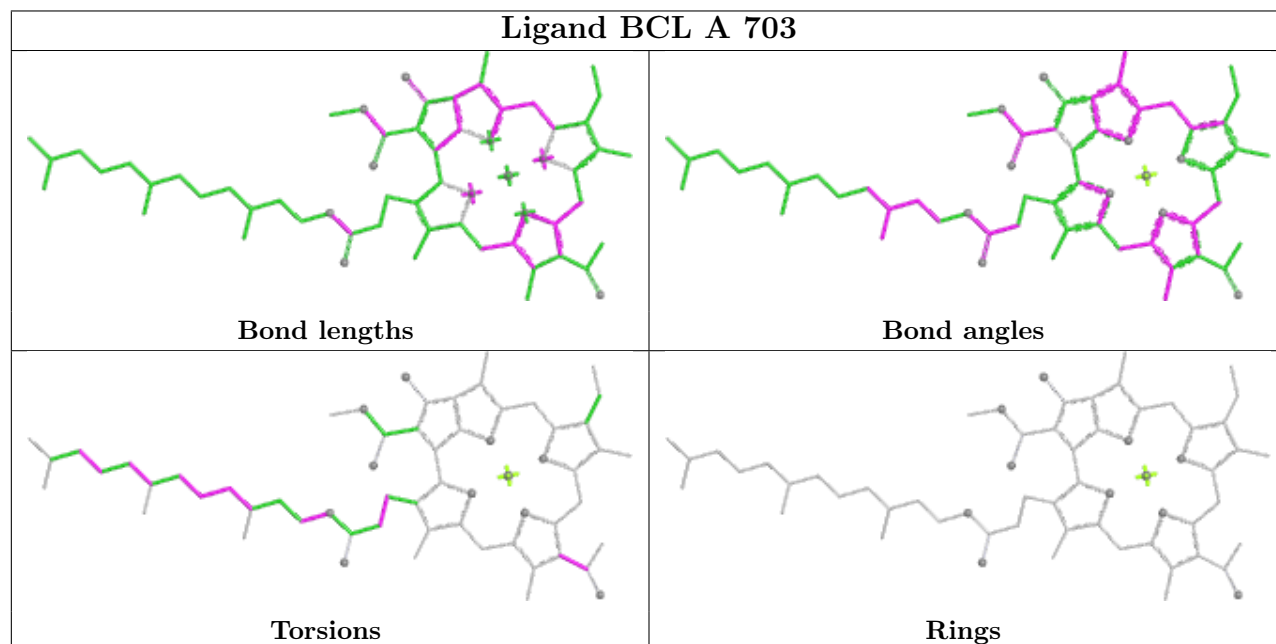
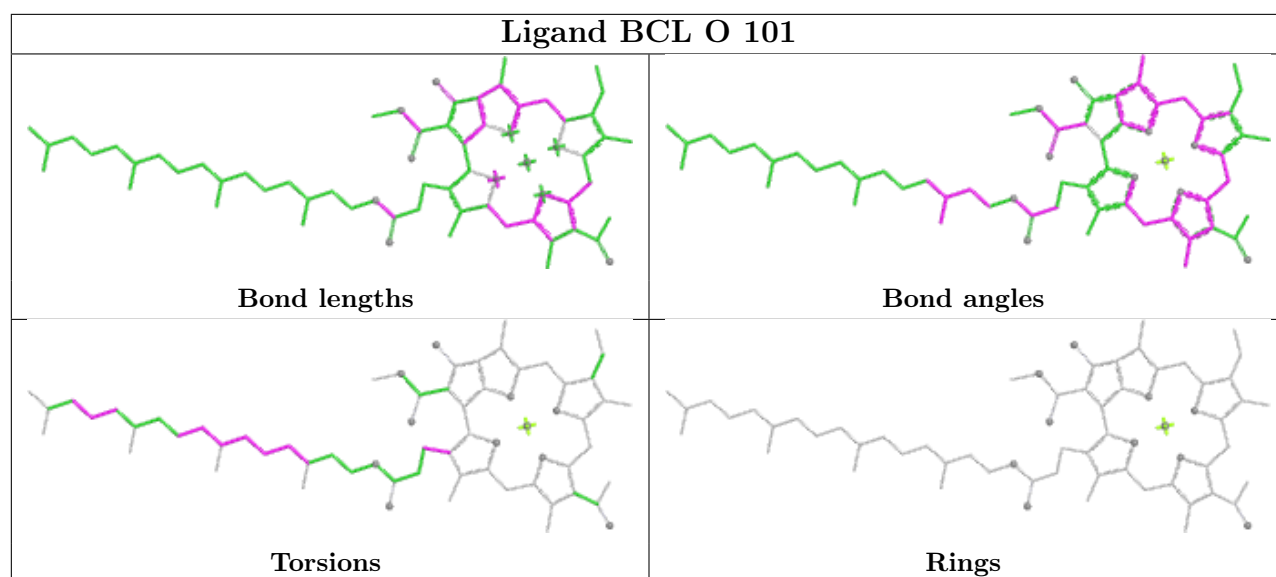


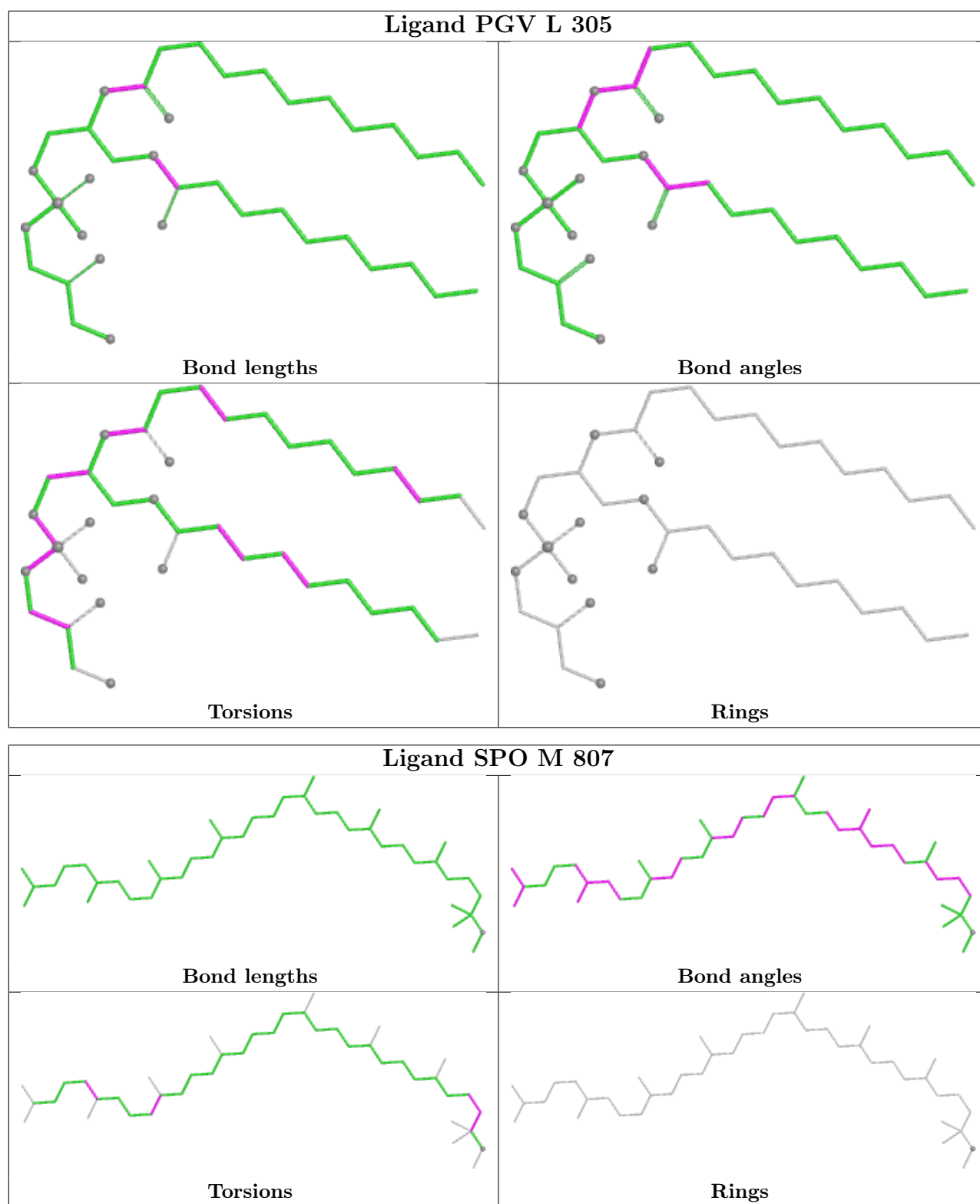


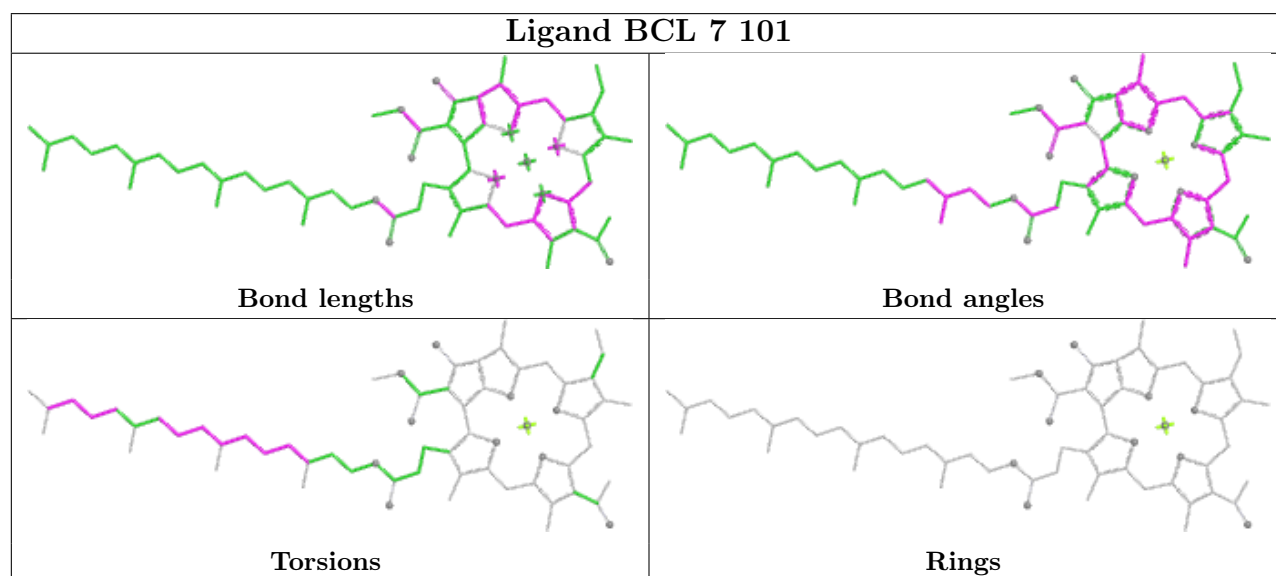
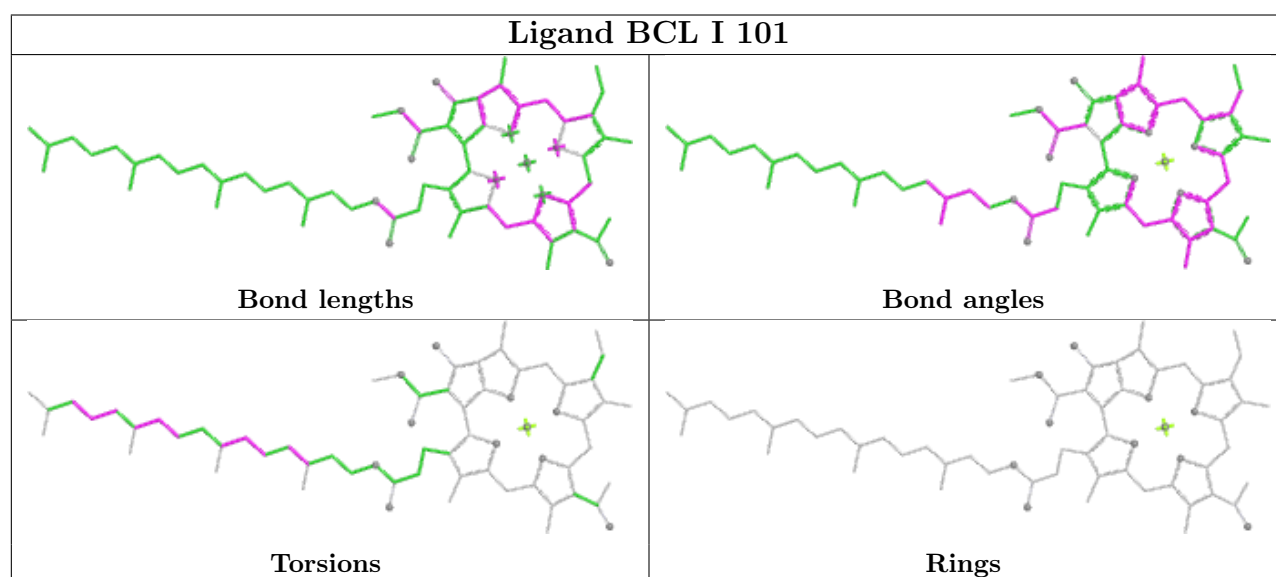
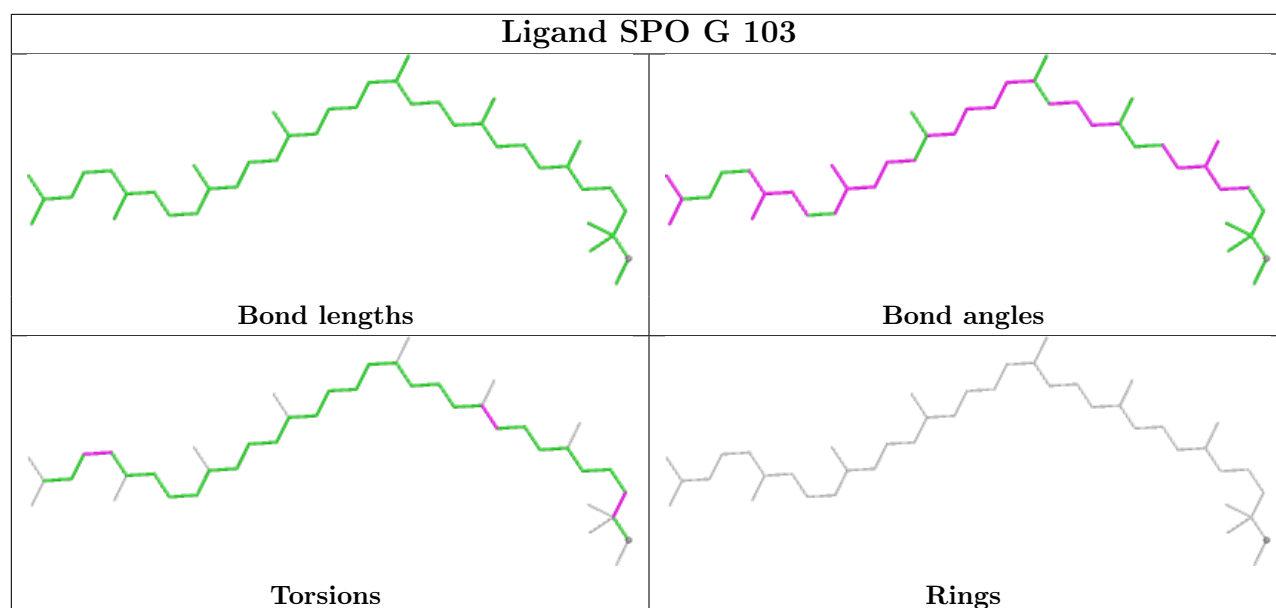


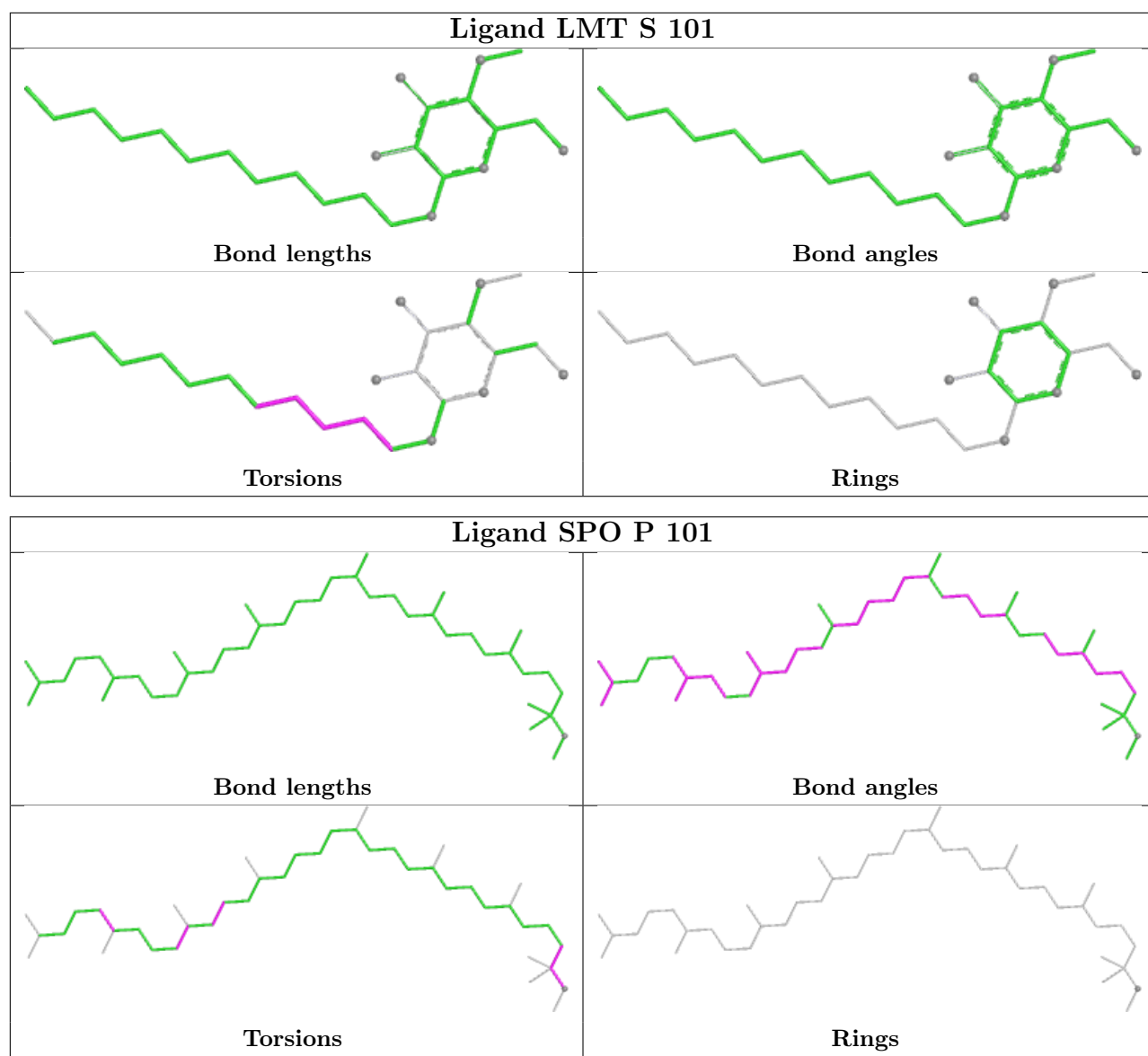


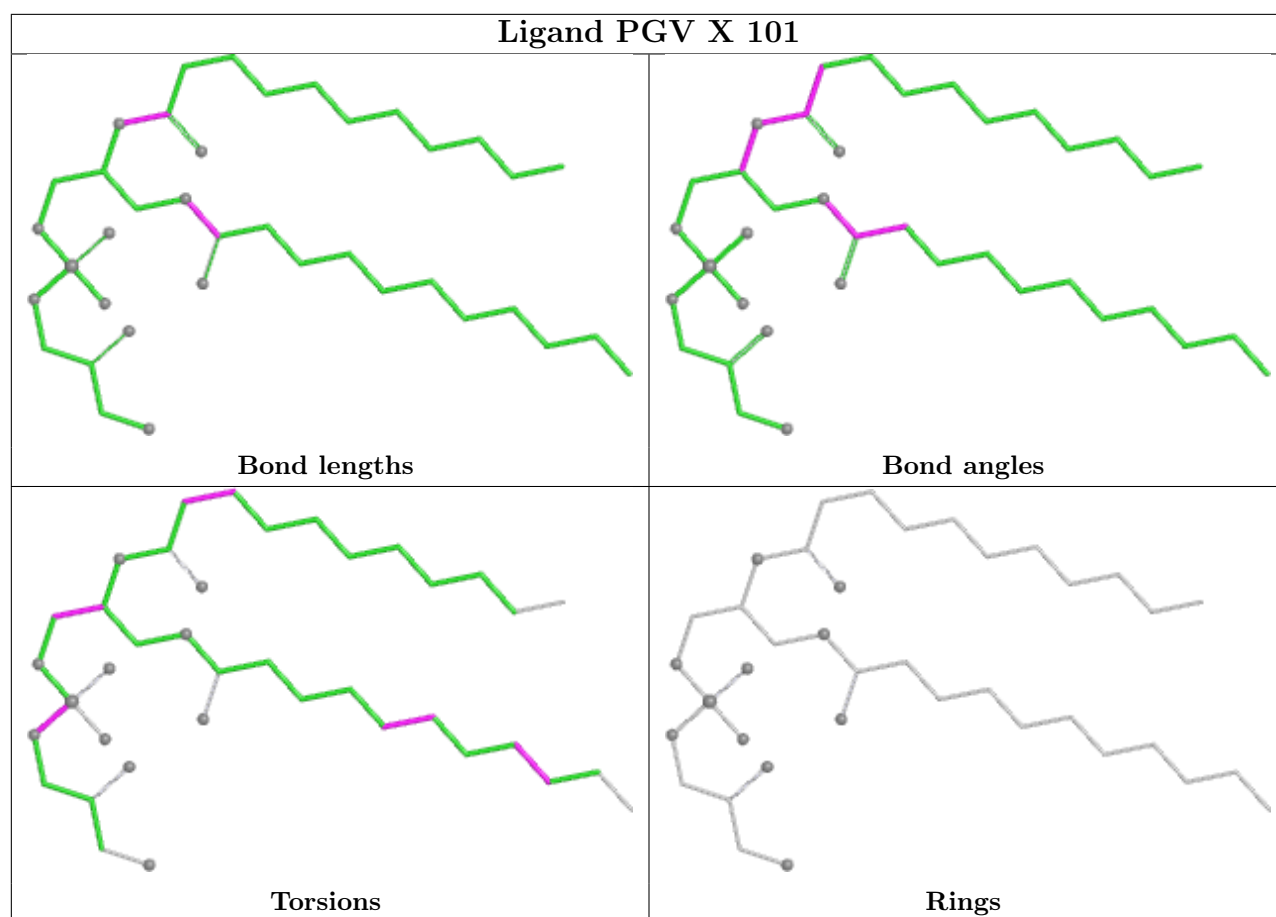


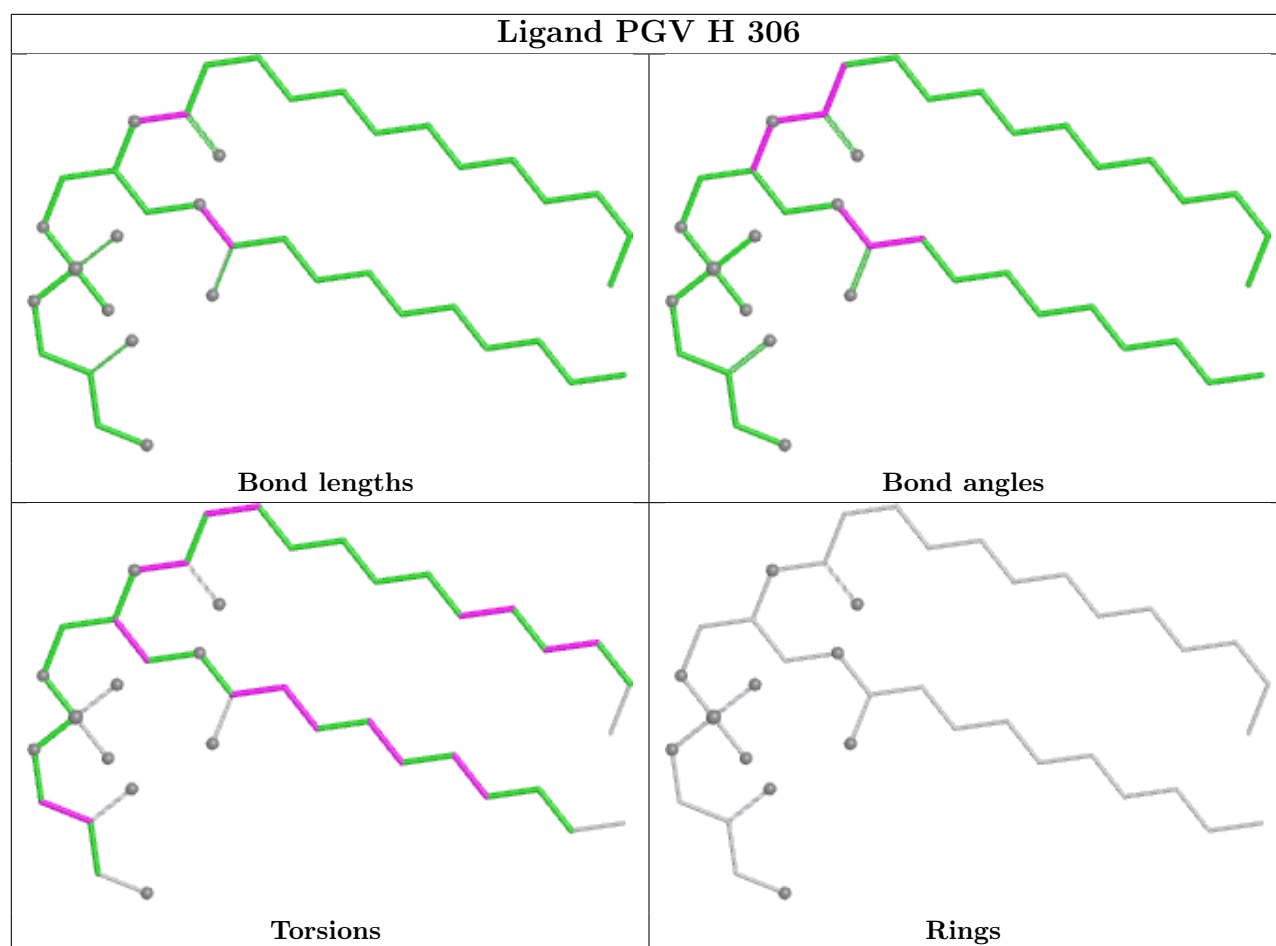












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

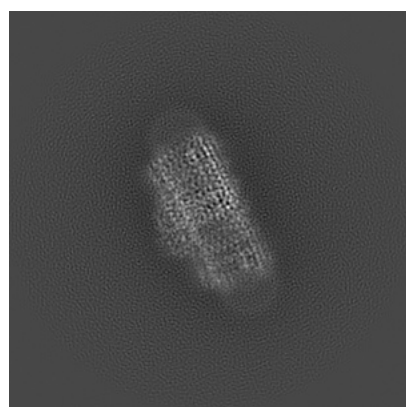
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31400. These allow visual inspection of the internal detail of the map and identification of artifacts.

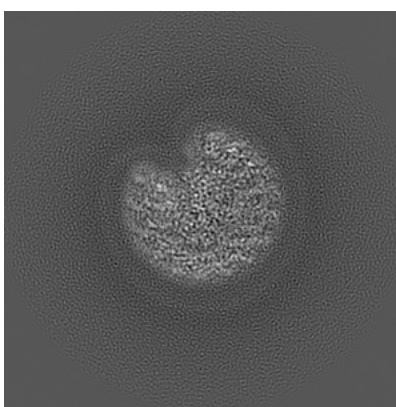
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

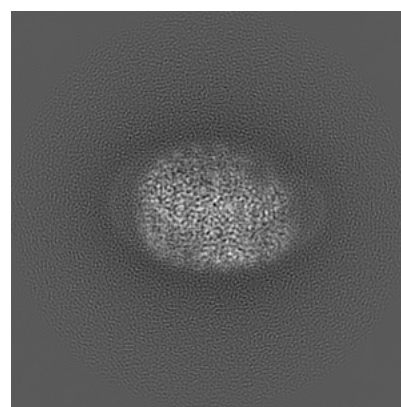
6.1.1 Primary map



X



Y

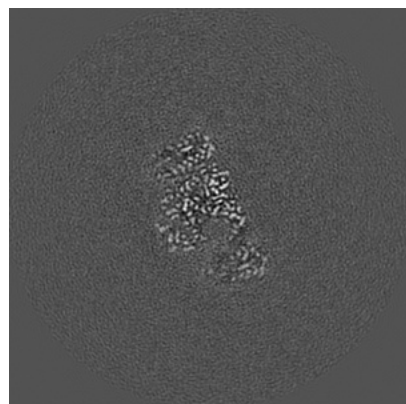


Z

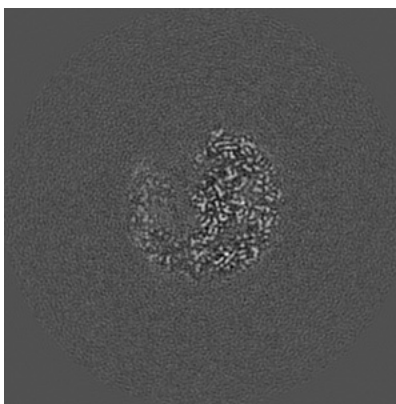
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

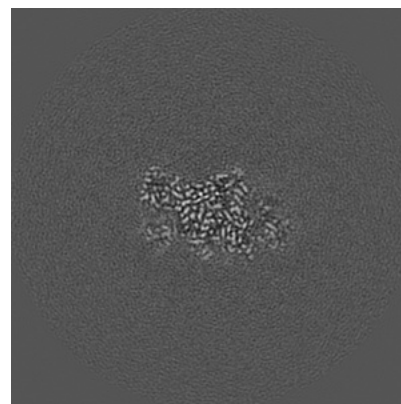
6.2.1 Primary map



X Index: 140



Y Index: 140

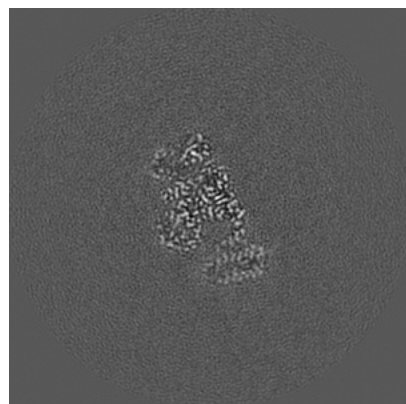


Z Index: 140

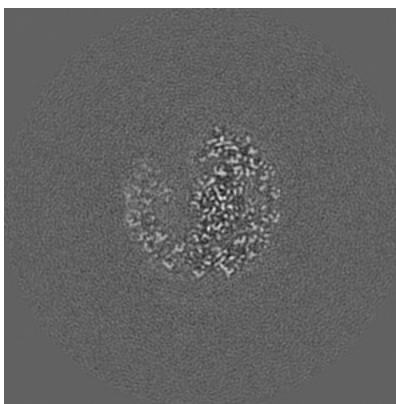
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

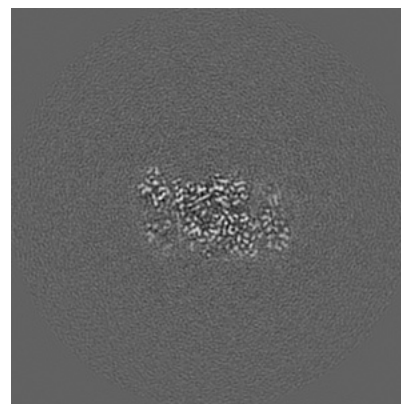
6.3.1 Primary map



X Index: 142



Y Index: 142

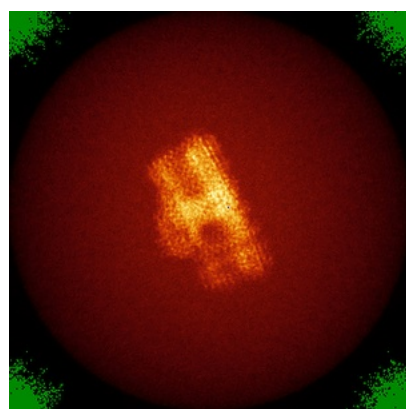


Z Index: 142

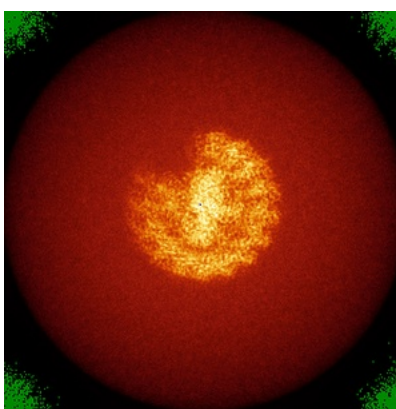
The images above show the largest variance slices of the map in three orthogonal directions.

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

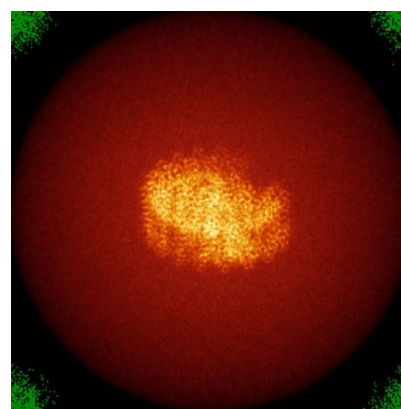
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

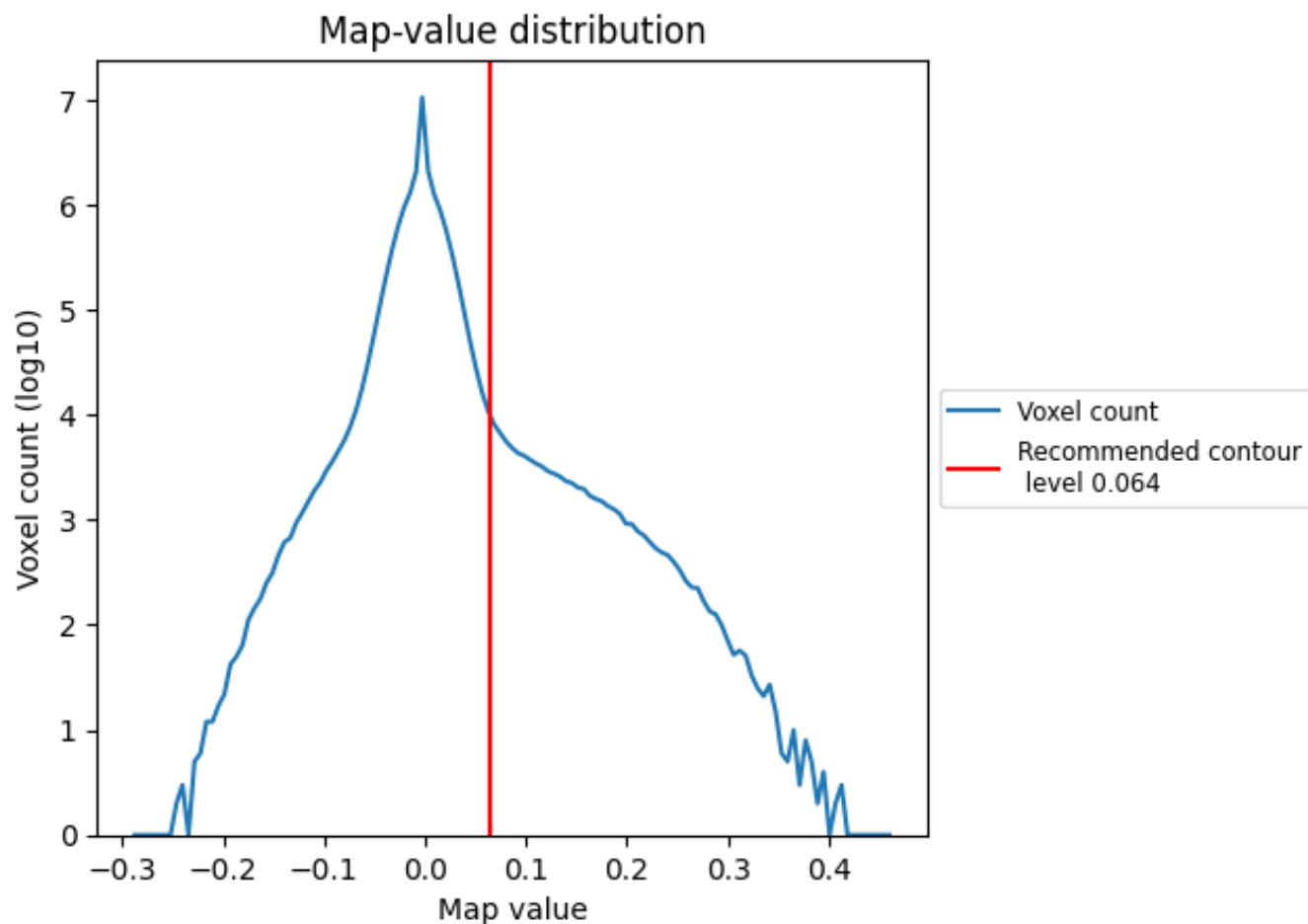
6.6 Mask visualisation

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

7 Map analysis [i](#)

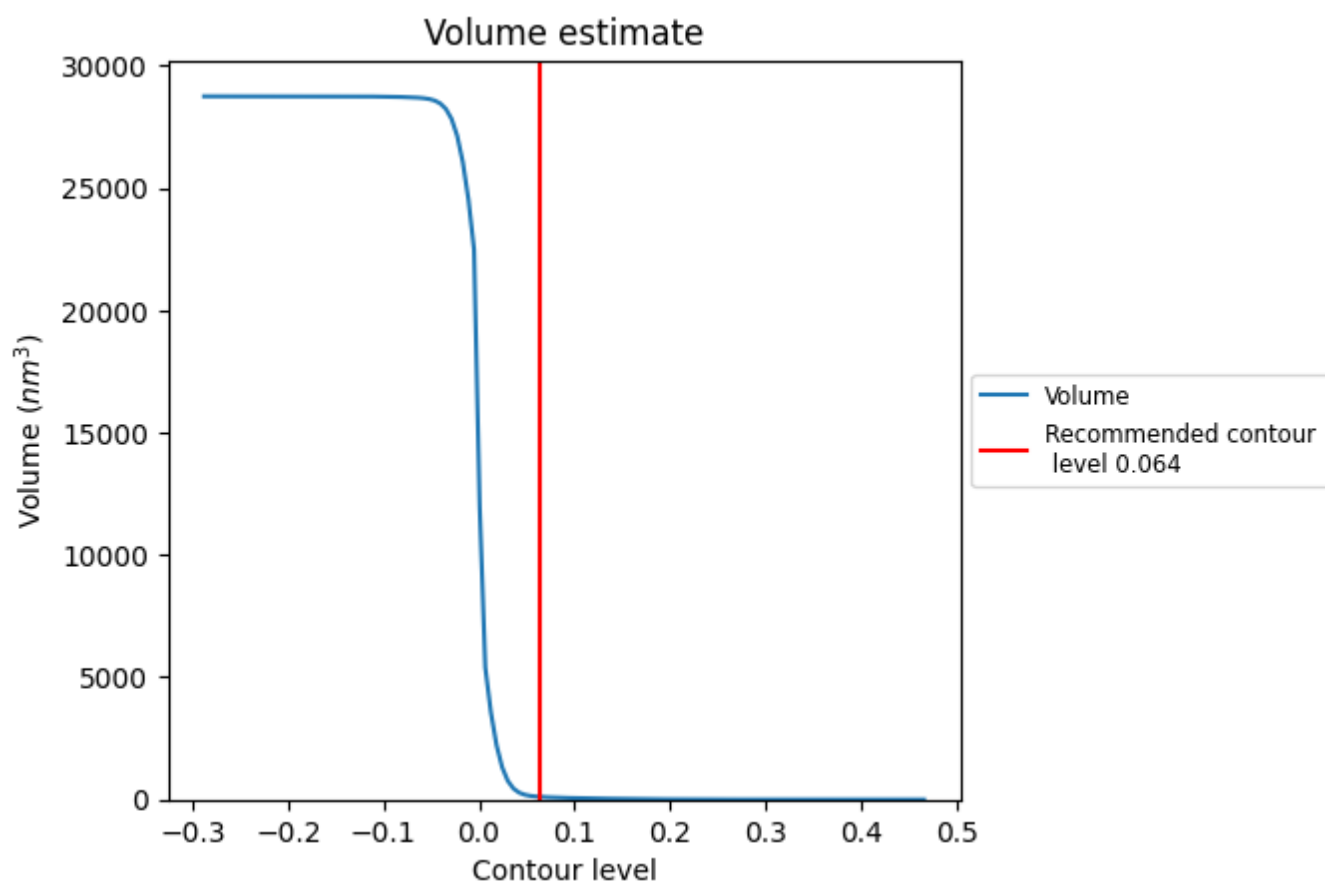
This section contains the results of statistical analysis of the map.

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.

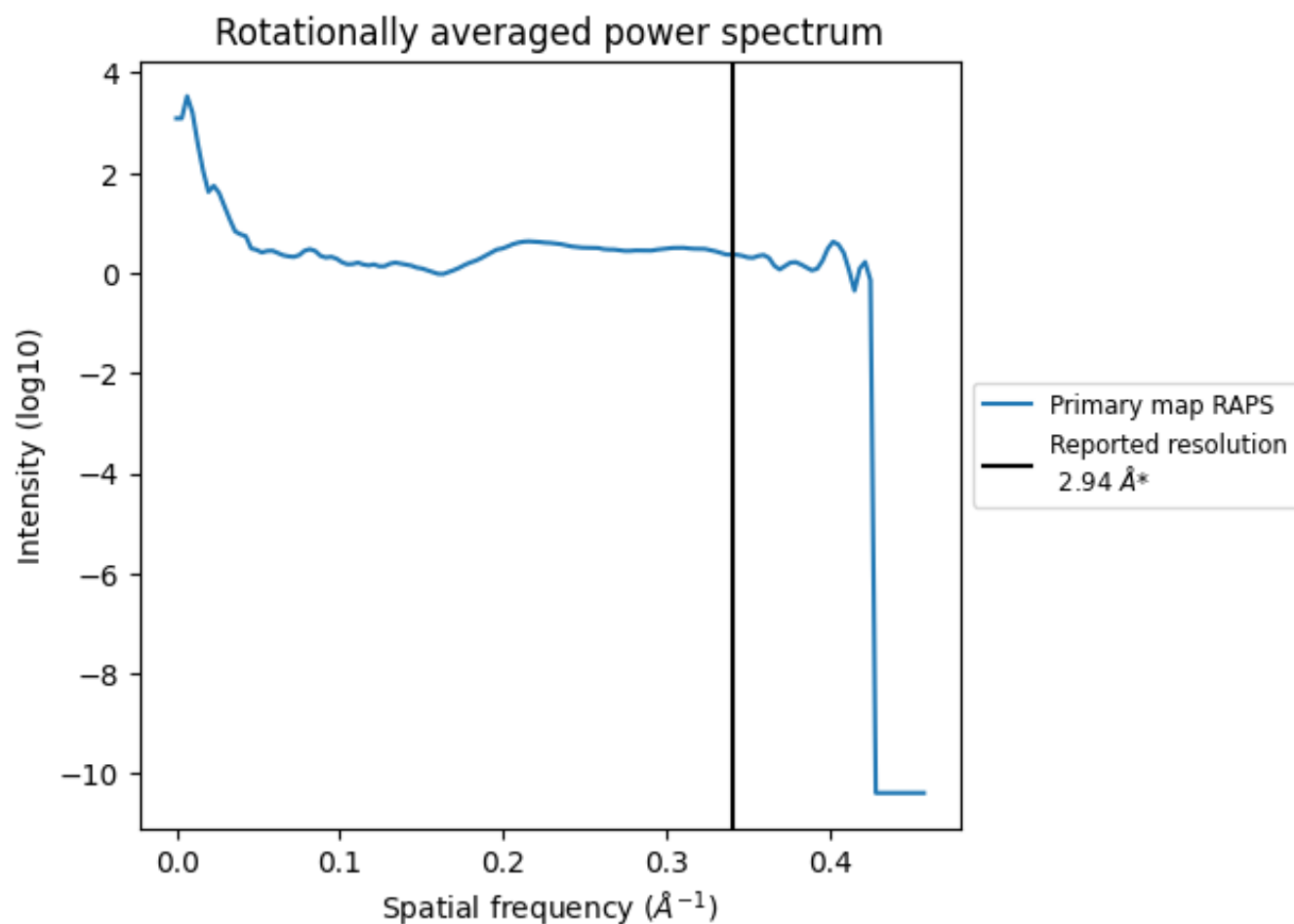
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 112 nm³; this corresponds to an approximate mass of 101 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 ⓘ

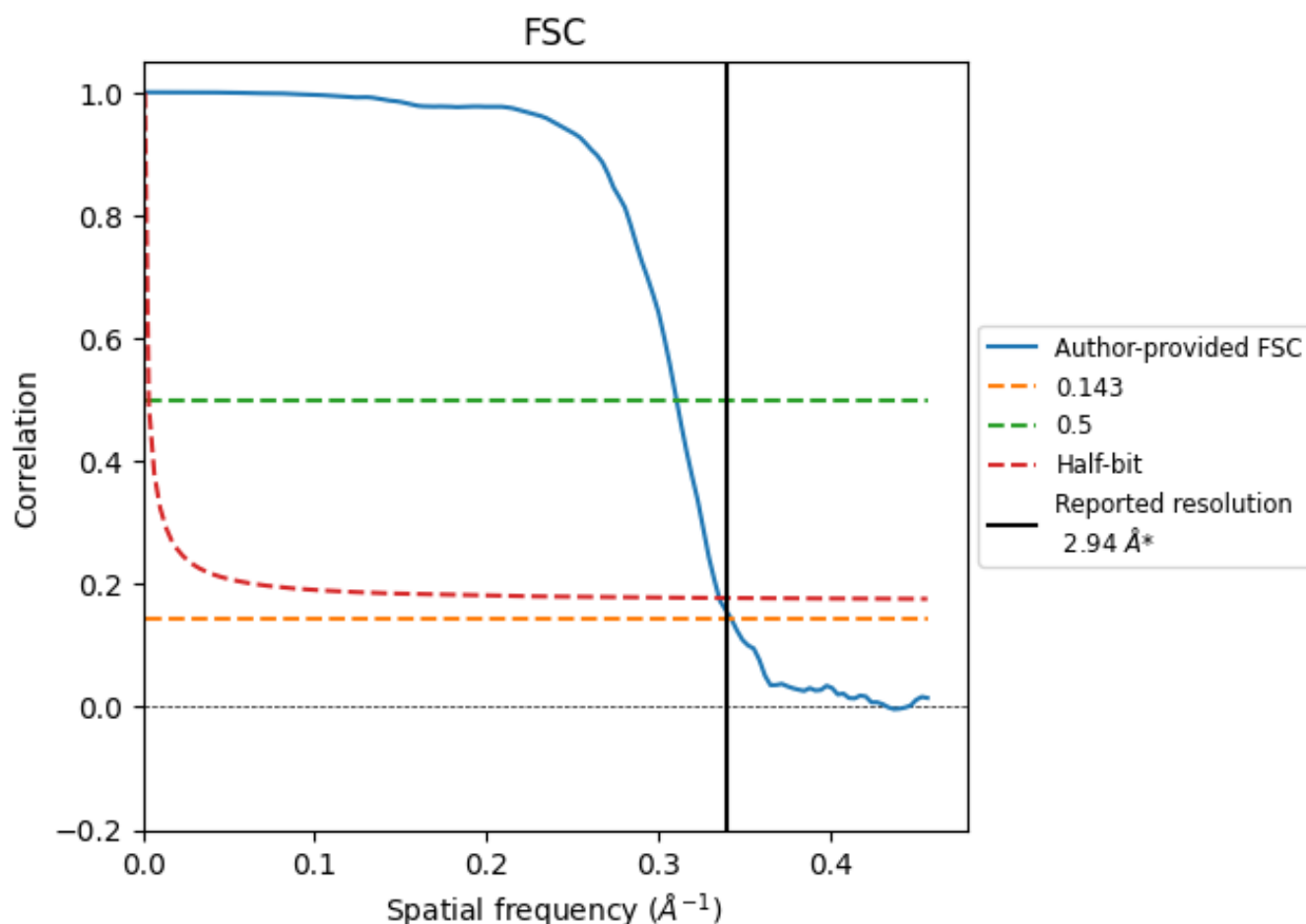


*Reported resolution corresponds to spatial frequency of 0.340 Å⁻¹

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 0.340 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	2.92	3.22	2.98
Unmasked-calculated*	-	-	-

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

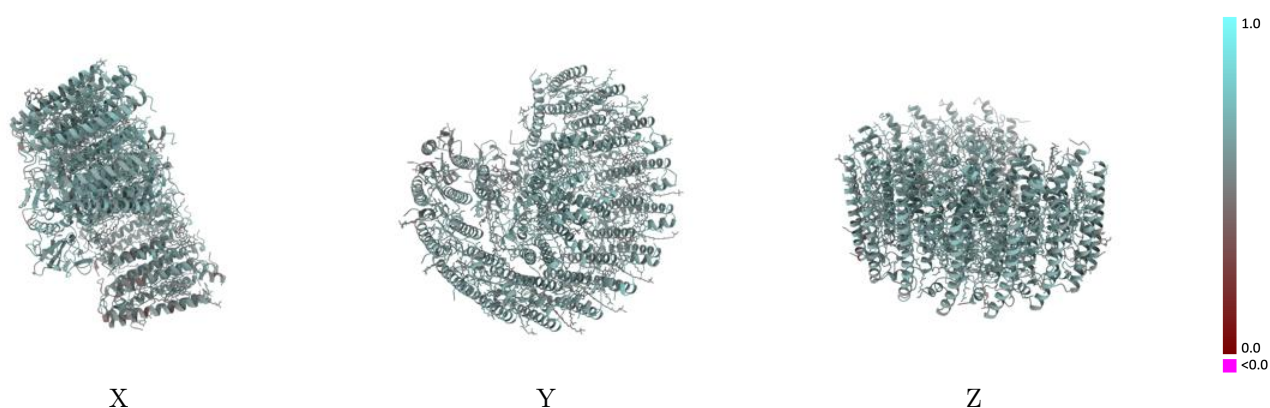
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-31400 and PDB model 7F0L. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)

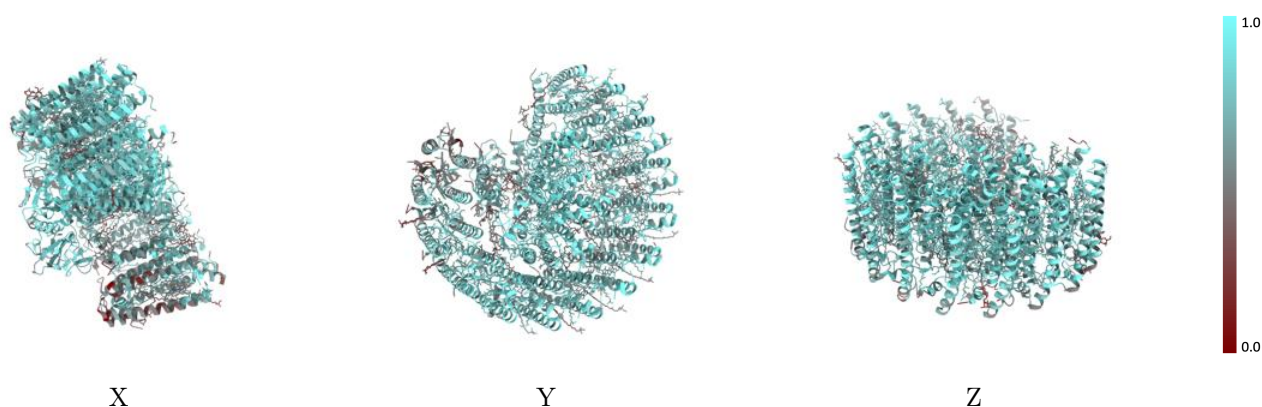
This section was not generated.

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



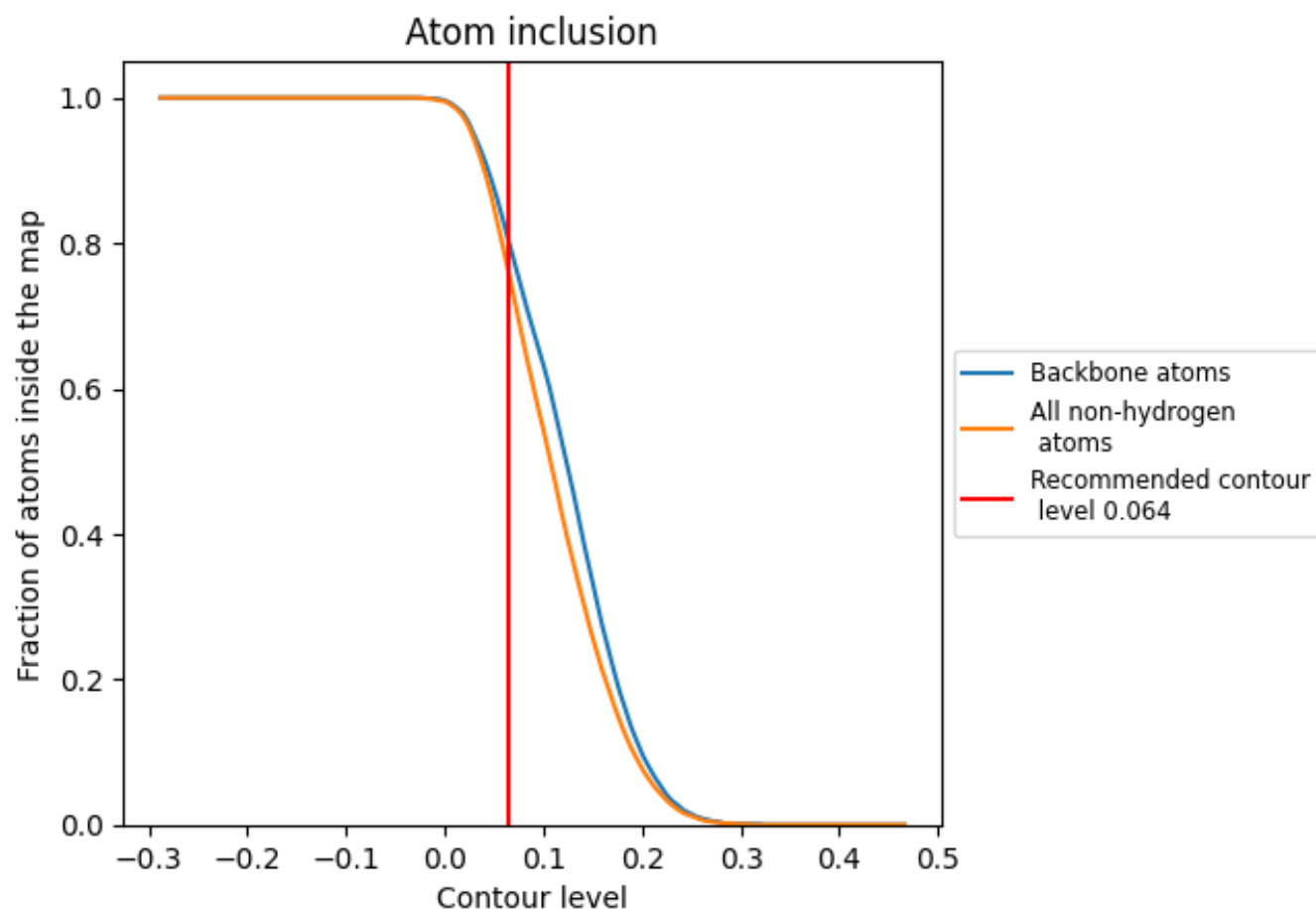
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.064).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 77% 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 (0.064) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7660	 0.5970
1	 0.7660	 0.5980
2	 0.7530	 0.5810
3	 0.6840	 0.5720
4	 0.6830	 0.5670
5	 0.6540	 0.5810
6	 0.6330	 0.5530
7	 0.5420	 0.5360
8	 0.4700	 0.5080
A	 0.7480	 0.5780
B	 0.7600	 0.5800
D	 0.8090	 0.6140
E	 0.8010	 0.6060
F	 0.7860	 0.6070
G	 0.7610	 0.5920
H	 0.7630	 0.5980
I	 0.8070	 0.6070
J	 0.8000	 0.5950
K	 0.7560	 0.6060
L	 0.8690	 0.6310
M	 0.8680	 0.6330
N	 0.7520	 0.5950
O	 0.7870	 0.6020
P	 0.7320	 0.5920
Q	 0.7220	 0.5870
R	 0.7520	 0.5770
S	 0.7760	 0.5990
T	 0.7320	 0.5640
U	 0.5910	 0.5540
V	 0.7620	 0.5940
W	 0.7540	 0.5710
X	 0.6690	 0.5750
Y	 0.7400	 0.5960
Z	 0.7530	 0.5810

