



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 07:05 AM JST

PDB ID : 7EQD / pdb_00007eqd
EMDB ID : EMD-31258
Title : STRUCTURE OF PHOTOSYNTHETIC LH1-RC SUPER-COMPLEX OF RHODOSPIRILLUM RUBRUM
Authors : Tani, K.; Kanno, R.; Ji, X.-C.; Yu, L.-J.; Hall, M.; Kimura, Y.; Madigan, M.T.; Mizoguchi, A.; Humbel, B.M.; Wang-Otomo, Z.-Y.
Deposited on : 2021-05-01
Resolution : 2.76 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:

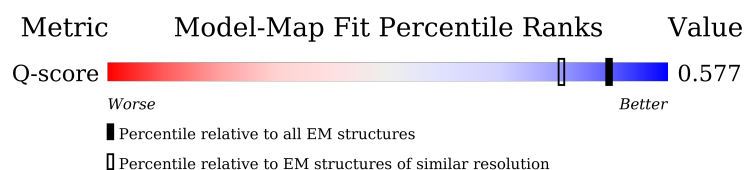
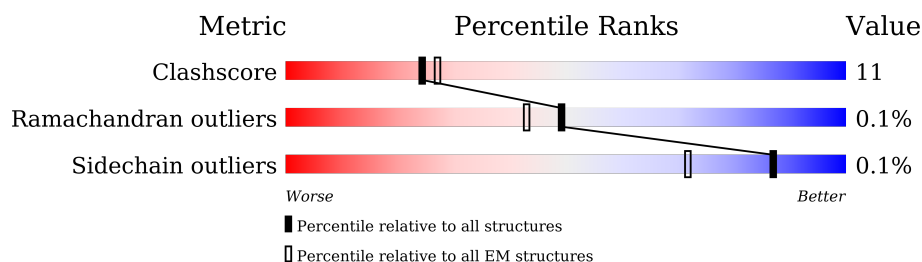
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 2.76 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	10642 (2.26 - 3.26)

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	275	
2	M	305	
3	H	256	
4	1	62	

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Mol	Chain	Length	Quality of chain
4	3	62	
4	5	62	
4	7	62	
4	9	62	
4	A	62	
4	D	62	
4	F	62	
4	I	62	
4	K	62	
4	O	62	
4	Q	62	
4	S	62	
4	U	62	
4	W	62	
4	Y	62	
5	0	55	
5	2	55	
5	4	55	
5	6	55	
5	8	55	
5	B	55	
5	E	55	
5	G	55	
5	J	55	
5	N	55	

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Mol	Chain	Length	Quality of chain
5	P	55	
5	R	55	
5	T	55	
5	V	55	
5	X	55	
5	Z	55	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	07D	0	102	X	-	-	-
6	07D	1	101	X	-	-	-
6	07D	2	102	X	-	-	-
6	07D	3	101	X	-	-	-
6	07D	4	102	X	-	-	-
6	07D	5	202	X	-	-	-
6	07D	6	102	X	-	-	-
6	07D	7	101	X	-	-	-
6	07D	8	102	X	-	-	-
6	07D	9	101	X	-	-	-
6	07D	A	101	X	-	-	-
6	07D	B	101	X	-	-	-
6	07D	D	101	X	-	-	-
6	07D	E	102	X	-	-	-
6	07D	F	101	X	-	-	-
6	07D	G	102	X	-	-	-
6	07D	I	101	X	-	-	-
6	07D	J	102	X	-	-	-
6	07D	K	101	X	-	-	-
6	07D	L	301	X	-	-	-
6	07D	M	404	X	-	-	-
6	07D	N	102	X	-	-	-
6	07D	O	101	X	-	-	-
6	07D	P	102	X	-	-	-
6	07D	Q	101	X	-	-	-
6	07D	Q	102	X	-	-	-
6	07D	S	101	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	07D	T	102	X	-	-	-
6	07D	U	101	X	-	-	-
6	07D	V	102	X	-	-	-
6	07D	W	101	X	-	-	-
6	07D	X	102	X	-	-	-
6	07D	Y	101	X	-	-	-
6	07D	Z	102	X	-	-	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 23122 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	275	Total	C	N	O	S	0	0
			2169	1458	345	356	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	304	Total	C	N	O	S	0	0
			2408	1608	396	395	9		

- Molecule 3 is a protein called Photoreaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	256	Total	C	N	O	S	0	0
			1951	1248	339	361	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	47	Total	C	N	O	S	0	0
			397	269	65	62	1		
4	D	47	Total	C	N	O	S	0	0
			397	269	65	62	1		
4	F	47	Total	C	N	O	S	0	0
			397	269	65	62	1		
4	I	47	Total	C	N	O	S	0	0
			391	266	62	62	1		
4	K	47	Total	C	N	O	S	0	0
			391	266	62	62	1		
4	O	47	Total	C	N	O	S	0	0
			387	264	61	61	1		
4	Q	47	Total	C	N	O	S	0	0
			391	266	62	62	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	47	Total	C	N	O	S	0	0
			382	258	61	62	1		
4	U	47	Total	C	N	O	S	0	0
			391	266	62	62	1		
4	W	47	Total	C	N	O	S	0	0
			397	269	65	62	1		
4	Y	47	Total	C	N	O	S	0	0
			391	266	62	62	1		
4	1	47	Total	C	N	O	S	0	0
			393	266	64	62	1		
4	3	47	Total	C	N	O	S	0	0
			393	266	64	62	1		
4	5	47	Total	C	N	O	S	0	0
			393	266	64	62	1		
4	7	47	Total	C	N	O	S	0	0
			382	258	61	62	1		
4	9	47	Total	C	N	O	S	0	0
			391	266	62	62	1		

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

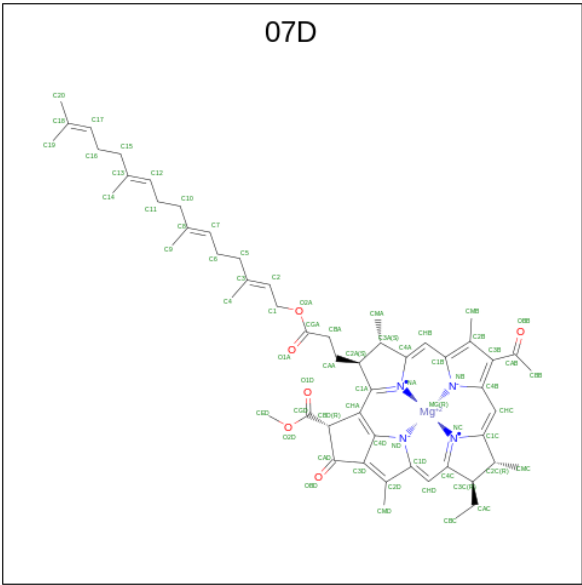
Mol	Chain	Residues	Atoms				AltConf	Trace
5	B	45	Total	C	N	O	0	0
			367	250	58	59		
5	E	44	Total	C	N	O	0	0
			351	240	57	54		
5	G	45	Total	C	N	O	0	0
			367	250	58	59		
5	J	45	Total	C	N	O	0	0
			367	250	58	59		
5	N	45	Total	C	N	O	0	0
			367	250	58	59		
5	P	44	Total	C	N	O	0	0
			359	244	57	58		
5	R	45	Total	C	N	O	0	0
			363	248	58	57		
5	T	45	Total	C	N	O	0	0
			350	239	57	54		
5	V	45	Total	C	N	O	0	0
			354	242	58	54		
5	X	45	Total	C	N	O	0	0
			362	246	58	58		

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	Z	44	Total	C	N	O	0	0
			355	242	57	56		
5	2	44	Total	C	N	O	0	0
			351	239	56	56		
5	4	45	Total	C	N	O	0	0
			350	239	57	54		
5	6	45	Total	C	N	O	0	0
			346	237	57	52		
5	8	44	Total	C	N	O	0	0
			349	239	57	53		
5	0	45	Total	C	N	O	0	0
			367	250	58	59		

- Molecule 6 is Trans-Geranyl BACTERIOCHLOROPHYLL A (CCD ID: 07D) (formula: $C_{55}H_{68}MgN_4O_6$).



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

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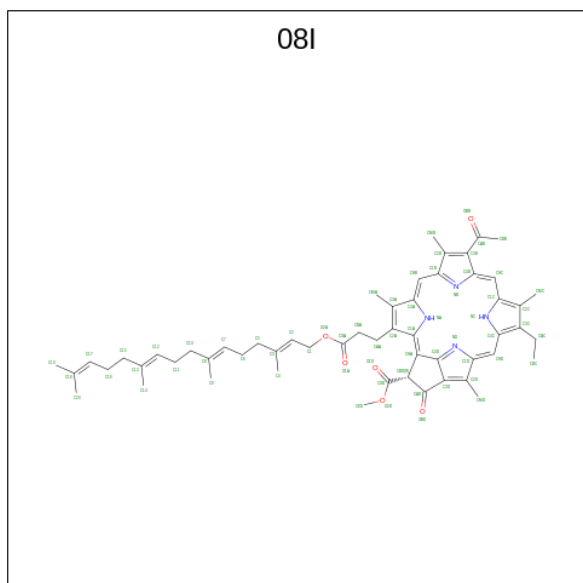
Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0

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

- Molecule 7 is Trans-Geranyl BACTERIOPHEOPHYTIN A (CCD ID: 08I) (formula: $C_{55}H_{66}N_4O_6$).



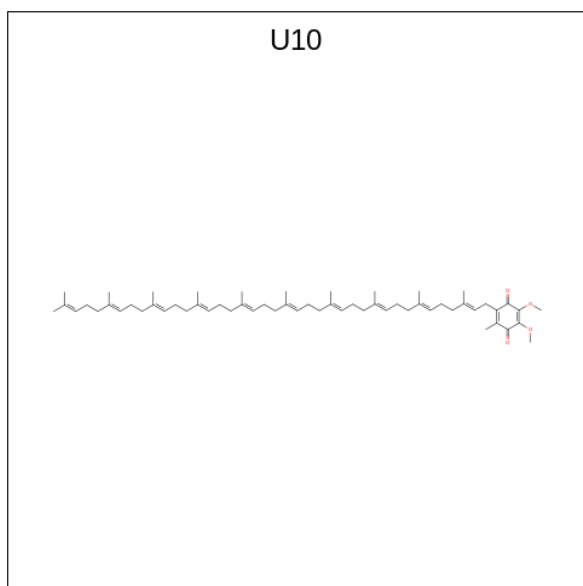
Mol	Chain	Residues	Atoms				AltConf
7	L	1	Total	C	N	O	0
			65	55	4	6	

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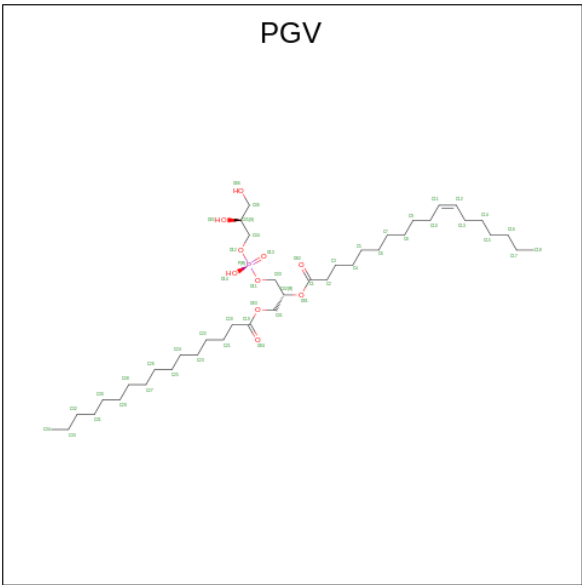
Mol	Chain	Residues	Atoms				AltConf
7	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 8 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



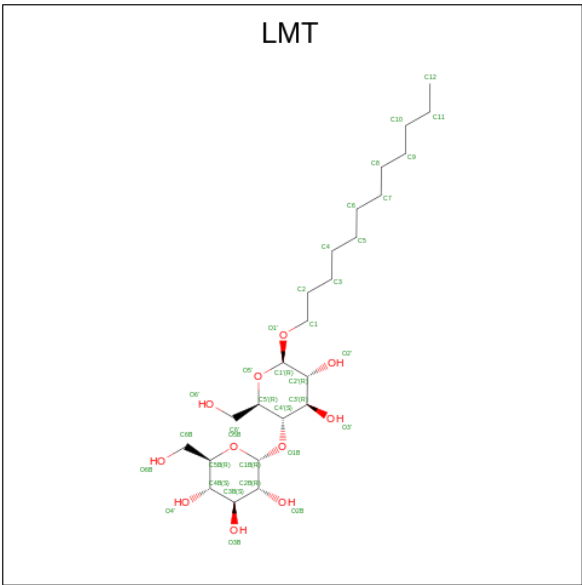
Mol	Chain	Residues	Atoms				AltConf
8	L	1	Total	C	O		0
			28	24	4		
8	M	1	Total	C	O		0
			18	14	4		

- Molecule 9 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
9	L	1	Total	C	O	P	0
			43	32	10	1	
9	H	1	Total	C	O	P	0
			36	25	10	1	

- Molecule 10 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
10	L	1	Total	C	O	0
			28	17	11	
10	L	1	Total	C	O	0
			32	21	11	

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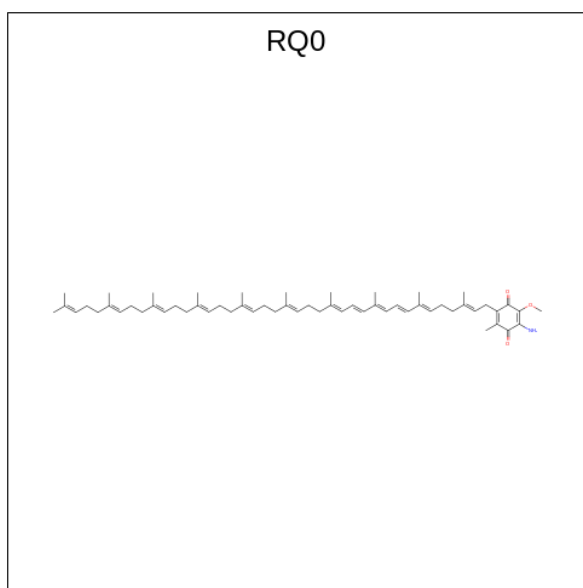
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Mol	Chain	Residues	Atoms			AltConf
10	M	1	Total	C	O	0
			35	24	11	
10	M	1	Total	C	O	0
			29	18	11	
10	H	1	Total	C	O	0
			35	24	11	
10	B	1	Total	C	O	0
			35	24	11	
10	E	1	Total	C	O	0
			35	24	11	
10	G	1	Total	C	O	0
			35	24	11	
10	J	1	Total	C	O	0
			35	24	11	
10	N	1	Total	C	O	0
			35	24	11	
10	P	1	Total	C	O	0
			35	24	11	
10	R	1	Total	C	O	0
			35	24	11	
10	T	1	Total	C	O	0
			35	24	11	
10	V	1	Total	C	O	0
			35	24	11	
10	X	1	Total	C	O	0
			35	24	11	
10	Z	1	Total	C	O	0
			35	24	11	
10	2	1	Total	C	O	0
			35	24	11	
10	4	1	Total	C	O	0
			35	24	11	
10	5	1	Total	C	O	0
			31	20	11	
10	5	1	Total	C	O	0
			35	24	11	
10	6	1	Total	C	O	0
			35	24	11	
10	8	1	Total	C	O	0
			35	24	11	
10	0	1	Total	C	O	0
			35	24	11	

- Molecule 11 is FE (III) ION (CCD ID: FE) (formula: Fe).

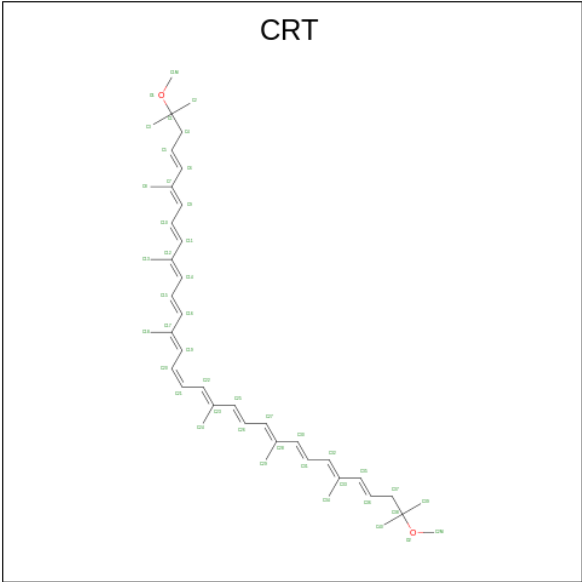
Mol	Chain	Residues	Atoms			AltConf
11	M	1	Total	Fe		0
			1	1		

- Molecule 12 is 2-azanyl-5-[(2 {E},6 {E},8 {E},10 {E},12 {E},14 {E},18 {E},22 {E},26 {E},30 {E},34 {E})-3,7,11,15,19,23,27,31,35,39-decamethyltetraconta-2,6,8,10,12,14,18,22,26,30,34,38-dodecaenyl]-3-methoxy-6-methyl-cyclohexa-2,5-diene-1,4-dione (CCD ID: RQ0) (formula: C₅₈H₈₅NO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
12	M	1	Total	C	N	O	0
			62	58	1	3	

- Molecule 13 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: C₄₂H₆₀O₂).



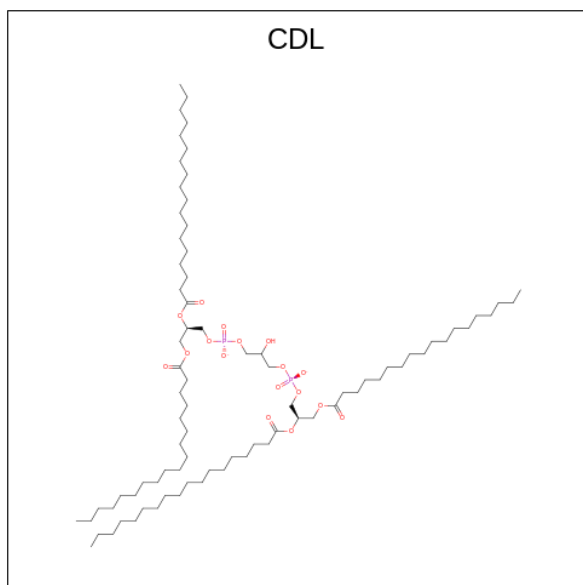
Mol	Chain	Residues	Atoms			AltConf
13	M	1	Total	C	O	0
			44	42	2	
13	A	1	Total	C	O	0
			44	42	2	
13	E	1	Total	C	O	0
			44	42	2	
13	G	1	Total	C	O	0
			44	42	2	
13	J	1	Total	C	O	0
			44	42	2	
13	N	1	Total	C	O	0
			44	42	2	
13	P	1	Total	C	O	0
			44	42	2	
13	R	1	Total	C	O	0
			44	42	2	
13	T	1	Total	C	O	0
			44	42	2	
13	V	1	Total	C	O	0
			44	42	2	
13	X	1	Total	C	O	0
			44	42	2	
13	Z	1	Total	C	O	0
			44	42	2	
13	2	1	Total	C	O	0
			44	42	2	
13	4	1	Total	C	O	0
			44	42	2	

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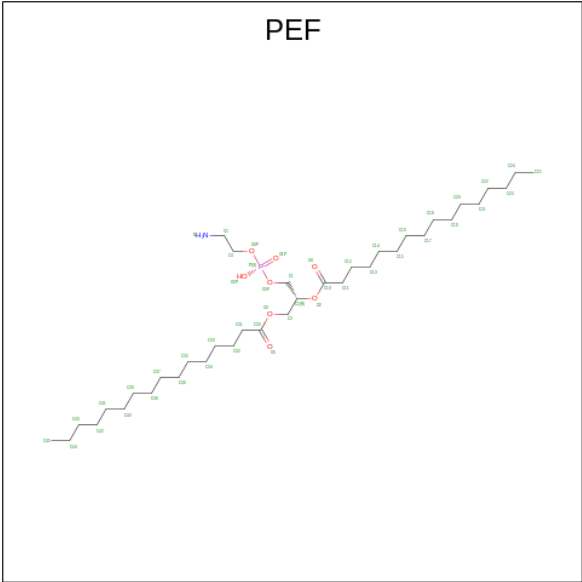
Mol	Chain	Residues	Atoms			AltConf
13	6	1	Total	C	O	0
			44	42	2	
13	8	1	Total	C	O	0
			44	42	2	
13	0	1	Total	C	O	0
			44	42	2	

- Molecule 14 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
14	M	1	Total	C	O	P	0
			68	49	17	2	
14	M	1	Total	C	O	P	0
			68	49	17	2	
14	H	1	Total	C	O	P	0
			64	45	17	2	
14	H	1	Total	C	O	P	0
			59	40	17	2	
14	H	1	Total	C	O	P	0
			33	15	16	2	

- Molecule 15 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: $C_{37}H_{74}NO_8P$).

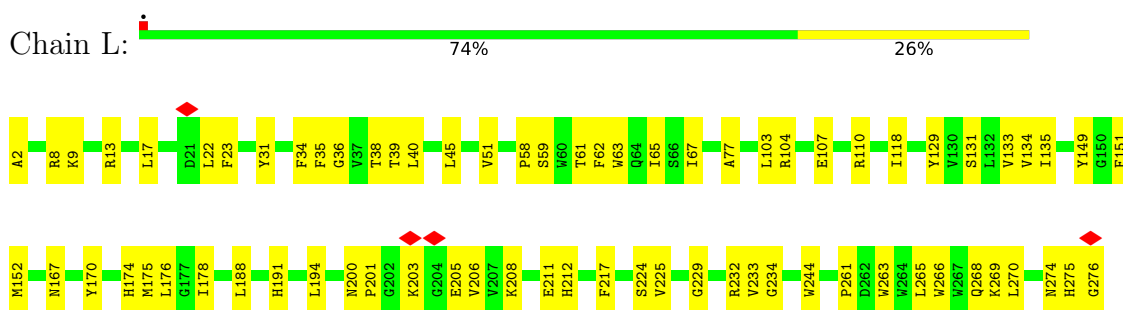


Mol	Chain	Residues	Atoms					AltConf
15	H	1	Total	C	N	O	P	0
			13	5	1	6	1	
15	K	1	Total	C	N	O	P	0
			31	21	1	8	1	
15	K	1	Total	C	N	O	P	0
			42	32	1	8	1	

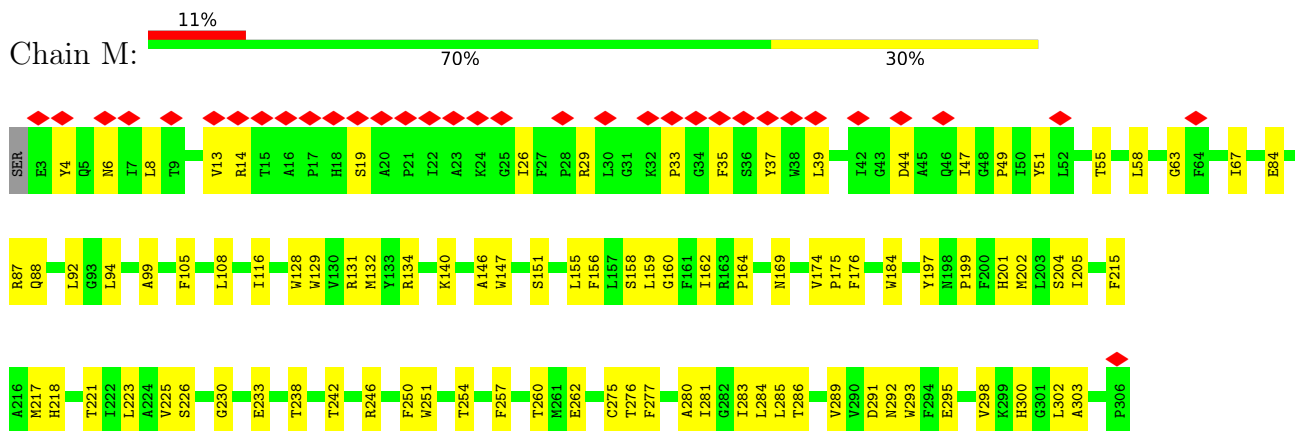
3 Residue-property plots

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

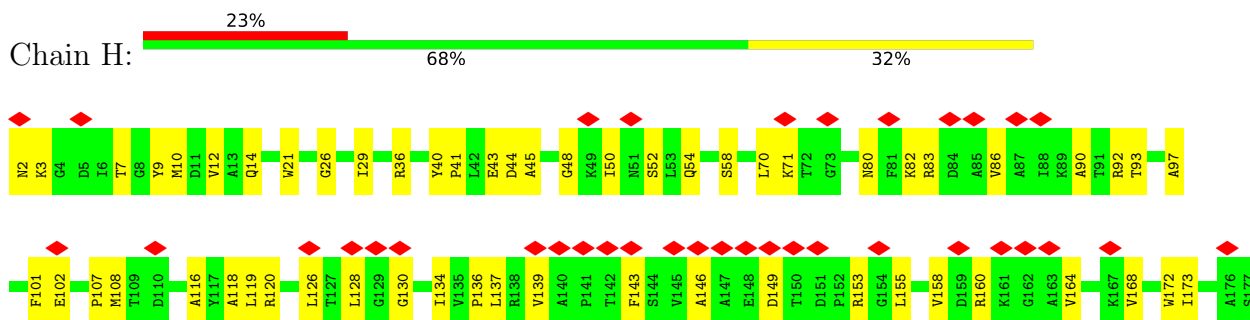
- Molecule 1: Reaction center protein L chain

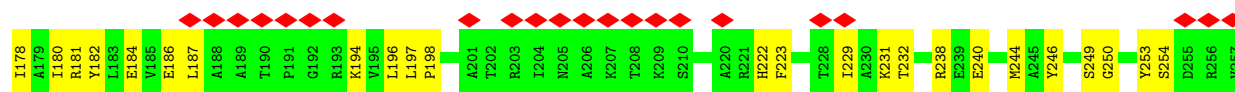


- Molecule 2: Reaction center protein M chain

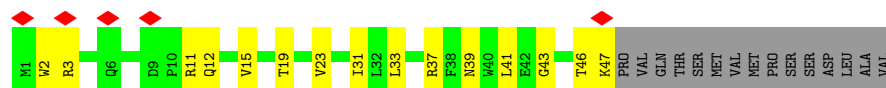


- Molecule 3: Photoreaction center protein H





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



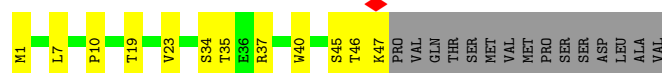
- Molecule 4: Light-harvesting protein B-870 alpha chain



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



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



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



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



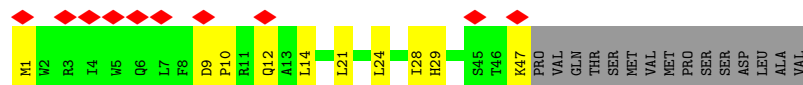
- Molecule 4: Light-harvesting protein B-870 alpha chain



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



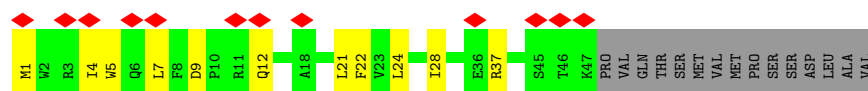
- Molecule 4: Light-harvesting protein B-870 alpha chain



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



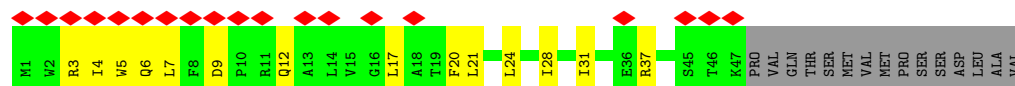
- Molecule 4: Light-harvesting protein B-870 alpha chain



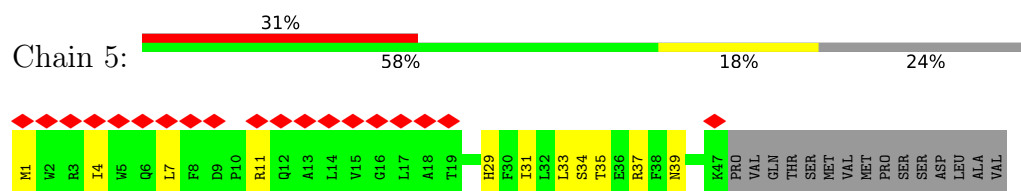
- Molecule 4: Light-harvesting protein B-870 alpha chain



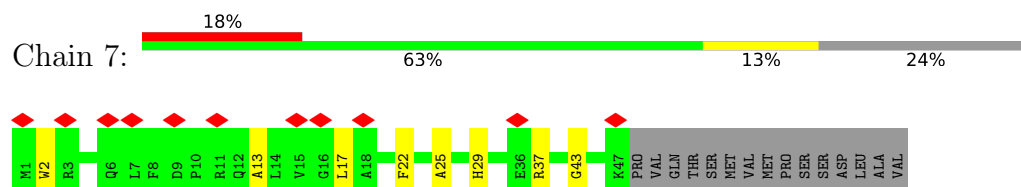
- Molecule 4: Light-harvesting protein B-870 alpha chain



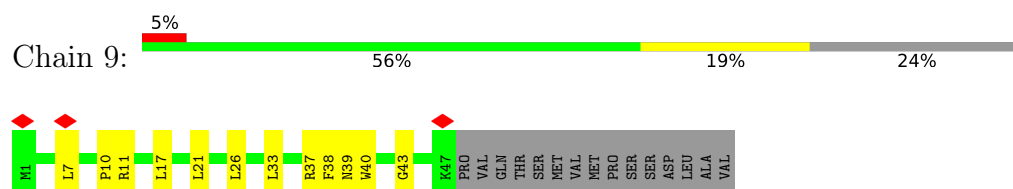
- Molecule 4: Light-harvesting protein B-870 alpha chain



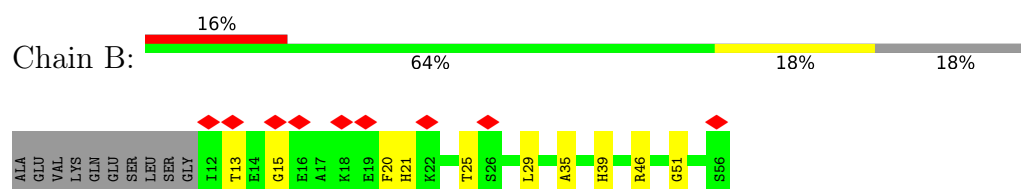
- Molecule 4: Light-harvesting protein B-870 alpha chain



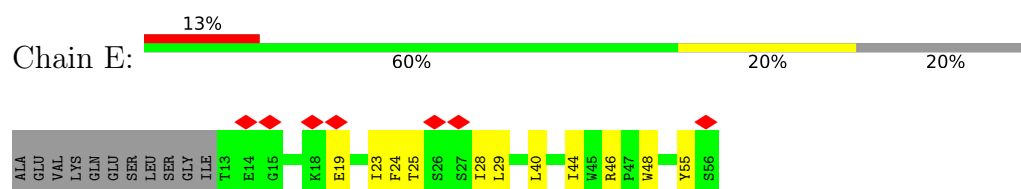
- Molecule 4: Light-harvesting protein B-870 alpha chain



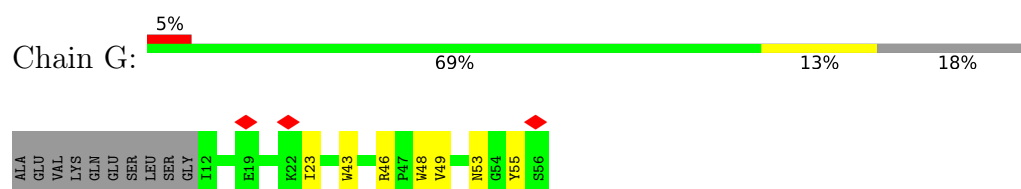
- Molecule 5: Light-harvesting protein B-870 beta chain



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

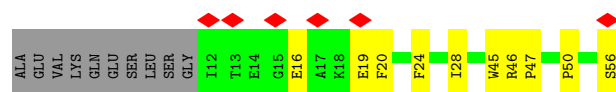


- Molecule 5: Light-harvesting protein B-870 beta chain

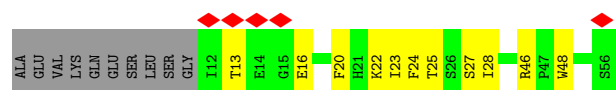


- Molecule 5: Light-harvesting protein B-870 beta chain

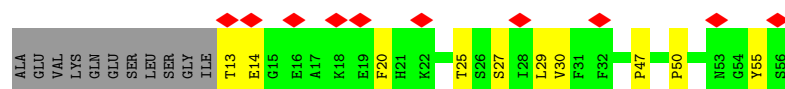




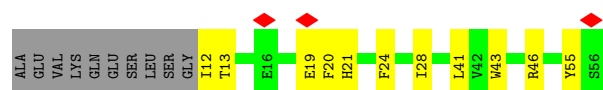
- Molecule 5: Light-harvesting protein B-870 beta chain



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



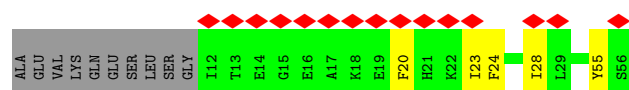
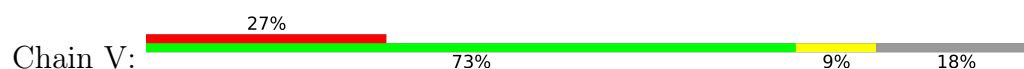
- Molecule 5: Light-harvesting protein B-870 beta chain



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



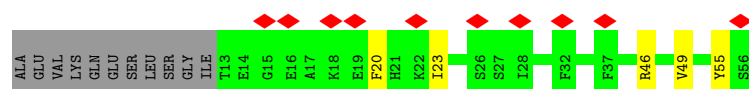
- Molecule 5: Light-harvesting protein B-870 beta chain



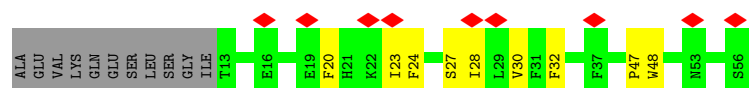
- Molecule 5: Light-harvesting protein B-870 beta chain



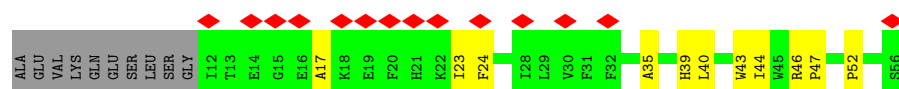
- Molecule 5: Light-harvesting protein B-870 beta chain



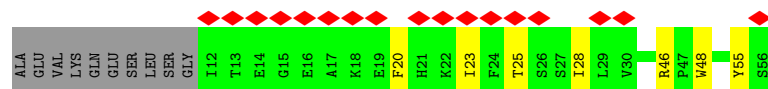
- Molecule 5: Light-harvesting protein B-870 beta chain



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



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



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	145033	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	0.238	Depositor
Minimum map value	-0.137	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.033	Depositor
Map size ($\text{\AA}$)	295.2, 295.2, 295.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82000005, 0.82000005, 0.82000005	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 07D, CRT, RQ0, FE, PGV, LMT, FME, U10, 08I, CDL, PEF

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	0.19	0/2253	0.39	0/3082
2	M	0.20	0/2499	0.35	0/3408
3	H	0.16	0/1993	0.33	0/2714
4	1	0.14	0/395	0.24	0/539
4	3	0.15	0/395	0.30	0/539
4	5	0.16	0/395	0.31	0/539
4	7	0.14	0/382	0.26	0/520
4	9	0.16	0/393	0.30	0/536
4	A	0.16	0/399	0.27	0/543
4	D	0.17	0/399	0.28	0/543
4	F	0.17	0/399	0.29	0/543
4	I	0.17	0/393	0.27	0/536
4	K	0.21	0/393	0.43	1/536 (0.2%)
4	O	0.21	0/389	0.52	1/531 (0.2%)
4	Q	0.18	0/393	0.27	0/536
4	S	0.15	0/382	0.26	0/520
4	U	0.15	0/393	0.25	0/536
4	W	0.16	0/399	0.31	0/543
4	Y	0.16	0/393	0.38	0/536
5	0	0.16	0/383	0.26	0/522
5	2	0.18	0/367	0.34	0/502
5	4	0.18	0/366	0.43	0/501
5	6	0.15	0/362	0.24	0/496
5	8	0.17	0/365	0.37	0/498
5	B	0.15	0/383	0.33	0/522
5	E	0.16	0/367	0.31	0/501
5	G	0.16	0/383	0.27	0/522
5	J	0.17	0/383	0.30	0/522
5	N	0.16	0/383	0.27	0/522
5	P	0.17	0/375	0.32	0/511
5	R	0.16	0/379	0.29	0/517
5	T	0.15	0/366	0.26	0/501

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	V	0.15	0/370	0.23	0/505
5	X	0.15	0/378	0.27	0/515
5	Z	0.16	0/371	0.33	0/506
All	All	0.17	0/19018	0.33	2/25943 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	10	PRO	CA-N-CD	-8.43	100.20	112.00
4	K	10	PRO	CA-N-CD	-6.07	103.50	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2169	0	2129	59	0
2	M	2408	0	2336	71	0
3	H	1951	0	1973	69	0
4	1	393	0	396	10	0
4	3	393	0	396	11	0
4	5	393	0	396	10	0
4	7	382	0	388	7	0
4	9	391	0	396	14	0
4	A	397	0	407	13	0
4	D	397	0	407	10	0
4	F	397	0	407	9	0
4	I	391	0	396	12	0
4	K	391	0	396	12	0
4	O	387	0	390	5	0
4	Q	391	0	396	14	0
4	S	382	0	388	6	0
4	U	391	0	396	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	W	397	0	407	11	0
4	Y	391	0	396	11	0
5	0	367	0	355	8	0
5	2	351	0	329	11	0
5	4	350	0	322	9	0
5	6	346	0	318	8	0
5	8	349	0	331	11	0
5	B	367	0	355	7	0
5	E	351	0	336	9	0
5	G	367	0	355	9	0
5	J	367	0	355	11	0
5	N	367	0	355	12	0
5	P	359	0	344	8	0
5	R	363	0	351	9	0
5	T	350	0	322	7	0
5	V	354	0	333	5	0
5	X	362	0	341	10	0
5	Z	355	0	340	6	0
6	0	66	0	0	0	0
6	1	66	0	0	0	0
6	2	66	0	0	3	0
6	3	66	0	0	0	0
6	4	66	0	0	0	0
6	5	66	0	0	0	0
6	6	66	0	0	0	0
6	7	66	0	0	1	0
6	8	66	0	0	2	0
6	9	66	0	0	0	0
6	A	66	0	0	0	0
6	B	66	0	0	0	0
6	D	66	0	0	0	0
6	E	66	0	0	1	0
6	F	66	0	0	0	0
6	G	66	0	0	1	0
6	I	66	0	0	0	0
6	J	66	0	0	0	0
6	K	66	0	0	0	0
6	L	132	0	0	0	0
6	M	132	0	0	0	0
6	N	66	0	0	1	0
6	O	66	0	0	0	0
6	P	66	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Q	132	0	0	0	0
6	S	66	0	0	0	0
6	T	66	0	0	0	0
6	U	66	0	0	0	0
6	V	66	0	0	0	0
6	W	66	0	0	0	0
6	X	66	0	0	0	0
6	Y	66	0	0	1	0
6	Z	66	0	0	0	0
7	L	65	0	0	0	0
7	M	65	0	0	0	0
8	L	28	0	31	4	0
8	M	18	0	15	1	0
9	H	36	0	42	6	0
9	L	43	0	59	4	0
10	0	35	0	46	1	0
10	2	35	0	46	1	0
10	4	35	0	46	0	0
10	5	66	0	81	4	0
10	6	35	0	46	2	0
10	8	35	0	46	1	0
10	B	35	0	46	2	0
10	E	35	0	46	2	0
10	G	35	0	46	3	0
10	H	35	0	46	5	0
10	J	35	0	46	2	0
10	L	60	0	66	0	0
10	M	64	0	77	4	0
10	N	35	0	46	0	0
10	P	35	0	46	1	0
10	R	35	0	46	2	0
10	T	35	0	46	1	0
10	V	35	0	46	0	0
10	X	35	0	46	1	0
10	Z	35	0	46	2	0
11	M	1	0	0	0	0
12	M	62	0	0	0	0
13	0	44	0	60	5	0
13	2	44	0	60	9	0
13	4	44	0	60	8	0
13	6	44	0	60	7	0
13	8	44	0	60	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	A	44	0	60	3	0
13	E	44	0	60	7	0
13	G	44	0	60	6	0
13	J	44	0	60	8	0
13	M	44	0	60	6	0
13	N	44	0	60	9	0
13	P	44	0	60	4	0
13	R	44	0	60	6	0
13	T	44	0	60	4	0
13	V	44	0	60	6	0
13	X	44	0	60	8	0
13	Z	44	0	60	7	0
14	H	156	0	155	8	0
14	M	136	0	160	7	0
15	H	13	0	11	3	0
15	K	73	0	95	5	0
All	All	23122	0	20832	469	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (469) 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)
3:H:172:TRP:HB2	3:H:182:TYR:HB2	1.59	0.84
5:Z:23:ILE:HD11	13:Z:101:CRT:H6	1.57	0.84
5:2:23:ILE:HD11	13:2:101:CRT:H6	1.64	0.78
4:9:37:ARG:NH1	5:0:47:PRO:O	2.16	0.77
4:I:37:ARG:NH1	5:J:47:PRO:O	2.18	0.76
1:L:188:LEU:HD13	2:M:215:PHE:HB2	1.68	0.75
2:M:51:TYR:O	2:M:131:ARG:NH2	2.19	0.75
13:A:102:CRT:H82	4:9:7:LEU:HD12	1.70	0.73
3:H:7:THR:HG22	3:H:10:MET:HE2	1.70	0.72
2:M:6:ASN:ND2	2:M:226:SER:OG	2.23	0.72
1:L:2:ALA:N	3:H:43:GLU:O	2.23	0.71
1:L:201:PRO:HB2	1:L:205:GLU:HB3	1.72	0.71
5:X:23:ILE:HD11	13:X:101:CRT:H6	1.72	0.70
4:O:37:ARG:NH1	5:P:47:PRO:O	2.24	0.70
2:M:134:ARG:NH2	10:M:410:LMT:O2B	2.24	0.69
3:H:54:GLN:HE21	15:H:305:PEF:H52	1.55	0.69
3:H:158:VAL:HG12	3:H:164:VAL:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:63:TRP:CH2	9:H:302:PGV:H012	2.27	0.69
4:3:31:ILE:HG12	10:5:201:LMT:H32	1.76	0.68
3:H:54:GLN:HG2	3:H:58:SER:HB3	1.75	0.68
4:W:33:LEU:O	4:W:39:ASN:ND2	2.27	0.68
4:Y:9:ASP:OD2	4:Y:12:GLN:NE2	2.27	0.67
4:7:37:ARG:NH1	5:8:47:PRO:O	2.25	0.66
4:Q:33:LEU:O	4:Q:39:ASN:ND2	2.30	0.65
4:5:33:LEU:O	4:5:39:ASN:ND2	2.29	0.65
1:L:200:ASN:HB3	14:M:408:CDL:HB22	1.77	0.65
1:L:23:PHE:HD1	1:L:34:PHE:HA	1.62	0.65
4:9:37:ARG:O	5:0:46:ARG:NH1	2.30	0.65
5:2:20:PHE:HB2	13:2:101:CRT:H23	1.78	0.65
14:M:408:CDL:H771	3:H:26:GLY:HA3	1.78	0.64
3:H:41:PRO:HG2	3:H:50:ILE:HD12	1.79	0.64
4:O:14:LEU:HD22	13:P:101:CRT:H81	1.79	0.64
3:H:173:ILE:HG22	3:H:180:ILE:HA	1.79	0.64
4:D:33:LEU:O	4:D:39:ASN:ND2	2.30	0.64
2:M:129:TRP:NE1	2:M:146:ALA:O	2.31	0.64
3:H:58:SER:OG	4:D:12:GLN:NE2	2.31	0.63
4:F:33:LEU:O	4:F:39:ASN:ND2	2.32	0.62
10:J:103:LMT:H6'	10:J:103:LMT:H2O1	1.47	0.62
4:I:7:LEU:HD22	4:K:11:ARG:HB2	1.80	0.62
5:J:20:PHE:HA	13:J:101:CRT:H6	1.80	0.62
5:G:43:TRP:HZ2	10:G:103:LMT:H2'	1.65	0.62
5:2:24:PHE:O	5:2:28:ILE:HG12	1.99	0.62
4:K:33:LEU:O	4:K:39:ASN:ND2	2.29	0.61
1:L:191:HIS:ND1	8:L:303:U10:O2	2.27	0.61
4:Q:17:LEU:HD11	13:R:101:CRT:H243	1.82	0.61
5:Z:49:VAL:HG21	10:Z:103:LMT:H21	1.83	0.61
1:L:131:SER:HA	1:L:135:ILE:HB	1.83	0.61
5:R:19:GLU:HB2	13:R:101:CRT:H21A	1.83	0.60
5:V:23:ILE:HG21	13:V:101:CRT:H6	1.82	0.60
3:H:52:SER:HB2	14:H:303:CDL:HA22	1.82	0.60
2:M:238:THR:HG21	3:H:70:LEU:HD11	1.83	0.60
3:H:80:ASN:HD22	3:H:82:LYS:HD3	1.67	0.60
3:H:134:ILE:HD12	3:H:181:ARG:HG3	1.83	0.60
5:R:24:PHE:O	5:R:28:ILE:HG12	2.02	0.60
13:Z:101:CRT:H372	4:1:29:HIS:CG	2.37	0.60
2:M:55:THR:HG22	10:M:410:LMT:H6'2	1.84	0.59
5:R:55:TYR:OH	4:S:40:TRP:O	2.18	0.59
4:K:10:PRO:HB3	5:N:20:PHE:CE1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:37:ARG:O	5:X:46:ARG:NH1	2.36	0.58
4:5:37:ARG:O	5:6:46:ARG:NH1	2.36	0.58
3:H:14:GLN:NE2	9:H:302:PGV:O13	2.36	0.58
2:M:291:ASP:OD1	3:H:3:LYS:NZ	2.33	0.58
3:H:44:ASP:HB3	3:H:48:GLY:H	1.68	0.58
2:M:204:SER:OG	2:M:275:CYS:O	2.18	0.58
4:D:9:ASP:HB3	4:D:12:GLN:HG3	1.83	0.58
3:H:137:LEU:HD13	3:H:153:ARG:HH21	1.67	0.58
5:N:13:THR:HB	5:N:16:GLU:HG2	1.84	0.58
2:M:58:LEU:HD23	4:Q:19:THR:HG23	1.84	0.58
4:K:39:ASN:HD21	15:K:102:PEF:H52	1.68	0.58
5:J:16:GLU:HB2	13:J:101:CRT:H31A	1.86	0.57
2:M:37:TYR:OH	3:H:149:ASP:OD1	2.19	0.57
2:M:108:LEU:HD11	4:Q:31:ILE:HG23	1.85	0.57
4:A:12:GLN:HA	4:A:15:VAL:HG12	1.87	0.57
2:M:286:THR:HB	2:M:293:TRP:HE1	1.70	0.57
5:E:48:TRP:HZ2	10:E:103:LMT:H71	1.69	0.57
1:L:31:TYR:O	1:L:104:ARG:NH1	2.36	0.57
1:L:174:HIS:CE1	1:L:178:ILE:HD11	2.40	0.56
5:T:43:TRP:HZ2	10:T:103:LMT:H2'	1.70	0.56
4:3:9:ASP:HB3	4:3:12:GLN:HB3	1.86	0.56
4:3:37:ARG:O	5:4:46:ARG:NH1	2.38	0.56
1:L:225:VAL:O	2:M:44:ASP:N	2.35	0.56
13:A:102:CRT:H21A	5:B:20:PHE:HB2	1.86	0.56
4:U:12:GLN:HE22	4:W:11:ARG:HH22	1.52	0.56
5:0:24:PHE:O	5:0:28:ILE:HG12	2.06	0.56
2:M:128:TRP:O	2:M:132:MET:HG2	2.06	0.56
10:H:306:LMT:O2'	15:K:102:PEF:O4	2.23	0.56
2:M:284:LEU:HD13	15:K:102:PEF:H352	1.86	0.56
4:A:37:ARG:O	5:B:46:ARG:NH1	2.39	0.56
4:S:37:ARG:HH12	4:S:46:THR:HG23	1.71	0.55
5:X:19:GLU:HG3	5:X:22:LYS:HE3	1.87	0.55
5:0:19:GLU:HA	5:0:22:LYS:HD3	1.88	0.55
1:L:203:LYS:O	1:L:205:GLU:HG2	2.06	0.55
4:3:4:ILE:HG23	13:6:101:CRT:H83	1.88	0.55
5:6:48:TRP:HZ2	10:6:103:LMT:H82	1.71	0.55
4:1:1:FME:HA	4:1:4:ILE:HD11	1.89	0.55
1:L:170:TYR:HA	1:L:175:MET:HE3	1.88	0.55
4:W:3:ARG:HD2	4:W:6:GLN:HE22	1.72	0.55
1:L:275:HIS:H	2:M:87:ARG:NH2	2.04	0.55
5:X:24:PHE:O	5:X:28:ILE:HG13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:251:TRP:HA	2:M:254:THR:HG22	1.89	0.55
3:H:182:TYR:HD1	3:H:198:PRO:HA	1.71	0.55
4:5:1:FME:SD	4:5:1:FME:N	2.80	0.55
5:X:24:PHE:CZ	5:X:28:ILE:HD11	2.42	0.54
1:L:133:VAL:HG23	1:L:134:VAL:HG23	1.89	0.54
4:W:14:LEU:HD21	5:X:20:PHE:HZ	1.72	0.54
4:1:9:ASP:HB3	4:1:12:GLN:HG2	1.88	0.54
2:M:39:LEU:HD12	2:M:47:ILE:HD11	1.89	0.54
1:L:188:LEU:HD13	2:M:215:PHE:CB	2.38	0.54
3:H:108:MET:HE1	3:H:250:GLY:HA2	1.89	0.54
5:V:24:PHE:O	5:V:28:ILE:HG12	2.08	0.54
5:4:23:ILE:HG21	13:4:101:CRT:H9	1.89	0.53
1:L:268:GLN:NE2	2:M:87:ARG:O	2.41	0.53
10:H:306:LMT:O2'	15:K:102:PEF:N	2.36	0.53
4:K:15:VAL:O	4:K:19:THR:HG23	2.07	0.53
1:L:274:ASN:HA	2:M:87:ARG:HH21	1.72	0.53
5:G:49:VAL:HG21	10:G:103:LMT:H31	1.90	0.53
4:Q:7:LEU:HD12	13:T:101:CRT:H82	1.91	0.53
5:4:40:LEU:O	5:4:44:ILE:HG12	2.08	0.53
5:X:20:PHE:HB2	13:X:101:CRT:H23	1.90	0.53
5:T:24:PHE:O	5:T:28:ILE:HG12	2.08	0.53
4:U:10:PRO:HB3	5:V:20:PHE:CZ	2.42	0.53
3:H:93:THR:HG22	3:H:102:GLU:HG2	1.91	0.53
5:P:50:PRO:HA	10:P:103:LMT:H6'1	1.91	0.53
4:W:3:ARG:HB3	13:Z:101:CRT:H21A	1.91	0.52
4:3:7:LEU:HD21	4:5:11:ARG:HB3	1.91	0.52
3:H:120:ARG:O	3:H:238:ARG:NH1	2.43	0.52
4:I:19:THR:O	4:I:23:VAL:HG23	2.09	0.52
5:8:55:TYR:OH	4:9:40:TRP:O	2.25	0.52
1:L:17:LEU:HD23	1:L:110:ARG:HH11	1.75	0.52
4:D:37:ARG:O	5:E:46:ARG:NH1	2.42	0.52
5:G:53:ASN:O	4:I:45:SER:OG	2.27	0.52
2:M:242:THR:HB	3:H:118:ALA:H	1.74	0.52
4:I:7:LEU:HD12	13:N:101:CRT:H82	1.91	0.52
1:L:104:ARG:NH2	2:M:254:THR:O	2.42	0.52
4:Q:32:LEU:O	4:Q:35:THR:OG1	2.26	0.52
5:Z:55:TYR:OH	4:1:40:TRP:O	2.26	0.52
4:3:20:PHE:HD2	4:3:21:LEU:HD22	1.75	0.52
1:L:103:LEU:O	1:L:107:GLU:HG3	2.10	0.51
4:W:10:PRO:HG2	13:X:101:CRT:H1M1	1.93	0.51
1:L:67:ILE:HB	1:L:149:TYR:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:4:ILE:HA	13:8:101:CRT:H83	1.92	0.51
1:L:13:ARG:HD3	3:H:102:GLU:OE2	2.11	0.51
4:I:47:LYS:NZ	5:J:56:SER:HB2	2.25	0.51
4:K:35:THR:HG21	4:O:41:LEU:HB3	1.93	0.51
4:9:10:PRO:HB3	5:0:20:PHE:CZ	2.46	0.51
4:1:37:ARG:NH2	5:2:47:PRO:O	2.39	0.51
5:8:23:ILE:HG21	13:8:101:CRT:H6	1.92	0.51
2:M:260:THR:HG22	2:M:262:GLU:H	1.76	0.51
2:M:285:LEU:HD12	10:M:411:LMT:H32	1.91	0.51
4:I:46:THR:HG23	5:J:46:ARG:HH21	1.75	0.51
2:M:4:TYR:OH	2:M:8:LEU:O	2.20	0.51
4:A:33:LEU:O	4:A:39:ASN:ND2	2.44	0.51
5:N:48:TRP:NE1	6:N:102:07D:OBB	2.43	0.51
4:Y:9:ASP:OD1	4:Y:9:ASP:N	2.44	0.51
5:J:45:TRP:CZ2	5:J:46:ARG:HD2	2.46	0.51
4:1:32:LEU:O	4:1:35:THR:OG1	2.25	0.51
1:L:36:GLY:O	1:L:40:LEU:HG	2.11	0.50
5:B:13:THR:HG22	5:B:15:GLY:H	1.76	0.50
5:N:23:ILE:HG13	13:N:101:CRT:H9	1.93	0.50
4:5:34:SER:O	10:5:203:LMT:O6B	2.21	0.50
5:2:27:SER:HA	5:2:30:VAL:HG12	1.92	0.50
4:3:5:TRP:HB2	5:4:17:ALA:HB1	1.92	0.50
5:4:24:PHE:CD1	13:4:101:CRT:H16	2.46	0.50
5:X:48:TRP:HZ2	10:X:103:LMT:H61	1.75	0.50
4:Y:5:TRP:CD2	5:Z:20:PHE:HE2	2.30	0.50
2:M:202:MET:HE1	2:M:302:LEU:HD13	1.93	0.50
3:H:182:TYR:OH	3:H:240:GLU:HB2	2.11	0.50
5:B:51:GLY:HA3	10:B:102:LMT:H6'1	1.93	0.50
5:G:23:ILE:CG2	13:G:101:CRT:H9	2.42	0.50
5:6:20:PHE:HB2	13:6:101:CRT:H31A	1.92	0.50
1:L:9:LYS:HE3	3:H:116:ALA:HB1	1.93	0.50
4:K:3:ARG:O	4:K:6:GLN:HB2	2.11	0.50
5:P:55:TYR:CD2	4:Q:43:GLY:HA3	2.47	0.50
5:6:23:ILE:HD12	13:6:101:CRT:H9	1.94	0.50
5:6:25:THR:HA	5:6:28:ILE:HG22	1.93	0.50
1:L:265:LEU:O	1:L:269:LYS:HG2	2.12	0.50
3:H:21:TRP:NE1	9:H:302:PGV:H201	2.26	0.50
5:P:20:PHE:HE1	13:P:101:CRT:H82	1.77	0.50
4:D:21:LEU:HD21	13:E:101:CRT:H22	1.94	0.50
2:M:14:ARG:HE	2:M:35:PHE:HB3	1.77	0.49
1:L:62:PHE:HA	1:L:65:ILE:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:37:ARG:O	5:Z:46:ARG:NH1	2.45	0.49
1:L:45:LEU:HD11	4:9:26:LEU:HD23	1.94	0.49
4:A:3:ARG:HB3	13:E:101:CRT:H31A	1.94	0.49
2:M:147:TRP:CZ2	14:M:408:CDL:H111	2.47	0.49
13:6:101:CRT:H35	6:7:101:07D:CHB	2.42	0.49
5:R:20:PHE:HB2	13:R:101:CRT:H23	1.93	0.49
5:G:48:TRP:NE1	6:G:102:07D:OBB	2.43	0.49
5:Z:23:ILE:HD11	13:Z:101:CRT:C6	2.36	0.49
10:M:410:LMT:H121	4:Q:22:PHE:HZ	1.76	0.49
1:L:152:MET:HE2	2:M:197:TYR:CE2	2.47	0.49
4:D:32:LEU:O	4:D:35:THR:OG1	2.31	0.49
2:M:158:SER:HA	2:M:162:ILE:HB	1.95	0.49
4:A:2:TRP:HB3	5:B:21:HIS:CD2	2.48	0.49
13:A:102:CRT:H372	4:D:29:HIS:CG	2.48	0.49
1:L:63:TRP:HA	1:L:151:PHE:HB3	1.94	0.49
3:H:136:PRO:HG2	3:H:139:VAL:HG22	1.95	0.49
5:8:23:ILE:HG23	13:8:101:CRT:H9	1.94	0.49
1:L:36:GLY:HA2	1:L:39:THR:HG22	1.95	0.48
4:D:7:LEU:HD21	4:F:10:PRO:HB2	1.95	0.48
5:E:25:THR:HA	5:E:28:ILE:HG22	1.95	0.48
5:8:23:ILE:CG2	13:8:101:CRT:H9	2.42	0.48
1:L:232:ARG:HG2	2:M:223:LEU:HD21	1.93	0.48
2:M:225:VAL:HG23	2:M:230:GLY:HA3	1.96	0.48
4:Y:4:ILE:HA	13:2:101:CRT:H83	1.95	0.48
5:E:23:ILE:HB	13:E:101:CRT:H6	1.95	0.48
4:9:33:LEU:O	4:9:39:ASN:ND2	2.47	0.48
2:M:94:LEU:HB3	2:M:176:PHE:HB2	1.95	0.48
2:M:199:PRO:HA	2:M:202:MET:HE3	1.96	0.48
4:7:37:ARG:O	5:8:46:ARG:NH1	2.45	0.48
2:M:199:PRO:HB3	9:H:302:PGV:H22	1.96	0.48
3:H:36:ARG:HG2	3:H:40:TYR:CZ	2.48	0.48
13:V:101:CRT:H372	4:W:29:HIS:CG	2.49	0.48
4:U:21:LEU:HD11	13:V:101:CRT:H20	1.96	0.48
3:H:108:MET:SD	3:H:249:SER:OG	2.66	0.48
4:S:37:ARG:O	5:T:46:ARG:NH1	2.46	0.48
2:M:63:GLY:O	2:M:67:ILE:HG12	2.14	0.48
3:H:108:MET:HB3	3:H:246:TYR:CE1	2.49	0.48
1:L:22:LEU:HA	4:9:11:ARG:NH2	2.29	0.47
5:N:23:ILE:HD11	13:N:101:CRT:C6	2.43	0.47
13:2:101:CRT:H25	6:2:102:07D:O1A	2.14	0.47
1:L:208:LYS:HD2	1:L:212:HIS:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:211:GLU:HG3	3:H:128:LEU:HD22	1.96	0.47
3:H:197:LEU:HD12	3:H:223:PHE:HE2	1.79	0.47
5:2:32:PHE:HE1	6:2:102:07D:CGA	2.27	0.47
13:2:101:CRT:H20	13:2:101:CRT:H181	1.78	0.47
2:M:292:ASN:OD1	2:M:295:GLU:HG2	2.13	0.47
3:H:187:LEU:HD11	3:H:223:PHE:HB3	1.96	0.47
4:Y:1:FME:HE3	4:Y:1:FME:HB2	1.63	0.47
13:6:101:CRT:H343	4:7:22:PHE:CE1	2.49	0.47
2:M:13:VAL:HB	3:H:178:ILE:HG22	1.97	0.47
4:D:20:PHE:HD2	4:D:21:LEU:HD12	1.78	0.47
2:M:88:GLN:O	2:M:92:LEU:HG	2.14	0.47
13:M:407:CRT:H181	13:M:407:CRT:H20	1.75	0.47
3:H:155:LEU:O	3:H:168:VAL:HG12	2.15	0.47
4:A:3:ARG:HE	13:E:101:CRT:H31A	1.79	0.47
15:K:103:PEF:H312	4:O:30:PHE:HD1	1.80	0.47
5:8:50:PRO:HG3	4:9:43:GLY:HA2	1.97	0.47
5:0:49:VAL:HG21	10:0:103:LMT:H11	1.97	0.47
3:H:196:LEU:HD11	3:H:229:ILE:HD13	1.97	0.47
4:A:41:LEU:HA	4:9:38:PHE:HE2	1.80	0.47
4:U:9:ASP:N	4:U:9:ASP:OD1	2.45	0.47
5:6:20:PHE:CD2	13:6:101:CRT:H21A	2.50	0.47
1:L:266:TRP:O	1:L:270:LEU:HD12	2.14	0.47
5:6:25:THR:O	5:6:28:ILE:HG22	2.15	0.47
4:9:17:LEU:HD11	13:0:101:CRT:H243	1.96	0.47
5:4:35:ALA:O	5:4:39:HIS:ND1	2.45	0.47
4:K:21:LEU:HD11	13:N:101:CRT:H22	1.96	0.46
3:H:186:GLU:HB2	3:H:194:LYS:HE2	1.97	0.46
3:H:250:GLY:O	3:H:254:SER:HB2	2.15	0.46
14:H:303:CDL:H331	15:H:305:PEF:H31	1.96	0.46
13:4:101:CRT:H372	4:5:29:HIS:CG	2.50	0.46
5:J:24:PHE:CD2	13:J:101:CRT:H14	2.49	0.46
13:Z:101:CRT:H5	13:Z:101:CRT:H23	1.64	0.46
3:H:231:LYS:O	3:H:232:THR:OG1	2.29	0.46
4:F:3:ARG:NE	5:J:19:GLU:OE2	2.49	0.46
10:6:103:LMT:H1B	10:6:103:LMT:H3'	1.62	0.46
5:6:55:TYR:CE2	4:7:43:GLY:HA3	2.51	0.46
5:4:43:TRP:CE2	5:4:47:PRO:HB3	2.51	0.46
2:M:160:GLY:O	2:M:164:PRO:HG2	2.16	0.46
2:M:246:ARG:NH2	3:H:116:ALA:O	2.48	0.46
13:P:101:CRT:H20	13:P:101:CRT:H181	1.79	0.46
2:M:14:ARG:HH11	3:H:146:ALA:HB1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:116:ILE:HG12	4:Q:30:PHE:HB3	1.98	0.46
3:H:90:ALA:HB1	3:H:101:PHE:HB3	1.97	0.46
5:E:55:TYR:OH	4:F:40:TRP:O	2.34	0.45
4:Q:37:ARG:O	5:R:46:ARG:NH1	2.45	0.45
5:R:12:ILE:HG23	5:R:13:THR:HG23	1.98	0.45
2:M:99:ALA:HB1	2:M:169:ASN:HD21	1.81	0.45
10:E:103:LMT:H5B	10:E:103:LMT:H6E	1.99	0.45
5:J:24:PHE:O	5:J:28:ILE:HG22	2.16	0.45
1:L:206:VAL:HG21	3:H:71:LYS:HB3	1.98	0.45
14:M:409:CDL:H761	14:M:409:CDL:H131	1.97	0.45
5:2:23:ILE:HD11	13:2:101:CRT:C6	2.40	0.45
1:L:176:LEU:HD23	1:L:244:TRP:CE2	2.52	0.45
1:L:35:PHE:HA	1:L:38:THR:OG1	2.17	0.45
5:N:23:ILE:HD11	13:N:101:CRT:H6	1.98	0.45
1:L:22:LEU:HA	4:9:11:ARG:HH21	1.82	0.45
2:M:19:SER:OG	2:M:29:ARG:NH1	2.50	0.45
1:L:263:TRP:O	1:L:266:TRP:HD1	2.00	0.45
2:M:289:VAL:HG11	3:H:12:VAL:HB	1.99	0.45
3:H:45:ALA:HB3	3:H:97:ALA:HB1	1.99	0.45
4:I:35:THR:HG21	4:K:41:LEU:HB3	1.99	0.45
1:L:63:TRP:CD1	1:L:151:PHE:CD2	3.05	0.45
2:M:33:PRO:HG3	2:M:49:PRO:HD3	1.99	0.44
5:N:22:LYS:HB2	5:N:22:LYS:HE2	1.72	0.44
4:S:27:LEU:O	4:S:31:ILE:HG13	2.17	0.44
5:T:53:ASN:OD1	4:U:47:LYS:NZ	2.43	0.44
10:2:103:LMT:H52	10:2:103:LMT:H21	1.86	0.44
2:M:257:PHE:HB3	14:H:303:CDL:HB4	1.99	0.44
3:H:7:THR:HG23	3:H:7:THR:O	2.17	0.44
3:H:29:ILE:HG12	14:H:304:CDL:H1	1.98	0.44
3:H:40:TYR:OH	14:H:303:CDL:OB3	2.24	0.44
5:E:40:LEU:O	5:E:44:ILE:HG12	2.16	0.44
4:1:7:LEU:HD21	13:4:101:CRT:H1M1	1.99	0.44
1:L:229:GLY:O	1:L:233:VAL:HG13	2.17	0.44
5:G:55:TYR:OH	4:I:40:TRP:O	2.35	0.44
4:3:3:ARG:HA	4:3:6:GLN:HG2	2.00	0.44
14:M:408:CDL:HA62	14:M:408:CDL:H511	1.98	0.44
3:H:3:LYS:O	10:H:306:LMT:O6'	2.18	0.44
5:G:43:TRP:CZ2	10:G:103:LMT:H2'	2.50	0.44
13:J:101:CRT:H20	13:J:101:CRT:H181	1.84	0.44
5:T:30:VAL:O	5:T:34:VAL:HG23	2.16	0.44
4:W:12:GLN:HA	4:W:15:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:101:CRT:H372	4:1:29:HIS:CD2	2.51	0.44
1:L:224:SER:OG	8:L:303:U10:H4M2	2.18	0.44
2:M:159:LEU:HD23	2:M:283:ILE:HG21	2.00	0.44
13:J:101:CRT:H10	13:J:101:CRT:H81	1.90	0.44
13:X:101:CRT:H342	6:Y:101:07D:O1A	2.17	0.44
13:X:101:CRT:H343	4:Y:22:PHE:CE1	2.53	0.44
5:8:20:PHE:HB2	13:8:101:CRT:H23	1.99	0.44
13:8:101:CRT:H25	6:8:102:07D:O1A	2.17	0.44
3:H:184:GLU:HG2	3:H:194:LYS:HD2	2.00	0.44
13:X:101:CRT:H10	13:X:101:CRT:H81	1.74	0.44
13:0:101:CRT:H15	13:0:101:CRT:H131	1.86	0.44
5:T:27:SER:HA	5:T:30:VAL:HG22	1.99	0.44
13:T:101:CRT:H372	4:U:29:HIS:CD2	2.53	0.44
2:M:156:PHE:CZ	13:M:407:CRT:H293	2.51	0.44
4:F:9:ASP:HB3	4:F:12:GLN:HG2	2.00	0.44
13:J:101:CRT:H372	4:K:29:HIS:CG	2.52	0.43
4:S:10:PRO:HB3	5:T:20:PHE:CZ	2.52	0.43
5:8:27:SER:HA	5:8:30:VAL:HG12	2.00	0.43
3:H:143:PHE:HE2	3:H:178:ILE:HG23	1.83	0.43
4:F:17:LEU:HD11	13:G:101:CRT:H243	1.99	0.43
4:I:10:PRO:HB3	5:J:20:PHE:CE2	2.52	0.43
5:P:13:THR:OG1	5:P:14:GLU:N	2.51	0.43
4:Y:28:ILE:HG12	13:Z:101:CRT:H2M1	2.00	0.43
13:6:101:CRT:H372	4:7:29:HIS:CG	2.54	0.43
13:8:101:CRT:H15	13:8:101:CRT:H131	1.85	0.43
14:H:303:CDL:H782	14:H:303:CDL:H752	1.70	0.43
1:L:118:ILE:HD11	2:M:221:THR:HA	2.01	0.43
2:M:159:LEU:HD22	2:M:184:TRP:CH2	2.53	0.43
10:H:306:LMT:O6B	4:I:34:SER:O	2.32	0.43
4:U:14:LEU:HD11	5:V:20:PHE:HZ	1.83	0.43
4:1:4:ILE:HD12	4:1:4:ILE:H	1.84	0.43
1:L:234:GLY:HA3	2:M:215:PHE:CZ	2.53	0.43
4:A:37:ARG:NH1	4:A:46:THR:OG1	2.51	0.43
10:5:201:LMT:H12	10:5:201:LMT:H41	1.89	0.43
4:7:13:ALA:O	4:7:17:LEU:HD23	2.19	0.43
1:L:194:LEU:HD22	1:L:217:PHE:CE2	2.53	0.43
2:M:155:LEU:HA	2:M:280:ALA:HB2	2.01	0.43
2:M:160:GLY:HA3	13:M:407:CRT:H292	2.00	0.43
3:H:182:TYR:OH	3:H:244:MET:HE3	2.18	0.43
4:F:37:ARG:O	5:G:46:ARG:NH1	2.50	0.43
10:R:102:LMT:H1B	10:R:102:LMT:H3'	1.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:160:ARG:HH22	3:H:254:SER:HB3	1.83	0.43
4:5:31:ILE:O	4:5:35:THR:HG23	2.19	0.43
1:L:77:ALA:HB2	10:5:203:LMT:H3'	2.00	0.43
3:H:21:TRP:CD1	9:H:302:PGV:H201	2.54	0.43
2:M:201:HIS:CE1	2:M:205:ILE:HD11	2.54	0.43
3:H:80:ASN:ND2	3:H:82:LYS:HD3	2.32	0.43
4:A:43:GLY:HA3	5:0:55:TYR:CE2	2.54	0.43
4:O:33:LEU:O	4:O:39:ASN:ND2	2.43	0.43
5:P:27:SER:HA	5:P:30:VAL:HG12	2.01	0.43
2:M:151:SER:HG	2:M:276:THR:HG1	1.59	0.42
3:H:41:PRO:O	3:H:83:ARG:NH2	2.46	0.42
4:A:47:LYS:HE3	5:0:52:PRO:HB2	2.01	0.42
5:E:19:GLU:O	5:E:23:ILE:HG13	2.18	0.42
4:9:21:LEU:HD11	13:0:101:CRT:H20	2.01	0.42
3:H:2:ASN:O	10:H:306:LMT:O4'	2.31	0.42
13:E:101:CRT:H5	13:E:101:CRT:H23	1.54	0.42
13:X:101:CRT:H15	13:X:101:CRT:H131	1.87	0.42
4:1:1:FME:H	5:4:23:ILE:HD12	1.83	0.42
13:2:101:CRT:H10	13:2:101:CRT:H81	1.88	0.42
2:M:174:VAL:HA	2:M:175:PRO:HD3	1.88	0.42
13:N:101:CRT:H10	13:N:101:CRT:H81	1.78	0.42
13:P:101:CRT:H15	13:P:101:CRT:H131	1.78	0.42
4:U:24:LEU:O	4:U:28:ILE:HG13	2.19	0.42
3:H:92:ARG:HH12	3:H:97:ALA:C	2.28	0.42
5:N:24:PHE:CD2	13:N:101:CRT:H14	2.55	0.42
4:3:24:LEU:O	4:3:28:ILE:HG13	2.20	0.42
5:B:25:THR:O	5:B:29:LEU:HD23	2.20	0.42
13:G:101:CRT:H15	13:G:101:CRT:H131	1.75	0.42
5:N:25:THR:O	5:N:28:ILE:HG22	2.20	0.42
3:H:10:MET:HA	3:H:14:GLN:OE1	2.19	0.42
5:E:25:THR:O	5:E:29:LEU:HD23	2.20	0.42
5:P:25:THR:O	5:P:29:LEU:HD23	2.19	0.42
4:Y:21:LEU:HD23	4:Y:21:LEU:HA	1.87	0.42
13:G:101:CRT:H26	13:G:101:CRT:H241	1.93	0.42
5:8:43:TRP:HZ2	10:8:103:LMT:H2'	1.84	0.42
1:L:8:ARG:CZ	3:H:86:VAL:HG13	2.50	0.42
8:L:303:U10:H122	8:L:303:U10:H101	1.81	0.42
2:M:26:ILE:HA	4:Q:11:ARG:NH1	2.35	0.42
2:M:99:ALA:CB	2:M:169:ASN:HD21	2.33	0.42
2:M:218:HIS:CE1	2:M:233:GLU:OE2	2.73	0.42
3:H:222:HIS:O	3:H:246:TYR:OH	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:50:PRO:HG3	4:K:43:GLY:HA2	2.00	0.42
13:N:101:CRT:H15	13:N:101:CRT:H131	1.94	0.42
4:Y:7:LEU:CD1	13:2:101:CRT:H5	2.50	0.42
13:0:101:CRT:H20	13:0:101:CRT:H181	1.87	0.42
2:M:105:PHE:CE2	13:M:407:CRT:H401	2.55	0.42
5:R:41:LEU:HD23	5:R:41:LEU:HA	1.92	0.42
13:R:101:CRT:H10	13:R:101:CRT:H81	1.87	0.42
5:V:55:TYR:CE2	4:W:43:GLY:HA3	2.55	0.42
5:2:24:PHE:CD1	13:2:101:CRT:H14	2.55	0.42
9:L:304:PGV:H202	4:A:31:ILE:HG12	2.02	0.42
13:M:407:CRT:H10	13:M:407:CRT:H81	1.88	0.42
4:Q:2:TRP:HA	5:R:21:HIS:ND1	2.35	0.42
1:L:118:ILE:HD13	2:M:250:PHE:CE2	2.56	0.41
5:B:35:ALA:O	5:B:39:HIS:ND1	2.42	0.41
4:F:7:LEU:HD11	13:J:101:CRT:H23	2.01	0.41
4:Q:7:LEU:HD23	4:Q:7:LEU:HA	1.94	0.41
13:R:101:CRT:H15	13:R:101:CRT:H131	1.86	0.41
13:V:101:CRT:H20	13:V:101:CRT:H181	1.86	0.41
4:Y:24:LEU:O	4:Y:28:ILE:HG13	2.20	0.41
1:L:58:PRO:HA	9:L:304:PGV:H061	2.01	0.41
14:H:303:CDL:H771	14:H:303:CDL:H802	1.89	0.41
14:M:409:CDL:H571	14:M:409:CDL:H601	1.85	0.41
4:A:11:ARG:HB2	4:9:7:LEU:HD22	2.01	0.41
4:F:25:ALA:O	4:F:29:HIS:ND1	2.40	0.41
5:X:35:ALA:O	5:X:39:HIS:ND1	2.50	0.41
10:Z:103:LMT:H3'	10:Z:103:LMT:H1B	1.80	0.41
5:2:48:TRP:NE1	6:2:102:07D:OBB	2.48	0.41
4:5:1:FME:HB2	4:5:4:ILE:HD11	2.02	0.41
8:L:303:U10:H151	8:L:303:U10:H171	1.67	0.41
9:L:304:PGV:H61	9:L:304:PGV:H92	1.89	0.41
2:M:300:HIS:ND1	9:H:302:PGV:O14	2.48	0.41
3:H:119:LEU:HD12	3:H:238:ARG:NH1	2.35	0.41
5:E:24:PHE:CD2	13:E:101:CRT:H14	2.56	0.41
13:R:101:CRT:H20	13:R:101:CRT:H181	1.90	0.41
5:X:28:ILE:HG12	13:X:101:CRT:H19	2.02	0.41
1:L:205:GLU:OE1	2:M:140:LYS:HD3	2.21	0.41
14:M:408:CDL:H352	14:M:408:CDL:H321	1.81	0.41
3:H:108:MET:HB3	3:H:246:TYR:HE1	1.85	0.41
3:H:172:TRP:CE2	3:H:196:LEU:HD21	2.56	0.41
5:G:23:ILE:HG21	13:G:101:CRT:H9	2.01	0.41
1:L:211:GLU:HG2	1:L:212:HIS:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:126:LEU:HD12	3:H:130:GLY:HA2	2.03	0.41
14:H:304:CDL:OA2	15:H:305:PEF:N	2.54	0.41
13:V:101:CRT:H15	13:V:101:CRT:H131	1.83	0.41
1:L:59:SER:C	1:L:61:THR:H	2.28	0.41
1:L:129:TYR:O	1:L:133:VAL:HG22	2.20	0.41
1:L:167:ASN:HB3	1:L:261:PRO:HG3	2.02	0.41
2:M:277:PHE:O	2:M:281:ILE:HG12	2.21	0.41
2:M:298:VAL:HG22	2:M:303:ALA:HB3	2.02	0.41
3:H:7:THR:O	3:H:9:TYR:N	2.53	0.41
13:G:101:CRT:H20	13:G:101:CRT:H181	1.85	0.41
3:H:107:PRO:HB2	3:H:253:TYR:CZ	2.56	0.41
13:J:101:CRT:H26	13:J:101:CRT:H241	1.89	0.41
5:2:28:ILE:HG23	5:2:32:PHE:CE2	2.56	0.41
5:4:24:PHE:CE1	13:4:101:CRT:H16	2.55	0.41
4:5:7:LEU:H	4:5:7:LEU:HD23	1.86	0.41
2:M:84:GLU:OE2	2:M:87:ARG:HD2	2.21	0.41
4:D:20:PHE:CD2	4:D:21:LEU:HD12	2.55	0.41
5:N:24:PHE:HA	13:N:101:CRT:H14	2.03	0.41
5:P:55:TYR:CE2	4:Q:43:GLY:HA3	2.56	0.41
13:T:101:CRT:H181	13:T:101:CRT:H20	1.78	0.41
1:L:51:VAL:HG22	9:L:304:PGV:H272	2.02	0.41
1:L:175:MET:HB2	8:M:401:U10:H1M2	2.03	0.40
1:L:274:ASN:O	1:L:276:GLY:N	2.53	0.40
4:K:37:ARG:O	5:N:46:ARG:NH1	2.54	0.40
4:S:39:ASN:ND2	4:S:42:GLU:OE1	2.53	0.40
13:M:407:CRT:H26	13:M:407:CRT:H241	1.93	0.40
10:J:103:LMT:O1B	10:J:103:LMT:O6'	2.39	0.40
13:T:101:CRT:H10	13:T:101:CRT:H81	1.85	0.40
5:8:32:PHE:HE1	6:8:102:07D:CGA	2.33	0.40
4:A:19:THR:O	4:A:23:VAL:HG23	2.20	0.40
13:E:101:CRT:H25	6:E:102:07D:O1A	2.21	0.40
13:V:101:CRT:H392	4:W:29:HIS:CB	2.52	0.40
4:3:17:LEU:HD11	13:4:101:CRT:H243	2.03	0.40
13:4:101:CRT:H26	13:4:101:CRT:H241	1.93	0.40
13:0:101:CRT:H10	13:0:101:CRT:H81	1.87	0.40
4:I:1:FME:HE1	5:N:27:SER:HB2	2.04	0.40
4:7:25:ALA:O	4:7:29:HIS:ND1	2.48	0.40
2:M:217:MET:HE3	2:M:251:TRP:CH2	2.57	0.40
10:B:102:LMT:H3'	10:B:102:LMT:H1B	1.78	0.40
5:R:43:TRP:CH2	10:R:102:LMT:H11	2.56	0.40
5:2:28:ILE:HG23	5:2:32:PHE:HE2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:21:LEU:HD11	13:4:101:CRT:C25	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	273/275 (99%)	258 (94%)	15 (6%)	0	100	100
2	M	302/305 (99%)	292 (97%)	10 (3%)	0	100	100
3	H	254/256 (99%)	233 (92%)	21 (8%)	0	100	100
4	1	45/62 (73%)	44 (98%)	0	1 (2%)	5	10
4	3	45/62 (73%)	45 (100%)	0	0	100	100
4	5	45/62 (73%)	42 (93%)	3 (7%)	0	100	100
4	7	45/62 (73%)	44 (98%)	0	1 (2%)	5	10
4	9	45/62 (73%)	45 (100%)	0	0	100	100
4	A	45/62 (73%)	45 (100%)	0	0	100	100
4	D	45/62 (73%)	45 (100%)	0	0	100	100
4	F	45/62 (73%)	45 (100%)	0	0	100	100
4	I	45/62 (73%)	45 (100%)	0	0	100	100
4	K	45/62 (73%)	45 (100%)	0	0	100	100
4	O	45/62 (73%)	45 (100%)	0	0	100	100
4	Q	45/62 (73%)	44 (98%)	1 (2%)	0	100	100
4	S	45/62 (73%)	45 (100%)	0	0	100	100
4	U	45/62 (73%)	42 (93%)	3 (7%)	0	100	100
4	W	45/62 (73%)	43 (96%)	2 (4%)	0	100	100
4	Y	45/62 (73%)	41 (91%)	4 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	0	43/55 (78%)	43 (100%)	0	0	100	100
5	2	42/55 (76%)	40 (95%)	2 (5%)	0	100	100
5	4	43/55 (78%)	42 (98%)	1 (2%)	0	100	100
5	6	43/55 (78%)	43 (100%)	0	0	100	100
5	8	42/55 (76%)	41 (98%)	1 (2%)	0	100	100
5	B	43/55 (78%)	41 (95%)	2 (5%)	0	100	100
5	E	42/55 (76%)	41 (98%)	1 (2%)	0	100	100
5	G	43/55 (78%)	43 (100%)	0	0	100	100
5	J	43/55 (78%)	42 (98%)	1 (2%)	0	100	100
5	N	43/55 (78%)	41 (95%)	2 (5%)	0	100	100
5	P	42/55 (76%)	42 (100%)	0	0	100	100
5	R	43/55 (78%)	43 (100%)	0	0	100	100
5	T	43/55 (78%)	43 (100%)	0	0	100	100
5	V	43/55 (78%)	42 (98%)	1 (2%)	0	100	100
5	X	43/55 (78%)	42 (98%)	1 (2%)	0	100	100
5	Z	42/55 (76%)	40 (95%)	2 (5%)	0	100	100
All	All	2232/2708 (82%)	2157 (97%)	73 (3%)	2 (0%)	49	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	7	2	TRP
4	1	2	TRP

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	219/219 (100%)	219 (100%)	0	100	100
2	M	235/239 (98%)	235 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	199/203 (98%)	199 (100%)	0	100	100
4	1	39/54 (72%)	39 (100%)	0	100	100
4	3	39/54 (72%)	39 (100%)	0	100	100
4	5	39/54 (72%)	39 (100%)	0	100	100
4	7	38/54 (70%)	38 (100%)	0	100	100
4	9	39/54 (72%)	39 (100%)	0	100	100
4	A	40/54 (74%)	40 (100%)	0	100	100
4	D	40/54 (74%)	40 (100%)	0	100	100
4	F	40/54 (74%)	40 (100%)	0	100	100
4	I	39/54 (72%)	39 (100%)	0	100	100
4	K	39/54 (72%)	39 (100%)	0	100	100
4	O	38/54 (70%)	38 (100%)	0	100	100
4	Q	39/54 (72%)	39 (100%)	0	100	100
4	S	38/54 (70%)	38 (100%)	0	100	100
4	U	39/54 (72%)	39 (100%)	0	100	100
4	W	40/54 (74%)	40 (100%)	0	100	100
4	Y	39/54 (72%)	39 (100%)	0	100	100
5	0	37/45 (82%)	37 (100%)	0	100	100
5	2	34/45 (76%)	34 (100%)	0	100	100
5	4	32/45 (71%)	31 (97%)	1 (3%)	35	59
5	6	31/45 (69%)	31 (100%)	0	100	100
5	8	33/45 (73%)	33 (100%)	0	100	100
5	B	37/45 (82%)	37 (100%)	0	100	100
5	E	34/45 (76%)	34 (100%)	0	100	100
5	G	37/45 (82%)	37 (100%)	0	100	100
5	J	37/45 (82%)	37 (100%)	0	100	100
5	N	37/45 (82%)	37 (100%)	0	100	100
5	P	36/45 (80%)	36 (100%)	0	100	100
5	R	36/45 (80%)	36 (100%)	0	100	100
5	T	32/45 (71%)	32 (100%)	0	100	100
5	V	33/45 (73%)	33 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	X	35/45 (78%)	35 (100%)	0	100	100
5	Z	35/45 (78%)	35 (100%)	0	100	100
All	All	1834/2245 (82%)	1833 (100%)	1 (0%)	87	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	4	52	PRO

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

Mol	Chain	Res	Type
1	L	167	ASN
1	L	200	ASN
2	M	5	GLN
2	M	6	ASN
2	M	88	GLN
3	H	54	GLN
3	H	106	ASN
4	D	12	GLN
4	K	6	GLN
4	S	39	ASN
4	U	12	GLN
4	Y	12	GLN
5	4	53	ASN
5	6	21	HIS
5	8	53	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	FME	F	1	4	8,9,10	0.87	0	7,9,11	0.90	0
4	FME	Q	1	4	8,9,10	0.84	0	7,9,11	1.63	2 (28%)
4	FME	5	1	4	8,9,10	0.95	0	7,9,11	0.85	0
4	FME	K	1	4	8,9,10	0.92	0	7,9,11	0.83	0
4	FME	A	1	4	8,9,10	0.95	0	7,9,11	0.97	0
4	FME	D	1	4	8,9,10	0.91	0	7,9,11	0.98	0
4	FME	7	1	4	8,9,10	0.93	0	7,9,11	0.88	0
4	FME	S	1	4	8,9,10	0.91	0	7,9,11	0.86	0
4	FME	3	1	4	8,9,10	0.92	0	7,9,11	0.97	0
4	FME	9	1	4	8,9,10	0.94	0	7,9,11	0.89	0
4	FME	W	1	4	8,9,10	0.91	0	7,9,11	1.56	2 (28%)
4	FME	Y	1	4	8,9,10	0.92	0	7,9,11	0.81	0
4	FME	1	1	4	8,9,10	0.91	0	7,9,11	0.98	0
4	FME	O	1	4	8,9,10	0.88	0	7,9,11	1.26	2 (28%)
4	FME	U	1	4	8,9,10	0.92	0	7,9,11	1.03	1 (14%)
4	FME	I	1	4	8,9,10	0.93	0	7,9,11	0.92	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FME	F	1	4	-	3/7/9/11	-
4	FME	Q	1	4	-	3/7/9/11	-
4	FME	5	1	4	-	0/7/9/11	-
4	FME	K	1	4	-	5/7/9/11	-
4	FME	A	1	4	-	2/7/9/11	-
4	FME	D	1	4	-	4/7/9/11	-
4	FME	7	1	4	-	4/7/9/11	-
4	FME	S	1	4	-	2/7/9/11	-
4	FME	3	1	4	-	4/7/9/11	-
4	FME	9	1	4	-	4/7/9/11	-
4	FME	W	1	4	-	3/7/9/11	-
4	FME	Y	1	4	-	4/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FME	1	1	4	-	0/7/9/11	-
4	FME	O	1	4	-	2/7/9/11	-
4	FME	U	1	4	-	5/7/9/11	-
4	FME	I	1	4	-	6/7/9/11	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	1	FME	C-CA-N	3.03	115.20	109.73
4	W	1	FME	CA-N-CN	2.75	127.05	122.82
4	W	1	FME	C-CA-N	2.66	114.53	109.73
4	Q	1	FME	CA-N-CN	2.53	126.72	122.82
4	U	1	FME	C-CA-N	2.22	113.74	109.73
4	O	1	FME	C-CA-N	2.12	113.56	109.73
4	O	1	FME	CA-N-CN	2.11	126.07	122.82

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	FME	O-C-CA-CB
4	D	1	FME	N-CA-CB-CG
4	I	1	FME	CB-CA-N-CN
4	I	1	FME	N-CA-CB-CG
4	I	1	FME	O-C-CA-CB
4	I	1	FME	CA-CB-CG-SD
4	K	1	FME	O1-CN-N-CA
4	K	1	FME	CB-CA-N-CN
4	K	1	FME	C-CA-CB-CG
4	O	1	FME	CB-CA-N-CN
4	O	1	FME	O-C-CA-CB
4	Q	1	FME	CB-CA-N-CN
4	Q	1	FME	C-CA-CB-CG
4	S	1	FME	O-C-CA-CB
4	U	1	FME	CB-CA-N-CN
4	W	1	FME	CB-CA-N-CN
4	W	1	FME	C-CA-CB-CG
4	Y	1	FME	O1-CN-N-CA
4	Y	1	FME	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
4	3	1	FME	N-CA-CB-CG
4	7	1	FME	O1-CN-N-CA
4	7	1	FME	N-CA-CB-CG
4	7	1	FME	C-CA-CB-CG
4	9	1	FME	O1-CN-N-CA
4	9	1	FME	N-CA-CB-CG
4	I	1	FME	CB-CG-SD-CE
4	Y	1	FME	CB-CG-SD-CE
4	A	1	FME	N-CA-CB-CG
4	F	1	FME	N-CA-CB-CG
4	U	1	FME	N-CA-CB-CG
4	W	1	FME	N-CA-CB-CG
4	F	1	FME	CB-CG-SD-CE
4	S	1	FME	CB-CG-SD-CE
4	U	1	FME	CB-CG-SD-CE
4	9	1	FME	CB-CG-SD-CE
4	F	1	FME	CA-CB-CG-SD
4	Q	1	FME	N-CA-CB-CG
4	D	1	FME	CB-CG-SD-CE
4	3	1	FME	CA-CB-CG-SD
4	K	1	FME	N-CA-CB-CG
4	U	1	FME	CA-CB-CG-SD
4	7	1	FME	CB-CG-SD-CE
4	D	1	FME	CB-CA-N-CN
4	3	1	FME	CB-CA-N-CN
4	D	1	FME	C-CA-CB-CG
4	I	1	FME	C-CA-CB-CG
4	U	1	FME	C-CA-CB-CG
4	Y	1	FME	C-CA-CB-CG
4	3	1	FME	C-CA-CB-CG
4	K	1	FME	CB-CG-SD-CE
4	9	1	FME	CB-CA-N-CN

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	5	1	FME	2	0
4	Y	1	FME	1	0
4	1	1	FME	2	0
4	I	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 92 ligands modelled in this entry, 1 is monoatomic - leaving 91 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	PEF	H	305	-	12,12,46	0.45	0	13,15,51	0.47	0
13	CRT	P	101	-	41,43,43	0.70	0	50,54,54	1.71	11 (22%)
15	PEF	K	103	-	41,41,46	1.01	2 (4%)	44,46,51	1.11	4 (9%)
7	08I	L	302	-	60,70,70	2.65	10 (16%)	56,101,101	2.82	16 (28%)
6	07D	N	102	5	69,74,74	1.17	4 (5%)	83,115,115	1.63	17 (20%)
13	CRT	M	407	-	41,43,43	0.75	0	50,54,54	3.81	16 (32%)
10	LMT	T	103	-	36,36,36	0.42	0	47,47,47	0.87	2 (4%)
6	07D	I	101	4	69,74,74	1.22	7 (10%)	83,115,115	1.72	15 (18%)
10	LMT	5	203	-	36,36,36	0.41	0	47,47,47	0.74	0
6	07D	K	101	4	69,74,74	1.19	5 (7%)	83,115,115	1.55	15 (18%)
10	LMT	B	102	-	36,36,36	0.43	0	47,47,47	0.76	1 (2%)
14	CDL	H	301	-	63,63,99	1.14	4 (6%)	69,75,111	1.21	4 (5%)
10	LMT	E	103	-	36,36,36	0.41	0	47,47,47	0.79	0
10	LMT	G	103	-	36,36,36	0.44	0	47,47,47	0.76	0
10	LMT	8	103	-	36,36,36	0.42	0	47,47,47	0.79	1 (2%)
10	LMT	L	305	-	29,29,36	0.41	0	40,40,47	0.76	1 (2%)
9	PGV	H	302	-	35,35,50	1.09	2 (5%)	38,41,56	1.29	4 (10%)
6	07D	P	102	5	69,74,74	1.18	5 (7%)	83,115,115	1.51	15 (18%)
13	CRT	T	101	-	41,43,43	0.70	0	50,54,54	1.79	11 (22%)
13	CRT	V	101	-	41,43,43	0.75	0	50,54,54	1.80	13 (26%)
14	CDL	M	408	-	67,67,99	1.10	4 (5%)	73,79,111	1.23	8 (10%)
14	CDL	H	304	-	32,32,99	1.37	3 (9%)	35,42,111	1.52	4 (11%)
13	CRT	0	101	-	41,43,43	0.70	0	50,54,54	1.62	13 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	07D	5	202	4	69,74,74	1.24	6 (8%)	83,115,115	1.78	19 (22%)
15	PEF	K	102	-	30,30,46	1.17	2 (6%)	33,35,51	1.17	2 (6%)
6	07D	E	102	5	69,74,74	1.16	5 (7%)	83,115,115	1.47	12 (14%)
6	07D	2	102	5	69,74,74	1.17	5 (7%)	83,115,115	1.52	13 (15%)
10	LMT	H	306	-	36,36,36	0.44	0	47,47,47	0.88	1 (2%)
12	RQ0	M	406	-	62,62,62	2.87	28 (45%)	69,78,78	2.37	27 (39%)
10	LMT	L	306	-	33,33,36	0.42	0	44,44,47	0.65	1 (2%)
10	LMT	4	103	-	36,36,36	0.47	0	47,47,47	0.79	0
6	07D	4	102	5	69,74,74	1.21	5 (7%)	83,115,115	1.56	16 (19%)
6	07D	1	101	4	69,74,74	1.22	5 (7%)	83,115,115	1.56	12 (14%)
10	LMT	0	103	-	36,36,36	0.38	0	47,47,47	0.70	1 (2%)
13	CRT	8	101	-	41,43,43	0.69	0	50,54,54	1.58	9 (18%)
6	07D	8	102	5	69,74,74	1.16	5 (7%)	83,115,115	1.78	16 (19%)
13	CRT	A	102	-	41,43,43	0.71	0	50,54,54	1.71	14 (28%)
6	07D	O	101	4	69,74,74	1.22	6 (8%)	83,115,115	1.52	14 (16%)
6	07D	D	101	4	69,74,74	1.24	6 (8%)	83,115,115	1.64	15 (18%)
10	LMT	M	410	-	36,36,36	0.42	0	47,47,47	0.90	1 (2%)
10	LMT	5	201	-	32,32,36	0.50	0	43,43,47	0.92	2 (4%)
10	LMT	P	103	-	36,36,36	0.43	0	47,47,47	0.68	1 (2%)
6	07D	Q	101	4	69,74,74	1.19	5 (7%)	83,115,115	1.61	16 (19%)
10	LMT	J	103	-	36,36,36	0.45	0	47,47,47	0.83	1 (2%)
6	07D	6	102	5	69,74,74	1.23	6 (8%)	83,115,115	1.53	14 (16%)
6	07D	G	102	5	69,74,74	1.16	5 (7%)	83,115,115	1.47	13 (15%)
10	LMT	X	103	-	36,36,36	0.44	0	47,47,47	0.78	1 (2%)
6	07D	J	102	5	69,74,74	1.18	5 (7%)	83,115,115	1.55	15 (18%)
6	07D	X	102	5	69,74,74	1.18	6 (8%)	83,115,115	1.52	14 (16%)
10	LMT	V	103	-	36,36,36	0.48	0	47,47,47	0.96	4 (8%)
6	07D	0	102	5	69,74,74	1.18	5 (7%)	83,115,115	1.47	12 (14%)
10	LMT	2	103	-	36,36,36	0.47	0	47,47,47	0.84	1 (2%)
13	CRT	4	101	-	41,43,43	0.72	0	50,54,54	1.64	9 (18%)
6	07D	A	101	4	69,74,74	1.20	5 (7%)	83,115,115	1.56	13 (15%)
6	07D	L	301	1	69,74,74	1.21	7 (10%)	83,115,115	1.40	12 (14%)
9	PGV	L	304	-	42,42,50	0.98	2 (4%)	45,48,56	1.23	4 (8%)
6	07D	T	102	5	69,74,74	1.17	6 (8%)	83,115,115	1.70	11 (13%)
13	CRT	2	101	-	41,43,43	0.73	0	50,54,54	1.64	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	07D	U	101	4	69,74,74	1.23	5 (7%)	83,115,115	1.53	15 (18%)
14	CDL	H	303	-	58,58,99	1.24	4 (6%)	64,70,111	1.22	5 (7%)
6	07D	S	101	4	69,74,74	1.22	5 (7%)	83,115,115	1.54	14 (16%)
6	07D	M	404	2	69,74,74	1.20	5 (7%)	83,115,115	1.57	14 (16%)
8	U10	L	303	-	28,28,63	0.90	2 (7%)	34,37,79	0.65	0
6	07D	Q	102	5	69,74,74	1.18	6 (8%)	83,115,115	1.52	10 (12%)
6	07D	Z	102	5	69,74,74	1.16	5 (7%)	83,115,115	1.44	10 (12%)
6	07D	V	102	5	69,74,74	1.16	5 (7%)	83,115,115	1.50	13 (15%)
13	CRT	E	101	-	41,43,43	0.70	0	50,54,54	1.68	14 (28%)
6	07D	7	101	4	69,74,74	1.23	5 (7%)	83,115,115	1.49	14 (16%)
6	07D	B	101	5	69,74,74	1.18	5 (7%)	83,115,115	1.78	16 (19%)
6	07D	Y	101	4	69,74,74	1.23	6 (8%)	83,115,115	1.57	16 (19%)
10	LMT	R	102	-	36,36,36	0.38	0	47,47,47	0.91	2 (4%)
8	U10	M	401	-	18,18,63	1.02	2 (11%)	22,25,79	0.69	0
10	LMT	6	103	-	36,36,36	0.45	0	47,47,47	0.83	0
10	LMT	N	103	-	36,36,36	0.43	0	47,47,47	0.97	3 (6%)
6	07D	L	307	1	69,74,74	1.19	5 (7%)	83,115,115	1.68	15 (18%)
13	CRT	6	101	-	41,43,43	0.71	0	50,54,54	1.57	9 (18%)
7	08I	M	405	-	60,70,70	2.72	9 (15%)	56,101,101	2.65	12 (21%)
10	LMT	Z	103	-	36,36,36	0.45	0	47,47,47	0.76	0
6	07D	9	101	4	69,74,74	1.23	6 (8%)	83,115,115	1.57	16 (19%)
13	CRT	Z	101	-	41,43,43	0.71	0	50,54,54	1.67	13 (26%)
13	CRT	R	101	-	41,43,43	0.71	0	50,54,54	1.52	9 (18%)
6	07D	W	101	4	69,74,74	1.22	5 (7%)	83,115,115	1.56	13 (15%)
6	07D	M	403	2	69,74,74	1.20	6 (8%)	83,115,115	1.51	8 (9%)
13	CRT	G	101	-	41,43,43	0.72	0	50,54,54	1.77	10 (20%)
13	CRT	J	101	-	41,43,43	0.69	0	50,54,54	1.61	9 (18%)
14	CDL	M	409	-	67,67,99	1.14	4 (5%)	73,79,111	1.10	5 (6%)
6	07D	F	101	4	69,74,74	1.21	5 (7%)	83,115,115	1.61	16 (19%)
6	07D	3	101	4	69,74,74	1.23	6 (8%)	83,115,115	1.46	12 (14%)
10	LMT	M	411	-	30,30,36	0.46	0	41,41,47	0.76	0
13	CRT	X	101	-	41,43,43	0.69	0	50,54,54	1.74	9 (18%)
13	CRT	N	101	-	41,43,43	0.70	0	50,54,54	1.58	8 (16%)

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	PEF	H	305	-	-	4/13/13/50	-
13	CRT	P	101	-	-	15/51/51/51	-
15	PEF	K	103	-	-	14/45/45/50	-
7	08I	L	302	-	-	13/41/105/105	0/5/6/6
6	07D	N	102	5	1/1/21/28	4/41/137/137	-
13	CRT	M	407	-	-	10/51/51/51	-
10	LMT	T	103	-	-	7/21/61/61	0/2/2/2
6	07D	I	101	4	1/1/21/28	8/41/137/137	-
10	LMT	5	203	-	-	5/21/61/61	0/2/2/2
6	07D	K	101	4	1/1/21/28	1/41/137/137	-
10	LMT	B	102	-	-	8/21/61/61	0/2/2/2
14	CDL	H	301	-	-	19/74/74/110	-
10	LMT	E	103	-	-	4/21/61/61	0/2/2/2
10	LMT	G	103	-	-	2/21/61/61	0/2/2/2
10	LMT	8	103	-	-	3/21/61/61	0/2/2/2
10	LMT	L	305	-	-	0/14/54/61	0/2/2/2
9	PGV	H	302	-	-	16/40/40/55	-
6	07D	P	102	5	1/1/21/28	10/41/137/137	-
13	CRT	T	101	-	-	7/51/51/51	-
13	CRT	V	101	-	-	7/51/51/51	-
14	CDL	M	408	-	-	23/78/78/110	-
14	CDL	H	304	-	-	20/40/40/110	-
13	CRT	0	101	-	-	7/51/51/51	-
6	07D	5	202	4	1/1/21/28	8/41/137/137	-
15	PEF	K	102	-	-	11/34/34/50	-
6	07D	E	102	5	1/1/21/28	8/41/137/137	-
6	07D	2	102	5	1/1/21/28	7/41/137/137	-
10	LMT	H	306	-	-	10/21/61/61	0/2/2/2
12	RQ0	M	406	-	-	22/61/85/85	0/1/1/1
10	LMT	L	306	-	-	6/18/58/61	0/2/2/2
10	LMT	4	103	-	-	8/21/61/61	0/2/2/2
6	07D	4	102	5	1/1/21/28	6/41/137/137	-
6	07D	1	101	4	1/1/21/28	8/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	LMT	0	103	-	-	3/21/61/61	0/2/2/2
13	CRT	8	101	-	-	7/51/51/51	-
6	07D	8	102	5	1/1/21/28	9/41/137/137	-
13	CRT	A	102	-	-	0/51/51/51	-
6	07D	O	101	4	1/1/21/28	11/41/137/137	-
6	07D	D	101	4	1/1/21/28	3/41/137/137	-
10	LMT	M	410	-	-	8/21/61/61	0/2/2/2
10	LMT	5	201	-	-	13/17/57/61	0/2/2/2
10	LMT	P	103	-	-	9/21/61/61	0/2/2/2
6	07D	Q	101	4	1/1/21/28	7/41/137/137	-
10	LMT	J	103	-	-	5/21/61/61	0/2/2/2
6	07D	6	102	5	1/1/21/28	9/41/137/137	-
6	07D	G	102	5	1/1/21/28	5/41/137/137	-
10	LMT	X	103	-	-	3/21/61/61	0/2/2/2
6	07D	J	102	5	1/1/21/28	5/41/137/137	-
6	07D	X	102	5	1/1/21/28	7/41/137/137	-
10	LMT	V	103	-	-	3/21/61/61	0/2/2/2
6	07D	0	102	5	1/1/21/28	7/41/137/137	-
10	LMT	2	103	-	-	7/21/61/61	0/2/2/2
13	CRT	4	101	-	-	4/51/51/51	-
6	07D	A	101	4	1/1/21/28	3/41/137/137	-
6	07D	L	301	1	1/1/21/28	2/41/137/137	-
9	PGV	L	304	-	-	9/47/47/55	-
6	07D	T	102	5	1/1/21/28	6/41/137/137	-
13	CRT	2	101	-	-	11/51/51/51	-
6	07D	U	101	4	1/1/21/28	4/41/137/137	-
14	CDL	H	303	-	-	30/68/68/110	-
6	07D	S	101	4	1/1/21/28	5/41/137/137	-
6	07D	M	404	2	1/1/21/28	5/41/137/137	-
8	U10	L	303	-	-	6/21/45/87	0/1/1/1
6	07D	Q	102	5	1/1/21/28	8/41/137/137	-
6	07D	Z	102	5	1/1/21/28	9/41/137/137	-
6	07D	V	102	5	1/1/21/28	4/41/137/137	-
13	CRT	E	101	-	-	11/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	07D	7	101	4	1/1/21/28	8/41/137/137	-
6	07D	B	101	5	1/1/21/28	8/41/137/137	-
6	07D	Y	101	4	1/1/21/28	7/41/137/137	-
10	LMT	R	102	-	-	4/21/61/61	0/2/2/2
8	U10	M	401	-	-	1/9/33/87	0/1/1/1
10	LMT	6	103	-	-	4/21/61/61	0/2/2/2
10	LMT	N	103	-	-	4/21/61/61	0/2/2/2
6	07D	L	307	1	-	4/41/137/137	-
13	CRT	6	101	-	-	13/51/51/51	-
7	08I	M	405	-	-	4/41/105/105	0/5/6/6
10	LMT	Z	103	-	-	6/21/61/61	0/2/2/2
6	07D	9	101	4	1/1/21/28	3/41/137/137	-
13	CRT	Z	101	-	-	10/51/51/51	-
13	CRT	R	101	-	-	7/51/51/51	-
6	07D	W	101	4	1/1/21/28	4/41/137/137	-
6	07D	M	403	2	-	5/41/137/137	-
13	CRT	G	101	-	-	10/51/51/51	-
13	CRT	J	101	-	-	2/51/51/51	-
14	CDL	M	409	-	-	23/78/78/110	-
6	07D	F	101	4	1/1/21/28	6/41/137/137	-
6	07D	3	101	4	1/1/21/28	8/41/137/137	-
10	LMT	M	411	-	-	5/15/55/61	0/2/2/2
13	CRT	X	101	-	-	7/51/51/51	-
13	CRT	N	101	-	-	5/51/51/51	-

All (272) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	405	08I	C4C-C3C	10.69	1.51	1.39
7	L	302	08I	C4C-C3C	10.47	1.51	1.39
12	M	406	RQ0	C18-C14	9.55	1.59	1.34
12	M	406	RQ0	C11-C07	9.55	1.59	1.34
7	M	405	08I	C4A-C3A	9.04	1.49	1.39
7	L	302	08I	C4A-C3A	8.55	1.49	1.39
7	M	405	08I	C1C-C2C	8.22	1.48	1.39
7	L	302	08I	C1C-C2C	7.83	1.48	1.39
7	M	405	08I	C1A-C2A	6.69	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	302	08I	C1A-C2A	6.30	1.49	1.39
7	L	302	08I	C2A-C3A	5.60	1.54	1.37
12	M	406	RQ0	C07-C19	5.52	1.57	1.45
7	L	302	08I	C3C-C2C	5.48	1.53	1.37
7	M	405	08I	C2A-C3A	5.42	1.53	1.37
7	M	405	08I	C3C-C2C	5.34	1.53	1.37
12	M	406	RQ0	C41-C42	5.33	1.58	1.50
12	M	406	RQ0	C14-C23	5.31	1.57	1.45
14	H	304	CDL	OB6-CB5	4.89	1.46	1.35
6	1	101	07D	MG-NA	4.84	2.17	2.06
14	H	303	CDL	OA6-CA5	4.80	1.46	1.35
6	4	102	07D	MG-NA	4.75	2.17	2.06
6	W	101	07D	MG-NA	4.71	2.17	2.06
6	N	102	07D	MG-NA	4.69	2.17	2.06
6	T	102	07D	MG-NA	4.65	2.17	2.06
6	M	404	07D	MG-NA	4.63	2.17	2.06
6	L	301	07D	MG-NA	4.63	2.17	2.06
6	F	101	07D	MG-NA	4.62	2.17	2.06
6	D	101	07D	MG-NA	4.60	2.17	2.06
6	Y	101	07D	MG-NA	4.58	2.17	2.06
6	L	307	07D	MG-NA	4.57	2.17	2.06
6	B	101	07D	MG-NA	4.57	2.17	2.06
6	U	101	07D	MG-NA	4.55	2.17	2.06
6	O	101	07D	MG-NA	4.55	2.17	2.06
6	Z	102	07D	MG-NA	4.55	2.17	2.06
6	5	202	07D	MG-NA	4.54	2.17	2.06
6	X	102	07D	MG-NA	4.52	2.17	2.06
7	M	405	08I	CBD-CGD	-4.52	1.46	1.52
6	M	403	07D	MG-NA	4.52	2.17	2.06
6	A	101	07D	MG-NA	4.52	2.17	2.06
6	V	102	07D	MG-NA	4.51	2.17	2.06
6	S	101	07D	MG-NA	4.50	2.17	2.06
6	I	101	07D	MG-NA	4.48	2.16	2.06
6	8	102	07D	MG-NA	4.48	2.16	2.06
6	2	102	07D	MG-NA	4.47	2.16	2.06
14	M	409	CDL	OA6-CA5	4.47	1.46	1.34
6	Q	102	07D	MG-NA	4.46	2.16	2.06
6	J	102	07D	MG-NA	4.44	2.16	2.06
6	G	102	07D	MG-NA	4.44	2.16	2.06
6	6	102	07D	MG-NA	4.43	2.16	2.06
6	P	102	07D	MG-NA	4.42	2.16	2.06
6	E	102	07D	MG-NA	4.41	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	9	101	07D	MG-NA	4.40	2.16	2.06
6	3	101	07D	MG-NA	4.39	2.16	2.06
6	K	101	07D	MG-NA	4.39	2.16	2.06
6	0	102	07D	MG-NA	4.38	2.16	2.06
6	Q	101	07D	MG-NA	4.36	2.16	2.06
6	7	101	07D	MG-NA	4.36	2.16	2.06
14	H	303	CDL	OA8-CA7	4.35	1.46	1.33
14	M	409	CDL	OB8-CB7	4.31	1.45	1.33
14	H	301	CDL	OB6-CB5	4.30	1.46	1.34
14	H	303	CDL	OB6-CB5	4.28	1.46	1.34
14	M	409	CDL	OA8-CA7	4.24	1.45	1.33
9	H	302	PGV	O03-C19	4.22	1.45	1.33
14	M	408	CDL	OA8-CA7	4.21	1.45	1.33
15	K	102	PEF	O2-C10	4.20	1.46	1.34
15	K	103	PEF	O3-C30	4.18	1.45	1.33
14	M	409	CDL	OB6-CB5	4.17	1.46	1.34
14	H	301	CDL	OA8-CA7	4.14	1.45	1.33
9	L	304	PGV	O01-C1	4.12	1.45	1.34
15	K	102	PEF	O3-C30	4.12	1.45	1.33
14	M	408	CDL	OB8-CB7	4.11	1.45	1.33
14	H	301	CDL	OB8-CB7	4.11	1.45	1.33
9	H	302	PGV	O01-C1	4.11	1.45	1.34
14	M	408	CDL	OB6-CB5	4.10	1.45	1.34
7	L	302	08I	CBD-CGD	-4.07	1.46	1.52
14	M	408	CDL	OA6-CA5	4.07	1.45	1.34
15	K	103	PEF	O2-C10	4.06	1.45	1.34
9	L	304	PGV	O03-C19	4.01	1.45	1.33
14	H	304	CDL	OA6-CA5	4.01	1.45	1.34
14	H	301	CDL	OA6-CA5	3.99	1.45	1.34
14	H	303	CDL	OB8-CB7	3.98	1.45	1.33
12	M	406	RQ0	C08-C17	3.88	1.59	1.51
12	M	406	RQ0	C18-C27	3.84	1.55	1.43
12	M	406	RQ0	C11-C25	3.81	1.55	1.43
7	L	302	08I	C3D-CAD	-3.77	1.41	1.48
12	M	406	RQ0	C30-C31	3.69	1.59	1.51
7	M	405	08I	C3D-CAD	-3.60	1.41	1.48
12	M	406	RQ0	C29-C35	3.58	1.58	1.51
12	M	406	RQ0	C15-C21	3.57	1.58	1.51
6	Z	102	07D	MG-NC	3.38	2.14	2.06
6	X	102	07D	MG-NC	3.37	2.14	2.06
6	4	102	07D	MG-NC	3.34	2.14	2.06
12	M	406	RQ0	C47-C45	3.34	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	T	102	07D	MG-NC	3.32	2.14	2.06
6	Y	101	07D	MG-NC	3.29	2.14	2.06
6	V	102	07D	MG-NC	3.28	2.14	2.06
6	1	101	07D	MG-NC	3.27	2.14	2.06
6	M	403	07D	MG-NC	3.26	2.14	2.06
12	M	406	RQ0	C56-C55	-3.23	1.34	1.39
6	0	102	07D	MG-NC	3.23	2.13	2.06
6	J	102	07D	MG-NC	3.22	2.13	2.06
6	O	101	07D	MG-NC	3.20	2.13	2.06
12	M	406	RQ0	C05-C13	3.18	1.57	1.51
6	5	202	07D	MG-NC	3.16	2.13	2.06
6	6	102	07D	MG-NC	3.16	2.13	2.06
6	B	101	07D	MG-NC	3.16	2.13	2.06
6	2	102	07D	MG-NC	3.16	2.13	2.06
6	L	301	07D	MG-NC	3.15	2.13	2.06
14	H	304	CDL	OA8-CA7	3.15	1.45	1.33
6	Q	102	07D	MG-NC	3.15	2.13	2.06
6	G	102	07D	MG-NC	3.14	2.13	2.06
6	7	101	07D	MG-NC	3.14	2.13	2.06
6	W	101	07D	MG-NC	3.13	2.13	2.06
6	L	307	07D	MG-NC	3.12	2.13	2.06
6	U	101	07D	MG-NC	3.12	2.13	2.06
12	M	406	RQ0	C06-C16	3.12	1.57	1.51
6	8	102	07D	MG-NC	3.12	2.13	2.06
6	Q	101	07D	MG-NC	3.12	2.13	2.06
12	M	406	RQ0	C25-C16	3.10	1.37	1.34
6	I	101	07D	MG-NC	3.10	2.13	2.06
6	F	101	07D	MG-NC	3.08	2.13	2.06
6	D	101	07D	C3B-C4B	3.08	1.46	1.41
6	S	101	07D	MG-NC	3.07	2.13	2.06
6	E	102	07D	MG-NC	3.06	2.13	2.06
6	9	101	07D	MG-NC	3.06	2.13	2.06
6	N	102	07D	MG-NC	3.06	2.13	2.06
6	A	101	07D	MG-NC	3.05	2.13	2.06
6	P	102	07D	MG-NC	3.05	2.13	2.06
8	L	303	U10	C3-C2	-3.04	1.40	1.48
6	U	101	07D	C3B-C4B	3.04	1.46	1.41
6	D	101	07D	MG-NC	3.00	2.13	2.06
6	3	101	07D	MG-NC	3.00	2.13	2.06
6	K	101	07D	MG-NC	2.97	2.13	2.06
6	S	101	07D	C3B-C4B	2.94	1.46	1.41
6	Q	101	07D	C3B-C4B	2.92	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	3	101	07D	C3B-C4B	2.90	1.46	1.41
6	7	101	07D	C3B-C4B	2.90	1.46	1.41
12	M	406	RQ0	O01-C62	-2.89	1.38	1.45
6	9	101	07D	C3B-C4B	2.87	1.46	1.41
6	M	404	07D	C3B-C4B	2.87	1.46	1.41
6	A	101	07D	C3B-C4B	2.87	1.46	1.41
6	M	404	07D	MG-NC	2.85	2.13	2.06
6	5	202	07D	C3B-C4B	2.82	1.46	1.41
6	Y	101	07D	C3B-C4B	2.78	1.46	1.41
6	F	101	07D	C3B-C4B	2.78	1.46	1.41
6	I	101	07D	C3B-C4B	2.77	1.46	1.41
6	W	101	07D	C3B-C4B	2.73	1.46	1.41
6	K	101	07D	C3B-C4B	2.72	1.46	1.41
6	P	102	07D	C3B-C4B	2.72	1.46	1.41
6	O	101	07D	C3B-C4B	2.70	1.46	1.41
6	J	102	07D	C3B-C4B	2.58	1.45	1.41
8	M	401	U10	C4-C5	-2.56	1.41	1.48
6	L	301	07D	C3B-C4B	2.51	1.45	1.41
6	2	102	07D	C3B-C4B	2.50	1.45	1.41
7	M	405	08I	C4D-C3D	-2.50	1.39	1.44
7	L	302	08I	C4D-C3D	-2.46	1.39	1.44
6	S	101	07D	CHD-C1D	2.46	1.43	1.38
6	0	102	07D	C3B-C4B	2.45	1.45	1.41
6	Z	102	07D	C3B-C4B	2.44	1.45	1.41
12	M	406	RQ0	C46-C52	-2.43	1.39	1.46
6	M	403	07D	C3B-C4B	2.40	1.45	1.41
6	N	102	07D	C3B-C4B	2.40	1.45	1.41
6	L	307	07D	CHD-C1D	2.39	1.43	1.38
6	4	102	07D	C1D-C2D	-2.39	1.40	1.45
6	Y	101	07D	O1A-CGA	-2.38	1.15	1.22
6	X	102	07D	C3B-C4B	2.38	1.45	1.41
6	8	102	07D	C3B-C4B	2.37	1.45	1.41
6	M	403	07D	CHD-C1D	2.37	1.43	1.38
6	1	101	07D	C3B-C4B	2.36	1.45	1.41
6	4	102	07D	C3B-C4B	2.35	1.45	1.41
6	J	102	07D	C3D-C4D	-2.34	1.38	1.44
6	L	301	07D	CHD-C1D	2.33	1.42	1.38
6	6	102	07D	C3B-C4B	2.29	1.45	1.41
6	1	101	07D	CHD-C1D	2.27	1.42	1.38
6	V	102	07D	C3B-C4B	2.26	1.45	1.41
6	Q	102	07D	C3D-C4D	-2.26	1.39	1.44
6	G	102	07D	C3B-C4B	2.26	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	9	101	07D	C3D-C4D	-2.26	1.39	1.44
6	4	102	07D	C3D-C4D	-2.25	1.39	1.44
6	E	102	07D	C3B-C4B	2.25	1.45	1.41
6	U	101	07D	CHD-C1D	2.25	1.42	1.38
6	T	102	07D	C3D-C4D	-2.24	1.39	1.44
6	G	102	07D	C3D-C4D	-2.24	1.39	1.44
12	M	406	RQ0	C08-C12	2.23	1.61	1.53
6	0	102	07D	C3D-C4D	-2.23	1.39	1.44
6	X	102	07D	C3D-C4D	-2.23	1.39	1.44
6	M	404	07D	C3D-C4D	-2.23	1.39	1.44
12	M	406	RQ0	C26-C21	2.22	1.38	1.33
6	Q	102	07D	CHD-C1D	2.22	1.42	1.38
6	9	101	07D	CHD-C1D	2.22	1.42	1.38
6	8	102	07D	C3D-C4D	-2.21	1.39	1.44
8	L	303	U10	C4-C5	-2.21	1.42	1.48
6	U	101	07D	C3D-C4D	-2.21	1.39	1.44
6	E	102	07D	C3D-C4D	-2.21	1.39	1.44
6	3	101	07D	O1A-CGA	-2.21	1.16	1.22
6	Q	101	07D	CHD-C1D	2.21	1.42	1.38
6	B	101	07D	CHD-C1D	2.20	1.42	1.38
6	I	101	07D	O1A-CGA	-2.20	1.16	1.22
6	V	102	07D	C3D-C4D	-2.20	1.39	1.44
7	L	302	08I	CHA-CBD	2.20	1.54	1.51
6	6	102	07D	C1D-C2D	-2.20	1.41	1.45
6	3	101	07D	CHD-C1D	2.19	1.42	1.38
6	D	101	07D	C3D-C4D	-2.19	1.39	1.44
6	P	102	07D	C3D-C4D	-2.19	1.39	1.44
6	B	101	07D	C3B-C4B	2.18	1.45	1.41
6	Z	102	07D	C3D-C4D	-2.18	1.39	1.44
8	M	401	U10	C3-C2	-2.17	1.42	1.48
6	A	101	07D	C3D-C4D	-2.17	1.39	1.44
6	S	101	07D	C3D-C4D	-2.16	1.39	1.44
6	F	101	07D	C3D-C4D	-2.16	1.39	1.44
6	P	102	07D	CHD-C1D	2.15	1.42	1.38
6	2	102	07D	C3D-C4D	-2.14	1.39	1.44
6	L	301	07D	O1A-CGA	-2.14	1.16	1.22
6	M	404	07D	CBD-CGD	-2.14	1.45	1.52
6	M	403	07D	C3D-C4D	-2.13	1.39	1.44
6	7	101	07D	C3D-C4D	-2.13	1.39	1.44
6	K	101	07D	C3D-C4D	-2.13	1.39	1.44
6	5	202	07D	C3D-C4D	-2.13	1.39	1.44
6	B	101	07D	C3D-C4D	-2.13	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Y	101	07D	C3D-C4D	-2.13	1.39	1.44
6	Q	102	07D	C3B-C4B	2.13	1.45	1.41
6	J	102	07D	C1D-C2D	-2.12	1.41	1.45
6	L	307	07D	C3D-C4D	-2.12	1.39	1.44
6	X	102	07D	CHD-C1D	2.12	1.42	1.38
6	O	101	07D	C3D-C4D	-2.11	1.39	1.44
12	M	406	RQ0	C32-C31	2.11	1.38	1.33
6	N	102	07D	C3D-C4D	-2.11	1.39	1.44
12	M	406	RQ0	C57-C50	-2.11	1.46	1.50
6	0	102	07D	CHD-C1D	2.11	1.42	1.38
6	I	101	07D	C15-C13	2.10	1.55	1.51
6	I	101	07D	CHD-C1D	2.10	1.42	1.38
6	T	102	07D	C3B-C4B	2.10	1.44	1.41
6	6	102	07D	C3D-C4D	-2.10	1.39	1.44
6	W	101	07D	O1A-CGA	-2.10	1.16	1.22
6	T	102	07D	C1D-C2D	-2.09	1.41	1.45
6	E	102	07D	CHD-C1D	2.09	1.42	1.38
12	M	406	RQ0	C42-C35	2.09	1.38	1.33
6	D	101	07D	CHD-C1D	2.08	1.42	1.38
6	F	101	07D	C1D-C2D	-2.08	1.41	1.45
6	G	102	07D	CHD-C1D	2.08	1.42	1.38
6	O	101	07D	CHD-C1D	2.07	1.42	1.38
6	X	102	07D	C1D-C2D	-2.07	1.41	1.45
6	V	102	07D	C1D-C2D	-2.06	1.41	1.45
6	T	102	07D	CHD-C1D	2.06	1.42	1.38
6	L	301	07D	C1D-C2D	-2.06	1.41	1.45
6	I	101	07D	C3D-C4D	-2.06	1.39	1.44
6	L	301	07D	C3D-C4D	-2.05	1.39	1.44
6	2	102	07D	CHD-C1D	2.05	1.42	1.38
6	7	101	07D	CHD-C1D	2.04	1.42	1.38
12	M	406	RQ0	C24-C17	2.04	1.37	1.33
6	D	101	07D	C1D-C2D	-2.04	1.41	1.45
12	M	406	RQ0	C22-C13	2.04	1.37	1.33
6	L	307	07D	C3B-C4B	2.04	1.44	1.41
6	Y	101	07D	CHD-C1D	2.04	1.42	1.38
6	W	101	07D	C3D-C4D	-2.03	1.39	1.44
6	Q	101	07D	C3D-C4D	-2.03	1.39	1.44
6	O	101	07D	O1A-CGA	-2.03	1.16	1.22
6	K	101	07D	CHD-C1D	2.03	1.42	1.38
12	M	406	RQ0	C34-C43	2.03	1.57	1.50
6	Q	102	07D	C1D-C2D	-2.02	1.41	1.45
6	9	101	07D	O1A-CGA	-2.02	1.16	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	403	07D	O1A-CGA	-2.02	1.16	1.22
6	A	101	07D	CHD-C1D	2.02	1.42	1.38
12	M	406	RQ0	C43-C45	2.02	1.37	1.33
6	8	102	07D	C1D-C2D	-2.01	1.41	1.45
6	3	101	07D	C3D-C4D	-2.01	1.39	1.44
6	Z	102	07D	CHD-C1D	2.01	1.42	1.38
6	1	101	07D	C3D-C4D	-2.01	1.39	1.44
6	5	202	07D	C15-C13	2.01	1.55	1.51
6	5	202	07D	CHD-C1D	2.01	1.42	1.38
6	6	102	07D	CHD-C1D	2.00	1.42	1.38
12	M	406	RQ0	C30-C34	2.00	1.60	1.53

All (807) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	407	CRT	C2-C1-C4	-15.77	86.64	110.86
13	M	407	CRT	C3-C1-C4	-15.66	86.81	110.86
7	L	302	08I	C4D-CHA-CBD	-13.64	103.49	110.42
7	M	405	08I	C4D-CHA-CBD	-13.25	103.69	110.42
12	M	406	RQ0	C50-C46-C52	-8.47	111.60	119.58
6	T	102	07D	C11-C10-C8	7.01	136.03	112.98
7	M	405	08I	CMA-C3A-C2A	-6.87	111.98	124.94
7	L	302	08I	CMA-C3A-C2A	-6.76	112.20	124.94
6	8	102	07D	C11-C10-C8	6.52	134.43	112.98
7	M	405	08I	CMC-C2C-C3C	-5.99	113.65	124.94
13	T	101	CRT	C5-C6-C7	-5.96	116.88	125.89
6	B	101	07D	C16-C15-C13	5.84	132.18	112.98
6	8	102	07D	C6-C7-C8	5.79	141.60	127.66
6	I	101	07D	C16-C15-C13	5.75	131.91	112.98
6	M	403	07D	CHD-C1D-ND	-5.69	119.23	124.45
6	M	404	07D	C4D-CHA-C1A	5.61	128.08	121.25
12	M	406	RQ0	C54-C56-N04	5.48	128.15	114.38
13	M	407	CRT	C3-C1-C2	5.47	120.66	110.37
6	L	307	07D	CHD-C1D-ND	-5.43	119.47	124.45
6	D	101	07D	C4D-CHA-C1A	5.40	127.82	121.25
6	O	101	07D	C4D-CHA-C1A	5.37	127.78	121.25
7	L	302	08I	CMC-C2C-C3C	-5.37	114.82	124.94
6	B	101	07D	C4D-CHA-C1A	5.32	127.72	121.25
7	L	302	08I	CAA-C2A-C3A	-5.31	111.99	127.25
6	Q	102	07D	C4D-CHA-C1A	5.30	127.70	121.25
6	Q	101	07D	CHD-C1D-ND	-5.30	119.58	124.45
6	Q	101	07D	C4D-CHA-C1A	5.29	127.69	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	101	07D	C4D-CHA-C1A	5.29	127.69	121.25
6	U	101	07D	C4D-CHA-C1A	5.29	127.68	121.25
6	3	101	07D	C4D-CHA-C1A	5.25	127.64	121.25
6	9	101	07D	C4D-CHA-C1A	5.24	127.63	121.25
6	I	101	07D	C4D-CHA-C1A	5.22	127.60	121.25
6	7	101	07D	C4D-CHA-C1A	5.21	127.59	121.25
6	5	202	07D	C11-C10-C8	5.20	130.10	112.98
6	A	101	07D	C4D-CHA-C1A	5.20	127.57	121.25
6	K	101	07D	CHD-C1D-ND	-5.19	119.68	124.45
6	9	101	07D	CHD-C1D-ND	-5.19	119.69	124.45
6	4	102	07D	C4D-CHA-C1A	5.18	127.55	121.25
6	0	102	07D	C4D-CHA-C1A	5.18	127.55	121.25
6	5	202	07D	C4D-CHA-C1A	5.18	127.55	121.25
6	V	102	07D	C4D-CHA-C1A	5.17	127.54	121.25
6	X	102	07D	C4D-CHA-C1A	5.17	127.54	121.25
6	S	101	07D	C4D-CHA-C1A	5.17	127.54	121.25
13	M	407	CRT	C21-C22-C23	-5.16	119.94	127.31
6	T	102	07D	C4D-CHA-C1A	5.15	127.51	121.25
6	3	101	07D	CHD-C1D-ND	-5.14	119.73	124.45
6	0	102	07D	CHD-C1D-ND	-5.14	119.73	124.45
6	W	101	07D	C4D-CHA-C1A	5.14	127.51	121.25
6	S	101	07D	CHD-C1D-ND	-5.14	119.73	124.45
12	M	406	RQ0	O02-C52-C46	-5.14	112.53	121.55
6	A	101	07D	CHD-C1D-ND	-5.14	119.73	124.45
6	N	102	07D	C4D-CHA-C1A	5.14	127.50	121.25
6	K	101	07D	C4D-CHA-C1A	5.13	127.50	121.25
6	B	101	07D	CHD-C1D-ND	-5.13	119.74	124.45
6	8	102	07D	C4D-CHA-C1A	5.13	127.50	121.25
14	H	304	CDL	OB6-CB5-C51	5.12	120.51	111.09
6	U	101	07D	CHD-C1D-ND	-5.12	119.75	124.45
6	D	101	07D	CHD-C1D-ND	-5.12	119.75	124.45
6	O	101	07D	CHD-C1D-ND	-5.11	119.76	124.45
6	I	101	07D	CHD-C1D-ND	-5.11	119.76	124.45
6	F	101	07D	CHD-C1D-ND	-5.10	119.77	124.45
6	E	102	07D	C4D-CHA-C1A	5.10	127.45	121.25
6	M	403	07D	C4D-CHA-C1A	5.09	127.44	121.25
6	Z	102	07D	CHD-C1D-ND	-5.07	119.80	124.45
6	P	102	07D	C4D-CHA-C1A	5.07	127.41	121.25
6	G	102	07D	CHD-C1D-ND	-5.06	119.80	124.45
6	P	102	07D	CHD-C1D-ND	-5.05	119.81	124.45
7	M	405	08I	CAA-C2A-C3A	-5.05	112.73	127.25
6	5	202	07D	CHD-C1D-ND	-5.05	119.81	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	8	102	07D	CHD-C1D-ND	-5.03	119.83	124.45
6	T	102	07D	CHD-C1D-ND	-5.02	119.84	124.45
6	Q	102	07D	CHD-C1D-ND	-5.01	119.85	124.45
6	Y	101	07D	C4D-CHA-C1A	5.00	127.33	121.25
6	7	101	07D	CHD-C1D-ND	-5.00	119.86	124.45
6	V	102	07D	CHD-C1D-ND	-4.98	119.87	124.45
6	M	404	07D	CHD-C1D-ND	-4.98	119.88	124.45
6	Y	101	07D	CHD-C1D-ND	-4.98	119.88	124.45
6	E	102	07D	CHD-C1D-ND	-4.98	119.88	124.45
13	M	407	CRT	C20-C19-C17	-4.97	120.21	127.31
6	J	102	07D	CHD-C1D-ND	-4.95	119.90	124.45
6	2	102	07D	CHD-C1D-ND	-4.95	119.91	124.45
6	1	101	07D	C4D-CHA-C1A	4.92	127.24	121.25
6	L	307	07D	C11-C10-C8	4.91	129.14	112.98
6	G	102	07D	C4D-CHA-C1A	4.90	127.22	121.25
6	4	102	07D	CHD-C1D-ND	-4.90	119.95	124.45
6	X	102	07D	CHD-C1D-ND	-4.90	119.95	124.45
6	N	102	07D	CHD-C1D-ND	-4.87	119.98	124.45
6	6	102	07D	C4D-CHA-C1A	4.87	127.18	121.25
6	J	102	07D	C4D-CHA-C1A	4.86	127.16	121.25
6	Z	102	07D	C4D-CHA-C1A	4.86	127.16	121.25
6	L	307	07D	C4D-CHA-C1A	4.83	127.12	121.25
6	6	102	07D	CHD-C1D-ND	-4.80	120.04	124.45
6	W	101	07D	CHD-C1D-ND	-4.78	120.06	124.45
6	L	301	07D	CHD-C1D-ND	-4.77	120.07	124.45
13	M	407	CRT	C8-C7-C6	4.74	125.55	118.08
6	L	301	07D	C4D-CHA-C1A	4.70	126.97	121.25
6	B	101	07D	C1-C2-C3	-4.68	117.94	126.04
13	M	407	CRT	C5-C6-C7	4.65	132.92	125.89
13	X	101	CRT	C10-C9-C7	-4.64	120.69	127.31
6	1	101	07D	CHD-C1D-ND	-4.62	120.20	124.45
9	L	304	PGV	O01-C1-C2	4.60	121.41	111.50
14	H	303	CDL	OA6-CA5-C11	4.58	119.51	111.09
13	G	101	CRT	C15-C14-C12	-4.56	120.81	127.31
12	M	406	RQ0	C57-C50-C46	-4.50	117.06	124.40
13	2	101	CRT	C21-C22-C23	-4.50	120.89	127.31
13	V	101	CRT	C21-C22-C23	-4.49	120.90	127.31
7	L	302	08I	C1-C2-C3	-4.49	118.28	126.04
6	2	102	07D	C4D-CHA-C1A	4.49	126.71	121.25
13	G	101	CRT	C21-C22-C23	-4.49	120.91	127.31
14	H	301	CDL	OB6-CB5-C51	4.43	121.05	111.50
6	L	307	07D	C11-C12-C13	-4.43	116.99	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Z	101	CRT	C21-C22-C23	-4.42	121.00	127.31
6	N	102	07D	C11-C10-C8	-4.42	98.44	112.98
13	P	101	CRT	C10-C9-C7	-4.40	121.03	127.31
13	E	101	CRT	C21-C22-C23	-4.39	121.05	127.31
6	F	101	07D	C15-C16-C17	4.37	126.23	111.88
6	D	101	07D	C11-C10-C8	4.35	127.28	112.98
6	B	101	07D	C15-C16-C17	4.34	126.15	111.88
9	H	302	PGV	O01-C1-C2	4.33	120.83	111.50
6	2	102	07D	C11-C10-C8	4.30	127.13	112.98
13	8	101	CRT	C21-C22-C23	-4.29	121.19	127.31
14	M	408	CDL	OA6-CA5-C11	4.27	120.70	111.50
13	N	101	CRT	C10-C9-C7	-4.25	121.24	127.31
13	X	101	CRT	C20-C19-C17	-4.22	121.29	127.31
13	J	101	CRT	C21-C22-C23	-4.20	121.31	127.31
14	H	303	CDL	OB6-CB5-C51	4.20	120.55	111.50
6	5	202	07D	C16-C15-C13	4.19	126.75	112.98
12	M	406	RQ0	C07-C19-C27	4.19	125.36	118.94
7	M	405	08I	C2C-C1C-NC	4.18	112.41	109.53
15	K	103	PEF	O2-C10-C11	4.17	120.48	111.50
7	L	302	08I	C2C-C1C-NC	4.14	112.39	109.53
13	4	101	CRT	C21-C22-C23	-4.10	121.46	127.31
13	A	102	CRT	C21-C22-C23	-4.10	121.46	127.31
15	K	102	PEF	O2-C10-C11	4.08	120.29	111.50
6	L	307	07D	C1D-ND-C4D	-4.07	103.44	106.33
14	H	301	CDL	OA6-CA5-C11	4.06	120.25	111.50
13	X	101	CRT	C5-C6-C7	-4.02	119.82	125.89
13	G	101	CRT	C20-C19-C17	-4.01	121.58	127.31
13	N	101	CRT	C21-C22-C23	-4.00	121.60	127.31
13	P	101	CRT	C20-C19-C17	-4.00	121.60	127.31
6	1	101	07D	C16-C15-C13	3.99	126.10	112.98
14	M	409	CDL	OB6-CB5-C51	3.97	120.06	111.50
12	M	406	RQ0	C11-C07-C19	-3.95	115.32	126.42
13	P	101	CRT	C15-C14-C12	-3.92	121.71	127.31
13	2	101	CRT	C20-C19-C17	-3.90	121.74	127.31
13	V	101	CRT	C15-C14-C12	-3.90	121.74	127.31
7	L	302	08I	CBA-CAA-C2A	-3.89	105.98	112.62
13	R	101	CRT	C21-C22-C23	-3.89	121.76	127.31
13	T	101	CRT	C20-C19-C17	-3.89	121.76	127.31
9	L	304	PGV	C02-O01-C1	-3.86	108.28	117.79
13	4	101	CRT	C26-C27-C28	-3.85	121.81	127.31
6	F	101	07D	C1D-ND-C4D	-3.85	103.60	106.33
13	X	101	CRT	C21-C22-C23	-3.84	121.83	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	102	CRT	C10-C9-C7	-3.84	121.83	127.31
13	0	101	CRT	C21-C22-C23	-3.83	121.85	127.31
6	W	101	07D	C4A-NA-C1A	3.82	108.42	106.71
6	5	202	07D	C15-C16-C17	3.81	124.41	111.88
13	T	101	CRT	C10-C9-C7	-3.81	121.88	127.31
12	M	406	RQ0	C39-C19-C27	-3.80	117.60	122.92
6	F	101	07D	C4A-NA-C1A	3.80	108.42	106.71
13	4	101	CRT	C15-C14-C12	-3.79	121.90	127.31
7	M	405	08I	OBD-CAD-C3D	3.78	130.80	126.82
14	M	408	CDL	OB6-CB5-C51	3.77	119.62	111.50
6	M	404	07D	C4A-NA-C1A	3.75	108.39	106.71
6	A	101	07D	C1D-ND-C4D	-3.69	103.71	106.33
13	N	101	CRT	C5-C6-C7	-3.69	120.32	125.89
12	M	406	RQ0	C56-C54-C50	3.65	125.46	118.84
6	L	307	07D	C15-C16-C17	3.64	123.85	111.88
12	M	406	RQ0	O03-C54-C56	-3.64	112.98	118.29
6	1	101	07D	C15-C16-C17	3.63	123.82	111.88
6	D	101	07D	C1D-ND-C4D	-3.63	103.76	106.33
6	D	101	07D	C16-C15-C13	3.63	124.91	112.98
13	6	101	CRT	C5-C6-C7	-3.62	120.42	125.89
13	4	101	CRT	C20-C19-C17	-3.62	122.15	127.31
14	H	304	CDL	CB4-OB6-CB5	-3.62	111.16	117.90
13	6	101	CRT	C21-C22-C23	-3.61	122.15	127.31
6	I	101	07D	C1D-ND-C4D	-3.61	103.77	106.33
6	T	102	07D	C11-C12-C13	-3.61	118.96	127.66
13	M	407	CRT	C14-C15-C16	-3.60	111.97	123.22
6	9	101	07D	C1D-ND-C4D	-3.60	103.78	106.33
13	E	101	CRT	C8-C7-C6	3.58	123.72	118.08
6	D	101	07D	C4A-NA-C1A	3.58	108.32	106.71
13	Z	101	CRT	C20-C19-C17	-3.56	122.23	127.31
6	U	101	07D	C1D-ND-C4D	-3.55	103.81	106.33
6	O	101	07D	C1D-ND-C4D	-3.55	103.82	106.33
6	Q	101	07D	C6-C7-C8	3.54	136.19	127.66
13	6	101	CRT	C10-C9-C7	-3.54	122.26	127.31
6	X	102	07D	C1-C2-C3	-3.53	119.94	126.04
13	A	102	CRT	C20-C19-C17	-3.52	122.28	127.31
13	V	101	CRT	C10-C9-C7	-3.52	122.29	127.31
6	Y	101	07D	C6-C7-C8	-3.52	119.19	127.66
6	N	102	07D	C4A-NA-C1A	3.50	108.28	106.71
6	2	102	07D	C11-C12-C13	-3.50	119.24	127.66
6	S	101	07D	C1D-ND-C4D	-3.48	103.86	106.33
7	M	405	08I	C1D-C2D-C3D	-3.47	105.22	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	4	102	07D	C1D-ND-C4D	-3.46	103.87	106.33
13	V	101	CRT	C5-C6-C7	-3.46	120.66	125.89
6	M	403	07D	C1D-ND-C4D	-3.46	103.88	106.33
6	6	102	07D	C1D-ND-C4D	-3.45	103.89	106.33
6	Q	101	07D	C1D-ND-C4D	-3.44	103.89	106.33
6	Q	102	07D	C16-C15-C13	3.44	124.28	112.98
7	L	302	08I	C1D-C2D-C3D	-3.43	105.26	108.46
6	7	101	07D	C1D-ND-C4D	-3.43	103.90	106.33
14	H	304	CDL	OA6-CA5-C11	3.43	120.35	110.80
6	M	404	07D	C1D-ND-C4D	-3.42	103.90	106.33
6	Y	101	07D	C1D-ND-C4D	-3.41	103.91	106.33
6	J	102	07D	C11-C12-C13	-3.41	119.45	127.66
6	N	102	07D	C15-C16-C17	-3.39	100.73	111.88
13	J	101	CRT	C20-C19-C17	-3.39	122.47	127.31
6	4	102	07D	C4A-NA-C1A	3.39	108.23	106.71
6	K	101	07D	C1D-ND-C4D	-3.39	103.93	106.33
6	3	101	07D	C1D-ND-C4D	-3.38	103.93	106.33
6	Y	101	07D	C4A-NA-C1A	3.38	108.22	106.71
13	J	101	CRT	C5-C6-C7	-3.38	120.79	125.89
6	S	101	07D	C4A-NA-C1A	3.37	108.22	106.71
10	N	103	LMT	O1B-C4'-C3'	3.37	116.25	107.28
6	Q	102	07D	C11-C12-C13	-3.37	119.54	127.66
14	M	409	CDL	OA6-CA5-C11	3.37	118.76	111.50
6	5	202	07D	C6-C7-C8	-3.36	119.56	127.66
6	A	101	07D	C4A-NA-C1A	3.36	108.22	106.71
14	M	408	CDL	OB8-CB7-C71	3.36	122.45	111.91
7	L	302	08I	OBD-CAD-C3D	3.35	130.34	126.82
6	8	102	07D	C1D-ND-C4D	-3.35	103.96	106.33
13	P	101	CRT	C5-C6-C7	-3.34	120.84	125.89
6	1	101	07D	C4A-NA-C1A	3.32	108.20	106.71
6	E	102	07D	C1D-ND-C4D	-3.32	103.98	106.33
6	5	202	07D	C1D-ND-C4D	-3.29	104.00	106.33
6	P	102	07D	C1D-ND-C4D	-3.28	104.00	106.33
7	L	302	08I	C11-C10-C8	-3.28	102.18	112.98
13	8	101	CRT	C15-C14-C12	-3.28	122.63	127.31
13	E	101	CRT	C32-C31-C30	-3.28	113.00	123.22
6	L	301	07D	C1D-ND-C4D	-3.26	104.02	106.33
6	I	101	07D	C1-C2-C3	-3.26	120.41	126.04
6	V	102	07D	C1D-ND-C4D	-3.25	104.03	106.33
6	B	101	07D	C1D-ND-C4D	-3.24	104.03	106.33
13	T	101	CRT	C15-C14-C12	-3.23	122.70	127.31
6	0	102	07D	C1D-ND-C4D	-3.23	104.04	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	G	101	CRT	C5-C6-C7	-3.23	121.01	125.89
13	P	101	CRT	C21-C22-C23	-3.22	122.71	127.31
6	G	102	07D	C1D-ND-C4D	-3.22	104.05	106.33
6	Z	102	07D	C1D-ND-C4D	-3.21	104.05	106.33
6	J	102	07D	C1D-ND-C4D	-3.21	104.06	106.33
6	4	102	07D	CAB-C3B-C2B	3.20	133.14	128.34
6	4	102	07D	CHA-C1A-NA	-3.20	119.07	126.40
6	6	102	07D	C11-C10-C8	3.20	123.51	112.98
6	N	102	07D	C16-C15-C13	3.20	123.50	112.98
6	X	102	07D	C1D-ND-C4D	-3.20	104.06	106.33
6	Q	102	07D	C1D-ND-C4D	-3.19	104.07	106.33
6	N	102	07D	C1D-ND-C4D	-3.19	104.07	106.33
6	I	101	07D	C4A-NA-C1A	3.19	108.14	106.71
6	T	102	07D	C1D-ND-C4D	-3.19	104.07	106.33
13	8	101	CRT	C32-C31-C30	-3.17	113.32	123.22
13	8	101	CRT	C5-C6-C7	-3.16	121.11	125.89
6	W	101	07D	C1D-ND-C4D	-3.16	104.09	106.33
6	2	102	07D	C1D-ND-C4D	-3.15	104.09	106.33
13	0	101	CRT	C32-C31-C30	-3.15	113.39	123.22
13	0	101	CRT	C15-C14-C12	-3.15	122.82	127.31
12	M	406	RQ0	C06-C09-C22	3.15	122.22	111.88
6	Z	102	07D	CHA-C1A-NA	-3.14	119.20	126.40
13	4	101	CRT	C10-C9-C7	-3.14	122.82	127.31
6	J	102	07D	C14-C13-C15	-3.14	110.00	115.27
6	2	102	07D	C2A-C1A-CHA	3.14	129.34	123.86
6	J	102	07D	CHA-C1A-NA	-3.13	119.23	126.40
6	M	403	07D	C4A-NA-C1A	3.12	108.11	106.71
6	4	102	07D	C1-C2-C3	-3.11	120.67	126.04
6	M	404	07D	CHA-C1A-NA	-3.09	119.31	126.40
13	X	101	CRT	C15-C14-C12	-3.09	122.90	127.31
6	2	102	07D	CHA-C1A-NA	-3.09	119.32	126.40
13	2	101	CRT	C5-C6-C7	-3.08	121.24	125.89
6	X	102	07D	CHA-C1A-NA	-3.08	119.35	126.40
7	M	405	08I	C15-C16-C17	3.08	122.00	111.88
10	V	103	LMT	C1B-O1B-C4'	-3.08	110.35	117.96
6	1	101	07D	C1D-ND-C4D	-3.08	104.15	106.33
6	Q	101	07D	CHA-C1A-NA	-3.07	119.36	126.40
6	1	101	07D	CHA-C1A-NA	-3.07	119.36	126.40
6	W	101	07D	CHA-C1A-NA	-3.06	119.39	126.40
6	L	307	07D	C4A-NA-C1A	3.06	108.08	106.71
13	Z	101	CRT	C26-C27-C28	-3.06	122.94	127.31
10	L	305	LMT	C1B-O1B-C4'	-3.06	110.40	117.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	101	07D	CHA-C1A-NA	-3.05	119.41	126.40
6	O	101	07D	CHA-C1A-NA	-3.05	119.41	126.40
6	U	101	07D	CHA-C1A-NA	-3.05	119.42	126.40
13	R	101	CRT	C15-C14-C12	-3.05	122.96	127.31
6	Q	102	07D	CHA-C1A-NA	-3.04	119.43	126.40
6	5	202	07D	CHA-C1A-NA	-3.04	119.43	126.40
6	K	101	07D	C6-C7-C8	3.04	134.99	127.66
13	V	101	CRT	C20-C19-C17	-3.04	122.97	127.31
13	X	101	CRT	C32-C31-C30	-3.04	113.74	123.22
6	6	102	07D	CHA-C1A-NA	-3.03	119.46	126.40
6	N	102	07D	CHA-C1A-NA	-3.02	119.47	126.40
6	G	102	07D	CHA-C1A-NA	-3.01	119.50	126.40
6	P	102	07D	CHA-C1A-NA	-3.01	119.52	126.40
13	E	101	CRT	C9-C10-C11	-3.00	113.84	123.22
6	B	101	07D	C14-C13-C15	-3.00	110.22	115.27
13	G	101	CRT	C10-C9-C7	-3.00	123.02	127.31
6	T	102	07D	CHA-C1A-NA	-3.00	119.53	126.40
6	3	101	07D	CHA-C1A-NA	-3.00	119.54	126.40
6	F	101	07D	CHA-C1A-NA	-3.00	119.54	126.40
6	W	101	07D	CAB-C3B-C2B	2.99	132.82	128.34
6	A	101	07D	CHA-C1A-NA	-2.99	119.56	126.40
13	G	101	CRT	C32-C31-C30	-2.99	113.90	123.22
6	8	102	07D	CHA-C1A-NA	-2.98	119.56	126.40
6	W	101	07D	C15-C16-C17	2.98	121.67	111.88
13	R	101	CRT	C32-C31-C30	-2.97	113.94	123.22
6	7	101	07D	C6-C7-C8	-2.97	120.50	127.66
6	7	101	07D	CHA-C1A-NA	-2.97	119.60	126.40
13	0	101	CRT	C10-C9-C7	-2.97	123.07	127.31
6	I	101	07D	CHA-C1A-NA	-2.96	119.61	126.40
6	0	102	07D	CHA-C1A-NA	-2.96	119.62	126.40
13	V	101	CRT	C32-C31-C30	-2.95	114.00	123.22
6	V	102	07D	CHA-C1A-NA	-2.95	119.63	126.40
6	E	102	07D	CHA-C1A-NA	-2.95	119.64	126.40
12	M	406	RQ0	C08-C12-C26	2.94	121.56	111.88
13	E	101	CRT	C20-C19-C17	-2.94	123.11	127.31
9	H	302	PGV	O03-C19-C20	2.94	121.12	111.91
13	R	101	CRT	C10-C9-C7	-2.93	123.12	127.31
6	P	102	07D	C2A-C1A-CHA	2.93	128.99	123.86
14	M	408	CDL	OA8-CA7-C31	2.93	121.11	111.91
6	O	101	07D	C4A-NA-C1A	2.93	108.02	106.71
6	M	403	07D	C2A-C1A-CHA	2.93	128.98	123.86
6	T	102	07D	C4A-NA-C1A	2.93	108.02	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	101	07D	C15-C16-C17	2.93	121.51	111.88
13	6	101	CRT	C15-C14-C12	-2.93	123.14	127.31
6	S	101	07D	CHA-C1A-NA	-2.92	119.70	126.40
6	U	101	07D	C4A-NA-C1A	2.91	108.02	106.71
6	8	102	07D	C11-C12-C13	-2.91	120.65	127.66
13	J	101	CRT	C32-C31-C30	-2.91	114.13	123.22
6	9	101	07D	CHA-C1A-NA	-2.91	119.74	126.40
6	F	101	07D	CAB-C3B-C2B	2.91	132.69	128.34
6	B	101	07D	CHA-C1A-NA	-2.90	119.75	126.40
6	V	102	07D	C4A-NA-C1A	2.90	108.01	106.71
6	M	403	07D	CHA-C1A-NA	-2.89	119.79	126.40
6	Y	101	07D	CAB-C3B-C2B	2.87	132.64	128.34
6	S	101	07D	C11-C12-C13	-2.87	120.75	127.66
6	Y	101	07D	CHA-C1A-NA	-2.87	119.84	126.40
6	4	102	07D	C11-C12-C13	-2.86	120.77	127.66
12	M	406	RQ0	C18-C14-C23	-2.86	118.37	126.42
6	N	102	07D	CAB-C3B-C2B	2.86	132.62	128.34
13	T	101	CRT	C21-C22-C23	-2.86	123.23	127.31
13	Z	101	CRT	C8-C7-C6	2.86	122.58	118.08
6	0	102	07D	CAB-C3B-C2B	2.86	132.62	128.34
6	0	102	07D	C6-C7-C8	-2.85	120.79	127.66
14	H	301	CDL	OB8-CB7-C71	2.85	120.86	111.91
6	6	102	07D	CAB-C3B-C2B	2.85	132.61	128.34
6	G	102	07D	C4A-NA-C1A	2.85	107.99	106.71
6	8	102	07D	C2A-C1A-CHA	2.85	128.84	123.86
6	M	404	07D	C16-C15-C13	2.85	122.34	112.98
6	G	102	07D	C2A-C1A-CHA	2.84	128.82	123.86
6	L	307	07D	C6-C7-C8	-2.83	120.84	127.66
6	V	102	07D	C1-C2-C3	-2.83	121.15	126.04
6	Z	102	07D	C11-C12-C13	-2.83	120.85	127.66
6	K	101	07D	CHA-C1A-NA	-2.83	119.93	126.40
6	Q	101	07D	CAB-C3B-C2B	2.82	132.57	128.34
6	9	101	07D	CAB-C3B-C2B	2.82	132.57	128.34
6	G	102	07D	CAB-C3B-C2B	2.82	132.56	128.34
6	J	102	07D	C11-C10-C8	2.82	122.25	112.98
15	K	103	PEF	O3-C30-C31	2.82	120.75	111.91
9	H	302	PGV	C02-O01-C1	-2.82	110.85	117.79
6	T	102	07D	C2A-C1A-CHA	2.82	128.78	123.86
6	K	101	07D	C4A-NA-C1A	2.82	107.97	106.71
13	P	101	CRT	C31-C32-C33	-2.81	123.30	127.31
6	W	101	07D	CHC-C4B-NB	-2.81	121.28	124.26
6	L	301	07D	CHA-C1A-NA	-2.81	119.96	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	2	101	CRT	C10-C9-C7	-2.80	123.31	127.31
6	B	101	07D	C4A-NA-C1A	2.79	107.96	106.71
13	M	407	CRT	C32-C31-C30	-2.79	114.52	123.22
6	L	301	07D	CAB-C3B-C2B	2.78	132.51	128.34
13	6	101	CRT	C20-C19-C17	-2.78	123.34	127.31
6	P	102	07D	C11-C10-C8	2.78	122.12	112.98
13	8	101	CRT	C10-C9-C7	-2.78	123.34	127.31
6	X	102	07D	C11-C12-C13	-2.78	120.97	127.66
6	L	307	07D	CHA-C1A-NA	-2.77	120.05	126.40
6	E	102	07D	C2A-C1A-CHA	2.77	128.70	123.86
6	1	101	07D	C2A-C1A-CHA	2.76	128.69	123.86
6	U	101	07D	C2A-C1A-CHA	2.76	128.68	123.86
6	Q	101	07D	CHC-C4B-NB	-2.74	121.35	124.26
6	W	101	07D	C2A-C1A-CHA	2.74	128.65	123.86
6	K	101	07D	C1-C2-C3	-2.73	121.32	126.04
6	5	202	07D	CAB-C3B-C2B	2.73	132.43	128.34
6	A	101	07D	CHC-C4B-NB	-2.73	121.37	124.26
6	L	301	07D	C2A-C1A-CHA	2.72	128.62	123.86
6	I	101	07D	C2A-C1A-CHA	2.72	128.62	123.86
13	N	101	CRT	C32-C31-C30	-2.72	114.72	123.22
6	L	301	07D	C4A-NA-C1A	2.72	107.93	106.71
12	M	406	RQ0	C05-C10-C24	2.72	120.82	111.88
6	X	102	07D	C6-C7-C8	2.72	134.21	127.66
6	9	101	07D	CHC-C4B-NB	-2.72	121.38	124.26
13	0	101	CRT	C20-C19-C17	-2.72	123.43	127.31
6	X	102	07D	C2A-C1A-CHA	2.71	128.61	123.86
6	O	101	07D	CAB-C3B-C2B	2.71	132.41	128.34
15	K	102	PEF	O3-C30-C31	2.71	120.41	111.91
6	I	101	07D	CAB-C3B-C2B	2.70	132.39	128.34
13	T	101	CRT	C32-C31-C30	-2.70	114.78	123.22
6	9	101	07D	C4A-NA-C1A	2.70	107.92	106.71
6	M	403	07D	C11-C10-C8	2.69	121.83	112.98
6	J	102	07D	C2A-C1A-CHA	2.69	128.56	123.86
6	1	101	07D	CAB-C3B-C2B	2.69	132.37	128.34
6	P	102	07D	C1C-NC-C4C	2.69	107.91	106.71
6	Q	102	07D	C4A-NA-C1A	2.69	107.91	106.71
14	M	409	CDL	OB8-CB7-C71	2.69	120.33	111.91
7	M	405	08I	C3C-C4C-NC	2.69	111.38	109.53
6	A	101	07D	C2A-C1A-CHA	2.69	128.55	123.86
6	S	101	07D	CAB-C3B-C2B	2.68	132.36	128.34
6	4	102	07D	C2A-C1A-CHA	2.68	128.55	123.86
13	N	101	CRT	C20-C19-C17	-2.68	123.49	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	101	07D	C2A-C1A-CHA	2.68	128.54	123.86
6	5	202	07D	CHC-C4B-NB	-2.68	121.42	124.26
12	M	406	RQ0	C29-C28-C33	2.67	120.66	111.88
6	Y	101	07D	CHC-C4B-NB	-2.66	121.44	124.26
6	Z	102	07D	C2A-C1A-CHA	2.66	128.51	123.86
6	S	101	07D	CHC-C4B-NB	-2.66	121.44	124.26
13	M	407	CRT	C34-C33-C35	2.66	122.27	118.08
6	U	101	07D	CHC-C4B-NB	-2.66	121.44	124.26
13	J	101	CRT	C10-C9-C7	-2.66	123.51	127.31
10	0	103	LMT	C1B-O1B-C4'	-2.65	111.40	117.96
6	U	101	07D	CAB-C3B-C2B	2.65	132.31	128.34
6	A	101	07D	CAB-C3B-C2B	2.65	132.31	128.34
6	2	102	07D	C4A-NA-C1A	2.63	107.89	106.71
13	Z	101	CRT	C32-C31-C30	-2.63	115.00	123.22
13	M	407	CRT	C13-C12-C11	2.63	122.22	118.08
13	E	101	CRT	C6-C7-C9	-2.62	114.92	118.94
6	7	101	07D	C1C-NC-C4C	2.62	107.89	106.71
6	B	101	07D	CAB-C3B-C2B	2.62	132.27	128.34
6	D	101	07D	CHC-C4B-NB	-2.62	121.48	124.26
10	M	410	LMT	C2'-C3'-C4'	2.62	115.66	109.68
6	7	101	07D	CHC-C4B-NB	-2.61	121.49	124.26
6	E	102	07D	CAB-C3B-C2B	2.61	132.25	128.34
6	3	101	07D	CHC-C4B-NB	-2.61	121.49	124.26
10	N	103	LMT	C1'-C2'-C3'	2.61	115.44	110.00
6	V	102	07D	CAB-C3B-C2B	2.61	132.25	128.34
13	A	102	CRT	C5-C6-C7	-2.61	121.94	125.89
13	J	101	CRT	C26-C27-C28	-2.61	123.59	127.31
6	7	101	07D	C2A-C1A-CHA	2.60	128.41	123.86
6	V	102	07D	C2A-C1A-CHA	2.60	128.40	123.86
14	H	301	CDL	OA8-CA7-C31	2.60	120.06	111.91
6	3	101	07D	C1C-NC-C4C	2.59	107.87	106.71
13	R	101	CRT	C5-C6-C7	-2.59	121.98	125.89
6	S	101	07D	C2A-C1A-CHA	2.58	128.37	123.86
6	L	307	07D	C2A-C1A-CHA	2.57	128.36	123.86
6	0	102	07D	C4A-NA-C1A	2.57	107.86	106.71
13	T	101	CRT	C34-C33-C35	2.57	122.13	118.08
6	4	102	07D	CHC-C4B-NB	-2.57	121.54	124.26
13	E	101	CRT	C5-C6-C7	2.57	129.77	125.89
6	K	101	07D	CHC-C4B-NB	-2.57	121.54	124.26
6	M	404	07D	CMB-C2B-C1B	-2.57	121.46	125.37
6	B	101	07D	C1C-NC-C4C	2.56	107.86	106.71
7	L	302	08I	C3A-C4A-NA	2.56	111.30	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	V	102	07D	C16-C15-C13	2.56	121.41	112.98
13	8	101	CRT	C20-C19-C17	-2.56	123.66	127.31
6	O	101	07D	C6-C7-C8	-2.56	121.50	127.66
13	M	407	CRT	C6-C7-C9	-2.56	115.02	118.94
6	7	101	07D	CAB-C3B-C2B	2.55	132.16	128.34
14	H	303	CDL	OA8-CA7-C31	2.55	119.92	111.91
6	Q	101	07D	C2A-C1A-CHA	2.55	128.32	123.86
12	M	406	RQ0	C15-C20-C32	2.55	120.25	111.88
6	O	101	07D	CHC-C4B-NB	-2.54	121.56	124.26
13	V	101	CRT	C36-C35-C33	-2.54	122.05	125.89
6	I	101	07D	CHC-C4B-NB	-2.54	121.56	124.26
13	E	101	CRT	C27-C26-C25	-2.54	115.30	123.22
6	5	202	07D	C14-C13-C15	-2.53	111.01	115.27
13	6	101	CRT	C26-C27-C28	-2.53	123.69	127.31
13	A	102	CRT	C14-C15-C16	-2.53	115.32	123.22
14	M	409	CDL	OA8-CA7-C31	2.53	119.85	111.91
6	E	102	07D	C1C-NC-C4C	2.53	107.84	106.71
6	6	102	07D	C6-C5-C3	2.53	121.28	112.98
6	M	404	07D	CHC-C4B-NB	-2.52	121.59	124.26
6	F	101	07D	C2A-C1A-CHA	2.52	128.27	123.86
6	6	102	07D	C2A-C1A-CHA	2.52	128.27	123.86
13	M	407	CRT	C8-C7-C9	-2.52	119.40	122.92
6	K	101	07D	C2A-C1A-CHA	2.52	128.26	123.86
6	Q	102	07D	CAB-C3B-C2B	2.51	132.11	128.34
13	2	101	CRT	C15-C14-C12	-2.51	123.72	127.31
13	V	101	CRT	C27-C26-C25	-2.51	115.38	123.22
6	I	101	07D	C1C-NC-C4C	2.51	107.83	106.71
6	U	101	07D	C1C-NC-C4C	2.51	107.83	106.71
13	A	102	CRT	C31-C32-C33	-2.51	123.73	127.31
14	M	409	CDL	CB4-OB6-CB5	-2.51	111.62	117.79
13	Z	101	CRT	C10-C9-C7	-2.51	123.73	127.31
6	A	101	07D	C11-C10-C8	2.51	121.22	112.98
6	5	202	07D	C4A-NA-C1A	2.50	107.83	106.71
6	M	404	07D	CAB-C3B-C2B	2.49	132.08	128.34
13	A	102	CRT	C27-C26-C25	-2.49	115.44	123.22
6	M	404	07D	C2A-C1A-CHA	2.49	128.22	123.86
6	F	101	07D	CHC-C4B-NB	-2.49	121.62	124.26
6	9	101	07D	C2A-C1A-CHA	2.48	128.20	123.86
6	Q	101	07D	C1-C2-C3	2.48	130.33	126.04
13	M	407	CRT	C9-C10-C11	-2.48	115.48	123.22
6	Y	101	07D	C11-C10-C8	2.47	121.11	112.98
6	2	102	07D	CHC-C4B-NB	-2.47	121.64	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	8	102	07D	C10-C8-C7	-2.47	116.12	121.12
6	1	101	07D	CAA-CBA-CGA	2.45	120.43	113.25
7	M	405	08I	OBb-CAB-C3B	2.45	123.84	120.77
6	N	102	07D	C2A-C1A-CHA	2.45	128.14	123.86
6	G	102	07D	CHC-C4B-NB	-2.45	121.67	124.26
6	J	102	07D	CHC-C4B-NB	-2.45	121.67	124.26
13	G	101	CRT	C26-C27-C28	-2.44	123.82	127.31
6	D	101	07D	CAB-C3B-C2B	2.44	132.00	128.34
6	Y	101	07D	C2A-C1A-CHA	2.44	128.13	123.86
6	K	101	07D	CAB-C3B-C2B	2.44	131.99	128.34
6	A	101	07D	CMB-C2B-C1B	-2.43	121.66	125.37
13	G	101	CRT	C29-C28-C30	2.43	121.91	118.08
6	0	102	07D	C2A-C1A-CHA	2.43	128.11	123.86
6	3	101	07D	CAB-C3B-C2B	2.43	131.97	128.34
6	3	101	07D	C1-C2-C3	2.42	130.23	126.04
6	5	202	07D	C2A-C1A-CHA	2.42	128.09	123.86
6	Y	101	07D	O2A-CGA-O1A	-2.42	117.48	123.59
6	U	101	07D	C15-C16-C17	2.42	119.83	111.88
6	J	102	07D	C15-C13-C12	2.42	126.01	121.12
7	L	302	08I	C16-C15-C13	2.41	120.92	112.98
6	9	101	07D	O2A-C1-C2	-2.41	102.29	108.64
6	8	102	07D	C4A-NA-C1A	2.41	107.79	106.71
13	G	101	CRT	C34-C33-C35	2.41	121.88	118.08
13	P	101	CRT	C32-C31-C30	-2.41	115.69	123.22
7	L	302	08I	C3C-C4C-NC	2.41	111.19	109.53
13	R	101	CRT	C34-C33-C35	2.41	121.88	118.08
13	R	101	CRT	C27-C26-C25	-2.41	115.70	123.22
10	5	201	LMT	O1B-C4'-C3'	2.41	113.69	107.28
6	1	101	07D	C6-C7-C8	-2.41	121.87	127.66
13	4	101	CRT	C32-C31-C30	-2.41	115.71	123.22
6	Q	101	07D	OBb-CAB-CBB	-2.40	114.41	119.73
6	P	102	07D	CHC-C4B-NB	-2.40	121.72	124.26
13	N	101	CRT	C34-C33-C35	2.40	121.85	118.08
6	O	101	07D	C11-C12-C13	-2.40	121.89	127.66
13	A	102	CRT	C21-C20-C19	-2.39	118.57	123.47
6	E	102	07D	C4A-NA-C1A	2.39	107.78	106.71
15	K	103	PEF	C2-O2-C10	-2.39	111.90	117.79
12	M	406	RQ0	O01-C55-C52	2.39	124.65	116.56
6	Y	101	07D	OBb-CAB-CBB	-2.39	114.43	119.73
6	Q	102	07D	C2A-C1A-CHA	2.39	128.04	123.86
6	4	102	07D	C11-C10-C8	-2.39	105.12	112.98
13	V	101	CRT	C29-C28-C30	2.39	121.84	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	101	07D	C2A-C1A-CHA	2.38	128.03	123.86
6	S	101	07D	CMB-C2B-C1B	-2.38	121.74	125.37
6	N	102	07D	CHC-C4B-NB	-2.38	121.73	124.26
9	L	304	PGV	O03-C19-C20	2.38	119.39	111.91
6	U	101	07D	CBA-CAA-C2A	-2.38	106.83	113.86
6	Z	102	07D	CHC-C4B-NB	-2.38	121.74	124.26
12	M	406	RQ0	C29-C35-C42	2.38	125.93	121.12
13	T	101	CRT	C27-C26-C25	-2.37	115.81	123.22
13	P	101	CRT	C36-C35-C33	-2.37	122.31	125.89
6	F	101	07D	C11-C10-C8	2.37	120.78	112.98
10	V	103	LMT	C1'-C2'-C3'	2.37	114.93	110.00
6	W	101	07D	C4B-C3B-C2B	-2.37	104.55	108.36
6	4	102	07D	C1-O2A-CGA	2.37	122.66	116.44
12	M	406	RQ0	C44-C23-C33	-2.37	118.95	123.59
6	Q	101	07D	C4B-C3B-C2B	-2.36	104.56	108.36
6	W	101	07D	CMB-C2B-C1B	-2.36	121.77	125.37
6	V	102	07D	C6-C7-C8	-2.36	121.97	127.66
13	E	101	CRT	C21-C20-C19	-2.36	118.64	123.47
13	0	101	CRT	C34-C33-C35	2.36	121.79	118.08
6	W	101	07D	OBb-CAB-CBB	-2.36	114.51	119.73
6	X	102	07D	CAB-C3B-C2B	2.35	131.86	128.34
6	N	102	07D	C6-C7-C8	-2.35	122.00	127.66
13	6	101	CRT	C36-C35-C33	-2.34	122.36	125.89
6	1	101	07D	CHC-C4B-NB	-2.33	121.79	124.26
6	B	101	07D	C16-C17-C18	-2.33	119.79	127.75
13	V	101	CRT	C21-C20-C19	-2.33	118.71	123.47
13	2	101	CRT	C26-C27-C28	-2.33	123.99	127.31
6	U	101	07D	CMB-C2B-C1B	-2.33	121.83	125.37
6	9	101	07D	OBb-CAB-CBB	-2.33	114.58	119.73
6	F	101	07D	OBb-CAB-CBB	-2.32	114.58	119.73
6	A	101	07D	C1C-NC-C4C	2.32	107.75	106.71
6	3	101	07D	C4A-NA-C1A	2.32	107.75	106.71
6	Q	101	07D	CMB-C2B-C1B	-2.32	121.83	125.37
6	P	102	07D	C16-C15-C13	2.32	120.61	112.98
12	M	406	RQ0	C46-C50-C54	2.32	121.02	119.18
6	B	101	07D	C15-C13-C12	2.32	125.81	121.12
6	A	101	07D	C4B-C3B-C2B	-2.31	104.64	108.36
6	L	301	07D	C16-C15-C13	2.31	120.58	112.98
6	G	102	07D	C11-C12-C13	-2.31	122.10	127.66
13	A	102	CRT	C32-C31-C30	-2.31	116.01	123.22
6	6	102	07D	C1C-NC-C4C	2.31	107.74	106.71
13	J	101	CRT	C21-C20-C19	-2.31	118.75	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	102	07D	C15-C13-C12	-2.31	116.45	121.12
13	Z	101	CRT	C8-C7-C9	-2.30	119.69	122.92
6	9	101	07D	C15-C13-C12	2.30	125.77	121.12
6	2	102	07D	C1C-NC-C4C	2.30	107.74	106.71
6	V	102	07D	CHC-C4B-NB	-2.30	121.82	124.26
13	0	101	CRT	C27-C26-C25	-2.30	116.05	123.22
6	E	102	07D	CHC-C4B-NB	-2.29	121.83	124.26
6	9	101	07D	C4B-C3B-C2B	-2.29	104.67	108.36
10	T	103	LMT	O3'-C3'-C2'	-2.29	105.05	110.35
6	I	101	07D	OB8-CAB-CBB	-2.29	114.65	119.73
14	M	408	CDL	OB8-CB7-OB9	-2.29	117.81	123.59
6	I	101	07D	C4B-C3B-C2B	-2.29	104.67	108.36
6	K	101	07D	CMB-C2B-C1B	-2.29	121.89	125.37
6	Y	101	07D	C4B-C3B-C2B	-2.29	104.68	108.36
6	L	307	07D	C14-C13-C15	-2.28	111.43	115.27
6	7	101	07D	CMB-C2B-C1B	-2.28	121.89	125.37
13	Z	101	CRT	C15-C14-C12	-2.28	124.05	127.31
13	2	101	CRT	C34-C33-C35	2.28	121.67	118.08
14	M	408	CDL	CA4-OA6-CA5	-2.28	112.18	117.79
7	L	302	08I	C15-C13-C12	-2.28	116.51	121.12
6	G	102	07D	C1C-NC-C4C	2.28	107.73	106.71
6	0	102	07D	C1-C2-C3	-2.28	122.11	126.04
10	N	103	LMT	O3'-C3'-C2'	-2.28	105.09	110.35
6	N	102	07D	C1-C2-C3	-2.27	122.11	126.04
6	O	101	07D	OB8-CAB-CBB	-2.27	114.69	119.73
6	5	202	07D	C4B-C3B-C2B	-2.27	104.70	108.36
6	F	101	07D	C4B-C3B-C2B	-2.27	104.70	108.36
6	L	307	07D	CHC-C4B-NB	-2.27	121.85	124.26
13	G	101	CRT	C27-C26-C25	-2.27	116.13	123.22
6	L	301	07D	CHC-C4B-NB	-2.27	121.86	124.26
6	K	101	07D	C4B-C3B-C2B	-2.27	104.71	108.36
6	S	101	07D	C4B-C3B-C2B	-2.27	104.71	108.36
13	M	407	CRT	C26-C27-C28	-2.27	124.07	127.31
13	E	101	CRT	C35-C33-C32	-2.27	115.46	118.94
10	V	103	LMT	O5'-C1'-C2'	2.27	115.14	110.35
6	D	101	07D	CMB-C2B-C1B	-2.26	121.92	125.37
6	M	404	07D	C4B-C3B-C2B	-2.26	104.72	108.36
6	Q	101	07D	C1C-NC-C4C	2.26	107.72	106.71
6	8	102	07D	C6-C5-C3	2.26	120.42	112.98
6	0	102	07D	C1C-NC-C4C	2.26	107.72	106.71
6	5	202	07D	CMB-C2B-C1B	-2.26	121.93	125.37
6	Q	102	07D	CHC-C4B-NB	-2.26	121.87	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	102	07D	CHC-C4B-NB	-2.26	121.87	124.26
6	6	102	07D	CHC-C4B-NB	-2.26	121.87	124.26
6	D	101	07D	C1C-NC-C4C	2.26	107.72	106.71
6	E	102	07D	C11-C10-C8	2.26	120.40	112.98
10	X	103	LMT	C1B-O1B-C4'	-2.25	112.39	117.96
13	8	101	CRT	C34-C33-C35	2.25	121.62	118.08
6	B	101	07D	CHC-C4B-NB	-2.25	121.88	124.26
6	K	101	07D	OB B-CAB-CBB	-2.24	114.76	119.73
6	B	101	07D	C2A-C1A-CHA	2.24	127.78	123.86
6	6	102	07D	C16-C15-C13	2.24	120.34	112.98
6	M	404	07D	C6-C7-C8	-2.24	122.27	127.66
6	7	101	07D	C4B-C3B-C2B	-2.24	104.76	108.36
13	N	101	CRT	C27-C26-C25	-2.24	116.23	123.22
6	5	202	07D	C1-O2A-CGA	2.24	122.32	116.44
6	K	101	07D	C1C-NC-C4C	2.24	107.71	106.71
6	7	101	07D	C4A-NA-C1A	2.24	107.71	106.71
6	U	101	07D	C4B-C3B-C2B	-2.24	104.76	108.36
13	0	101	CRT	C29-C28-C30	2.24	121.60	118.08
6	X	102	07D	CHC-C4B-NB	-2.24	121.89	124.26
6	M	404	07D	OB B-CAB-CBB	-2.23	114.78	119.73
13	6	101	CRT	C31-C32-C33	-2.23	124.12	127.31
6	I	101	07D	CMB-C2B-C1B	-2.23	121.97	125.37
6	U	101	07D	OB B-CAB-CBB	-2.23	114.79	119.73
6	0	102	07D	CHC-C4B-NB	-2.23	121.89	124.26
6	D	101	07D	C11-C12-C13	-2.23	122.29	127.66
6	N	102	07D	C1C-NC-C4C	2.23	107.71	106.71
6	D	101	07D	C4B-C3B-C2B	-2.23	104.77	108.36
6	S	101	07D	C15-C16-C17	2.23	119.21	111.88
13	M	407	CRT	C11-C12-C14	-2.23	115.52	118.94
13	N	101	CRT	C21-C20-C19	-2.23	118.91	123.47
6	9	101	07D	C1C-NC-C4C	2.23	107.71	106.71
13	X	101	CRT	C8-C7-C9	-2.23	119.81	122.92
6	8	102	07D	CHC-C4B-NB	-2.22	121.90	124.26
6	9	101	07D	C14-C13-C15	-2.22	111.53	115.27
6	O	101	07D	C4B-C3B-C2B	-2.22	104.78	108.36
13	E	101	CRT	C34-C33-C35	2.22	121.58	118.08
6	3	101	07D	CMB-C2B-C1B	-2.22	121.99	125.37
14	H	303	CDL	OB8-CB7-C71	2.22	118.88	111.91
6	7	101	07D	OB B-CAB-CBB	-2.22	114.81	119.73
13	V	101	CRT	C18-C17-C16	2.22	121.58	118.08
10	8	103	LMT	O1B-C4'-C3'	2.22	113.19	107.28
6	L	307	07D	C15-C13-C12	2.22	125.61	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	202	07D	O2A-C1-C2	-2.22	102.81	108.64
6	9	101	07D	CMB-C2B-C1B	-2.22	121.99	125.37
6	L	301	07D	OBb-CAB-CBB	-2.22	114.82	119.73
13	E	101	CRT	C29-C28-C30	2.22	121.57	118.08
6	D	101	07D	OBb-CAB-CBB	-2.21	114.83	119.73
6	K	101	07D	C11-C10-C8	2.21	120.26	112.98
12	M	406	RQ0	C48-C31-C32	-2.21	118.00	123.68
14	H	303	CDL	CB6-CB4-CB3	-2.21	106.56	111.79
6	5	202	07D	OBb-CAB-CBB	-2.21	114.84	119.73
6	T	102	07D	C14-C13-C15	-2.20	111.56	115.27
6	8	102	07D	C1C-NC-C4C	2.20	107.70	106.71
6	O	101	07D	C1C-NC-C4C	2.20	107.70	106.71
6	O	101	07D	CMB-C2B-C1B	-2.20	122.02	125.37
13	J	101	CRT	C14-C15-C16	-2.20	116.36	123.22
6	A	101	07D	OBb-CAB-CBB	-2.19	114.87	119.73
13	0	101	CRT	C20-C21-C22	-2.19	118.98	123.47
12	M	406	RQ0	C30-C34-C43	2.19	119.09	111.88
6	S	101	07D	OBb-CAB-CBB	-2.19	114.87	119.73
6	P	102	07D	CAB-C3B-C2B	2.19	131.62	128.34
6	8	102	07D	CAB-C3B-C2B	2.19	131.62	128.34
10	T	103	LMT	O1B-C4'-C3'	2.19	113.10	107.28
6	F	101	07D	C1C-NC-C4C	2.18	107.69	106.71
6	5	202	07D	C15-C13-C12	2.18	125.53	121.12
6	3	101	07D	C4B-C3B-C2B	-2.18	104.85	108.36
10	L	306	LMT	C1B-O1B-C4'	-2.18	112.57	117.96
7	M	405	08I	C16-C15-C13	2.18	120.14	112.98
10	R	102	LMT	O1B-C4'-C3'	2.18	113.07	107.28
13	A	102	CRT	C34-C33-C35	2.18	121.51	118.08
6	X	102	07D	C1C-NC-C4C	2.18	107.68	106.71
6	Z	102	07D	C4A-NA-C1A	2.18	107.68	106.71
6	W	101	07D	C6-C7-C8	-2.17	122.43	127.66
13	Z	101	CRT	C36-C35-C33	-2.17	122.61	125.89
7	L	302	08I	OBb-CAB-CBB	-2.17	114.92	119.73
13	Z	101	CRT	C21-C20-C19	-2.17	119.03	123.47
6	Q	101	07D	C4A-NA-C1A	2.17	107.68	106.71
13	X	101	CRT	C27-C26-C25	-2.17	116.46	123.22
6	P	102	07D	C4B-C3B-C2B	-2.17	104.88	108.36
13	2	101	CRT	C32-C31-C30	-2.16	116.46	123.22
10	5	201	LMT	C1B-O5B-C5B	2.16	117.94	113.69
6	L	301	07D	C4B-C3B-C2B	-2.16	104.89	108.36
6	Q	101	07D	C11-C12-C13	-2.16	122.47	127.66
13	4	101	CRT	C13-C12-C14	-2.15	119.91	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	102	LMT	O1B-C4'-C3'	2.15	113.00	107.28
6	6	102	07D	C11-C12-C13	-2.15	122.49	127.66
14	H	304	CDL	CA6-CA4-CA3	-2.15	106.71	111.79
13	Z	101	CRT	C13-C12-C11	2.14	121.45	118.08
14	M	408	CDL	OA8-CA7-OA9	-2.14	118.18	123.59
12	M	406	RQ0	C12-C08-C17	2.14	120.03	112.98
6	P	102	07D	CMB-C2B-C1B	-2.14	122.11	125.37
6	L	307	07D	C16-C15-C13	2.14	120.02	112.98
6	P	102	07D	C4A-NA-C1A	2.14	107.67	106.71
6	V	102	07D	C11-C10-C8	2.14	120.01	112.98
6	Q	101	07D	C11-C10-C8	2.14	120.00	112.98
6	U	101	07D	CAA-CBA-CGA	2.14	119.49	113.25
6	Y	101	07D	CMB-C2B-C1B	-2.13	122.12	125.37
6	F	101	07D	C2D-C1D-ND	2.13	111.68	110.10
15	K	103	PEF	O3-C30-O5	-2.13	118.21	123.59
10	J	103	LMT	C1B-C2B-C3B	2.13	114.44	110.00
6	4	102	07D	OBB-CAB-CBB	-2.13	115.01	119.73
6	J	102	07D	C15-C16-C17	-2.13	104.89	111.88
6	M	404	07D	C16-C17-C18	-2.12	120.49	127.75
6	6	102	07D	C4A-NA-C1A	2.12	107.66	106.71
6	4	102	07D	C4B-C3B-C2B	-2.12	104.95	108.36
6	2	102	07D	C14-C13-C15	-2.12	111.70	115.27
6	Z	102	07D	C1C-NC-C4C	2.12	107.66	106.71
13	R	101	CRT	C29-C28-C30	2.12	121.42	118.08
6	N	102	07D	CMB-C2B-C1B	-2.12	122.14	125.37
6	3	101	07D	OBB-CAB-CBB	-2.12	115.04	119.73
10	2	103	LMT	C1B-O1B-C4'	-2.11	112.73	117.96
13	P	101	CRT	C13-C12-C14	-2.11	119.96	122.92
13	4	101	CRT	C5-C6-C7	-2.11	122.70	125.89
6	6	102	07D	C14-C13-C15	-2.11	111.72	115.27
6	X	102	07D	C4A-NA-C1A	2.11	107.66	106.71
12	M	406	RQ0	C41-C46-C52	-2.11	115.94	118.48
13	T	101	CRT	C26-C27-C28	-2.11	124.30	127.31
13	2	101	CRT	C31-C32-C33	-2.11	124.31	127.31
13	4	101	CRT	C36-C35-C33	-2.10	122.72	125.89
13	A	102	CRT	C13-C12-C11	2.10	121.38	118.08
13	J	101	CRT	C9-C10-C11	-2.10	116.67	123.22
13	0	101	CRT	C18-C17-C16	2.10	121.38	118.08
6	L	307	07D	C2D-C1D-ND	2.10	111.65	110.10
6	S	101	07D	C1C-NC-C4C	2.09	107.64	106.71
6	T	102	07D	CAB-C3B-C2B	2.09	131.47	128.34
6	B	101	07D	C11-C12-C13	-2.08	122.64	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	E	101	CRT	C13-C12-C11	2.08	121.36	118.08
6	Z	102	07D	CAB-C3B-C2B	2.08	131.45	128.34
6	N	102	07D	C4B-C3B-C2B	-2.08	105.02	108.36
13	A	102	CRT	C15-C14-C12	-2.08	124.35	127.31
6	9	101	07D	C11-C10-C8	2.08	119.80	112.98
13	8	101	CRT	C27-C26-C25	-2.07	116.75	123.22
6	P	102	07D	C15-C16-C17	-2.07	105.07	111.88
13	A	102	CRT	C26-C27-C28	-2.07	124.36	127.31
6	F	101	07D	CMB-C2B-C1B	-2.07	122.22	125.37
9	H	302	PGV	O01-C1-O02	-2.07	118.71	123.70
10	V	103	LMT	O5'-C5'-C4'	-2.07	105.40	109.75
6	G	102	07D	C4B-C3B-C2B	-2.06	105.04	108.36
6	G	102	07D	C6-C7-C8	-2.06	122.69	127.66
10	P	103	LMT	O1B-C4'-C3'	2.06	112.77	107.28
6	J	102	07D	CAB-C3B-C2B	2.06	131.43	128.34
6	E	102	07D	C15-C16-C17	-2.06	105.12	111.88
13	0	101	CRT	C5-C6-C7	-2.06	122.79	125.89
13	2	101	CRT	C18-C17-C19	-2.05	120.05	122.92
12	M	406	RQ0	C49-C35-C42	-2.05	118.41	123.68
6	J	102	07D	C1C-NC-C4C	2.05	107.63	106.71
13	R	101	CRT	C20-C19-C17	-2.05	124.38	127.31
6	8	102	07D	C5-C6-C7	-2.05	105.14	111.88
13	Z	101	CRT	C14-C15-C16	-2.05	116.82	123.22
13	T	101	CRT	C18-C17-C19	-2.05	120.05	122.92
13	V	101	CRT	C8-C7-C9	-2.05	120.05	122.92
13	6	101	CRT	C32-C31-C30	-2.05	116.82	123.22
6	M	403	07D	CHC-C4B-NB	-2.05	122.09	124.26
9	L	304	PGV	O01-C1-O02	-2.05	118.76	123.70
6	4	102	07D	CMB-C2B-C1B	-2.05	122.25	125.37
6	F	101	07D	C16-C15-C13	2.04	119.70	112.98
6	J	102	07D	CMB-C2B-C1B	-2.04	122.26	125.37
7	M	405	08I	O2A-C1-C2	-2.04	103.27	108.64
13	P	101	CRT	C20-C21-C22	-2.04	119.29	123.47
12	M	406	RQ0	C47-C51-C58	2.04	118.59	111.88
13	0	101	CRT	C35-C33-C32	-2.04	115.81	118.94
6	P	102	07D	OBB-CAB-CBB	-2.04	115.21	119.73
13	P	101	CRT	C27-C26-C25	-2.04	116.86	123.22
6	J	102	07D	C4B-C3B-C2B	-2.04	105.08	108.36
6	0	102	07D	C4B-C3B-C2B	-2.04	105.08	108.36
13	T	101	CRT	C20-C21-C22	-2.03	119.31	123.47
6	X	102	07D	C10-C8-C7	-2.03	117.00	121.12
13	8	101	CRT	C21-C20-C19	-2.03	119.31	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Y	101	07D	O2A-C1-C2	-2.03	103.29	108.64
10	H	306	LMT	C1'-C2'-C3'	2.03	114.23	110.00
13	A	102	CRT	C9-C10-C11	-2.03	116.88	123.22
14	M	408	CDL	OA6-CA5-OA7	-2.03	118.80	123.70
6	2	102	07D	C15-C13-C12	2.03	125.22	121.12
13	E	101	CRT	C14-C15-C16	-2.03	116.89	123.22
13	V	101	CRT	C14-C15-C16	-2.03	116.89	123.22
6	L	301	07D	CMB-C2B-C1B	-2.03	122.28	125.37
13	X	101	CRT	C29-C28-C30	2.03	121.27	118.08
13	0	101	CRT	C9-C10-C11	-2.02	116.91	123.22
7	L	302	08I	C1-O2A-CGA	2.02	121.75	116.44
6	4	102	07D	CHC-C1C-NC	-2.02	121.72	124.51
6	2	102	07D	C4B-C3B-C2B	-2.02	105.12	108.36
13	Z	101	CRT	C31-C32-C33	-2.02	124.43	127.31
6	E	102	07D	C16-C15-C13	2.02	119.61	112.98
10	R	102	LMT	C1-O1'-C1'	-2.01	110.50	113.84
6	X	102	07D	C4B-C3B-C2B	-2.01	105.12	108.36
12	M	406	RQ0	C38-C17-C24	-2.01	118.52	123.68
6	Y	101	07D	O2A-CGA-CBA	2.01	118.21	111.91
12	M	406	RQ0	C40-C21-C26	-2.01	118.53	123.68
6	7	101	07D	O2A-C1-C2	-2.01	103.36	108.64
6	8	102	07D	C4B-C3B-C2B	-2.00	105.14	108.36
6	V	102	07D	C4B-C3B-C2B	-2.00	105.14	108.36
6	G	102	07D	CMB-C2B-C1B	-2.00	122.32	125.37

All (34) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	L	301	07D	ND
6	M	404	07D	ND
6	A	101	07D	ND
6	B	101	07D	ND
6	D	101	07D	ND
6	E	102	07D	ND
6	F	101	07D	ND
6	G	102	07D	ND
6	I	101	07D	ND
6	J	102	07D	ND
6	K	101	07D	ND
6	N	102	07D	ND
6	O	101	07D	ND
6	P	102	07D	ND

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Mol	Chain	Res	Type	Atom
6	Q	101	07D	ND
6	Q	102	07D	ND
6	S	101	07D	ND
6	T	102	07D	ND
6	U	101	07D	ND
6	V	102	07D	ND
6	W	101	07D	ND
6	X	102	07D	ND
6	Y	101	07D	ND
6	Z	102	07D	ND
6	1	101	07D	ND
6	2	102	07D	ND
6	3	101	07D	ND
6	4	102	07D	ND
6	5	202	07D	ND
6	6	102	07D	ND
6	7	101	07D	ND
6	8	102	07D	ND
6	9	101	07D	ND
6	0	102	07D	ND

All (697) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	307	07D	C12-C13-C15-C16
6	L	307	07D	C14-C13-C15-C16
6	M	403	07D	C11-C10-C8-C9
6	M	404	07D	C11-C10-C8-C7
6	M	404	07D	C11-C10-C8-C9
6	E	102	07D	C12-C13-C15-C16
6	E	102	07D	C14-C13-C15-C16
6	I	101	07D	C8-C10-C11-C12
6	I	101	07D	C12-C13-C15-C16
6	I	101	07D	C14-C13-C15-C16
6	O	101	07D	C3A-C2A-CAA-CBA
6	O	101	07D	CHA-CBD-CGD-O1D
6	O	101	07D	CHA-CBD-CGD-O2D
6	P	102	07D	C12-C13-C15-C16
6	P	102	07D	C14-C13-C15-C16
6	Q	102	07D	C4-C3-C5-C6
6	Q	102	07D	C2-C3-C5-C6
6	S	101	07D	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
6	T	102	07D	C11-C10-C8-C7
6	T	102	07D	C11-C10-C8-C9
6	T	102	07D	C12-C13-C15-C16
6	T	102	07D	C14-C13-C15-C16
6	W	101	07D	C4-C3-C5-C6
6	W	101	07D	C2-C3-C5-C6
6	X	102	07D	C14-C13-C15-C16
6	Y	101	07D	CBA-CGA-O2A-C1
6	Y	101	07D	O1A-CGA-O2A-C1
6	2	102	07D	C12-C13-C15-C16
6	2	102	07D	C14-C13-C15-C16
6	3	101	07D	O2A-C1-C2-C3
6	3	101	07D	C1A-C2A-CAA-CBA
6	3	101	07D	CHA-CBD-CGD-O1D
6	3	101	07D	CHA-CBD-CGD-O2D
6	4	102	07D	C4-C3-C5-C6
6	5	202	07D	C2A-CAA-CBA-CGA
6	6	102	07D	C4-C3-C5-C6
6	6	102	07D	C2-C3-C5-C6
6	6	102	07D	C14-C13-C15-C16
6	8	102	07D	C11-C10-C8-C9
6	0	102	07D	C4-C3-C5-C6
6	0	102	07D	C2-C3-C5-C6
6	0	102	07D	C12-C13-C15-C16
6	0	102	07D	C14-C13-C15-C16
7	L	302	08I	C4-C3-C5-C6
7	L	302	08I	C2-C3-C5-C6
7	L	302	08I	C12-C13-C15-C16
7	L	302	08I	C14-C13-C15-C16
7	L	302	08I	C1A-C2A-CAA-CBA
7	L	302	08I	C2C-C3C-CAC-CBC
7	M	405	08I	C1A-C2A-CAA-CBA
7	M	405	08I	C4B-C3B-CAB-OB
7	M	405	08I	C2C-C3C-CAC-CBC
8	L	303	U10	C12-C11-C9-C10
8	L	303	U10	C15-C14-C16-C17
9	H	302	PGV	C03-O11-P-O14
9	H	302	PGV	O12-C04-C05-C06
9	H	302	PGV	O12-C04-C05-O05
10	H	306	LMT	O5'-C1'-O1'-C1
10	5	203	LMT	O5'-C1'-O1'-C1
12	M	406	RQ0	C09-C06-C16-C37

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Mol	Chain	Res	Type	Atoms
12	M	406	RQ0	C11-C07-C19-C27
12	M	406	RQ0	C11-C07-C19-C39
12	M	406	RQ0	C31-C30-C34-C43
13	M	407	CRT	C32-C33-C35-C36
13	M	407	CRT	C34-C33-C35-C36
13	M	407	CRT	C36-C37-C38-C39
13	M	407	CRT	C36-C37-C38-C40
13	E	101	CRT	C2-C1-C4-C5
13	E	101	CRT	C3-C1-C4-C5
13	E	101	CRT	C1-C4-C5-C6
13	E	101	CRT	C5-C6-C7-C8
13	E	101	CRT	C5-C6-C7-C9
13	E	101	CRT	C15-C16-C17-C18
13	E	101	CRT	C15-C16-C17-C19
13	G	101	CRT	C10-C11-C12-C13
13	G	101	CRT	C10-C11-C12-C14
13	G	101	CRT	C40-C38-O2-C2M
13	J	101	CRT	C10-C11-C12-C13
13	N	101	CRT	C10-C11-C12-C13
13	N	101	CRT	C10-C11-C12-C14
13	N	101	CRT	C15-C16-C17-C18
13	P	101	CRT	C10-C11-C12-C13
13	P	101	CRT	C10-C11-C12-C14
13	P	101	CRT	C32-C33-C35-C36
13	P	101	CRT	C34-C33-C35-C36
13	P	101	CRT	C36-C37-C38-C39
13	P	101	CRT	C36-C37-C38-C40
13	R	101	CRT	C2-C1-C4-C5
13	R	101	CRT	C3-C1-C4-C5
13	R	101	CRT	C10-C11-C12-C13
13	R	101	CRT	C10-C11-C12-C14
13	T	101	CRT	O1-C1-C4-C5
13	T	101	CRT	C2-C1-C4-C5
13	T	101	CRT	C3-C1-C4-C5
13	T	101	CRT	C10-C11-C12-C13
13	T	101	CRT	C10-C11-C12-C14
13	T	101	CRT	C15-C16-C17-C18
13	T	101	CRT	C15-C16-C17-C19
13	V	101	CRT	O1-C1-C4-C5
13	V	101	CRT	C2-C1-C4-C5
13	V	101	CRT	C3-C1-C4-C5
13	V	101	CRT	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
13	V	101	CRT	C10-C11-C12-C14
13	X	101	CRT	C2-C1-C4-C5
13	X	101	CRT	C3-C1-C4-C5
13	X	101	CRT	C10-C11-C12-C13
13	X	101	CRT	C10-C11-C12-C14
13	Z	101	CRT	C2-C1-C4-C5
13	Z	101	CRT	C1-C4-C5-C6
13	Z	101	CRT	C15-C16-C17-C18
13	2	101	CRT	C2-C1-C4-C5
13	2	101	CRT	C3-C1-C4-C5
13	2	101	CRT	C10-C11-C12-C13
13	2	101	CRT	C10-C11-C12-C14
13	2	101	CRT	C35-C36-C37-C38
13	6	101	CRT	O1-C1-C4-C5
13	6	101	CRT	C2-C1-C4-C5
13	6	101	CRT	C3-C1-C4-C5
13	6	101	CRT	C5-C6-C7-C8
13	6	101	CRT	C5-C6-C7-C9
13	6	101	CRT	C32-C33-C35-C36
13	6	101	CRT	C34-C33-C35-C36
13	6	101	CRT	C36-C37-C38-C39
13	6	101	CRT	C36-C37-C38-C40
13	6	101	CRT	C36-C37-C38-O2
13	8	101	CRT	O1-C1-C4-C5
13	8	101	CRT	C2-C1-C4-C5
13	8	101	CRT	C3-C1-C4-C5
13	8	101	CRT	C10-C11-C12-C13
13	8	101	CRT	C15-C16-C17-C18
13	8	101	CRT	C15-C16-C17-C19
14	M	408	CDL	CB2-OB2-PB2-OB5
14	M	408	CDL	CB3-OB5-PB2-OB3
14	M	409	CDL	CA2-OA2-PA1-OA3
14	M	409	CDL	CA2-OA2-PA1-OA4
14	H	301	CDL	CA2-OA2-PA1-OA4
14	H	301	CDL	CA3-OA5-PA1-OA3
14	H	301	CDL	CB2-OB2-PB2-OB5
14	H	301	CDL	CB3-OB5-PB2-OB3
14	H	301	CDL	C51-CB5-OB6-CB4
14	H	303	CDL	CA2-OA2-PA1-OA3
14	H	303	CDL	CA2-OA2-PA1-OA4
14	H	303	CDL	CA2-OA2-PA1-OA5
14	H	303	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
14	H	304	CDL	CA3-OA5-PA1-OA2
14	H	304	CDL	CA3-OA5-PA1-OA3
14	H	304	CDL	CB2-OB2-PB2-OB3
15	H	305	PEF	C4-O4P-P-O1P
15	K	102	PEF	C4-O4P-P-O2P
15	K	103	PEF	C4-O4P-P-O1P
15	K	103	PEF	C4-O4P-P-O3P
14	H	303	CDL	C11-CA5-OA6-CA4
10	N	103	LMT	C3'-C4'-O1B-C1B
10	R	102	LMT	C3'-C4'-O1B-C1B
10	P	103	LMT	C3'-C4'-O1B-C1B
10	J	103	LMT	O5B-C1B-O1B-C4'
10	5	201	LMT	O5B-C1B-O1B-C4'
14	H	301	CDL	OB7-CB5-OB6-CB4
14	H	303	CDL	OB7-CB5-OB6-CB4
10	6	103	LMT	C3'-C4'-O1B-C1B
14	H	304	CDL	C51-CB5-OB6-CB4
6	F	101	07D	C14-C13-C15-C16
6	P	102	07D	C11-C10-C8-C9
6	Z	102	07D	C4-C3-C5-C6
6	8	102	07D	C4-C3-C5-C6
6	9	101	07D	C4-C3-C5-C6
6	M	403	07D	C11-C10-C8-C7
6	F	101	07D	C12-C13-C15-C16
6	8	102	07D	C2-C3-C5-C6
8	L	303	U10	C12-C11-C9-C8
6	O	101	07D	C2A-CAA-CBA-CGA
10	B	102	LMT	C3'-C4'-O1B-C1B
14	H	303	CDL	OA7-CA5-OA6-CA4
12	M	406	RQ0	C14-C18-C27-C19
14	H	301	CDL	O1-C1-CB2-OB2
14	H	304	CDL	O1-C1-CA2-OA2
14	M	408	CDL	C31-CA7-OA8-CA6
10	4	103	LMT	O5B-C1B-O1B-C4'
10	T	103	LMT	C3'-C4'-O1B-C1B
10	Z	103	LMT	C3'-C4'-O1B-C1B
6	D	101	07D	C11-C10-C8-C9
6	J	102	07D	C4-C3-C5-C6
6	P	102	07D	C4-C3-C5-C6
6	Z	102	07D	C14-C13-C15-C16
6	8	102	07D	C14-C13-C15-C16
12	M	406	RQ0	C20-C15-C21-C40

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Mol	Chain	Res	Type	Atoms
12	M	406	RQ0	C34-C30-C31-C48
10	R	102	LMT	C4B-C5B-C6B-O6B
6	D	101	07D	C11-C10-C8-C7
6	J	102	07D	C2-C3-C5-C6
6	P	102	07D	C2-C3-C5-C6
6	X	102	07D	C12-C13-C15-C16
6	Z	102	07D	C12-C13-C15-C16
6	4	102	07D	C2-C3-C5-C6
6	6	102	07D	C12-C13-C15-C16
6	8	102	07D	C11-C10-C8-C7
6	8	102	07D	C12-C13-C15-C16
8	L	303	U10	C13-C14-C16-C17
12	M	406	RQ0	C09-C06-C16-C25
12	M	406	RQ0	C20-C15-C21-C26
12	M	406	RQ0	C34-C30-C31-C32
10	0	103	LMT	O5'-C5'-C6'-O6'
14	M	408	CDL	OA9-CA7-OA8-CA6
10	P	103	LMT	O5'-C1'-O1'-C1
7	L	302	08I	C8-C10-C11-C12
12	M	406	RQ0	C13-C05-C10-C24
12	M	406	RQ0	C16-C06-C09-C22
12	M	406	RQ0	C21-C15-C20-C32
10	H	306	LMT	O5B-C1B-O1B-C4'
14	M	409	CDL	CB2-C1-CA2-OA2
14	M	409	CDL	CA2-C1-CB2-OB2
14	H	301	CDL	CA2-C1-CB2-OB2
14	H	303	CDL	CA2-C1-CB2-OB2
10	0	103	LMT	C4'-C5'-C6'-O6'
14	M	409	CDL	O1-C1-CA2-OA2
14	H	303	CDL	O1-C1-CB2-OB2
10	X	103	LMT	C3'-C4'-O1B-C1B
6	P	102	07D	C11-C10-C8-C7
6	Z	102	07D	C2-C3-C5-C6
6	9	101	07D	C2-C3-C5-C6
13	R	101	CRT	C15-C16-C17-C18
13	Z	101	CRT	C5-C6-C7-C8
13	2	101	CRT	C15-C16-C17-C18
13	2	101	CRT	C29-C28-C30-C31
13	4	101	CRT	C10-C11-C12-C13
13	0	101	CRT	C5-C6-C7-C8
13	Z	101	CRT	C5-C6-C7-C9
13	4	101	CRT	C10-C11-C12-C14

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Mol	Chain	Res	Type	Atoms
15	K	102	PEF	C11-C10-O2-C2
15	K	103	PEF	C11-C10-O2-C2
10	5	203	LMT	C4-C5-C6-C7
10	M	411	LMT	O5B-C1B-O1B-C4'
10	X	103	LMT	C5'-C4'-O1B-C1B
10	4	103	LMT	C5'-C4'-O1B-C1B
10	Z	103	LMT	C5'-C4'-O1B-C1B
15	K	102	PEF	O4-C10-O2-C2
10	4	103	LMT	C3'-C4'-O1B-C1B
6	E	102	07D	C2A-CAA-CBA-CGA
10	L	306	LMT	O5'-C1'-O1'-C1
10	G	103	LMT	O5'-C1'-O1'-C1
10	Z	103	LMT	O1'-C1-C2-C3
14	M	409	CDL	O1-C1-CB2-OB2
10	P	103	LMT	O1'-C1-C2-C3
6	W	101	07D	C15-C16-C17-C18
9	H	302	PGV	C03-O11-P-O12
9	H	302	PGV	C04-O12-P-O11
14	M	409	CDL	CA2-OA2-PA1-OA5
14	H	301	CDL	CA2-OA2-PA1-OA5
14	H	301	CDL	CA3-OA5-PA1-OA2
14	H	303	CDL	CB2-OB2-PB2-OB5
14	H	304	CDL	CA2-OA2-PA1-OA5
14	H	304	CDL	CB3-OB5-PB2-OB2
15	K	102	PEF	C4-O4P-P-O3P
15	K	103	PEF	C1-O3P-P-O4P
10	B	102	LMT	C4'-C5'-C6'-O6'
15	K	103	PEF	O4-C10-O2-C2
6	L	307	07D	C11-C10-C8-C9
6	X	102	07D	C2A-CAA-CBA-CGA
10	E	103	LMT	O5B-C5B-C6B-O6B
10	M	411	LMT	O1'-C1-C2-C3
10	T	103	LMT	C5'-C4'-O1B-C1B
10	2	103	LMT	C5'-C4'-O1B-C1B
10	5	201	LMT	O5'-C5'-C6'-O6'
10	H	306	LMT	C7-C8-C9-C10
14	M	408	CDL	C11-CA5-OA6-CA4
10	R	102	LMT	O5B-C5B-C6B-O6B
10	N	103	LMT	C6-C7-C8-C9
14	H	301	CDL	CB6-CB4-OB6-CB5
14	M	408	CDL	OA7-CA5-OA6-CA4
10	M	410	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
14	M	408	CDL	O1-C1-CA2-OA2
15	H	305	PEF	O3P-C1-C2-O2
10	L	306	LMT	C2-C3-C4-C5
10	L	306	LMT	C2'-C1'-O1'-C1
10	M	410	LMT	C11-C10-C9-C8
10	0	103	LMT	O1'-C1-C2-C3
6	L	307	07D	C11-C10-C8-C7
14	M	409	CDL	CB5-C51-C52-C53
6	P	102	07D	C2A-CAA-CBA-CGA
12	M	406	RQ0	C18-C14-C23-C44
13	2	101	CRT	C34-C33-C35-C36
10	5	201	LMT	C2-C3-C4-C5
12	M	406	RQ0	C18-C14-C23-C33
13	N	101	CRT	C15-C16-C17-C19
13	2	101	CRT	C32-C33-C35-C36
14	H	304	CDL	C11-CA5-OA6-CA4
9	L	304	PGV	C1-C2-C3-C4
15	K	102	PEF	C30-C31-C32-C33
14	H	304	CDL	OB7-CB5-OB6-CB4
10	M	410	LMT	O5B-C5B-C6B-O6B
14	H	303	CDL	C82-C83-C84-C85
6	3	101	07D	C3A-C2A-CAA-CBA
6	0	102	07D	C3A-C2A-CAA-CBA
10	6	103	LMT	O5B-C5B-C6B-O6B
10	5	201	LMT	C2-C1-O1'-C1'
14	H	303	CDL	C73-C74-C75-C76
6	Z	102	07D	O2A-C1-C2-C3
10	2	103	LMT	C3'-C4'-O1B-C1B
6	B	101	07D	C11-C10-C8-C9
6	A	101	07D	C11-C10-C8-C7
6	B	101	07D	C2-C3-C5-C6
6	B	101	07D	C11-C10-C8-C7
14	H	304	CDL	OA7-CA5-OA6-CA4
6	4	102	07D	C2-C1-O2A-CGA
10	T	103	LMT	O5B-C1B-O1B-C4'
14	H	303	CDL	C79-C80-C81-C82
10	T	103	LMT	O5'-C5'-C6'-O6'
10	B	102	LMT	C5'-C4'-O1B-C1B
9	H	302	PGV	C1-C2-C3-C4
14	M	408	CDL	C75-C76-C77-C78
6	A	101	07D	C11-C10-C8-C9
6	B	101	07D	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
6	X	102	07D	C4-C3-C5-C6
6	1	101	07D	C4-C3-C5-C6
6	1	101	07D	C14-C13-C15-C16
6	O	101	07D	C2-C3-C5-C6
6	S	101	07D	C11-C10-C8-C7
6	V	102	07D	C11-C10-C8-C7
6	X	102	07D	C2-C3-C5-C6
6	1	101	07D	C12-C13-C15-C16
6	T	102	07D	C2A-CAA-CBA-CGA
10	Z	103	LMT	O5B-C1B-O1B-C4'
10	X	103	LMT	O5'-C5'-C6'-O6'
14	M	409	CDL	C12-C13-C14-C15
9	L	304	PGV	C2-C1-O01-C02
15	K	103	PEF	C12-C13-C14-C15
10	P	103	LMT	C4B-C5B-C6B-O6B
10	J	103	LMT	O5B-C5B-C6B-O6B
14	H	301	CDL	C55-C56-C57-C58
6	O	101	07D	C4-C3-C5-C6
6	S	101	07D	C11-C10-C8-C9
6	V	102	07D	C11-C10-C8-C9
12	M	406	RQ0	C28-C29-C35-C42
10	J	103	LMT	O5'-C5'-C6'-O6'
10	P	103	LMT	O5B-C5B-C6B-O6B
13	J	101	CRT	C10-C11-C12-C14
6	O	101	07D	C1A-C2A-CAA-CBA
6	0	102	07D	C1A-C2A-CAA-CBA
10	V	103	LMT	O5'-C5'-C6'-O6'
9	L	304	PGV	O02-C1-O01-C02
12	M	406	RQ0	C07-C11-C25-C16
14	H	303	CDL	CB3-OB5-PB2-OB2
15	H	305	PEF	C4-O4P-P-O3P
9	H	302	PGV	C2-C3-C4-C5
10	V	103	LMT	C2-C3-C4-C5
10	6	103	LMT	C5'-C4'-O1B-C1B
10	N	103	LMT	O5B-C5B-C6B-O6B
10	Z	103	LMT	O5B-C5B-C6B-O6B
13	0	101	CRT	C1-C4-C5-C6
10	J	103	LMT	C2-C3-C4-C5
10	L	306	LMT	C1-C2-C3-C4
10	V	103	LMT	O5B-C5B-C6B-O6B
10	8	103	LMT	O5'-C5'-C6'-O6'
14	M	408	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
6	1	101	07D	C11-C10-C8-C9
10	T	103	LMT	O5B-C5B-C6B-O6B
10	2	103	LMT	O5B-C5B-C6B-O6B
10	4	103	LMT	O5'-C5'-C6'-O6'
14	M	408	CDL	CB3-CB4-CB6-OB8
10	2	103	LMT	O5'-C5'-C6'-O6'
10	5	201	LMT	C3'-C4'-O1B-C1B
10	M	411	LMT	O5'-C5'-C6'-O6'
10	H	306	LMT	O5'-C5'-C6'-O6'
10	5	203	LMT	O5'-C5'-C6'-O6'
6	3	101	07D	C14-C13-C15-C16
12	M	406	RQ0	C28-C29-C35-C49
6	3	101	07D	C12-C13-C15-C16
6	M	403	07D	C2-C1-O2A-CGA
10	5	201	LMT	C5'-C4'-O1B-C1B
13	M	407	CRT	C2-C1-O1-C1M
13	M	407	CRT	C3-C1-O1-C1M
13	G	101	CRT	C39-C38-O2-C2M
15	K	103	PEF	O2-C2-C3-O3
10	B	102	LMT	O5'-C5'-C6'-O6'
13	E	101	CRT	C36-C37-C38-C39
13	G	101	CRT	C3-C1-C4-C5
13	G	101	CRT	C36-C37-C38-C39
13	P	101	CRT	C3-C1-C4-C5
13	X	101	CRT	C36-C37-C38-C39
13	Z	101	CRT	C3-C1-C4-C5
13	0	101	CRT	C36-C37-C38-C39
14	H	301	CDL	CA5-C11-C12-C13
6	5	202	07D	C11-C10-C8-C9
6	1	101	07D	C2-C3-C5-C6
6	5	202	07D	C11-C10-C8-C7
10	P	103	LMT	C4-C5-C6-C7
14	M	408	CDL	C71-C72-C73-C74
13	P	101	CRT	C36-C37-C38-O2
13	M	407	CRT	C15-C16-C17-C18
13	P	101	CRT	C24-C23-C25-C26
13	Z	101	CRT	C34-C33-C35-C36
13	4	101	CRT	C34-C33-C35-C36
10	H	306	LMT	C5'-C4'-O1B-C1B
6	2	102	07D	C4-C3-C5-C6
14	M	408	CDL	CB7-C71-C72-C73
15	K	103	PEF	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
9	H	302	PGV	C20-C21-C22-C23
10	J	103	LMT	C3-C4-C5-C6
6	I	101	07D	C10-C11-C12-C13
10	H	306	LMT	C3'-C4'-O1B-C1B
6	6	102	07D	C3A-C2A-CAA-CBA
15	K	103	PEF	C1-C2-C3-O3
10	5	201	LMT	C1-C2-C3-C4
10	L	306	LMT	C5-C6-C7-C8
10	B	102	LMT	O5B-C1B-O1B-C4'
6	Y	101	07D	C11-C10-C8-C9
6	1	101	07D	C11-C10-C8-C7
10	5	201	LMT	C4-C5-C6-C7
15	K	102	PEF	C32-C33-C34-C35
6	Q	102	07D	C8-C10-C11-C12
14	H	304	CDL	CB2-C1-CA2-OA2
6	Q	101	07D	C14-C13-C15-C16
6	2	102	07D	C2-C1-O2A-CGA
6	8	102	07D	C2A-CAA-CBA-CGA
10	8	103	LMT	O5B-C1B-O1B-C4'
13	R	101	CRT	C15-C16-C17-C19
13	Z	101	CRT	C15-C16-C17-C19
13	8	101	CRT	C10-C11-C12-C14
14	M	409	CDL	OB5-CB3-CB4-CB6
14	H	304	CDL	OA5-CA3-CA4-CA6
10	T	103	LMT	C4-C5-C6-C7
6	Q	101	07D	C12-C13-C15-C16
6	Y	101	07D	C11-C10-C8-C7
7	L	302	08I	C4B-C3B-CAB-OB
13	M	407	CRT	C20-C21-C22-C23
13	P	101	CRT	C11-C10-C9-C7
10	4	103	LMT	C4-C5-C6-C7
7	L	302	08I	CAD-CBD-CGD-O2D
10	M	410	LMT	O5'-C1'-O1'-C1
9	H	302	PGV	C02-C03-O11-P
9	H	302	PGV	C5-C6-C7-C8
15	K	103	PEF	C31-C30-O3-C3
6	1	101	07D	CHA-CBD-CGD-O1D
10	H	306	LMT	C2'-C1'-O1'-C1
14	H	301	CDL	C54-C55-C56-C57
10	4	103	LMT	C9-C10-C11-C12
10	6	103	LMT	C4-C5-C6-C7
13	P	101	CRT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
13	V	101	CRT	C24-C23-C25-C26
13	6	101	CRT	C10-C11-C12-C13
13	6	101	CRT	C10-C11-C12-C14
13	0	101	CRT	C5-C6-C7-C9
10	4	103	LMT	C2-C3-C4-C5
6	B	101	07D	C1A-C2A-CAA-CBA
14	M	408	CDL	CA3-OA5-PA1-OA2
14	H	304	CDL	CB2-OB2-PB2-OB5
15	K	102	PEF	C1-O3P-P-O4P
14	M	408	CDL	C14-C15-C16-C17
6	7	101	07D	C14-C13-C15-C16
15	K	103	PEF	O5-C30-O3-C3
9	H	302	PGV	C03-O11-P-O13
9	H	302	PGV	C04-O12-P-O13
14	M	408	CDL	CB2-OB2-PB2-OB4
14	H	301	CDL	CA3-OA5-PA1-OA4
14	H	301	CDL	CB2-OB2-PB2-OB4
14	H	303	CDL	CB2-OB2-PB2-OB3
14	H	304	CDL	CA2-OA2-PA1-OA3
14	H	304	CDL	CA2-OA2-PA1-OA4
14	H	304	CDL	CB3-OB5-PB2-OB3
15	H	305	PEF	C4-O4P-P-O2P
15	K	103	PEF	C1-O3P-P-O1P
15	K	103	PEF	C4-O4P-P-O2P
9	H	302	PGV	C01-C02-C03-O11
14	M	409	CDL	OA5-CA3-CA4-CA6
15	K	102	PEF	O3P-C1-C2-C3
14	M	409	CDL	CB7-C71-C72-C73
6	M	404	07D	CAD-CBD-CGD-O1D
13	M	407	CRT	C1-C4-C5-C6
6	E	102	07D	C4-C3-C5-C6
6	S	101	07D	C4-C3-C5-C6
9	H	302	PGV	O01-C02-C03-O11
14	M	409	CDL	OA5-CA3-CA4-OA6
14	H	304	CDL	OA5-CA3-CA4-OA6
14	M	408	CDL	OA6-CA4-CA6-OA8
14	M	408	CDL	OB6-CB4-CB6-OB8
14	H	303	CDL	OA6-CA4-CA6-OA8
10	P	103	LMT	C5'-C4'-O1B-C1B
6	Z	102	07D	C2A-CAA-CBA-CGA
10	8	103	LMT	C2B-C1B-O1B-C4'
10	5	203	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
10	5	201	LMT	C4B-C5B-C6B-O6B
14	M	409	CDL	CA5-C11-C12-C13
14	H	303	CDL	CA6-CA4-OA6-CA5
14	H	303	CDL	CB3-CB4-OB6-CB5
14	H	304	CDL	CA6-CA4-OA6-CA5
6	3	101	07D	C2A-CAA-CBA-CGA
10	M	410	LMT	C5'-C4'-O1B-C1B
15	K	102	PEF	O3P-C1-C2-O2
10	5	203	LMT	C3'-C4'-O1B-C1B
6	Q	102	07D	C11-C10-C8-C9
6	2	102	07D	C2-C3-C5-C6
15	K	102	PEF	O5-C30-O3-C3
10	5	201	LMT	O5'-C1'-O1'-C1
9	L	304	PGV	C03-O11-P-O12
9	L	304	PGV	C04-O12-P-O11
14	M	408	CDL	CA2-OA2-PA1-OA5
14	M	408	CDL	CB3-OB5-PB2-OB2
14	M	409	CDL	CB2-OB2-PB2-OB5
14	M	409	CDL	CB3-OB5-PB2-OB2
14	H	301	CDL	CB3-OB5-PB2-OB2
14	H	303	CDL	CA3-OA5-PA1-OA2
13	E	101	CRT	C36-C37-C38-C40
13	G	101	CRT	C2-C1-C4-C5
13	N	101	CRT	C36-C37-C38-C39
13	P	101	CRT	C2-C1-C4-C5
6	7	101	07D	C12-C13-C15-C16
10	B	102	LMT	C3-C4-C5-C6
6	G	102	07D	C2A-CAA-CBA-CGA
13	E	101	CRT	O1-C1-C4-C5
13	E	101	CRT	C36-C37-C38-O2
13	G	101	CRT	C36-C37-C38-O2
13	P	101	CRT	O1-C1-C4-C5
13	0	101	CRT	C36-C37-C38-O2
10	B	102	LMT	C2B-C1B-O1B-C4'
6	7	101	07D	C11-C10-C8-C9
6	M	403	07D	C5-C6-C7-C8
6	F	101	07D	C15-C16-C17-C18
15	K	103	PEF	C14-C15-C16-C17
15	K	102	PEF	C31-C30-O3-C3
10	5	201	LMT	C4'-C5'-C6'-O6'
13	6	101	CRT	C11-C10-C9-C7
10	P	103	LMT	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
14	H	301	CDL	OA7-CA5-OA6-CA4
6	4	102	07D	CAA-CBA-CGA-O2A
6	I	101	07D	C2-C1-O2A-CGA
6	8	102	07D	C2-C1-O2A-CGA
10	B	102	LMT	C2-C3-C4-C5
14	H	303	CDL	CB5-C51-C52-C53
6	B	101	07D	C3A-C2A-CAA-CBA
8	M	401	U10	C5-C4-O4-C4M
10	R	102	LMT	C11-C10-C9-C8
6	O	101	07D	C14-C13-C15-C16
14	H	303	CDL	CA3-CA4-CA6-OA8
14	H	303	CDL	CB3-CB4-CB6-OB8
6	4	102	07D	C2A-CAA-CBA-CGA
14	H	303	CDL	C71-C72-C73-C74
13	2	101	CRT	C15-C16-C17-C19
6	Q	101	07D	C11-C10-C8-C9
6	E	102	07D	C1A-C2A-CAA-CBA
6	Q	102	07D	C1A-C2A-CAA-CBA
6	6	102	07D	C1A-C2A-CAA-CBA
14	H	304	CDL	C1-CA2-OA2-PA1
9	L	304	PGV	C2-C3-C4-C5
10	2	103	LMT	O1'-C1-C2-C3
6	G	102	07D	C11-C10-C8-C7
10	Z	103	LMT	C2B-C1B-O1B-C4'
10	M	410	LMT	C3'-C4'-O1B-C1B
6	N	102	07D	C10-C11-C12-C13
10	T	103	LMT	C2B-C1B-O1B-C4'
6	T	102	07D	C13-C15-C16-C17
6	X	102	07D	C8-C10-C11-C12
6	L	301	07D	C14-C13-C15-C16
6	M	404	07D	C4-C3-C5-C6
6	F	101	07D	C11-C10-C8-C9
6	J	102	07D	C2-C1-O2A-CGA
6	Q	101	07D	C2-C1-O2A-CGA
6	Q	101	07D	C11-C10-C8-C7
6	7	101	07D	C11-C10-C8-C7
14	H	301	CDL	C11-CA5-OA6-CA4
10	M	411	LMT	C2-C3-C4-C5
6	G	102	07D	C11-C10-C8-C9
6	I	101	07D	C11-C10-C8-C9
6	N	102	07D	C11-C10-C8-C9
13	P	101	CRT	C22-C23-C25-C26

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Mol	Chain	Res	Type	Atoms
13	2	101	CRT	C27-C28-C30-C31
13	4	101	CRT	C32-C33-C35-C36
14	M	409	CDL	C73-C74-C75-C76
14	M	409	CDL	OB5-CB3-CB4-OB6
7	M	405	08I	C4B-C3B-CAB-CBB
6	M	404	07D	CAA-CBA-CGA-O2A
8	L	303	U10	C2-C3-O3-C3M
10	4	103	LMT	C3-C4-C5-C6
6	U	101	07D	C11-C10-C8-C9
6	Q	101	07D	C3-C5-C6-C7
6	Z	102	07D	C8-C10-C11-C12
10	2	103	LMT	C1-C2-C3-C4
14	H	303	CDL	C75-C76-C77-C78
14	M	409	CDL	C12-C11-CA5-OA6
10	M	411	LMT	C1-C2-C3-C4
7	L	302	08I	C4C-C3C-CAC-CBC
6	B	101	07D	C14-C13-C15-C16
6	O	101	07D	C11-C10-C8-C9
6	W	101	07D	C11-C10-C8-C9
7	L	302	08I	C11-C10-C8-C9
6	S	101	07D	C2-C3-C5-C6
14	M	408	CDL	C12-C11-CA5-OA6
14	H	303	CDL	C32-C31-CA7-OA8
14	M	409	CDL	CA6-CA4-OA6-CA5
6	U	101	07D	CAA-CBA-CGA-O2A
10	P	103	LMT	C2B-C1B-O1B-C4'
12	M	406	RQ0	C53-C45-C47-C51
6	B	101	07D	C12-C13-C15-C16
6	E	102	07D	C2-C3-C5-C6
13	P	101	CRT	C5-C6-C7-C9
13	V	101	CRT	C22-C23-C25-C26
13	Z	101	CRT	C32-C33-C35-C36
6	2	102	07D	C3-C5-C6-C7
6	E	102	07D	C5-C6-C7-C8
10	L	306	LMT	C6-C7-C8-C9
6	J	102	07D	O2A-C1-C2-C3
6	8	102	07D	O2A-C1-C2-C3
6	A	101	07D	CHA-CBD-CGD-O2D
6	F	101	07D	CHA-CBD-CGD-O2D
6	I	101	07D	CHA-CBD-CGD-O1D
6	I	101	07D	CHA-CBD-CGD-O2D
6	X	102	07D	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
6	Y	101	07D	CHA-CBD-CGD-O1D
6	Y	101	07D	CHA-CBD-CGD-O2D
6	1	101	07D	CHA-CBD-CGD-O2D
6	5	202	07D	CHA-CBD-CGD-O1D
6	5	202	07D	CHA-CBD-CGD-O2D
6	6	102	07D	CHA-CBD-CGD-O1D
6	6	102	07D	CHA-CBD-CGD-O2D
6	7	101	07D	CHA-CBD-CGD-O1D
6	7	101	07D	CHA-CBD-CGD-O2D
6	5	202	07D	C14-C13-C15-C16
10	H	306	LMT	C3-C4-C5-C6
13	R	101	CRT	C39-C38-O2-C2M
13	0	101	CRT	C3-C1-O1-C1M
10	H	306	LMT	C4-C5-C6-C7
7	L	302	08I	CHA-CBD-CGD-O1D
13	G	101	CRT	C36-C37-C38-C40
13	X	101	CRT	C36-C37-C38-C40
13	0	101	CRT	C36-C37-C38-C40
6	5	202	07D	C10-C11-C12-C13
10	E	103	LMT	C1-C2-C3-C4
6	O	101	07D	C11-C10-C8-C7
6	Q	102	07D	C11-C10-C8-C7
12	M	406	RQ0	C43-C45-C47-C51
9	L	304	PGV	C20-C21-C22-C23
10	M	410	LMT	O5B-C1B-O1B-C4'
6	L	301	07D	C15-C16-C17-C18
6	M	403	07D	C10-C11-C12-C13
6	D	101	07D	C10-C11-C12-C13
6	N	102	07D	C15-C16-C17-C18
6	V	102	07D	C15-C16-C17-C18
6	Z	102	07D	C10-C11-C12-C13
6	5	202	07D	C15-C16-C17-C18
12	M	406	RQ0	C06-C09-C22-C13
13	G	101	CRT	O1-C1-C4-C5
13	X	101	CRT	C36-C37-C38-O2
13	Z	101	CRT	O1-C1-C4-C5
14	M	408	CDL	C12-C11-CA5-OA7
6	U	101	07D	C11-C10-C8-C7
6	F	101	07D	C1A-C2A-CAA-CBA
6	J	102	07D	C1A-C2A-CAA-CBA
6	P	102	07D	C1A-C2A-CAA-CBA
6	V	102	07D	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
6	Z	102	07D	C1A-C2A-CAA-CBA
6	U	101	07D	CAA-CBA-CGA-O1A
10	H	306	LMT	C2-C3-C4-C5
6	7	101	07D	C2-C1-O2A-CGA
14	M	408	CDL	CA3-CA4-CA6-OA8
10	N	103	LMT	O5B-C1B-O1B-C4'
14	M	409	CDL	C12-C11-CA5-OA7
14	H	303	CDL	C32-C31-CA7-OA9
10	E	103	LMT	C7-C8-C9-C10
8	L	303	U10	C6-C7-C8-C9
9	L	304	PGV	C03-O11-P-O13
9	L	304	PGV	C04-O12-P-O13
14	M	409	CDL	CB2-OB2-PB2-OB3
14	H	303	CDL	CB3-OB5-PB2-OB3
10	E	103	LMT	O5'-C1'-O1'-C1
14	M	408	CDL	OA5-CA3-CA4-CA6
6	4	102	07D	C3-C5-C6-C7
12	M	406	RQ0	C45-C47-C51-C58
9	H	302	PGV	O01-C1-C2-C3
14	H	303	CDL	C51-C52-C53-C54
6	2	102	07D	C2A-CAA-CBA-CGA
10	M	410	LMT	C2B-C1B-O1B-C4'
6	N	102	07D	C14-C13-C15-C16
6	Y	101	07D	C4-C3-C5-C6
6	9	101	07D	C14-C13-C15-C16
6	P	102	07D	C10-C11-C12-C13
6	7	101	07D	C15-C16-C17-C18
14	M	409	CDL	C51-C52-C53-C54
6	K	101	07D	CAD-CBD-CGD-O1D
6	Q	102	07D	CAD-CBD-CGD-O1D
6	6	102	07D	CAD-CBD-CGD-O1D
14	H	303	CDL	CB6-CB4-OB6-CB5
10	5	201	LMT	O5B-C5B-C6B-O6B
6	G	102	07D	CAA-CBA-CGA-O2A
10	G	103	LMT	C5'-C4'-O1B-C1B
6	P	102	07D	C5-C6-C7-C8
14	H	304	CDL	CA2-C1-CB2-OB2
6	Q	101	07D	C4-C3-C5-C6
6	E	102	07D	C3A-C2A-CAA-CBA
6	O	101	07D	C12-C13-C15-C16
6	Q	102	07D	C3A-C2A-CAA-CBA
10	5	201	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
13	M	407	CRT	C15-C16-C17-C19
6	G	102	07D	CAA-CBA-CGA-O1A
9	H	302	PGV	O02-C1-C2-C3
7	L	302	08I	C5-C6-C7-C8
14	H	303	CDL	C72-C73-C74-C75
10	2	103	LMT	C4-C5-C6-C7
6	0	102	07D	CAA-CBA-CGA-O2A

There are no ring outliers.

53 monomers are involved in 183 short contacts:

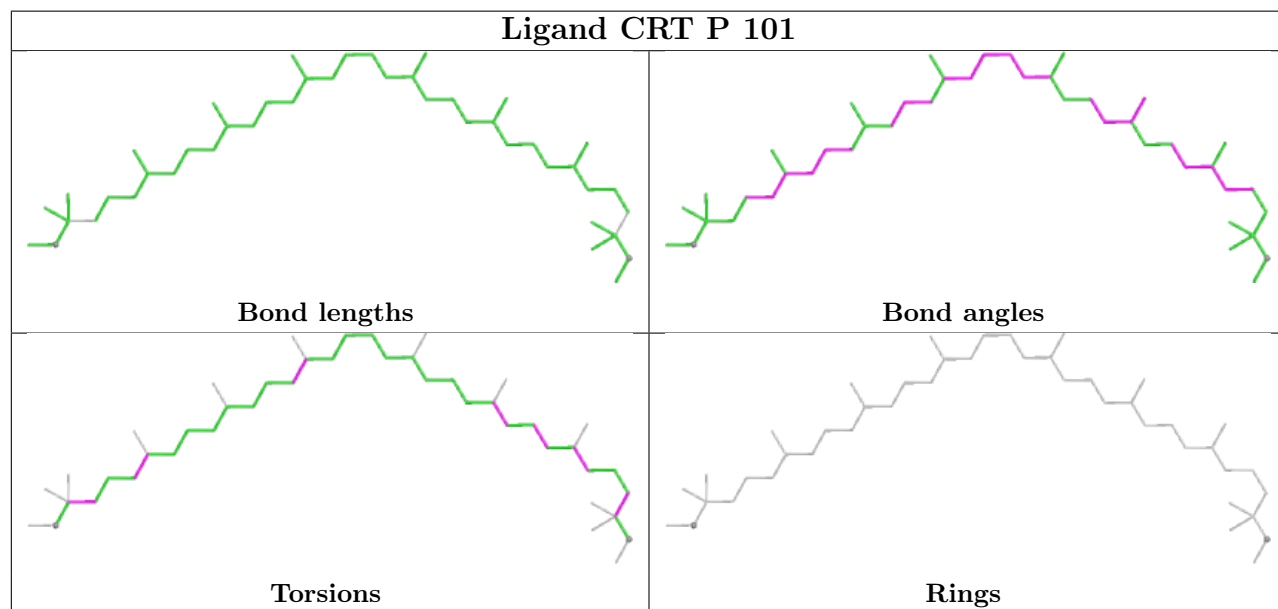
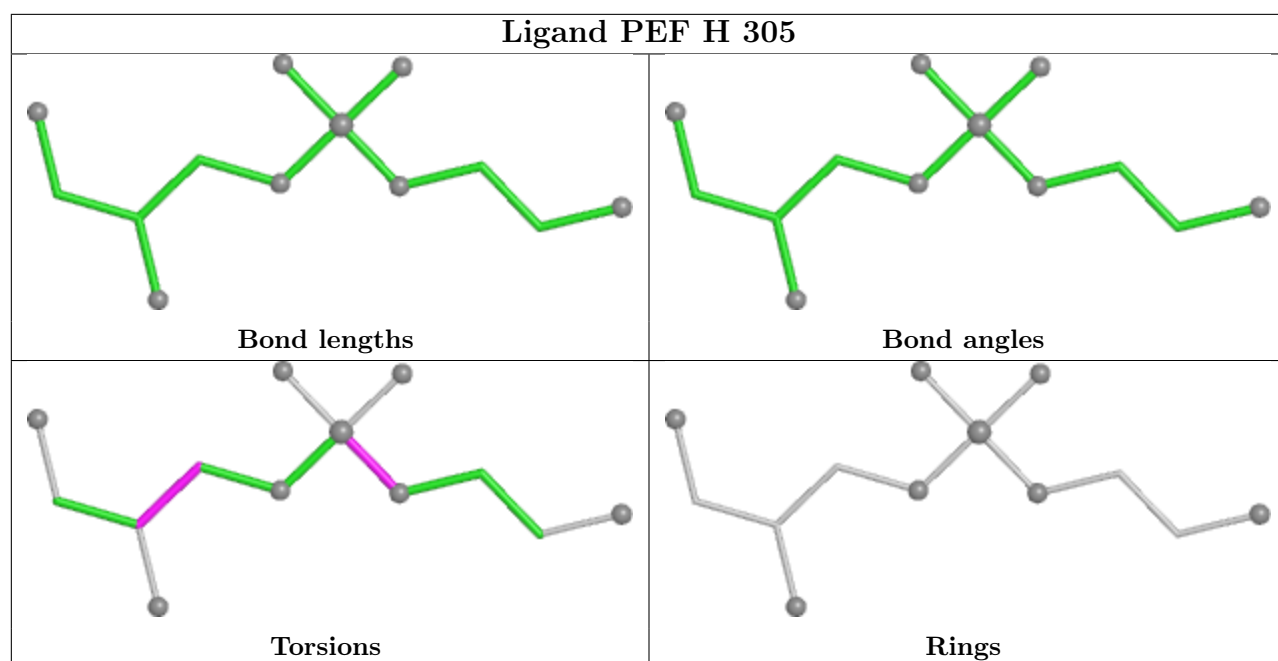
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	H	305	PEF	3	0
13	P	101	CRT	4	0
15	K	103	PEF	1	0
6	N	102	07D	1	0
13	M	407	CRT	6	0
10	T	103	LMT	1	0
10	5	203	LMT	2	0
10	B	102	LMT	2	0
10	E	103	LMT	2	0
10	G	103	LMT	3	0
10	8	103	LMT	1	0
9	H	302	PGV	6	0
13	T	101	CRT	4	0
13	V	101	CRT	6	0
14	M	408	CDL	5	0
14	H	304	CDL	2	0
13	0	101	CRT	5	0
15	K	102	PEF	4	0
6	E	102	07D	1	0
6	2	102	07D	3	0
10	H	306	LMT	5	0
10	0	103	LMT	1	0
13	8	101	CRT	7	0
6	8	102	07D	2	0
13	A	102	CRT	3	0
10	M	410	LMT	3	0
10	5	201	LMT	2	0
10	P	103	LMT	1	0
10	J	103	LMT	2	0
6	G	102	07D	1	0

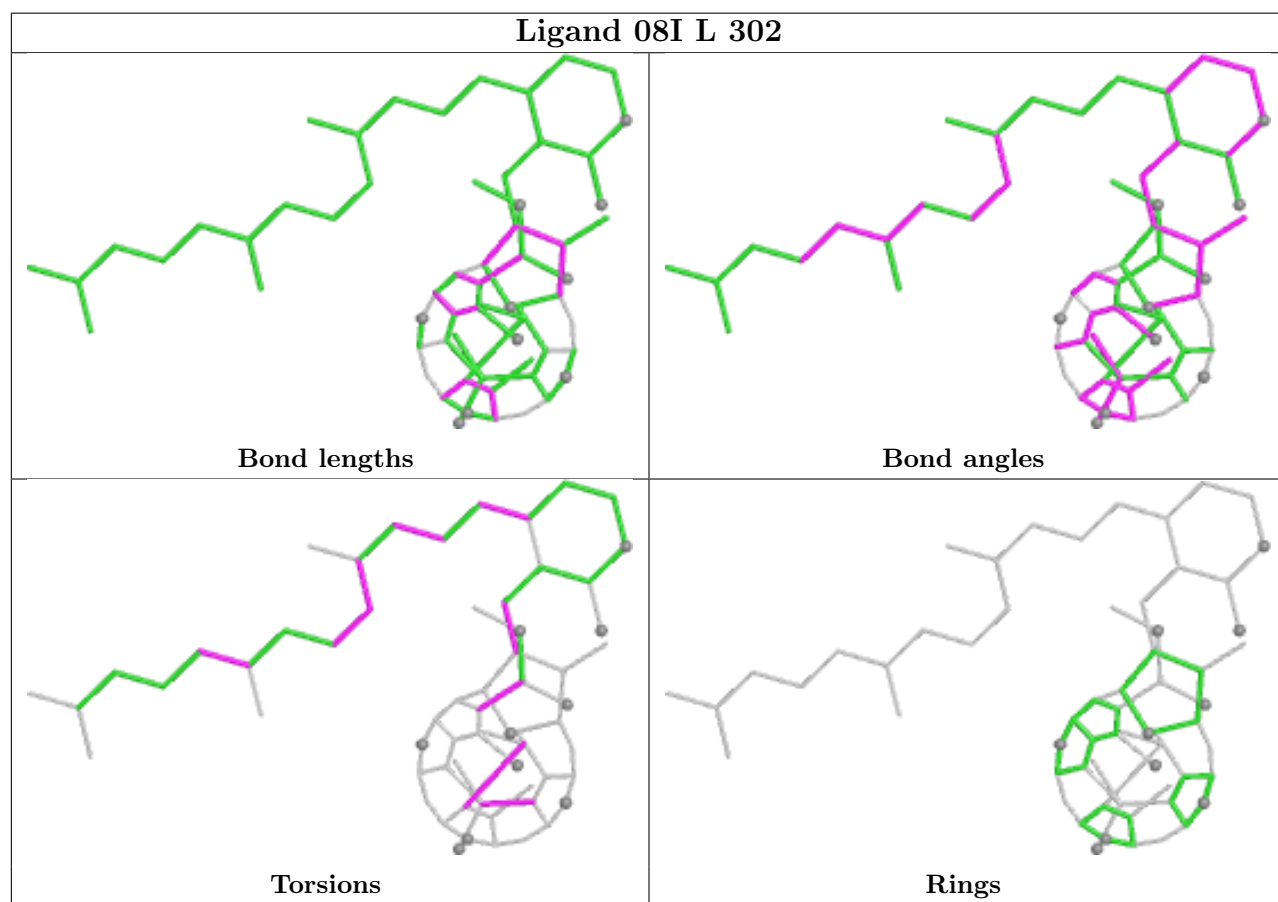
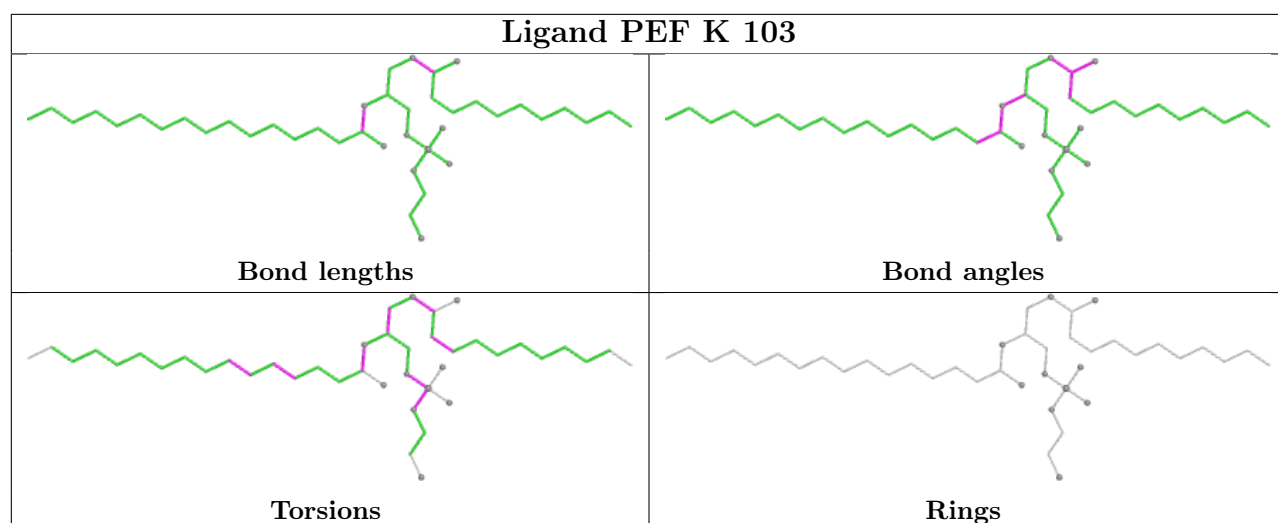
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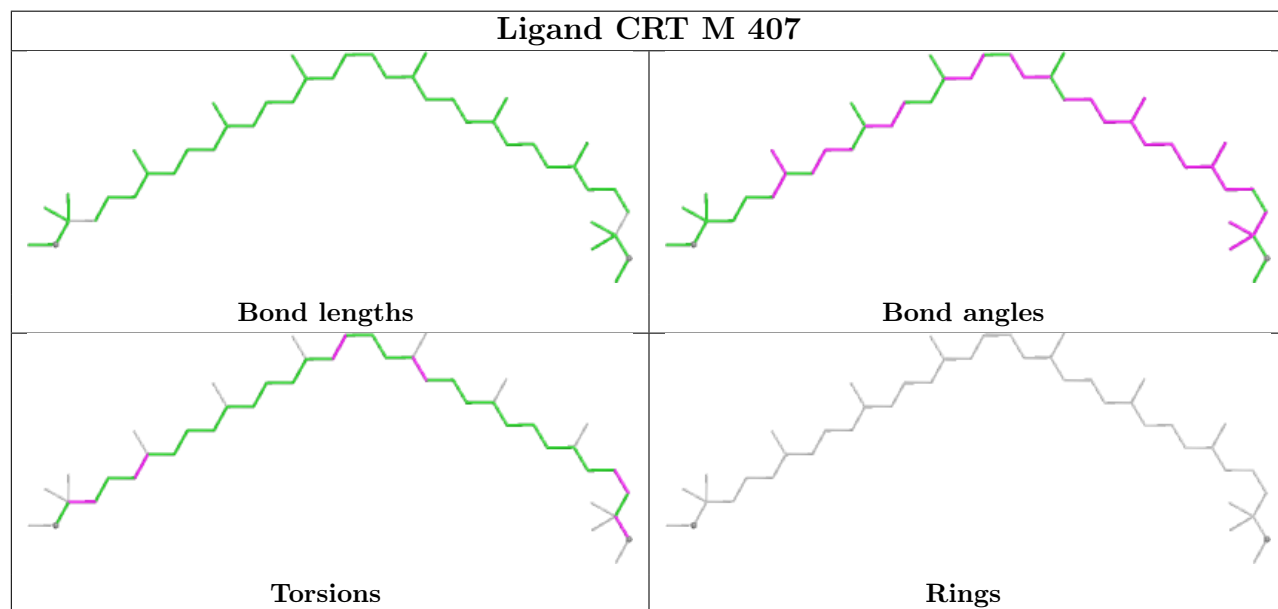
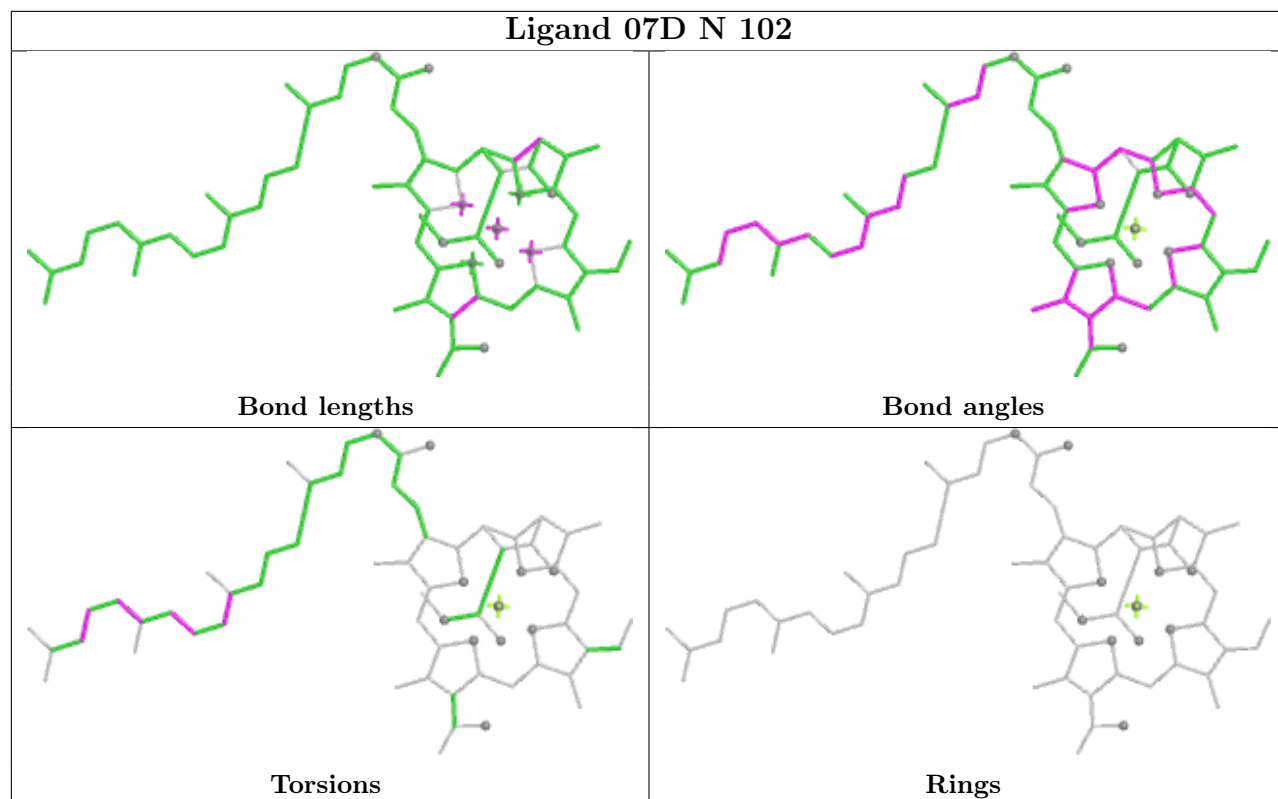
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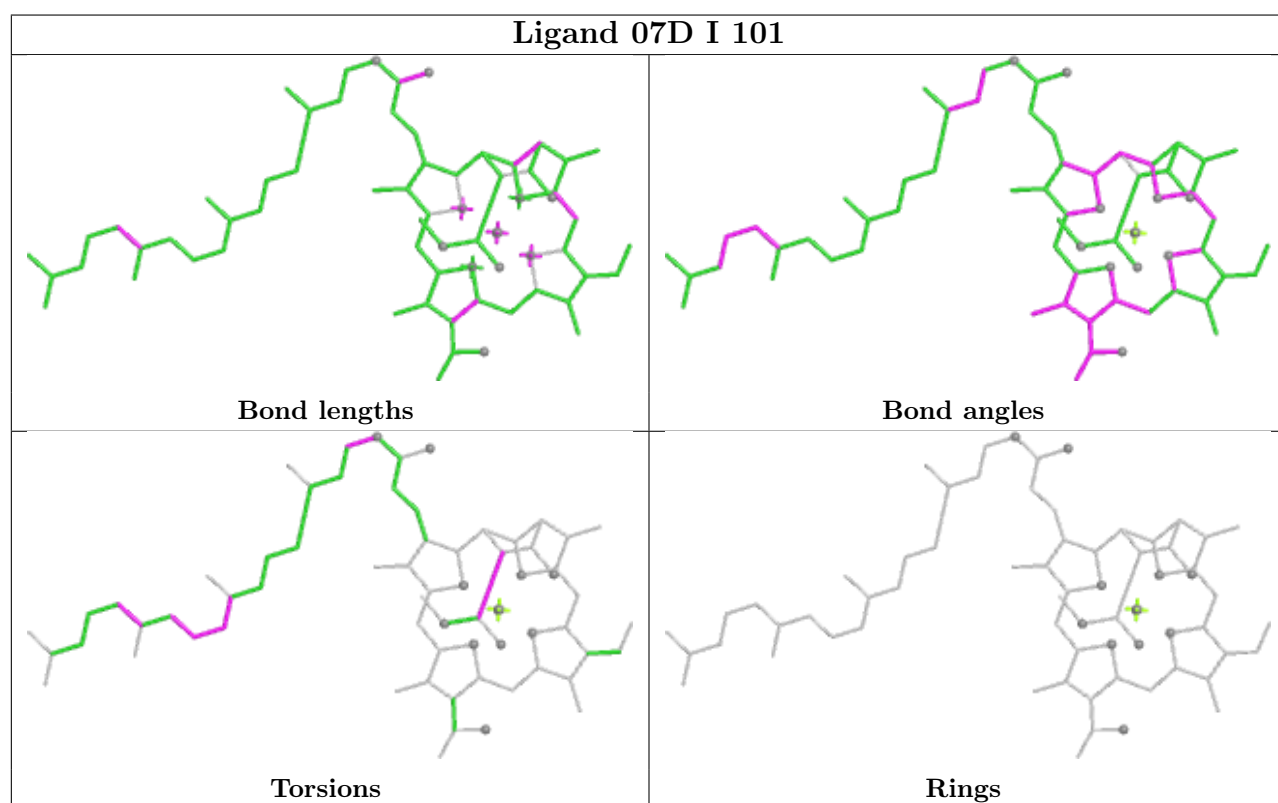
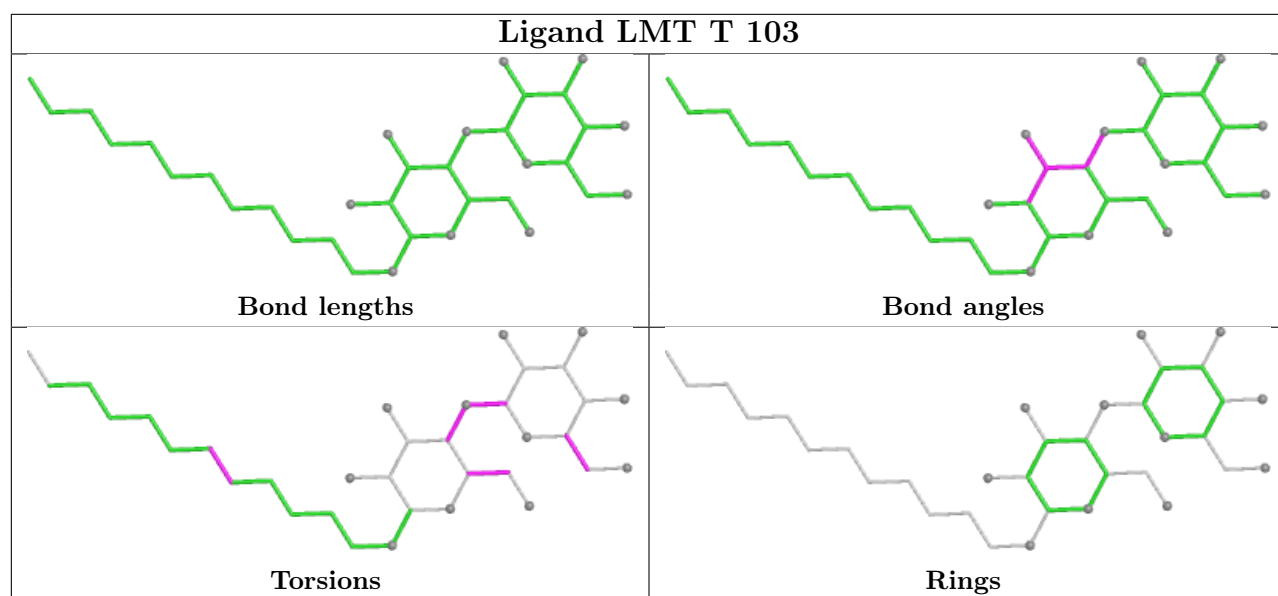
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	X	103	LMT	1	0
10	2	103	LMT	1	0
13	4	101	CRT	8	0
9	L	304	PGV	4	0
13	2	101	CRT	9	0
14	H	303	CDL	6	0
8	L	303	U10	4	0
13	E	101	CRT	7	0
6	7	101	07D	1	0
6	Y	101	07D	1	0
10	R	102	LMT	2	0
8	M	401	U10	1	0
10	6	103	LMT	2	0
13	6	101	CRT	7	0
10	Z	103	LMT	2	0
13	Z	101	CRT	7	0
13	R	101	CRT	6	0
13	G	101	CRT	6	0
13	J	101	CRT	8	0
14	M	409	CDL	2	0
10	M	411	LMT	1	0
13	X	101	CRT	8	0
13	N	101	CRT	9	0

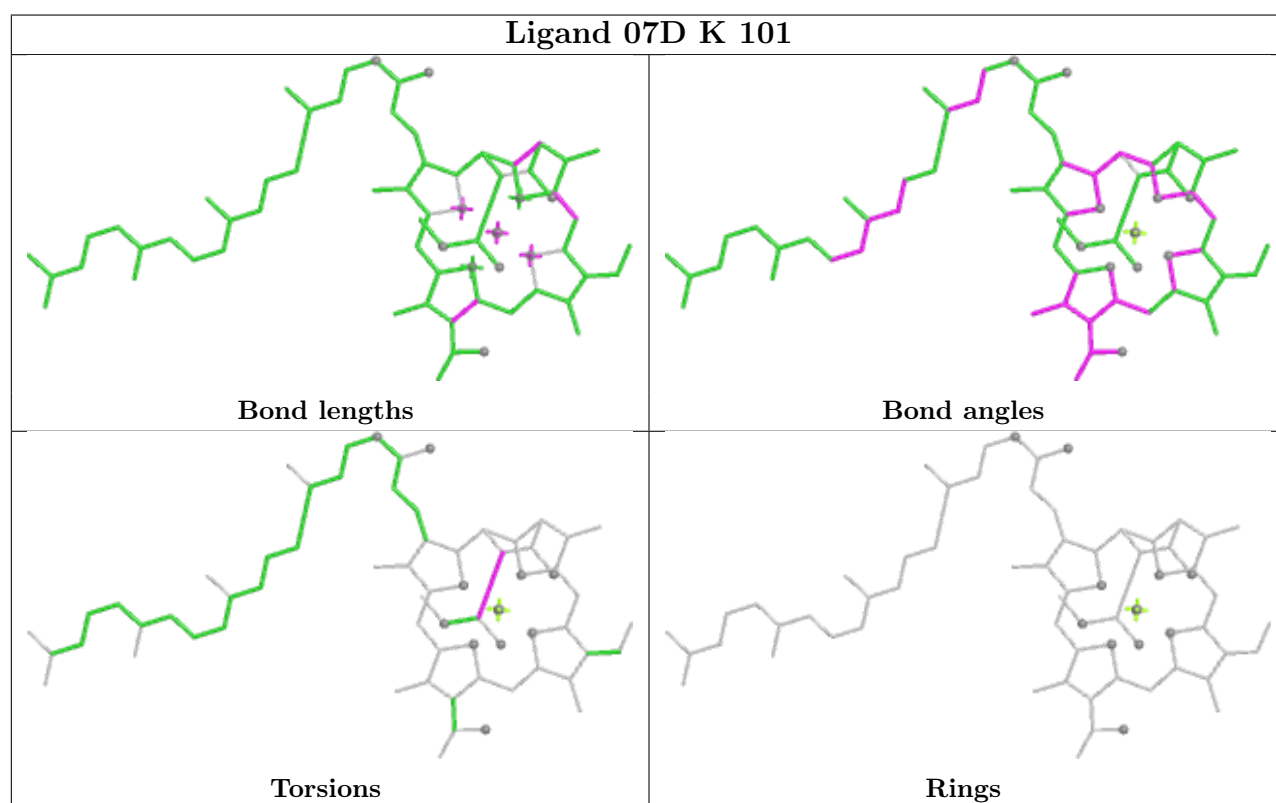
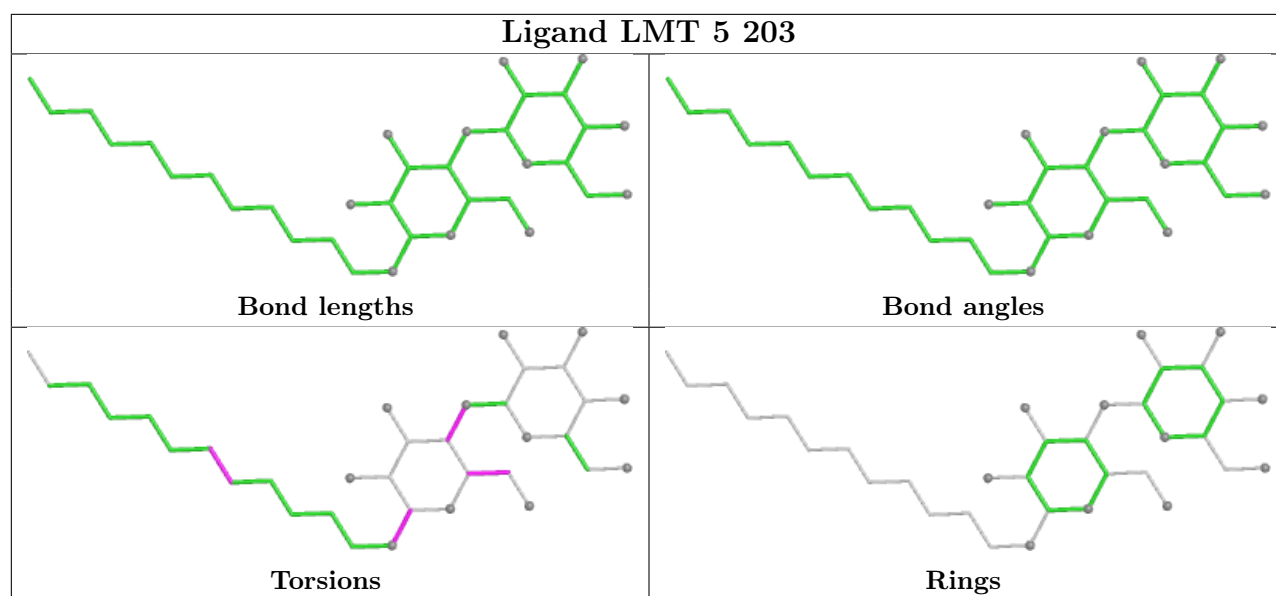
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

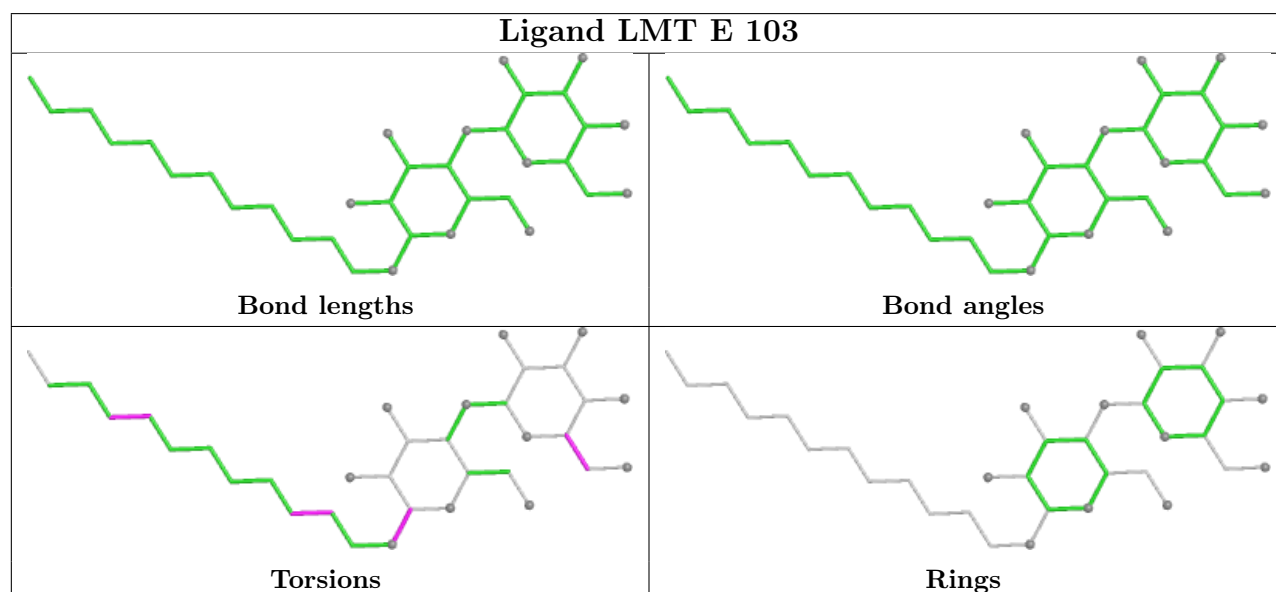
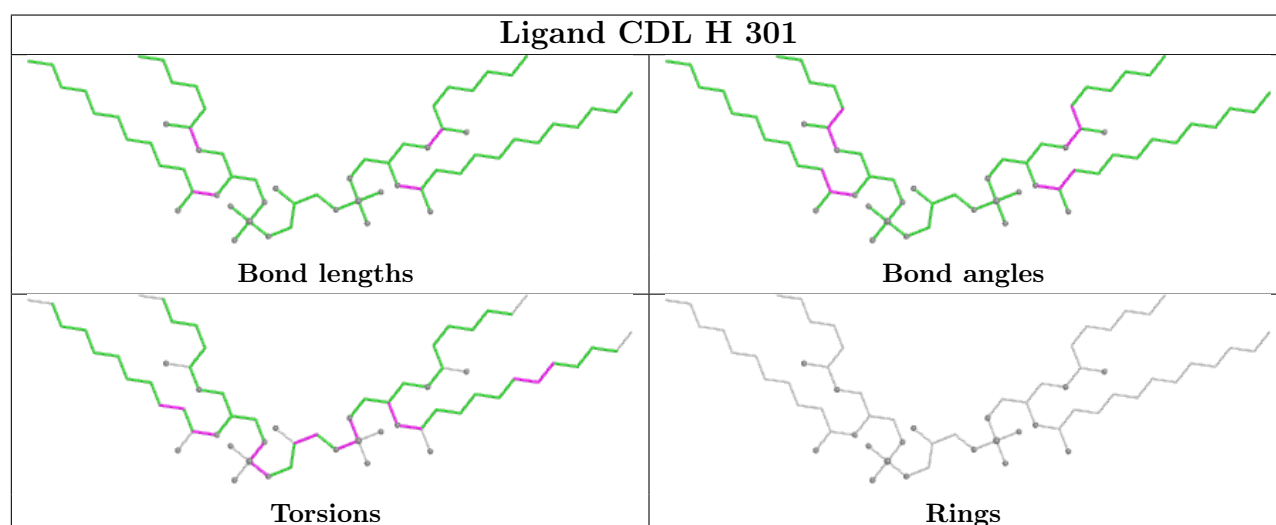
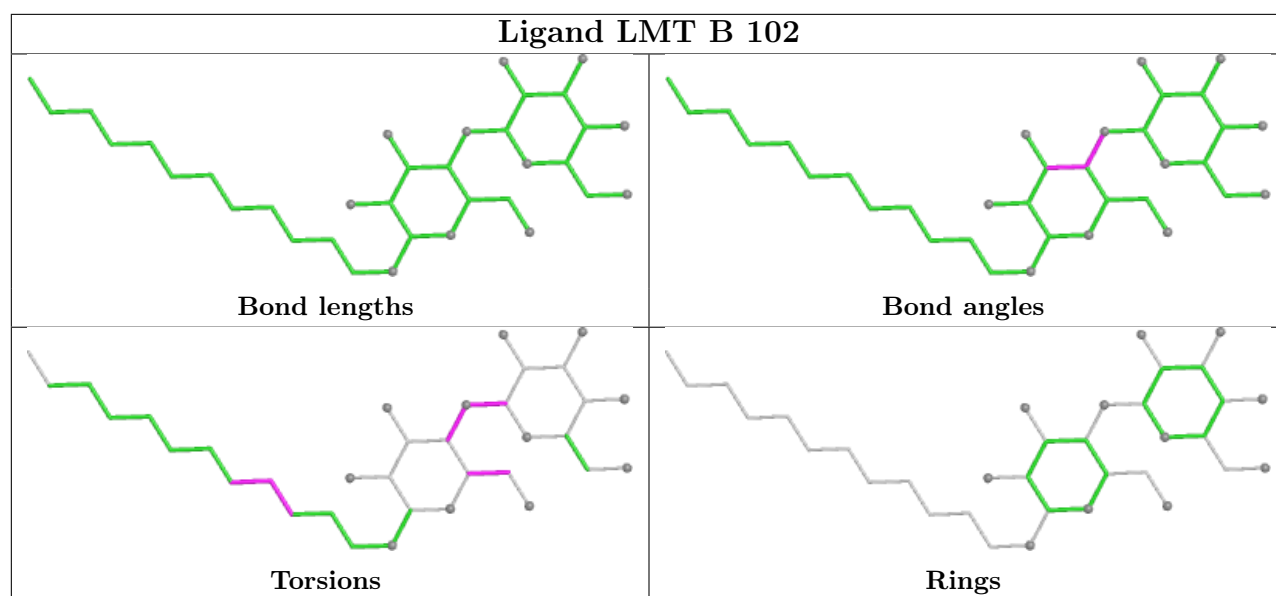


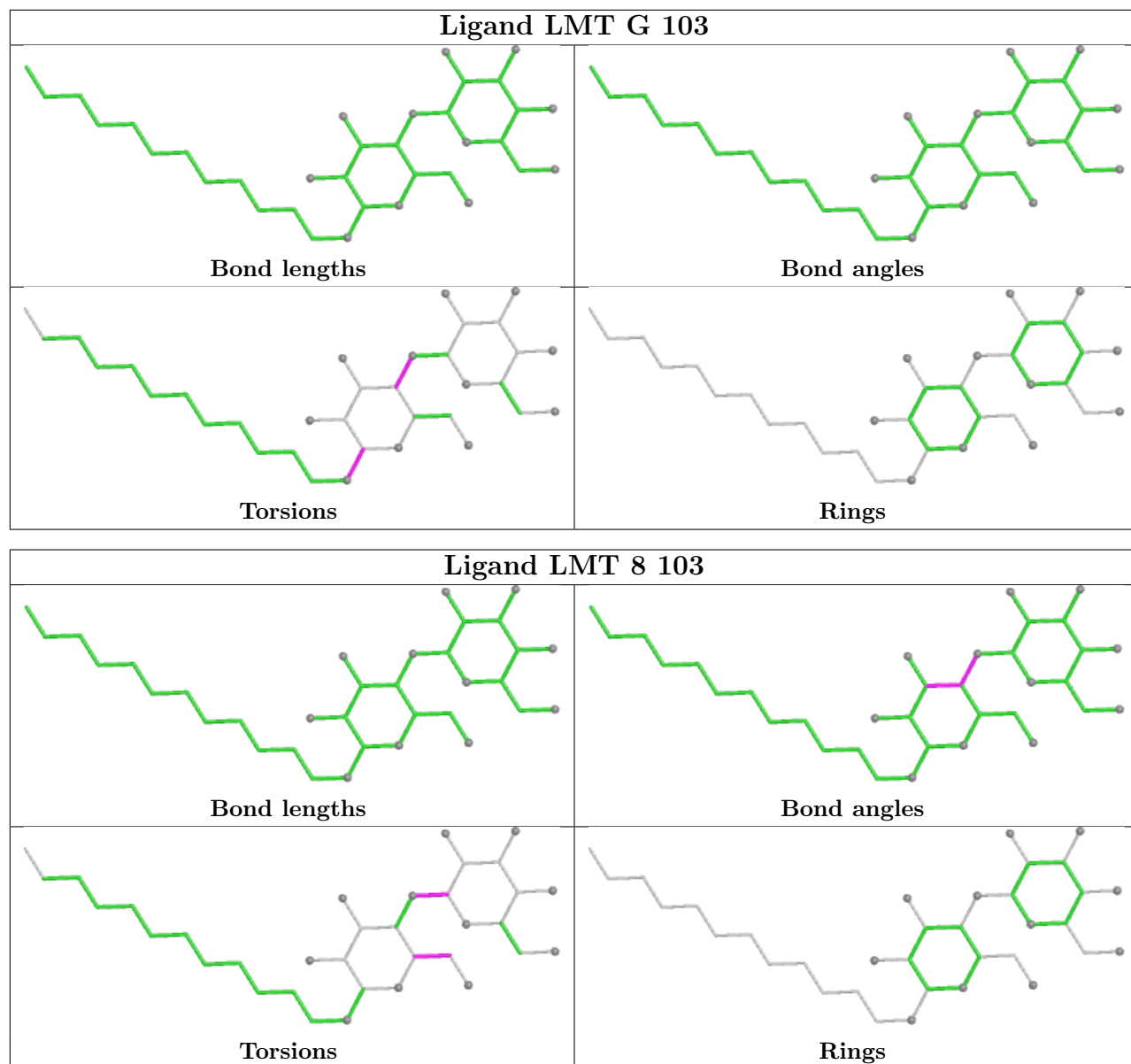


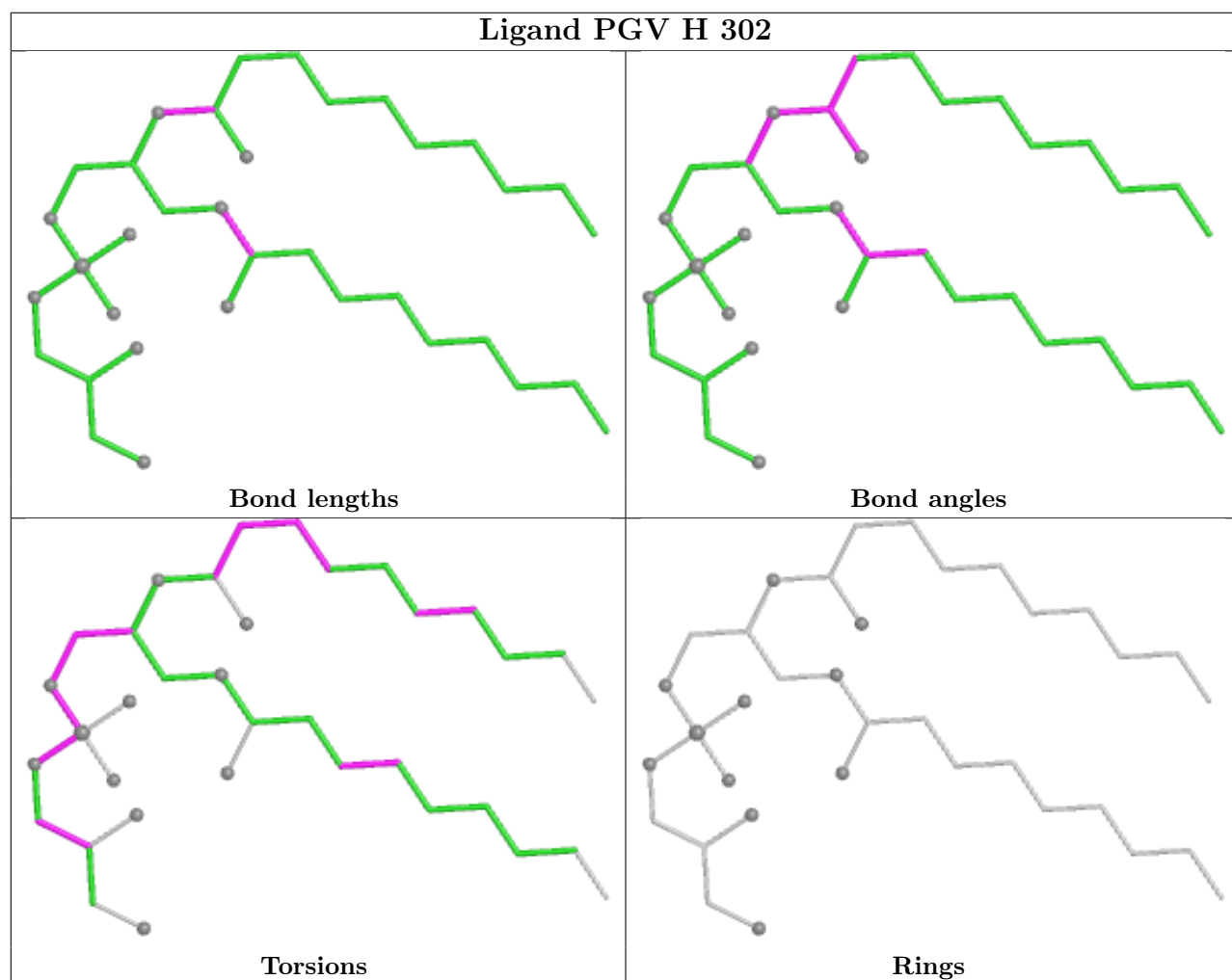
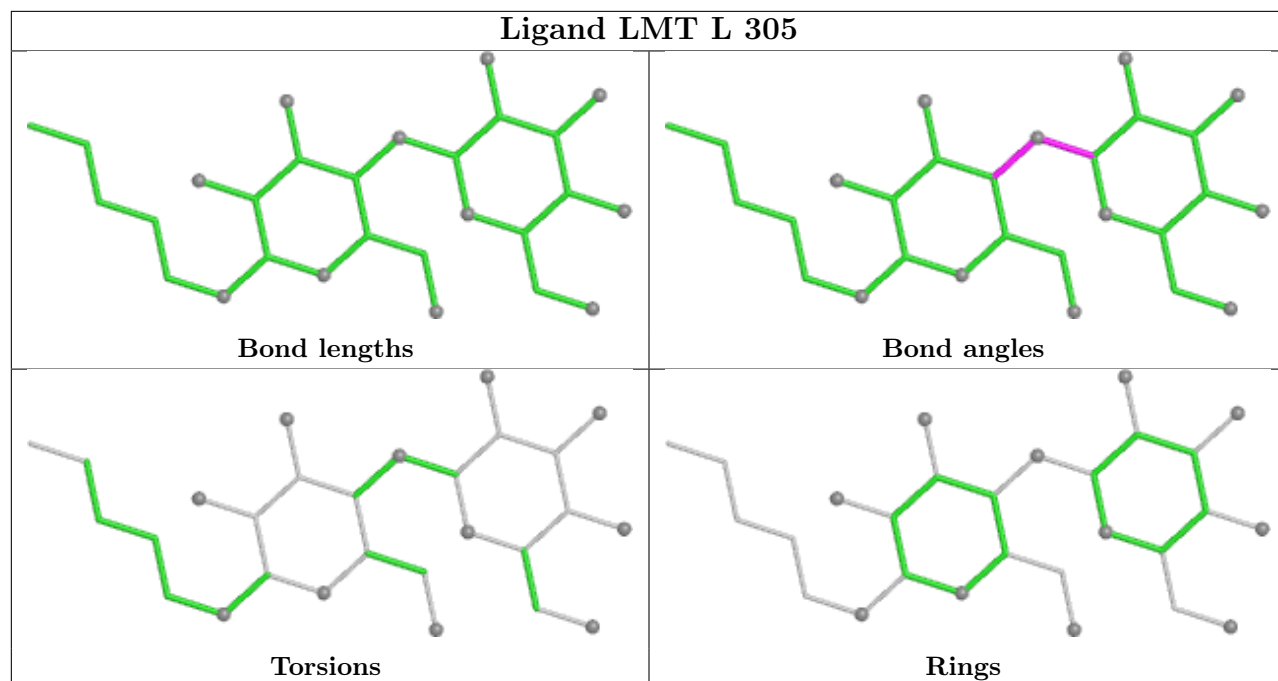


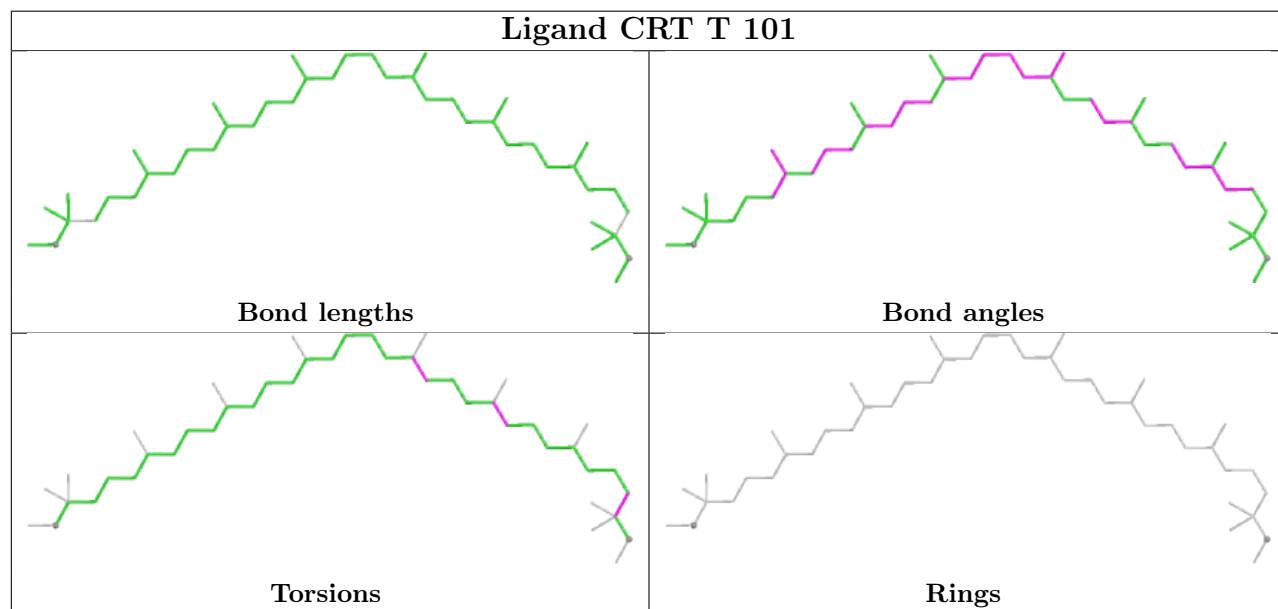
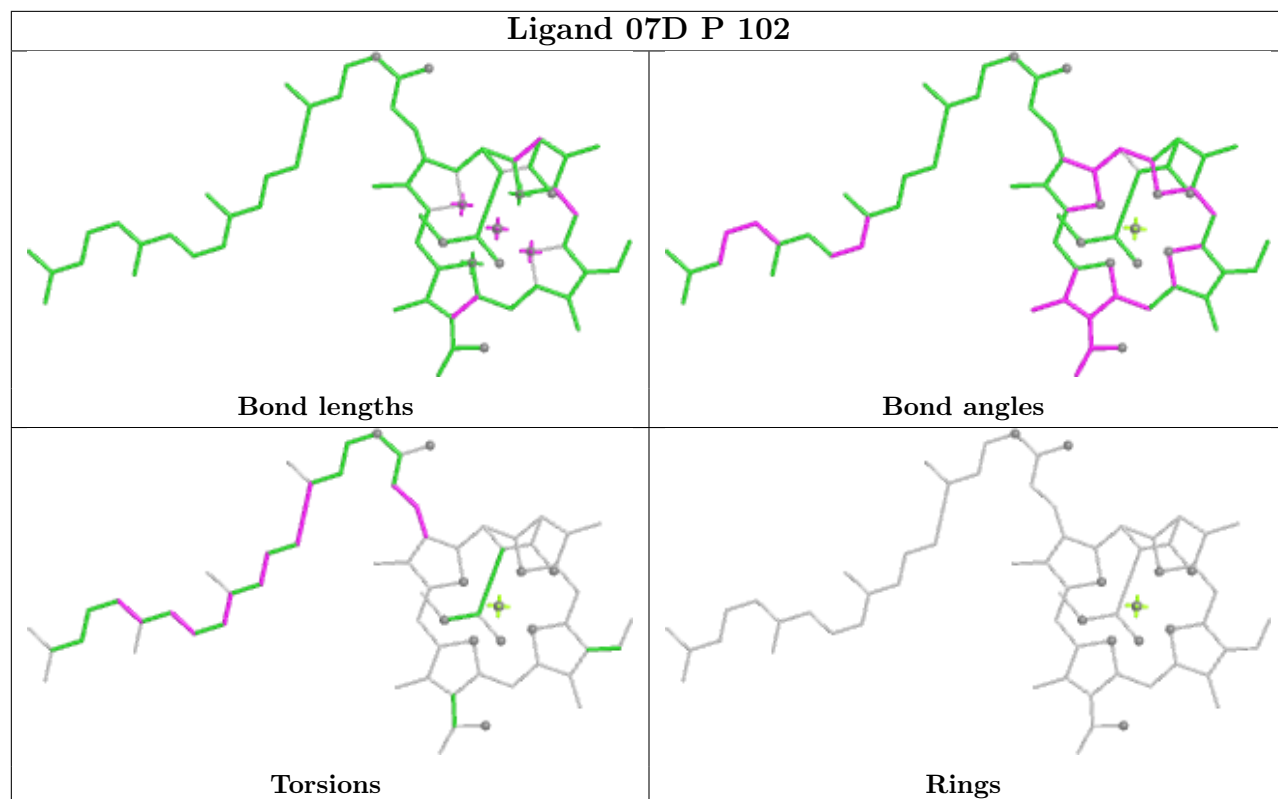


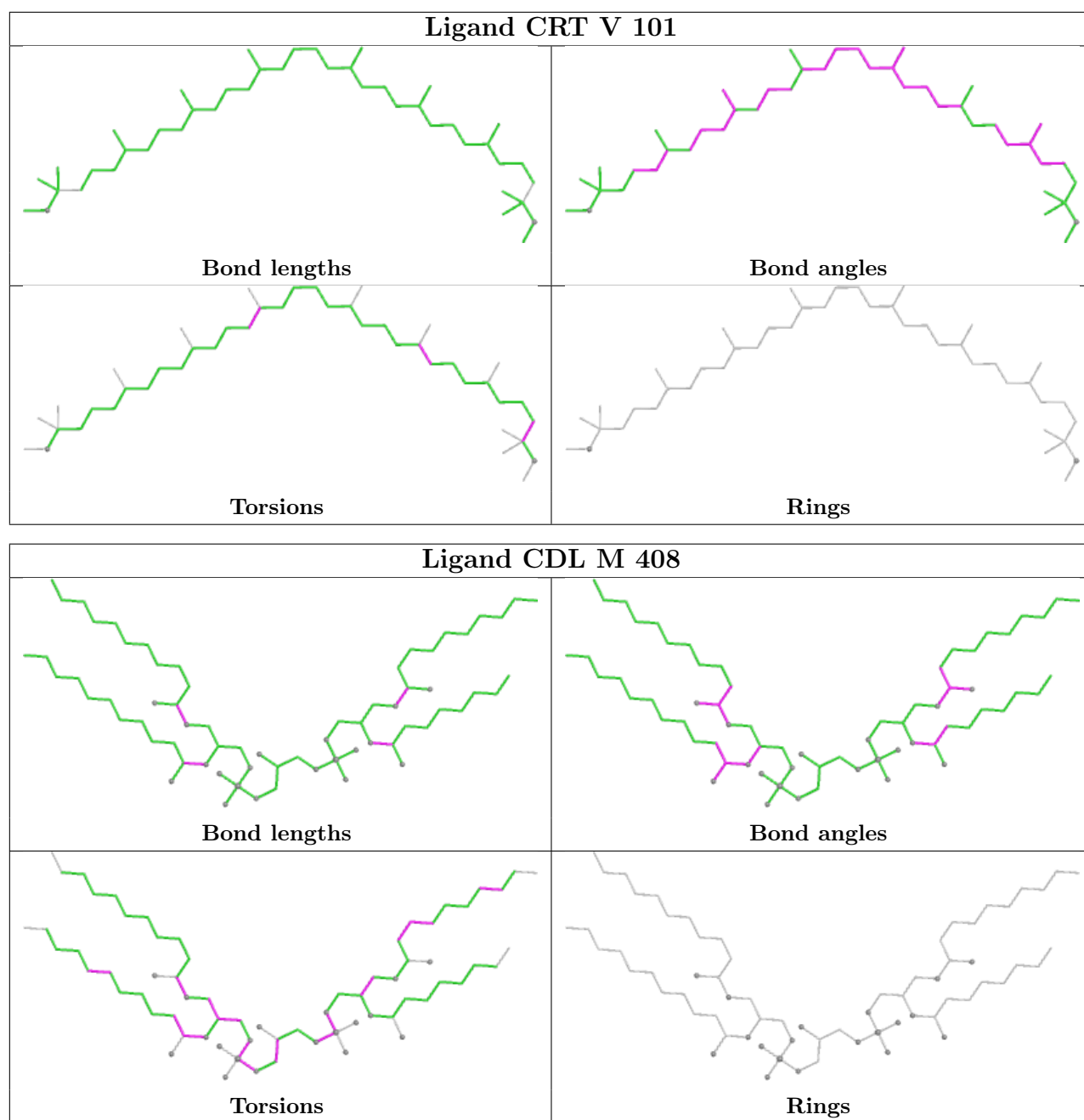


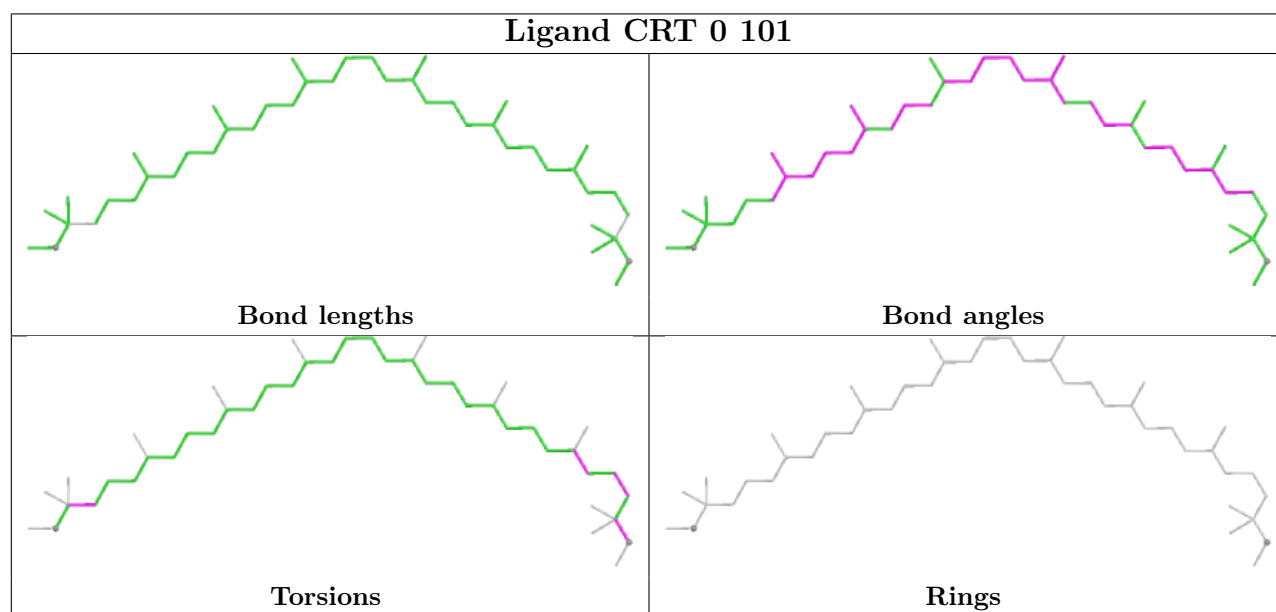
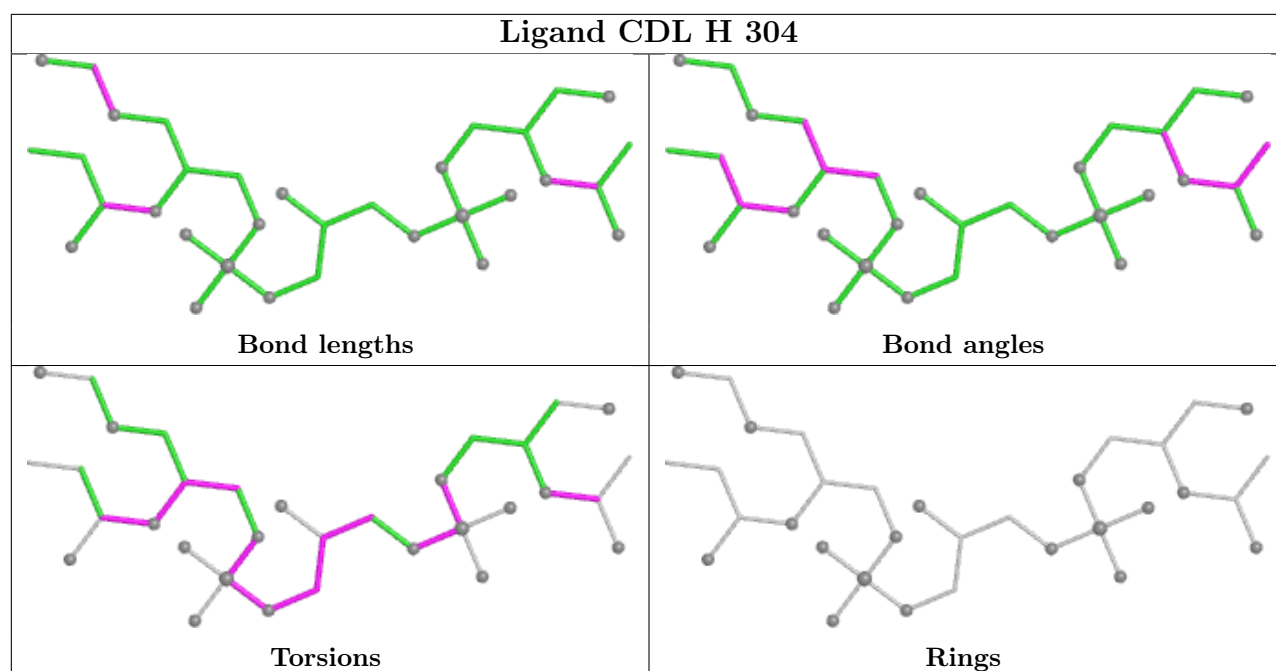


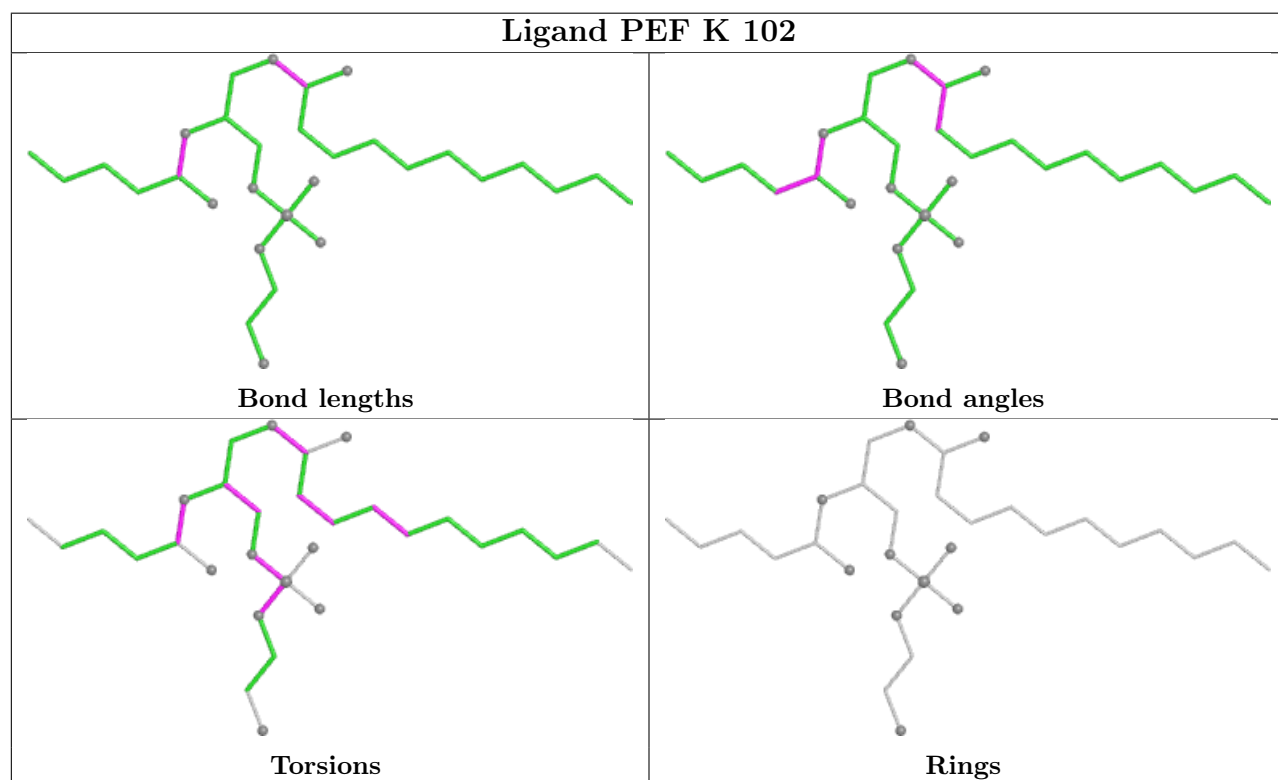
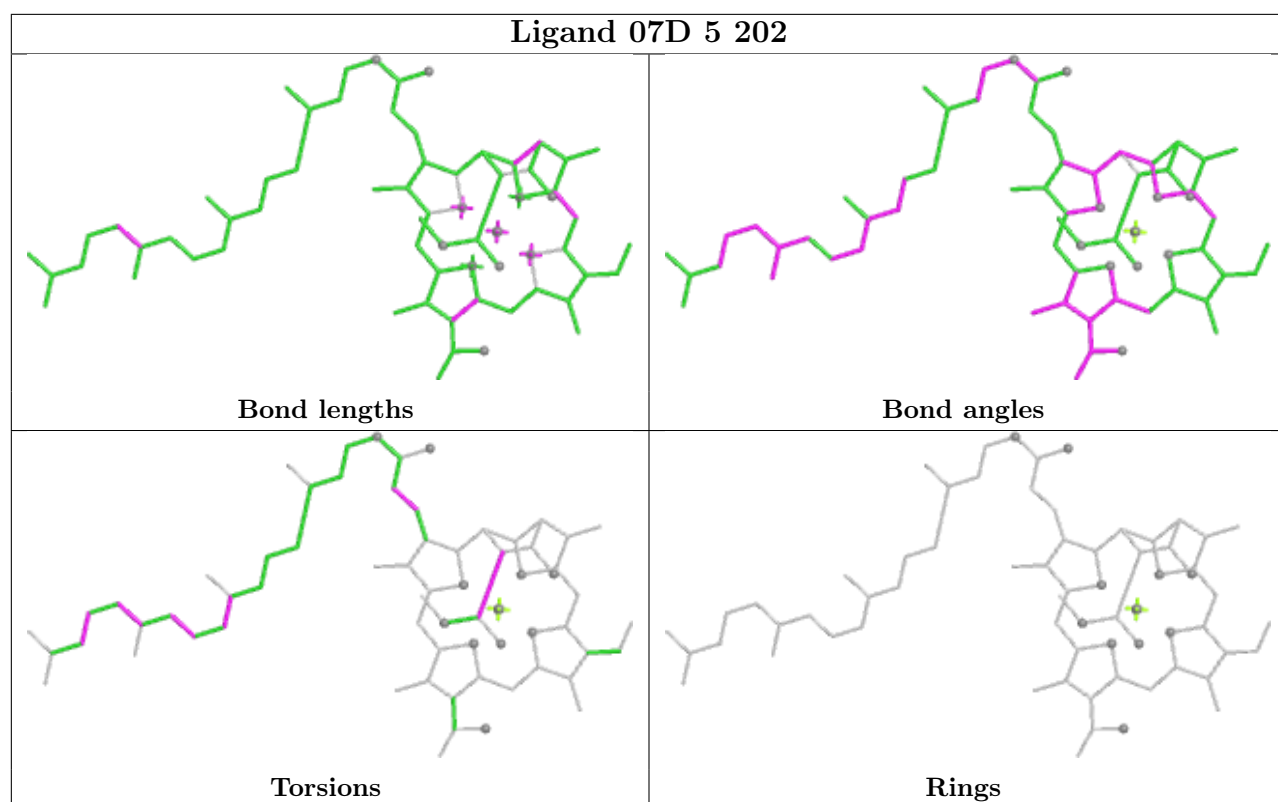


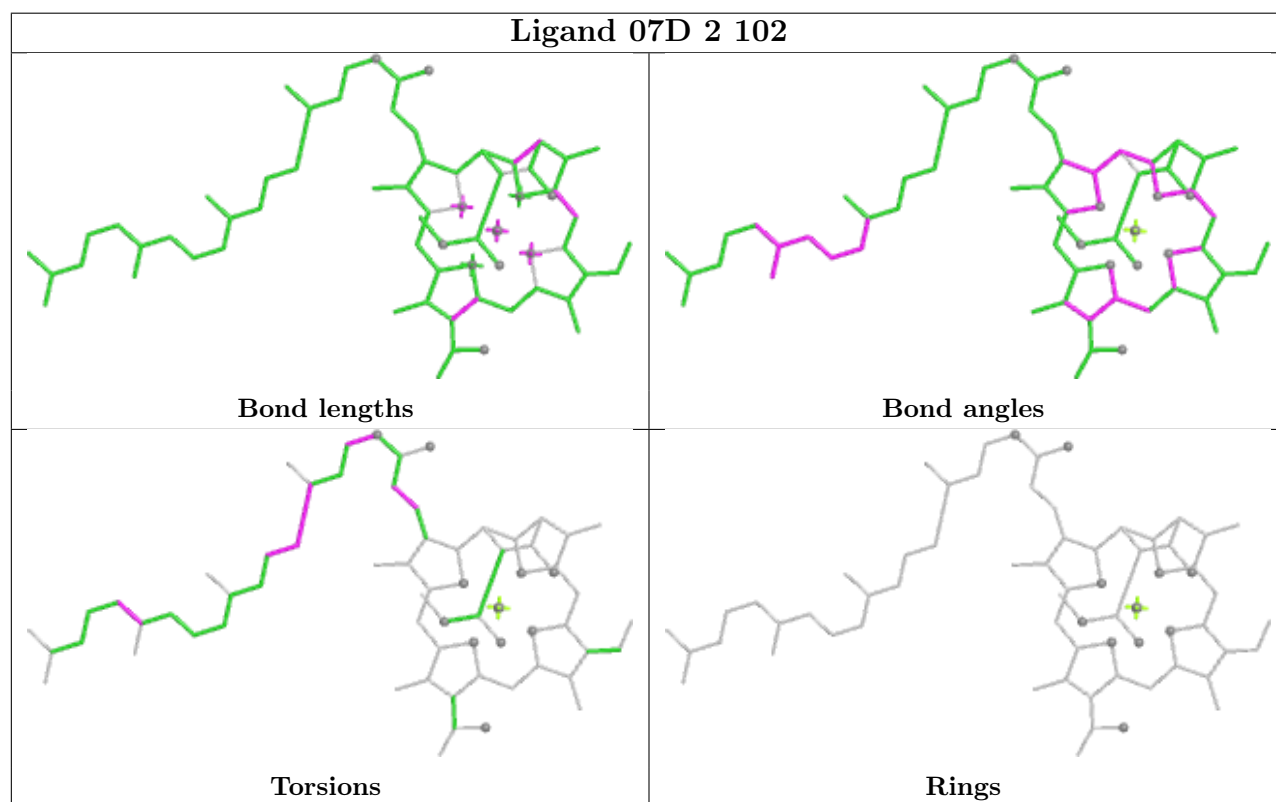
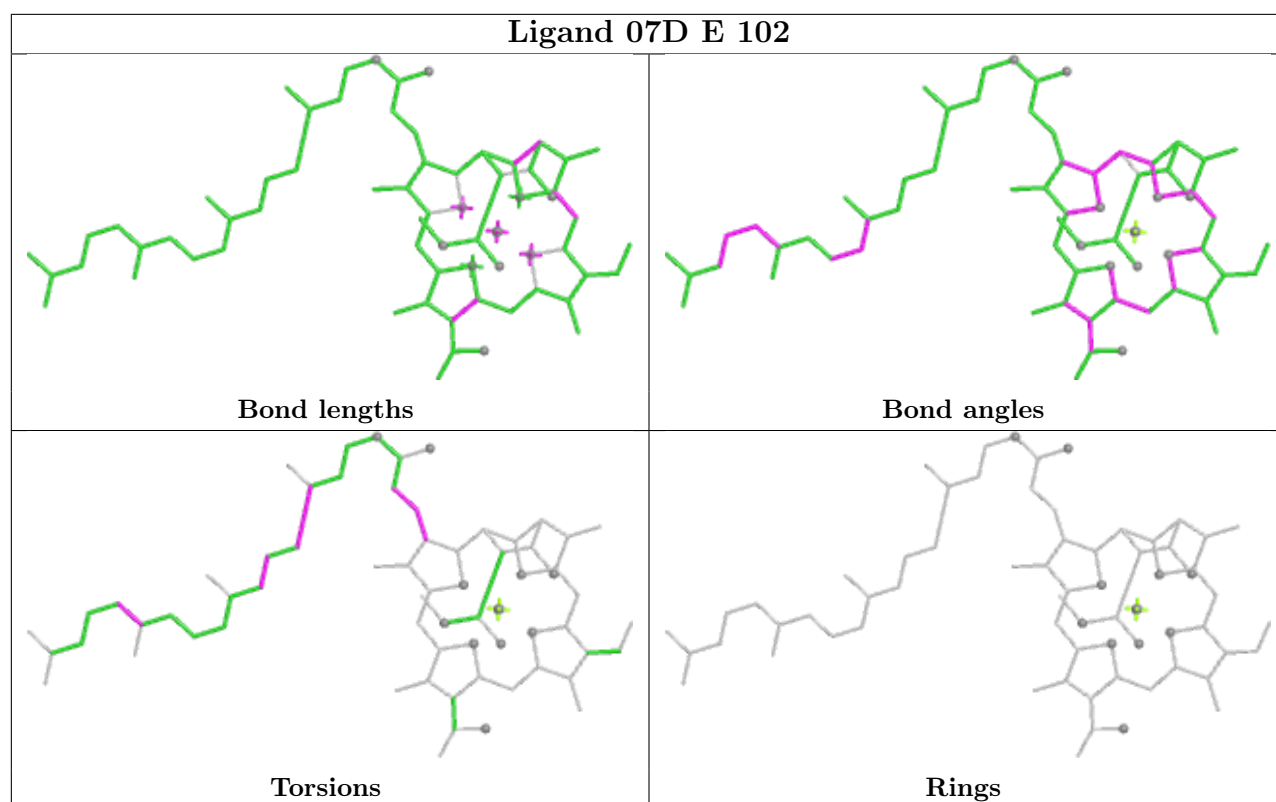


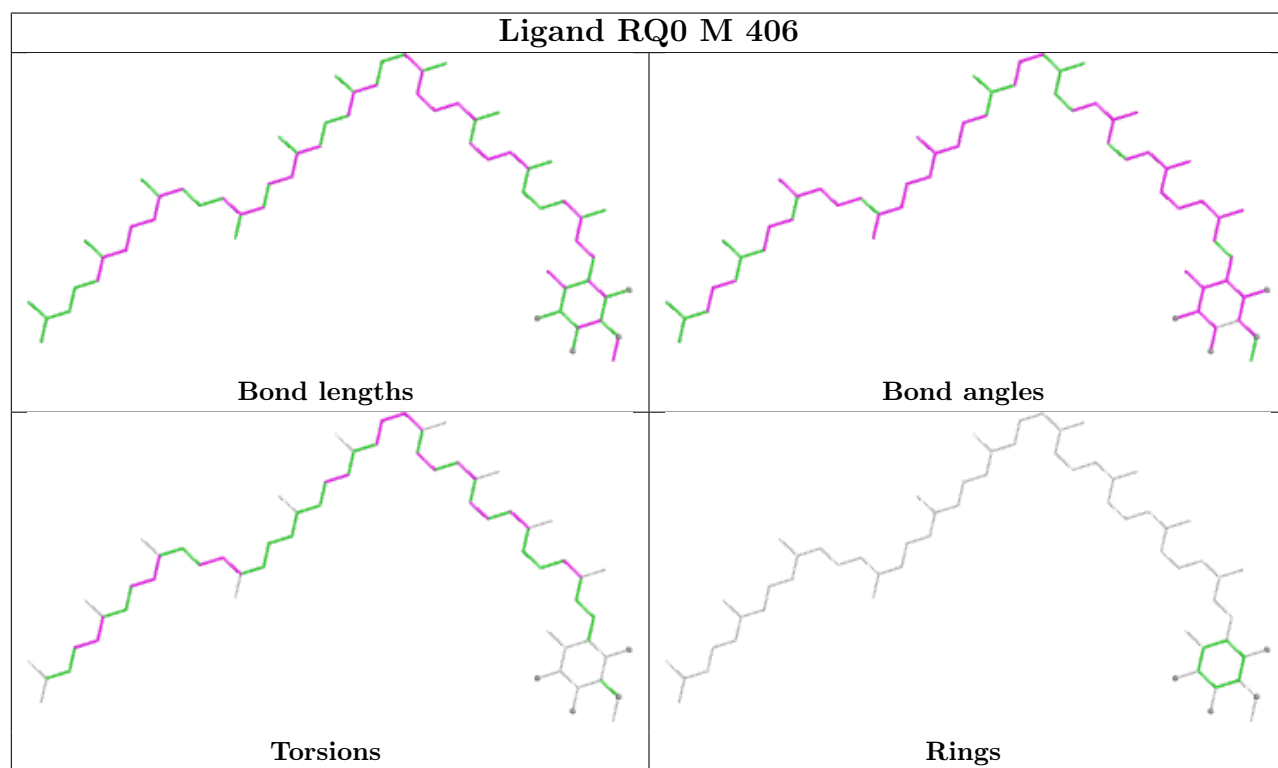
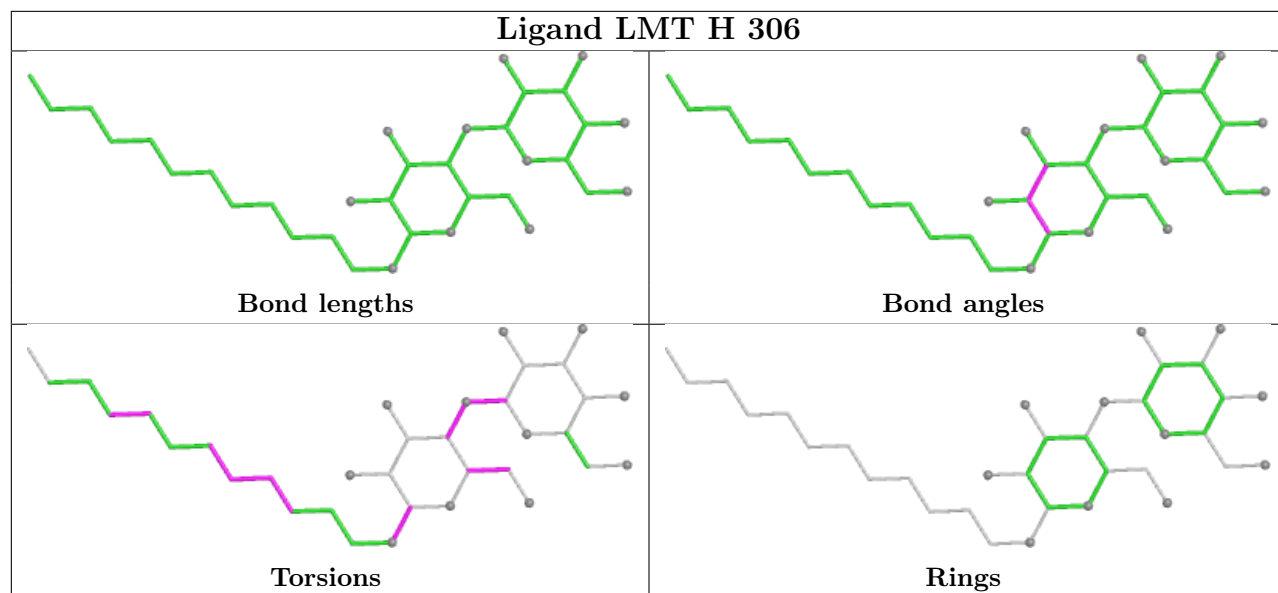


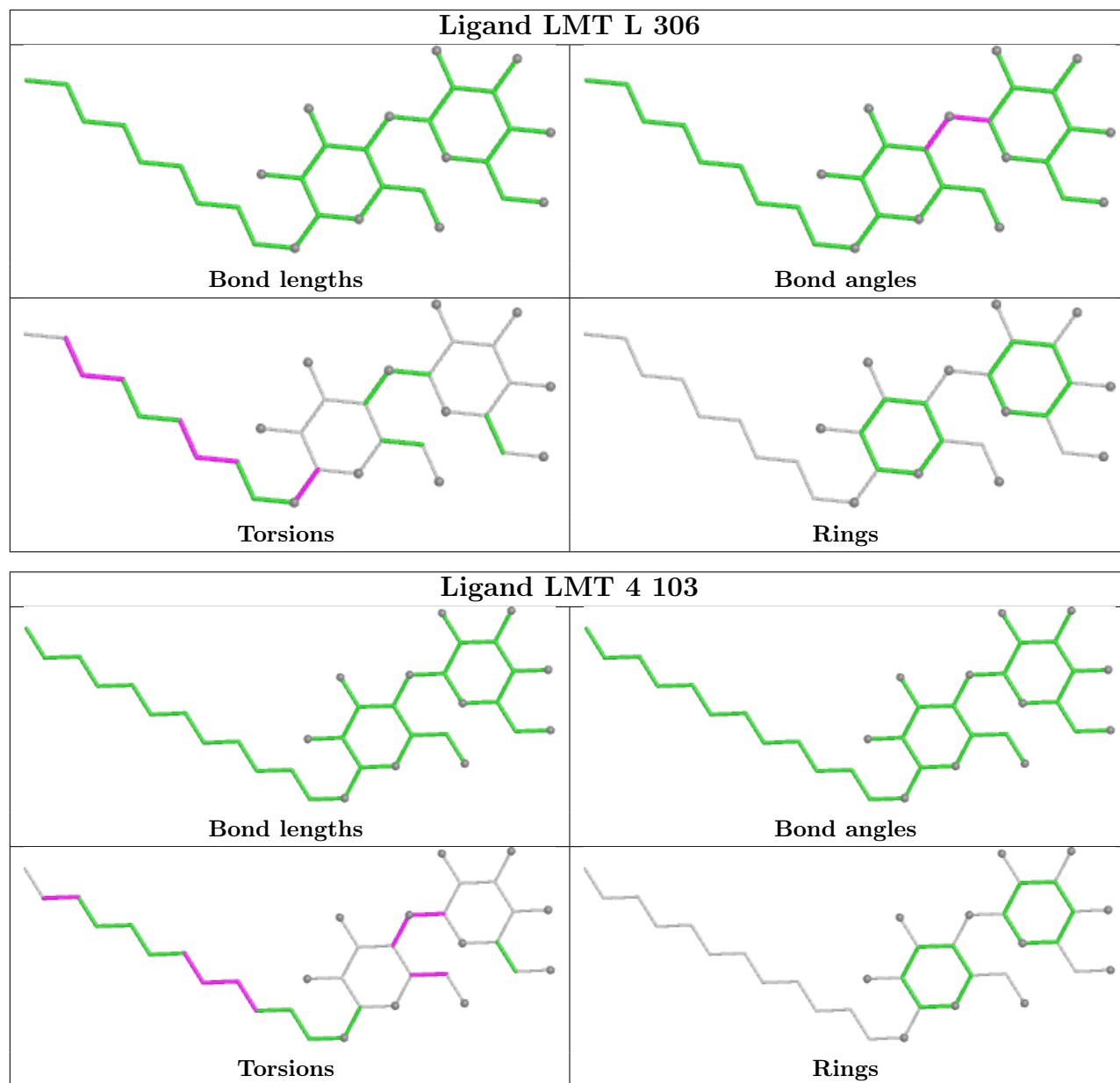


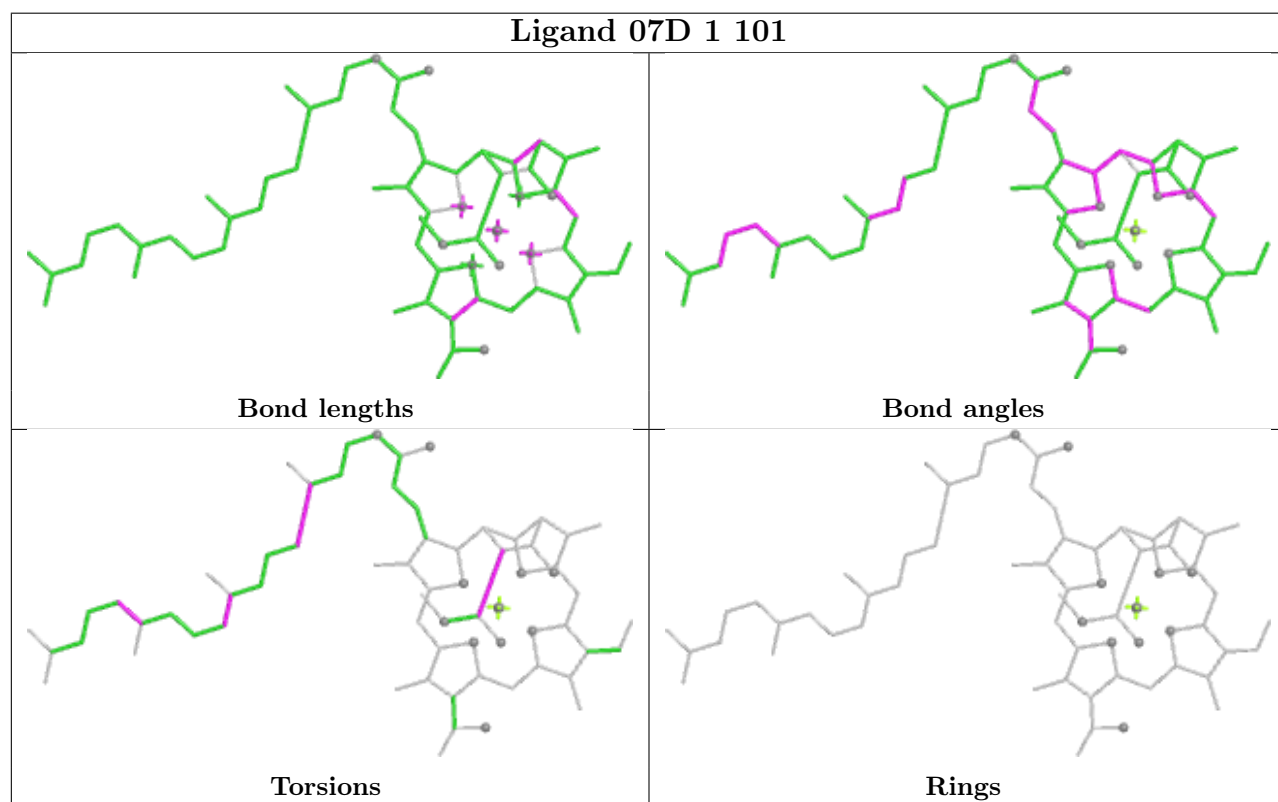
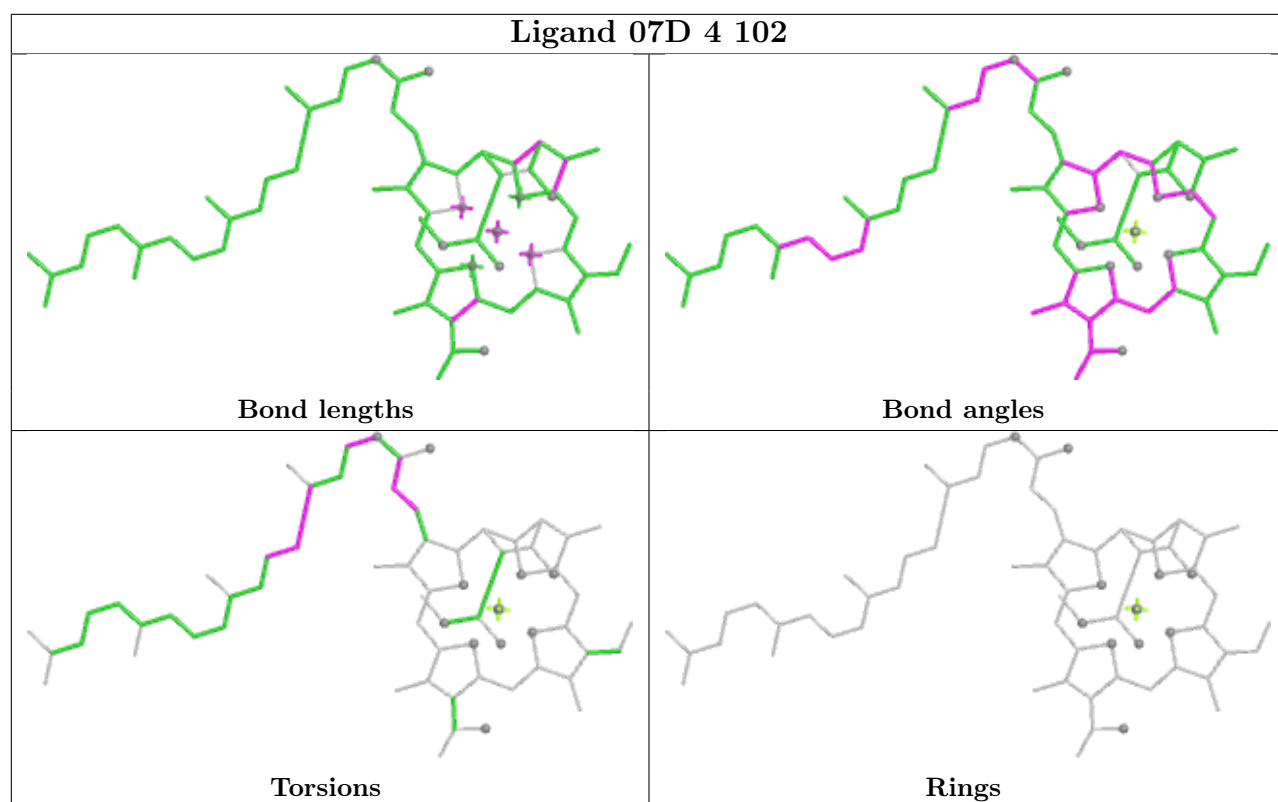


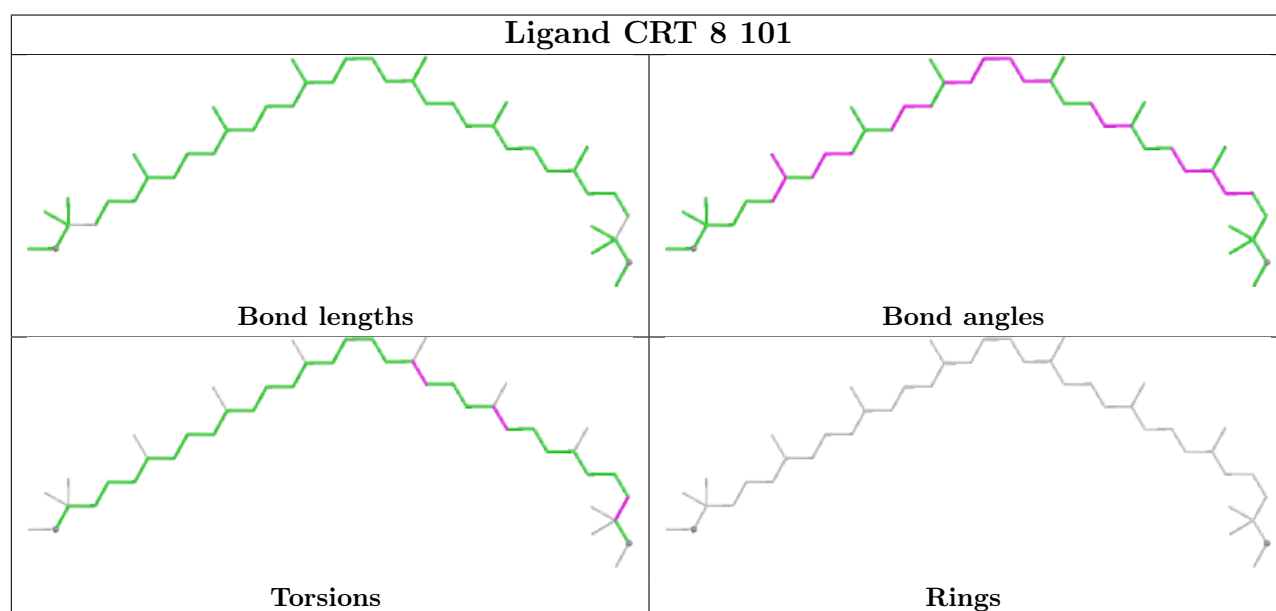
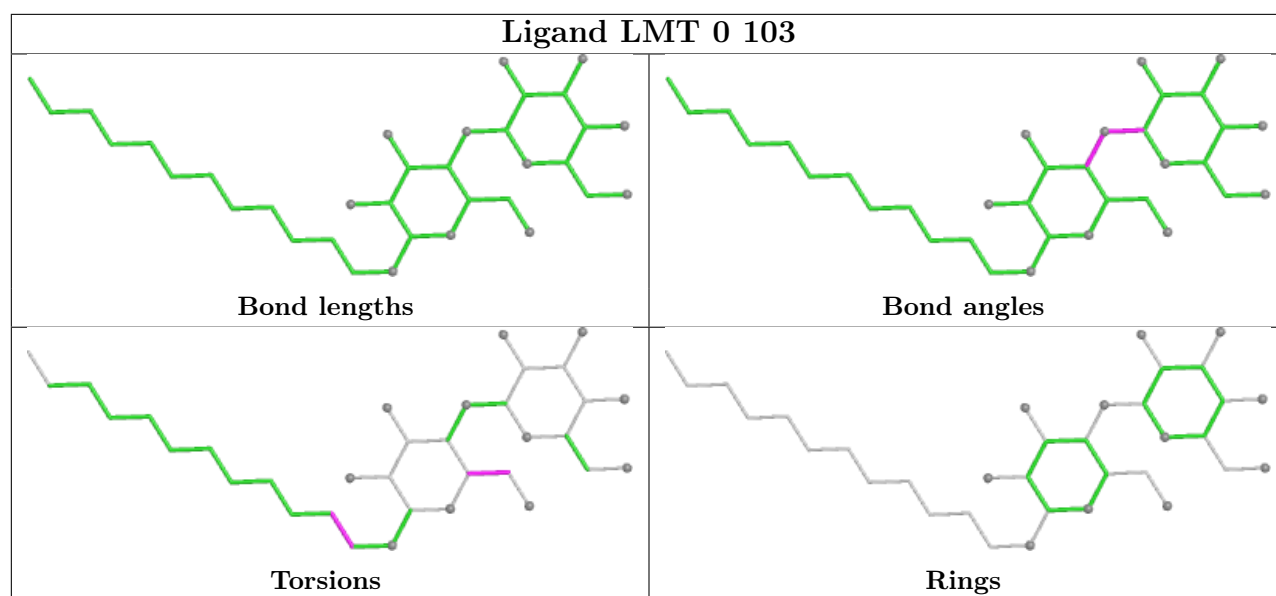


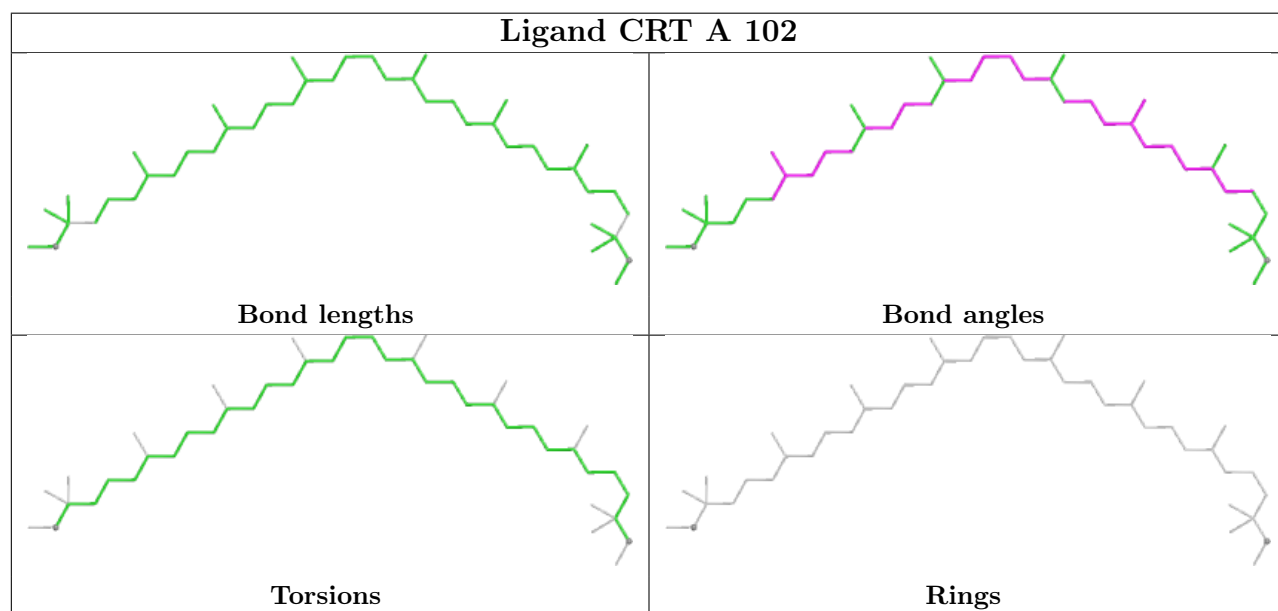
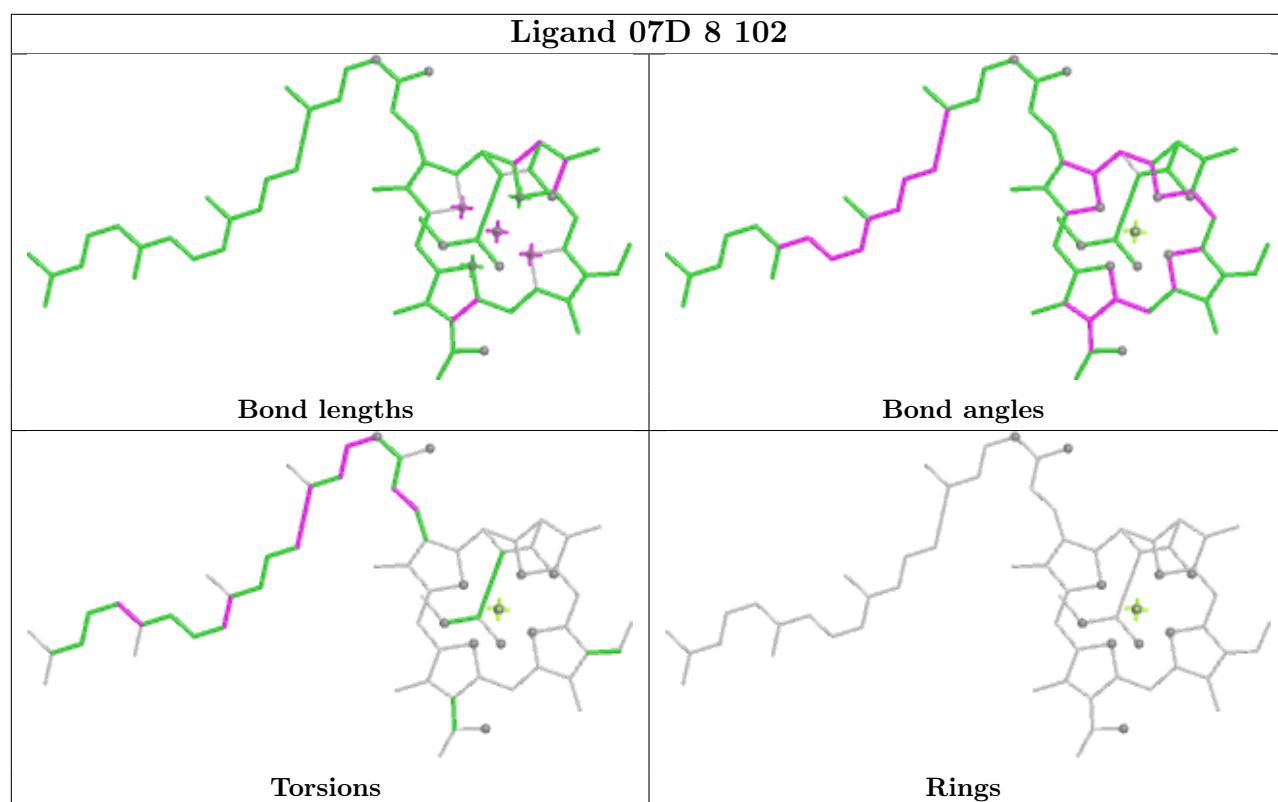


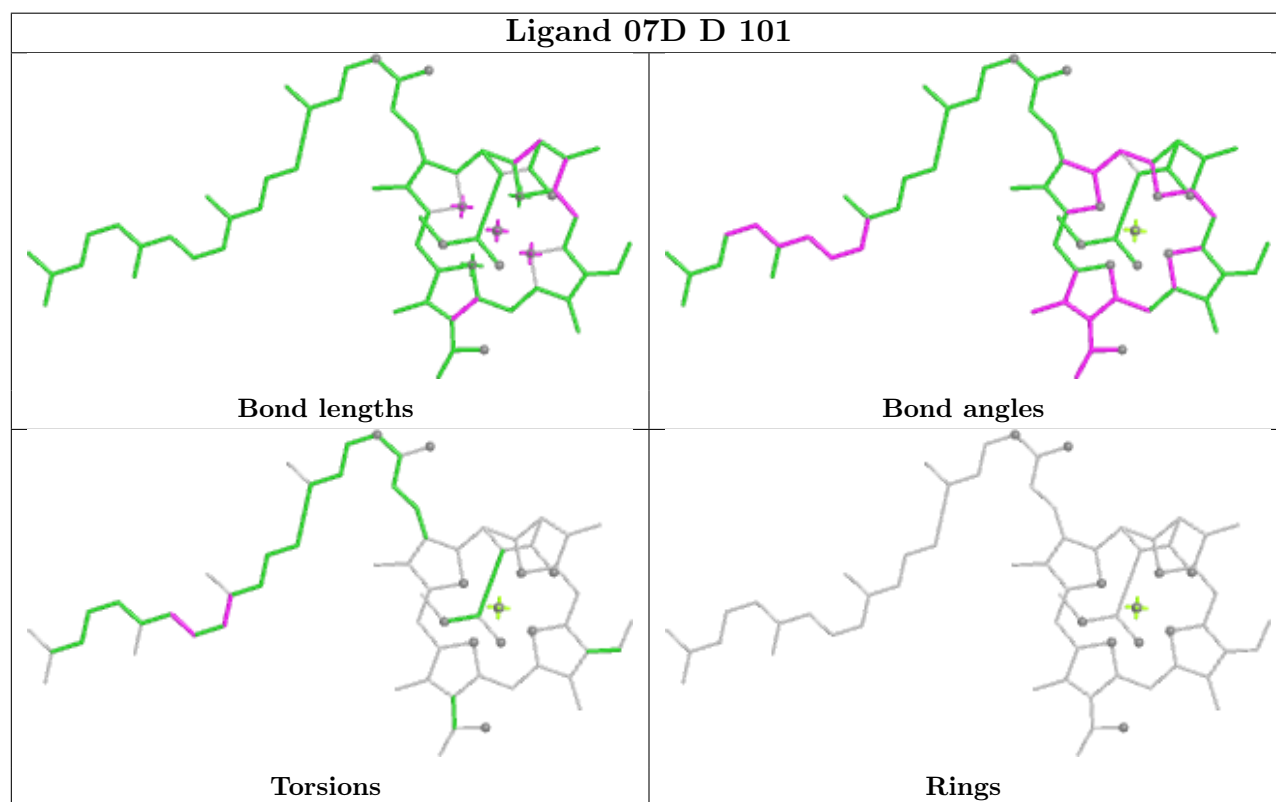
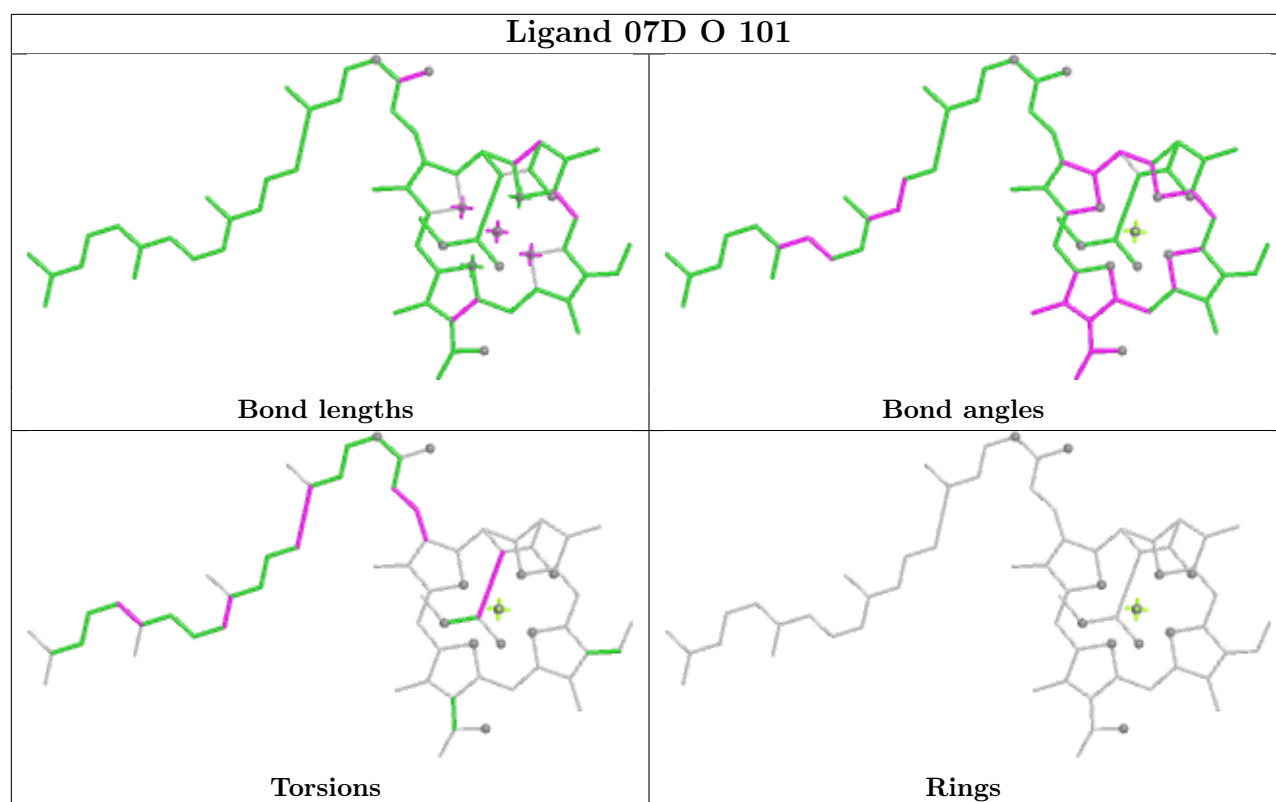


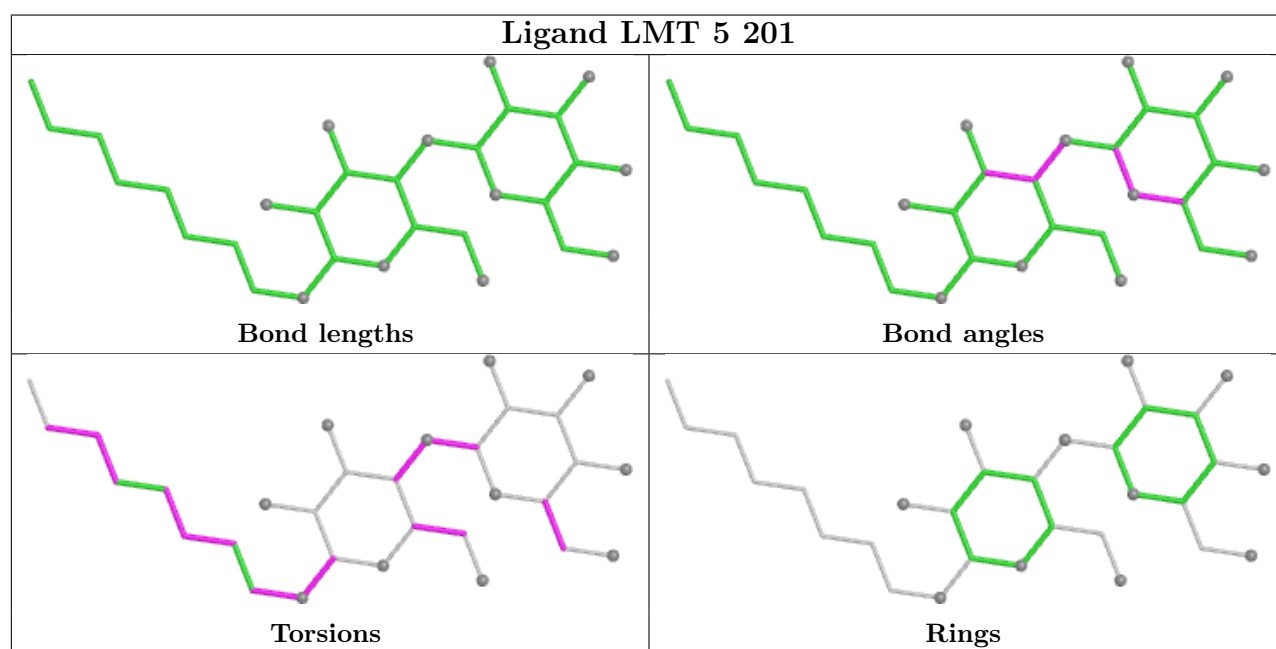
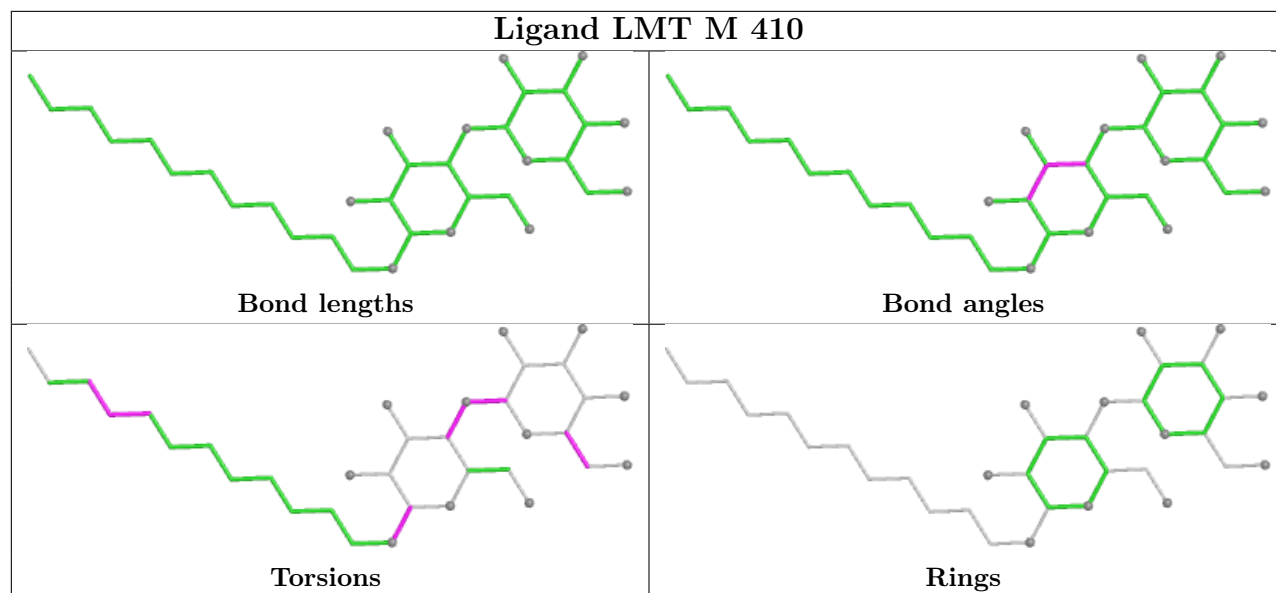


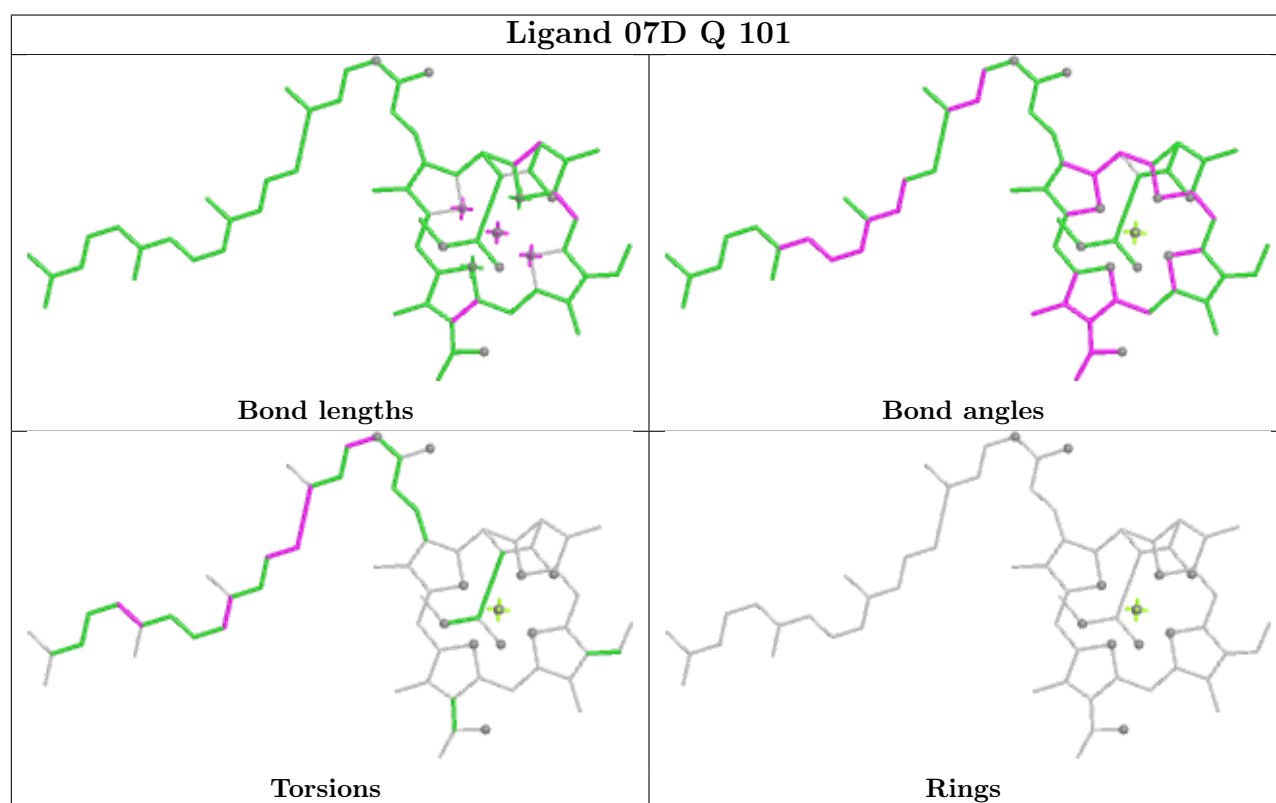
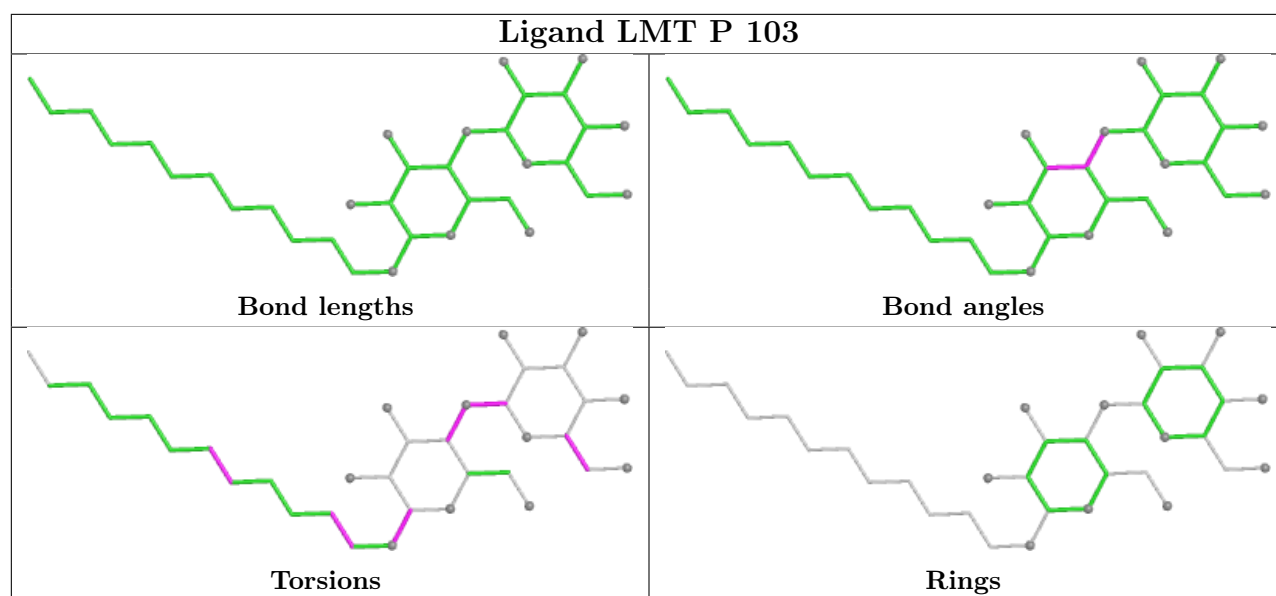


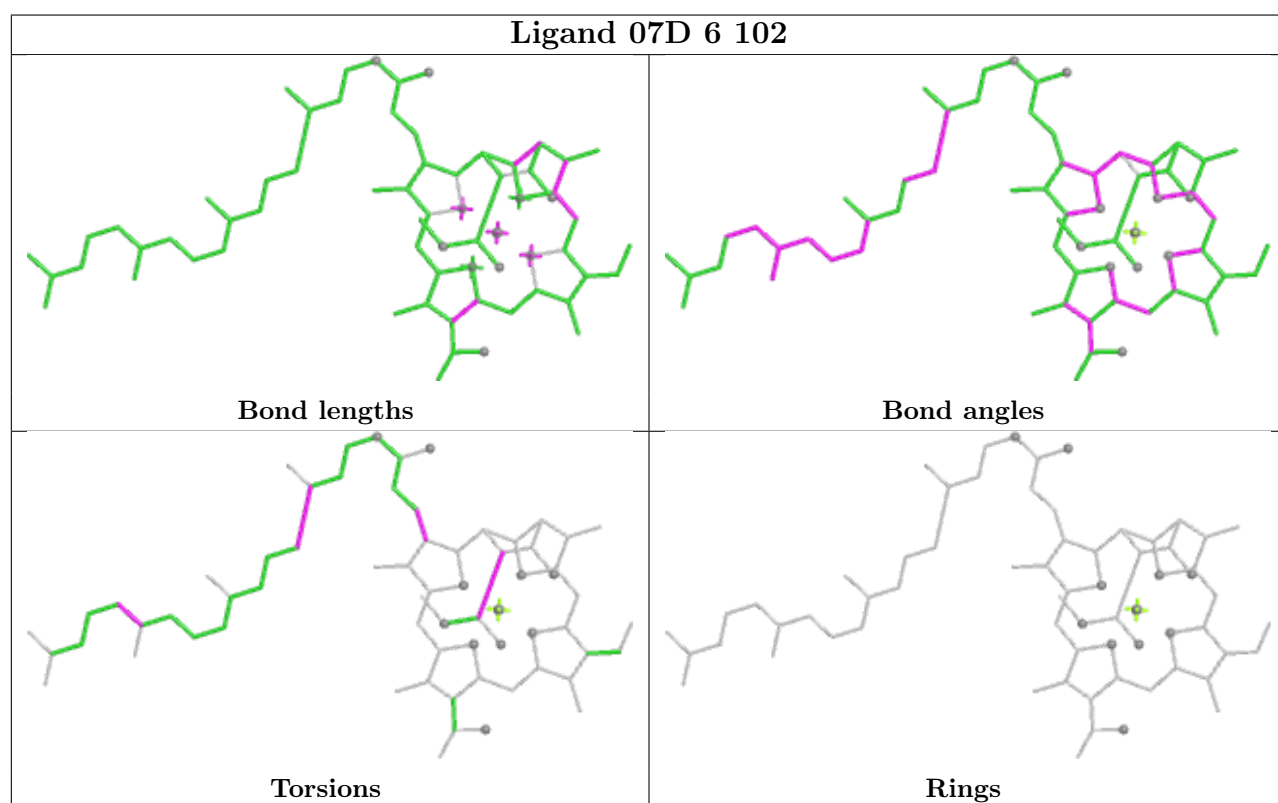
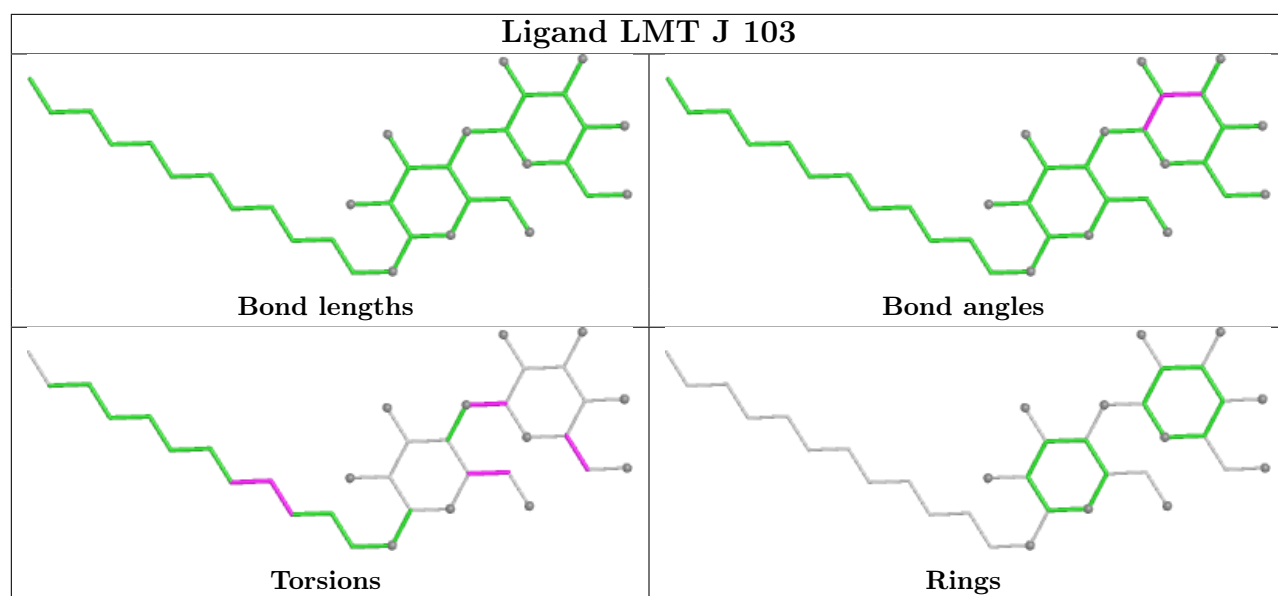


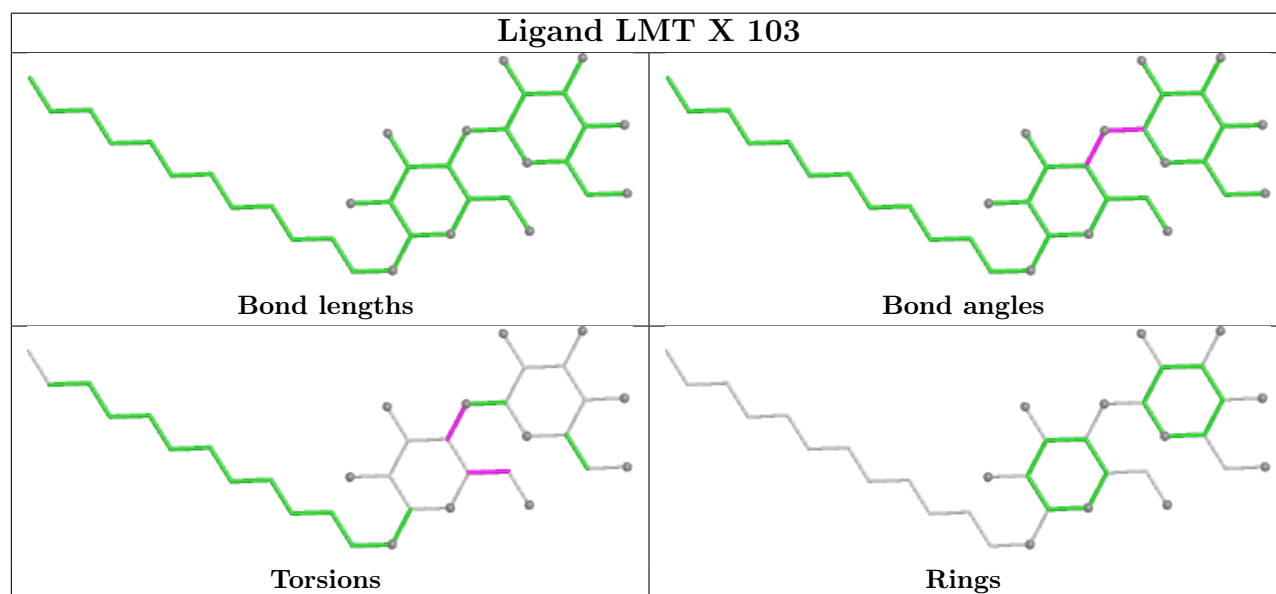
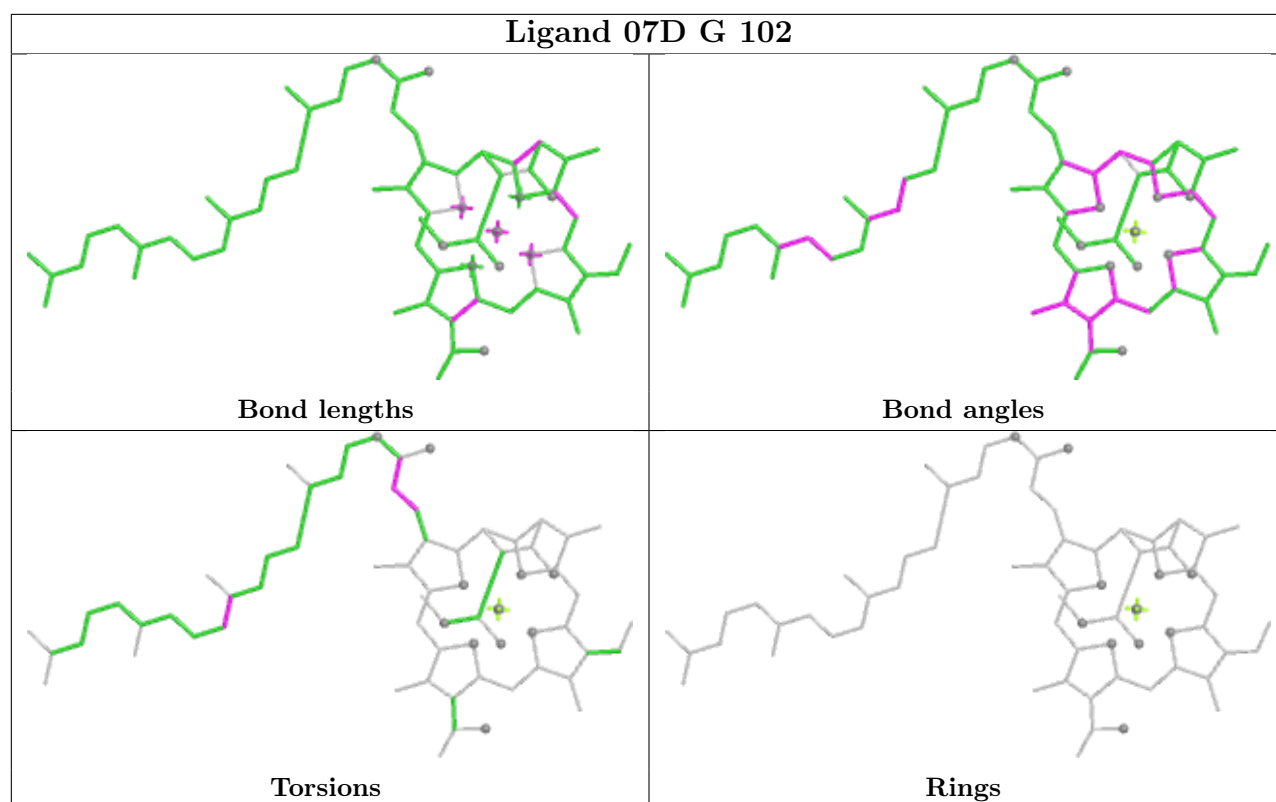


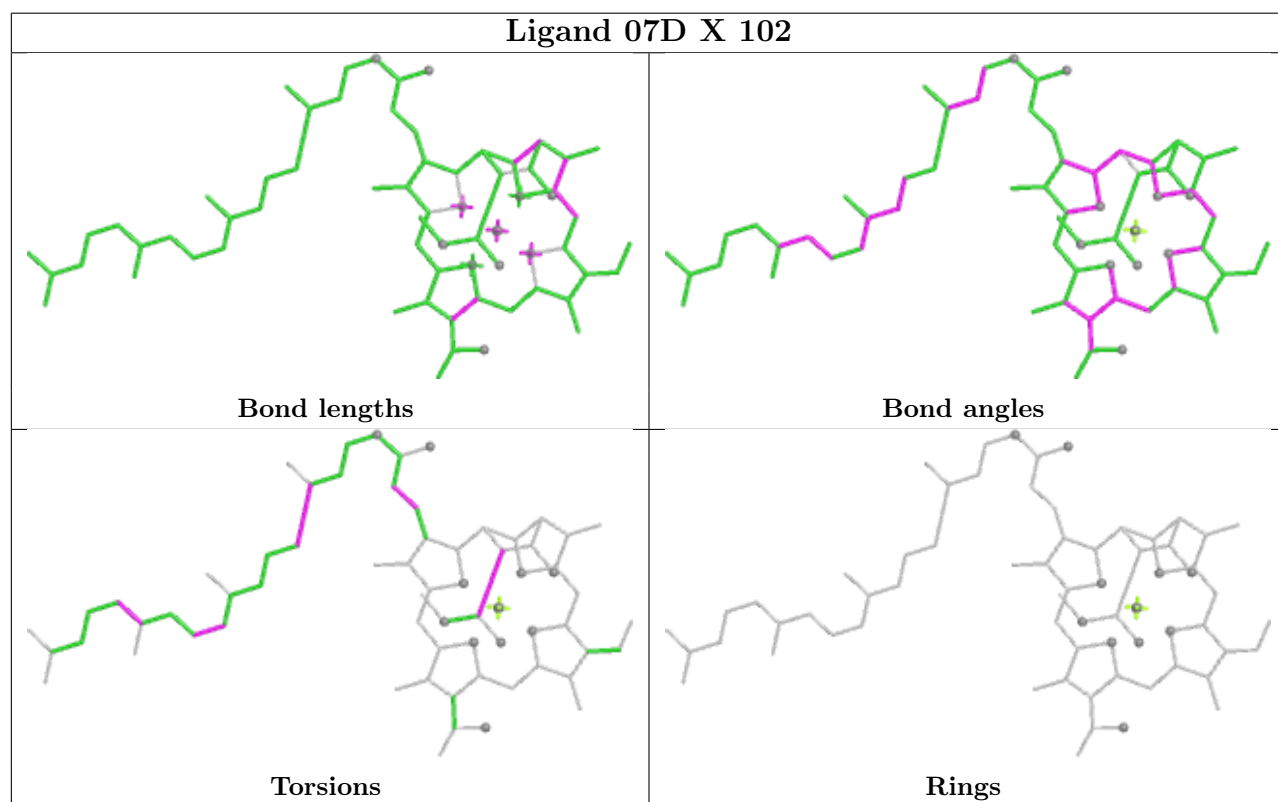
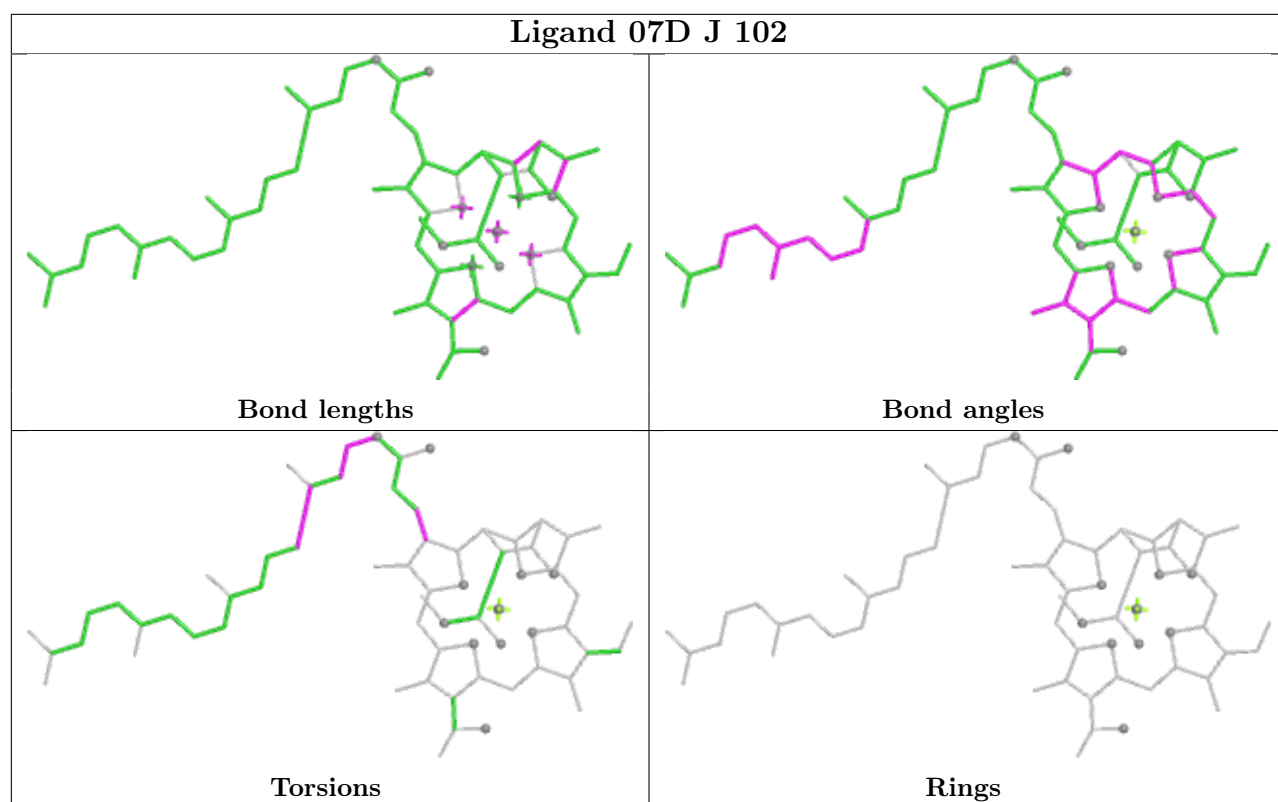


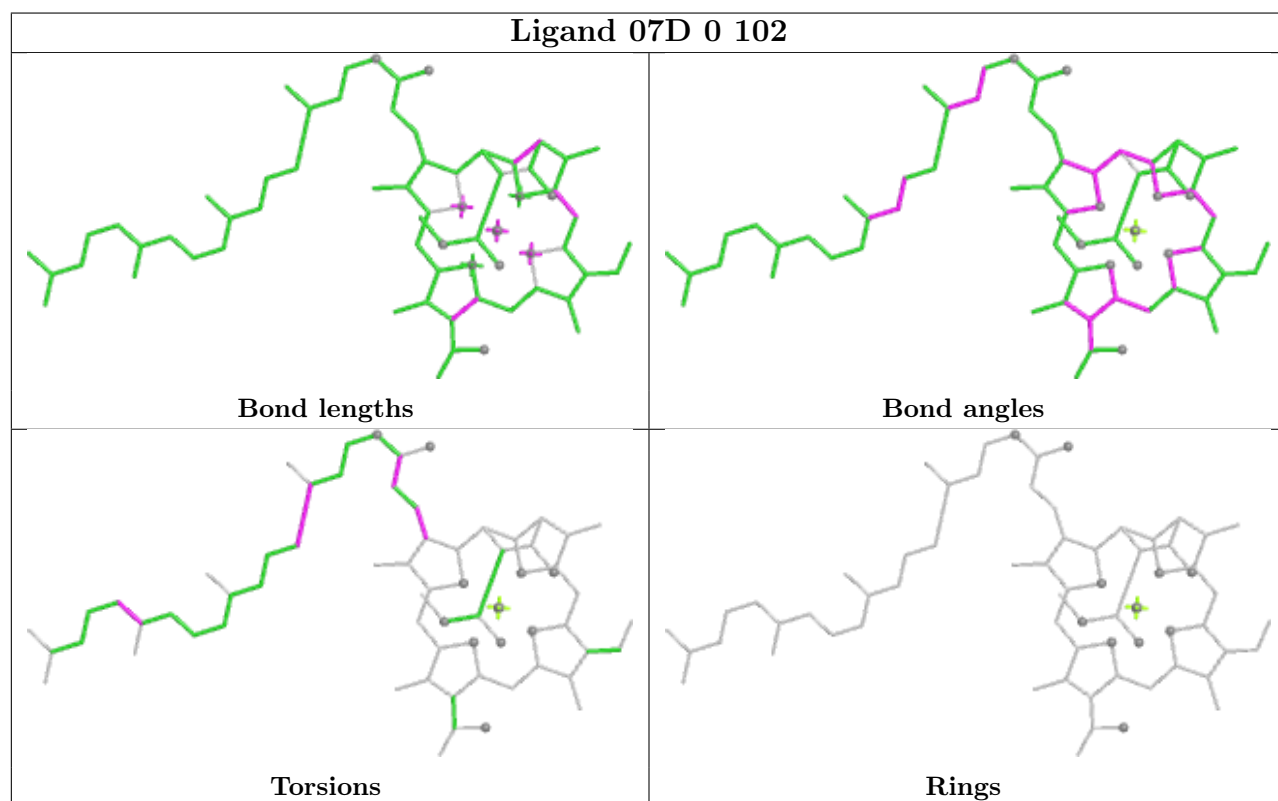
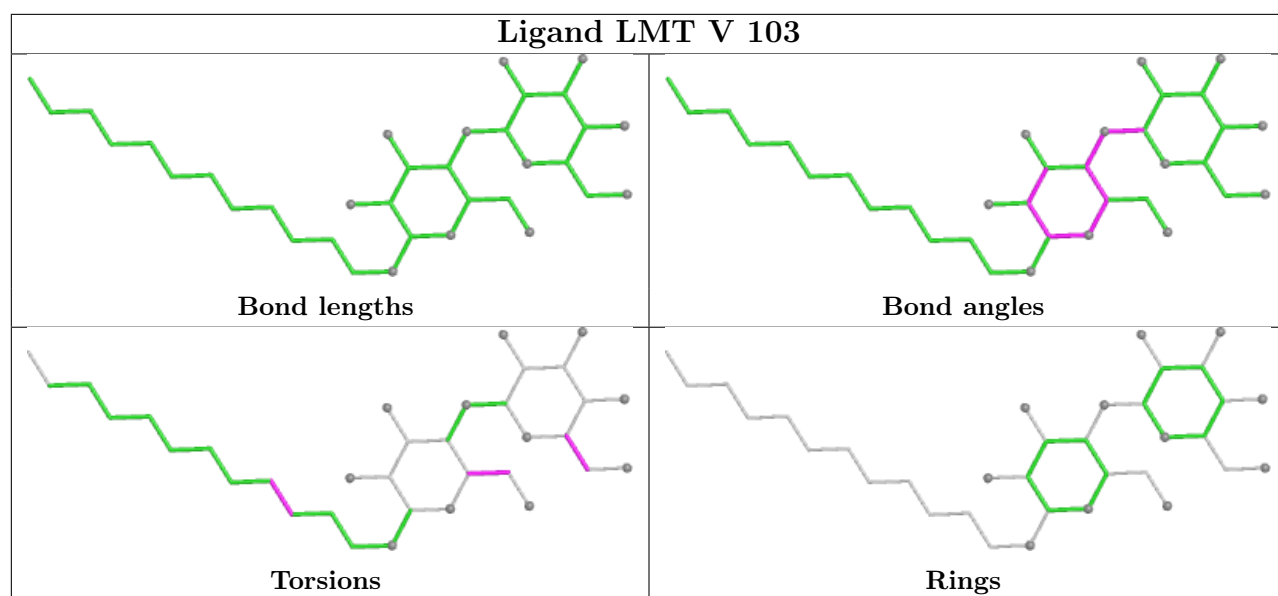


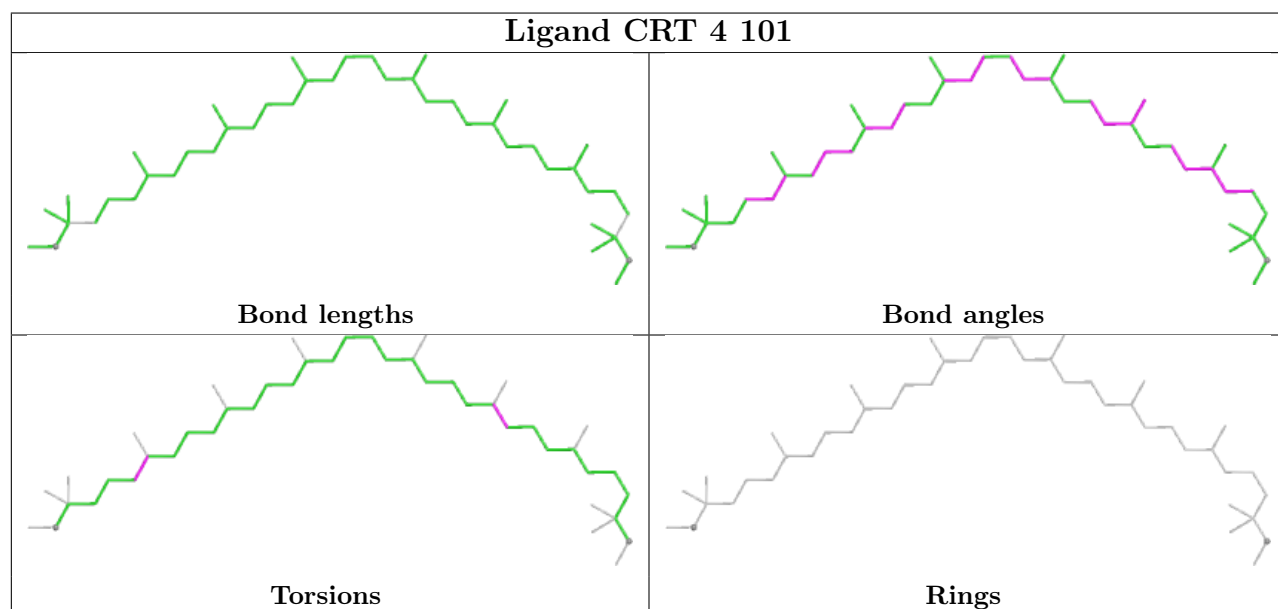
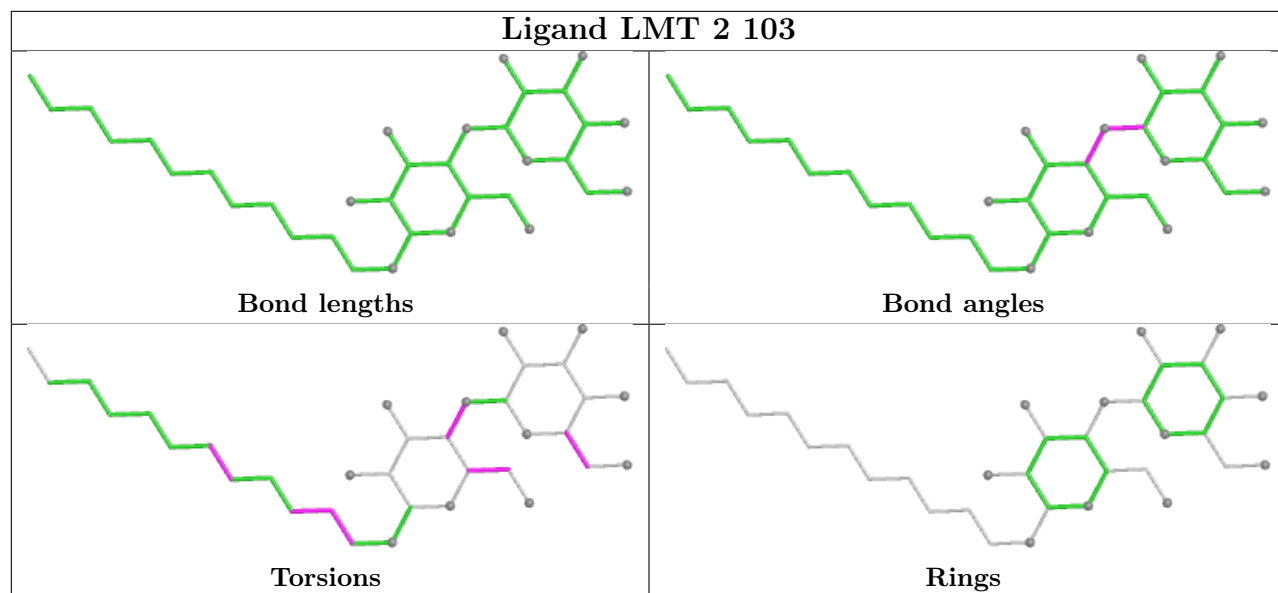


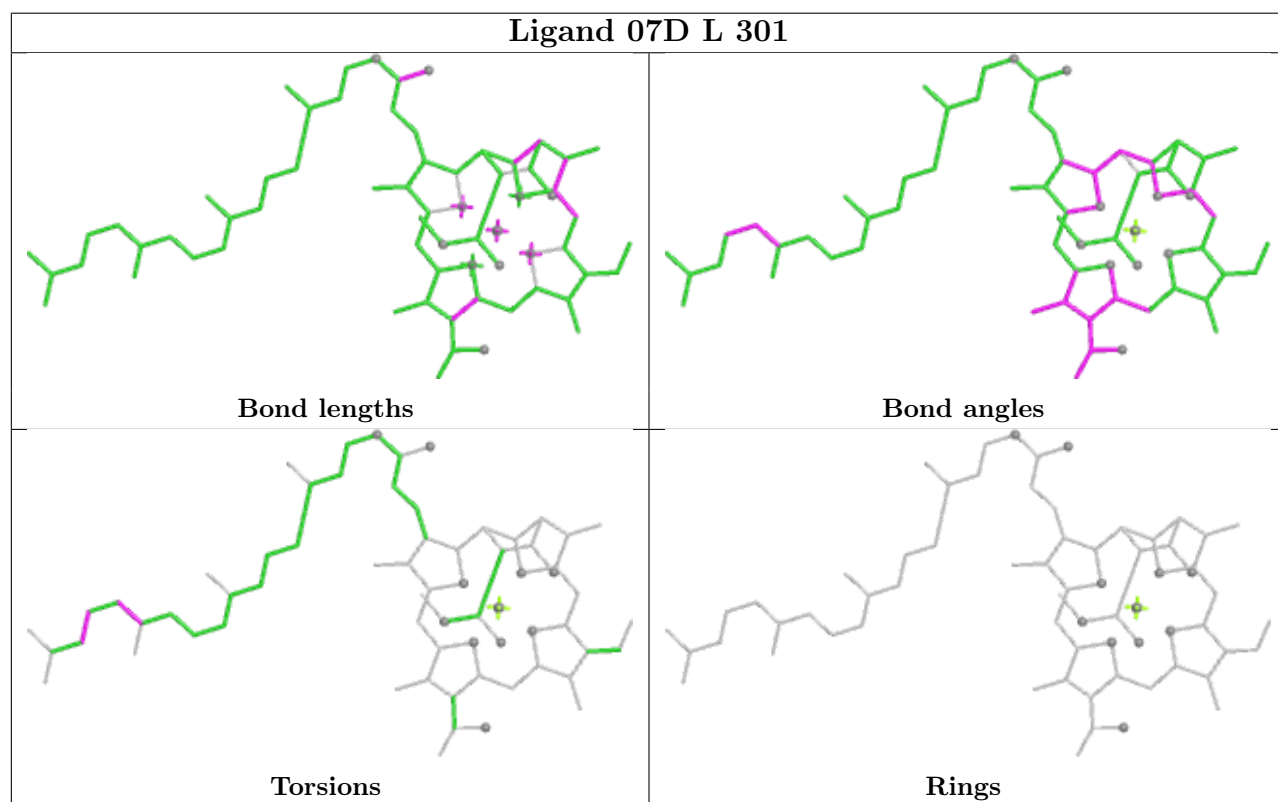
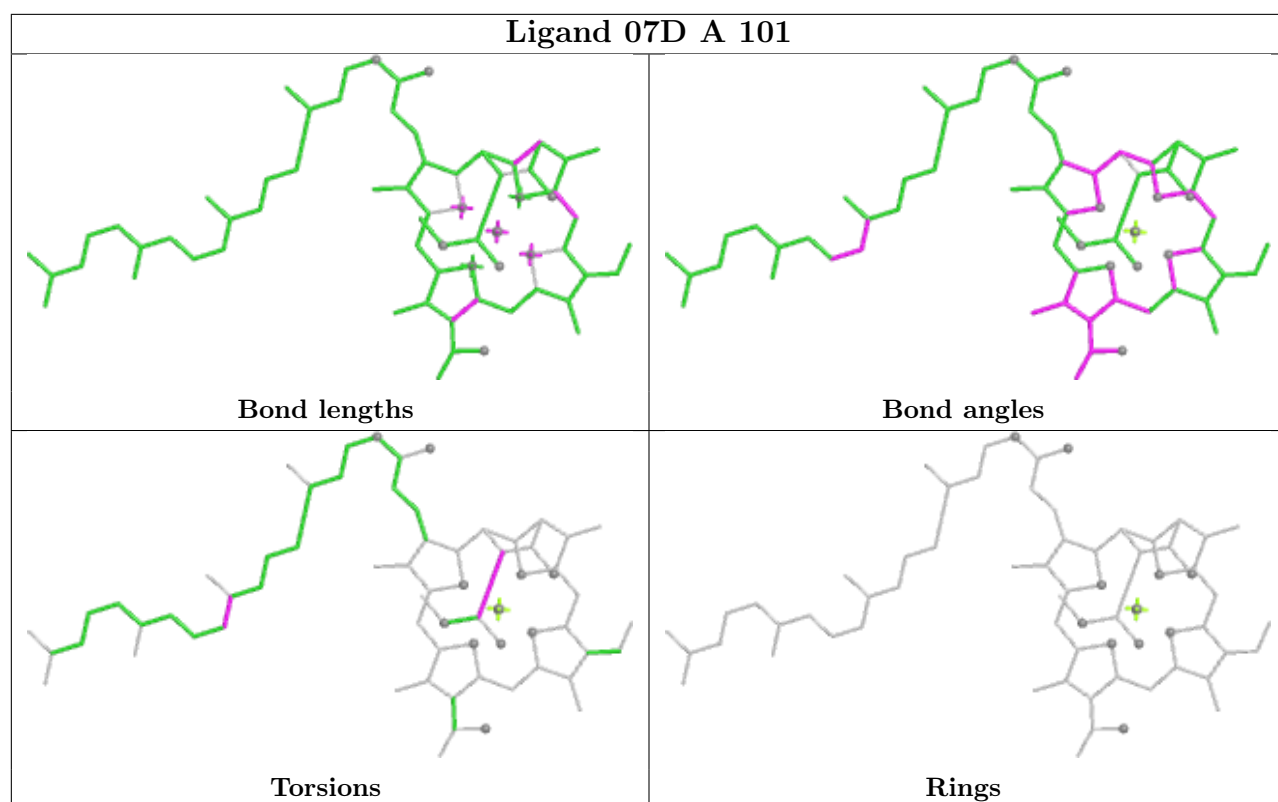


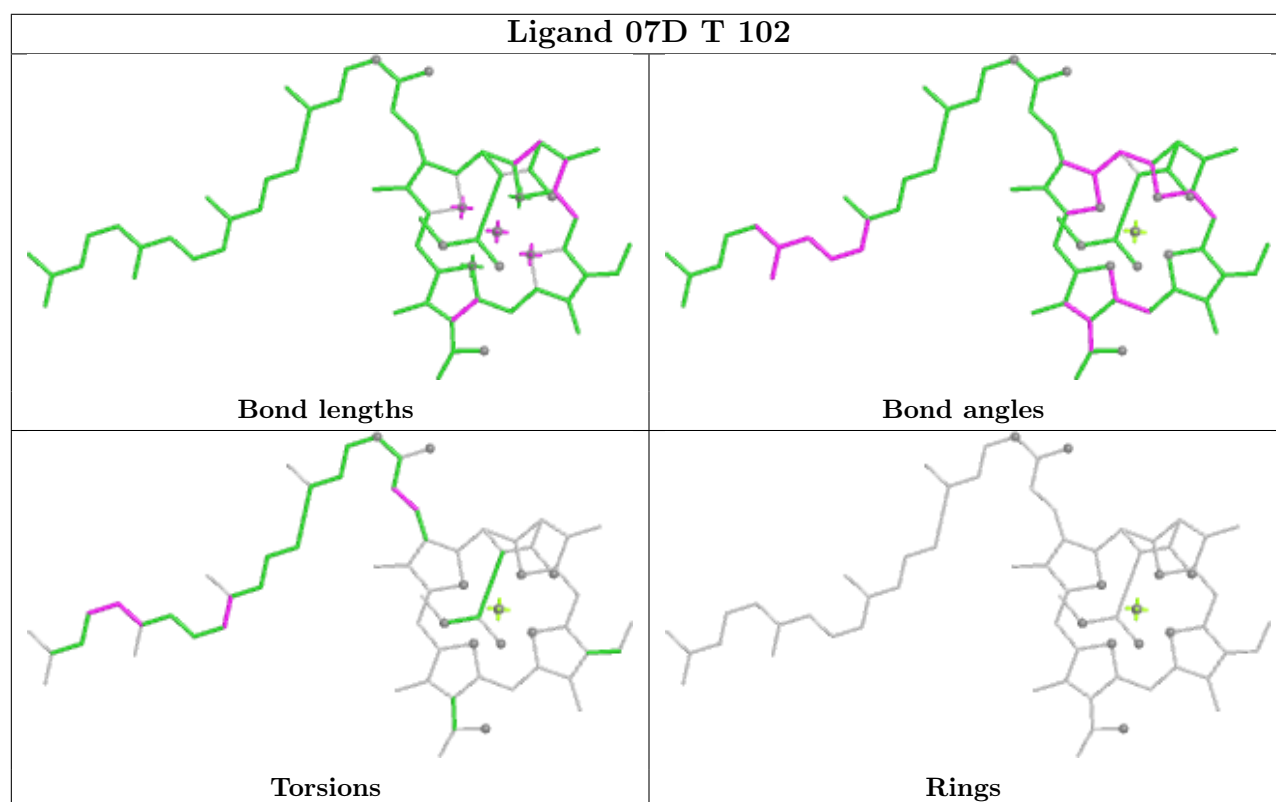
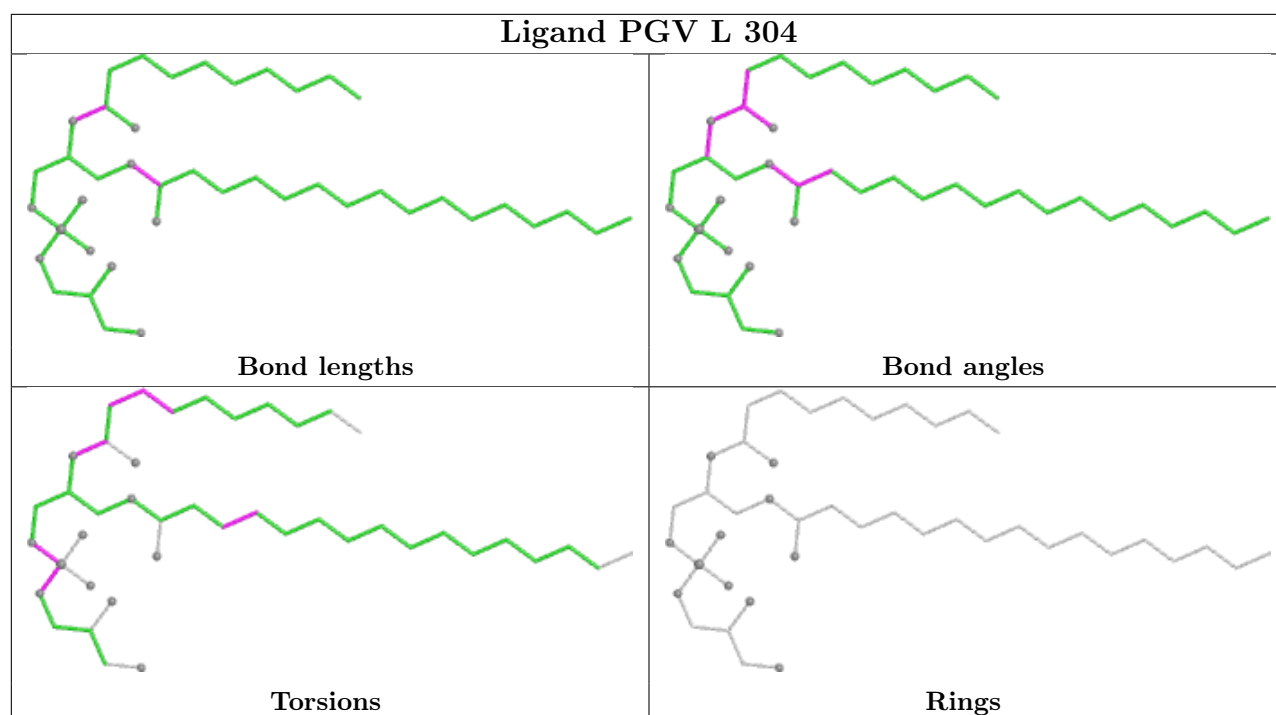


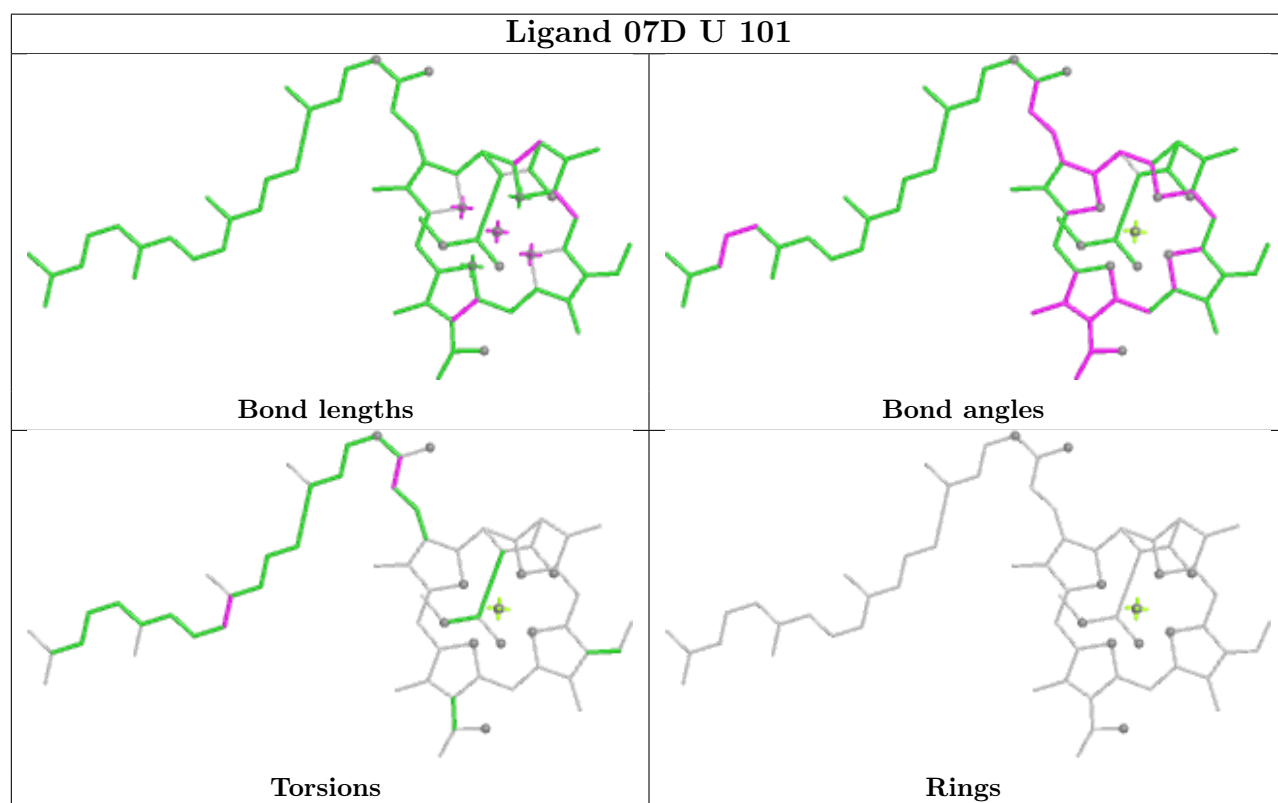
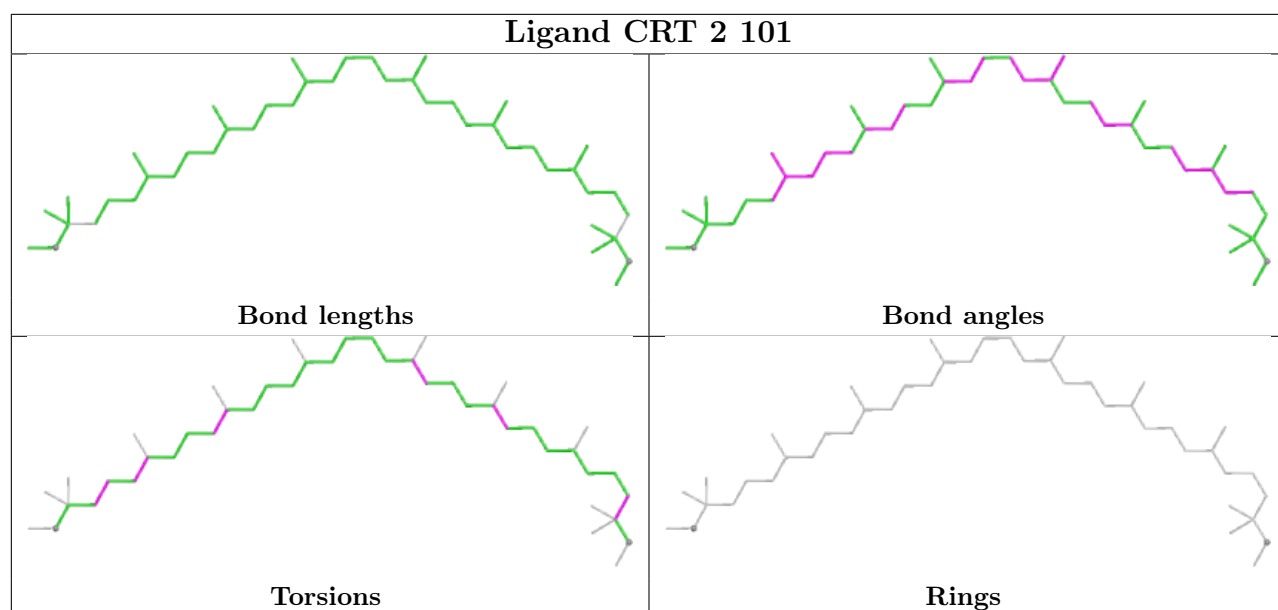


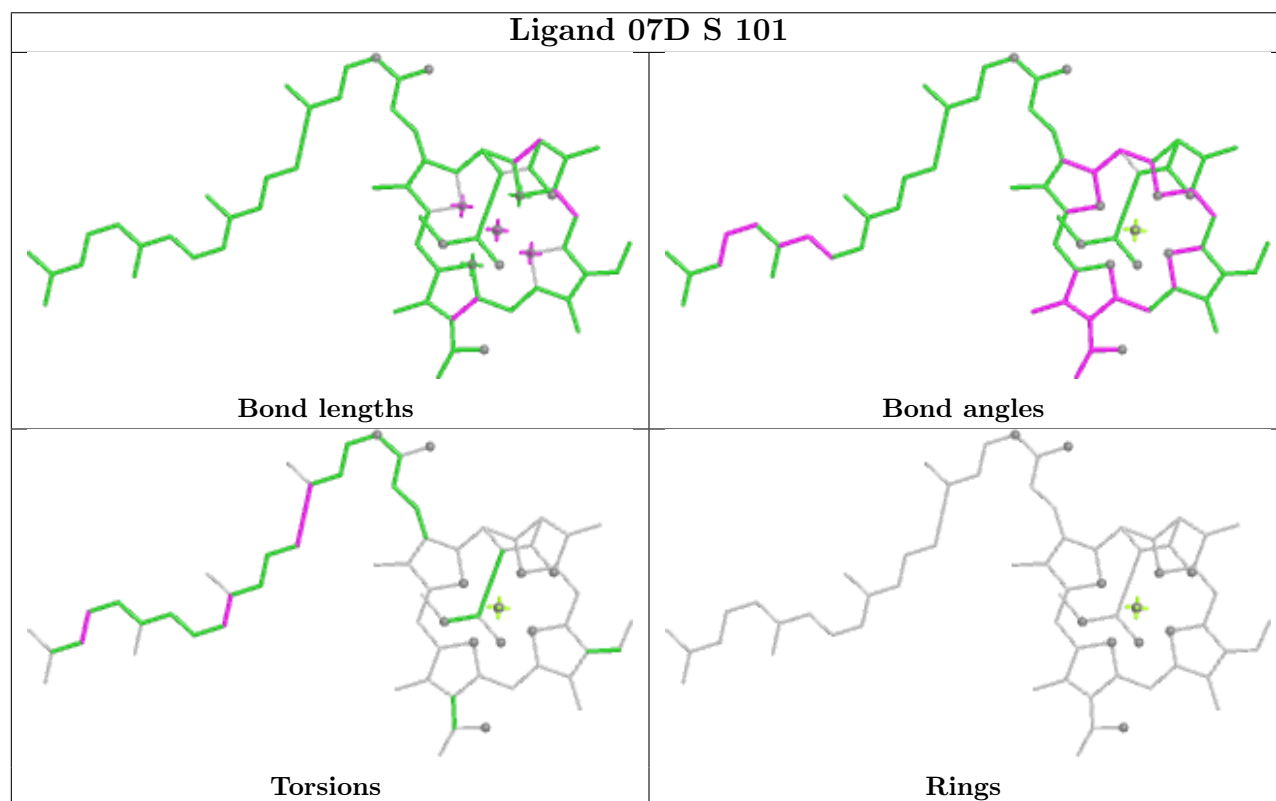
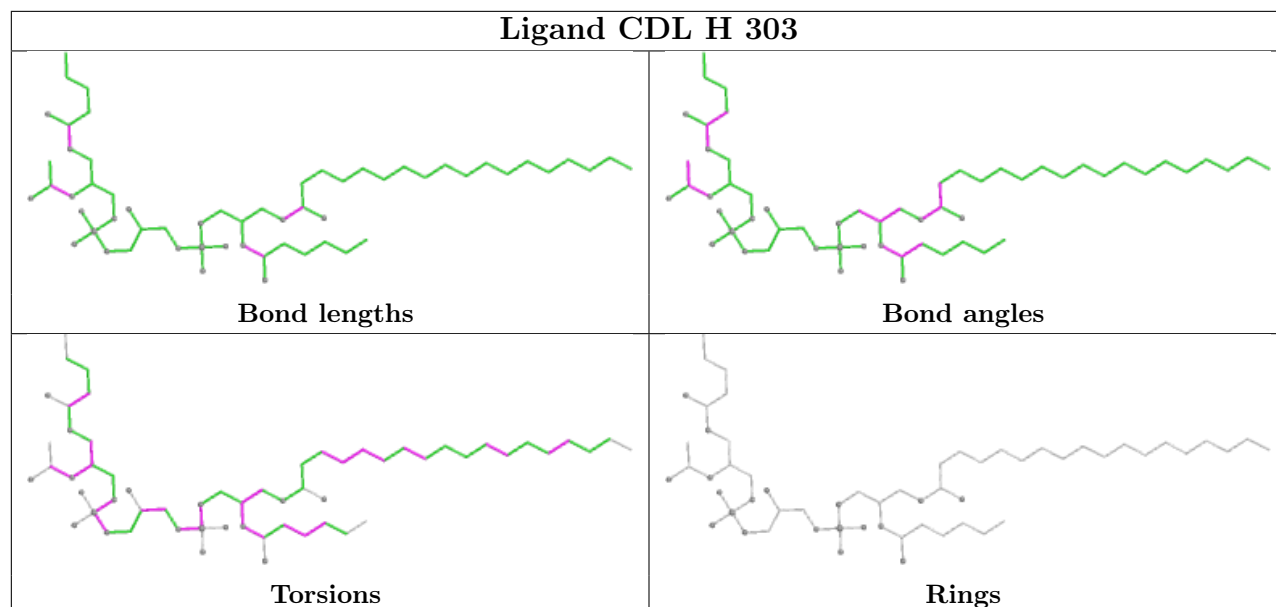


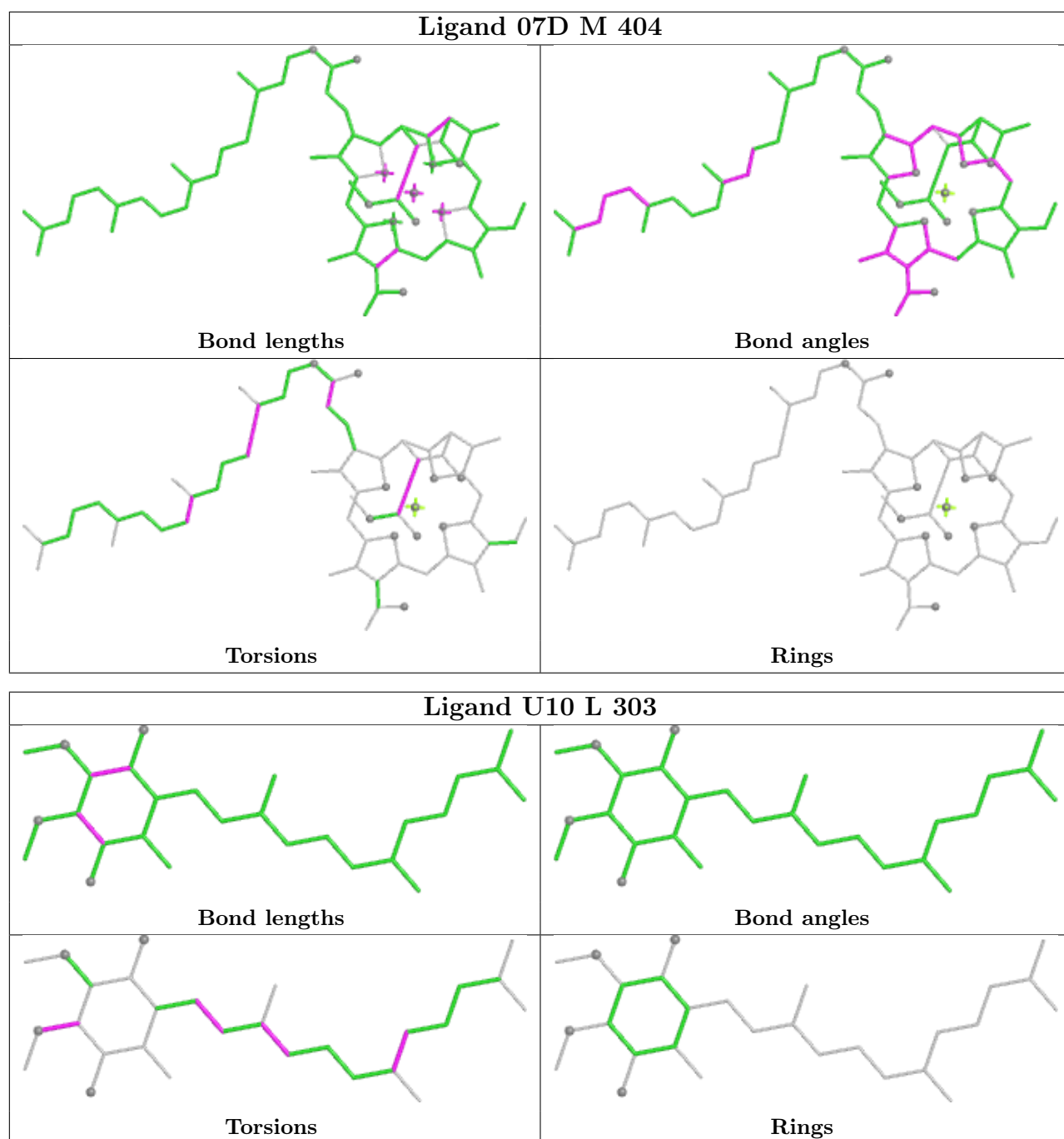


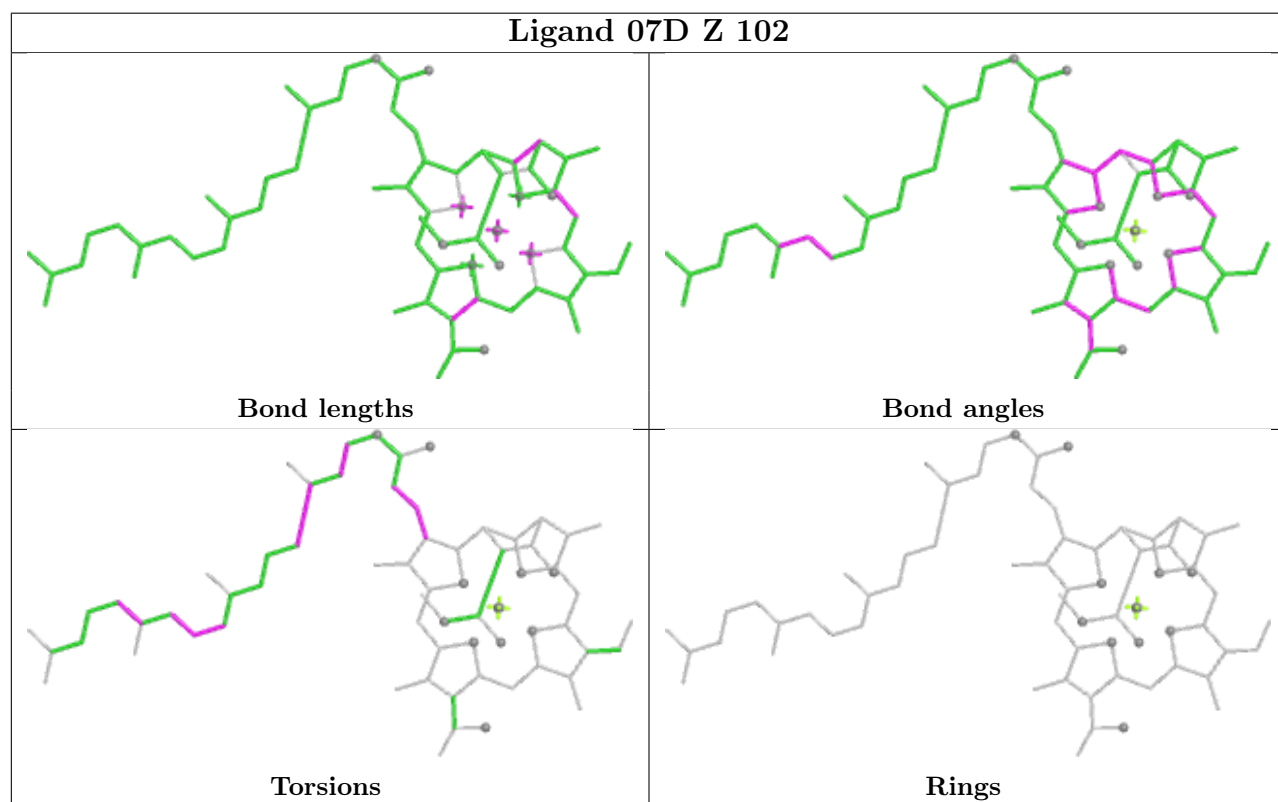
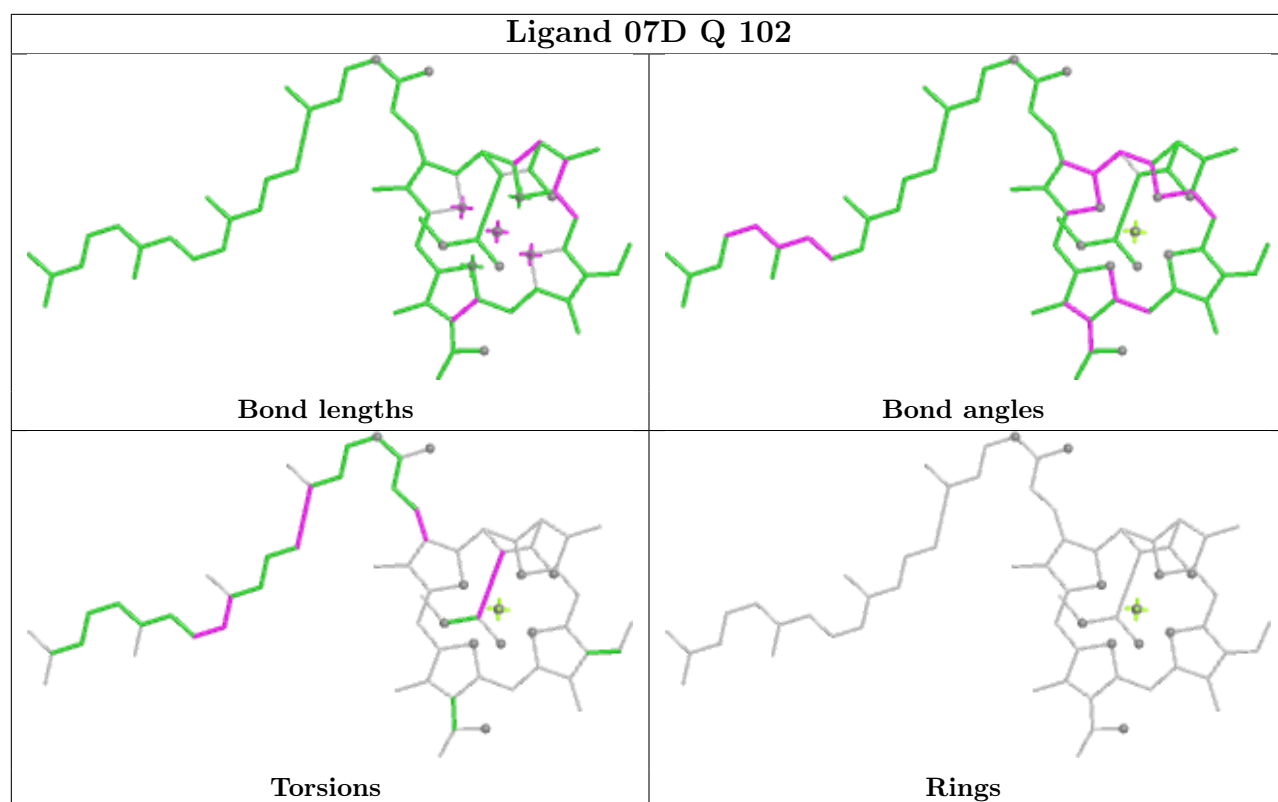


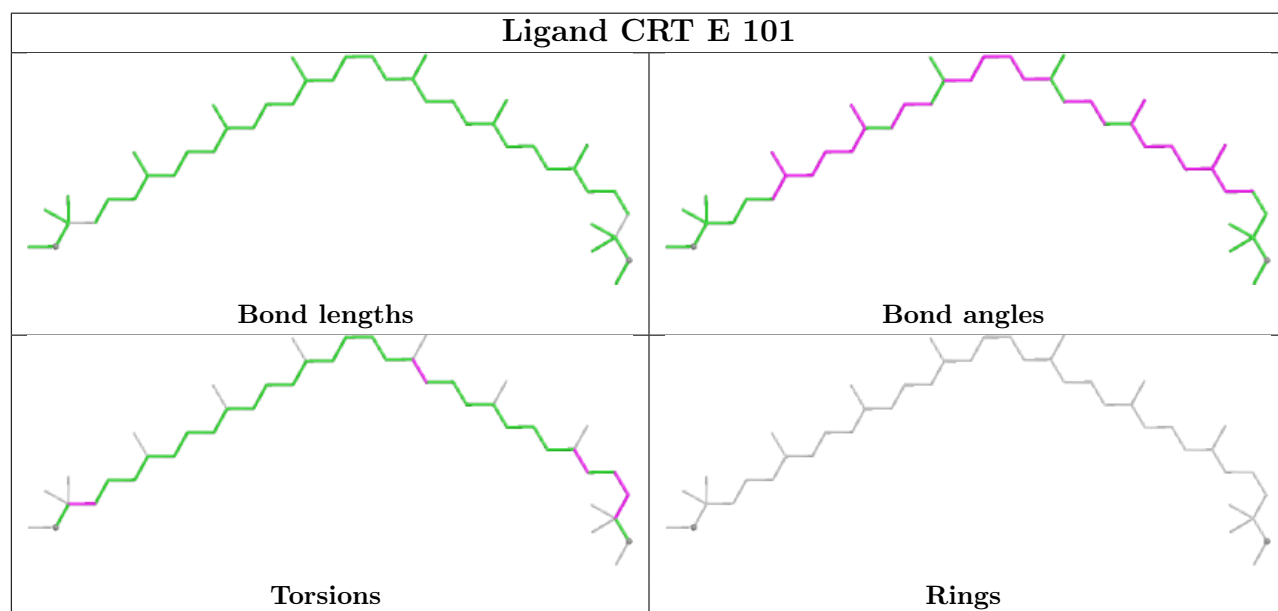
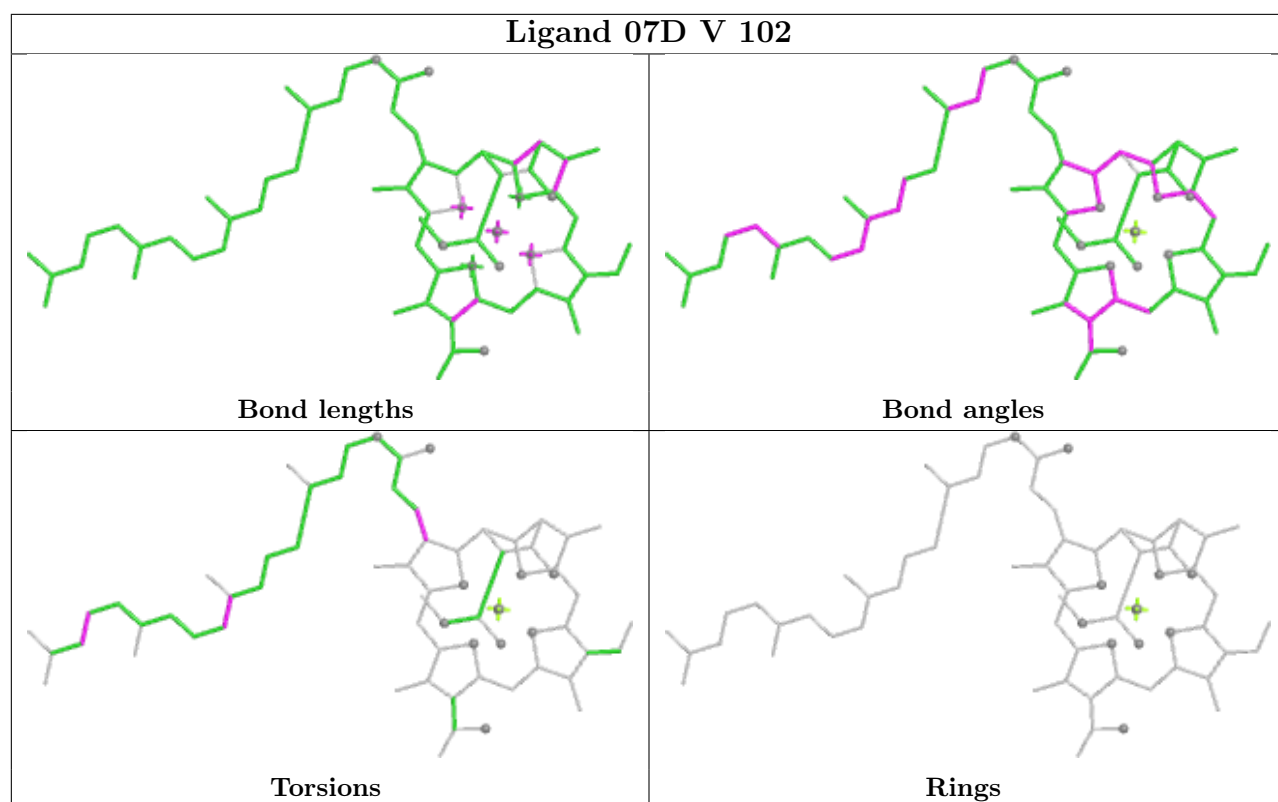


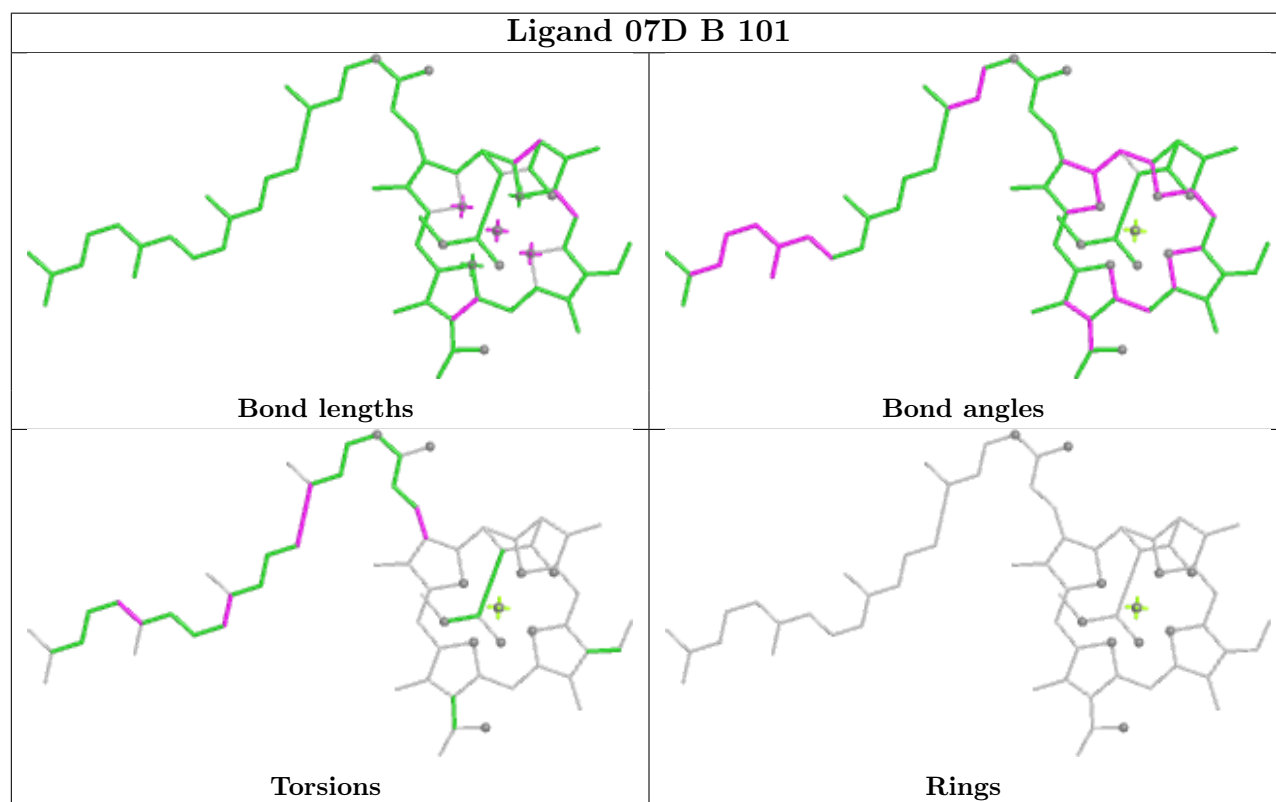
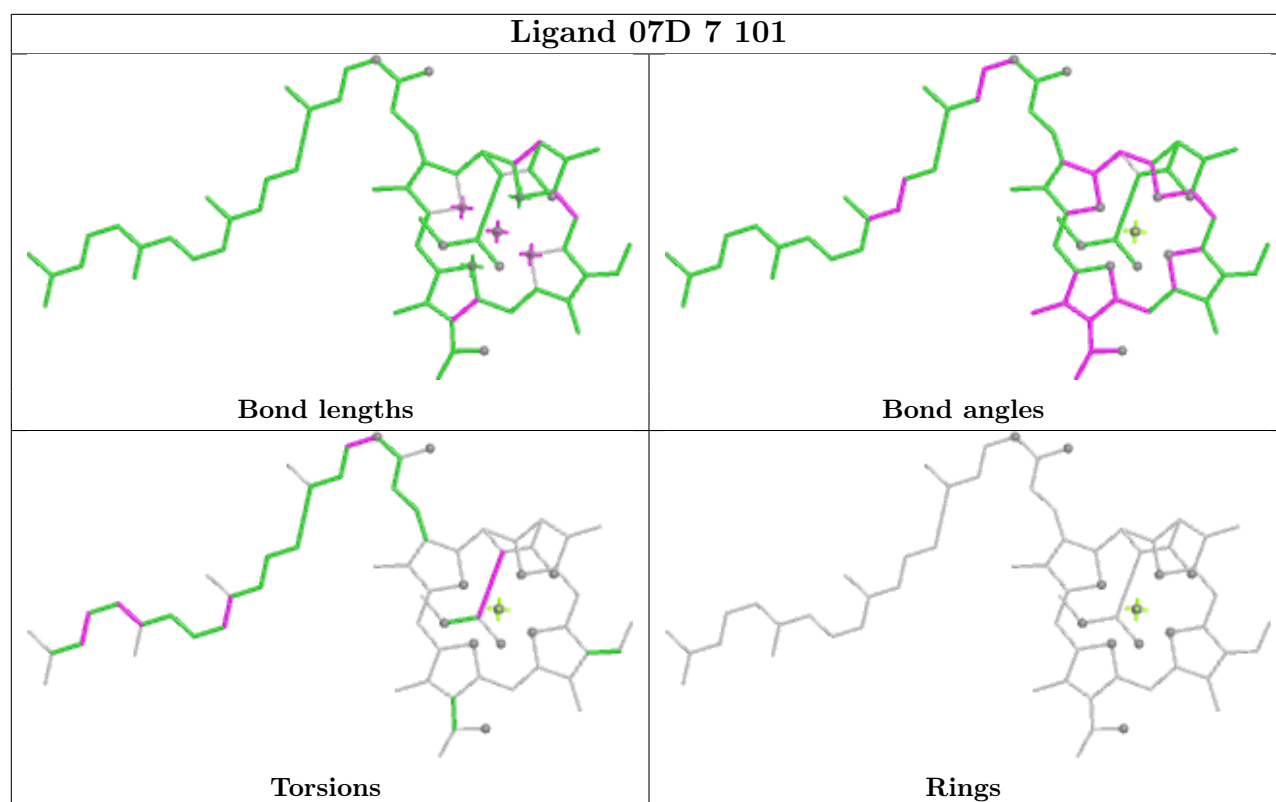


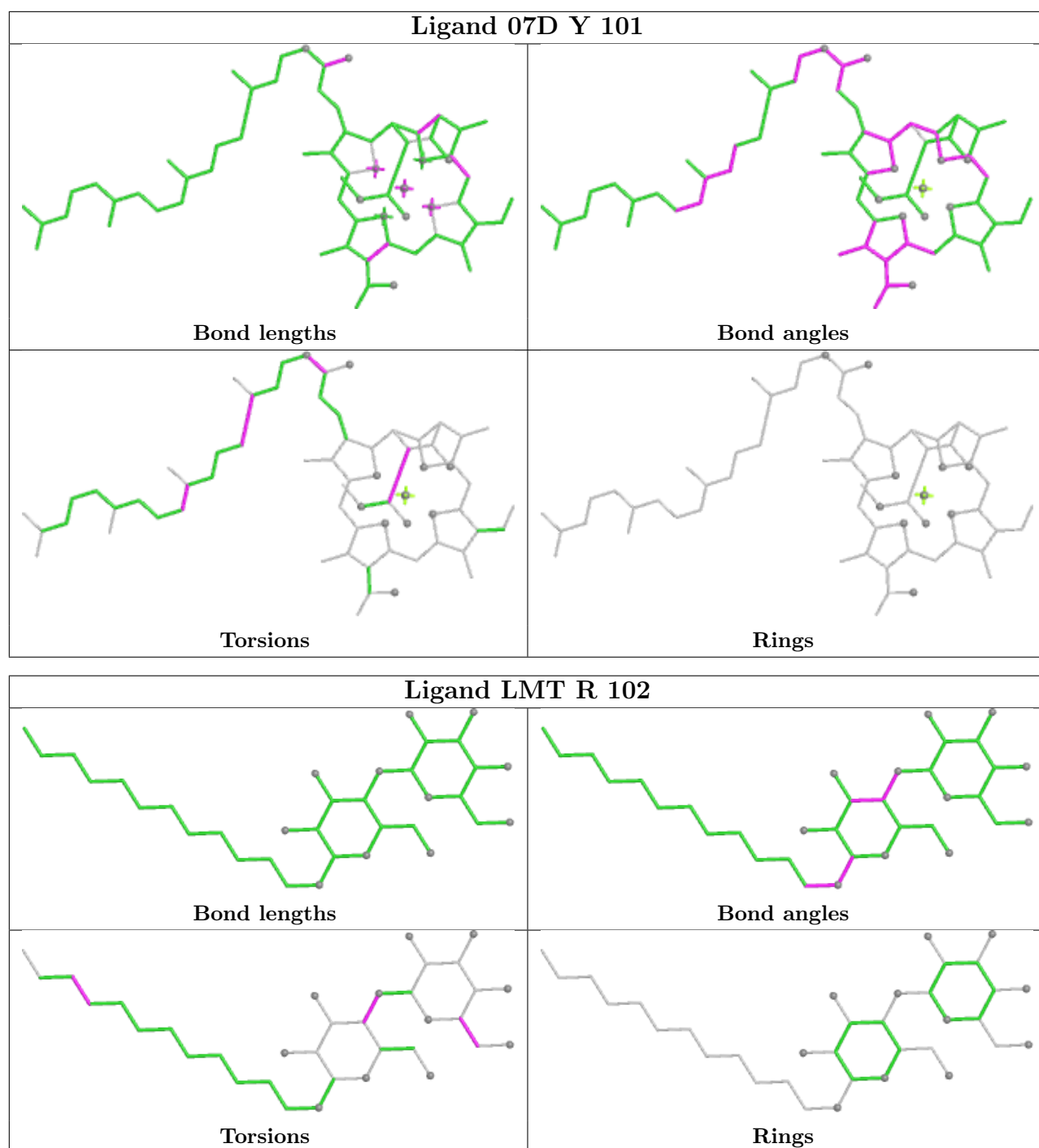


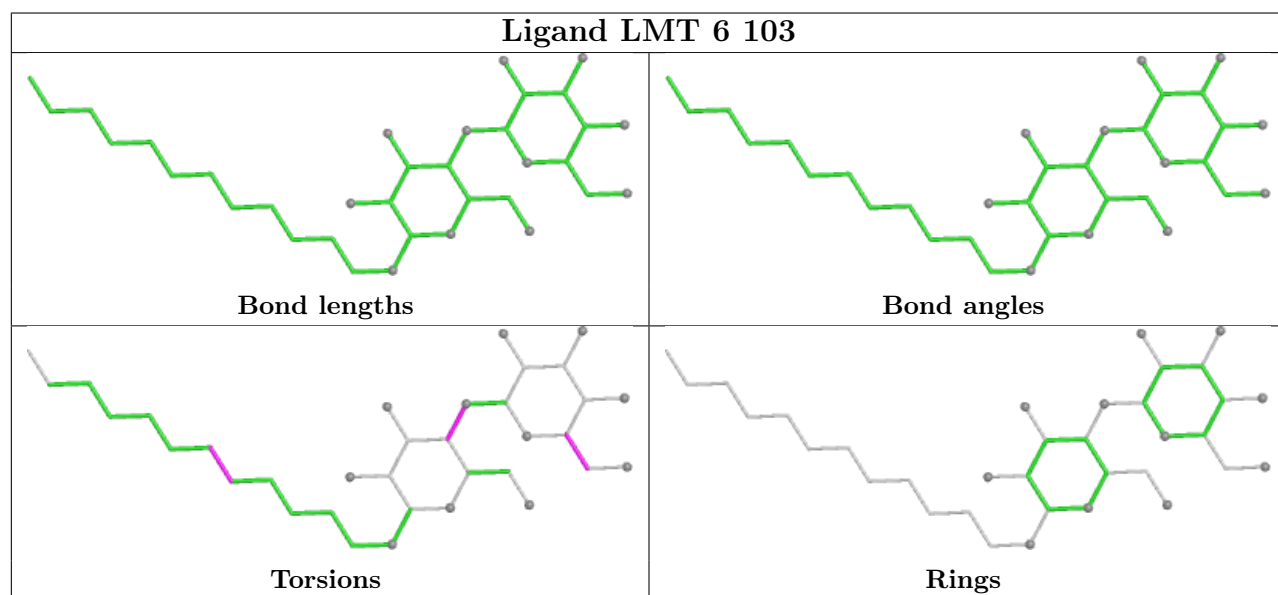
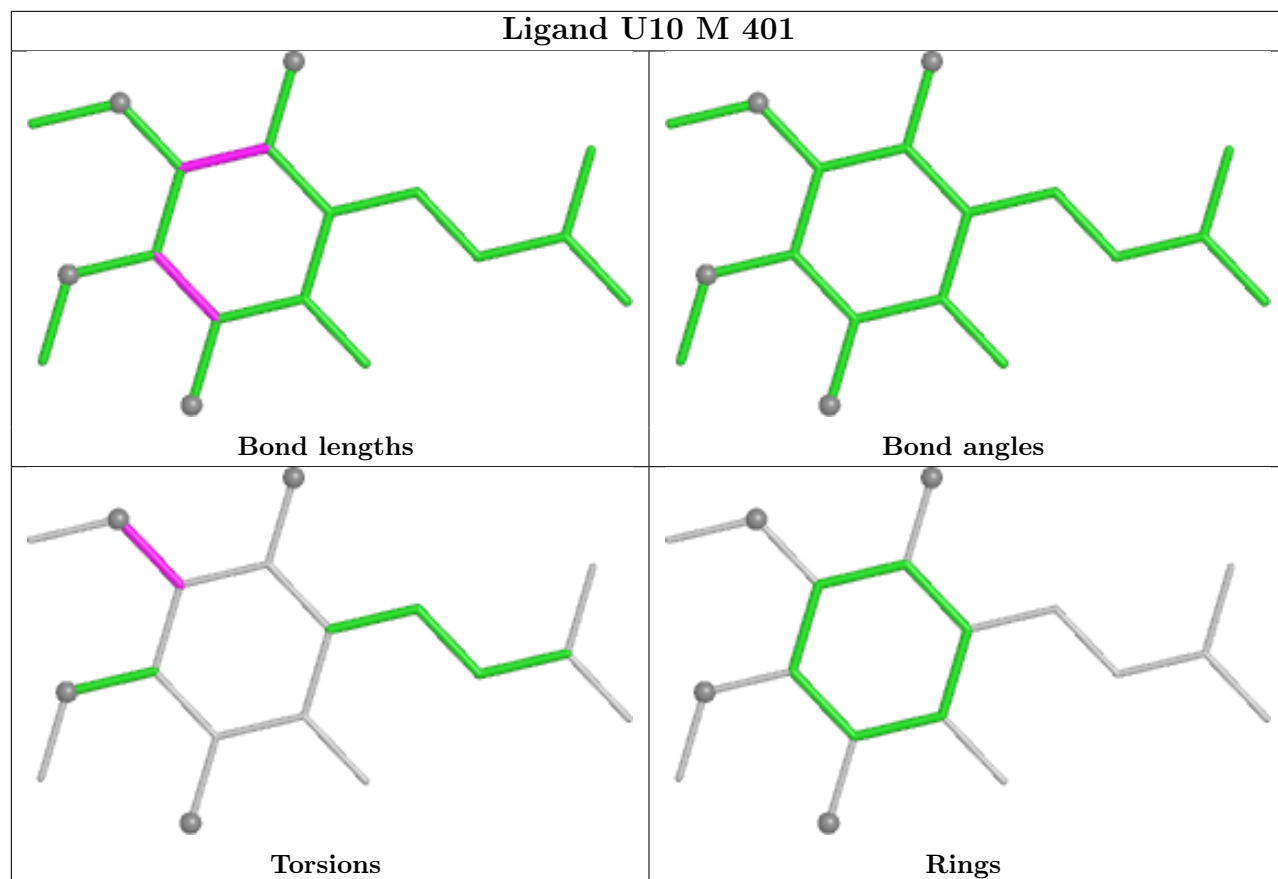


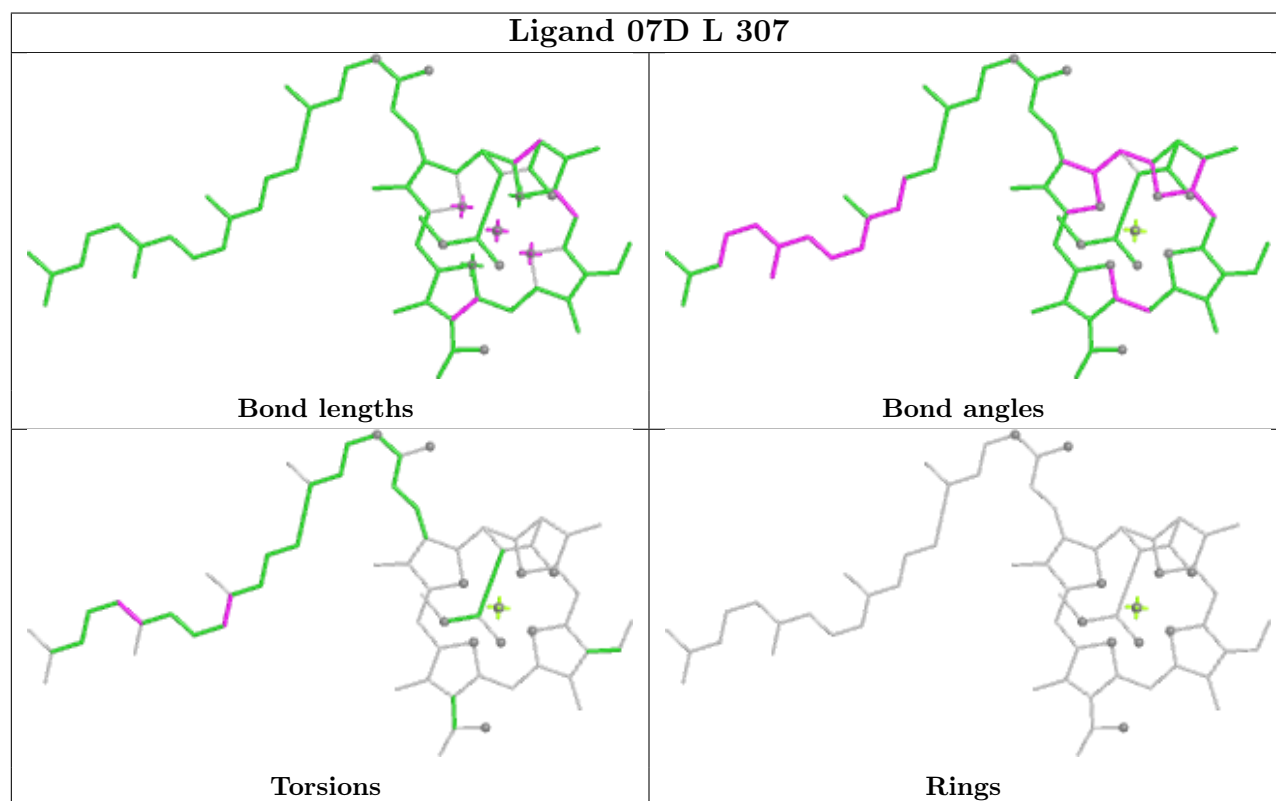
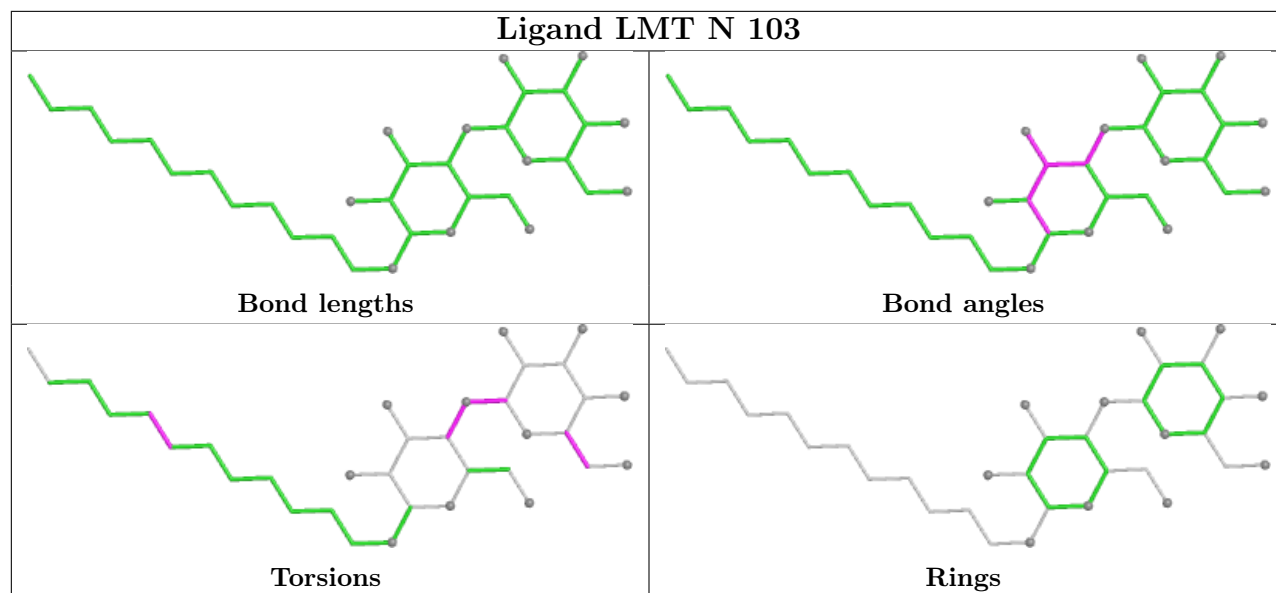


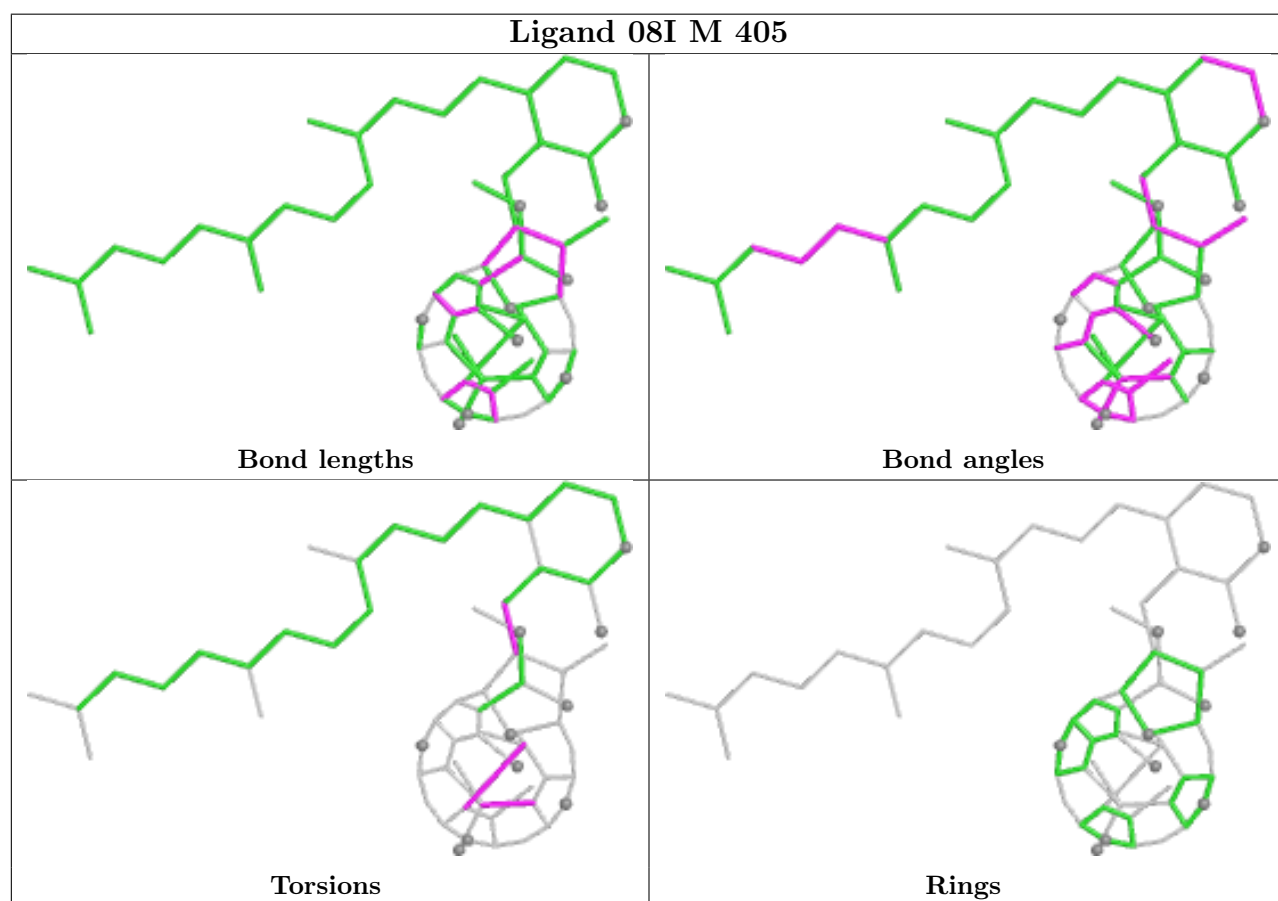
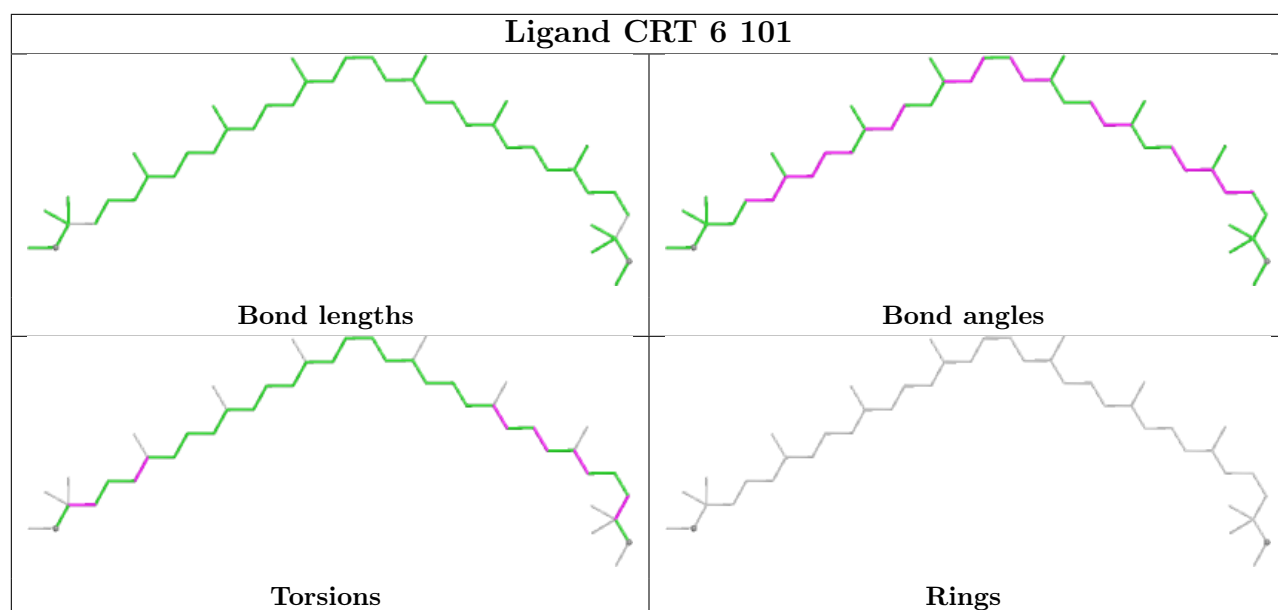


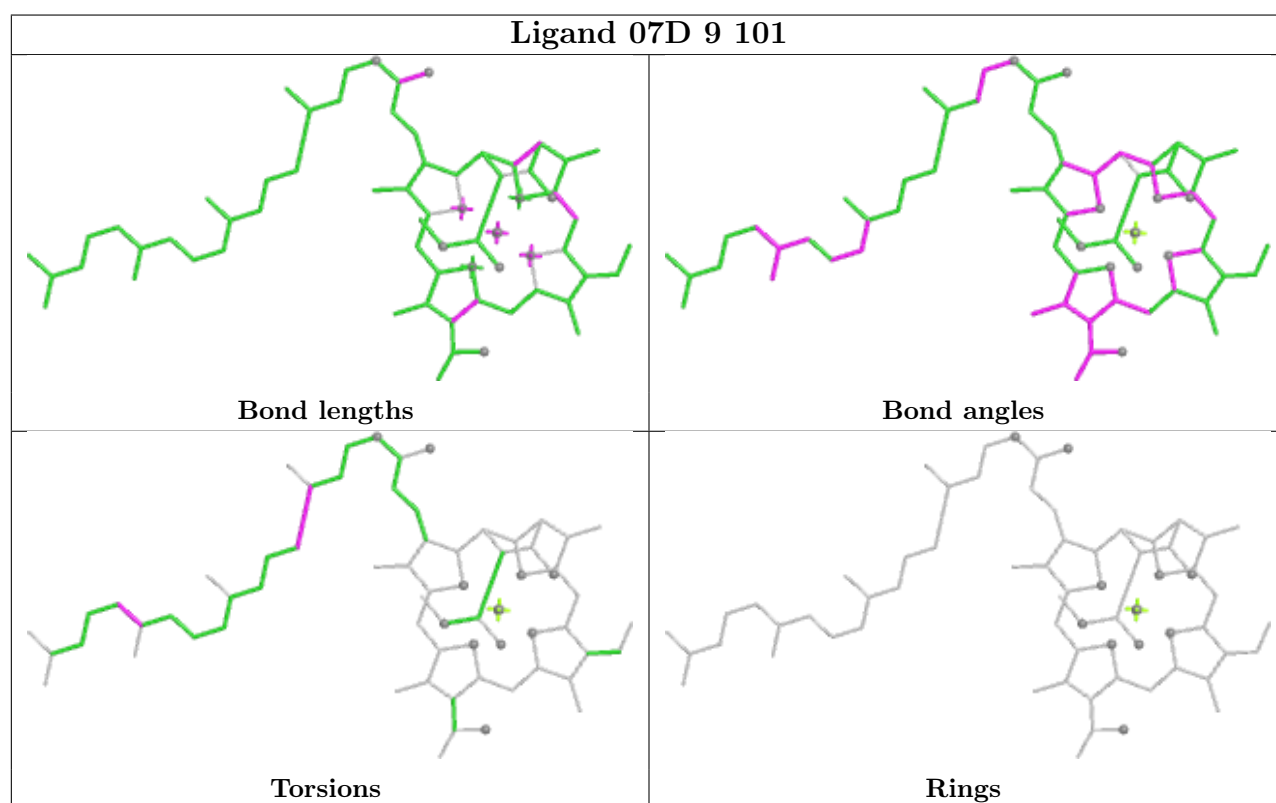
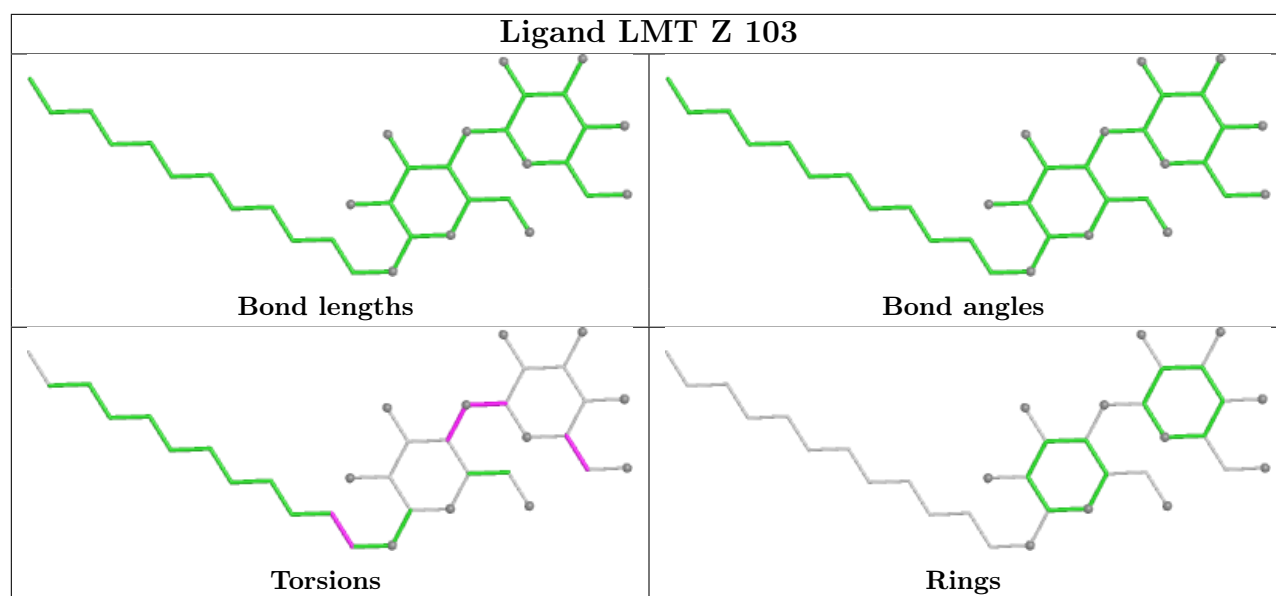


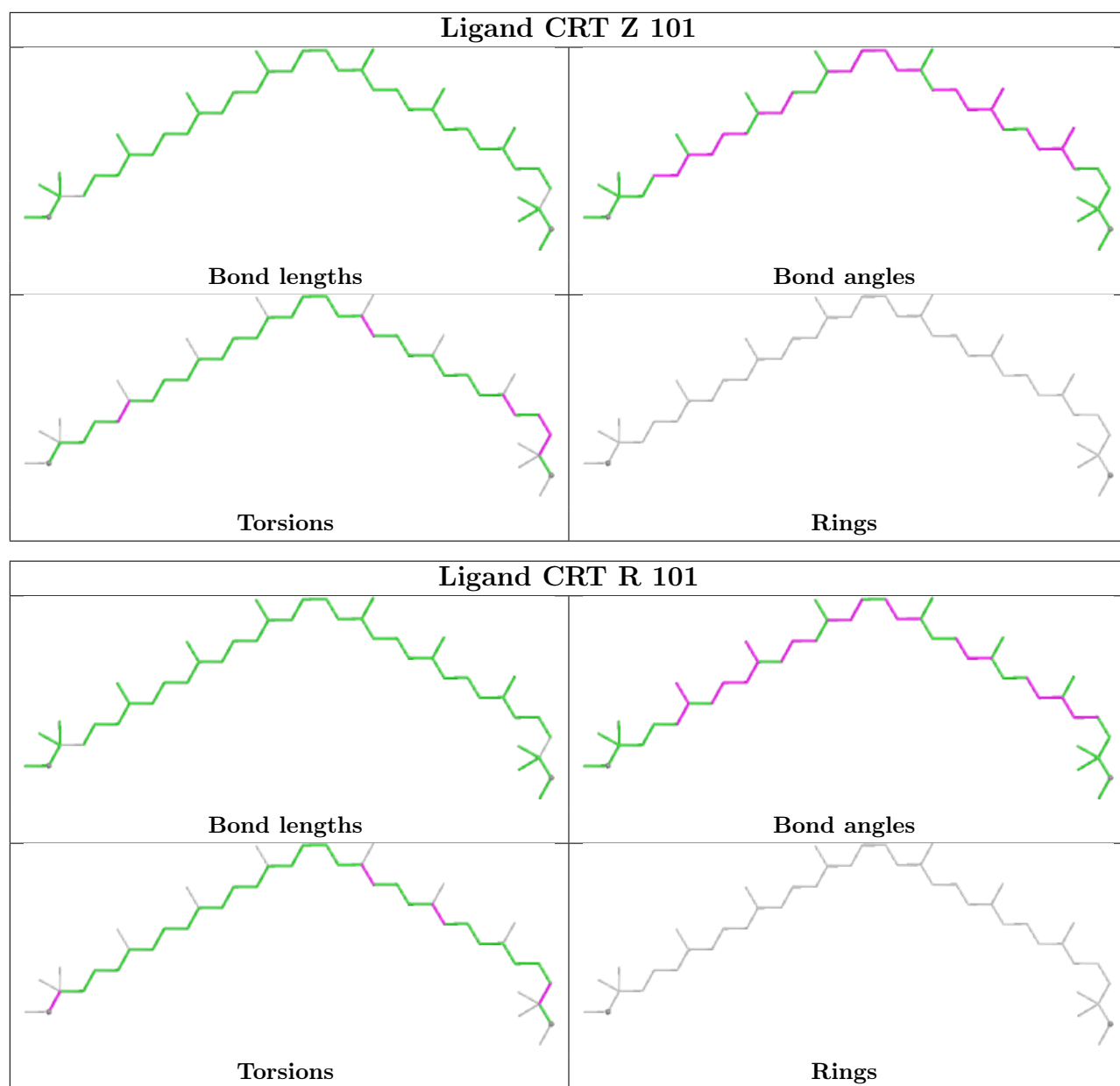


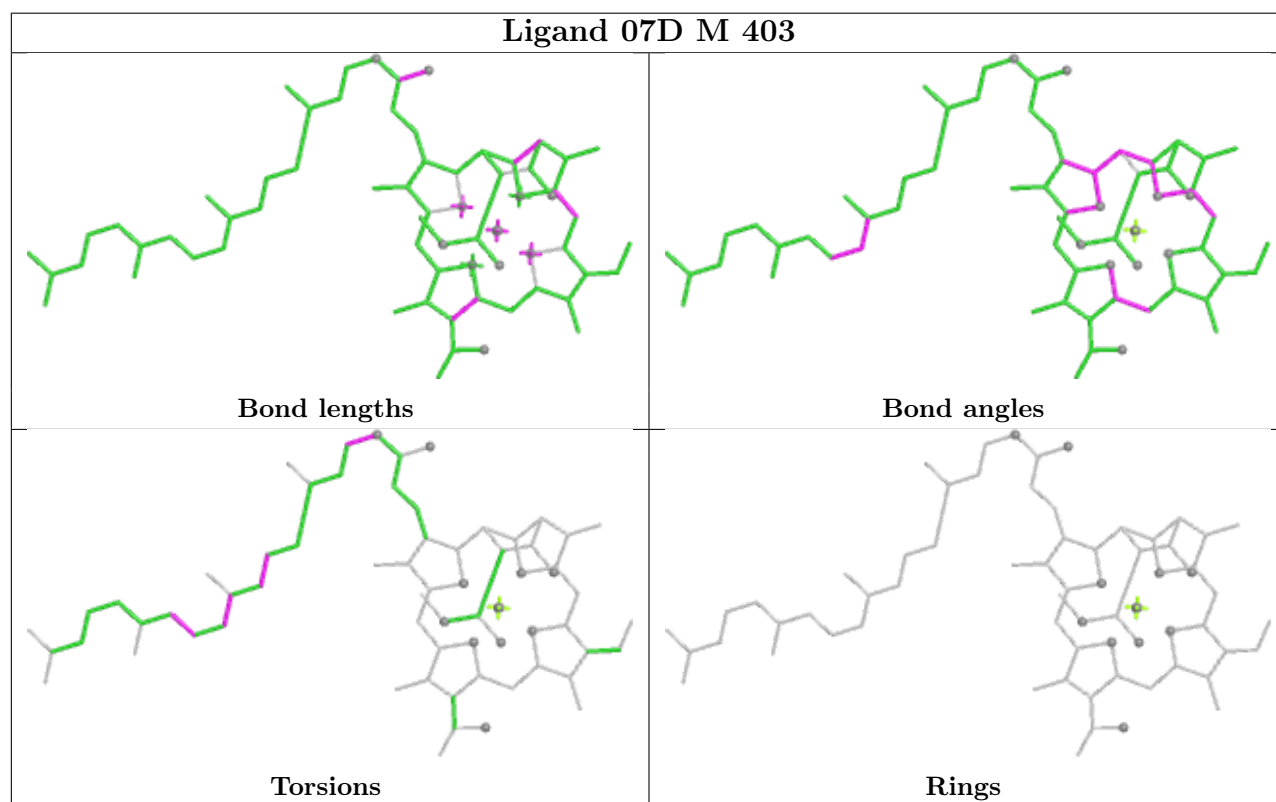
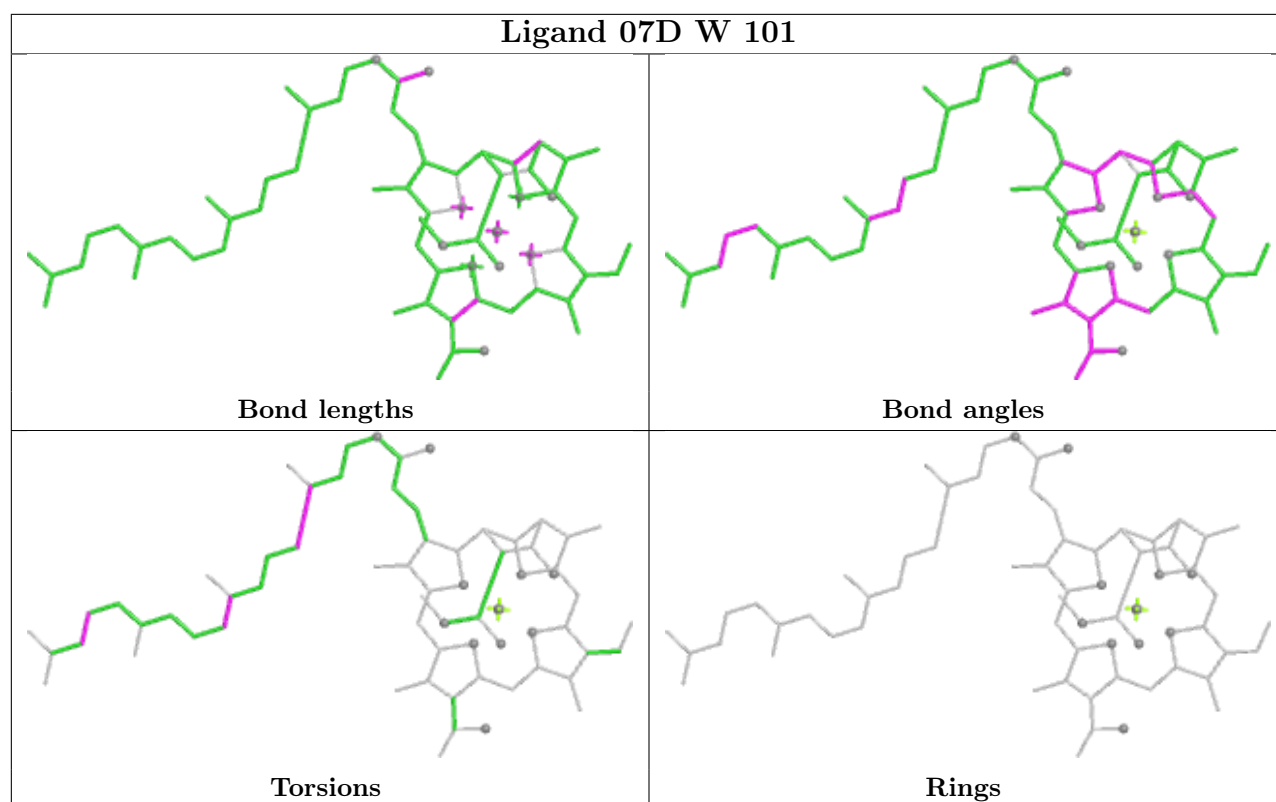


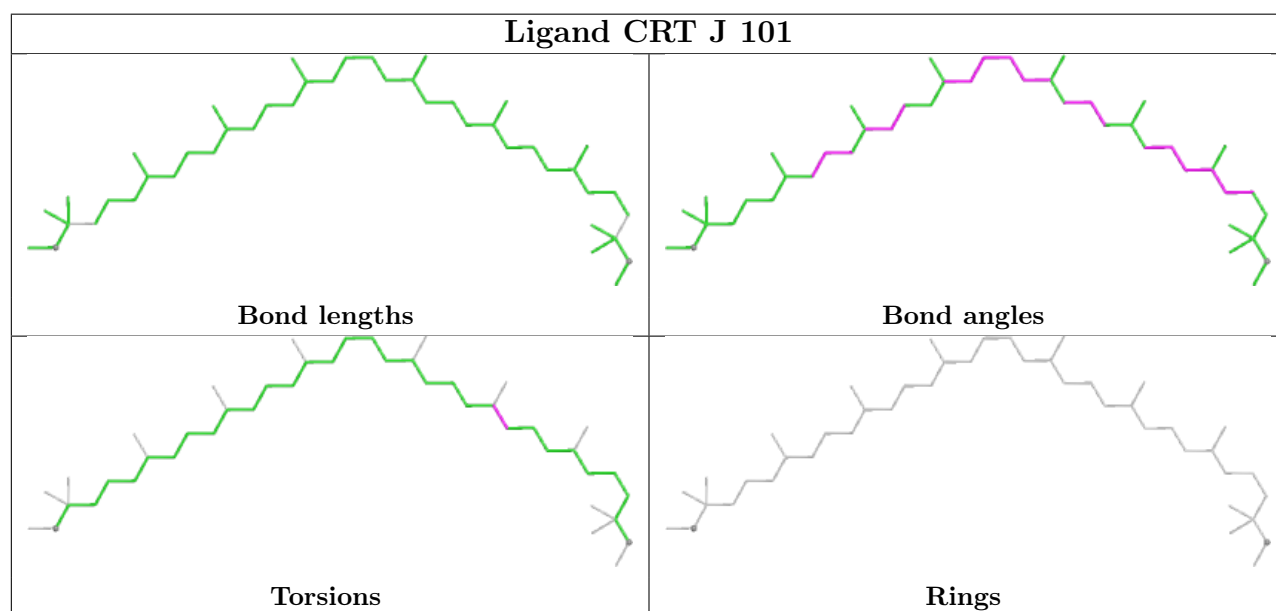
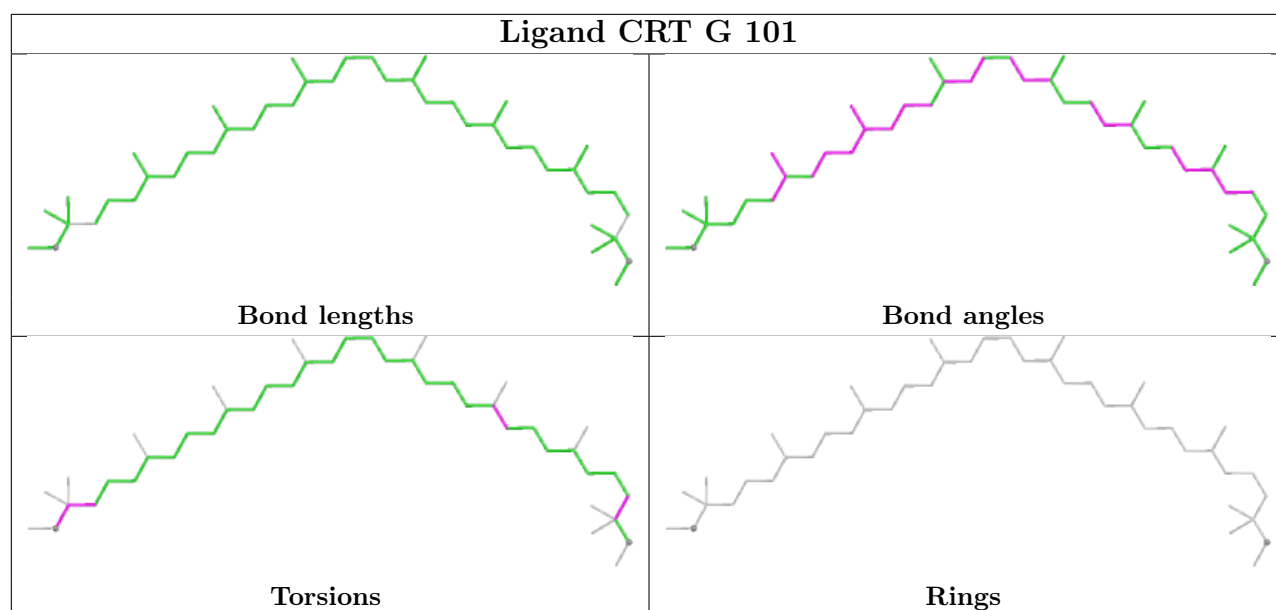


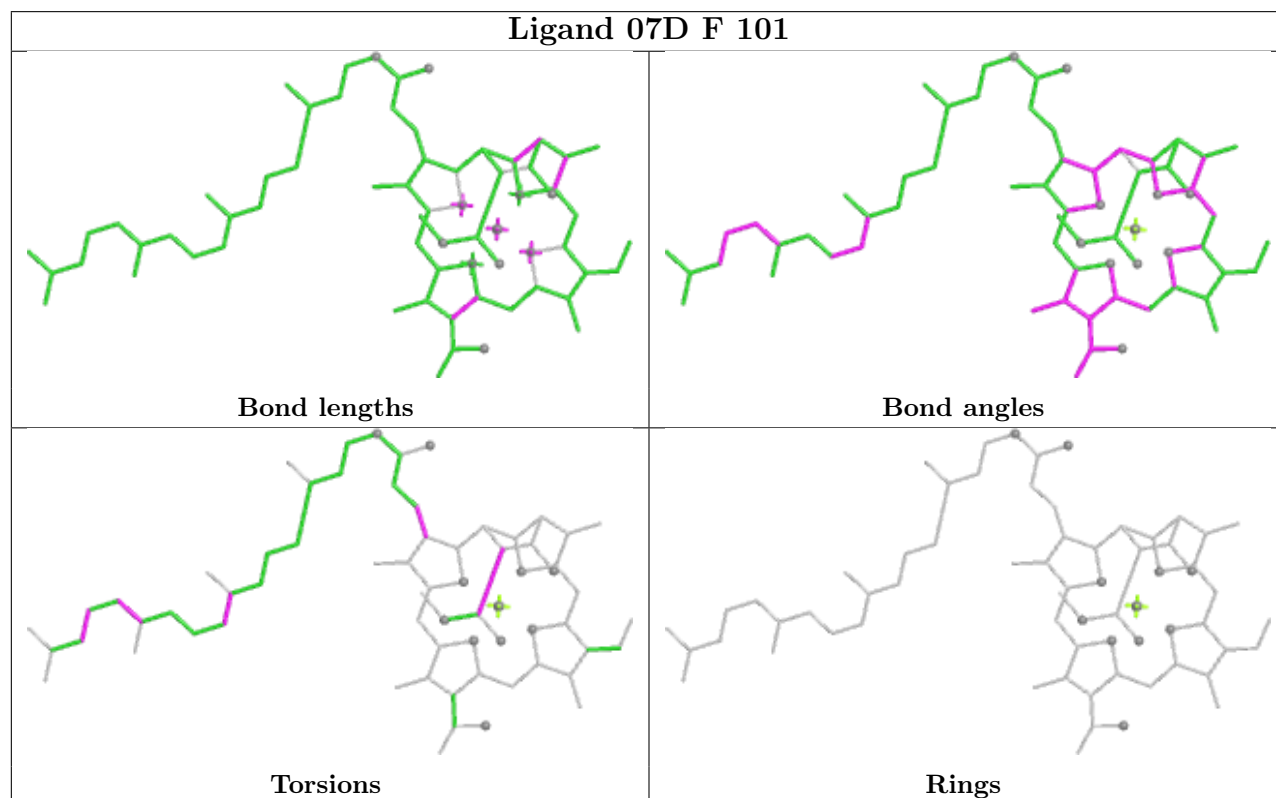
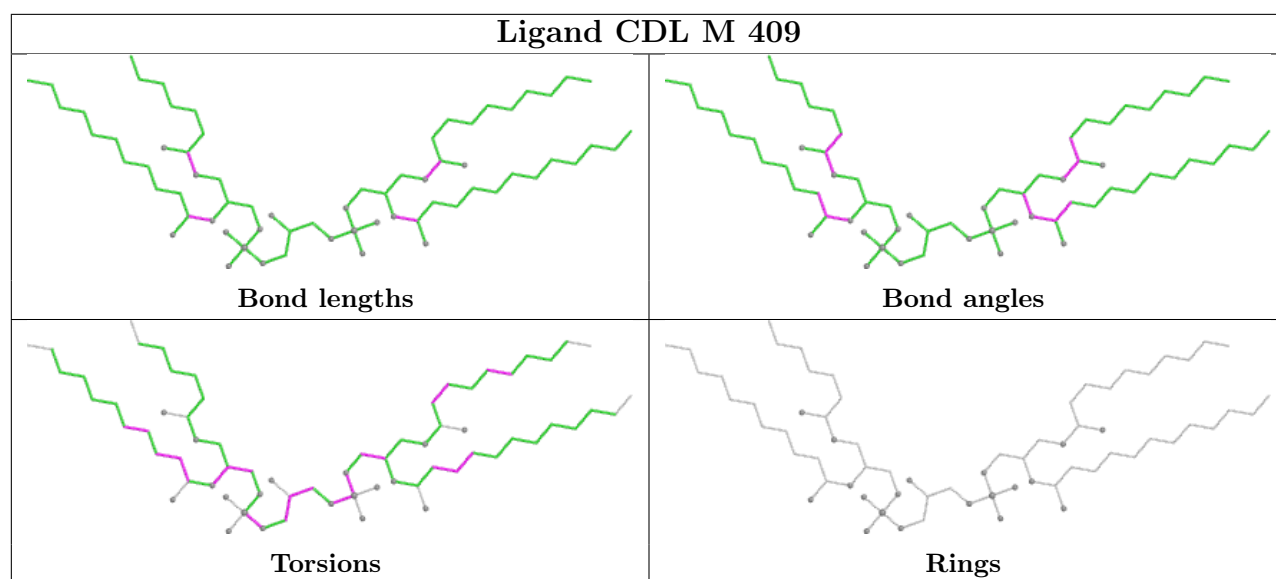


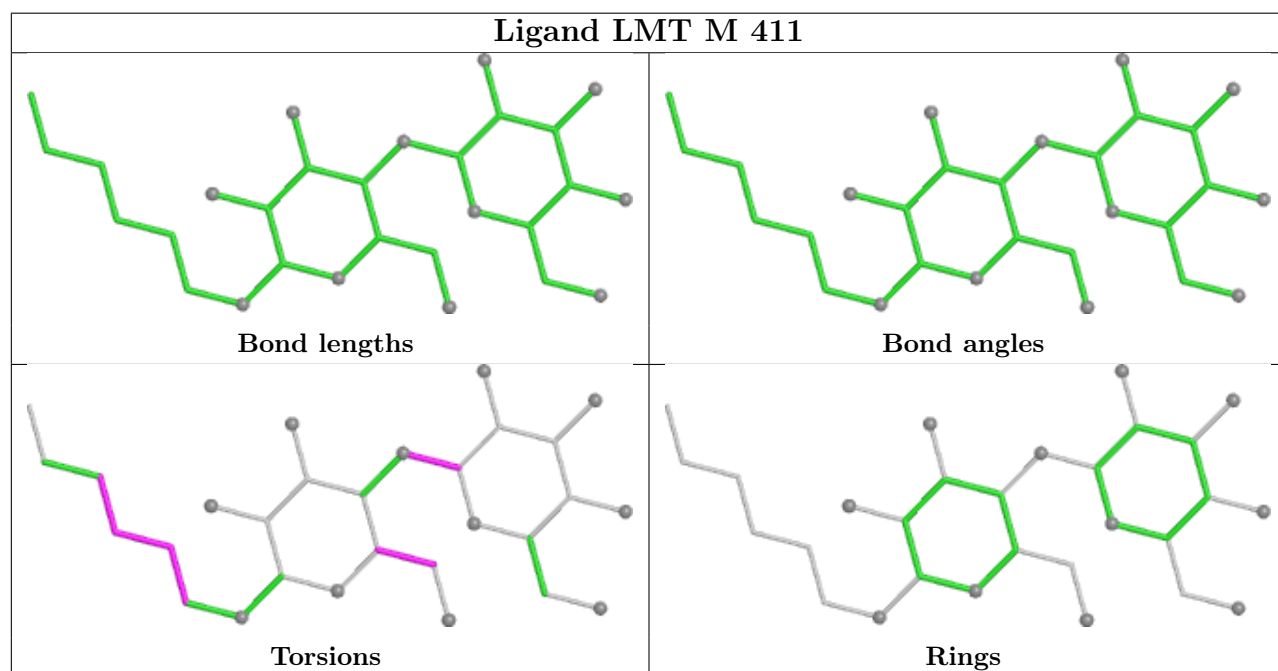
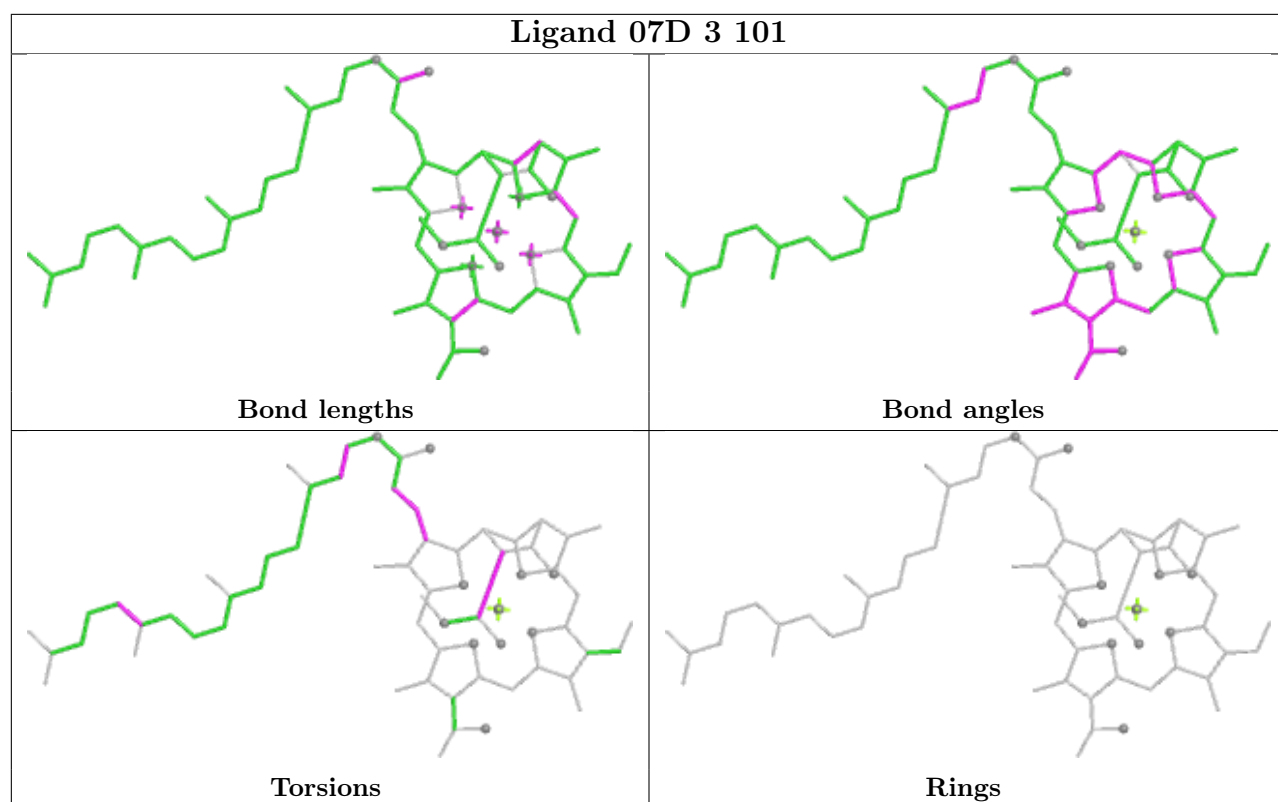


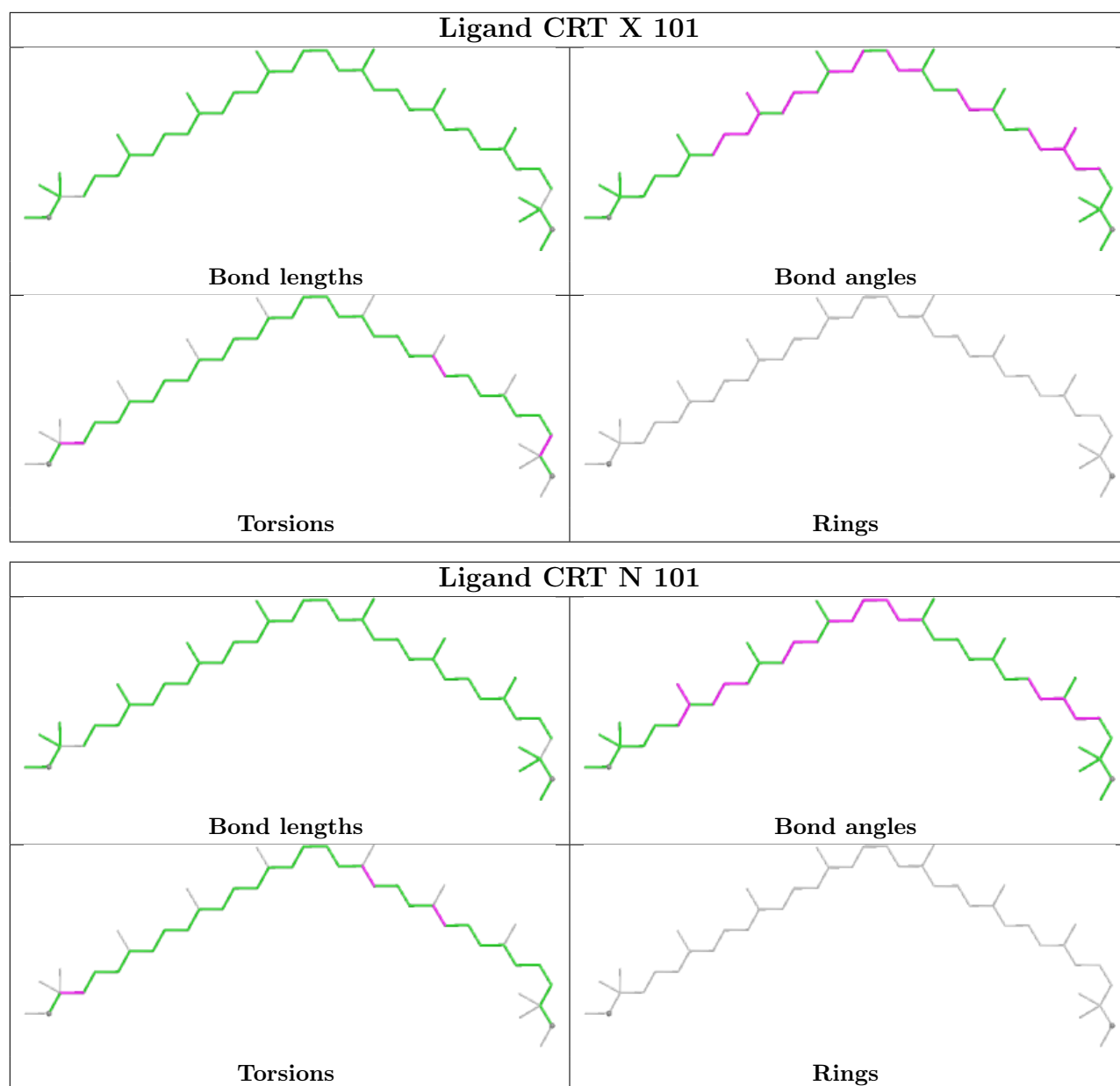












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

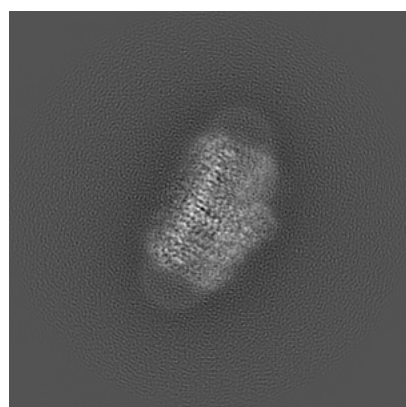
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31258. These allow visual inspection of the internal detail of the map and identification of artifacts.

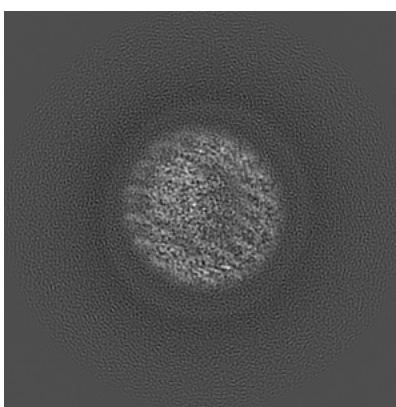
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

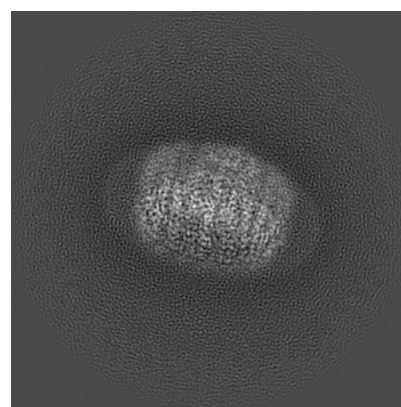
6.1.1 Primary map



X



Y

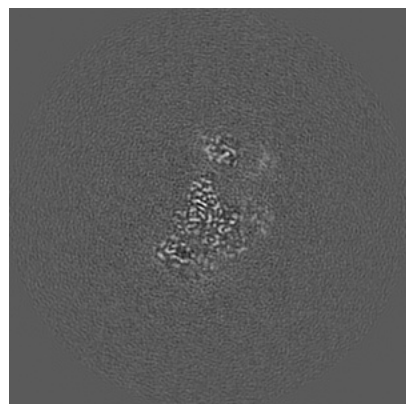


Z

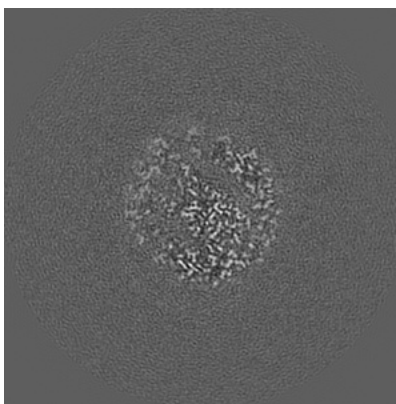
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

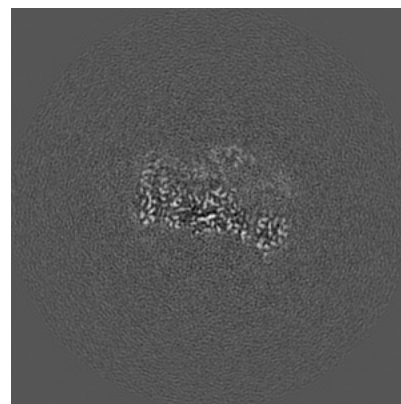
6.2.1 Primary map



X Index: 180



Y Index: 180

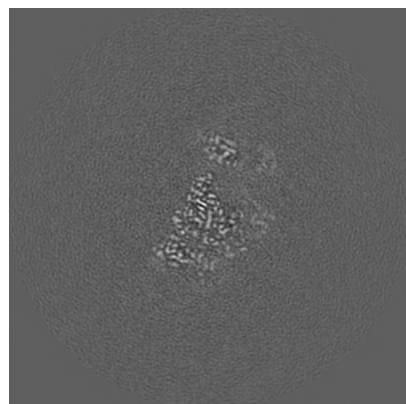


Z Index: 180

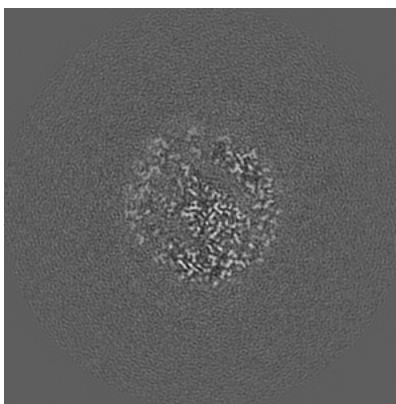
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

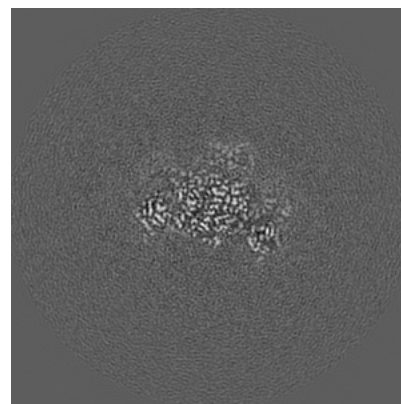
6.3.1 Primary map



X Index: 179



Y Index: 180

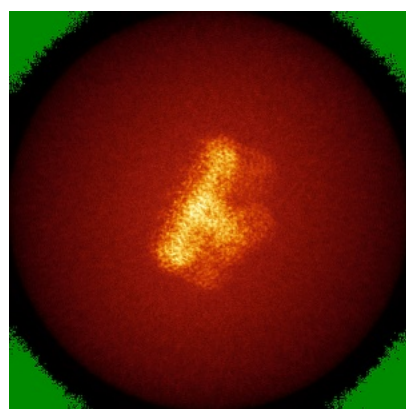


Z Index: 171

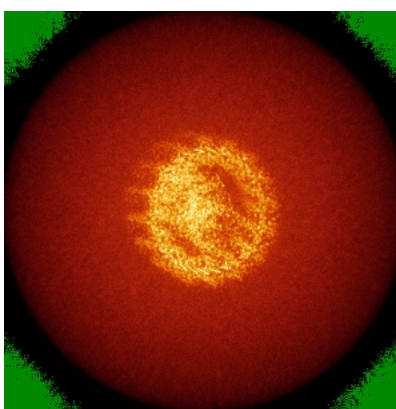
The images above show the largest variance slices of the map in three orthogonal directions.

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

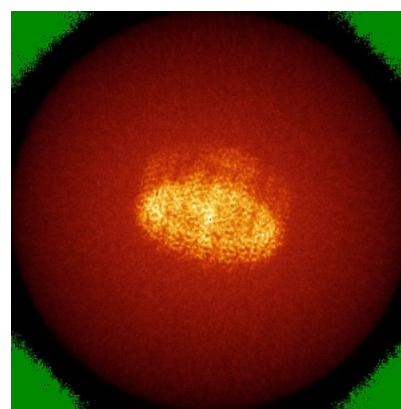
6.4.1 Primary map



X



Y

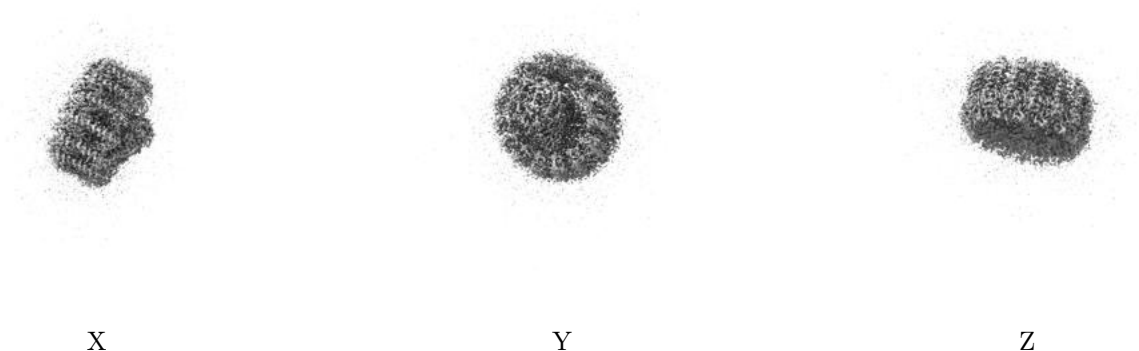


Z

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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.033. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

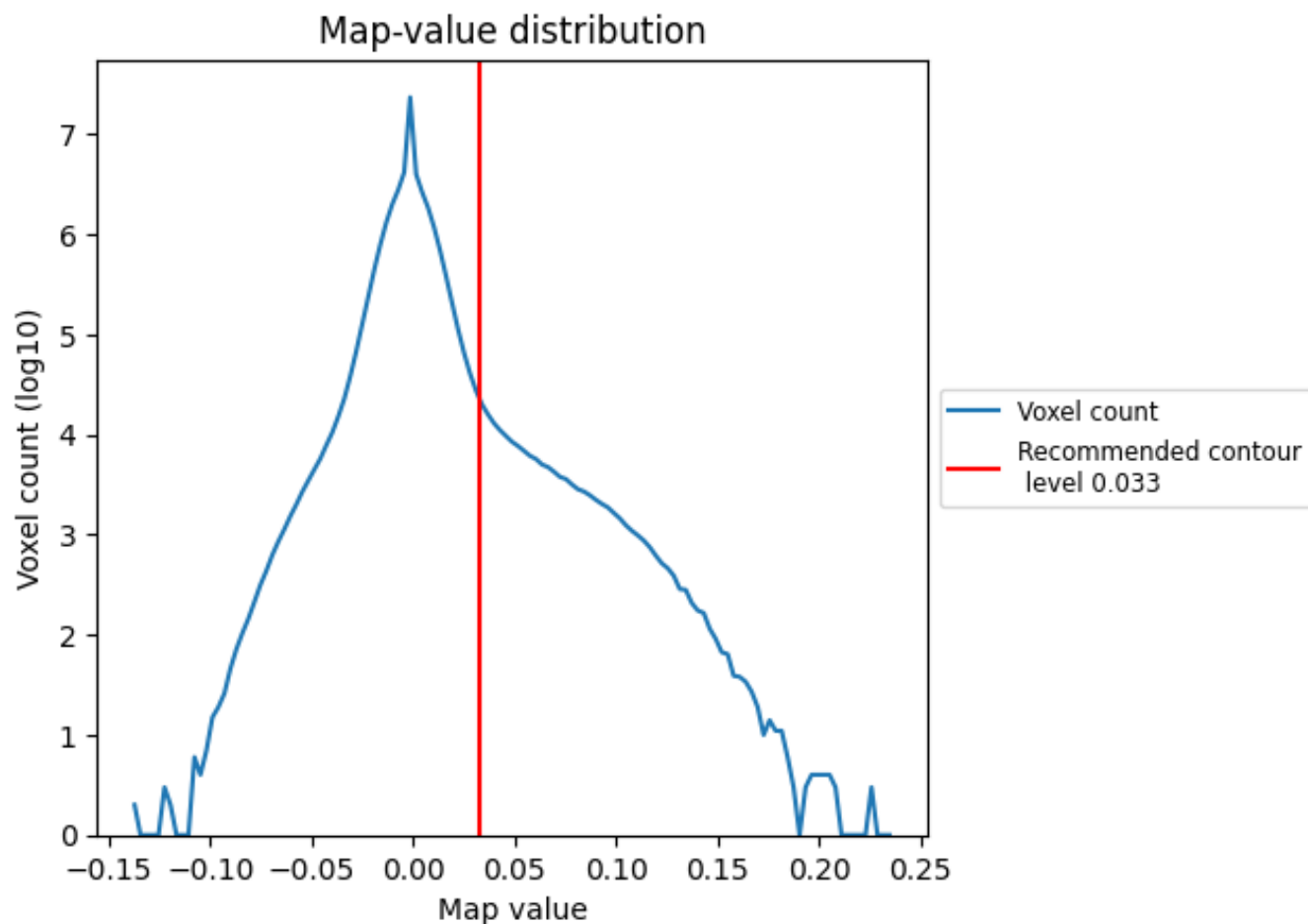
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

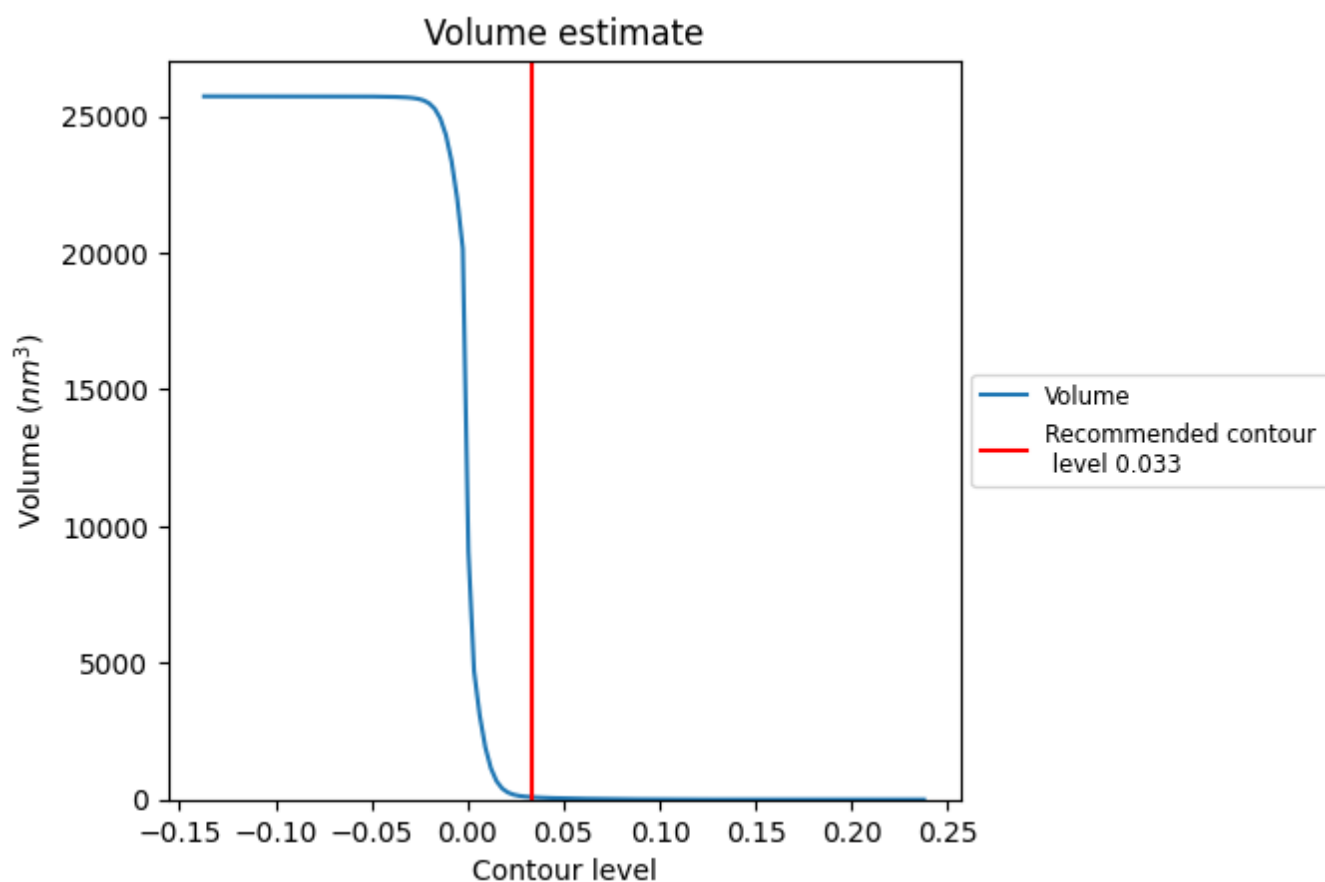
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

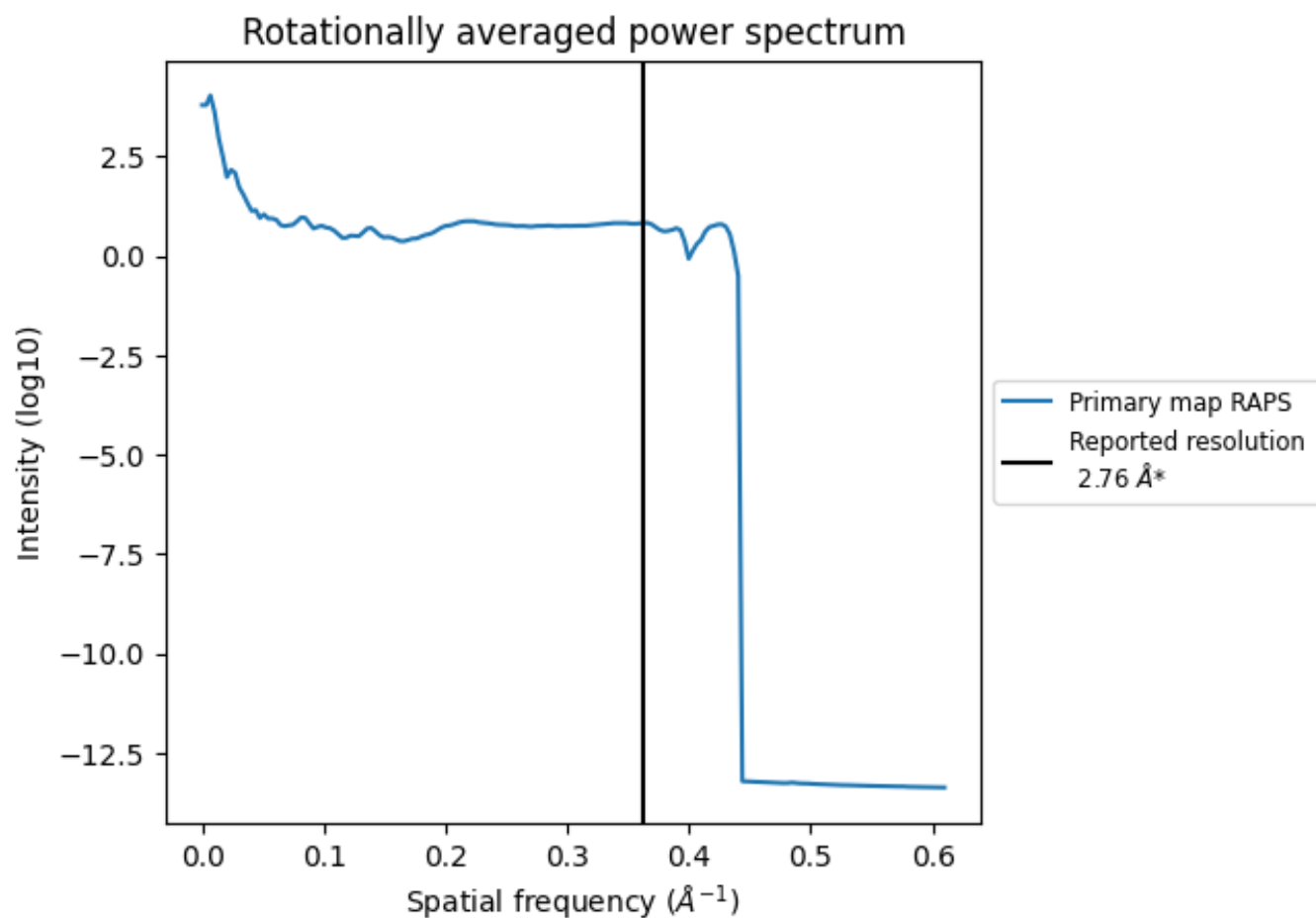
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 90 nm^3 ; this corresponds to an approximate mass of 81 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 ⓘ

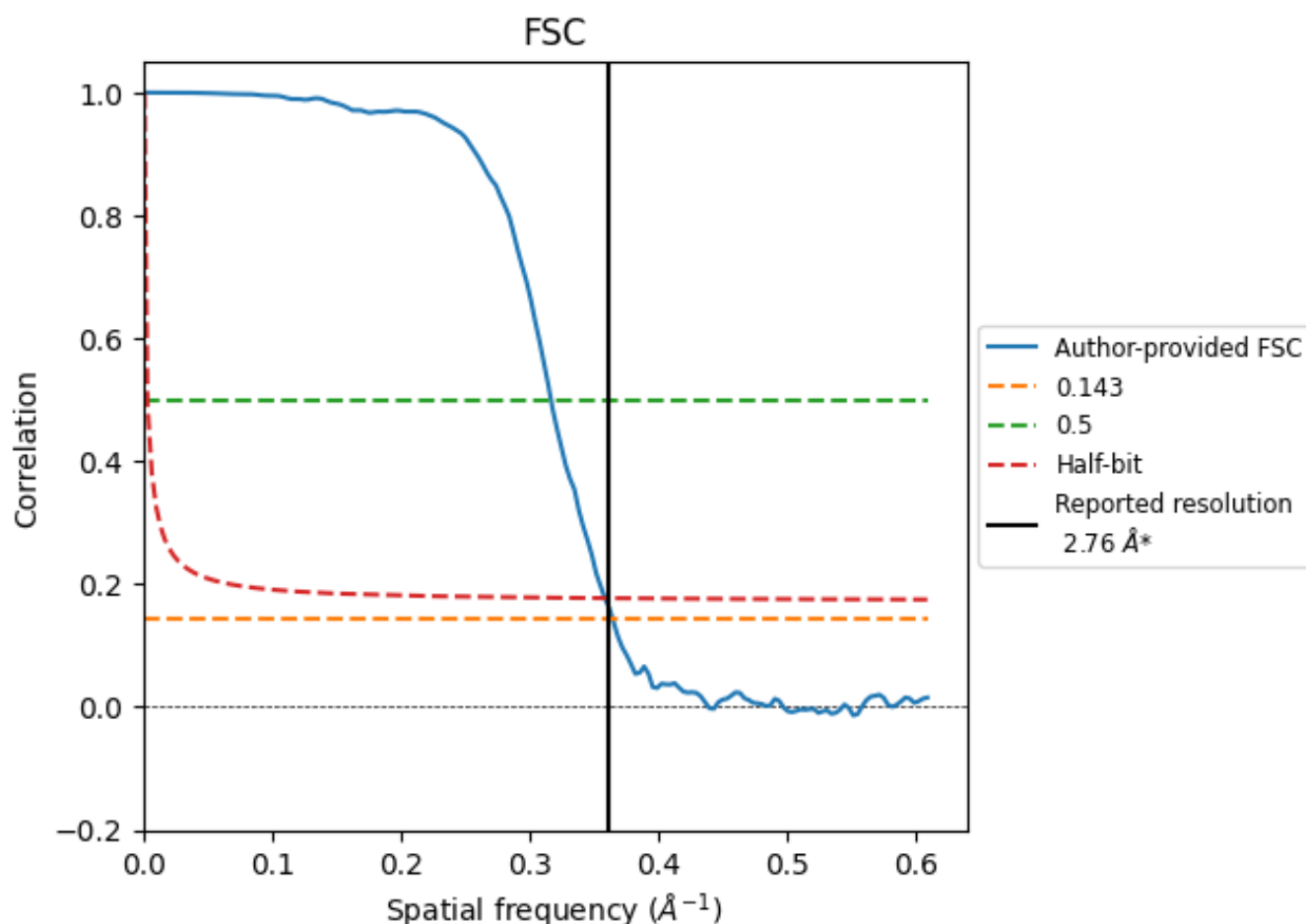


*Reported resolution corresponds to spatial frequency of 0.362 Å⁻¹

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 0.362 Å⁻¹

8.2 Resolution estimates [i](#)

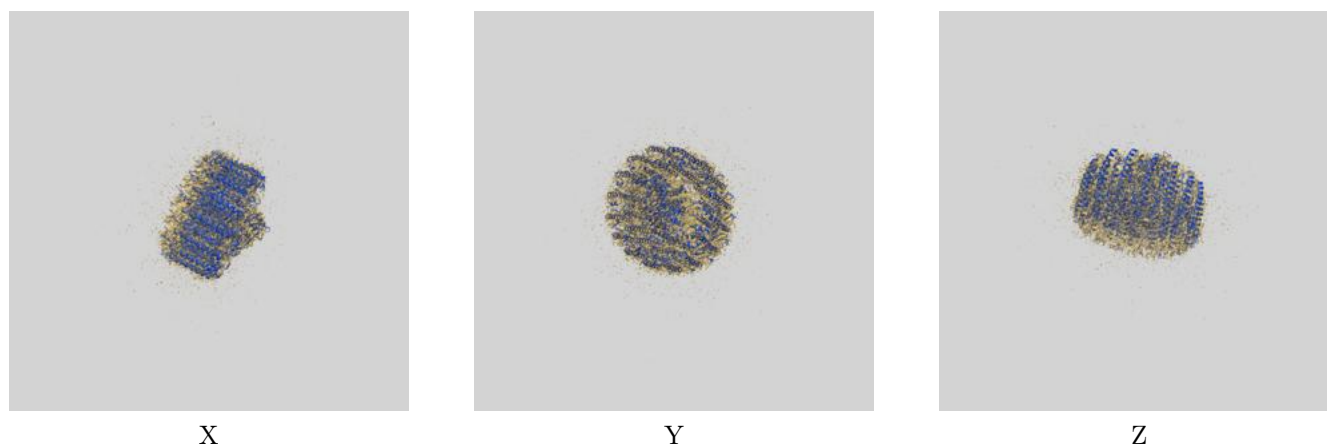
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.76	-	-
Author-provided FSC curve	2.74	3.15	2.79
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

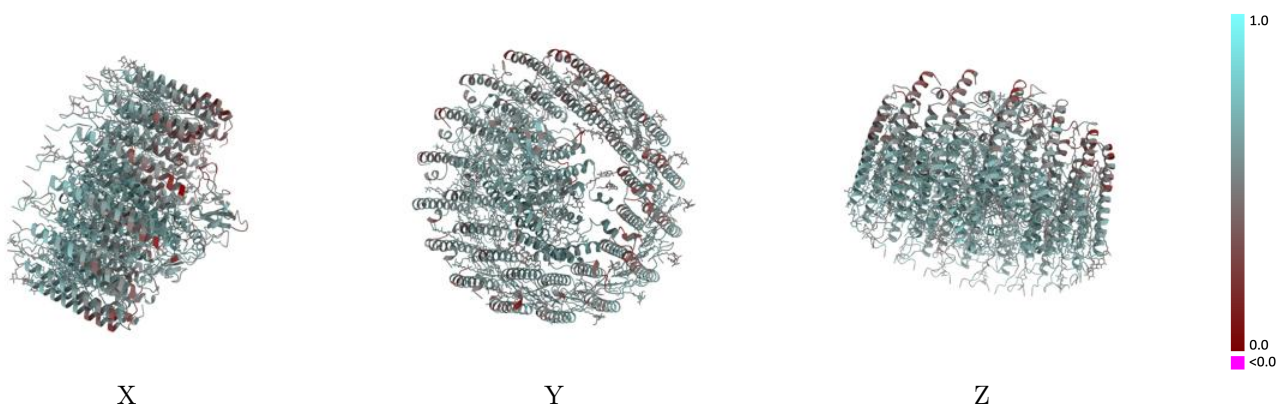
This section contains information regarding the fit between EMDB map EMD-31258 and PDB model 7EQD. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



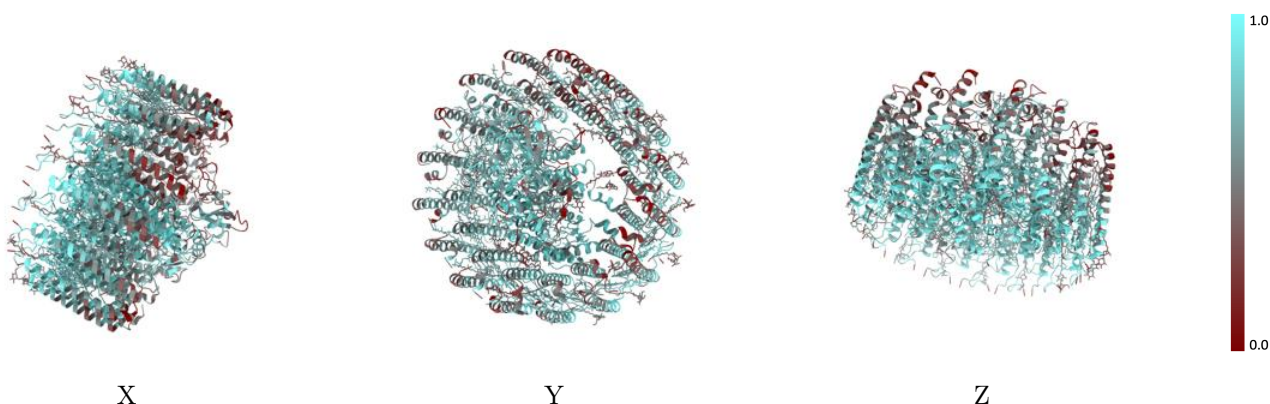
The images above show the 3D surface view of the map at the recommended contour level 0.033 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



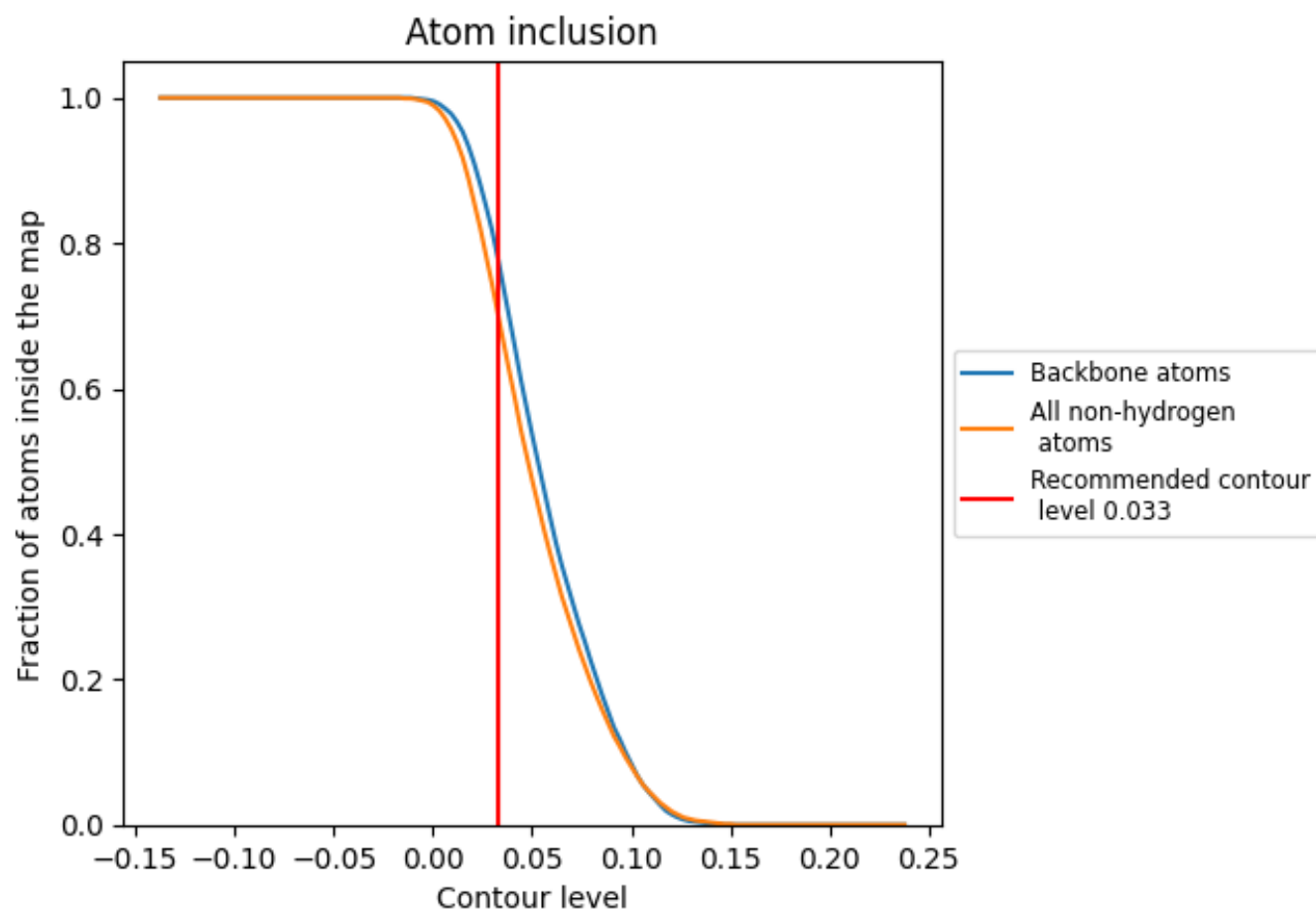
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.033).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 70% 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 (0.033) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7000	 0.5770
0	 0.6870	 0.5780
1	 0.6170	 0.5370
2	 0.5890	 0.5370
3	 0.5810	 0.5370
4	 0.5610	 0.5020
5	 0.5590	 0.5320
6	 0.5610	 0.5080
7	 0.6800	 0.5750
8	 0.6590	 0.5560
9	 0.7380	 0.5940
A	 0.7290	 0.5910
B	 0.6680	 0.5540
D	 0.7530	 0.6020
E	 0.7040	 0.5670
F	 0.7580	 0.5990
G	 0.7430	 0.5960
H	 0.6100	 0.5460
I	 0.7580	 0.5970
J	 0.7070	 0.5900
K	 0.7400	 0.5920
L	 0.8650	 0.6400
M	 0.7990	 0.6240
N	 0.6910	 0.5730
O	 0.7350	 0.5830
P	 0.6270	 0.5550
Q	 0.7280	 0.6010
R	 0.7130	 0.5660
S	 0.6760	 0.5680
T	 0.6560	 0.5560
U	 0.6660	 0.5600
V	 0.5990	 0.5250
W	 0.6690	 0.5650
X	 0.5860	 0.5350
Y	 0.6370	 0.5270
Z	 0.6220	 0.5290

