



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:02 pm BST

PDB ID : 5Y5S
Title : Structure of photosynthetic LH1-RC super-complex at 1.9 angstrom resolution
Authors : Yu, L.-J.; Suga, M.; Wang-Otomo, Z.-Y.; Shen, J.-R.
Deposited on : 2017-08-09
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

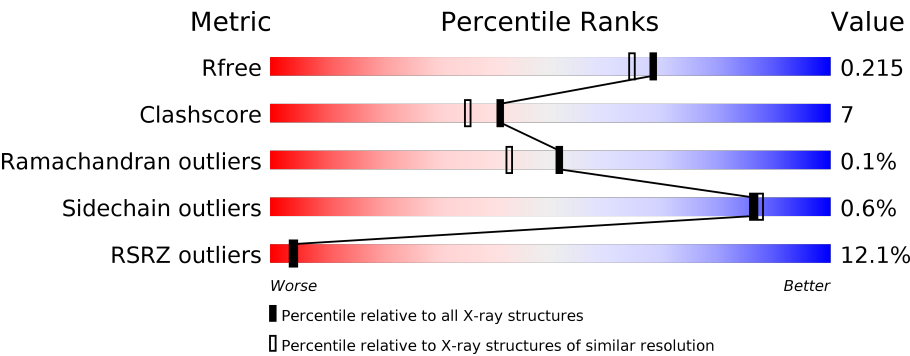
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	404	<div><div>2%</div><div><div></div><div>72%</div><div>5%</div><div>23%</div></div></div>
2	L	281	<div><div>7%</div><div><div></div><div>92%</div><div>7%</div></div></div>
3	M	325	<div><div>3%</div><div><div></div><div>90%</div><div>8%</div><div>•</div></div></div>
4	H	259	<div><div>3%</div><div><div></div><div>90%</div><div>8%</div><div>•</div></div></div>
5	1	61	<div><div>18%</div><div><div></div><div>79%</div><div>13%</div><div>8%</div></div></div>
5	3	61	<div><div>13%</div><div><div></div><div>87%</div><div>5%</div><div>8%</div></div></div>





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Mol	Chain	Length	Quality of chain
5	5	61	
5	7	61	
5	9	61	
5	A	61	
5	D	61	
5	F	61	
5	I	61	
5	K	61	
5	O	61	
5	Q	61	
5	S	61	
5	U	61	
5	W	61	
5	Y	61	
6	0	47	
6	2	47	
6	4	47	
6	6	47	
6	8	47	
6	B	47	
6	E	47	
6	G	47	
6	J	47	
6	N	47	
6	P	47	

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Mol	Chain	Length	Quality of chain
6	R	47	
6	T	47	
6	V	47	
6	X	47	
6	Z	47	

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
20	PEF	1	104	-	X	-	-
20	PEF	3	103	-	X	-	-
20	PEF	5	103	-	X	-	-
20	PEF	I	103	-	X	-	-
20	PEF	M	407	-	X	-	-
20	PEF	M	409	-	X	-	-
20	PEF	U	104	-	X	-	-
20	PEF	U	105	-	X	-	-
20	PEF	W	103	-	X	-	-

2 Entry composition [i](#)

There are 25 unique types of molecules in this entry. The entry contains 27981 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	311	Total	C	N	O	S	0	0	0
			2417	1524	424	453	16			

- Molecule 2 is a protein called Photosynthetic reaction center L subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	280	Total	C	N	O	S	0	1	0
			2236	1505	359	361	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	318	Total	C	N	O	S	0	2	0
			2555	1715	417	412	11			

- Molecule 4 is a protein called Photosynthetic reaction center H subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	255	Total	C	N	O	S	0	2	0
			1976	1272	337	361	6			

- Molecule 5 is a protein called LH1 alpha polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	54	Total	C	N	O	S	0	0	0
			434	290	70	73	1			
5	D	55	Total	C	N	O	S	0	1	0
			445	296	72	76	1			
5	F	55	Total	C	N	O	S	0	1	0
			445	296	72	76	1			
5	I	57	Total	C	N	O	S	0	1	0
			460	305	74	79	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	57	Total	C	N	O	S	0	0	0
			457	303	74	78	2			
5	O	56	Total	C	N	O	S	0	1	0
			455	303	73	76	3			
5	Q	57	Total	C	N	O	S	0	0	0
			457	303	74	78	2			
5	S	56	Total	C	N	O	S	0	3	0
			468	312	74	79	3			
5	U	58	Total	C	N	O	S	0	0	0
			466	309	76	79	2			
5	W	56	Total	C	N	O	S	0	0	0
			451	300	74	76	1			
5	Y	57	Total	C	N	O	S	0	0	0
			457	303	74	78	2			
5	1	56	Total	C	N	O	S	0	0	0
			450	299	73	76	2			
5	3	56	Total	C	N	O	S	0	1	0
			455	303	73	76	3			
5	5	54	Total	C	N	O	S	0	0	0
			434	290	70	73	1			
5	7	57	Total	C	N	O	S	0	0	0
			457	303	74	78	2			
5	9	57	Total	C	N	O	S	0	0	0
			457	303	74	78	2			

- Molecule 6 is a protein called LH1 beta polypeptide.

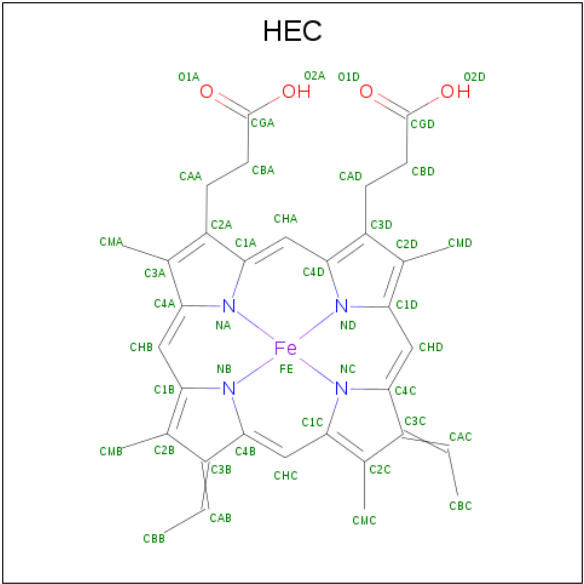
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	42	Total	C	N	O	S	0	0	0
			351	237	54	58	2			
6	E	38	Total	C	N	O	S	0	0	0
			326	222	50	52	2			
6	G	42	Total	C	N	O	S	0	0	0
			351	237	54	58	2			
6	J	42	Total	C	N	O	S	0	0	0
			351	237	54	58	2			
6	N	42	Total	C	N	O	S	0	0	0
			351	237	54	58	2			
6	P	42	Total	C	N	O	S	0	0	0
			351	237	54	58	2			
6	R	41	Total	C	N	O	S	0	0	0
			345	234	53	56	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	T	43	Total	C	N	O	S	0	0	0
			360	243	56	59	2			
6	V	42	Total	C	N	O	S	0	0	0
			351	237	54	58	2			
6	X	41	Total	C	N	O	S	0	0	0
			345	234	53	56	2			
6	Z	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	2	41	Total	C	N	O	S	0	0	0
			345	234	53	56	2			
6	4	42	Total	C	N	O	S	0	0	0
			351	237	54	58	2			
6	6	42	Total	C	N	O	S	0	0	0
			351	237	54	58	2			
6	8	41	Total	C	N	O	S	0	0	0
			345	234	53	56	2			
6	0	43	Total	C	N	O	S	0	0	0
			360	243	56	59	2			

- Molecule 7 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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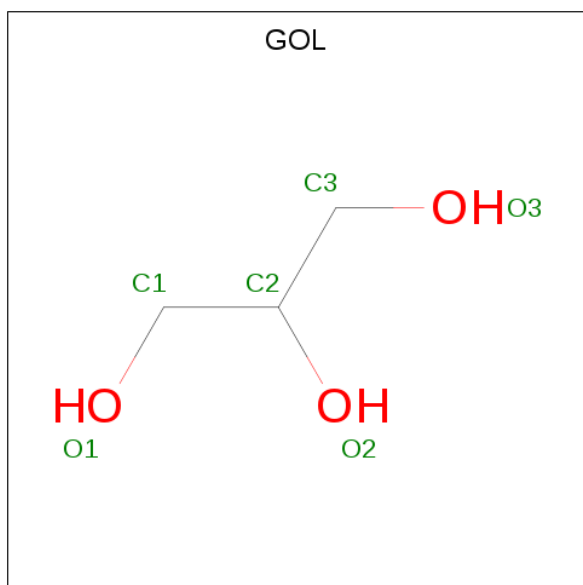
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
7	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

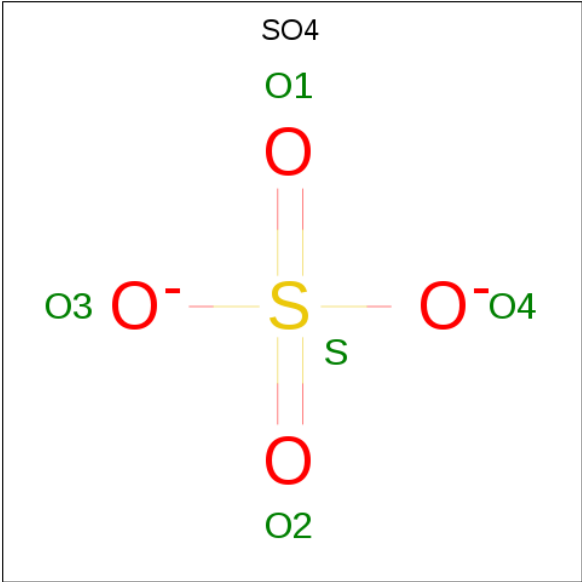
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total Mg 1 1	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



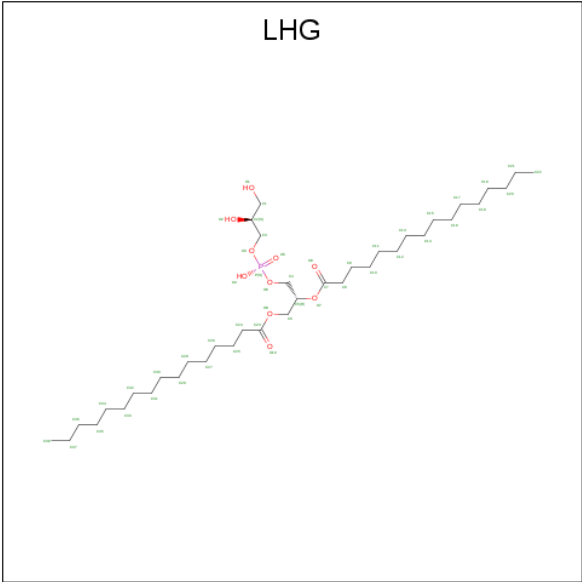
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O		
			6	3	3		
9	H	1	Total	C	O		
			6	3	3		

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



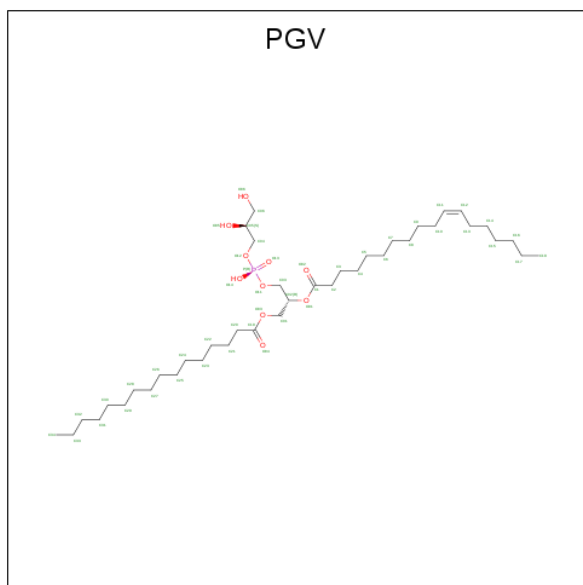
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	O	S	0	0
			5	4	1		
10	L	1	Total	O	S	0	0
			5	4	1		
10	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 11 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



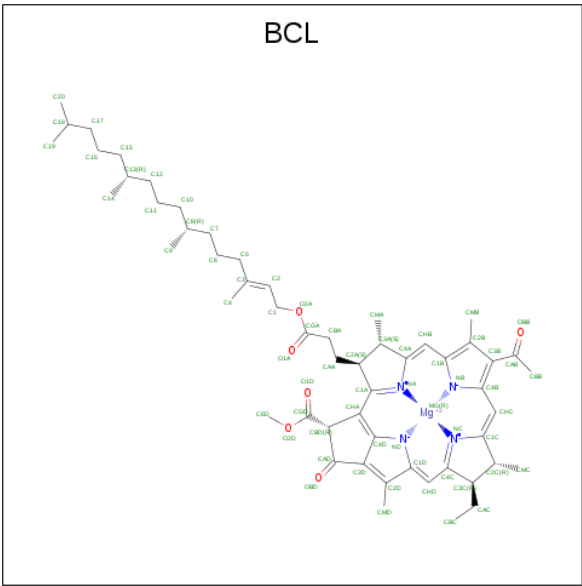
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O	0	0
			9	8	1		

- Molecule 12 is (1R)-2-{{[[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	O		0	0
			21	17	4			
12	L	1	Total	C	O	P	0	0
			43	32	10	1		
12	L	1	Total	C	O	P	0	0
			44	33	10	1		
12	M	1	Total	C	O	P	0	0
			46	37	8	1		
12	M	1	Total	C	O	P	0	0
			37	26	10	1		
12	H	1	Total	C	O	P	0	0
			36	25	10	1		
12	A	1	Total	C	O	P	0	0
			33	22	10	1		
12	D	1	Total	C	O	P	0	0
			35	24	10	1		
12	1	1	Total	C	O	P	0	0
			31	20	10	1		
12	3	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 13 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	D	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	D	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	F	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	F	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	I	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	I	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	K	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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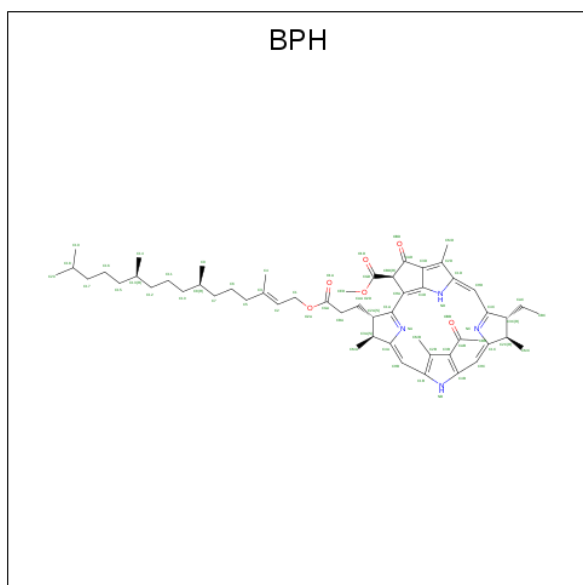
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	K	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	O	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	O	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	S	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	S	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	U	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	U	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	W	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	W	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	1	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	1	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	3	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	3	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	5	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	5	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	7	1	Total 61	C 50	Mg 1	N 4	O 6	0	0
13	7	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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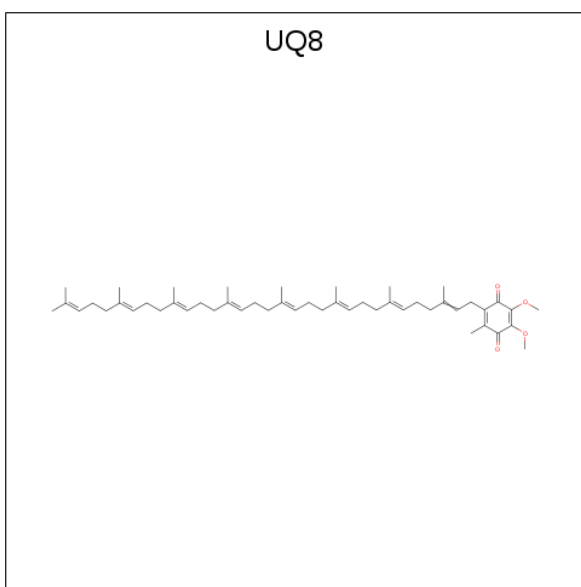
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	9	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
13	0	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 14 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



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

- Molecule 15 is Ubiquinone-8 (three-letter code: UQ8) (formula: $C_{49}H_{74}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	L	1	Total	C	O	0	0
			33	29	4		
15	L	1	Total	C	O	0	0
			53	49	4		
15	L	1	Total	C	O	0	0
			18	14	4		
15	M	1	Total	C	O	0	0
			18	14	4		
15	7	1	Total	C	O	0	0
			33	29	4		

- Molecule 16 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	P	1	Total	C	0	0
			12	12		
16	G	1	Total	C	0	0
			12	12		
16	J	1	Total	C	0	0
			12	12		
16	E	1	Total	C	0	0
			12	12		
16	B	1	Total	C	0	0
			12	12		
16	6	1	Total	C	0	0
			12	12		
16	8	1	Total	C	0	0
			12	12		

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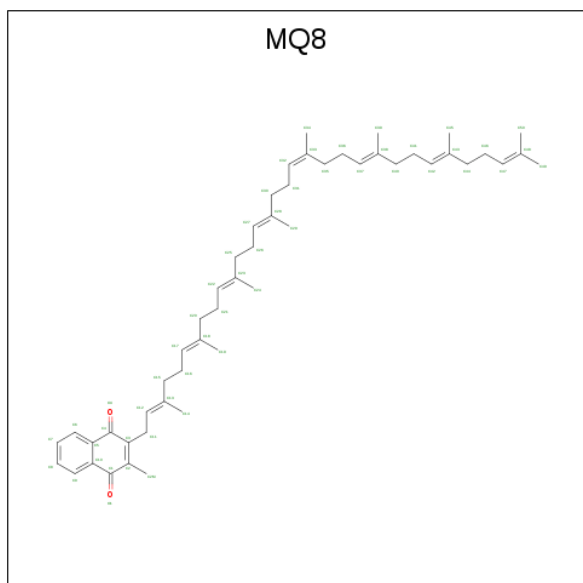
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	Z	1	Total C 12 12	0	0
16	T	1	Total C 12 12	0	0
16	O	1	Total C 12 12	0	0
16	X	1	Total C 12 12	0	0
16	4	1	Total C 12 12	0	0
16	R	1	Total C 12 12	0	0
16	L	1	Total C 12 12	0	0
16	2	1	Total C 12 12	0	0
16	M	1	Total C 9 9	0	0

- Molecule 17 is FE (III) ION (three-letter code: FE) (formula: Fe).

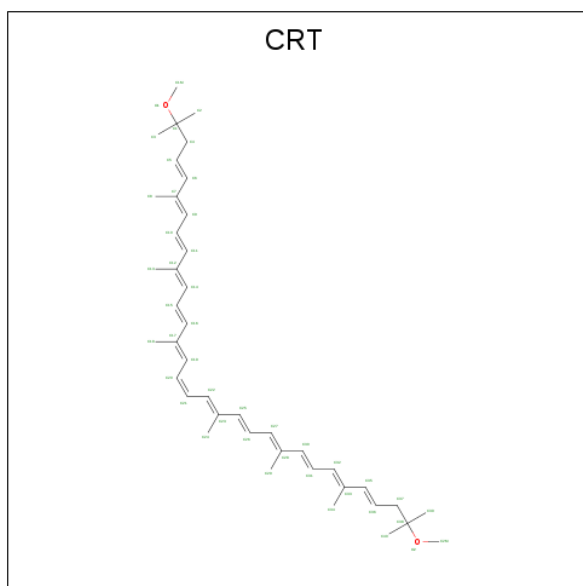
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	L	1	Total Fe 1 1	0	0

- Molecule 18 is MENAQUINONE 8 (three-letter code: MQ8) (formula: C₅₁H₇₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	M	1	Total	C	O	0	0
			53	51	2		

- Molecule 19 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: C₄₂H₆₀O₂).



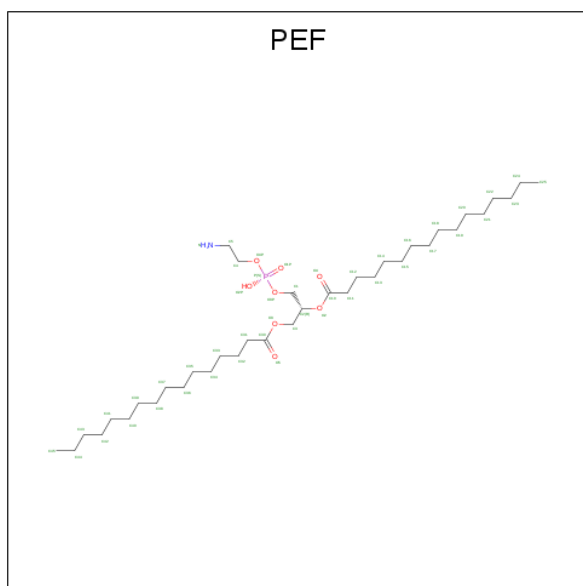
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	M	1	Total	C	O	0	0
			44	42	2		
19	A	1	Total	C	O	0	0
			44	42	2		
19	G	1	Total	C	O	0	0
			44	42	2		
19	J	1	Total	C	O	0	0
			44	42	2		
19	N	1	Total	C	O	0	0
			44	42	2		
19	O	1	Total	C	O	0	0
			44	42	2		
19	P	1	Total	C	O	0	0
			44	42	2		
19	Q	1	Total	C	O	0	0
			44	42	2		
19	U	1	Total	C	O	0	0
			44	42	2		
19	V	1	Total	C	O	0	0
			44	42	2		
19	Z	1	Total	C	O	0	0
			44	42	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	1	1	Total	C	O	0	0
			44	42	2		
19	2	1	Total	C	O	0	0
			44	42	2		
19	6	1	Total	C	O	0	0
			44	42	2		
19	9	1	Total	C	O	0	0
			44	42	2		
19	9	1	Total	C	O	0	0
			44	42	2		
19	0	1	Total	C	O	0	0
			44	42	2		

- Molecule 20 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: $C_{37}H_{74}NO_8P$).



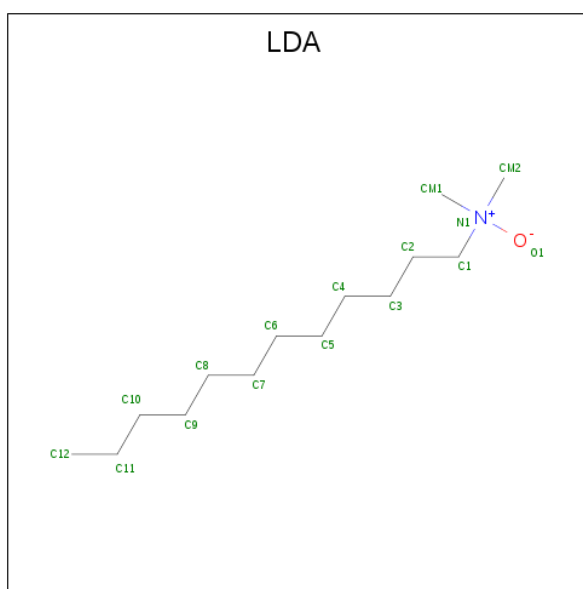
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	M	1	Total	O	P			0	0
			5	4	1				
20	M	1	Total	O	P			0	0
			5	4	1				
20	M	1	Total	O	P			0	0
			5	4	1				
20	M	1	Total	O	P			0	0
			5	4	1				
20	M	1	Total	C	N	O	P	0	0
			47	37	1	8	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	I	1	Total	O	P		0	0
			5	4	1			
20	K	1	Total	C	N	O	P	
			27	17	1	8	1	
20	U	1	Total	O	P			
			5	4	1			
20	U	1	Total	O	P			
			5	4	1			
20	W	1	Total	O	P			
			5	4	1			
20	1	1	Total	O	P			
			5	4	1			
20	3	1	Total	O	P			
			5	4	1			
20	5	1	Total	O	P			
			5	4	1			

- Molecule 21 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



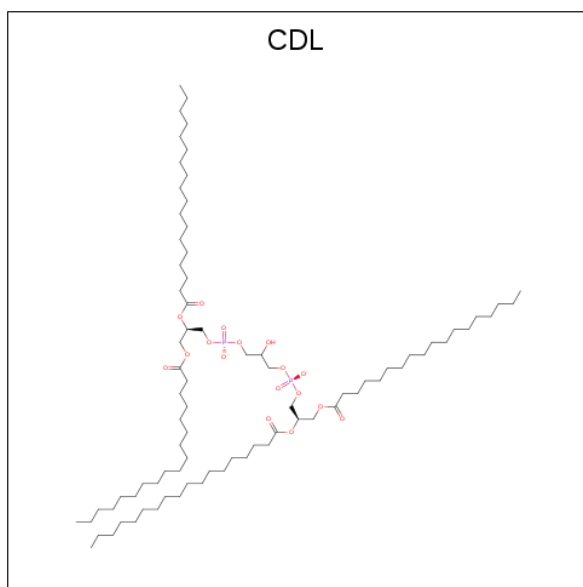
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	M	1	Total	C	N	O	0	0
			14	12	1	1		
21	I	1	Total	C	N	O	0	0
			16	14	1	1		
21	J	1	Total	C	N	O	0	0
			16	14	1	1		

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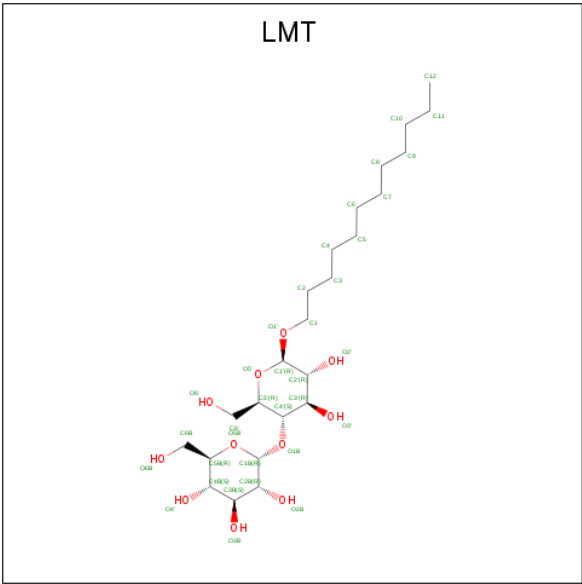
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	O	1	Total	C	N	O	0	0
			14	12	1	1		
21	V	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 22 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	M	1	Total	C	O	P	0	0
			39	21	16	2		
22	H	1	Total	C	O	P	0	0
			64	45	17	2		
22	H	1	Total	C	O	P	0	0
			79	60	17	2		
22	D	1	Total	C	O	P	0	0
			40	21	17	2		
22	K	1	Total	C	O	P	0	0
			86	67	17	2		
22	Q	1	Total	C	O	P	0	0
			75	56	17	2		
22	S	1	Total	C	O	P	0	0
			62	43	17	2		
22	Y	1	Total	C	O	P	0	0
			40	21	17	2		
22	Y	1	Total	C	O	P	0	0
			13	5	7	1		

- Molecule 23 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	M	1	Total	C	O	0	0
			35	24	11		
23	F	1	Total	C	O	0	0
			35	24	11		

- Molecule 24 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	P	1	Total	Ca	0	0
			1	1		
24	G	1	Total	Ca	0	0
			1	1		
24	J	1	Total	Ca	0	0
			1	1		
24	E	1	Total	Ca	0	0
			1	1		
24	B	1	Total	Ca	0	0
			1	1		
24	V	1	Total	Ca	0	0
			1	1		
24	8	1	Total	Ca	0	0
			1	1		
24	Z	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	1	Total 1	Ca 1	0	0
24	T	1	Total 1	Ca 1	0	0
24	6	1	Total 1	Ca 1	0	0
24	N	1	Total 1	Ca 1	0	0
24	X	1	Total 1	Ca 1	0	0
24	4	1	Total 1	Ca 1	0	0
24	R	1	Total 1	Ca 1	0	0
24	2	1	Total 1	Ca 1	0	0

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	C	275	Total 277	O 277	0	2
25	L	108	Total 108	O 108	0	0
25	M	162	Total 162	O 162	0	0
25	H	158	Total 158	O 158	0	0
25	A	8	Total 8	O 8	0	0
25	B	5	Total 5	O 5	0	0
25	D	11	Total 11	O 11	0	0
25	E	5	Total 5	O 5	0	0
25	F	12	Total 12	O 12	0	0
25	G	2	Total 2	O 2	0	0
25	I	11	Total 11	O 11	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	J	4	Total 4	O 4	0	0
25	K	8	Total 8	O 8	0	0
25	N	3	Total 3	O 3	0	0
25	O	13	Total 13	O 13	0	0
25	P	7	Total 7	O 7	0	0
25	Q	18	Total 18	O 18	0	0
25	R	9	Total 9	O 9	0	0
25	S	12	Total 12	O 12	0	0
25	T	11	Total 11	O 11	0	0
25	U	15	Total 15	O 15	0	0
25	V	5	Total 5	O 5	0	0
25	W	11	Total 11	O 11	0	0
25	X	3	Total 3	O 3	0	0
25	Y	9	Total 9	O 9	0	0
25	Z	5	Total 5	O 5	0	0
25	1	3	Total 3	O 3	0	0
25	2	3	Total 3	O 3	0	0
25	3	6	Total 6	O 6	0	0
25	4	2	Total 2	O 2	0	0
25	5	10	Total 10	O 10	0	0
25	6	4	Total 4	O 4	0	0

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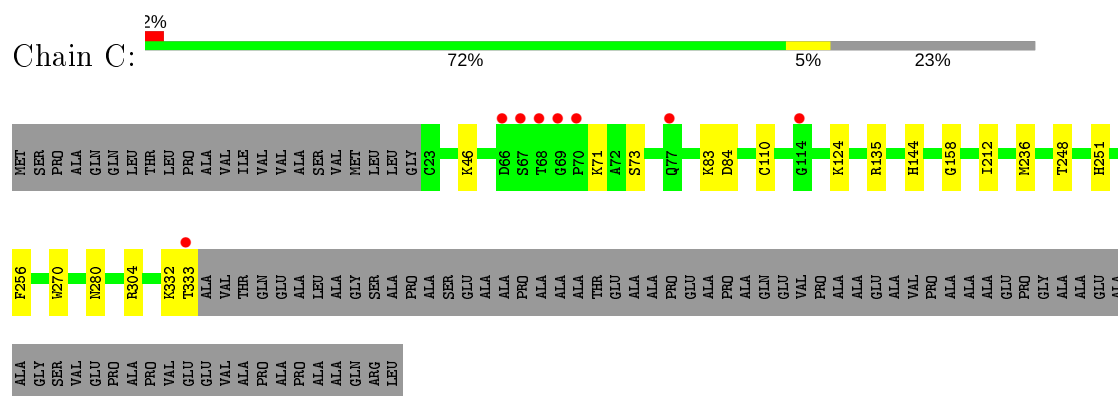
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	7	4	Total 4	O 4	0	0
25	8	11	Total 11	O 11	0	0
25	9	13	Total 13	O 13	0	0
25	0	8	Total 8	O 8	0	0

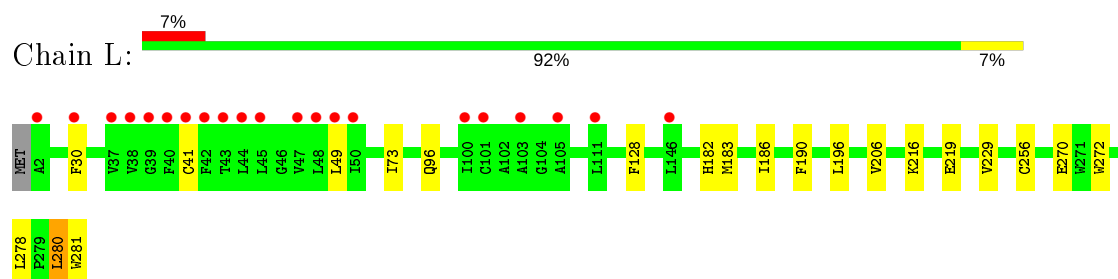
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

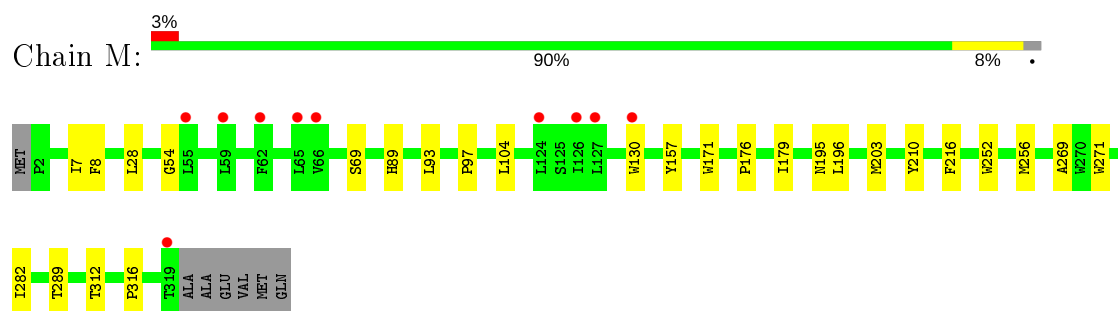
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



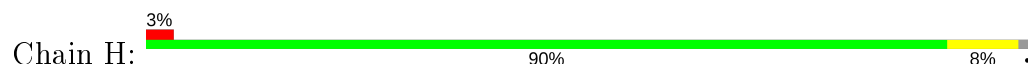
- Molecule 2: Photosynthetic reaction center L subunit

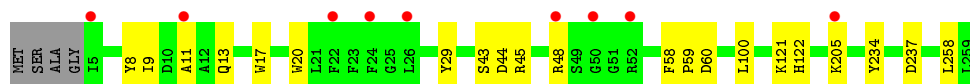


- Molecule 3: Photosynthetic reaction center M subunit

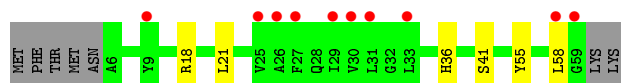
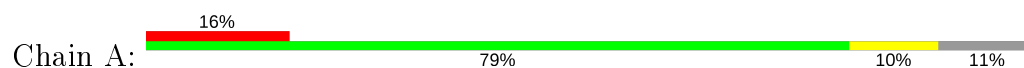


- Molecule 4: Photosynthetic reaction center H subunit

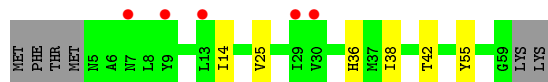
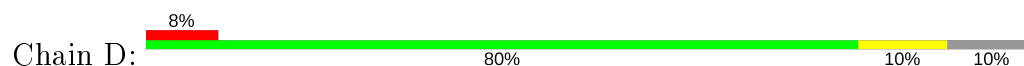




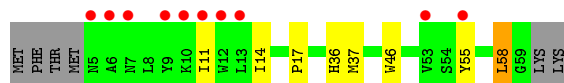
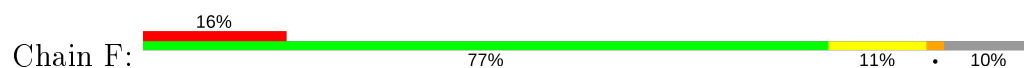
- Molecule 5: LH1 alpha polypeptide



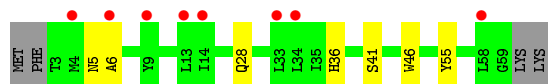
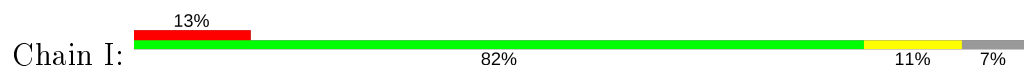
- Molecule 5: LH1 alpha polypeptide



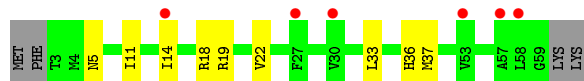
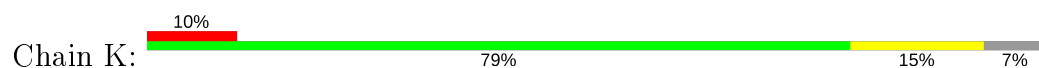
- Molecule 5: LH1 alpha polypeptide



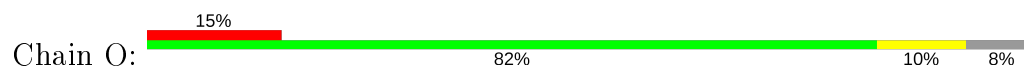
- Molecule 5: LH1 alpha polypeptide



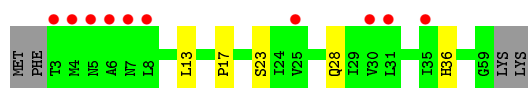
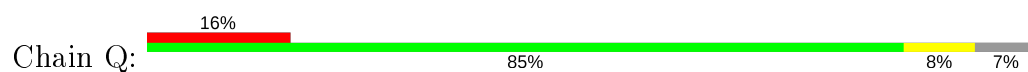
- Molecule 5: LH1 alpha polypeptide



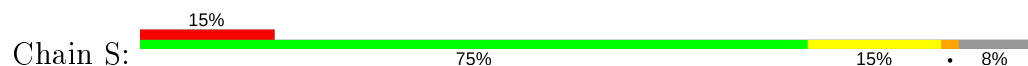
- Molecule 5: LH1 alpha polypeptide



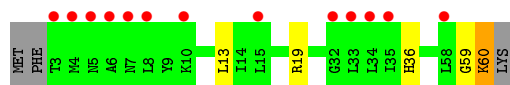
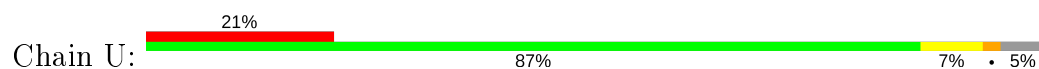
- Molecule 5: LH1 alpha polypeptide



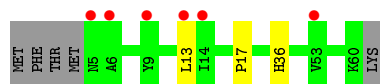
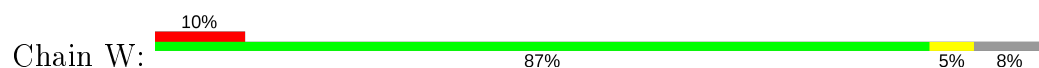
- Molecule 5: LH1 alpha polypeptide



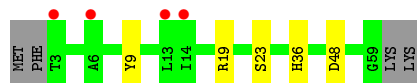
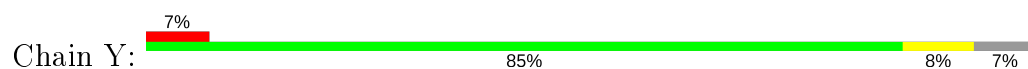
- Molecule 5: LH1 alpha polypeptide



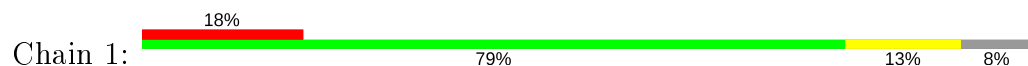
- Molecule 5: LH1 alpha polypeptide



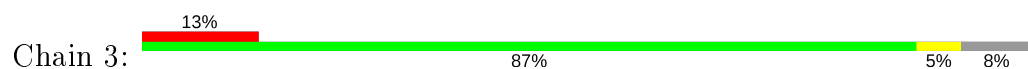
- Molecule 5: LH1 alpha polypeptide



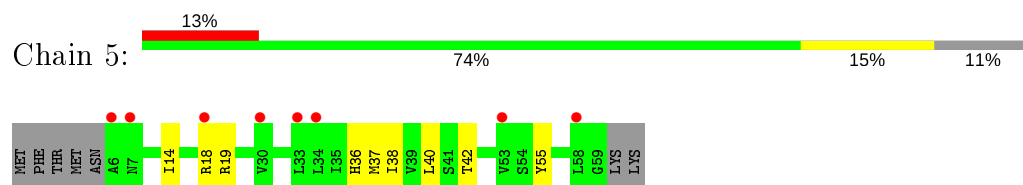
- Molecule 5: LH1 alpha polypeptide



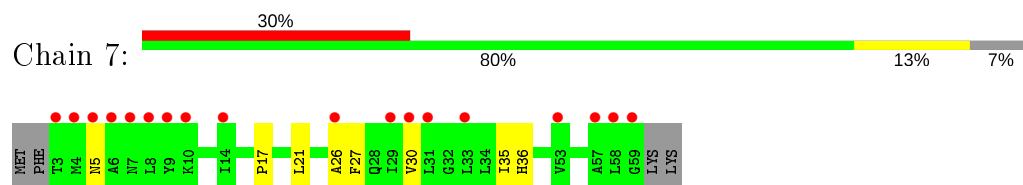
- Molecule 5: LH1 alpha polypeptide



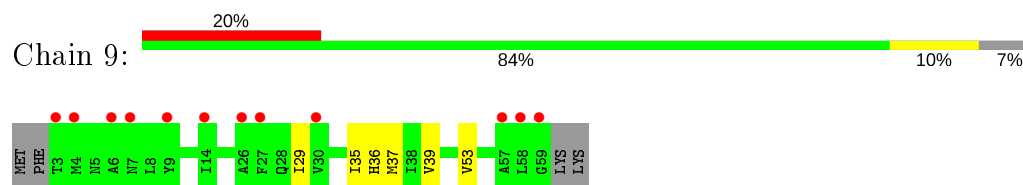
- Molecule 5: LH1 alpha polypeptide



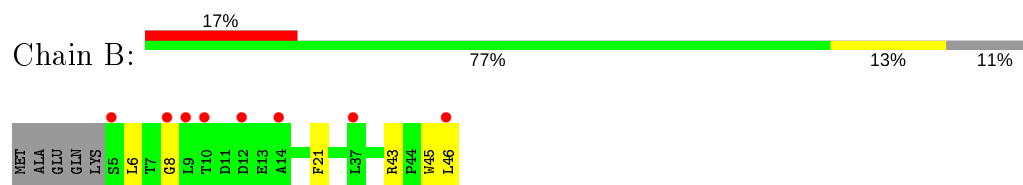
- Molecule 5: LH1 alpha polypeptide



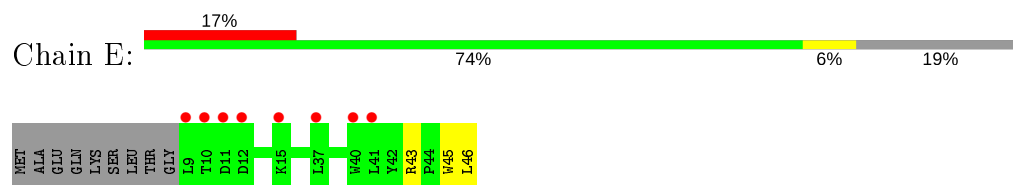
- Molecule 5: LH1 alpha polypeptide



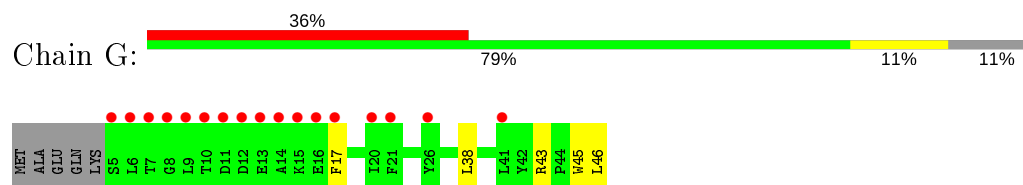
- Molecule 6: LH1 beta polypeptide



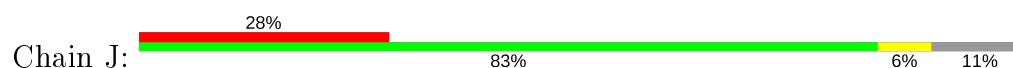
- Molecule 6: LH1 beta polypeptide

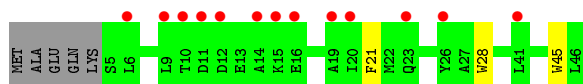


- Molecule 6: LH1 beta polypeptide

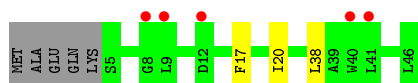
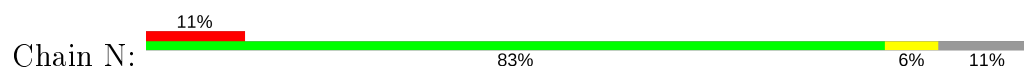


- Molecule 6: LH1 beta polypeptide

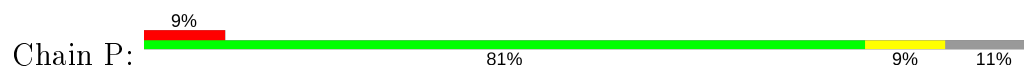




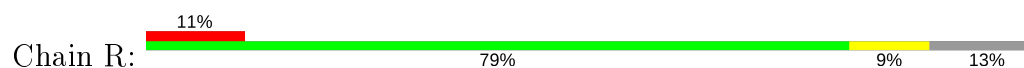
- Molecule 6: LH1 beta polypeptide



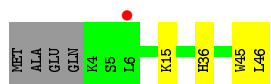
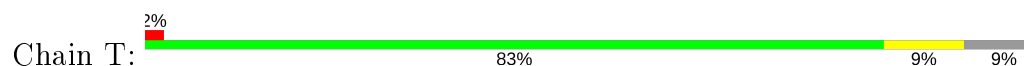
- Molecule 6: LH1 beta polypeptide



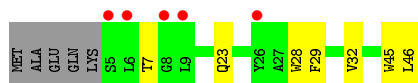
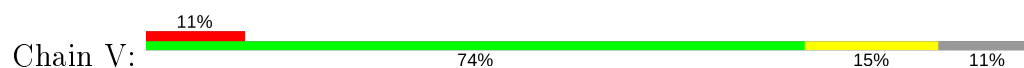
- Molecule 6: LH1 beta polypeptide



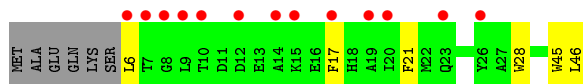
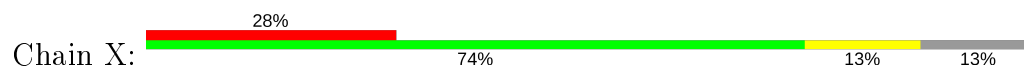
- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



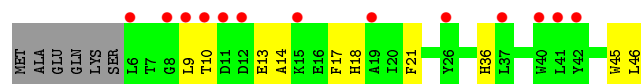
- Molecule 6: LH1 beta polypeptide



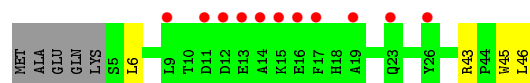
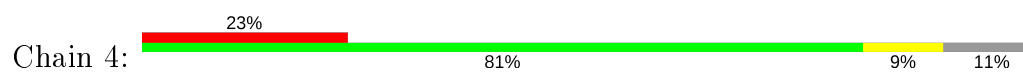
- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



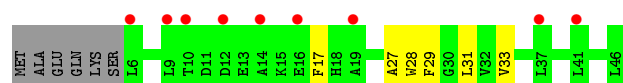
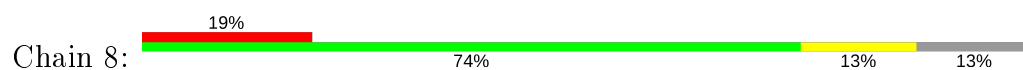
- Molecule 6: LH1 beta polypeptide



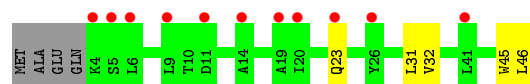
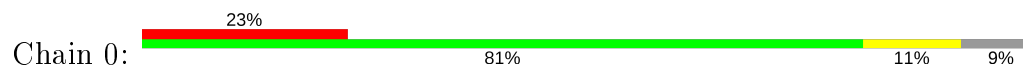
- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.28Å 143.81Å 210.28Å 90.00° 90.74° 90.00°	Depositor
Resolution (Å)	46.92 – 1.90 46.92 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.92-1.90) 91.8 (46.92-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.63 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.12rc0_2787	Depositor
R, R_{free}	0.181 , 0.215 0.181 , 0.215	Depositor DCC
R_{free} test set	16921 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 80.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l 0.019 for -k,-h,-l 0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	27981	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, LHG, LDA, CRT, GOL, CDL, BPH, CA, LMT, MG, PGV, UQ8, FE, HEC, MQ8, PEF, UNL, SO4

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	C	0.42	0/2487	0.55	0/3396
2	L	0.51	0/2326	0.55	0/3177
3	M	0.50	0/2658	0.56	0/3637
4	H	0.45	0/2034	0.57	0/2773
5	1	0.44	0/459	0.47	0/628
5	3	0.27	0/467	0.44	0/638
5	5	0.30	0/443	0.45	0/607
5	7	0.34	0/466	0.47	0/638
5	9	0.30	0/466	0.46	0/638
5	A	0.31	0/443	0.48	0/607
5	D	0.27	0/457	0.44	0/626
5	F	0.31	0/457	0.43	0/626
5	I	0.28	0/472	0.44	0/646
5	K	0.29	0/466	0.42	0/638
5	O	0.34	0/467	0.47	0/638
5	Q	0.44	0/466	0.53	0/638
5	S	0.41	0/483	0.51	0/661
5	U	0.34	0/475	0.49	0/649
5	W	0.30	0/460	0.46	0/629
5	Y	0.27	0/466	0.45	0/638
6	0	0.30	0/373	0.42	0/506
6	2	0.25	0/358	0.37	0/487
6	4	0.27	0/364	0.40	0/495
6	6	0.32	0/364	0.40	0/495
6	8	0.32	0/358	0.43	0/487
6	B	0.28	0/364	0.36	0/495
6	E	0.26	0/339	0.36	0/461
6	G	0.24	0/364	0.37	0/495
6	J	0.25	0/364	0.38	0/495
6	N	0.26	0/364	0.40	0/495
6	P	0.30	0/364	0.42	0/495

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	R	0.37	0/358	0.48	0/487
6	T	0.38	0/373	0.42	0/506
6	V	0.31	0/364	0.40	0/495
6	X	0.28	0/358	0.37	0/487
6	Z	0.25	0/350	0.40	0/476
All	All	0.39	0/22697	0.49	0/30985

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2417	0	2328	12	0
2	L	2236	0	2201	18	0
3	M	2555	0	2530	23	0
4	H	1976	0	1977	20	0
5	1	450	0	475	7	0
5	3	455	0	484	3	0
5	5	434	0	460	8	0
5	7	457	0	482	9	0
5	9	457	0	482	6	0
5	A	434	0	460	6	0
5	D	445	0	471	7	0
5	F	445	0	471	8	0
5	I	460	0	487	10	0
5	K	457	0	482	7	0
5	O	455	0	484	4	0
5	Q	457	0	482	6	0
5	S	468	0	501	11	0
5	U	466	0	495	5	0
5	W	451	0	479	3	0
5	Y	457	0	480	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	0	360	0	352	4	0
6	2	345	0	334	19	0
6	4	351	0	339	3	0
6	6	351	0	339	8	0
6	8	345	0	334	4	0
6	B	351	0	339	7	0
6	E	326	0	313	2	0
6	G	351	0	339	6	0
6	J	351	0	339	3	0
6	N	351	0	339	4	0
6	P	351	0	339	4	0
6	R	345	0	334	4	0
6	T	360	0	352	3	0
6	V	351	0	339	8	0
6	X	345	0	334	5	0
6	Z	337	0	323	7	0
7	C	172	0	120	3	0
8	C	1	0	0	0	0
9	C	6	0	8	0	0
9	H	6	0	8	1	0
10	C	5	0	0	0	0
10	L	5	0	0	0	0
10	M	5	0	0	0	0
11	C	9	0	12	0	0
12	1	31	0	32	0	0
12	3	51	0	76	3	0
12	A	33	0	36	5	0
12	C	21	0	23	0	0
12	D	35	0	40	2	0
12	H	36	0	42	1	0
12	L	87	0	120	8	0
12	M	83	0	116	7	0
13	0	66	0	72	8	0
13	1	132	0	144	12	0
13	3	132	0	144	8	0
13	5	132	0	144	14	0
13	7	127	0	131	8	0
13	9	66	0	72	4	0
13	A	132	0	144	8	0
13	D	132	0	144	6	0
13	F	132	0	144	5	0
13	I	132	0	144	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	K	132	0	144	5	0
13	L	66	0	72	4	0
13	M	198	0	216	9	0
13	O	132	0	144	8	0
13	Q	132	0	144	10	0
13	S	132	0	144	11	0
13	U	132	0	144	12	0
13	W	132	0	144	7	0
13	Y	66	0	72	5	0
13	Z	66	0	72	7	0
14	L	65	0	74	6	0
14	M	65	0	74	6	0
15	7	33	0	39	8	0
15	L	104	0	128	10	0
15	M	18	0	15	3	0
16	0	12	0	0	0	0
16	2	12	0	0	0	0
16	4	12	0	0	0	0
16	6	12	0	0	0	0
16	8	12	0	0	0	0
16	B	12	0	0	0	0
16	E	12	0	0	0	0
16	G	12	0	0	0	0
16	J	12	0	0	0	0
16	L	12	0	0	0	0
16	M	9	0	0	0	0
16	P	12	0	0	0	0
16	R	12	0	0	0	0
16	T	12	0	0	0	0
16	X	12	0	0	0	0
16	Z	12	0	0	0	0
17	L	1	0	0	0	0
18	M	53	0	72	5	0
19	0	44	0	60	2	0
19	1	44	0	60	3	0
19	2	44	0	60	6	0
19	6	44	0	60	2	0
19	9	88	0	120	6	0
19	A	44	0	60	3	0
19	G	44	0	60	5	0
19	J	44	0	60	3	0
19	M	44	0	60	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	N	44	0	60	4	0
19	O	44	0	60	2	0
19	P	44	0	60	2	0
19	Q	44	0	60	2	0
19	U	44	0	60	2	0
19	V	44	0	60	1	0
19	Z	44	0	60	3	0
20	1	5	0	0	0	0
20	3	5	0	0	0	0
20	5	5	0	0	1	0
20	I	5	0	0	1	0
20	K	27	0	27	1	0
20	M	67	0	73	3	0
20	U	10	0	0	0	0
20	W	5	0	0	0	0
21	I	16	0	31	6	0
21	J	16	0	31	1	0
21	M	14	0	24	1	0
21	O	14	0	24	1	0
21	V	16	0	31	0	0
22	D	40	0	24	2	0
22	H	143	0	177	6	0
22	K	86	0	119	4	0
22	M	39	0	28	1	0
22	Q	75	0	94	3	0
22	S	62	0	68	10	0
22	Y	53	0	31	1	0
23	F	35	0	46	5	0
23	M	35	0	46	3	0
24	2	1	0	0	0	0
24	4	1	0	0	0	0
24	6	1	0	0	0	0
24	8	1	0	0	0	0
24	A	1	0	0	0	0
24	B	1	0	0	0	0
24	E	1	0	0	0	0
24	G	1	0	0	0	0
24	J	1	0	0	0	0
24	N	1	0	0	0	0
24	P	1	0	0	0	0
24	R	1	0	0	0	0
24	T	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	V	1	0	0	0	0
24	X	1	0	0	0	0
24	Z	1	0	0	0	0
25	0	8	0	0	0	0
25	1	3	0	0	0	0
25	2	3	0	0	0	0
25	3	6	0	0	0	0
25	4	2	0	0	0	0
25	5	10	0	0	0	0
25	6	4	0	0	0	0
25	7	4	0	0	0	0
25	8	11	0	0	0	0
25	9	13	0	0	0	0
25	A	8	0	0	0	0
25	B	5	0	0	0	0
25	C	277	0	0	1	0
25	D	11	0	0	0	0
25	E	5	0	0	0	0
25	F	12	0	0	0	0
25	G	2	0	0	0	0
25	H	158	0	0	1	1
25	I	11	0	0	0	0
25	J	4	0	0	0	0
25	K	8	0	0	0	0
25	L	108	0	0	1	0
25	M	162	0	0	2	0
25	N	3	0	0	0	0
25	O	13	0	0	0	0
25	P	7	0	0	0	0
25	Q	18	0	0	0	0
25	R	9	0	0	0	0
25	S	12	0	0	0	1
25	T	11	0	0	0	0
25	U	15	0	0	1	0
25	V	5	0	0	0	0
25	W	11	0	0	0	0
25	X	3	0	0	0	0
25	Y	9	0	0	0	0
25	Z	5	0	0	0	0
All	All	27981	0	27607	386	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (386) 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)
5:S:19:ARG:CZ	22:S:103:CDL:OA4	1.88	1.20
6:2:9:LEU:HD21	6:2:14:ALA:N	1.54	1.19
22:S:103:CDL:C19	13:U:101:BCL:H51	1.83	1.08
5:S:19:ARG:NH1	22:S:103:CDL:OA4	1.91	1.03
6:2:9:LEU:CD2	6:2:14:ALA:N	2.23	1.00
6:2:9:LEU:HD22	6:2:14:ALA:HB2	1.50	0.92
6:2:9:LEU:HD21	6:2:13:GLU:C	1.96	0.86
14:L:302:BPH:HHC	14:L:302:BPH:HBB3	1.62	0.81
4:H:48:ARG:HG2	6:B:8:GLY:HA3	1.63	0.80
2:L:96:GLN:HG2	15:L:308:UQ8:H4M	1.63	0.79
4:H:11:ALA:H	21:I:104:LDA:HM21	1.46	0.79
23:M:419:LMT:H42	21:I:104:LDA:H42	1.65	0.78
19:1:103:CRT:H371	13:5:101:BCL:HMB2	1.64	0.78
6:2:9:LEU:HD23	6:2:10:THR:O	1.84	0.76
14:M:404:BPH:HHC	14:M:404:BPH:HBB3	1.69	0.75
22:S:103:CDL:C19	13:U:101:BCL:C5	2.65	0.74
13:D:102:BCL:H202	6:G:38:LEU:HD13	1.70	0.74
6:2:9:LEU:CD2	6:2:14:ALA:H	2.01	0.72
5:F:58:LEU:N	5:F:58:LEU:HD23	2.05	0.70
5:U:36:HIS:CE1	13:U:102:BCL:HMD1	2.28	0.69
19:U:103:CRT:H371	13:Y:101:BCL:HMB2	1.74	0.68
13:1:102:BCL:HMB2	13:1:102:BCL:H72	1.75	0.68
6:2:9:LEU:HD22	6:2:14:ALA:CB	2.24	0.67
5:D:36:HIS:CE1	13:D:102:BCL:HMD1	2.30	0.67
2:L:190:PHE:HB3	14:M:404:BPH:HBB2	1.76	0.67
5:W:36:HIS:CE1	13:W:102:BCL:HMD1	2.29	0.67
22:Q:104:CDL:H142	22:Q:104:CDL:H362	1.76	0.66
4:H:121:LYS:HD2	4:H:234:TYR:HB3	1.78	0.66
15:M:417:UQ8:H1MA	22:S:103:CDL:C43	2.26	0.66
19:6:101:CRT:H371	13:7:101:BCL:HMB2	1.78	0.65
5:K:36:HIS:CE1	13:K:102:BCL:HMD1	2.31	0.65
13:0:102:BCL:H72	13:0:102:BCL:HMB2	1.77	0.65
5:7:36:HIS:CE1	13:7:102:BCL:HMD1	2.31	0.64
19:J:101:CRT:H371	13:K:101:BCL:HMB2	1.78	0.64
5:1:36:HIS:CE1	13:1:102:BCL:HMD1	2.32	0.64
13:Q:102:BCL:H51	13:S:101:BCL:H18	1.79	0.64
5:F:36:HIS:CE1	13:F:102:BCL:HMD1	2.33	0.64
15:L:309:UQ8:H3M	13:M:402:BCL:H161	1.80	0.64
5:Q:36:HIS:CE1	13:Q:102:BCL:HMD1	2.33	0.64
5:O:36:HIS:CE1	13:O:102:BCL:HMD1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:5:101:BCL:H172	6:6:31:LEU:HD21	1.80	0.63
5:9:36:HIS:CE1	13:0:102:BCL:HMD1	2.33	0.63
2:L:206:VAL:HB	2:L:216:LYS:HB2	1.81	0.63
5:I:36:HIS:CE1	13:I:102:BCL:HMD1	2.34	0.62
3:M:256:MET:HE1	18:M:405:MQ8:H142	1.80	0.62
5:A:18:ARG:HH22	12:A:105:PGV:H041	1.64	0.62
5:Y:23:SER:HB3	13:1:101:BCL:H172	1.80	0.62
5:3:14:ILE:HG22	6:4:6:LEU:HD23	1.81	0.61
5:5:36:HIS:CE1	13:5:102:BCL:HMD1	2.36	0.60
19:V:101:CRT:H371	13:W:101:BCL:HMB2	1.83	0.60
5:Y:36:HIS:CE1	13:Z:102:BCL:HMD1	2.36	0.60
14:L:302:BPH:HHC	14:L:302:BPH:CBB	2.30	0.60
5:3:36:HIS:CE1	13:3:102:BCL:HMD1	2.37	0.59
5:D:14:ILE:HD11	19:G:101:CRT:H23	1.84	0.59
4:H:258:LEU:O	5:5:19:ARG:HD2	2.01	0.59
6:Z:17:PHE:HA	19:Z:101:CRT:H6	1.84	0.59
13:Q:101:BCL:H43	6:R:28:TRP:CZ2	2.37	0.59
18:M:405:MQ8:H241	22:H:304:CDL:H772	1.84	0.59
22:H:302:CDL:H551	22:H:302:CDL:H751	1.84	0.59
19:Q:103:CRT:H371	13:U:101:BCL:HMB2	1.84	0.59
5:A:36:HIS:CE1	13:A:103:BCL:HMD1	2.38	0.58
13:K:102:BCL:H101	13:K:102:BCL:HMB2	1.85	0.58
6:2:9:LEU:CD2	6:2:13:GLU:HB2	2.33	0.58
14:M:404:BPH:HHH	14:M:404:BPH:HBC3	1.85	0.58
5:S:36:HIS:CE1	13:S:102:BCL:HMD1	2.38	0.58
21:M:411:LDA:H41	21:O:104:LDA:H71	1.85	0.58
4:H:9:ILE:HA	4:H:13:GLN:OE1	2.04	0.58
6:0:32:VAL:HG12	13:0:102:BCL:H92	1.86	0.58
22:S:103:CDL:OB4	5:U:19:ARG:NH2	2.37	0.57
4:H:44:ASP:H	12:A:105:PGV:H062	1.68	0.57
5:7:26:ALA:HB3	15:7:103:UQ8:C4M	2.34	0.57
1:C:46:LYS:HD3	12:3:104:PGV:H062	1.87	0.57
6:B:43:ARG:HG3	5:D:55:TYR:CZ	2.40	0.57
6:E:45:TRP:CD1	6:E:46:LEU:HG	2.40	0.57
5:Q:28:GLN:HB3	13:Q:101:BCL:H42	1.88	0.56
19:A:104:CRT:H371	13:F:101:BCL:HMB2	1.88	0.56
5:K:18:ARG:O	5:K:22:VAL:HG12	2.06	0.56
13:W:101:BCL:HED3	13:W:101:BCL:H172	1.88	0.55
12:L:305:PGV:H81	12:D:104:PGV:H81	1.88	0.55
5:F:11:ILE:HD12	5:F:14:ILE:HD11	1.87	0.55
2:L:278:LEU:HB3	2:L:280:LEU:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:69[A]:SER:OG	15:M:417:UQ8:H8	2.06	0.55
19:N:101:CRT:H371	13:O:101:BCL:HMB2	1.88	0.54
1:C:135:ARG:HB3	1:C:332:LYS:HG3	1.88	0.54
6:E:43:ARG:HG3	5:F:55:TYR:CZ	2.43	0.54
5:7:27:PHE:N	15:7:103:UQ8:H4MA	2.22	0.54
4:H:60:ASP:HB2	22:D:103:CDL:HB22	1.89	0.53
5:1:39:VAL:HG21	13:1:102:BCL:HHD	1.90	0.53
6:2:9:LEU:CD2	6:2:14:ALA:CA	2.86	0.53
19:2:101:CRT:H35	13:3:101:BCL:HMB2	1.91	0.53
2:L:183:MET:HE3	2:L:272:TRP:HZ2	1.74	0.53
6:V:45:TRP:CD1	6:V:46:LEU:HG	2.44	0.53
5:A:55:TYR:HA	5:A:58:LEU:HD13	1.90	0.52
5:7:5:ASN:ND2	6:0:23:GLN:OE1	2.38	0.52
3:M:256:MET:CE	18:M:405:MQ8:H142	2.39	0.52
13:Z:102:BCL:H142	13:Z:102:BCL:H102	1.91	0.52
6:G:17:PHE:HB2	19:G:101:CRT:H21A	1.92	0.52
5:I:41[A]:SER:HB2	21:I:104:LDA:H11	1.90	0.52
5:Q:28:GLN:CB	13:Q:101:BCL:H42	2.40	0.52
13:D:102:BCL:HMB2	13:D:102:BCL:H72	1.92	0.52
5:A:18:ARG:NH1	12:A:105:PGV:H012	2.25	0.52
5:I:41[B]:SER:HB3	21:I:104:LDA:H11	1.90	0.51
13:O:102:BCL:H121	6:P:45:TRP:HZ2	1.74	0.51
13:Y:101:BCL:HED3	13:Y:101:BCL:H172	1.92	0.51
12:M:414:PGV:H05	5:S:19:ARG:NH2	2.25	0.51
3:M:271:TRP:HZ2	20:M:418:PEF:H112	1.76	0.51
6:N:17:PHE:HA	19:N:101:CRT:H6	1.92	0.51
6:2:9:LEU:HD21	6:2:14:ALA:CA	2.38	0.51
6:G:17:PHE:HA	19:G:101:CRT:H6	1.93	0.51
13:S:102:BCL:H42	13:U:101:BCL:H151	1.91	0.51
13:5:101:BCL:H143	13:5:101:BCL:HBA1	1.93	0.51
2:L:128:PHE:CE2	12:M:413:PGV:H51	2.45	0.51
1:C:144:HIS:HE1	7:C:504:HEC:NC	2.05	0.51
5:S:5:ASN:ND2	6:V:23:GLN:OE1	2.44	0.51
5:7:17:PRO:HB3	6:8:17:PHE:CE2	2.47	0.50
1:C:158:GLY:O	25:C:601:HOH:O	2.19	0.50
13:I:101:BCL:H43	6:J:28:TRP:CZ2	2.46	0.50
2:L:186:ILE:HG12	13:L:301:BCL:HMB3	1.93	0.50
5:K:5:ASN:ND2	6:P:23:GLN:OE1	2.38	0.50
6:X:45:TRP:CD1	6:X:46:LEU:HG	2.46	0.50
3:M:28:LEU:HD12	3:M:54:GLY:HA2	1.93	0.50
3:M:312:THR:O	25:M:501:HOH:O	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:289:THR:HB	23:M:419:LMT:H12	1.93	0.50
6:2:17:PHE:HA	19:2:101:CRT:H6	1.94	0.49
5:F:46:TRP:CE3	13:F:101:BCL:HAC2	2.47	0.49
2:L:270:GLU:OE2	25:L:401:HOH:O	2.20	0.49
14:L:302:BPH:HBB2	3:M:210:TYR:HB3	1.93	0.49
12:3:104:PGV:H211	5:5:40:LEU:HB3	1.95	0.49
19:O:103:CRT:H292	13:S:101:BCL:H111	1.94	0.49
5:3:5:ASN:ND2	6:6:23:GLN:OE1	2.42	0.49
5:9:29:ILE:HD11	13:9:103:BCL:H203	1.94	0.49
1:C:73:SER:HB2	1:C:83:LYS:HB3	1.94	0.49
2:L:190:PHE:HB3	14:M:404:BPH:CBB	2.42	0.49
19:G:101:CRT:H371	13:I:101:BCL:HMB2	1.95	0.48
6:Z:45:TRP:CD1	6:Z:46:LEU:HG	2.47	0.48
2:L:41:CYS:SG	15:7:103:UQ8:H1M	2.53	0.48
4:H:17:TRP:CD1	23:F:103:LMT:H61	2.48	0.48
2:L:196:LEU:HD11	3:M:269:ALA:HB1	1.94	0.48
3:M:130:TRP:HZ3	22:K:103:CDL:H511	1.78	0.48
5:S:21:LEU:O	5:S:25:VAL:HG13	2.13	0.48
22:S:103:CDL:C51	22:S:103:CDL:H721	2.43	0.48
13:5:101:BCL:H8	13:5:101:BCL:H51	1.58	0.48
19:M:406:CRT:H2M3	5:O:38:ILE:HA	1.94	0.48
5:U:13:LEU:O	6:V:7:THR:HG23	2.14	0.48
5:7:26:ALA:HB3	15:7:103:UQ8:H4M	1.96	0.48
3:M:282:ILE:HG12	23:M:419:LMT:H101	1.96	0.48
4:H:20:TRP:NE1	12:H:303:PGV:H202	2.28	0.47
13:Y:101:BCL:H43	6:Z:28:TRP:CZ2	2.49	0.47
13:1:102:BCL:HMA3	13:3:101:BCL:HMB3	1.96	0.47
13:O:102:BCL:H93	13:O:102:BCL:H61	1.65	0.47
5:5:18:ARG:NH1	20:5:103:PEF:O2P	2.42	0.47
13:A:103:BCL:HAC2	6:B:45:TRP:CE3	2.49	0.47
6:Z:45:TRP:CE3	13:Z:102:BCL:HAC2	2.49	0.47
5:1:8:LEU:HD12	6:2:18:HIS:CE1	2.49	0.47
14:L:302:BPH:HBB1	3:M:210:TYR:CD2	2.50	0.47
3:M:252:TRP:CE3	3:M:256:MET:HE2	2.50	0.47
3:M:7:ILE:HD12	12:M:413:PGV:H92	1.95	0.47
13:M:402:BCL:HBB2	13:M:402:BCL:HMB1	1.97	0.47
15:L:308:UQ8:H46A	6:6:21:PHE:CE1	2.50	0.47
13:D:101:BCL:H202	13:D:101:BCL:H162	1.79	0.47
6:4:43:ARG:HG3	5:5:55:TYR:CZ	2.49	0.47
13:5:102:BCL:H13	6:6:45:TRP:HZ2	1.79	0.47
20:M:418:PEF:H111	4:H:29:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:46:TRP:CE3	13:1:101:BCL:HAC2	2.50	0.47
13:9:103:BCL:H72	13:9:103:BCL:H111	1.51	0.47
12:L:306:PGV:C11	15:L:308:UQ8:H26A	2.45	0.47
13:Z:102:BCL:H72	13:Z:102:BCL:HMB2	1.96	0.47
15:7:103:UQ8:H13	15:7:103:UQ8:H17	1.70	0.47
6:2:9:LEU:HD23	6:2:13:GLU:HB2	1.96	0.46
1:C:71:LYS:NZ	1:C:84:ASP:O	2.44	0.46
5:F:37:MET:HB3	23:F:103:LMT:H42	1.97	0.46
13:Y:101:BCL:H112	13:Y:101:BCL:H91	1.65	0.46
5:5:38:ILE:O	5:5:42:THR:HG23	2.15	0.46
14:M:404:BPH:CHC	14:M:404:BPH:HBB3	2.43	0.46
13:W:101:BCL:HED1	6:X:28:TRP:CZ3	2.50	0.46
6:Z:29:PHE:CE1	13:Z:102:BCL:H2	2.50	0.46
6:B:45:TRP:CD1	6:B:46:LEU:HG	2.50	0.46
13:M:403:BCL:HAA2	13:M:403:BCL:HBD	1.96	0.46
5:I:5:ASN:ND2	6:N:20:ILE:HA	2.30	0.46
1:C:270:TRP:CG	3:M:316:PRO:HG2	2.51	0.46
12:3:104:PGV:H251	5:5:37:MET:HG3	1.98	0.46
21:J:102:LDA:H81	6:N:38:LEU:HB3	1.97	0.46
13:9:103:BCL:HHC	13:9:103:BCL:OBB	2.15	0.46
19:P:101:CRT:H371	13:Q:101:BCL:HMB2	1.96	0.46
5:I:28:GLN:CB	13:I:101:BCL:H42	2.46	0.46
13:K:101:BCL:H8	13:K:101:BCL:H51	1.66	0.46
13:3:102:BCL:H71	13:3:102:BCL:HMB2	1.98	0.46
5:K:33:LEU:O	5:K:37:MET:HG3	2.16	0.46
19:Z:101:CRT:H371	13:1:101:BCL:HMB2	1.97	0.46
19:1:103:CRT:H10	19:1:103:CRT:H81	1.85	0.46
22:D:103:CDL:O1	22:D:103:CDL:OA7	2.33	0.46
13:S:102:BCL:H41	13:U:101:BCL:H203	1.97	0.46
13:W:101:BCL:H141	13:W:101:BCL:H161	1.73	0.46
5:7:30:VAL:HG12	15:7:103:UQ8:H13	1.98	0.45
12:D:104:PGV:H05	23:F:103:LMT:H2B	1.97	0.45
12:M:414:PGV:H05	5:S:19:ARG:HH22	1.80	0.45
13:Q:102:BCL:H91	6:R:36:HIS:CG	2.51	0.45
13:1:102:BCL:C2B	13:1:102:BCL:H101	2.46	0.45
15:7:103:UQ8:H7A	15:7:103:UQ8:H10	1.62	0.45
2:L:219:GLU:OE1	2:L:219:GLU:N	2.46	0.45
22:Q:104:CDL:H171	22:Q:104:CDL:H131	1.98	0.45
6:2:10:THR:OG1	6:2:13:GLU:HG3	2.16	0.45
13:F:102:BCL:H112	13:F:102:BCL:H152	1.53	0.45
5:S:16:ASP:HB2	5:S:19:ARG:HH11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:5:101:BCL:H43	6:6:28:TRP:CZ2	2.51	0.45
5:U:60:LYS:NZ	25:U:201:HOH:O	2.40	0.45
6:2:45:TRP:CD1	6:2:46:LEU:HG	2.52	0.45
5:1:38:ILE:O	5:1:42:THR:HG23	2.17	0.45
13:A:101:BCL:H18	13:0:102:BCL:H51	1.99	0.45
6:T:45:TRP:CD1	6:T:46:LEU:HG	2.52	0.45
13:3:102:BCL:H42	13:5:101:BCL:H151	1.99	0.45
4:H:45:ARG:NH2	6:B:6:LEU:O	2.49	0.45
15:L:308:UQ8:H25	15:L:308:UQ8:H22	1.73	0.45
20:I:103:PEF:O3P	5:K:18:ARG:NH1	2.50	0.45
5:Q:23:SER:HB2	22:Q:104:CDL:H132	1.99	0.45
13:W:101:BCL:H41	13:W:101:BCL:H62	1.72	0.45
15:7:103:UQ8:H12	15:7:103:UQ8:H15	1.71	0.44
6:6:17:PHE:HA	19:6:101:CRT:H6	1.98	0.44
13:7:101:BCL:H43	6:8:28:TRP:CZ2	2.52	0.44
13:7:102:BCL:HMB2	13:7:102:BCL:H101	1.99	0.44
19:9:101:CRT:H20	19:9:101:CRT:H181	1.89	0.44
4:H:17:TRP:CG	23:F:103:LMT:H61	2.52	0.44
22:H:302:CDL:H521	5:D:25:VAL:HG11	1.99	0.44
2:L:182:HIS:CE1	2:L:186:ILE:HD11	2.52	0.44
13:L:301:BCL:HBB3	13:L:301:BCL:HMB1	2.00	0.44
13:S:101:BCL:H13	13:S:101:BCL:H102	1.65	0.44
5:5:14:ILE:HG22	6:6:6:LEU:HD12	2.00	0.44
19:J:101:CRT:H20	19:J:101:CRT:H181	1.81	0.44
5:9:35:ILE:O	5:9:39:VAL:HG23	2.17	0.44
13:I:102:BCL:HAC2	6:J:45:TRP:CE3	2.52	0.44
22:K:103:CDL:H521	22:K:103:CDL:H362	1.99	0.44
13:A:101:BCL:H102	13:A:101:BCL:H13	1.80	0.44
13:A:103:BCL:H152	13:A:103:BCL:H112	1.66	0.44
5:A:21:LEU:HA	5:A:21:LEU:HD12	1.83	0.44
3:M:157:TYR:CZ	19:M:406:CRT:H293	2.53	0.44
14:L:302:BPH:H202	13:M:401:BCL:C2B	2.47	0.44
5:S:9:TYR:CE1	6:T:15:LYS:HG3	2.52	0.44
5:1:10:LYS:HD3	19:1:103:CRT:H31A	1.99	0.44
5:I:46:TRP:CD2	13:I:101:BCL:HAC2	2.53	0.44
13:L:301:BCL:CGA	13:M:401:BCL:HBC1	2.48	0.44
6:0:45:TRP:CD1	6:0:46:LEU:HG	2.53	0.44
5:K:19:ARG:HD3	22:K:103:CDL:OA5	2.17	0.44
19:Z:101:CRT:H181	19:Z:101:CRT:H20	1.86	0.44
1:C:248:THR:HA	1:C:251:HIS:O	2.17	0.43
19:Q:103:CRT:H81	19:Q:103:CRT:H10	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:102:BCL:H102	6:2:36:HIS:CD2	2.53	0.43
6:4:45:TRP:CD1	6:4:46:LEU:HG	2.53	0.43
21:I:104:LDA:H61	20:K:104:PEF:H311	2.00	0.43
19:G:101:CRT:H372	5:I:36:HIS:CG	2.54	0.43
15:L:303:UQ8:H22A	15:L:303:UQ8:H20A	1.85	0.43
15:L:308:UQ8:H30	15:L:308:UQ8:H27	1.72	0.43
3:M:104:LEU:HA	3:M:171:TRP:CD1	2.53	0.43
2:L:190:PHE:CD2	14:M:404:BPH:HBB1	2.53	0.43
12:M:413:PGV:H281	12:M:413:PGV:H312	1.81	0.43
13:S:102:BCL:H93	13:S:102:BCL:H61	1.69	0.43
5:9:36:HIS:CG	19:9:102:CRT:H372	2.54	0.43
1:C:280:ASN:OD1	1:C:304:ARG:HB2	2.19	0.43
5:F:58:LEU:H	5:F:58:LEU:HD23	1.78	0.43
5:S:38:ILE:O	5:S:42:THR:HG23	2.18	0.43
13:5:101:BCL:H62	13:5:101:BCL:H41	1.79	0.43
5:D:38:ILE:O	5:D:42:THR:HG23	2.19	0.43
6:G:43:ARG:HG3	5:I:55:TYR:CZ	2.53	0.43
13:5:101:BCL:H202	13:5:101:BCL:H162	1.80	0.43
19:A:104:CRT:H181	19:A:104:CRT:H20	1.89	0.43
3:M:203:MET:HB3	13:M:401:BCL:O1D	2.18	0.43
18:M:405:MQ8:H412	18:M:405:MQ8:H441	1.78	0.43
13:1:101:BCL:H111	13:1:101:BCL:H142	1.73	0.43
5:D:36:HIS:CG	19:9:101:CRT:H372	2.54	0.43
13:U:102:BCL:H141	6:V:45:TRP:HZ2	1.84	0.43
13:0:102:BCL:H161	13:0:102:BCL:H122	1.93	0.43
1:C:236:MET:HB3	7:C:503:HEC:C4B	2.48	0.43
15:L:308:UQ8:H42A	15:L:308:UQ8:H40A	1.91	0.43
13:K:102:BCL:O1A	19:N:101:CRT:H27	2.18	0.43
13:A:103:BCL:HHC	13:A:103:BCL:OB	2.19	0.43
13:L:301:BCL:HAA2	13:M:401:BCL:HAC2	2.01	0.43
13:1:102:BCL:H12	13:1:102:BCL:H52	1.77	0.42
5:F:17:PRO:HB3	6:G:17:PHE:CZ	2.54	0.42
4:H:205:LYS:HA	4:H:205:LYS:HD2	1.80	0.42
5:I:5:ASN:OD1	5:I:6:ALA:N	2.52	0.42
2:L:229:VAL:O	12:M:414:PGV:H261	2.19	0.42
15:M:417:UQ8:C1M	22:S:103:CDL:C43	2.94	0.42
13:S:101:BCL:HMD1	6:T:36:HIS:CE1	2.54	0.42
6:0:45:TRP:CE3	13:0:102:BCL:HAC2	2.54	0.42
6:8:27:ALA:O	6:8:31:LEU:HD13	2.19	0.42
5:K:11:ILE:HD12	5:K:14:ILE:HD12	2.01	0.42
12:L:306:PGV:H52	12:L:306:PGV:H81	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:271:TRP:CZ2	20:M:418:PEF:H112	2.53	0.42
5:Q:17:PRO:HB3	6:R:17:PHE:CZ	2.54	0.42
5:Q:13:LEU:O	6:R:6:LEU:HA	2.19	0.42
6:2:9:LEU:HD22	6:2:14:ALA:CA	2.49	0.42
13:M:401:BCL:H13	13:M:401:BCL:H172	1.89	0.42
13:5:101:BCL:H141	13:5:101:BCL:H161	1.67	0.42
13:A:101:BCL:H41	13:A:101:BCL:H62	1.69	0.42
4:H:8:TYR:CE1	23:F:103:LMT:H5B	2.55	0.42
6:B:21:PHE:HA	19:9:101:CRT:H14	2.00	0.42
13:F:102:BCL:HHC	13:F:102:BCL:OBB	2.20	0.42
22:H:304:CDL:H862	22:H:304:CDL:H592	2.00	0.42
15:L:303:UQ8:H25	15:L:303:UQ8:H22	1.74	0.42
3:M:8:PHE:CE2	22:M:415:CDL:H312	2.55	0.42
6:P:17:PHE:HA	19:P:101:CRT:H6	2.01	0.42
13:Q:101:BCL:H162	13:Q:101:BCL:H203	1.78	0.42
12:L:305:PGV:O06	5:A:41:SER:O	2.37	0.42
5:W:17:PRO:HB3	6:X:17:PHE:CZ	2.55	0.42
13:5:102:BCL:H192	13:5:102:BCL:H162	1.76	0.42
4:H:121:LYS:HD2	4:H:234:TYR:CB	2.46	0.42
13:U:101:BCL:H61	13:U:101:BCL:H92	1.87	0.42
13:D:101:BCL:H62	13:D:101:BCL:H41	1.90	0.42
4:H:100:LEU:HD11	9:H:301:GOL:H12	2.02	0.42
4:H:43:SER:HB2	12:A:105:PGV:O06	2.20	0.42
3:M:196:LEU:HA	3:M:196:LEU:HD12	1.74	0.42
13:S:102:BCL:HHC	13:S:102:BCL:OBB	2.20	0.42
6:8:29:PHE:O	6:8:33:VAL:HG23	2.20	0.41
5:I:5:ASN:HD22	6:N:20:ILE:HA	1.85	0.41
12:L:306:PGV:H302	12:M:413:PGV:H262	2.02	0.41
5:S:19:ARG:NE	22:S:103:CDL:OA4	2.43	0.41
13:U:101:BCL:HED1	6:V:28:TRP:CZ3	2.55	0.41
19:U:103:CRT:H14	6:X:21:PHE:HA	2.02	0.41
13:U:102:BCL:H2	6:V:29:PHE:CE1	2.55	0.41
13:1:101:BCL:H62	13:1:101:BCL:H41	1.82	0.41
6:J:21:PHE:CD2	19:J:101:CRT:H14	2.55	0.41
22:K:103:CDL:H711	5:O:26:ALA:HB3	2.02	0.41
2:L:30:PHE:CD2	22:H:304:CDL:H142	2.55	0.41
13:U:102:BCL:H92	6:V:32:VAL:HG12	2.00	0.41
5:U:59:GLY:C	5:U:60:LYS:HD2	2.41	0.41
13:O:101:BCL:H41	13:O:101:BCL:H62	1.87	0.41
19:2:101:CRT:H20	19:2:101:CRT:H181	1.86	0.41
13:5:101:BCL:HMD1	6:6:36:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:7:21:LEU:HD21	19:9:102:CRT:C14	2.49	0.41
1:C:110:CYS:O	1:C:124:LYS:HB2	2.20	0.41
6:G:45:TRP:CD1	6:G:46:LEU:HG	2.56	0.41
13:I:102:BCL:H161	13:I:102:BCL:H192	1.84	0.41
3:M:97:PRO:HD3	3:M:176:PRO:HB3	2.02	0.41
19:O:103:CRT:H10	19:O:103:CRT:H81	1.88	0.41
13:Q:101:BCL:H112	13:Q:101:BCL:H143	1.77	0.41
5:Y:19:ARG:HD3	22:Y:102:CDL:HA32	2.03	0.41
2:L:49:LEU:HD21	5:9:37:MET:HE3	2.03	0.41
19:A:104:CRT:H241	19:A:104:CRT:H26	1.94	0.41
4:H:44:ASP:HB2	12:A:105:PGV:H062	2.02	0.41
2:L:73:ILE:HD13	12:L:305:PGV:H272	2.01	0.41
18:M:405:MQ8:H401	18:M:405:MQ8:H362	1.82	0.41
3:M:89:HIS:O	3:M:93:LEU:HG	2.20	0.41
19:N:101:CRT:H31	19:N:101:CRT:H291	1.95	0.41
5:Y:9:TYR:CE2	6:Z:15:LYS:HG3	2.56	0.41
13:D:102:BCL:H18	13:D:102:BCL:H151	1.74	0.41
19:M:406:CRT:H81	19:M:406:CRT:H10	1.92	0.41
5:O:33:LEU:O	5:O:37[A]:MET:HG3	2.20	0.41
13:Q:102:BCL:HMB3	13:S:101:BCL:CHB	2.51	0.41
6:2:21:PHE:HA	19:2:101:CRT:H11	2.03	0.41
13:O:101:BCL:H8	13:O:101:BCL:H51	1.77	0.41
13:Y:101:BCL:H161	13:Y:101:BCL:H141	1.94	0.41
13:Z:102:BCL:H52	13:Z:102:BCL:H12	1.71	0.41
1:C:256:PHE:CZ	7:C:503:HEC:HMB3	2.56	0.41
4:H:58:PHE:CD1	4:H:59:PRO:HA	2.56	0.41
22:S:103:CDL:C51	22:S:103:CDL:C72	2.99	0.41
19:O:101:CRT:H27	13:O:102:BCL:O1A	2.21	0.41
6:Z:43:ARG:HG3	5:1:55:TYR:CZ	2.56	0.41
13:3:102:BCL:H93	13:3:102:BCL:H111	1.86	0.41
22:H:302:CDL:H742	22:H:302:CDL:H772	1.95	0.41
13:O:102:BCL:OBB	13:O:102:BCL:HHC	2.21	0.41
13:5:102:BCL:H111	13:5:102:BCL:H142	1.80	0.41
25:M:584:HOH:O	4:H:122:HIS:HE1	2.04	0.41
13:I:102:BCL:H152	13:I:102:BCL:H111	1.88	0.41
12:L:305:PGV:H52	12:L:305:PGV:H231	2.03	0.41
12:L:306:PGV:C11	15:L:308:UQ8:H23	2.51	0.41
13:U:101:BCL:H43	6:V:28:TRP:CZ2	2.56	0.41
13:Z:102:BCL:H162	13:Z:102:BCL:H141	1.73	0.41
13:3:101:BCL:H41	13:3:101:BCL:H62	1.79	0.40
13:7:102:BCL:H112	13:7:102:BCL:H152	1.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:7:35:ILE:HD12	13:7:102:BCL:O1D	2.21	0.40
13:S:102:BCL:H111	13:S:102:BCL:H91	1.78	0.40
19:2:101:CRT:H15	19:2:101:CRT:H131	1.98	0.40
6:2:9:LEU:HD21	6:2:13:GLU:CB	2.51	0.40
19:9:101:CRT:H341	19:9:101:CRT:H36	1.89	0.40
5:9:29:ILE:HG13	13:9:103:BCL:H43	2.04	0.40
13:O:102:BCL:OBB	13:O:102:BCL:HHC	2.21	0.40
5:W:13:LEU:O	6:X:6:LEU:HB3	2.21	0.40
13:7:101:BCL:H41	13:7:101:BCL:H61	1.90	0.40
13:7:102:BCL:HBA2	13:7:102:BCL:HED3	2.04	0.40
6:B:43:ARG:HG3	5:D:55:TYR:CE1	2.57	0.40
19:M:406:CRT:H241	19:M:406:CRT:H26	1.96	0.40
13:W:102:BCL:H161	13:W:102:BCL:H121	1.79	0.40
13:A:101:BCL:HMB2	19:0:101:CRT:H371	2.03	0.40
25:H:431:HOH:O	21:I:104:LDA:HM13	2.21	0.40
14:L:302:BPH:HMB3	13:M:401:BCL:HMB2	2.03	0.40
13:O:101:BCL:H43	6:P:28:TRP:CZ2	2.56	0.40
19:2:101:CRT:C35	13:3:101:BCL:HMB2	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:H:558:HOH:O	25:S:210:HOH:O[3_455]	2.08	0.12

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	C	309/404 (76%)	295 (96%)	14 (4%)	0	100	100
2	L	279/281 (99%)	272 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	318/325 (98%)	311 (98%)	5 (2%)	2 (1%)	25	15
4	H	255/259 (98%)	254 (100%)	1 (0%)	0	100	100
5	1	54/61 (88%)	54 (100%)	0	0	100	100
5	3	55/61 (90%)	54 (98%)	1 (2%)	0	100	100
5	5	52/61 (85%)	50 (96%)	2 (4%)	0	100	100
5	7	55/61 (90%)	54 (98%)	1 (2%)	0	100	100
5	9	55/61 (90%)	54 (98%)	1 (2%)	0	100	100
5	A	52/61 (85%)	51 (98%)	1 (2%)	0	100	100
5	D	54/61 (88%)	54 (100%)	0	0	100	100
5	F	54/61 (88%)	52 (96%)	2 (4%)	0	100	100
5	I	56/61 (92%)	55 (98%)	1 (2%)	0	100	100
5	K	55/61 (90%)	55 (100%)	0	0	100	100
5	O	55/61 (90%)	54 (98%)	1 (2%)	0	100	100
5	Q	55/61 (90%)	55 (100%)	0	0	100	100
5	S	57/61 (93%)	57 (100%)	0	0	100	100
5	U	56/61 (92%)	54 (96%)	2 (4%)	0	100	100
5	W	54/61 (88%)	54 (100%)	0	0	100	100
5	Y	55/61 (90%)	54 (98%)	1 (2%)	0	100	100
6	0	41/47 (87%)	41 (100%)	0	0	100	100
6	2	39/47 (83%)	39 (100%)	0	0	100	100
6	4	40/47 (85%)	40 (100%)	0	0	100	100
6	6	40/47 (85%)	40 (100%)	0	0	100	100
6	8	39/47 (83%)	39 (100%)	0	0	100	100
6	B	40/47 (85%)	40 (100%)	0	0	100	100
6	E	36/47 (77%)	36 (100%)	0	0	100	100
6	G	40/47 (85%)	40 (100%)	0	0	100	100
6	J	40/47 (85%)	40 (100%)	0	0	100	100
6	N	40/47 (85%)	40 (100%)	0	0	100	100
6	P	40/47 (85%)	40 (100%)	0	0	100	100
6	R	39/47 (83%)	39 (100%)	0	0	100	100
6	T	41/47 (87%)	41 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	V	40/47 (85%)	40 (100%)	0	0	100	100
6	X	39/47 (83%)	39 (100%)	0	0	100	100
6	Z	38/47 (81%)	38 (100%)	0	0	100	100
All	All	2667/2997 (89%)	2625 (98%)	40 (2%)	2 (0%)	51	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	195	ASN
3	M	179	ILE

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 X-ray entries followed by that with respect to entries of similar resolution.

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	C	260/317 (82%)	258 (99%)	2 (1%)	81	82
2	L	229/229 (100%)	226 (99%)	3 (1%)	69	68
3	M	258/261 (99%)	257 (100%)	1 (0%)	91	91
4	H	211/211 (100%)	210 (100%)	1 (0%)	88	89
5	1	51/56 (91%)	51 (100%)	0	100	100
5	3	52/56 (93%)	52 (100%)	0	100	100
5	5	49/56 (88%)	49 (100%)	0	100	100
5	7	52/56 (93%)	52 (100%)	0	100	100
5	9	52/56 (93%)	51 (98%)	1 (2%)	57	53
5	A	49/56 (88%)	49 (100%)	0	100	100
5	D	51/56 (91%)	51 (100%)	0	100	100
5	F	51/56 (91%)	50 (98%)	1 (2%)	55	51
5	I	53/56 (95%)	53 (100%)	0	100	100
5	K	52/56 (93%)	52 (100%)	0	100	100
5	O	52/56 (93%)	51 (98%)	1 (2%)	57	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Q	52/56 (93%)	52 (100%)	0	100	100
5	S	55/56 (98%)	53 (96%)	2 (4%)	35	26
5	U	53/56 (95%)	52 (98%)	1 (2%)	57	53
5	W	51/56 (91%)	51 (100%)	0	100	100
5	Y	52/56 (93%)	51 (98%)	1 (2%)	57	53
6	0	36/39 (92%)	35 (97%)	1 (3%)	43	36
6	2	34/39 (87%)	34 (100%)	0	100	100
6	4	35/39 (90%)	35 (100%)	0	100	100
6	6	35/39 (90%)	35 (100%)	0	100	100
6	8	34/39 (87%)	34 (100%)	0	100	100
6	B	35/39 (90%)	35 (100%)	0	100	100
6	E	32/39 (82%)	32 (100%)	0	100	100
6	G	35/39 (90%)	35 (100%)	0	100	100
6	J	35/39 (90%)	35 (100%)	0	100	100
6	N	35/39 (90%)	35 (100%)	0	100	100
6	P	35/39 (90%)	35 (100%)	0	100	100
6	R	34/39 (87%)	34 (100%)	0	100	100
6	T	36/39 (92%)	36 (100%)	0	100	100
6	V	35/39 (90%)	35 (100%)	0	100	100
6	X	34/39 (87%)	34 (100%)	0	100	100
6	Z	33/39 (85%)	33 (100%)	0	100	100
All	All	2338/2538 (92%)	2323 (99%)	15 (1%)	86	87

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	212	ILE
1	C	333	THR
2	L	256	CYS
2	L	280	LEU
2	L	281	TRP
3	M	216	PHE
4	H	237	ASP
5	F	58	LEU
5	O	53	VAL

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Mol	Chain	Res	Type
5	S	8	LEU
5	S	25	VAL
5	U	60	LYS
5	Y	48	ASP
5	9	53	VAL
6	0	31	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 144 ligands modelled in this entry, 16 are unknown and 18 are monoatomic - leaving 110 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	$\# Z > 2$
20	PEF	K	104	-	26,26,46	1.25	2 (7%)	29,31,51	1.45	4 (13%)
12	PGV	A	105	-	32,32,50	1.18	2 (6%)	35,38,56	1.18	3 (8%)
13	BCL	7	101	-	53,69,74	1.74	9 (16%)	63,109,115	2.36	20 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PEF	3	103	-	4,4,46	2.62	2 (50%)	6,6,51	1.88	2 (33%)
12	PGV	L	305	-	42,42,50	1.04	2 (4%)	45,48,56	1.26	3 (6%)
19	CRT	6	101	-	41,43,43	0.73	0	50,54,54	1.52	8 (16%)
22	CDL	Y	103	-	12,12,99	0.47	0	13,15,111	0.49	0
13	BCL	O	102	-	58,74,74	1.64	9 (15%)	69,115,115	2.15	18 (26%)
23	LMT	F	103	-	36,36,36	0.49	0	47,47,47	1.44	9 (19%)
15	UQ8	M	417	-	18,18,53	2.07	2 (11%)	22,25,67	1.44	4 (18%)
18	MQ8	M	405	-	54,54,54	1.38	3 (5%)	66,69,69	1.48	14 (21%)
12	PGV	L	306	-	43,43,50	0.99	2 (4%)	46,49,56	1.12	2 (4%)
13	BCL	S	101	-	58,74,74	1.78	9 (15%)	69,115,115	2.22	18 (26%)
11	LHG	C	508	1	8,8,48	0.39	0	7,7,54	0.47	0
10	SO4	C	507	-	4,4,4	0.13	0	6,6,6	0.10	0
22	CDL	H	304	-	78,78,99	1.04	4 (5%)	84,90,111	1.15	8 (9%)
12	PGV	1	105	-	30,30,50	1.21	2 (6%)	33,36,56	1.18	3 (9%)
21	LDA	O	104	-	10,13,15	2.28	1 (10%)	12,15,17	0.49	0
15	UQ8	7	103	-	33,33,53	1.41	2 (6%)	40,43,67	2.09	14 (35%)
19	CRT	G	101	-	41,43,43	0.73	0	50,54,54	1.49	11 (22%)
13	BCL	Z	102	-	58,74,74	1.71	9 (15%)	69,115,115	2.27	19 (27%)
10	SO4	M	412	-	4,4,4	0.14	0	6,6,6	0.09	0
22	CDL	H	302	-	63,63,99	1.08	4 (6%)	69,75,111	1.33	9 (13%)
13	BCL	0	102	-	58,74,74	1.70	8 (13%)	69,115,115	2.26	19 (27%)
20	PEF	W	103	-	4,4,46	2.64	2 (50%)	6,6,51	1.82	2 (33%)
12	PGV	3	104	-	50,50,50	0.94	2 (4%)	53,56,56	0.92	2 (3%)
19	CRT	Z	101	-	41,43,43	0.70	0	50,54,54	1.74	11 (22%)
13	BCL	W	101	-	58,74,74	1.68	9 (15%)	69,115,115	2.43	20 (28%)
19	CRT	V	101	-	41,43,43	0.74	0	50,54,54	1.56	9 (18%)
13	BCL	K	102	-	58,74,74	1.71	9 (15%)	69,115,115	2.31	19 (27%)
20	PEF	1	104	-	4,4,46	2.71	2 (50%)	6,6,51	1.81	2 (33%)
12	PGV	H	303	-	35,35,50	1.10	2 (5%)	38,41,56	1.27	4 (10%)
19	CRT	P	101	-	41,43,43	0.81	0	50,54,54	1.44	10 (20%)
9	GOL	C	506	-	5,5,5	0.89	0	5,5,5	0.87	0
13	BCL	Q	102	-	58,74,74	1.71	8 (13%)	69,115,115	2.27	19 (27%)
19	CRT	9	101	-	41,43,43	0.74	0	50,54,54	1.63	13 (26%)
12	PGV	M	414	-	36,36,50	1.07	2 (5%)	39,42,56	1.21	3 (7%)
19	CRT	N	101	-	41,43,43	0.70	0	50,54,54	1.56	13 (26%)
20	PEF	I	103	-	4,4,46	2.62	2 (50%)	6,6,51	1.81	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BCL	U	101	-	58,74,74	1.70	9 (15%)	69,115,115	2.27	23 (33%)
7	HEC	C	501	1	26,50,50	1.62	4 (15%)	18,82,82	1.66	3 (16%)
13	BCL	I	101	-	58,74,74	1.71	9 (15%)	69,115,115	2.25	18 (26%)
13	BCL	W	102	-	58,74,74	1.71	8 (13%)	69,115,115	2.24	17 (24%)
13	BCL	D	102	-	58,74,74	1.69	9 (15%)	69,115,115	2.25	19 (27%)
13	BCL	1	101	-	58,74,74	1.73	8 (13%)	69,115,115	2.23	18 (26%)
13	BCL	L	301	-	58,74,74	1.59	8 (13%)	69,115,115	1.93	18 (26%)
13	BCL	A	103	-	58,74,74	1.71	9 (15%)	69,115,115	2.20	17 (24%)
19	CRT	0	101	-	41,43,43	0.70	0	50,54,54	1.37	7 (14%)
13	BCL	5	102	-	58,74,74	1.69	8 (13%)	69,115,115	2.13	19 (27%)
7	HEC	C	504	1	26,50,50	1.59	4 (15%)	18,82,82	1.41	3 (16%)
20	PEF	U	104	-	4,4,46	2.53	2 (50%)	6,6,51	1.85	2 (33%)
13	BCL	F	102	-	58,74,74	1.73	8 (13%)	69,115,115	2.26	19 (27%)
12	PGV	C	509	-	20,20,50	1.44	3 (15%)	22,22,56	1.58	3 (13%)
19	CRT	U	103	-	41,43,43	0.74	0	50,54,54	1.52	12 (24%)
20	PEF	M	407	-	4,4,46	2.62	2 (50%)	6,6,51	1.82	2 (33%)
15	UQ8	L	309	-	18,18,53	2.07	2 (11%)	22,25,67	1.01	2 (9%)
13	BCL	M	401	-	58,74,74	1.66	9 (15%)	69,115,115	2.19	22 (31%)
21	LDA	I	104	-	12,15,15	1.95	1 (8%)	14,17,17	0.46	0
12	PGV	D	104	-	34,34,50	1.07	2 (5%)	37,40,56	1.20	5 (13%)
13	BCL	Q	101	-	58,74,74	1.65	9 (15%)	69,115,115	2.12	21 (30%)
19	CRT	2	101	-	41,43,43	0.71	0	50,54,54	1.46	9 (18%)
14	BPH	L	302	-	64,70,70	2.00	13 (20%)	76,101,101	1.86	20 (26%)
9	GOL	H	301	-	5,5,5	0.87	0	5,5,5	0.95	0
13	BCL	S	102	-	58,74,74	1.68	7 (12%)	69,115,115	2.22	20 (28%)
13	BCL	A	101	-	58,74,74	1.73	9 (15%)	69,115,115	2.28	21 (30%)
13	BCL	I	102	-	58,74,74	1.71	8 (13%)	69,115,115	2.19	21 (30%)
22	CDL	Q	104	-	74,74,99	1.09	4 (5%)	80,86,111	1.13	7 (8%)
14	BPH	M	404	-	64,70,70	1.96	12 (18%)	76,101,101	1.89	20 (26%)
19	CRT	J	101	-	41,43,43	0.75	0	50,54,54	1.56	12 (24%)
13	BCL	U	102	-	58,74,74	1.70	8 (13%)	69,115,115	2.22	20 (28%)
20	PEF	U	105	-	4,4,46	2.65	2 (50%)	6,6,51	1.84	2 (33%)
13	BCL	M	402	-	58,74,74	1.59	8 (13%)	69,115,115	2.17	21 (30%)
13	BCL	5	101	-	58,74,74	1.62	8 (13%)	69,115,115	2.24	19 (27%)
23	LMT	M	419	-	36,36,36	0.47	1 (2%)	47,47,47	0.93	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CRT	O	103	-	41,43,43	0.78	0	50,54,54	1.52	12 (24%)
19	CRT	M	406	-	41,43,43	0.88	0	50,54,54	1.35	9 (18%)
19	CRT	A	104	-	41,43,43	0.71	0	50,54,54	1.56	10 (20%)
13	BCL	Y	101	-	58,74,74	1.71	9 (15%)	69,115,115	2.33	20 (28%)
21	LDA	V	102	-	12,15,15	2.07	1 (8%)	14,17,17	0.38	0
22	CDL	M	415	-	38,38,99	1.32	3 (7%)	43,49,111	1.27	3 (6%)
7	HEC	C	502	1	26,50,50	1.53	4 (15%)	18,82,82	1.55	2 (11%)
20	PEF	5	103	-	4,4,46	2.63	2 (50%)	6,6,51	1.79	2 (33%)
22	CDL	D	103	-	39,39,99	1.45	4 (10%)	45,51,111	1.43	6 (13%)
21	LDA	M	411	-	10,13,15	2.26	1 (10%)	12,15,17	0.48	0
20	PEF	M	410	-	4,4,46	2.37	1 (25%)	6,6,51	1.39	1 (16%)
12	PGV	M	413	-	45,45,50	1.06	2 (4%)	49,50,56	0.97	4 (8%)
13	BCL	9	103	-	58,74,74	1.69	9 (15%)	69,115,115	2.32	16 (23%)
13	BCL	M	403	-	58,74,74	1.65	8 (13%)	69,115,115	2.13	18 (26%)
22	CDL	K	103	-	85,85,99	1.00	4 (4%)	91,97,111	1.17	9 (9%)
21	LDA	J	102	-	12,15,15	2.07	1 (8%)	14,17,17	0.45	0
13	BCL	D	101	-	58,74,74	1.69	9 (15%)	69,115,115	2.32	18 (26%)
22	CDL	S	103	-	61,61,99	1.10	4 (6%)	67,73,111	1.31	8 (11%)
13	BCL	3	102	-	58,74,74	1.75	8 (13%)	69,115,115	2.22	19 (27%)
13	BCL	1	102	-	58,74,74	1.72	8 (13%)	69,115,115	2.34	18 (26%)
7	HEC	C	503	1	26,50,50	1.53	4 (15%)	18,82,82	1.58	5 (27%)
13	BCL	3	101	-	58,74,74	1.69	9 (15%)	69,115,115	2.12	17 (24%)
19	CRT	Q	103	-	41,43,43	0.77	0	50,54,54	1.49	7 (14%)
15	UQ8	L	303	-	33,33,53	1.62	2 (6%)	40,43,67	1.57	7 (17%)
20	PEF	M	409	-	4,4,46	2.65	2 (50%)	6,6,51	1.84	2 (33%)
13	BCL	7	102	-	58,74,74	1.68	8 (13%)	69,115,115	2.03	18 (26%)
13	BCL	O	101	-	58,74,74	1.67	8 (13%)	69,115,115	2.40	20 (28%)
19	CRT	9	102	-	41,43,43	0.72	0	50,54,54	1.52	9 (18%)
20	PEF	M	408	-	4,4,46	1.84	2 (50%)	6,6,51	1.18	1 (16%)
20	PEF	M	418	-	46,46,46	0.96	2 (4%)	49,51,51	1.07	3 (6%)
19	CRT	1	103	-	41,43,43	0.72	0	50,54,54	1.48	8 (16%)
15	UQ8	L	308	-	53,53,53	1.19	2 (3%)	64,67,67	1.69	19 (29%)
13	BCL	F	101	-	58,74,74	1.73	10 (17%)	69,115,115	2.25	19 (27%)
13	BCL	K	101	-	58,74,74	1.72	10 (17%)	69,115,115	2.28	18 (26%)
10	SO4	L	304	-	4,4,4	0.13	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CDL	Y	102	5	39,39,99	1.48	4 (10%)	45,51,111	1.33	4 (8%)

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
20	PEF	K	104	-	-	2/30/30/50	-
12	PGV	A	105	-	-	13/37/37/55	-
13	BCL	7	101	-	-	7/31/131/137	-
12	PGV	L	305	-	-	15/47/47/55	-
19	CRT	6	101	-	-	0/51/51/51	-
22	CDL	Y	103	-	-	7/13/13/110	-
13	BCL	O	102	-	-	16/37/137/137	-
23	LMT	F	103	-	-	9/21/61/61	0/2/2/2
15	UQ8	M	417	-	-	1/9/33/75	0/1/1/1
18	MQ8	M	405	-	-	2/47/67/67	0/2/2/2
12	PGV	L	306	-	-	17/48/48/55	-
13	BCL	S	101	-	-	10/37/137/137	-
11	LHG	C	508	1	-	1/5/6/53	-
22	CDL	H	304	-	-	22/89/89/110	-
12	PGV	1	105	-	-	10/35/35/55	-
21	LDA	O	104	-	-	8/11/11/13	-
15	UQ8	7	103	-	-	9/27/51/75	0/1/1/1
19	CRT	G	101	-	-	2/51/51/51	-
12	PGV	M	413	-	-	16/47/47/55	-
22	CDL	H	302	-	-	23/73/73/110	-
13	BCL	0	102	-	-	7/37/137/137	-
12	PGV	3	104	-	-	16/55/55/55	-
19	CRT	Z	101	-	-	0/51/51/51	-
13	BCL	W	101	-	-	10/37/137/137	-
19	CRT	V	101	-	-	6/51/51/51	-
13	BCL	K	102	-	-	14/37/137/137	-
12	PGV	H	303	-	-	16/40/40/55	-
19	CRT	P	101	-	-	1/51/51/51	-
13	BCL	3	101	-	-	18/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCL	Q	102	-	-	9/37/137/137	-
19	CRT	9	101	-	-	5/51/51/51	-
12	PGV	M	414	-	-	16/41/41/55	-
19	CRT	N	101	-	-	0/51/51/51	-
13	BCL	U	101	-	-	4/37/137/137	-
7	HEC	C	501	1	-	0/6/54/54	-
13	BCL	I	101	-	-	9/37/137/137	-
13	BCL	W	102	-	-	8/37/137/137	-
13	BCL	D	102	-	-	7/37/137/137	-
13	BCL	1	101	-	-	15/37/137/137	-
13	BCL	L	301	-	-	2/37/137/137	-
13	BCL	A	103	-	-	10/37/137/137	-
19	CRT	0	101	-	-	5/51/51/51	-
13	BCL	5	102	-	-	13/37/137/137	-
7	HEC	C	504	1	-	0/6/54/54	-
13	BCL	F	102	-	-	11/37/137/137	-
12	PGV	C	509	-	-	4/21/21/55	-
19	CRT	U	103	-	-	3/51/51/51	-
15	UQ8	L	309	-	-	1/9/33/75	0/1/1/1
13	BCL	M	401	-	-	4/37/137/137	-
21	LDA	I	104	-	-	4/13/13/13	-
12	PGV	D	104	-	-	11/39/39/55	-
13	BCL	Q	101	-	-	15/37/137/137	-
19	CRT	2	101	-	-	3/51/51/51	-
14	BPH	L	302	-	-	7/54/105/105	0/5/6/6
9	GOL	H	301	-	-	0/4/4/4	-
13	BCL	S	102	-	-	18/37/137/137	-
13	BCL	A	101	-	-	15/37/137/137	-
13	BCL	I	102	-	-	10/37/137/137	-
22	CDL	Q	104	-	-	36/85/85/110	-
14	BPH	M	404	-	-	10/54/105/105	0/5/6/6
19	CRT	J	101	-	-	1/51/51/51	-
13	BCL	U	102	-	-	15/37/137/137	-
13	BCL	M	402	-	-	15/37/137/137	-
13	BCL	5	101	-	-	11/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LMT	M	419	-	-	6/21/61/61	0/2/2/2
19	CRT	O	103	-	-	4/51/51/51	-
19	CRT	M	406	-	-	5/51/51/51	-
19	CRT	A	104	-	-	0/51/51/51	-
13	BCL	Y	101	-	-	11/37/137/137	-
21	LDA	V	102	-	-	5/13/13/13	-
22	CDL	M	415	-	-	15/48/48/110	-
7	HEC	C	502	1	-	0/6/54/54	-
22	CDL	D	103	-	-	18/50/50/110	-
21	LDA	M	411	-	-	6/11/11/13	-
13	BCL	Z	102	-	-	15/37/137/137	-
13	BCL	9	103	-	-	16/37/137/137	-
13	BCL	M	403	-	-	6/37/137/137	-
22	CDL	K	103	-	-	32/96/96/110	-
21	LDA	J	102	-	-	3/13/13/13	-
13	BCL	D	101	-	-	13/37/137/137	-
22	CDL	S	103	-	-	29/71/71/110	-
13	BCL	3	102	-	-	18/37/137/137	-
13	BCL	1	102	-	-	14/37/137/137	-
7	HEC	C	503	1	-	0/6/54/54	-
9	GOL	C	506	-	-	2/4/4/4	-
19	CRT	Q	103	-	-	3/51/51/51	-
15	UQ8	L	303	-	-	3/27/51/75	0/1/1/1
13	BCL	7	102	-	-	13/37/137/137	-
13	BCL	O	101	-	-	5/37/137/137	-
19	CRT	9	102	-	-	4/51/51/51	-
20	PEF	M	418	-	-	19/50/50/50	-
19	CRT	1	103	-	-	1/51/51/51	-
15	UQ8	L	308	-	-	9/51/75/75	0/1/1/1
13	BCL	F	101	-	-	12/37/137/137	-
13	BCL	K	101	-	-	13/37/137/137	-
22	CDL	Y	102	5	-	25/50/50/110	-

All (445) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	L	303	UQ8	C6-C1	8.04	1.49	1.35
15	M	417	UQ8	C6-C1	7.75	1.49	1.35
15	L	309	UQ8	C6-C1	7.72	1.49	1.35
18	M	405	MQ8	C3-C2	7.48	1.48	1.35
21	O	104	LDA	O1-N1	-7.15	1.25	1.42
15	L	308	UQ8	C6-C1	7.12	1.48	1.35
21	M	411	LDA	O1-N1	-7.10	1.25	1.42
21	J	102	LDA	O1-N1	-7.10	1.25	1.42
21	V	102	LDA	O1-N1	-7.10	1.25	1.42
21	I	104	LDA	O1-N1	-6.72	1.26	1.42
15	7	103	UQ8	C6-C1	6.54	1.47	1.35
13	M	403	BCL	C3B-C2B	6.53	1.51	1.39
13	A	101	BCL	C3B-C2B	6.28	1.50	1.39
13	U	101	BCL	C3B-C2B	6.25	1.50	1.39
13	1	102	BCL	C3B-C2B	6.16	1.50	1.39
13	I	102	BCL	C3B-C2B	6.12	1.50	1.39
13	S	101	BCL	C3B-C2B	6.08	1.50	1.39
13	5	102	BCL	C3B-C2B	6.08	1.50	1.39
13	U	102	BCL	C3B-C2B	6.06	1.50	1.39
13	K	101	BCL	C3B-C2B	6.05	1.50	1.39
13	O	101	BCL	C3B-C2B	6.03	1.50	1.39
13	Z	102	BCL	C3B-C2B	6.01	1.50	1.39
13	D	101	BCL	C3B-C2B	6.00	1.50	1.39
13	Q	101	BCL	C3B-C2B	5.98	1.50	1.39
13	1	101	BCL	C3B-C2B	5.97	1.50	1.39
13	7	102	BCL	C3B-C2B	5.95	1.50	1.39
13	W	102	BCL	C3B-C2B	5.94	1.50	1.39
13	Y	101	BCL	C3B-C2B	5.93	1.50	1.39
14	M	404	BPH	C1A-NA	-5.92	1.25	1.37
13	3	101	BCL	C3B-C2B	5.90	1.50	1.39
13	F	102	BCL	C3B-C2B	5.90	1.50	1.39
13	S	102	BCL	C3B-C2B	5.88	1.50	1.39
13	9	103	BCL	C3B-C2B	5.88	1.50	1.39
13	W	101	BCL	C3B-C2B	5.87	1.50	1.39
13	3	102	BCL	C3B-C2B	5.87	1.50	1.39
13	F	101	BCL	C3B-C2B	5.86	1.49	1.39
13	7	101	BCL	C3B-C2B	5.84	1.49	1.39
13	I	101	BCL	C3B-C2B	5.82	1.49	1.39
13	5	101	BCL	C3B-C2B	5.80	1.49	1.39
13	D	102	BCL	C3B-C2B	5.76	1.49	1.39
13	K	102	BCL	C3B-C2B	5.76	1.49	1.39
13	M	401	BCL	C3B-C2B	5.75	1.49	1.39
13	Q	102	BCL	C3B-C2B	5.74	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	0	102	BCL	C3B-C2B	5.71	1.49	1.39
13	A	103	BCL	C3B-C2B	5.66	1.49	1.39
13	S	101	BCL	OBD-CAD	5.62	1.30	1.22
13	Q	102	BCL	OBD-CAD	5.51	1.30	1.22
18	M	405	MQ8	C10-C5	5.45	1.49	1.40
13	M	402	BCL	C3B-C2B	5.45	1.49	1.39
13	S	101	BCL	C3D-C2D	5.42	1.49	1.39
13	3	102	BCL	OBD-CAD	5.36	1.29	1.22
13	F	102	BCL	C3D-C2D	5.32	1.49	1.39
13	5	102	BCL	C3D-C2D	5.31	1.49	1.39
13	O	102	BCL	C3B-C2B	5.29	1.48	1.39
13	K	102	BCL	O2D-CGD	5.28	1.46	1.33
13	Z	102	BCL	C3D-C2D	5.26	1.48	1.39
13	A	101	BCL	C3D-C2D	5.26	1.48	1.39
13	9	103	BCL	C3D-C2D	5.20	1.48	1.39
13	U	102	BCL	O2D-CGD	5.19	1.45	1.33
13	3	102	BCL	C3D-C2D	5.19	1.48	1.39
13	L	301	BCL	C3B-C2B	5.18	1.48	1.39
13	D	102	BCL	C3D-C2D	5.16	1.48	1.39
13	D	101	BCL	C3D-C2D	5.16	1.48	1.39
13	O	101	BCL	C3D-C2D	5.16	1.48	1.39
14	L	302	BPH	CHA-C1A	5.15	1.49	1.38
13	1	102	BCL	O2D-CGD	5.14	1.45	1.33
13	S	102	BCL	OBD-CAD	5.13	1.29	1.22
13	0	102	BCL	C3D-C2D	5.13	1.48	1.39
13	7	102	BCL	O2D-CGD	5.12	1.45	1.33
13	U	101	BCL	C3D-C2D	5.11	1.48	1.39
14	L	302	BPH	CHB-C1B	5.10	1.48	1.38
13	A	103	BCL	O2D-CGD	5.10	1.45	1.33
13	7	102	BCL	OBD-CAD	5.10	1.29	1.22
13	I	101	BCL	C3D-C2D	5.09	1.48	1.39
13	1	101	BCL	O2D-CGD	5.09	1.45	1.33
13	1	101	BCL	OBD-CAD	5.08	1.29	1.22
13	W	102	BCL	C3D-C2D	5.08	1.48	1.39
14	M	404	BPH	O2D-CGD	5.06	1.45	1.33
13	M	401	BCL	C3D-C2D	5.06	1.48	1.39
14	L	302	BPH	C3D-C2D	5.06	1.48	1.39
13	W	102	BCL	O2D-CGD	5.05	1.45	1.33
13	Q	101	BCL	C3D-C2D	5.05	1.48	1.39
13	3	101	BCL	O2D-CGD	5.05	1.45	1.33
13	F	102	BCL	O2D-CGD	5.04	1.45	1.33
13	W	101	BCL	C3D-C2D	5.03	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	0	102	BCL	OBD-CAD	5.02	1.29	1.22
13	F	101	BCL	C3D-C2D	5.01	1.48	1.39
13	I	102	BCL	C3D-C2D	5.01	1.48	1.39
13	K	102	BCL	C3D-C2D	4.99	1.48	1.39
13	S	102	BCL	C3D-C2D	4.98	1.48	1.39
13	F	101	BCL	OBD-CAD	4.97	1.29	1.22
14	M	404	BPH	CHB-C1B	4.97	1.48	1.38
13	0	102	BCL	O2D-CGD	4.96	1.45	1.33
13	3	102	BCL	O2D-CGD	4.96	1.45	1.33
13	A	103	BCL	OBD-CAD	4.96	1.29	1.22
13	U	102	BCL	C3D-C2D	4.95	1.48	1.39
13	Y	101	BCL	C3D-C2D	4.95	1.48	1.39
13	I	101	BCL	O2D-CGD	4.95	1.45	1.33
13	9	103	BCL	OBD-CAD	4.94	1.29	1.22
13	K	101	BCL	OBD-CAD	4.94	1.29	1.22
13	D	102	BCL	O2D-CGD	4.93	1.45	1.33
13	I	102	BCL	O2D-CGD	4.93	1.45	1.33
13	L	301	BCL	OBD-CAD	4.88	1.29	1.22
13	A	101	BCL	OBD-CAD	4.86	1.29	1.22
13	K	101	BCL	C3D-C2D	4.84	1.48	1.39
13	1	101	BCL	C3D-C2D	4.84	1.48	1.39
13	Q	102	BCL	C3D-C2D	4.84	1.48	1.39
13	F	102	BCL	OBD-CAD	4.83	1.29	1.22
13	F	101	BCL	O2D-CGD	4.83	1.45	1.33
13	A	103	BCL	C3D-C2D	4.81	1.48	1.39
13	5	101	BCL	O2D-CGD	4.81	1.44	1.33
14	L	302	BPH	C4C-NC	-4.81	1.27	1.37
13	Q	101	BCL	O2D-CGD	4.81	1.44	1.33
13	7	102	BCL	C3D-C2D	4.79	1.48	1.39
13	1	102	BCL	C3D-C2D	4.77	1.48	1.39
13	1	102	BCL	OBD-CAD	4.76	1.29	1.22
13	Z	102	BCL	O2D-CGD	4.76	1.44	1.33
13	S	102	BCL	O2D-CGD	4.76	1.44	1.33
13	3	101	BCL	C3D-C2D	4.75	1.48	1.39
13	A	101	BCL	O2D-CGD	4.75	1.44	1.33
13	D	101	BCL	O2D-CGD	4.74	1.44	1.33
13	7	101	BCL	OBD-CAD	4.73	1.28	1.22
13	7	101	BCL	C3D-C2D	4.73	1.47	1.39
13	W	102	BCL	OBD-CAD	4.72	1.28	1.22
14	L	302	BPH	CHC-C4B	4.72	1.51	1.40
13	5	102	BCL	OBD-CAD	4.72	1.28	1.22
13	7	101	BCL	O2D-CGD	4.72	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	404	BPH	C4C-NC	-4.71	1.27	1.37
13	W	101	BCL	O2D-CGD	4.70	1.44	1.33
13	O	102	BCL	C3D-C2D	4.70	1.47	1.39
13	O	101	BCL	O2D-CGD	4.67	1.44	1.33
14	M	404	BPH	CHA-C1A	4.67	1.48	1.38
13	O	102	BCL	OBD-CAD	4.66	1.28	1.22
13	Y	101	BCL	O2D-CGD	4.66	1.44	1.33
20	1	104	PEF	P-O1P	4.66	1.61	1.50
13	Y	101	BCL	OBD-CAD	4.65	1.28	1.22
13	D	101	BCL	OBD-CAD	4.65	1.28	1.22
13	Z	102	BCL	OBD-CAD	4.63	1.28	1.22
14	L	302	BPH	C1A-NA	-4.63	1.28	1.37
13	D	102	BCL	OBD-CAD	4.62	1.28	1.22
13	5	101	BCL	C3D-C2D	4.61	1.47	1.39
13	3	101	BCL	OBD-CAD	4.60	1.28	1.22
13	Q	102	BCL	O2D-CGD	4.60	1.44	1.33
13	U	102	BCL	OBD-CAD	4.60	1.28	1.22
13	K	101	BCL	O2D-CGD	4.60	1.44	1.33
13	I	102	BCL	OBD-CAD	4.60	1.28	1.22
7	C	501	HEC	C3B-C2B	-4.60	1.35	1.40
13	5	102	BCL	O2D-CGD	4.59	1.44	1.33
12	L	305	PGV	O01-C1	4.58	1.47	1.34
22	Q	104	CDL	OA8-CA7	4.56	1.46	1.33
13	O	102	BCL	O2D-CGD	4.56	1.44	1.33
13	U	101	BCL	OBD-CAD	4.54	1.28	1.22
22	M	415	CDL	OA8-CA7	4.54	1.46	1.33
20	U	105	PEF	P-O1P	4.54	1.61	1.50
13	S	101	BCL	O2D-CGD	4.53	1.44	1.33
20	W	103	PEF	P-O1P	4.53	1.61	1.50
20	M	409	PEF	P-O1P	4.53	1.61	1.50
13	L	301	BCL	O2D-CGD	4.53	1.44	1.33
20	3	103	PEF	P-O1P	4.52	1.61	1.50
20	M	407	PEF	P-O1P	4.51	1.61	1.50
22	H	304	CDL	OA6-CA5	4.51	1.47	1.34
13	I	101	BCL	OBD-CAD	4.50	1.28	1.22
12	M	413	PGV	O03-C19	4.50	1.46	1.33
22	H	302	CDL	OA6-CA5	4.49	1.47	1.34
12	H	303	PGV	O03-C19	4.49	1.46	1.33
13	K	102	BCL	OBD-CAD	4.49	1.28	1.22
13	U	101	BCL	O2D-CGD	4.48	1.44	1.33
20	5	103	PEF	P-O1P	4.48	1.61	1.50
20	I	103	PEF	P-O1P	4.46	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	W	101	BCL	OBD-CAD	4.45	1.28	1.22
13	1	102	BCL	O2A-CGA	4.44	1.46	1.33
14	L	302	BPH	O2D-CGD	4.44	1.44	1.33
13	9	103	BCL	O2D-CGD	4.43	1.44	1.33
13	O	101	BCL	O2A-CGA	4.42	1.46	1.33
13	M	401	BCL	O2A-CGA	4.42	1.46	1.33
13	Y	101	BCL	O2A-CGA	4.42	1.46	1.33
13	M	401	BCL	OBD-CAD	4.41	1.28	1.22
13	M	403	BCL	C3D-C2D	4.41	1.47	1.39
13	F	101	BCL	O2A-CGA	4.39	1.46	1.33
20	M	410	PEF	P-O1P	4.38	1.61	1.50
13	M	401	BCL	O2D-CGD	4.37	1.43	1.33
13	F	102	BCL	O2A-CGA	4.37	1.46	1.33
13	I	101	BCL	O2A-CGA	4.37	1.46	1.33
22	Y	102	CDL	OA8-CA7	4.37	1.46	1.33
22	H	302	CDL	OB8-CB7	4.35	1.46	1.33
13	A	103	BCL	O2A-CGA	4.34	1.46	1.33
12	A	105	PGV	O03-C19	4.33	1.46	1.33
13	K	101	BCL	O2A-CGA	4.33	1.46	1.33
22	Q	104	CDL	OB8-CB7	4.33	1.46	1.33
22	H	304	CDL	OA8-CA7	4.33	1.46	1.33
12	1	105	PGV	O03-C19	4.32	1.46	1.33
13	3	101	BCL	O2A-CGA	4.31	1.45	1.33
22	Y	102	CDL	OB8-CB7	4.31	1.45	1.33
20	M	418	PEF	O3-C30	4.31	1.45	1.33
13	1	101	BCL	O2A-CGA	4.31	1.45	1.33
22	Y	102	CDL	OB6-CB5	4.31	1.46	1.34
22	K	103	CDL	OB8-CB7	4.31	1.45	1.33
13	7	101	BCL	O2A-CGA	4.30	1.45	1.33
13	W	102	BCL	O2A-CGA	4.29	1.45	1.33
13	5	101	BCL	O2A-CGA	4.29	1.45	1.33
12	1	105	PGV	O01-C1	4.29	1.46	1.34
13	I	102	BCL	O2A-CGA	4.28	1.45	1.33
12	3	104	PGV	O01-C1	4.28	1.46	1.34
13	S	101	BCL	O2A-CGA	4.28	1.45	1.33
22	Y	102	CDL	OA6-CA5	4.28	1.46	1.34
13	3	102	BCL	O2A-CGA	4.28	1.45	1.33
7	C	503	HEC	C3B-C2B	-4.28	1.36	1.40
13	O	102	BCL	O2A-CGA	4.28	1.45	1.33
12	L	306	PGV	O03-C19	4.27	1.45	1.33
20	U	104	PEF	P-O1P	4.27	1.60	1.50
13	Z	102	BCL	O2A-CGA	4.26	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	103	CDL	OB8-CB7	4.25	1.45	1.33
22	D	103	CDL	OA6-CA5	4.24	1.46	1.34
22	K	103	CDL	OA6-CA5	4.24	1.46	1.34
14	M	404	BPH	CHC-C4B	4.22	1.50	1.40
13	D	101	BCL	O2A-CGA	4.22	1.45	1.33
22	D	103	CDL	OA8-CA7	4.22	1.45	1.33
13	L	301	BCL	C3D-C2D	4.21	1.47	1.39
13	K	102	BCL	O2A-CGA	4.21	1.45	1.33
12	3	104	PGV	O03-C19	4.21	1.45	1.33
13	0	102	BCL	O2A-CGA	4.21	1.45	1.33
12	L	305	PGV	O03-C19	4.20	1.45	1.33
13	A	101	BCL	O2A-CGA	4.19	1.45	1.33
22	M	415	CDL	OA6-CA5	4.17	1.46	1.34
22	D	103	CDL	OB6-CB5	4.17	1.46	1.34
22	Q	104	CDL	OB6-CB5	4.16	1.46	1.34
12	M	414	PGV	O01-C1	4.16	1.46	1.34
13	W	101	BCL	O2A-CGA	4.16	1.45	1.33
13	U	101	BCL	O2A-CGA	4.16	1.45	1.33
12	A	105	PGV	O01-C1	4.15	1.46	1.34
12	C	509	PGV	O03-C19	4.15	1.45	1.33
12	L	306	PGV	O01-C1	4.14	1.46	1.34
12	M	413	PGV	O01-C1	4.13	1.46	1.34
13	M	403	BCL	O2D-CGD	4.13	1.43	1.33
20	M	418	PEF	O2-C10	4.12	1.45	1.34
22	K	103	CDL	OA8-CA7	4.12	1.45	1.33
20	K	104	PEF	O3-C30	4.12	1.45	1.33
13	M	402	BCL	O2A-CGA	4.11	1.45	1.33
22	Q	104	CDL	OA6-CA5	4.11	1.45	1.34
7	C	501	HEC	CBB-CAB	-4.10	1.34	1.49
12	M	414	PGV	O03-C19	4.09	1.45	1.33
22	H	304	CDL	OB8-CB7	4.09	1.45	1.33
13	U	102	BCL	O2A-CGA	4.08	1.45	1.33
13	Q	101	BCL	O2A-CGA	4.08	1.45	1.33
22	M	415	CDL	OB6-CB5	4.08	1.45	1.34
13	Q	102	BCL	O2A-CGA	4.07	1.45	1.33
14	M	404	BPH	C3D-C2D	4.07	1.46	1.39
13	D	102	BCL	O2A-CGA	4.06	1.45	1.33
7	C	502	HEC	CBC-CAC	-4.06	1.34	1.49
13	M	402	BCL	C3D-C2D	4.06	1.46	1.39
13	5	101	BCL	OBD-CAD	4.06	1.28	1.22
13	M	403	BCL	OBD-CAD	4.04	1.28	1.22
7	C	502	HEC	CBB-CAB	-4.03	1.34	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	504	HEC	C3B-C2B	-4.02	1.36	1.40
13	9	103	BCL	O2A-CGA	4.02	1.45	1.33
12	H	303	PGV	O01-C1	4.00	1.45	1.34
22	H	304	CDL	OB6-CB5	3.99	1.45	1.34
13	5	102	BCL	O2A-CGA	3.99	1.45	1.33
22	K	103	CDL	OB6-CB5	3.99	1.45	1.34
20	K	104	PEF	O2-C10	3.99	1.45	1.34
12	C	509	PGV	O01-C1	3.97	1.45	1.34
13	O	101	BCL	OBD-CAD	3.97	1.27	1.22
7	C	501	HEC	CBC-CAC	-3.95	1.34	1.49
12	D	104	PGV	O03-C19	3.94	1.44	1.33
22	H	302	CDL	OB6-CB5	3.94	1.45	1.34
7	C	504	HEC	CBB-CAB	-3.93	1.34	1.49
13	7	102	BCL	O2A-CGA	3.92	1.44	1.33
7	C	504	HEC	CBC-CAC	-3.89	1.34	1.49
22	S	103	CDL	OB6-CB5	3.89	1.44	1.35
7	C	503	HEC	CBC-CAC	-3.87	1.35	1.49
13	M	402	BCL	OBD-CAD	3.86	1.27	1.22
14	L	302	BPH	O2A-CGA	3.84	1.44	1.33
22	S	103	CDL	OB8-CB7	3.83	1.44	1.33
13	Q	101	BCL	OBD-CAD	3.82	1.27	1.22
22	S	103	CDL	OA8-CA7	3.82	1.44	1.33
13	S	102	BCL	O2A-CGA	3.81	1.44	1.33
13	M	403	BCL	O2A-CGA	3.68	1.44	1.33
12	D	104	PGV	O01-C1	3.67	1.44	1.34
14	M	404	BPH	O2A-CGA	3.64	1.44	1.33
14	M	404	BPH	CHD-C4C	3.61	1.47	1.38
13	L	301	BCL	O2A-CGA	3.58	1.43	1.33
7	C	502	HEC	C3B-C2B	-3.56	1.37	1.40
14	L	302	BPH	OBD-CAD	3.50	1.27	1.22
7	C	504	HEC	C3B-C4B	3.47	1.49	1.43
7	C	502	HEC	C3B-C4B	3.46	1.49	1.43
14	M	404	BPH	OBD-CAD	3.45	1.27	1.22
13	M	402	BCL	O2D-CGD	3.44	1.41	1.33
15	L	308	UQ8	C4-C3	3.35	1.50	1.36
15	L	309	UQ8	C4-C3	3.32	1.49	1.36
14	L	302	BPH	C3B-C2B	3.31	1.48	1.39
7	C	503	HEC	C3B-C4B	3.28	1.49	1.43
15	M	417	UQ8	C4-C3	3.25	1.49	1.36
15	L	303	UQ8	C4-C3	3.24	1.49	1.36
14	L	302	BPH	CHD-C4C	3.22	1.46	1.38
13	S	102	BCL	C4B-CHC	3.21	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	402	BCL	C1D-C2D	3.17	1.49	1.42
7	C	503	HEC	CBB-CAB	-3.15	1.37	1.49
13	S	101	BCL	C4B-CHC	3.13	1.49	1.41
13	M	402	BCL	C4B-CHC	3.08	1.49	1.41
13	Q	102	BCL	C1B-CHB	3.05	1.49	1.41
13	M	402	BCL	C1B-CHB	3.05	1.49	1.41
13	9	103	BCL	C4B-CHC	3.04	1.49	1.41
15	7	103	UQ8	C4-C3	3.03	1.48	1.36
13	U	102	BCL	C4B-CHC	3.02	1.49	1.41
13	K	102	BCL	C4B-CHC	3.01	1.49	1.41
13	1	101	BCL	C1D-C2D	3.00	1.49	1.42
13	3	101	BCL	C1D-C2D	3.00	1.49	1.42
22	S	103	CDL	OA6-CA5	2.99	1.42	1.34
13	5	102	BCL	C4B-CHC	2.98	1.49	1.41
13	U	101	BCL	C4B-CHC	2.98	1.49	1.41
13	Q	102	BCL	C4B-CHC	2.98	1.49	1.41
13	O	102	BCL	C4B-CHC	2.96	1.49	1.41
13	L	301	BCL	C1B-CHB	2.96	1.49	1.41
13	M	403	BCL	C4B-CHC	2.91	1.49	1.41
13	I	102	BCL	C4B-CHC	2.90	1.49	1.41
13	Q	101	BCL	C4B-CHC	2.90	1.49	1.41
13	3	102	BCL	C4B-CHC	2.87	1.49	1.41
13	Y	101	BCL	C1D-C2D	2.81	1.48	1.42
13	W	102	BCL	C4B-CHC	2.81	1.48	1.41
13	K	101	BCL	C4B-CHC	2.81	1.48	1.41
13	D	102	BCL	C4B-CHC	2.77	1.48	1.41
14	M	404	BPH	C3B-C2B	2.77	1.46	1.39
13	M	401	BCL	C4B-CHC	2.76	1.48	1.41
13	7	101	BCL	C4B-CHC	2.75	1.48	1.41
13	0	102	BCL	C4B-CHC	2.75	1.48	1.41
13	1	101	BCL	C4B-CHC	2.74	1.48	1.41
13	O	101	BCL	C4B-CHC	2.74	1.48	1.41
13	M	403	BCL	C1B-CHB	2.73	1.48	1.41
13	Y	101	BCL	C4B-CHC	2.73	1.48	1.41
7	C	501	HEC	C3B-C4B	2.72	1.48	1.43
13	3	102	BCL	C1B-CHB	2.72	1.48	1.41
13	A	101	BCL	C4B-CHC	2.72	1.48	1.41
13	W	101	BCL	C1D-C2D	2.71	1.48	1.42
14	L	302	BPH	CBB-CAB	-2.71	1.44	1.50
13	1	102	BCL	C4B-CHC	2.70	1.48	1.41
13	5	102	BCL	C1B-CHB	2.70	1.48	1.41
13	7	102	BCL	C1B-CHB	2.70	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	W	101	BCL	C1B-CHB	2.70	1.48	1.41
13	A	101	BCL	C1D-C2D	2.69	1.48	1.42
13	L	301	BCL	C4B-CHC	2.66	1.48	1.41
13	W	102	BCL	C1B-CHB	2.65	1.48	1.41
13	1	102	BCL	C1B-CHB	2.65	1.48	1.41
13	Z	102	BCL	C4B-CHC	2.64	1.48	1.41
13	O	101	BCL	C1B-CHB	2.64	1.48	1.41
13	F	101	BCL	C4B-CHC	2.64	1.48	1.41
13	O	102	BCL	C1B-CHB	2.63	1.48	1.41
13	D	101	BCL	C4B-CHC	2.63	1.48	1.41
13	I	102	BCL	C1B-CHB	2.63	1.48	1.41
13	S	101	BCL	C1B-CHB	2.63	1.48	1.41
13	Q	101	BCL	C1D-C2D	2.62	1.48	1.42
13	I	101	BCL	C1D-C2D	2.62	1.48	1.42
13	M	403	BCL	C1D-C2D	2.62	1.48	1.42
13	S	102	BCL	C1B-CHB	2.61	1.48	1.41
13	D	101	BCL	C1D-C2D	2.61	1.48	1.42
13	U	102	BCL	C1B-CHB	2.59	1.48	1.41
13	W	101	BCL	C4B-CHC	2.59	1.48	1.41
13	A	103	BCL	C4B-CHC	2.59	1.48	1.41
13	5	101	BCL	C4B-CHC	2.58	1.48	1.41
13	9	103	BCL	C1D-C2D	2.58	1.48	1.42
13	S	101	BCL	C1D-C2D	2.57	1.48	1.42
13	F	102	BCL	C4B-CHC	2.57	1.48	1.41
13	A	103	BCL	C1B-CHB	2.57	1.48	1.41
13	F	101	BCL	C1D-C2D	2.56	1.48	1.42
13	F	102	BCL	C1B-CHB	2.55	1.48	1.41
13	K	102	BCL	C1B-CHB	2.55	1.48	1.41
13	M	401	BCL	C1B-CHB	2.54	1.48	1.41
13	K	101	BCL	C1B-CHB	2.54	1.48	1.41
13	3	101	BCL	C1B-CHB	2.53	1.48	1.41
13	I	101	BCL	C4B-CHC	2.52	1.48	1.41
13	K	101	BCL	C1D-C2D	2.52	1.48	1.42
13	U	101	BCL	C1D-C2D	2.52	1.48	1.42
13	5	101	BCL	C1B-CHB	2.51	1.48	1.41
13	7	101	BCL	C1B-CHB	2.50	1.47	1.41
22	H	302	CDL	OA8-CA7	2.47	1.45	1.33
20	M	408	PEF	P-O4P	2.47	1.62	1.54
13	Q	102	BCL	MG-NA	2.46	2.12	2.06
13	1	101	BCL	C1B-CHB	2.46	1.47	1.41
13	9	103	BCL	C1B-CHB	2.44	1.47	1.41
13	7	102	BCL	C4B-CHC	2.44	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F	101	BCL	C1B-CHB	2.42	1.47	1.41
20	M	408	PEF	P-O3P	2.42	1.61	1.54
13	Z	102	BCL	C1B-CHB	2.41	1.47	1.41
13	D	101	BCL	C1B-CHB	2.41	1.47	1.41
13	0	102	BCL	C1B-CHB	2.41	1.47	1.41
13	A	103	BCL	C1D-C2D	2.41	1.48	1.42
13	I	101	BCL	C1B-CHB	2.40	1.47	1.41
13	D	102	BCL	C1B-CHB	2.40	1.47	1.41
13	3	101	BCL	C4B-CHC	2.38	1.47	1.41
13	O	102	BCL	C4B-NB	-2.37	1.33	1.35
13	5	101	BCL	C1D-C2D	2.37	1.47	1.42
13	U	101	BCL	C1B-CHB	2.35	1.47	1.41
20	1	104	PEF	P-O3P	2.35	1.61	1.54
13	O	101	BCL	C1D-C2D	2.35	1.47	1.42
13	U	101	BCL	CHD-C4C	2.34	1.47	1.41
13	Y	101	BCL	C1B-CHB	2.34	1.47	1.41
20	I	103	PEF	P-O4P	2.34	1.61	1.54
13	D	102	BCL	C1D-C2D	2.33	1.47	1.42
13	I	102	BCL	C1D-C2D	2.32	1.47	1.42
20	U	104	PEF	P-O4P	2.31	1.61	1.54
12	C	509	PGV	O01-C02	-2.31	1.43	1.47
14	L	302	BPH	C3B-C4B	2.31	1.51	1.43
13	S	101	BCL	CHD-C4C	2.30	1.47	1.41
20	U	105	PEF	P-O3P	2.30	1.61	1.54
20	5	103	PEF	P-O4P	2.29	1.61	1.54
20	W	103	PEF	P-O4P	2.29	1.61	1.54
20	M	407	PEF	P-O4P	2.28	1.61	1.54
20	M	409	PEF	P-O3P	2.28	1.61	1.54
13	Z	102	BCL	C1D-C2D	2.28	1.47	1.42
13	A	101	BCL	CHD-C4C	2.27	1.47	1.41
13	7	101	BCL	C1D-C2D	2.26	1.47	1.42
13	Q	101	BCL	C1B-CHB	2.25	1.47	1.41
14	M	404	BPH	CBB-CAB	-2.25	1.45	1.50
13	O	102	BCL	C1D-C2D	2.25	1.47	1.42
13	A	101	BCL	C1B-CHB	2.24	1.47	1.41
20	3	103	PEF	P-O3P	2.24	1.61	1.54
13	3	101	BCL	CHD-C4C	2.23	1.47	1.41
13	1	102	BCL	C1D-C2D	2.23	1.47	1.42
13	3	102	BCL	C1D-C2D	2.21	1.47	1.42
13	M	401	BCL	C1D-C2D	2.20	1.47	1.42
13	F	101	BCL	CHD-C4C	2.17	1.47	1.41
13	W	101	BCL	CHD-C4C	2.17	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	7	101	BCL	CHD-C4C	2.15	1.47	1.41
13	K	102	BCL	C1D-C2D	2.15	1.47	1.42
13	K	101	BCL	C4B-NB	-2.14	1.33	1.35
13	I	101	BCL	CHD-C4C	2.12	1.47	1.41
13	D	101	BCL	CHD-C4C	2.12	1.47	1.41
13	W	102	BCL	C1D-C2D	2.11	1.47	1.42
13	5	102	BCL	C1D-C2D	2.11	1.47	1.42
13	0	102	BCL	C1D-C2D	2.11	1.47	1.42
13	A	103	BCL	CHD-C4C	2.10	1.47	1.41
13	Y	101	BCL	CHD-C4C	2.10	1.47	1.41
13	7	102	BCL	C1D-C2D	2.10	1.47	1.42
13	U	102	BCL	C1D-C2D	2.08	1.47	1.42
13	D	102	BCL	CHD-C4C	2.08	1.47	1.41
13	L	301	BCL	C1D-C2D	2.06	1.47	1.42
13	F	102	BCL	C1D-C2D	2.05	1.47	1.42
23	M	419	LMT	O1'-C1'	2.05	1.43	1.40
18	M	405	MQ8	O4-C4	2.05	1.27	1.23
13	F	101	BCL	C4B-NB	-2.04	1.33	1.35
13	M	401	BCL	C3C-C4C	-2.03	1.49	1.51
13	K	101	BCL	CHD-C4C	2.03	1.47	1.41
13	Q	101	BCL	CHD-C4C	2.03	1.47	1.41
13	9	103	BCL	CHD-C4C	2.02	1.47	1.41
13	Z	102	BCL	CHD-C4C	2.01	1.47	1.41
13	K	102	BCL	CHD-C4C	2.00	1.47	1.41

All (1094) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	102	BCL	C1D-CHD-C4C	-8.82	112.86	125.88
13	3	102	BCL	C1D-CHD-C4C	-8.24	113.71	125.88
13	M	402	BCL	C4A-NA-C1A	-7.80	103.20	106.71
13	A	101	BCL	C4A-NA-C1A	-7.67	103.26	106.71
13	K	102	BCL	C1D-CHD-C4C	-7.66	114.57	125.88
13	W	101	BCL	O2D-CGD-CBD	7.52	124.63	111.27
13	Z	102	BCL	C1D-CHD-C4C	-7.50	114.81	125.88
13	O	101	BCL	C4A-NA-C1A	-7.50	103.34	106.71
13	W	101	BCL	C4A-NA-C1A	-7.40	103.38	106.71
13	S	102	BCL	C4A-NA-C1A	-7.32	103.42	106.71
13	D	101	BCL	C4A-NA-C1A	-7.31	103.42	106.71
13	I	102	BCL	C1D-CHD-C4C	-7.30	115.11	125.88
13	W	102	BCL	C1D-CHD-C4C	-7.28	115.13	125.88
13	M	401	BCL	C1D-CHD-C4C	-7.21	115.24	125.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	F	102	BCL	C1D-CHD-C4C	-7.21	115.24	125.88
13	D	101	BCL	C1D-CHD-C4C	-7.11	115.39	125.88
13	0	102	BCL	C1D-CHD-C4C	-7.05	115.47	125.88
13	Q	102	BCL	C1D-CHD-C4C	-7.02	115.52	125.88
13	U	101	BCL	O2D-CGD-CBD	7.01	123.73	111.27
13	M	403	BCL	C1D-CHD-C4C	-7.00	115.55	125.88
13	K	101	BCL	C1D-CHD-C4C	-6.97	115.59	125.88
13	D	102	BCL	C4A-NA-C1A	-6.92	103.60	106.71
13	A	103	BCL	C4A-NA-C1A	-6.90	103.60	106.71
13	I	101	BCL	C1D-CHD-C4C	-6.88	115.72	125.88
13	9	103	BCL	C4A-NA-C1A	-6.87	103.62	106.71
13	O	101	BCL	C1D-CHD-C4C	-6.87	115.74	125.88
13	D	102	BCL	C1D-CHD-C4C	-6.86	115.75	125.88
13	Y	101	BCL	C1D-CHD-C4C	-6.86	115.76	125.88
13	W	101	BCL	CAC-C3C-C4C	6.85	127.80	112.58
13	S	101	BCL	O2D-CGD-CBD	6.80	123.36	111.27
13	S	102	BCL	C1D-CHD-C4C	-6.75	115.92	125.88
13	9	103	BCL	C1D-CHD-C4C	-6.75	115.92	125.88
13	7	101	BCL	C1D-CHD-C4C	-6.71	115.98	125.88
13	M	401	BCL	C4A-NA-C1A	-6.71	103.69	106.71
13	5	101	BCL	C1D-CHD-C4C	-6.61	116.13	125.88
13	7	102	BCL	C1D-CHD-C4C	-6.59	116.15	125.88
13	U	102	BCL	C1D-CHD-C4C	-6.59	116.16	125.88
13	Q	102	BCL	C4A-NA-C1A	-6.58	103.75	106.71
13	1	101	BCL	C4A-NA-C1A	-6.57	103.75	106.71
13	Y	101	BCL	C4A-NA-C1A	-6.55	103.76	106.71
13	Z	102	BCL	C4A-NA-C1A	-6.55	103.76	106.71
13	Q	101	BCL	O2D-CGD-CBD	6.54	122.88	111.27
13	1	102	BCL	C1C-NC-C4C	-6.51	103.78	106.71
13	F	101	BCL	C4A-NA-C1A	-6.48	103.79	106.71
13	F	101	BCL	C1D-CHD-C4C	-6.47	116.33	125.88
13	O	102	BCL	C1D-CHD-C4C	-6.44	116.38	125.88
13	9	103	BCL	O2D-CGD-CBD	6.43	122.70	111.27
13	U	101	BCL	C1D-CHD-C4C	-6.39	116.45	125.88
13	W	102	BCL	C1C-NC-C4C	-6.36	103.85	106.71
13	A	101	BCL	C1D-CHD-C4C	-6.34	116.52	125.88
13	1	101	BCL	C1D-CHD-C4C	-6.33	116.54	125.88
13	K	102	BCL	C4A-NA-C1A	-6.30	103.87	106.71
13	Y	101	BCL	O2D-CGD-CBD	6.29	122.44	111.27
13	A	103	BCL	C1D-CHD-C4C	-6.28	116.61	125.88
13	W	101	BCL	CMC-C2C-C1C	6.27	128.63	111.77
13	K	101	BCL	C4A-NA-C1A	-6.25	103.90	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Q	101	BCL	C4A-NA-C1A	-6.24	103.90	106.71
13	7	101	BCL	O2D-CGD-CBD	6.23	122.34	111.27
13	O	102	BCL	C4A-NA-C1A	-6.23	103.91	106.71
13	5	102	BCL	C1D-CHD-C4C	-6.22	116.70	125.88
13	0	102	BCL	CMC-C2C-C1C	6.21	128.46	111.77
13	I	101	BCL	C4A-NA-C1A	-6.19	103.92	106.71
13	1	102	BCL	CMC-C2C-C1C	6.18	128.37	111.77
13	5	101	BCL	O2D-CGD-CBD	6.16	122.21	111.27
13	3	101	BCL	C4A-NA-C1A	-6.15	103.94	106.71
13	I	101	BCL	CMC-C2C-C1C	6.13	128.24	111.77
13	0	102	BCL	C1C-NC-C4C	-6.12	103.96	106.71
13	D	102	BCL	CAC-C3C-C4C	6.11	126.15	112.58
13	F	101	BCL	CMC-C2C-C1C	6.10	128.16	111.77
13	1	102	BCL	CAC-C3C-C4C	6.10	126.12	112.58
13	K	102	BCL	CMC-C2C-C1C	6.09	128.13	111.77
13	5	102	BCL	CMC-C2C-C1C	6.08	128.12	111.77
13	F	101	BCL	CAC-C3C-C4C	6.08	126.08	112.58
13	3	101	BCL	O2D-CGD-CBD	6.06	122.04	111.27
13	M	402	BCL	CAC-C3C-C4C	6.06	126.03	112.58
13	O	101	BCL	CMC-C2C-C1C	6.05	128.03	111.77
13	7	102	BCL	CAC-C3C-C4C	6.02	125.94	112.58
13	D	101	BCL	CAC-C3C-C4C	5.99	125.88	112.58
13	O	101	BCL	O2D-CGD-CBD	5.99	121.92	111.27
13	D	102	BCL	CMC-C2C-C1C	5.98	127.84	111.77
13	3	102	BCL	CMC-C2C-C1C	5.97	127.82	111.77
13	1	101	BCL	CMC-C2C-C1C	5.97	127.81	111.77
13	U	101	BCL	C4A-NA-C1A	-5.96	104.03	106.71
13	F	102	BCL	CMC-C2C-C1C	5.96	127.79	111.77
13	A	103	BCL	CMC-C2C-C1C	5.95	127.76	111.77
13	A	101	BCL	O2D-CGD-CBD	5.95	121.84	111.27
13	Y	101	BCL	CAC-C3C-C4C	5.95	125.78	112.58
13	7	101	BCL	C4A-NA-C1A	-5.94	104.04	106.71
13	5	101	BCL	CMC-C2C-C1C	5.92	127.69	111.77
13	Y	101	BCL	CMC-C2C-C1C	5.92	127.69	111.77
13	F	102	BCL	CAC-C3C-C4C	5.91	125.69	112.58
13	U	102	BCL	C1C-NC-C4C	-5.90	104.05	106.71
13	3	102	BCL	C4A-NA-C1A	-5.86	104.07	106.71
13	S	101	BCL	C1D-CHD-C4C	-5.86	117.24	125.88
13	Z	102	BCL	CMC-C2C-C1C	5.84	127.46	111.77
13	I	102	BCL	C4A-NA-C1A	-5.82	104.09	106.71
13	D	101	BCL	CMC-C2C-C1C	5.82	127.42	111.77
13	A	103	BCL	CAC-C3C-C4C	5.82	125.50	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	S	101	BCL	CAC-C3C-C4C	5.80	125.47	112.58
13	I	101	BCL	CAC-C3C-C4C	5.78	125.41	112.58
13	K	102	BCL	CAC-C3C-C4C	5.77	125.38	112.58
13	Z	102	BCL	CAC-C3C-C4C	5.77	125.38	112.58
13	1	101	BCL	CAC-C3C-C4C	5.74	125.32	112.58
13	3	101	BCL	C1D-CHD-C4C	-5.73	117.42	125.88
13	K	101	BCL	O2D-CGD-CBD	5.71	121.42	111.27
13	5	101	BCL	C4A-NA-C1A	-5.69	104.15	106.71
13	I	102	BCL	CMC-C2C-C1C	5.69	127.05	111.77
19	Z	101	CRT	C21-C22-C23	-5.66	119.23	127.31
13	A	101	BCL	CMC-C2C-C1C	5.64	126.94	111.77
13	Z	102	BCL	C1C-NC-C4C	-5.64	104.17	106.71
13	K	101	BCL	CAC-C3C-C4C	5.61	125.03	112.58
13	K	101	BCL	CMC-C2C-C1C	5.61	126.84	111.77
13	O	101	BCL	C1C-NC-C4C	-5.60	104.19	106.71
13	5	101	BCL	CAC-C3C-C4C	5.60	125.00	112.58
13	9	103	BCL	C1C-NC-C4C	-5.59	104.19	106.71
13	W	101	BCL	C1D-CHD-C4C	-5.58	117.64	125.88
13	W	102	BCL	CMC-C2C-C1C	5.57	126.75	111.77
13	W	102	BCL	C4A-NA-C1A	-5.56	104.20	106.71
13	I	102	BCL	CAC-C3C-C4C	5.50	124.78	112.58
13	0	102	BCL	C4A-NA-C1A	-5.49	104.24	106.71
13	9	103	BCL	CMC-C2C-C1C	5.48	126.49	111.77
13	3	102	BCL	CAC-C3C-C4C	5.42	124.62	112.58
13	S	102	BCL	CMC-C2C-C1C	5.42	126.33	111.77
13	U	102	BCL	C4A-NA-C1A	-5.41	104.28	106.71
13	1	102	BCL	C4A-NA-C1A	-5.40	104.28	106.71
13	S	101	BCL	C4A-NA-C1A	-5.38	104.29	106.71
13	5	102	BCL	C4A-NA-C1A	-5.37	104.29	106.71
13	0	102	BCL	CAC-C3C-C4C	5.36	124.49	112.58
15	L	303	UQ8	C15-C14-C16	5.36	124.28	115.27
13	1	101	BCL	O2D-CGD-CBD	5.35	120.77	111.27
13	L	301	BCL	C1D-CHD-C4C	-5.32	118.02	125.88
13	7	102	BCL	CMC-C2C-C1C	5.32	126.07	111.77
13	W	102	BCL	CAC-C3C-C4C	5.31	124.37	112.58
13	3	101	BCL	CAC-C3C-C4C	5.31	124.36	112.58
13	3	101	BCL	CMC-C2C-C1C	5.30	126.02	111.77
13	F	102	BCL	C1C-NC-C4C	-5.29	104.33	106.71
13	7	102	BCL	C1C-NC-C4C	-5.29	104.33	106.71
13	F	101	BCL	C1C-NC-C4C	-5.28	104.33	106.71
13	5	102	BCL	C1C-NC-C4C	-5.27	104.34	106.71
13	U	102	BCL	CAC-C3C-C4C	5.25	124.23	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	101	BCL	C1C-NC-C4C	-5.22	104.36	106.71
13	K	101	BCL	C1C-NC-C4C	-5.20	104.37	106.71
13	S	102	BCL	C1C-NC-C4C	-5.20	104.37	106.71
13	F	101	BCL	O2D-CGD-CBD	5.19	120.50	111.27
13	O	102	BCL	CAC-C3C-C4C	5.19	124.11	112.58
13	I	101	BCL	C1C-NC-C4C	-5.16	104.39	106.71
13	7	101	BCL	CAC-C3C-C4C	5.16	124.04	112.58
13	7	101	BCL	CMC-C2C-C1C	5.15	125.62	111.77
13	U	102	BCL	CMC-C2C-C1C	5.15	125.61	111.77
13	I	101	BCL	O2D-CGD-CBD	5.14	120.39	111.27
13	D	101	BCL	O2D-CGD-CBD	5.10	120.33	111.27
13	M	402	BCL	C1D-CHD-C4C	-5.10	118.36	125.88
14	L	302	BPH	CMC-C2C-C1C	5.10	126.34	112.09
13	M	403	BCL	C4A-NA-C1A	-5.10	104.42	106.71
13	Q	102	BCL	C3C-C4C-CHD	-5.09	112.51	123.39
13	K	102	BCL	C1C-NC-C4C	-5.06	104.43	106.71
15	7	103	UQ8	C1M-C1-C6	-5.06	116.15	124.40
13	F	102	BCL	C4A-NA-C1A	-5.05	104.44	106.71
13	A	101	BCL	CAC-C3C-C4C	5.03	123.75	112.58
13	5	101	BCL	C1C-NC-C4C	-5.02	104.45	106.71
13	5	102	BCL	CAC-C3C-C4C	5.00	123.68	112.58
13	S	101	BCL	CMC-C2C-C1C	4.99	125.19	111.77
13	M	402	BCL	CMC-C2C-C1C	4.94	125.05	111.77
14	M	404	BPH	CMB-C2B-C1B	4.89	132.60	125.06
22	H	302	CDL	OA6-CA5-C11	4.89	122.03	111.50
13	Q	101	BCL	C1D-CHD-C4C	-4.88	118.67	125.88
13	U	101	BCL	CMC-C2C-C1C	4.87	124.87	111.77
15	7	103	UQ8	C6-C1-C2	4.86	123.03	119.18
12	L	305	PGV	O01-C1-C2	4.84	121.94	111.50
13	1	101	BCL	C1C-NC-C4C	-4.83	104.53	106.71
13	O	102	BCL	CMC-C2C-C1C	4.83	124.74	111.77
13	F	102	BCL	O2D-CGD-CBD	4.82	119.84	111.27
13	L	301	BCL	C3C-C4C-CHD	-4.81	113.12	123.39
13	S	102	BCL	CAC-C3C-C4C	4.80	123.25	112.58
13	W	101	BCL	O2D-CGD-O1D	-4.80	114.46	123.84
22	S	103	CDL	OB6-CB5-C51	4.79	119.89	111.09
13	3	102	BCL	C1C-NC-C4C	-4.78	104.56	106.71
7	C	501	HEC	CAD-CBD-CGD	4.77	120.67	112.67
13	Q	102	BCL	C1C-NC-C4C	-4.77	104.56	106.71
19	N	101	CRT	C21-C22-C23	-4.74	120.55	127.31
13	O	101	BCL	CAC-C3C-C4C	4.73	123.07	112.58
13	1	102	BCL	O2D-CGD-CBD	4.71	119.63	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	401	BCL	CMC-C2C-C1C	4.70	124.41	111.77
13	L	301	BCL	C4A-NA-C1A	-4.70	104.59	106.71
19	V	101	CRT	C21-C22-C23	-4.69	120.61	127.31
20	K	104	PEF	O2-C10-C11	4.68	121.59	111.50
13	Y	101	BCL	C1C-NC-C4C	-4.66	104.61	106.71
14	L	302	BPH	CAC-C3C-C4C	4.64	124.59	112.67
13	Q	101	BCL	CMC-C2C-C1C	4.60	124.14	111.77
22	H	304	CDL	OB6-CB5-C51	4.58	121.38	111.50
13	A	103	BCL	C1C-NC-C4C	-4.57	104.65	106.71
13	D	102	BCL	C1C-NC-C4C	-4.56	104.65	106.71
19	Q	103	CRT	C21-C22-C23	-4.56	120.80	127.31
13	L	301	BCL	O2D-CGD-CBD	4.55	119.36	111.27
12	M	414	PGV	O01-C1-C2	4.55	121.31	111.50
13	W	101	BCL	C1C-NC-C4C	-4.54	104.66	106.71
19	9	101	CRT	C21-C22-C23	-4.54	120.83	127.31
13	W	102	BCL	C3C-C4C-CHD	-4.53	113.72	123.39
13	9	103	BCL	C3C-C4C-CHD	-4.51	113.76	123.39
13	O	102	BCL	CMB-C2B-C3B	4.51	133.11	124.68
14	M	404	BPH	C2A-C1A-NA	4.50	117.03	111.86
13	U	101	BCL	C1C-NC-C4C	-4.50	104.68	106.71
19	J	101	CRT	C21-C22-C23	-4.50	120.89	127.31
13	M	403	BCL	CAC-C3C-C4C	4.50	122.56	112.58
13	Q	102	BCL	CMC-C2C-C1C	4.49	123.84	111.77
19	6	101	CRT	C5-C6-C7	-4.49	119.11	125.89
13	S	102	BCL	C3C-C4C-CHD	-4.47	113.83	123.39
13	7	101	BCL	C1C-NC-C4C	-4.47	104.70	106.71
13	U	101	BCL	C3C-C4C-CHD	-4.47	113.84	123.39
22	S	103	CDL	CB4-OB6-CB5	-4.46	109.59	117.90
13	M	402	BCL	C3C-C4C-CHD	-4.41	113.97	123.39
12	H	303	PGV	O01-C1-C2	4.41	121.00	111.50
19	9	102	CRT	C21-C22-C23	-4.40	121.02	127.31
14	M	404	BPH	C1-C2-C3	-4.39	118.45	126.04
12	L	306	PGV	O01-C1-C2	4.39	120.95	111.50
22	K	103	CDL	OA6-CA5-C11	4.39	120.95	111.50
13	7	101	BCL	C3C-C4C-CHD	-4.38	114.04	123.39
22	K	103	CDL	OB6-CB5-C51	4.36	120.89	111.50
13	U	101	BCL	O2D-CGD-O1D	-4.36	115.32	123.84
15	7	103	UQ8	C7-C8-C9	-4.35	119.55	126.79
23	F	103	LMT	C1'-O5'-C5'	4.31	122.14	113.69
19	G	101	CRT	C21-C22-C23	-4.29	121.19	127.31
19	A	104	CRT	C21-C22-C23	-4.28	121.20	127.31
13	I	102	BCL	O2D-CGD-CBD	4.28	118.87	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	9	103	BCL	CAC-C3C-C4C	4.26	122.04	112.58
13	M	403	BCL	O2D-CGD-CBD	4.25	118.83	111.27
13	F	102	BCL	C3C-C4C-CHD	-4.25	114.31	123.39
13	Q	102	BCL	CAC-C3C-C2C	4.23	124.84	114.26
14	L	302	BPH	C2A-C1A-NA	4.23	116.72	111.86
13	Z	102	BCL	O2D-CGD-CBD	4.22	118.78	111.27
22	H	302	CDL	OB6-CB5-C51	4.22	120.60	111.50
13	O	101	BCL	C3C-C4C-CHD	-4.21	114.40	123.39
13	O	102	BCL	C3C-C4C-CHD	-4.20	114.42	123.39
13	K	102	BCL	O2D-CGD-CBD	4.19	118.71	111.27
13	5	102	BCL	C3C-C4C-CHD	-4.17	114.47	123.39
14	L	302	BPH	C3B-C2B-C1B	-4.17	99.80	105.87
22	Q	104	CDL	OA6-CA5-C11	4.17	120.48	111.50
13	I	102	BCL	C1C-NC-C4C	-4.17	104.83	106.71
13	Q	102	BCL	O2D-CGD-CBD	4.16	118.66	111.27
14	M	404	BPH	O2D-CGD-CBD	4.16	118.66	111.27
13	U	102	BCL	C3C-C4C-CHD	-4.13	114.56	123.39
13	S	101	BCL	C3C-C4C-CHD	-4.11	114.61	123.39
22	Q	104	CDL	OB6-CB5-C51	4.10	120.34	111.50
7	C	503	HEC	CAD-CBD-CGD	4.10	119.55	112.67
12	C	509	PGV	C02-O01-C1	-4.10	112.61	117.88
14	M	404	BPH	CAC-C3C-C4C	4.08	123.14	112.67
13	U	101	BCL	CMB-C2B-C3B	4.07	132.29	124.68
13	O	101	BCL	CMB-C2B-C3B	4.06	132.27	124.68
13	M	403	BCL	C2C-C3C-C4C	-4.05	95.27	101.34
13	U	101	BCL	CAC-C3C-C4C	4.03	121.54	112.58
12	1	105	PGV	O01-C1-C2	4.01	120.15	111.50
13	M	401	BCL	C2C-C3C-C4C	-4.01	95.34	101.34
13	Q	101	BCL	C3C-C4C-CHD	-4.01	114.83	123.39
13	M	403	BCL	C1C-NC-C4C	-3.99	104.91	106.71
13	9	103	BCL	O2D-CGD-O1D	-3.98	116.06	123.84
19	P	101	CRT	C21-C22-C23	-3.98	121.63	127.31
13	A	101	BCL	C3C-C4C-CHD	-3.96	114.93	123.39
13	Q	101	BCL	CMB-C2B-C3B	3.96	132.08	124.68
13	M	401	BCL	CAC-C3C-C4C	3.94	121.33	112.58
13	M	401	BCL	CHD-C4C-NC	3.94	129.45	125.08
13	K	102	BCL	C3C-C4C-CHD	-3.92	115.02	123.39
13	M	401	BCL	C3C-C4C-CHD	-3.89	115.08	123.39
22	M	415	CDL	OA8-CA7-C31	3.88	121.55	111.38
13	M	403	BCL	CHD-C4C-NC	3.87	129.38	125.08
14	M	404	BPH	C4-C3-C5	3.87	121.78	115.27
13	W	101	BCL	C3C-C4C-CHD	-3.87	115.13	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	403	BCL	O2D-CGD-O1D	-3.86	116.29	123.84
13	5	102	BCL	O2D-CGD-CBD	3.85	118.11	111.27
13	D	102	BCL	O2D-CGD-CBD	3.84	118.10	111.27
13	W	102	BCL	CHD-C4C-NC	3.83	129.33	125.08
13	3	102	BCL	C3C-C4C-CHD	-3.83	115.21	123.39
13	D	102	BCL	C3C-C4C-CHD	-3.82	115.24	123.39
13	Q	102	BCL	CHD-C4C-NC	3.81	129.31	125.08
13	O	102	BCL	O2D-CGD-CBD	3.81	118.03	111.27
20	3	103	PEF	O4P-P-O2P	3.80	120.18	107.97
13	K	102	BCL	CMB-C2B-C1B	-3.79	122.63	128.46
13	A	103	BCL	C3C-C4C-CHD	-3.79	115.29	123.39
13	5	101	BCL	O2D-CGD-O1D	-3.78	116.44	123.84
20	U	104	PEF	O3P-P-O2P	3.78	120.11	107.97
20	U	105	PEF	O4P-P-O2P	3.77	120.08	107.97
19	6	101	CRT	C21-C22-C23	-3.76	121.94	127.31
13	M	403	BCL	C3C-C4C-CHD	-3.76	115.35	123.39
13	I	102	BCL	C3C-C4C-CHD	-3.74	115.40	123.39
22	H	304	CDL	OA6-CA5-C11	3.74	119.55	111.50
20	I	103	PEF	O3P-P-O2P	3.73	119.96	107.97
13	F	101	BCL	C3C-C4C-CHD	-3.72	115.44	123.39
20	1	104	PEF	O4P-P-O2P	3.72	119.91	107.97
13	K	101	BCL	C3C-C4C-CHD	-3.71	115.46	123.39
20	W	103	PEF	O3P-P-O2P	3.71	119.89	107.97
20	M	407	PEF	O3P-P-O2P	3.70	119.85	107.97
13	7	101	BCL	CHD-C4C-NC	3.70	129.19	125.08
13	A	101	BCL	C1C-NC-C4C	-3.69	105.05	106.71
13	O	102	BCL	C1C-NC-C4C	-3.68	105.05	106.71
13	3	101	BCL	C3C-C4C-CHD	-3.68	115.53	123.39
22	M	415	CDL	OB6-CB5-C51	3.67	119.42	111.50
13	L	301	BCL	CAC-C3C-C4C	3.67	120.73	112.58
20	M	409	PEF	O4P-P-O2P	3.66	119.73	107.97
13	S	101	BCL	O2D-CGD-O1D	-3.66	116.67	123.84
12	3	104	PGV	O01-C1-C2	3.65	119.37	111.50
14	M	404	BPH	O2A-C1-C2	-3.65	99.05	108.64
13	Y	101	BCL	CMB-C2B-C1B	-3.65	122.86	128.46
13	U	101	BCL	CHD-C4C-NC	3.65	129.13	125.08
20	M	418	PEF	O2-C10-C11	3.65	119.36	111.50
20	5	103	PEF	O3P-P-O2P	3.65	119.67	107.97
13	U	102	BCL	CMB-C2B-C3B	3.64	131.49	124.68
13	K	102	BCL	CHD-C4C-NC	3.64	129.12	125.08
22	D	103	CDL	OA6-CA5-C11	3.64	120.94	110.80
13	0	102	BCL	O2D-CGD-CBD	3.63	117.72	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	S	101	BCL	CHD-C4C-NC	3.63	129.10	125.08
13	3	101	BCL	C1C-NC-C4C	-3.62	105.08	106.71
19	1	103	CRT	C21-C22-C23	-3.61	122.15	127.31
12	A	105	PGV	O01-C1-C2	3.61	119.29	111.50
13	W	102	BCL	O2D-CGD-CBD	3.61	117.68	111.27
13	Y	101	BCL	C3C-C4C-CHD	-3.61	115.69	123.39
13	M	401	BCL	C1C-NC-C4C	-3.60	105.09	106.71
13	0	102	BCL	C3C-C4C-CHD	-3.59	115.72	123.39
19	2	101	CRT	C21-C22-C23	-3.58	122.20	127.31
12	C	509	PGV	O01-C1-C2	3.58	119.22	111.50
13	O	101	BCL	CHD-C4C-NC	3.58	129.05	125.08
19	U	103	CRT	C21-C22-C23	-3.57	122.21	127.31
13	Q	102	BCL	C4-C3-C5	3.57	121.28	115.27
13	S	102	BCL	CHD-C4C-NC	3.57	129.04	125.08
13	7	102	BCL	O2D-CGD-CBD	3.54	117.56	111.27
13	3	102	BCL	O2D-CGD-CBD	3.54	117.55	111.27
13	D	101	BCL	C3C-C4C-CHD	-3.53	115.84	123.39
13	A	103	BCL	CMB-C2B-C3B	3.53	131.28	124.68
22	D	103	CDL	OB6-CB5-C51	3.53	120.63	110.80
12	H	303	PGV	C02-O01-C1	-3.52	109.12	117.79
13	K	101	BCL	CMB-C2B-C1B	-3.52	123.05	128.46
13	M	403	BCL	CMC-C2C-C1C	3.52	121.22	111.77
13	A	101	BCL	O2D-CGD-O1D	-3.51	116.97	123.84
14	L	302	BPH	OBD-CAD-C3D	-3.51	122.15	127.98
22	S	103	CDL	OA6-CA5-C11	3.51	119.06	111.50
7	C	502	HEC	CAD-CBD-CGD	3.50	118.55	112.67
13	F	102	BCL	CHD-C4C-NC	3.50	128.97	125.08
13	M	402	BCL	C1C-NC-C4C	-3.50	105.13	106.71
13	5	101	BCL	C3C-C4C-CHD	-3.49	115.93	123.39
12	L	305	PGV	C03-C02-C01	-3.49	103.53	111.79
22	Y	102	CDL	OA8-CA7-C31	3.49	120.54	111.38
14	M	404	BPH	CMC-C2C-C3C	3.49	127.89	113.83
14	L	302	BPH	C4D-CHA-C1A	-3.49	121.91	130.51
13	Q	102	BCL	CAC-C3C-C4C	3.47	120.30	112.58
13	A	103	BCL	CHD-C4C-NC	3.47	128.93	125.08
13	3	102	BCL	CMB-C2B-C3B	3.47	131.17	124.68
13	L	301	BCL	CHD-C4C-NC	3.47	128.93	125.08
13	7	102	BCL	C3C-C4C-CHD	-3.46	116.00	123.39
13	M	401	BCL	O2D-CGD-CBD	3.46	117.41	111.27
13	9	103	BCL	CHD-C4C-NC	3.45	128.91	125.08
13	0	102	BCL	CMB-C2B-C3B	3.45	131.13	124.68
19	O	103	CRT	C5-C6-C7	-3.45	120.68	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Q	101	BCL	CAC-C3C-C4C	3.43	120.19	112.58
14	M	404	BPH	CMC-C2C-C1C	3.42	121.65	112.09
13	A	103	BCL	CBC-CAC-C3C	-3.41	105.88	113.47
19	Q	103	CRT	C10-C9-C7	-3.40	122.45	127.31
13	Y	101	BCL	O2D-CGD-O1D	-3.40	117.19	123.84
13	D	102	BCL	CMB-C2B-C3B	3.39	131.02	124.68
13	A	103	BCL	O2D-CGD-CBD	3.39	117.29	111.27
13	U	102	BCL	CMD-C2D-C3D	3.38	131.01	124.68
13	U	102	BCL	O2D-CGD-CBD	3.38	117.28	111.27
13	A	103	BCL	C4-C3-C5	3.38	120.96	115.27
13	L	301	BCL	CMB-C2B-C3B	3.37	130.98	124.68
19	9	102	CRT	C10-C9-C7	-3.37	122.50	127.31
13	Q	102	BCL	CMD-C2D-C3D	3.37	130.98	124.68
13	S	102	BCL	CMB-C2B-C3B	3.36	130.97	124.68
13	O	101	BCL	O2D-CGD-O1D	-3.36	117.27	123.84
13	3	102	BCL	C1-C2-C3	-3.35	120.25	126.04
19	0	101	CRT	C21-C22-C23	-3.35	122.53	127.31
13	W	101	BCL	C1-C2-C3	-3.34	120.26	126.04
13	A	101	BCL	CHD-C4C-NC	3.33	128.78	125.08
22	K	103	CDL	OB8-CB7-C71	3.32	122.33	111.91
13	3	101	BCL	CMC-C2C-C3C	3.32	127.22	113.83
19	M	406	CRT	C26-C27-C28	-3.32	122.57	127.31
13	M	401	BCL	CAC-C3C-C2C	3.30	122.51	114.26
22	Y	102	CDL	OB8-CB7-C71	3.30	120.03	111.38
13	3	101	BCL	O2D-CGD-O1D	-3.29	117.40	123.84
13	S	102	BCL	C1-C2-C3	-3.29	120.35	126.04
13	U	102	BCL	C2C-C3C-C4C	-3.29	96.41	101.34
13	Q	101	BCL	CMC-C2C-C3C	3.29	127.10	113.83
12	D	104	PGV	C02-O01-C1	-3.29	109.69	117.79
20	K	104	PEF	C2-O2-C10	-3.28	109.70	117.79
15	L	308	UQ8	O5-C5-C6	-3.27	115.81	121.55
22	Y	102	CDL	OA6-CA5-C11	3.27	119.91	110.80
13	Y	101	BCL	CBC-CAC-C3C	-3.26	106.20	113.47
22	Y	102	CDL	OB6-CB5-C51	3.26	119.89	110.80
13	U	102	BCL	CHD-C4C-NC	3.26	128.69	125.08
19	A	104	CRT	C5-C6-C7	-3.26	120.97	125.89
23	F	103	LMT	C4B-C3B-C2B	-3.25	105.14	110.82
13	I	101	BCL	CBC-CAC-C3C	-3.25	106.24	113.47
19	1	103	CRT	C10-C9-C7	-3.25	122.68	127.31
13	A	101	BCL	CMB-C2B-C3B	3.24	130.75	124.68
13	D	101	BCL	CMB-C2B-C3B	3.24	130.75	124.68
13	O	101	BCL	C1-O2A-CGA	3.24	124.94	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	M	405	MQ8	C29-C28-C30	3.24	120.71	115.27
13	5	102	BCL	O2D-CGD-O1D	-3.23	117.52	123.84
13	I	101	BCL	CMC-C2C-C3C	3.22	126.84	113.83
22	K	103	CDL	CB4-OB6-CB5	-3.22	109.86	117.79
22	M	415	CDL	OA6-CA5-C11	3.22	119.78	110.80
22	H	302	CDL	CB4-OB6-CB5	-3.22	109.86	117.79
22	D	103	CDL	OA8-CA7-C31	3.21	119.81	111.38
19	Z	101	CRT	C20-C19-C17	-3.21	122.72	127.31
19	J	101	CRT	C20-C19-C17	-3.21	122.73	127.31
13	1	101	BCL	C3C-C4C-CHD	-3.21	116.54	123.39
20	M	418	PEF	O3-C30-C31	3.20	121.95	111.91
13	O	102	BCL	CHD-C4C-NC	3.20	128.62	125.08
13	D	101	BCL	C4-C3-C5	3.19	120.64	115.27
13	M	402	BCL	CMB-C2B-C3B	3.19	130.65	124.68
13	S	101	BCL	CBA-CAA-C2A	-3.18	104.46	113.86
13	Q	101	BCL	CHD-C4C-NC	3.18	128.61	125.08
13	Y	101	BCL	CHD-C4C-NC	3.17	128.60	125.08
13	I	101	BCL	C3C-C4C-CHD	-3.17	116.62	123.39
19	O	103	CRT	C21-C20-C19	-3.17	116.99	123.47
13	D	102	BCL	CHD-C4C-NC	3.16	128.59	125.08
15	7	103	UQ8	C12-C13-C14	-3.16	120.06	127.66
15	L	303	UQ8	C16-C14-C13	-3.14	114.76	121.12
19	1	103	CRT	C5-C6-C7	-3.13	121.16	125.89
13	D	101	BCL	CMC-C2C-C3C	3.13	126.46	113.83
13	L	301	BCL	CAC-C3C-C2C	3.12	122.05	114.26
22	D	103	CDL	OB8-CB7-C71	3.12	119.55	111.38
13	1	102	BCL	CBC-CAC-C3C	-3.12	106.53	113.47
13	Q	101	BCL	O2D-CGD-O1D	-3.11	117.75	123.84
15	7	103	UQ8	C17-C18-C19	-3.11	120.17	127.66
13	5	102	BCL	CHD-C4C-NC	3.11	128.53	125.08
13	S	101	BCL	CMC-C2C-C3C	3.11	126.36	113.83
13	Q	101	BCL	CBA-CAA-C2A	-3.11	104.69	113.86
13	A	101	BCL	CMC-C2C-C3C	3.11	126.35	113.83
13	M	402	BCL	C2A-C1A-CHA	-3.10	118.43	123.86
13	I	102	BCL	CHD-C4C-NC	3.10	128.52	125.08
19	V	101	CRT	C21-C20-C19	-3.10	117.12	123.47
13	9	103	BCL	C4-C3-C5	3.10	120.48	115.27
13	K	101	BCL	CMC-C2C-C3C	3.10	126.32	113.83
19	Q	103	CRT	C5-C6-C7	-3.09	121.22	125.89
13	F	102	BCL	CMD-C2D-C3D	3.09	130.47	124.68
13	5	102	BCL	C4-C3-C5	3.09	120.47	115.27
13	7	101	BCL	C1-C2-C3	-3.08	120.71	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	301	BCL	CMC-C2C-C3C	3.08	126.25	113.83
13	5	101	BCL	C1-O2A-CGA	3.08	124.52	116.44
13	S	102	BCL	C4-C3-C5	3.07	120.43	115.27
19	P	101	CRT	C10-C9-C7	-3.06	122.94	127.31
13	F	101	BCL	CHD-C4C-NC	3.06	128.48	125.08
19	Z	101	CRT	C21-C20-C19	-3.06	117.20	123.47
13	U	102	BCL	CED-O2D-CGD	3.06	122.86	115.94
13	Z	102	BCL	CMC-C2C-C3C	3.06	126.16	113.83
13	0	102	BCL	CHD-C4C-NC	3.06	128.47	125.08
13	0	102	BCL	O2A-CGA-CBA	3.05	121.49	111.91
13	F	102	BCL	CBC-CAC-C3C	-3.04	106.69	113.47
13	F	102	BCL	CMB-C2B-C1B	-3.04	123.79	128.46
13	5	102	BCL	CMD-C2D-C3D	3.04	130.36	124.68
13	S	101	BCL	CMB-C2B-C3B	3.04	130.36	124.68
13	9	103	BCL	CMB-C2B-C3B	3.03	130.35	124.68
22	H	302	CDL	OB8-CB7-C71	3.03	121.41	111.91
13	K	101	BCL	CBC-CAC-C3C	-3.03	106.73	113.47
19	9	102	CRT	C5-C6-C7	-3.02	121.32	125.89
15	L	308	UQ8	C35-C34-C36	3.02	120.36	115.27
13	M	401	BCL	CMB-C2B-C1B	-3.02	123.82	128.46
13	Q	102	BCL	C1-C2-C3	-3.02	120.82	126.04
15	7	103	UQ8	O5-C5-C6	-3.02	116.25	121.55
13	S	102	BCL	O2D-CGD-CBD	3.02	116.63	111.27
13	U	102	BCL	C4-C3-C5	3.02	120.34	115.27
13	Z	102	BCL	C1-C2-C3	-3.01	120.83	126.04
14	M	404	BPH	CBB-CAB-C3B	-3.01	114.00	120.43
13	K	101	BCL	O2D-CGD-O1D	-3.00	117.97	123.84
13	S	101	BCL	C1C-NC-C4C	-3.00	105.36	106.71
13	O	101	BCL	CMC-C2C-C3C	3.00	125.93	113.83
13	W	101	BCL	CMB-C2B-C3B	3.00	130.29	124.68
19	9	101	CRT	C10-C9-C7	-3.00	123.03	127.31
13	I	102	BCL	CMC-C2C-C3C	2.99	125.90	113.83
13	D	102	BCL	C4-C3-C5	2.99	120.30	115.27
13	7	102	BCL	C4A-NA-C1A	-2.98	105.36	106.71
19	9	101	CRT	C20-C19-C17	-2.98	123.05	127.31
19	V	101	CRT	C10-C9-C7	-2.98	123.06	127.31
13	1	101	BCL	CMC-C2C-C3C	2.98	125.85	113.83
22	H	302	CDL	CA6-CA4-CA3	-2.98	104.74	111.79
13	0	102	BCL	C4-C3-C5	2.98	120.28	115.27
13	D	101	BCL	O2D-CGD-O1D	-2.98	118.01	123.84
13	Z	102	BCL	C3C-C4C-CHD	-2.98	117.03	123.39
13	W	102	BCL	C4-C3-C5	2.97	120.28	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	9	101	CRT	C21-C20-C19	-2.97	117.39	123.47
18	M	405	MQ8	C24-C23-C25	2.97	120.27	115.27
23	F	103	LMT	O5'-C1'-C2'	2.97	116.63	110.35
13	M	401	BCL	O2A-CGA-CBA	2.96	121.21	111.91
19	M	406	CRT	C14-C15-C16	-2.96	113.97	123.22
15	L	308	UQ8	C22-C23-C24	-2.96	120.53	127.66
13	F	101	BCL	CMC-C2C-C3C	2.96	125.75	113.83
13	I	101	BCL	CMB-C2B-C1B	-2.95	123.93	128.46
13	W	102	BCL	CMC-C2C-C3C	2.94	125.71	113.83
13	1	102	BCL	C2C-C3C-C4C	-2.94	96.93	101.34
19	Z	101	CRT	C5-C6-C7	-2.94	121.45	125.89
13	W	101	BCL	C4-C3-C5	2.94	120.22	115.27
14	M	404	BPH	CBA-CAA-C2A	-2.94	105.19	113.86
23	F	103	LMT	C1'-C2'-C3'	2.94	116.12	110.00
19	J	101	CRT	C5-C6-C7	-2.94	121.45	125.89
13	5	101	BCL	CMC-C2C-C3C	2.94	125.67	113.83
22	Q	104	CDL	CA4-OA6-CA5	-2.93	110.57	117.79
13	W	102	BCL	CMB-C2B-C3B	2.93	130.17	124.68
13	L	301	BCL	O2D-CGD-O1D	-2.93	118.10	123.84
14	L	302	BPH	CMB-C2B-C1B	2.93	129.57	125.06
12	L	306	PGV	O03-C19-C20	2.93	121.09	111.91
13	F	101	BCL	CMB-C2B-C3B	2.93	130.15	124.68
13	S	101	BCL	CBC-CAC-C3C	-2.92	106.96	113.47
13	K	102	BCL	C4-C3-C5	2.92	120.19	115.27
19	N	101	CRT	C34-C33-C35	2.92	122.67	118.08
13	I	101	BCL	C1-O2A-CGA	2.92	124.09	116.44
15	L	308	UQ8	C27-C28-C29	-2.91	120.64	127.66
13	7	102	BCL	C4-C3-C5	2.91	120.17	115.27
15	7	103	UQ8	C20-C19-C21	2.91	120.17	115.27
13	Q	102	BCL	C2C-C3C-C4C	-2.91	96.98	101.34
13	M	402	BCL	CHD-C4C-NC	2.91	128.31	125.08
13	I	102	BCL	O2D-CGD-O1D	-2.91	118.15	123.84
13	K	102	BCL	CBC-CAC-C3C	-2.90	107.00	113.47
13	7	101	BCL	CMC-C2C-C3C	2.90	125.54	113.83
13	M	402	BCL	C1-C2-C3	-2.90	121.03	126.04
13	1	102	BCL	CMB-C2B-C3B	2.90	130.10	124.68
19	J	101	CRT	C32-C31-C30	-2.89	114.19	123.22
13	F	102	BCL	C4-C3-C5	2.89	120.14	115.27
15	L	308	UQ8	C10-C9-C11	2.89	120.14	115.27
13	9	103	BCL	CMC-C2C-C3C	2.89	125.49	113.83
13	1	101	BCL	CBC-CAC-C3C	-2.89	107.04	113.47
13	M	401	BCL	CMC-C2C-C3C	2.88	125.45	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L	302	BPH	C4A-NA-C1A	-2.88	105.81	108.14
13	5	102	BCL	CMB-C2B-C1B	-2.87	124.05	128.46
13	7	102	BCL	CHD-C4C-NC	2.87	128.26	125.08
13	U	102	BCL	CMC-C2C-C3C	2.87	125.39	113.83
13	M	402	BCL	C1B-CHB-C4A	-2.86	124.44	130.12
13	1	101	BCL	C4-C3-C5	2.86	120.09	115.27
15	7	103	UQ8	O4-C4-C3	-2.86	112.86	123.64
13	D	102	BCL	CMC-C2C-C3C	2.85	125.34	113.83
13	F	102	BCL	O2D-CGD-O1D	-2.85	118.26	123.84
13	Y	101	BCL	CMC-C2C-C3C	2.85	125.33	113.83
13	A	103	BCL	CMC-C2C-C3C	2.85	125.32	113.83
13	M	402	BCL	C1-O2A-CGA	2.85	123.92	116.44
15	L	308	UQ8	C7-C8-C9	-2.85	122.05	126.79
13	3	101	BCL	C4-C3-C5	2.85	120.06	115.27
13	S	101	BCL	C4-C3-C5	2.84	120.06	115.27
22	H	304	CDL	CB4-OB6-CB5	-2.84	110.79	117.79
19	Z	101	CRT	C32-C31-C30	-2.84	114.36	123.22
13	I	102	BCL	CBC-CAC-C3C	-2.84	107.15	113.47
13	D	102	BCL	CBC-CAC-C3C	-2.84	107.15	113.47
12	M	413	PGV	O12-P-O11	-2.83	99.19	106.73
18	M	405	MQ8	C26-C27-C28	-2.83	120.84	127.66
19	1	103	CRT	C20-C19-C17	-2.83	123.28	127.31
15	M	417	UQ8	C10-C9-C11	2.82	120.84	114.60
13	W	102	BCL	CMD-C2D-C3D	2.82	129.96	124.68
14	L	302	BPH	O2D-CGD-O1D	-2.82	118.32	123.84
13	I	101	BCL	O2D-CGD-O1D	-2.82	118.32	123.84
19	Q	103	CRT	C14-C15-C16	-2.81	114.44	123.22
19	2	101	CRT	C20-C19-C17	-2.81	123.30	127.31
13	F	102	BCL	CMC-C2C-C3C	2.81	125.14	113.83
22	S	103	CDL	CB6-CB4-CB3	-2.80	105.16	111.79
13	O	102	BCL	C4-C3-C5	2.80	119.98	115.27
19	U	103	CRT	C18-C17-C16	2.80	122.49	118.08
13	Z	102	BCL	CBC-CAC-C3C	-2.80	107.24	113.47
14	M	404	BPH	C3B-C2B-C1B	-2.79	101.80	105.87
14	M	404	BPH	C6-C5-C3	-2.79	106.14	113.45
13	W	101	BCL	CMC-C2C-C3C	2.79	125.08	113.83
20	M	410	PEF	O3P-P-O2P	2.79	116.91	107.97
13	0	102	BCL	CMC-C2C-C3C	2.78	125.06	113.83
19	N	101	CRT	C5-C6-C7	-2.78	121.69	125.89
13	M	403	BCL	O2A-CGA-CBA	2.78	120.64	111.91
13	K	102	BCL	C2C-C3C-C4C	-2.78	97.17	101.34
15	L	308	UQ8	C15-C14-C16	2.78	119.95	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	W	101	BCL	CHD-C4C-NC	2.78	128.16	125.08
13	3	101	BCL	CHD-C4C-NC	2.78	128.16	125.08
12	A	105	PGV	O03-C19-C20	2.77	120.61	111.91
13	Z	102	BCL	C2C-C3C-C4C	-2.77	97.18	101.34
13	K	101	BCL	CHD-C4C-NC	2.77	128.16	125.08
19	6	101	CRT	C10-C9-C7	-2.77	123.35	127.31
14	L	302	BPH	O2D-CGD-CBD	2.77	116.19	111.27
13	I	102	BCL	CMB-C2B-C1B	-2.77	124.21	128.46
14	L	302	BPH	C2B-C1B-NB	2.76	113.95	109.79
13	5	101	BCL	OBD-CAD-C3D	-2.76	123.41	127.98
12	D	104	PGV	O01-C1-C2	2.76	117.44	111.50
19	6	101	CRT	C14-C15-C16	-2.75	114.63	123.22
19	O	103	CRT	C26-C27-C28	-2.75	123.38	127.31
13	D	101	BCL	CBC-CAC-C3C	-2.75	107.34	113.47
14	L	302	BPH	C4-C3-C5	2.75	119.89	115.27
22	H	304	CDL	OB8-CB7-C71	2.75	120.53	111.91
19	N	101	CRT	C21-C20-C19	-2.75	117.85	123.47
13	M	401	BCL	CBC-CAC-C3C	-2.75	107.36	113.47
13	Y	101	BCL	C1-O2A-CGA	2.74	123.64	116.44
13	1	101	BCL	CMB-C2B-C3B	2.74	129.81	124.68
14	M	404	BPH	C4D-CHA-C1A	-2.74	123.75	130.51
13	7	101	BCL	O2D-CGD-O1D	-2.74	118.48	123.84
13	Q	101	BCL	C1C-NC-C4C	-2.74	105.47	106.71
13	O	102	BCL	CBC-CAC-C3C	-2.74	107.37	113.47
13	3	102	BCL	CMC-C2C-C3C	2.74	124.88	113.83
12	D	104	PGV	O03-C19-O04	-2.74	116.68	123.59
15	7	103	UQ8	C7-C6-C5	2.74	121.77	118.48
13	O	102	BCL	C2A-C1A-CHA	-2.74	119.08	123.86
19	M	406	CRT	C5-C6-C7	-2.73	121.76	125.89
13	Z	102	BCL	CMB-C2B-C3B	2.73	129.79	124.68
19	U	103	CRT	C32-C31-C30	-2.73	114.70	123.22
13	1	102	BCL	CMC-C2C-C3C	2.73	124.83	113.83
13	K	102	BCL	CMD-C2D-C3D	2.73	129.78	124.68
15	L	308	UQ8	C1M-C1-C6	-2.72	119.96	124.40
13	F	101	BCL	O2D-CGD-O1D	-2.72	118.52	123.84
19	U	103	CRT	C20-C19-C17	-2.72	123.43	127.31
13	1	101	BCL	CHD-C4C-NC	2.72	128.09	125.08
13	A	101	BCL	C4-C3-C5	2.71	119.84	115.27
14	L	302	BPH	CBC-CAC-C3C	-2.71	107.42	113.47
19	J	101	CRT	C18-C17-C16	2.71	122.35	118.08
13	Q	102	BCL	CMC-C2C-C3C	2.71	124.77	113.83
15	7	103	UQ8	C22-C23-C24	-2.71	118.49	127.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	3	101	BCL	C2A-C1A-CHA	-2.71	119.12	123.86
19	9	102	CRT	C21-C20-C19	-2.71	117.93	123.47
19	V	101	CRT	C14-C15-C16	-2.70	114.78	123.22
14	L	302	BPH	CMC-C2C-C3C	2.70	124.73	113.83
13	1	101	BCL	O2D-CGD-O1D	-2.70	118.56	123.84
22	K	103	CDL	OA8-CA7-C31	2.69	120.36	111.91
13	Q	101	BCL	C6-C5-C3	-2.69	106.40	113.45
12	C	509	PGV	O03-C19-C20	2.69	120.35	111.91
13	U	101	BCL	CMC-C2C-C3C	2.69	124.68	113.83
13	5	102	BCL	CMC-C2C-C3C	2.69	124.67	113.83
12	H	303	PGV	O03-C19-C20	2.68	120.32	111.91
12	1	105	PGV	O03-C19-C20	2.68	120.31	111.91
13	L	301	BCL	CMC-C2C-C1C	2.68	118.97	111.77
18	M	405	MQ8	C41-C42-C43	-2.67	121.22	127.66
19	G	101	CRT	C14-C15-C16	-2.67	114.88	123.22
13	F	101	BCL	C1-O2A-CGA	2.67	123.45	116.44
13	0	102	BCL	C6-C5-C3	-2.67	106.46	113.45
19	A	104	CRT	C20-C19-C17	-2.66	123.51	127.31
13	F	101	BCL	C4-C3-C5	2.66	119.75	115.27
13	7	101	BCL	CMB-C2B-C1B	-2.66	124.37	128.46
19	M	406	CRT	C32-C31-C30	-2.66	114.90	123.22
15	L	308	UQ8	C20-C19-C21	2.66	119.75	115.27
13	K	102	BCL	CMC-C2C-C3C	2.66	124.56	113.83
19	U	103	CRT	C10-C9-C7	-2.66	123.51	127.31
12	D	104	PGV	O03-C19-C20	2.66	120.25	111.91
13	U	102	BCL	CAC-C3C-C2C	2.66	120.90	114.26
13	D	101	BCL	CHD-C4C-NC	2.66	128.03	125.08
12	A	105	PGV	C02-O01-C1	-2.65	111.25	117.79
13	7	102	BCL	CMC-C2C-C3C	2.65	124.52	113.83
13	1	102	BCL	C3C-C4C-CHD	-2.65	117.73	123.39
19	2	101	CRT	C32-C31-C30	-2.64	114.96	123.22
13	O	102	BCL	CMD-C2D-C3D	2.64	129.63	124.68
13	0	102	BCL	CMD-C2D-C3D	2.64	129.63	124.68
22	Q	104	CDL	OB8-CB7-C71	2.64	120.19	111.91
13	M	403	BCL	CAC-C3C-C2C	2.64	120.85	114.26
13	I	101	BCL	CHD-C4C-NC	2.64	128.01	125.08
12	M	414	PGV	C02-O01-C1	-2.64	111.30	117.79
13	D	101	BCL	O2A-CGA-CBA	2.63	120.17	111.91
19	Z	101	CRT	C29-C28-C30	2.62	122.21	118.08
13	M	402	BCL	CBC-CAC-C3C	-2.62	107.63	113.47
13	7	101	BCL	O1D-CGD-CBD	-2.62	119.12	124.48
13	S	101	BCL	CHC-C1C-NC	2.62	128.13	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	5	101	BCL	CBC-CAC-C3C	-2.62	107.64	113.47
13	Q	102	BCL	O2A-CGA-CBA	2.60	120.08	111.91
19	P	101	CRT	C32-C31-C30	-2.60	115.09	123.22
23	F	103	LMT	C1B-O5B-C5B	2.60	118.78	113.69
18	M	405	MQ8	C50-C48-C49	2.60	120.34	114.60
13	U	101	BCL	CGD-CBD-CAD	-2.59	102.33	110.73
13	1	102	BCL	O2D-CGD-O1D	-2.59	118.77	123.84
13	Z	102	BCL	C4-C3-C5	2.59	119.63	115.27
13	Z	102	BCL	CMD-C2D-C3D	2.59	129.53	124.68
19	M	406	CRT	C20-C19-C17	-2.59	123.61	127.31
19	0	101	CRT	C10-C9-C7	-2.59	123.61	127.31
13	3	102	BCL	CMD-C2D-C3D	2.59	129.52	124.68
13	I	102	BCL	C4-C3-C5	2.59	119.63	115.27
13	I	102	BCL	CMB-C2B-C3B	2.59	129.52	124.68
13	O	102	BCL	CAC-C3C-C2C	2.59	120.72	114.26
19	P	101	CRT	C14-C15-C16	-2.58	115.15	123.22
12	3	104	PGV	O03-C19-C20	2.58	120.01	111.91
7	C	502	HEC	C3B-C4B-NB	-2.58	106.08	110.94
19	A	104	CRT	C14-C15-C16	-2.58	115.18	123.22
19	9	101	CRT	C32-C31-C30	-2.57	115.18	123.22
13	M	401	BCL	C1-C2-C3	-2.57	121.59	126.04
13	O	102	BCL	O2D-CGD-O1D	-2.57	118.81	123.84
13	Z	102	BCL	O2D-CGD-O1D	-2.57	118.81	123.84
19	Z	101	CRT	C9-C10-C11	-2.57	115.19	123.22
22	D	103	CDL	CB4-OB6-CB5	-2.57	111.47	117.79
13	7	102	BCL	CBC-CAC-C3C	-2.57	107.75	113.47
7	C	504	HEC	C3B-C4B-NB	-2.57	106.10	110.94
14	L	302	BPH	CBB-CAB-C3B	-2.56	114.95	120.43
19	1	103	CRT	C21-C20-C19	-2.56	118.23	123.47
15	L	308	UQ8	C17-C18-C19	-2.56	121.50	127.66
19	O	103	CRT	C21-C22-C23	-2.56	123.66	127.31
19	G	101	CRT	C21-C20-C19	-2.56	118.24	123.47
13	M	402	BCL	O2D-CGD-O1D	-2.55	118.85	123.84
13	W	101	BCL	CBC-CAC-C3C	-2.55	107.78	113.47
13	U	101	BCL	C2A-C1A-CHA	-2.55	119.40	123.86
19	A	104	CRT	C10-C9-C7	-2.55	123.67	127.31
19	A	104	CRT	C32-C31-C30	-2.55	115.27	123.22
13	L	301	BCL	C1C-NC-C4C	-2.55	105.56	106.71
13	9	103	BCL	O2A-CGA-O1A	-2.54	117.18	123.59
22	S	103	CDL	OA8-CA7-C31	2.54	119.88	111.91
19	0	101	CRT	C32-C31-C30	-2.54	115.30	123.22
19	U	103	CRT	C5-C6-C7	-2.54	122.06	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	U	103	CRT	C14-C15-C16	-2.53	115.31	123.22
13	Q	101	BCL	O1D-CGD-CBD	-2.53	119.30	124.48
13	Q	101	BCL	OBD-CAD-C3D	-2.53	123.78	127.98
13	O	101	BCL	CMB-C2B-C1B	-2.53	124.57	128.46
12	L	305	PGV	O03-C19-C20	2.53	119.85	111.91
13	0	102	BCL	CBC-CAC-C3C	-2.53	107.83	113.47
15	7	103	UQ8	O4-C4-C5	2.53	125.11	116.56
18	M	405	MQ8	C39-C38-C40	2.53	119.52	115.27
13	K	101	BCL	O2A-CGA-CBA	2.52	119.83	111.91
12	M	413	PGV	O14-P-O13	2.52	120.56	110.68
13	S	101	BCL	C1-C2-C3	-2.52	121.68	126.04
19	U	103	CRT	C21-C20-C19	-2.52	118.31	123.47
13	I	102	BCL	O2A-CGA-CBA	2.52	119.81	111.91
12	H	303	PGV	O01-C1-O02	-2.52	117.61	123.70
13	M	403	BCL	CMB-C2B-C3B	2.52	129.39	124.68
19	6	101	CRT	C13-C12-C11	2.52	122.05	118.08
14	L	302	BPH	C6-C5-C3	-2.52	106.86	113.45
20	M	408	PEF	O2P-P-O1P	2.51	120.08	110.89
13	O	102	BCL	CMC-C2C-C3C	2.51	123.96	113.83
15	M	417	UQ8	C4M-O4-C4	2.51	125.36	116.47
23	F	103	LMT	O5'-C5'-C4'	2.51	115.04	109.75
13	5	101	BCL	CHD-C4C-NC	2.51	127.86	125.08
19	6	101	CRT	C21-C20-C19	-2.50	118.34	123.47
13	L	301	BCL	O2A-CGA-O1A	-2.50	117.29	123.59
13	1	102	BCL	O2A-CGA-CBA	2.50	119.75	111.91
22	H	304	CDL	OA8-CA7-C31	2.50	119.74	111.91
13	I	101	BCL	CMB-C2B-C3B	2.50	129.35	124.68
13	S	102	BCL	C2C-C3C-C4C	-2.50	97.60	101.34
13	D	102	BCL	O2A-CGA-CBA	2.49	119.74	111.91
13	M	403	BCL	O2A-CGA-O1A	-2.49	117.30	123.59
13	3	102	BCL	C4-C3-C5	2.49	119.46	115.27
13	7	102	BCL	CMD-C2D-C3D	2.49	129.34	124.68
13	M	402	BCL	C3A-C2A-C1A	-2.49	97.61	101.34
13	W	102	BCL	CBC-CAC-C3C	-2.49	107.93	113.47
13	I	102	BCL	C6-C5-C3	-2.48	106.94	113.45
7	C	504	HEC	CBA-CAA-C2A	-2.48	107.90	112.48
7	C	503	HEC	C3B-C4B-NB	-2.48	106.26	110.94
7	C	501	HEC	C3B-C4B-NB	-2.48	106.26	110.94
19	V	101	CRT	C29-C28-C30	2.48	121.99	118.08
19	G	101	CRT	C9-C10-C11	-2.48	115.48	123.22
12	M	413	PGV	O03-C19-C20	2.48	119.68	111.91
13	M	403	BCL	OBD-CAD-CBD	2.48	129.43	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	M	419	LMT	C1B-O1B-C4'	-2.47	111.84	117.96
19	9	102	CRT	C24-C23-C22	-2.47	119.46	122.92
19	9	101	CRT	C5-C6-C7	-2.47	122.16	125.89
13	7	101	BCL	CAC-C3C-C2C	2.47	120.43	114.26
15	L	303	UQ8	C10-C9-C11	2.47	119.42	115.27
13	7	101	BCL	CMB-C2B-C3B	2.47	129.29	124.68
13	7	102	BCL	CMB-C2B-C3B	2.47	129.29	124.68
13	F	101	BCL	CBC-CAC-C3C	-2.47	107.98	113.47
13	F	102	BCL	CMB-C2B-C3B	2.47	129.29	124.68
13	M	403	BCL	CHA-C1A-NA	-2.46	120.75	126.40
15	L	308	UQ8	C3M-O3-C3	2.46	125.20	116.47
18	M	405	MQ8	C36-C37-C38	-2.46	121.73	127.66
19	O	103	CRT	C32-C31-C30	-2.46	115.55	123.22
13	W	101	BCL	O2A-CGA-CBA	2.46	119.62	111.91
15	L	309	UQ8	C10-C9-C11	2.46	120.03	114.60
13	K	102	BCL	O2A-CGA-CBA	2.45	119.61	111.91
13	1	101	BCL	C2A-C1A-CHA	-2.45	119.57	123.86
18	M	405	MQ8	C45-C43-C44	2.45	119.40	115.27
19	O	103	CRT	C29-C28-C30	2.45	121.94	118.08
13	M	403	BCL	OBD-CAD-C3D	-2.45	123.92	127.98
20	M	409	PEF	O3P-P-O1P	-2.44	101.95	110.89
19	9	101	CRT	C13-C12-C11	2.44	121.93	118.08
19	2	101	CRT	C18-C17-C16	2.44	121.93	118.08
19	J	101	CRT	C18-C17-C19	-2.44	119.50	122.92
13	5	102	BCL	C1-C2-C3	-2.44	121.83	126.04
13	Z	102	BCL	CHD-C4C-NC	2.44	127.78	125.08
13	W	101	BCL	C2A-C1A-CHA	-2.44	119.60	123.86
20	K	104	PEF	O3-C30-C31	2.44	119.55	111.91
19	2	101	CRT	C5-C6-C7	-2.43	122.22	125.89
13	A	103	BCL	O2A-CGA-CBA	2.43	119.53	111.91
15	L	308	UQ8	C25-C24-C26	2.43	119.36	115.27
13	3	102	BCL	CBC-CAC-C3C	-2.43	108.06	113.47
15	7	103	UQ8	O5-C5-C4	2.43	126.08	120.93
13	Q	102	BCL	C2A-C1A-CHA	-2.43	119.62	123.86
19	9	102	CRT	C14-C15-C16	-2.42	115.66	123.22
13	O	101	BCL	C4-C3-C5	2.42	119.35	115.27
13	Q	101	BCL	C1-O2A-CGA	2.42	122.80	116.44
13	M	401	BCL	O2A-CGA-O1A	-2.42	117.48	123.59
19	9	101	CRT	C14-C15-C16	-2.42	115.68	123.22
13	W	102	BCL	CMB-C2B-C1B	-2.42	124.75	128.46
13	U	101	BCL	CAC-C3C-C2C	2.41	120.27	114.26
13	D	101	BCL	C1-C2-C3	-2.41	121.88	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	O	103	CRT	C14-C15-C16	-2.41	115.71	123.22
13	Y	101	BCL	CHA-C1A-NA	-2.40	120.89	126.40
13	3	101	BCL	CMB-C2B-C3B	2.40	129.18	124.68
13	Q	102	BCL	CED-O2D-CGD	2.40	121.36	115.94
19	A	104	CRT	C21-C20-C19	-2.40	118.56	123.47
19	9	101	CRT	C36-C35-C33	-2.40	122.27	125.89
13	S	102	BCL	CMC-C2C-C3C	2.39	123.48	113.83
19	O	103	CRT	C10-C9-C7	-2.39	123.90	127.31
13	K	101	BCL	C4-C3-C5	2.39	119.29	115.27
14	L	302	BPH	OBD-CAD-CBD	2.39	129.31	125.89
15	L	308	UQ8	C12-C13-C14	-2.39	121.91	127.66
13	M	402	BCL	OBD-CAD-C3D	-2.38	124.02	127.98
20	3	103	PEF	O3P-P-O1P	-2.38	102.17	110.89
19	P	101	CRT	C13-C12-C11	2.38	121.83	118.08
13	I	101	BCL	CHA-C1A-NA	-2.38	120.95	126.40
22	Q	104	CDL	OA6-CA5-OA7	-2.38	117.95	123.70
13	M	402	BCL	O2A-CGA-CBA	2.38	119.37	111.91
19	2	101	CRT	C9-C10-C11	-2.38	115.80	123.22
19	U	103	CRT	C34-C33-C35	2.38	121.82	118.08
13	S	102	BCL	CMD-C2D-C3D	2.38	129.12	124.68
13	M	402	BCL	C4-C3-C5	2.37	119.26	115.27
19	Q	103	CRT	C32-C31-C30	-2.37	115.81	123.22
13	Z	102	BCL	O2A-CGA-CBA	2.37	119.35	111.91
13	5	101	BCL	O2A-CGA-CBA	2.37	119.35	111.91
20	K	104	PEF	O2-C10-O4	-2.37	117.98	123.70
19	0	101	CRT	C5-C6-C7	-2.37	122.31	125.89
13	W	102	BCL	O2A-CGA-CBA	2.37	119.33	111.91
19	9	102	CRT	C32-C31-C30	-2.36	115.84	123.22
19	O	103	CRT	C8-C7-C9	-2.36	119.61	122.92
19	O	103	CRT	C20-C19-C17	-2.36	123.94	127.31
13	1	101	BCL	O2A-CGA-CBA	2.36	119.32	111.91
15	L	308	UQ8	C30-C29-C31	2.36	119.24	115.27
13	1	102	BCL	C1-C2-C3	-2.36	121.97	126.04
13	1	102	BCL	C4-C3-C5	2.36	119.23	115.27
13	F	101	BCL	O2A-CGA-CBA	2.35	119.29	111.91
13	D	102	BCL	CMD-C2D-C3D	2.35	129.08	124.68
13	D	101	BCL	CHA-C1A-NA	-2.35	121.02	126.40
13	U	101	BCL	O2A-CGA-CBA	2.35	119.28	111.91
19	0	101	CRT	C9-C10-C11	-2.35	115.89	123.22
13	7	101	BCL	C1-O2A-CGA	2.34	122.59	116.44
19	G	101	CRT	C32-C31-C30	-2.34	115.91	123.22
12	M	414	PGV	O03-C19-C20	2.34	119.24	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	403	BCL	C4B-CHC-C1C	-2.34	125.49	130.12
13	A	101	BCL	CHA-C1A-NA	-2.34	121.05	126.40
13	1	102	BCL	CMD-C2D-C3D	2.34	129.05	124.68
14	L	302	BPH	C1C-NC-C4C	-2.34	108.49	110.54
13	A	101	BCL	C1-C2-C3	-2.33	122.01	126.04
13	I	102	BCL	C2A-C1A-CHA	-2.33	119.78	123.86
13	5	101	BCL	C4-C3-C5	2.33	119.19	115.27
22	K	103	CDL	CA4-OA6-CA5	-2.33	112.05	117.79
18	M	405	MQ8	C34-C33-C35	2.33	119.19	115.27
13	U	102	BCL	CAA-CBA-CGA	-2.33	106.45	113.25
13	5	101	BCL	OBD-CAD-CBD	2.33	129.22	125.89
19	G	101	CRT	C18-C17-C16	2.32	121.73	118.08
13	S	102	BCL	CAC-C3C-C2C	2.32	120.05	114.26
22	H	304	CDL	OB6-CB5-OB7	-2.32	118.10	123.70
15	L	303	UQ8	C25-C24-C26	2.32	119.72	114.60
19	U	103	CRT	C26-C27-C28	-2.32	124.01	127.31
13	K	101	BCL	CHA-C1A-NA	-2.31	121.11	126.40
13	0	102	BCL	C1-C2-C3	-2.30	122.06	126.04
12	M	413	PGV	O01-C1-C2	2.30	116.46	111.50
13	Q	101	BCL	C1-C2-C3	-2.30	122.06	126.04
13	I	102	BCL	CMD-C2D-C3D	2.30	128.98	124.68
13	Z	102	BCL	CMB-C2B-C1B	-2.30	124.93	128.46
13	9	103	BCL	C2A-C1A-CHA	-2.30	119.84	123.86
19	6	101	CRT	C9-C10-C11	-2.30	116.04	123.22
13	Z	102	BCL	CHA-C1A-NA	-2.30	121.13	126.40
14	M	404	BPH	CGD-CBD-CAD	-2.30	103.28	110.73
19	6	101	CRT	C32-C31-C30	-2.30	116.04	123.22
23	F	103	LMT	O5B-C5B-C6B	2.30	112.15	106.44
23	F	103	LMT	O1B-C4'-C5'	-2.30	103.15	109.45
13	A	101	BCL	O2A-CGA-CBA	2.29	119.11	111.91
19	N	101	CRT	C24-C23-C22	-2.29	119.71	122.92
13	D	102	BCL	C1-C2-C3	-2.29	122.08	126.04
19	P	101	CRT	C21-C20-C19	-2.29	118.78	123.47
19	Q	103	CRT	C9-C10-C11	-2.29	116.07	123.22
13	3	102	BCL	CHD-C4C-NC	2.28	127.61	125.08
13	1	101	BCL	C2C-C3C-C4C	-2.28	97.92	101.34
13	M	401	BCL	C2A-C1A-CHA	-2.28	119.87	123.86
19	2	101	CRT	C29-C28-C30	2.28	121.67	118.08
15	7	103	UQ8	C10-C9-C11	2.28	119.10	115.27
13	A	101	BCL	CMB-C2B-C1B	-2.28	124.97	128.46
19	2	101	CRT	C35-C33-C32	-2.27	115.45	118.94
20	W	103	PEF	O4P-P-O1P	-2.27	102.58	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	3	101	BCL	CBC-CAC-C3C	-2.27	108.41	113.47
22	Q	104	CDL	CB4-OB6-CB5	-2.27	112.20	117.79
13	3	101	BCL	CHC-C1C-NC	2.27	127.65	124.51
13	S	101	BCL	O1D-CGD-CBD	-2.27	119.84	124.48
18	M	405	MQ8	C14-C13-C15	2.27	119.09	115.27
13	O	101	BCL	C2A-C1A-CHA	-2.27	119.89	123.86
13	O	101	BCL	CHA-C1A-NA	-2.27	121.21	126.40
19	J	101	CRT	C21-C20-C19	-2.27	118.83	123.47
13	U	101	BCL	C1-O2A-CGA	2.26	122.37	116.44
19	M	406	CRT	C10-C9-C7	-2.26	124.08	127.31
19	Z	101	CRT	C26-C27-C28	-2.26	124.09	127.31
20	M	407	PEF	O4P-P-O1P	-2.26	102.63	110.89
13	L	301	BCL	O2A-CGA-CBA	2.26	118.98	111.91
13	K	102	BCL	C1-C2-C3	-2.25	122.14	126.04
13	F	102	BCL	CHA-C1A-NA	-2.25	121.24	126.40
19	Z	101	CRT	C18-C17-C16	2.25	121.62	118.08
7	C	501	HEC	CBD-CAD-C3D	-2.25	108.33	112.49
19	1	103	CRT	C32-C31-C30	-2.25	116.19	123.22
13	1	101	BCL	CMB-C2B-C1B	-2.25	125.01	128.46
19	N	101	CRT	C9-C10-C11	-2.25	116.20	123.22
13	A	101	BCL	C2A-C1A-CHA	-2.25	119.93	123.86
18	M	405	MQ8	C2M-C2-C3	-2.24	120.74	124.40
13	5	102	BCL	O2A-CGA-CBA	2.24	118.95	111.91
13	K	102	BCL	O2D-CGD-O1D	-2.24	119.45	123.84
13	3	101	BCL	C1-O2A-CGA	2.24	122.33	116.44
19	1	103	CRT	C14-C15-C16	-2.24	116.22	123.22
19	O	103	CRT	C9-C10-C11	-2.24	116.22	123.22
13	A	101	BCL	C1-O2A-CGA	2.24	122.32	116.44
13	L	301	BCL	C2A-C1A-CHA	-2.24	119.94	123.86
19	Z	101	CRT	C14-C15-C16	-2.24	116.23	123.22
13	L	301	BCL	OBD-CAD-CBD	2.24	129.09	125.89
13	F	101	BCL	CHA-C1A-NA	-2.24	121.28	126.40
22	K	103	CDL	OB6-CB5-OB7	-2.24	118.30	123.70
23	F	103	LMT	C3B-C4B-C5B	-2.24	106.25	110.24
20	U	105	PEF	O3P-P-O1P	-2.24	102.72	110.89
14	L	302	BPH	C11-C10-C8	-2.23	108.70	115.92
13	7	101	BCL	C2A-C1A-CHA	-2.23	119.95	123.86
13	5	102	BCL	C2A-C1A-CHA	-2.23	119.96	123.86
22	H	304	CDL	OB4-PB2-OB3	2.23	123.26	112.24
7	C	503	HEC	CMC-C2C-C1C	-2.23	125.04	128.46
15	M	417	UQ8	O5-C5-C6	-2.22	117.65	121.55
13	M	401	BCL	CMD-C2D-C3D	2.22	128.84	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	5	102	BCL	C2C-C3C-C4C	-2.22	98.01	101.34
13	3	102	BCL	O2A-CGA-CBA	2.22	118.88	111.91
15	L	303	UQ8	C6-C1-C2	2.22	120.94	119.18
13	S	102	BCL	C2A-C3A-C4A	-2.22	98.28	101.87
13	5	101	BCL	CHA-C1A-NA	-2.22	121.31	126.40
19	N	101	CRT	C18-C17-C16	2.22	121.58	118.08
22	K	103	CDL	OB8-CB7-OB9	-2.22	117.99	123.59
13	9	103	BCL	O2A-CGA-CBA	2.22	118.87	111.91
19	1	103	CRT	C8-C7-C9	-2.22	119.82	122.92
13	O	102	BCL	O2A-CGA-CBA	2.22	118.86	111.91
13	O	102	BCL	C1B-CHB-C4A	-2.22	125.73	130.12
13	W	102	BCL	C2C-C3C-C4C	-2.21	98.02	101.34
13	U	101	BCL	CHA-C1A-NA	-2.21	121.33	126.40
13	Y	101	BCL	C4-C3-C5	2.21	118.98	115.27
13	F	102	BCL	CHC-C1C-NC	2.21	127.56	124.51
13	3	102	BCL	CHA-C1A-NA	-2.21	121.35	126.40
19	N	101	CRT	C10-C9-C7	-2.20	124.17	127.31
13	A	103	BCL	CED-O2D-CGD	2.20	120.92	115.94
22	H	302	CDL	OB6-CB5-OB7	-2.20	118.38	123.70
19	V	101	CRT	C31-C32-C33	-2.20	124.17	127.31
13	A	103	BCL	CMD-C2D-C3D	2.20	128.79	124.68
20	U	104	PEF	O4P-P-O1P	-2.20	102.84	110.89
22	S	103	CDL	OB4-PB2-OB3	2.20	123.12	112.24
13	1	102	BCL	CMB-C2B-C1B	-2.20	125.09	128.46
19	J	101	CRT	C34-C33-C35	2.20	121.54	118.08
14	M	404	BPH	CAC-C3C-C2C	2.19	119.74	114.26
19	J	101	CRT	C10-C9-C7	-2.19	124.18	127.31
13	0	102	BCL	O2A-CGA-O1A	-2.19	118.07	123.59
22	S	103	CDL	OA6-CA5-OA7	-2.19	118.41	123.70
13	7	101	BCL	C4-C3-C5	2.19	118.95	115.27
7	C	503	HEC	CMB-C2B-C1B	-2.19	125.10	128.46
22	D	103	CDL	CA4-OA6-CA5	-2.19	112.41	117.79
13	U	101	BCL	CHC-C1C-NC	2.18	127.53	124.51
15	7	103	UQ8	C25-C24-C26	2.18	119.42	114.60
13	1	101	BCL	C1-O2A-CGA	2.18	122.17	116.44
13	S	102	BCL	C1-O2A-CGA	2.18	122.17	116.44
19	9	101	CRT	C26-C27-C28	-2.18	124.20	127.31
20	1	104	PEF	O3P-P-O1P	-2.18	102.92	110.89
13	U	101	BCL	C4B-CHC-C1C	-2.18	125.80	130.12
13	Y	101	BCL	CMB-C2B-C3B	2.18	128.75	124.68
13	S	102	BCL	C2A-C1A-CHA	-2.17	120.06	123.86
13	A	101	BCL	O2A-CGA-O1A	-2.17	118.10	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	102	BCL	CHC-C1C-NC	2.17	127.52	124.51
20	5	103	PEF	O4P-P-O1P	-2.17	102.95	110.89
22	H	302	CDL	CA4-OA6-CA5	-2.17	112.44	117.79
19	N	101	CRT	C20-C19-C17	-2.17	124.21	127.31
13	U	101	BCL	O2A-CGA-O1A	-2.17	118.11	123.59
13	U	102	BCL	O2A-CGA-CBA	2.17	118.72	111.91
13	U	102	BCL	O2D-CGD-O1D	-2.17	119.59	123.84
19	N	101	CRT	C32-C31-C30	-2.17	116.45	123.22
13	F	102	BCL	O2A-CGA-CBA	2.17	118.71	111.91
7	C	503	HEC	CAA-CBA-CGA	-2.17	109.04	112.67
19	N	101	CRT	C35-C33-C32	-2.16	115.62	118.94
13	5	101	BCL	CMB-C2B-C1B	-2.16	125.14	128.46
13	A	101	BCL	CHC-C1C-NC	2.16	127.50	124.51
19	V	101	CRT	C18-C17-C16	2.16	121.48	118.08
13	A	101	BCL	CBC-CAC-C3C	-2.16	108.66	113.47
13	K	102	BCL	CHA-C1A-NA	-2.16	121.45	126.40
19	N	101	CRT	C27-C26-C25	-2.16	116.47	123.22
13	Q	101	BCL	O2A-CGA-CBA	2.16	118.69	111.91
15	L	308	UQ8	C42-C43-C44	-2.16	120.37	127.75
13	F	102	BCL	C1-C2-C3	-2.16	122.31	126.04
19	Z	101	CRT	C27-C26-C25	-2.16	116.48	123.22
19	V	101	CRT	C27-C26-C25	-2.16	116.48	123.22
13	Q	101	BCL	CHC-C1C-NC	2.16	127.50	124.51
13	L	301	BCL	CMB-C2B-C1B	-2.16	125.15	128.46
23	M	419	LMT	O5B-C5B-C4B	2.16	113.61	109.69
13	Y	101	BCL	O2A-CGA-CBA	2.16	118.67	111.91
20	I	103	PEF	O4P-P-O1P	-2.15	103.01	110.89
13	M	402	BCL	CMD-C2D-C3D	2.15	128.71	124.68
19	J	101	CRT	C26-C27-C28	-2.15	124.24	127.31
13	I	101	BCL	O2A-CGA-CBA	2.15	118.66	111.91
14	M	404	BPH	C4-C3-C2	-2.15	118.16	123.68
13	9	103	BCL	CHA-C1A-NA	-2.15	121.48	126.40
19	Q	103	CRT	C24-C23-C22	-2.15	119.92	122.92
13	D	102	BCL	CHA-C1A-NA	-2.15	121.48	126.40
13	W	101	BCL	O2A-CGA-O1A	-2.15	118.18	123.59
13	M	402	BCL	O2A-CGA-O1A	-2.14	118.18	123.59
19	A	104	CRT	C9-C10-C11	-2.14	116.53	123.22
23	M	419	LMT	C1B-O5B-C5B	2.14	117.89	113.69
22	Q	104	CDL	OA8-CA7-C31	2.14	118.63	111.91
19	9	101	CRT	C8-C7-C9	-2.14	119.92	122.92
18	M	405	MQ8	C21-C20-C18	-2.14	105.94	112.98
13	F	101	BCL	C2A-C1A-CHA	-2.14	120.12	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	9	102	CRT	C9-C10-C11	-2.14	116.55	123.22
19	G	101	CRT	C26-C27-C28	-2.13	124.26	127.31
15	L	303	UQ8	C7-C8-C9	-2.13	123.24	126.79
13	0	102	BCL	CHA-C1A-NA	-2.13	121.52	126.40
19	G	101	CRT	C5-C6-C7	-2.13	122.68	125.89
15	L	303	UQ8	C22-C21-C19	-2.13	105.98	112.98
13	3	101	BCL	O2A-CGA-CBA	2.12	118.57	111.91
19	N	101	CRT	C14-C15-C16	-2.12	116.59	123.22
7	C	504	HEC	CAA-CBA-CGA	2.12	116.23	112.67
13	7	102	BCL	O2A-CGA-CBA	2.12	118.56	111.91
13	A	103	BCL	C2A-C1A-CHA	-2.12	120.15	123.86
13	M	401	BCL	C4B-CHC-C1C	-2.12	125.92	130.12
13	Y	101	BCL	CGD-CBD-CAD	-2.12	103.88	110.73
19	O	103	CRT	C18-C17-C16	2.12	121.41	118.08
13	3	102	BCL	CMB-C2B-C1B	-2.11	125.21	128.46
13	I	101	BCL	CHC-C1C-NC	2.11	127.44	124.51
22	S	103	CDL	OB6-CB5-OB7	-2.11	118.77	122.96
13	I	102	BCL	CHC-C1C-NC	2.11	127.43	124.51
14	M	404	BPH	OBB-CAB-C3B	2.11	124.31	120.41
19	P	101	CRT	C18-C17-C16	2.11	121.40	118.08
22	K	103	CDL	OA6-CA5-OA7	-2.11	118.61	123.70
13	O	101	BCL	C11-C10-C8	-2.11	109.11	115.92
19	9	101	CRT	C39-C38-C37	-2.11	107.62	110.86
19	G	101	CRT	C24-C23-C22	-2.10	119.97	122.92
13	O	101	BCL	CGD-CBD-CAD	-2.10	103.92	110.73
19	U	103	CRT	C35-C33-C32	-2.10	115.71	118.94
19	P	101	CRT	C8-C7-C9	-2.10	119.98	122.92
19	A	104	CRT	C13-C12-C11	2.10	121.38	118.08
19	0	101	CRT	C14-C15-C16	-2.10	116.67	123.22
13	3	102	BCL	C2C-C3C-C4C	-2.10	98.20	101.34
13	5	102	BCL	CMB-C2B-C3B	2.09	128.59	124.68
13	K	102	BCL	OBD-CAD-C3D	-2.09	124.50	127.98
13	Y	101	BCL	CHC-C1C-NC	2.09	127.41	124.51
15	L	308	UQ8	C40-C39-C41	2.09	118.79	115.27
14	L	302	BPH	CMD-C2D-C3D	2.09	128.59	124.68
18	M	405	MQ8	C16-C17-C18	-2.09	122.62	127.66
14	M	404	BPH	C1C-NC-C4C	-2.09	108.70	110.54
13	A	103	BCL	CHA-C1A-NA	-2.09	121.61	126.40
19	M	406	CRT	C9-C10-C11	-2.09	116.70	123.22
13	Q	102	BCL	CAA-CBA-CGA	-2.09	107.16	113.25
13	W	101	BCL	CHA-C1A-NA	-2.09	121.62	126.40
13	Q	101	BCL	CHA-C1A-NA	-2.08	121.63	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	H	304	CDL	OB8-CB7-OB9	-2.08	118.34	123.59
13	M	402	BCL	CMC-C2C-C3C	2.08	122.22	113.83
19	J	101	CRT	C24-C23-C22	-2.08	120.01	122.92
13	D	101	BCL	CMB-C2B-C1B	-2.08	125.27	128.46
19	U	103	CRT	C27-C26-C25	-2.08	116.73	123.22
13	F	101	BCL	C1-C2-C3	-2.08	122.45	126.04
13	7	101	BCL	CHA-C1A-NA	-2.08	121.64	126.40
13	7	102	BCL	CAA-CBA-CGA	-2.08	107.18	113.25
13	U	101	BCL	CBC-CAC-C3C	-2.08	108.84	113.47
13	U	101	BCL	CMD-C2D-C3D	2.08	128.56	124.68
13	K	101	BCL	C1-C2-C3	-2.07	122.46	126.04
13	S	102	BCL	CAA-CBA-CGA	-2.07	107.19	113.25
13	0	102	BCL	C2C-C3C-C4C	-2.07	98.23	101.34
19	G	101	CRT	C29-C28-C30	2.07	121.34	118.08
22	H	302	CDL	C12-C11-CA5	-2.07	106.09	113.62
13	O	101	BCL	CMD-C2D-C3D	2.07	128.55	124.68
13	U	101	BCL	CMB-C2B-C1B	-2.07	125.29	128.46
13	L	301	BCL	CHC-C1C-NC	2.07	127.37	124.51
13	M	401	BCL	CHA-C1A-NA	-2.07	121.67	126.40
20	M	418	PEF	O3-C30-O5	-2.07	118.38	123.59
13	U	102	BCL	C2A-C1A-CHA	-2.07	120.25	123.86
13	I	102	BCL	CHA-C1A-NA	-2.06	121.67	126.40
19	P	101	CRT	C24-C23-C22	-2.06	120.03	122.92
13	K	101	BCL	OBD-CAD-C3D	-2.06	124.56	127.98
13	I	101	BCL	C4-C3-C5	2.06	118.73	115.27
13	D	102	BCL	O2D-CGD-O1D	-2.06	119.82	123.84
15	L	308	UQ8	C4M-O4-C4	2.06	123.76	116.47
19	V	101	CRT	C32-C31-C30	-2.06	116.80	123.22
13	K	101	BCL	CMB-C2B-C3B	2.05	128.52	124.68
13	Q	101	BCL	CBC-CAC-C3C	-2.05	108.90	113.47
19	M	406	CRT	C21-C22-C23	-2.05	124.38	127.31
13	7	102	BCL	C1-C2-C3	-2.05	122.50	126.04
15	L	308	UQ8	C37-C38-C39	-2.05	122.72	127.66
13	7	101	BCL	O2A-CGA-CBA	2.05	118.34	111.91
19	M	406	CRT	C20-C21-C22	2.05	127.67	123.47
15	L	308	UQ8	C46-C44-C45	2.05	119.13	114.60
13	U	102	BCL	C1-C2-C3	-2.05	122.50	126.04
13	M	401	BCL	C4-C3-C5	2.05	118.71	115.27
19	9	102	CRT	C29-C28-C30	2.05	121.30	118.08
13	W	102	BCL	CHC-C1C-NC	2.04	127.34	124.51
19	0	101	CRT	C21-C20-C19	-2.04	119.29	123.47
13	7	102	BCL	OBD-CAD-CBD	2.04	128.81	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	S	102	BCL	C4-C3-C2	-2.04	118.45	123.68
13	F	101	BCL	CHC-C1C-NC	2.04	127.33	124.51
13	D	101	BCL	C2A-C3A-C4A	-2.04	98.58	101.87
19	9	101	CRT	C27-C26-C25	-2.04	116.86	123.22
13	Y	101	BCL	O1D-CGD-CBD	-2.04	120.32	124.48
13	Q	102	BCL	OBD-CAD-CBD	2.03	128.80	125.89
12	D	104	PGV	C3-C2-C1	-2.03	106.24	113.62
13	3	102	BCL	CED-O2D-CGD	2.03	120.53	115.94
19	P	101	CRT	C9-C10-C11	-2.03	116.89	123.22
13	5	102	BCL	CHA-C1A-NA	-2.03	121.76	126.40
19	2	101	CRT	C10-C9-C7	-2.03	124.42	127.31
15	L	309	UQ8	C4M-O4-C4	2.03	123.65	116.47
13	5	101	BCL	C2A-C1A-CHA	-2.03	120.32	123.86
13	O	101	BCL	CBC-CAC-C3C	-2.02	108.96	113.47
13	D	102	BCL	CMB-C2B-C1B	-2.02	125.36	128.46
15	M	417	UQ8	O4-C4-C5	2.02	123.39	116.56
19	G	101	CRT	C24-C23-C25	2.02	121.26	118.08
13	M	401	BCL	O2D-CGD-O1D	-2.02	119.89	123.84
13	I	102	BCL	C1-C2-C3	-2.02	122.55	126.04
13	S	101	BCL	C2A-C1A-CHA	-2.02	120.33	123.86
18	M	405	MQ8	C21-C22-C23	-2.02	122.80	127.66
19	A	104	CRT	C34-C33-C35	2.01	121.25	118.08
19	J	101	CRT	C9-C10-C11	-2.01	116.94	123.22
13	W	101	BCL	CBA-CAA-C2A	-2.01	107.93	113.86
13	W	101	BCL	CGD-CBD-CAD	-2.01	104.23	110.73
22	H	302	CDL	CB2-C1-CA2	-2.01	106.88	112.79
14	M	404	BPH	C4A-NA-C1A	-2.01	106.52	108.14
13	1	102	BCL	CHA-C1A-NA	-2.00	121.81	126.40
13	7	102	BCL	C4B-CHC-C1C	-2.00	126.15	130.12
12	1	105	PGV	C02-O01-C1	-2.00	112.87	117.79

There are no chirality outliers.

All (900) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	K	104	PEF	O4P-C4-C5-N
13	7	101	BCL	C2-C3-C5-C6
13	7	101	BCL	C4-C3-C5-C6
12	L	305	PGV	C04-O12-P-O13
22	Y	103	CDL	CB2-OB2-PB2-OB3
22	Y	103	CDL	CB2-OB2-PB2-OB4
22	Y	103	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
22	Y	103	CDL	CB3-OB5-PB2-OB2
22	Y	103	CDL	CB3-OB5-PB2-OB3
22	Y	103	CDL	CB3-OB5-PB2-OB4
23	F	103	LMT	C2'-C1'-O1'-C1
23	F	103	LMT	O5'-C1'-O1'-C1
18	M	405	MQ8	C33-C35-C36-C37
18	M	405	MQ8	C38-C40-C41-C42
12	L	306	PGV	C03-O11-P-O14
12	L	306	PGV	C04-O12-P-O13
12	L	306	PGV	C04-O12-P-O14
12	L	306	PGV	O12-C04-C05-C06
22	H	304	CDL	O1-C1-CB2-OB2
22	H	304	CDL	CA2-OA2-PA1-OA4
22	H	304	CDL	CA3-OA5-PA1-OA3
12	1	105	PGV	C04-O12-P-O13
21	O	104	LDA	C2-C1-N1-CM1
21	O	104	LDA	C2-C1-N1-CM2
21	O	104	LDA	N1-C1-C2-C3
13	Z	102	BCL	C2C-C3C-CAC-CBC
13	Z	102	BCL	C4C-C3C-CAC-CBC
22	H	302	CDL	CA2-OA2-PA1-OA4
22	H	302	CDL	CA3-OA5-PA1-OA3
22	H	302	CDL	OA7-CA5-OA6-CA4
22	H	302	CDL	C11-CA5-OA6-CA4
22	H	302	CDL	CB2-OB2-PB2-OB3
22	H	302	CDL	CB2-OB2-PB2-OB4
22	H	302	CDL	CB2-OB2-PB2-OB5
13	0	102	BCL	C1A-C2A-CAA-CBA
13	0	102	BCL	C2C-C3C-CAC-CBC
13	0	102	BCL	C4C-C3C-CAC-CBC
12	3	104	PGV	C03-O11-P-O13
12	3	104	PGV	C03-O11-P-O14
12	3	104	PGV	C04-O12-P-O11
13	W	101	BCL	C2C-C3C-CAC-CBC
13	W	101	BCL	C4C-C3C-CAC-CBC
19	V	101	CRT	C5-C6-C7-C8
13	K	102	BCL	C4C-C3C-CAC-CBC
12	H	303	PGV	O03-C01-C02-O01
13	Q	102	BCL	C1A-C2A-CAA-CBA
19	9	101	CRT	C5-C6-C7-C8
12	M	414	PGV	C04-C05-C06-O06
13	I	101	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
13	W	102	BCL	C1A-C2A-CAA-CBA
13	W	102	BCL	C3A-C2A-CAA-CBA
13	W	102	BCL	C4C-C3C-CAC-CBC
13	D	102	BCL	C4C-C3C-CAC-CBC
13	1	101	BCL	C2C-C3C-CAC-CBC
13	1	101	BCL	C4C-C3C-CAC-CBC
13	A	103	BCL	C4C-C3C-CAC-CBC
19	0	101	CRT	C5-C6-C7-C8
13	5	102	BCL	C1A-C2A-CAA-CBA
13	5	102	BCL	C4C-C3C-CAC-CBC
13	5	102	BCL	C11-C12-C13-C14
13	F	102	BCL	C1A-C2A-CAA-CBA
13	F	102	BCL	C4C-C3C-CAC-CBC
12	C	509	PGV	C2-C1-O01-C02
12	D	104	PGV	C03-O11-P-O12
12	D	104	PGV	C03-O11-P-O13
12	D	104	PGV	C03-O11-P-O14
12	D	104	PGV	C04-O12-P-O14
12	D	104	PGV	O12-C04-C05-O05
12	D	104	PGV	O04-C19-O03-C01
12	D	104	PGV	C20-C19-O03-C01
13	Q	101	BCL	C2-C3-C5-C6
13	Q	101	BCL	C4-C3-C5-C6
13	S	102	BCL	C4C-C3C-CAC-CBC
13	A	101	BCL	C14-C13-C15-C16
13	I	102	BCL	C1A-C2A-CAA-CBA
13	I	102	BCL	C2C-C3C-CAC-CBC
13	I	102	BCL	C4C-C3C-CAC-CBC
22	Q	104	CDL	CA2-OA2-PA1-OA3
22	Q	104	CDL	CA2-OA2-PA1-OA5
22	Q	104	CDL	CA3-OA5-PA1-OA2
22	Q	104	CDL	CA3-OA5-PA1-OA3
22	Q	104	CDL	CB3-OB5-PB2-OB2
22	Q	104	CDL	CB3-OB5-PB2-OB3
22	Q	104	CDL	CB3-OB5-PB2-OB4
14	M	404	BPH	C2C-C3C-CAC-CBC
14	M	404	BPH	C4B-C3B-CAB-CBB
14	M	404	BPH	C4B-C3B-CAB-OB
13	U	102	BCL	C1A-C2A-CAA-CBA
13	U	102	BCL	C4C-C3C-CAC-CBC
13	U	102	BCL	C11-C10-C8-C9
13	M	402	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
13	M	402	BCL	C6-C7-C8-C9
23	M	419	LMT	C2'-C1'-O1'-C1
23	M	419	LMT	O5'-C1'-O1'-C1
19	M	406	CRT	O1-C1-C4-C5
19	M	406	CRT	C2-C1-C4-C5
19	M	406	CRT	C39-C38-O2-C2M
13	Y	101	BCL	C2C-C3C-CAC-CBC
13	Y	101	BCL	C4C-C3C-CAC-CBC
21	V	102	LDA	C2-C1-N1-CM1
21	V	102	LDA	N1-C1-C2-C3
22	M	415	CDL	O1-C1-CB2-OB2
22	M	415	CDL	CA2-OA2-PA1-OA3
22	M	415	CDL	CB2-OB2-PB2-OB3
22	M	415	CDL	CB2-OB2-PB2-OB4
22	M	415	CDL	CB3-OB5-PB2-OB2
22	M	415	CDL	CB3-OB5-PB2-OB3
22	M	415	CDL	CB3-OB5-PB2-OB4
22	M	415	CDL	OB6-CB4-CB6-OB8
22	D	103	CDL	CA2-OA2-PA1-OA3
22	D	103	CDL	CA3-OA5-PA1-OA3
22	D	103	CDL	CA3-OA5-PA1-OA4
22	D	103	CDL	CB2-OB2-PB2-OB3
22	D	103	CDL	CB3-OB5-PB2-OB4
21	M	411	LDA	C2-C1-N1-CM1
21	M	411	LDA	C2-C1-N1-CM2
12	M	413	PGV	C03-O11-P-O12
12	M	413	PGV	C03-O11-P-O13
12	M	413	PGV	C03-O11-P-O14
13	M	403	BCL	CHA-CBD-CGD-O2D
13	M	403	BCL	CAD-CBD-CGD-O1D
13	M	403	BCL	CAD-CBD-CGD-O2D
22	K	103	CDL	CB3-OB5-PB2-OB2
22	K	103	CDL	OB7-CB5-OB6-CB4
22	K	103	CDL	C51-CB5-OB6-CB4
13	D	101	BCL	C4C-C3C-CAC-CBC
22	S	103	CDL	OA9-CA7-OA8-CA6
22	S	103	CDL	C31-CA7-OA8-CA6
22	S	103	CDL	OB7-CB5-OB6-CB4
13	3	102	BCL	C4C-C3C-CAC-CBC
13	1	102	BCL	C2C-C3C-CAC-CBC
13	1	102	BCL	C4C-C3C-CAC-CBC
13	3	101	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
15	L	303	UQ8	C15-C14-C16-C17
15	L	303	UQ8	C13-C14-C16-C17
13	7	102	BCL	C4C-C3C-CAC-CBC
13	7	102	BCL	C11-C10-C8-C9
19	9	102	CRT	C10-C11-C12-C13
19	9	102	CRT	C10-C11-C12-C14
20	M	418	PEF	O4P-C4-C5-N
20	M	418	PEF	C1-O3P-P-O2P
15	L	308	UQ8	C35-C34-C36-C37
15	L	308	UQ8	C33-C34-C36-C37
15	L	308	UQ8	C15-C14-C16-C17
15	L	308	UQ8	C13-C14-C16-C17
13	F	101	BCL	C4C-C3C-CAC-CBC
13	K	101	BCL	C4C-C3C-CAC-CBC
22	Y	102	CDL	CA2-C1-CB2-OB2
22	Y	102	CDL	CA2-OA2-PA1-OA3
22	Y	102	CDL	CA3-OA5-PA1-OA3
22	Y	102	CDL	CB3-OB5-PB2-OB4
22	S	103	CDL	C51-CB5-OB6-CB4
12	C	509	PGV	O04-C19-O03-C01
12	C	509	PGV	C20-C19-O03-C01
12	3	104	PGV	O02-C1-O01-C02
12	C	509	PGV	O02-C1-O01-C02
15	7	103	UQ8	C12-C11-C9-C10
13	W	101	BCL	C4-C3-C5-C6
13	A	101	BCL	C4-C3-C5-C6
15	7	103	UQ8	C12-C11-C9-C8
13	W	101	BCL	C2-C3-C5-C6
13	3	101	BCL	C2-C3-C5-C6
13	3	101	BCL	C3-C5-C6-C7
13	S	101	BCL	CBD-CGD-O2D-CED
13	9	103	BCL	CBD-CGD-O2D-CED
12	L	306	PGV	O12-C04-C05-O05
22	Y	102	CDL	O1-C1-CA2-OA2
22	Y	102	CDL	O1-C1-CB2-OB2
12	3	104	PGV	C2-C1-O01-C02
23	F	103	LMT	C4'-C5'-C6'-O6'
22	S	103	CDL	CB4-CB6-OB8-CB7
22	S	103	CDL	C36-C37-C38-C39
13	1	101	BCL	C4-C3-C5-C6
14	M	404	BPH	C4-C3-C5-C6
13	1	101	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	M	404	BPH	C2-C3-C5-C6
15	7	103	UQ8	C19-C21-C22-C23
22	H	304	CDL	CA2-C1-CB2-OB2
12	3	104	PGV	O12-C04-C05-C06
13	O	102	BCL	C3-C5-C6-C7
13	1	102	BCL	C3-C5-C6-C7
13	O	102	BCL	CBA-CGA-O2A-C1
12	M	413	PGV	C20-C19-O03-C01
22	K	103	CDL	C31-CA7-OA8-CA6
13	5	101	BCL	C5-C6-C7-C8
13	3	102	BCL	C8-C10-C11-C12
13	O	102	BCL	C8-C10-C11-C12
13	Q	101	BCL	C5-C6-C7-C8
13	3	101	BCL	C5-C6-C7-C8
22	K	103	CDL	O1-C1-CB2-OB2
22	S	103	CDL	O1-C1-CA2-OA2
13	A	101	BCL	C2-C3-C5-C6
13	O	102	BCL	C6-C7-C8-C9
13	O	102	BCL	C11-C10-C8-C9
13	S	101	BCL	C14-C13-C15-C16
13	Z	102	BCL	C14-C13-C15-C16
13	K	102	BCL	C6-C7-C8-C9
13	K	102	BCL	C11-C10-C8-C9
13	Q	102	BCL	C14-C13-C15-C16
13	W	102	BCL	C6-C7-C8-C9
13	A	103	BCL	C6-C7-C8-C9
13	F	102	BCL	C6-C7-C8-C9
13	F	102	BCL	C11-C10-C8-C9
13	Q	101	BCL	C11-C12-C13-C14
13	S	102	BCL	C11-C10-C8-C9
13	U	102	BCL	C11-C12-C13-C14
13	M	402	BCL	C14-C13-C15-C16
13	3	102	BCL	C11-C10-C8-C9
13	3	101	BCL	C14-C13-C15-C16
13	7	102	BCL	C6-C7-C8-C9
13	K	101	BCL	C14-C13-C15-C16
19	G	101	CRT	C15-C16-C17-C18
19	U	103	CRT	C15-C16-C17-C18
19	9	102	CRT	C15-C16-C17-C18
22	K	103	CDL	OA9-CA7-OA8-CA6
13	W	102	BCL	C8-C10-C11-C12
12	L	305	PGV	C20-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
13	O	102	BCL	C5-C6-C7-C8
13	1	101	BCL	C5-C6-C7-C8
22	Q	104	CDL	CB5-C51-C52-C53
23	F	103	LMT	O5'-C5'-C6'-O6'
13	I	101	BCL	C5-C6-C7-C8
13	O	101	BCL	C13-C15-C16-C17
13	F	101	BCL	C15-C16-C17-C18
9	C	506	GOL	O1-C1-C2-O2
22	K	103	CDL	CB7-C71-C72-C73
13	1	101	BCL	C13-C15-C16-C17
13	Y	101	BCL	C8-C10-C11-C12
13	D	101	BCL	C13-C15-C16-C17
22	S	103	CDL	CA5-C11-C12-C13
22	S	103	CDL	CA7-C31-C32-C33
13	Q	101	BCL	CBD-CGD-O2D-CED
12	A	105	PGV	C2-C1-O01-C02
13	7	101	BCL	C8-C10-C11-C12
13	A	101	BCL	C13-C15-C16-C17
13	S	101	BCL	C12-C13-C15-C16
13	W	102	BCL	C6-C7-C8-C10
13	9	103	BCL	C11-C10-C8-C7
15	M	417	UQ8	C3-C4-O4-C4M
15	7	103	UQ8	C3-C4-O4-C4M
15	L	308	UQ8	C4-C3-O3-C3M
15	L	308	UQ8	C3-C4-O4-C4M
20	M	418	PEF	C10-C11-C12-C13
13	S	102	BCL	C5-C6-C7-C8
14	M	404	BPH	C5-C6-C7-C8
21	I	104	LDA	C4-C5-C6-C7
22	S	103	CDL	C34-C35-C36-C37
12	M	413	PGV	O04-C19-O03-C01
15	7	103	UQ8	C14-C16-C17-C18
15	L	303	UQ8	C14-C16-C17-C18
22	S	103	CDL	CB7-C71-C72-C73
12	3	104	PGV	O12-C04-C05-O05
22	D	103	CDL	O1-C1-CB2-OB2
13	S	101	BCL	C5-C6-C7-C8
13	Z	102	BCL	C8-C10-C11-C12
13	5	101	BCL	C13-C15-C16-C17
13	Y	101	BCL	C13-C15-C16-C17
13	Z	102	BCL	C13-C15-C16-C17
13	Z	102	BCL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
13	U	101	BCL	C5-C6-C7-C8
13	W	102	BCL	C13-C15-C16-C17
13	1	101	BCL	C15-C16-C17-C18
13	O	102	BCL	O1A-CGA-O2A-C1
13	W	101	BCL	C13-C15-C16-C17
13	A	103	BCL	C13-C15-C16-C17
12	L	306	PGV	C04-O12-P-O11
22	H	304	CDL	CA3-OA5-PA1-OA2
22	H	302	CDL	CA2-OA2-PA1-OA5
12	3	104	PGV	C03-O11-P-O12
12	M	414	PGV	C04-O12-P-O11
12	D	104	PGV	C04-O12-P-O11
22	Q	104	CDL	CB2-OB2-PB2-OB5
22	M	415	CDL	CB2-OB2-PB2-OB5
22	D	103	CDL	CA3-OA5-PA1-OA2
22	D	103	CDL	CB2-OB2-PB2-OB5
22	D	103	CDL	CB3-OB5-PB2-OB2
22	S	103	CDL	CA2-OA2-PA1-OA5
20	M	418	PEF	C1-O3P-P-O4P
22	Y	102	CDL	CA3-OA5-PA1-OA2
22	Y	102	CDL	CB2-OB2-PB2-OB5
22	Y	102	CDL	CB3-OB5-PB2-OB2
12	A	105	PGV	C1-C2-C3-C4
12	A	105	PGV	C20-C19-O03-C01
13	Q	102	BCL	C13-C15-C16-C17
13	I	102	BCL	C15-C16-C17-C18
12	D	104	PGV	O12-C04-C05-C06
22	M	415	CDL	CA2-C1-CB2-OB2
22	D	103	CDL	CA2-C1-CB2-OB2
22	K	103	CDL	CA2-C1-CB2-OB2
22	Y	102	CDL	CB2-C1-CA2-OA2
12	A	105	PGV	O02-C1-O01-C02
13	Q	102	BCL	C10-C11-C12-C13
22	K	103	CDL	C11-CA5-OA6-CA4
13	Q	101	BCL	C10-C11-C12-C13
12	1	105	PGV	C3-C4-C5-C6
21	I	104	LDA	C6-C7-C8-C9
22	Q	104	CDL	C37-C38-C39-C40
13	Q	101	BCL	C16-C17-C18-C19
13	9	103	BCL	C16-C17-C18-C19
22	K	103	CDL	OA7-CA5-OA6-CA4
21	O	104	LDA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
12	M	413	PGV	C2-C3-C4-C5
12	L	305	PGV	O04-C19-O03-C01
22	H	302	CDL	C73-C74-C75-C76
12	H	303	PGV	C6-C7-C8-C9
21	I	104	LDA	C2-C3-C4-C5
22	Q	104	CDL	C12-C13-C14-C15
12	M	414	PGV	O12-C04-C05-O05
21	J	102	LDA	C4-C5-C6-C7
12	L	305	PGV	C23-C24-C25-C26
12	M	414	PGV	C29-C30-C31-C32
13	U	102	BCL	C8-C10-C11-C12
13	F	101	BCL	C13-C15-C16-C17
13	O	102	BCL	C16-C17-C18-C20
14	L	302	BPH	C16-C17-C18-C19
13	S	102	BCL	C16-C17-C18-C19
12	H	303	PGV	C2-C3-C4-C5
22	Q	104	CDL	C72-C73-C74-C75
12	M	413	PGV	C14-C15-C16-C17
13	U	101	BCL	C11-C10-C8-C9
13	A	103	BCL	C11-C10-C8-C9
13	5	102	BCL	C11-C10-C8-C9
13	S	102	BCL	C11-C12-C13-C14
13	A	101	BCL	C11-C10-C8-C9
13	U	102	BCL	C6-C7-C8-C9
22	H	304	CDL	CA5-C11-C12-C13
12	M	413	PGV	C19-C20-C21-C22
22	Q	104	CDL	C51-C52-C53-C54
12	M	413	PGV	C30-C31-C32-C33
13	Q	101	BCL	C15-C16-C17-C18
13	1	102	BCL	C13-C15-C16-C17
22	H	304	CDL	C11-C12-C13-C14
21	O	104	LDA	C2-C3-C4-C5
12	M	413	PGV	C21-C22-C23-C24
20	M	418	PEF	C11-C12-C13-C14
9	C	506	GOL	O1-C1-C2-C3
12	L	305	PGV	C26-C27-C28-C29
22	Q	104	CDL	C14-C15-C16-C17
22	Q	104	CDL	C73-C74-C75-C76
22	K	103	CDL	C11-C12-C13-C14
22	S	103	CDL	C32-C33-C34-C35
12	L	306	PGV	C20-C21-C22-C23
22	H	302	CDL	C59-C60-C61-C62

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Mol	Chain	Res	Type	Atoms
12	H	303	PGV	C4-C5-C6-C7
21	J	102	LDA	C5-C6-C7-C8
20	M	418	PEF	C36-C37-C38-C39
23	F	103	LMT	C1-C2-C3-C4
13	9	103	BCL	C16-C17-C18-C20
13	F	102	BCL	C10-C11-C12-C13
13	7	102	BCL	C10-C11-C12-C13
22	S	103	CDL	C72-C73-C74-C75
12	L	306	PGV	C1-C2-C3-C4
13	1	101	BCL	C10-C11-C12-C13
22	H	304	CDL	C79-C80-C81-C82
12	M	414	PGV	C21-C22-C23-C24
22	S	103	CDL	C13-C14-C15-C16
13	O	102	BCL	C3A-C2A-CAA-CBA
13	Z	102	BCL	C3A-C2A-CAA-CBA
13	0	102	BCL	C3A-C2A-CAA-CBA
13	K	102	BCL	C3A-C2A-CAA-CBA
13	Q	102	BCL	C3A-C2A-CAA-CBA
13	D	102	BCL	C3A-C2A-CAA-CBA
13	A	103	BCL	C3A-C2A-CAA-CBA
13	5	102	BCL	C3A-C2A-CAA-CBA
13	F	102	BCL	C3A-C2A-CAA-CBA
13	S	102	BCL	C3A-C2A-CAA-CBA
13	I	102	BCL	C3A-C2A-CAA-CBA
13	U	102	BCL	C3A-C2A-CAA-CBA
13	3	102	BCL	C3A-C2A-CAA-CBA
13	1	102	BCL	C3A-C2A-CAA-CBA
13	7	102	BCL	C3A-C2A-CAA-CBA
13	F	101	BCL	C5-C6-C7-C8
13	I	101	BCL	C16-C17-C18-C19
13	F	101	BCL	CBD-CGD-O2D-CED
13	Z	102	BCL	C3-C5-C6-C7
13	K	102	BCL	C3-C5-C6-C7
12	L	305	PGV	C2-C1-O01-C02
22	Y	102	CDL	C51-CB5-OB6-CB4
12	L	305	PGV	C24-C25-C26-C27
12	L	306	PGV	C3-C4-C5-C6
12	A	105	PGV	O04-C19-O03-C01
13	3	102	BCL	CBA-CGA-O2A-C1
23	M	419	LMT	C4-C5-C6-C7
22	Q	104	CDL	C58-C59-C60-C61
12	L	305	PGV	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
22	Y	102	CDL	OB7-CB5-OB6-CB4
13	S	102	BCL	C15-C16-C17-C18
13	3	102	BCL	C5-C6-C7-C8
13	3	101	BCL	C13-C15-C16-C17
12	A	105	PGV	C20-C21-C22-C23
21	O	104	LDA	C1-C2-C3-C4
12	L	305	PGV	C19-C20-C21-C22
13	9	103	BCL	C5-C6-C7-C8
22	Q	104	CDL	C51-CB5-OB6-CB4
22	D	103	CDL	C11-CA5-OA6-CA4
22	Y	102	CDL	C11-CA5-OA6-CA4
22	S	103	CDL	C16-C17-C18-C19
20	M	418	PEF	C12-C13-C14-C15
13	U	102	BCL	C10-C11-C12-C13
15	7	103	UQ8	C13-C14-C16-C17
13	W	101	BCL	C11-C10-C8-C7
13	Q	102	BCL	C12-C13-C15-C16
13	Q	101	BCL	C11-C10-C8-C7
13	Q	101	BCL	C11-C12-C13-C15
14	L	302	BPH	C2-C3-C5-C6
13	S	102	BCL	C11-C12-C13-C15
13	A	101	BCL	C11-C10-C8-C7
13	U	102	BCL	C6-C7-C8-C10
13	Q	101	BCL	C16-C17-C18-C20
13	S	102	BCL	C16-C17-C18-C20
13	W	101	BCL	C5-C6-C7-C8
22	Q	104	CDL	C35-C36-C37-C38
22	K	103	CDL	C77-C78-C79-C80
13	K	101	BCL	C13-C15-C16-C17
13	A	103	BCL	C3-C5-C6-C7
22	H	304	CDL	OB6-CB4-CB6-OB8
12	M	414	PGV	C28-C29-C30-C31
13	3	102	BCL	O1A-CGA-O2A-C1
13	O	102	BCL	C16-C17-C18-C19
13	M	402	BCL	C16-C17-C18-C19
22	S	103	CDL	C14-C15-C16-C17
13	S	101	BCL	C15-C16-C17-C18
12	3	104	PGV	C11-C10-C9-C8
15	7	103	UQ8	C15-C14-C16-C17
14	L	302	BPH	C4-C3-C5-C6
13	7	101	BCL	C11-C10-C8-C9
13	W	101	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
13	Q	101	BCL	C11-C10-C8-C9
13	F	101	BCL	C11-C10-C8-C9
12	A	105	PGV	C23-C24-C25-C26
22	H	304	CDL	C78-C79-C80-C81
12	H	303	PGV	C21-C22-C23-C24
13	3	102	BCL	C3-C5-C6-C7
19	V	101	CRT	C10-C11-C12-C13
19	Q	103	CRT	C5-C6-C7-C8
13	O	102	BCL	C13-C15-C16-C17
19	9	101	CRT	C5-C6-C7-C9
19	0	101	CRT	C5-C6-C7-C9
13	O	102	BCL	C1A-C2A-CAA-CBA
13	K	102	BCL	C1A-C2A-CAA-CBA
13	D	102	BCL	C1A-C2A-CAA-CBA
13	S	102	BCL	C1A-C2A-CAA-CBA
22	Q	104	CDL	OB7-CB5-OB6-CB4
22	D	103	CDL	OA7-CA5-OA6-CA4
22	Y	102	CDL	OA7-CA5-OA6-CA4
22	K	103	CDL	C76-C77-C78-C79
12	L	306	PGV	C03-O11-P-O12
22	H	302	CDL	CA3-OA5-PA1-OA2
22	Y	102	CDL	CA2-OA2-PA1-OA5
13	W	102	BCL	C10-C11-C12-C13
23	F	103	LMT	O5B-C1B-O1B-C4'
12	3	104	PGV	C13-C14-C15-C16
12	H	303	PGV	C20-C19-O03-C01
13	I	101	BCL	C2C-C3C-CAC-CBC
13	A	103	BCL	C2C-C3C-CAC-CBC
13	Y	101	BCL	C15-C16-C17-C18
20	M	418	PEF	C40-C41-C42-C43
20	M	418	PEF	C11-C10-O2-C2
12	L	306	PGV	C26-C27-C28-C29
22	S	103	CDL	CA3-CA4-CA6-OA8
12	3	104	PGV	C25-C26-C27-C28
22	S	103	CDL	C74-C75-C76-C77
21	O	104	LDA	C7-C8-C9-C10
22	H	302	CDL	C71-CB7-OB8-CB6
12	M	414	PGV	O05-C05-C06-O06
13	A	101	BCL	C10-C11-C12-C13
22	D	103	CDL	C51-CB5-OB6-CB4
13	M	402	BCL	C13-C15-C16-C17
22	H	304	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
13	3	101	BCL	CBA-CGA-O2A-C1
12	H	303	PGV	O01-C02-C03-O11
22	Q	104	CDL	OB5-CB3-CB4-OB6
23	M	419	LMT	C5-C6-C7-C8
14	L	302	BPH	C8-C10-C11-C12
22	H	304	CDL	CB5-C51-C52-C53
13	Q	101	BCL	C13-C15-C16-C17
19	M	406	CRT	C40-C38-O2-C2M
22	Y	102	CDL	OA6-CA4-CA6-OA8
12	3	104	PGV	C7-C8-C9-C10
19	9	101	CRT	C2-C1-C4-C5
19	9	101	CRT	C3-C1-C4-C5
19	0	101	CRT	C2-C1-C4-C5
19	U	103	CRT	C2-C1-C4-C5
19	J	101	CRT	C2-C1-C4-C5
19	M	406	CRT	C3-C1-C4-C5
22	S	103	CDL	C11-C12-C13-C14
13	O	102	BCL	C6-C7-C8-C10
13	K	102	BCL	C6-C7-C8-C10
13	D	102	BCL	C12-C13-C15-C16
13	A	103	BCL	C6-C7-C8-C10
13	F	102	BCL	C6-C7-C8-C10
13	I	102	BCL	C12-C13-C15-C16
13	D	101	BCL	C11-C10-C8-C7
13	1	102	BCL	C12-C13-C15-C16
13	7	102	BCL	C6-C7-C8-C10
13	F	101	BCL	C11-C10-C8-C7
13	0	102	BCL	C6-C7-C8-C9
13	U	101	BCL	C14-C13-C15-C16
13	D	102	BCL	C14-C13-C15-C16
13	5	101	BCL	C11-C10-C8-C9
13	9	103	BCL	C11-C10-C8-C9
13	9	103	BCL	C11-C12-C13-C14
13	D	101	BCL	C11-C10-C8-C9
13	3	101	BCL	C11-C10-C8-C9
19	9	101	CRT	O1-C1-C4-C5
19	2	101	CRT	C10-C11-C12-C13
13	S	101	BCL	C10-C11-C12-C13
13	S	101	BCL	C13-C15-C16-C17
13	A	101	BCL	C15-C16-C17-C18
13	A	103	BCL	C10-C11-C12-C13
13	M	402	BCL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
20	M	418	PEF	O3P-C1-C2-C3
12	D	104	PGV	C19-C20-C21-C22
13	D	101	BCL	C4-C3-C5-C6
20	M	418	PEF	O4-C10-O2-C2
13	S	101	BCL	O1D-CGD-O2D-CED
13	1	101	BCL	C16-C17-C18-C19
13	S	102	BCL	CBA-CGA-O2A-C1
20	M	418	PEF	C31-C30-O3-C3
13	F	101	BCL	CBA-CGA-O2A-C1
12	A	105	PGV	C21-C22-C23-C24
22	H	304	CDL	C60-C61-C62-C63
12	M	414	PGV	C20-C21-C22-C23
20	M	418	PEF	C13-C14-C15-C16
22	K	103	CDL	C36-C37-C38-C39
23	M	419	LMT	C2-C1-O1'-C1'
13	I	101	BCL	C16-C17-C18-C20
13	1	102	BCL	CBA-CGA-O2A-C1
13	5	102	BCL	C10-C11-C12-C13
13	9	103	BCL	C15-C16-C17-C18
22	H	304	CDL	CB3-CB4-CB6-OB8
22	Q	104	CDL	CA3-CA4-CA6-OA8
22	Q	104	CDL	CB3-CB4-CB6-OB8
22	S	103	CDL	CB3-CB4-CB6-OB8
13	9	103	BCL	O1D-CGD-O2D-CED
13	7	102	BCL	C15-C16-C17-C18
22	Q	104	CDL	C74-C75-C76-C77
22	M	415	CDL	CA2-OA2-PA1-OA5
12	L	306	PGV	C24-C25-C26-C27
13	I	102	BCL	C13-C15-C16-C17
13	D	101	BCL	C15-C16-C17-C18
12	H	303	PGV	C5-C6-C7-C8
22	Q	104	CDL	OA5-CA3-CA4-OA6
20	M	418	PEF	O3P-C1-C2-O2
13	Z	102	BCL	CBA-CGA-O2A-C1
22	K	103	CDL	C34-C35-C36-C37
22	H	302	CDL	OB9-CB7-OB8-CB6
12	H	303	PGV	O04-C19-O03-C01
13	3	101	BCL	O1A-CGA-O2A-C1
22	Q	104	CDL	OA6-CA4-CA6-OA8
22	S	103	CDL	OA6-CA4-CA6-OA8
12	M	414	PGV	O12-C04-C05-C06
22	M	415	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
22	S	103	CDL	CB2-C1-CA2-OA2
20	M	418	PEF	C34-C35-C36-C37
22	D	103	CDL	OB7-CB5-OB6-CB4
13	9	103	BCL	C2-C1-O2A-CGA
13	S	102	BCL	C8-C10-C11-C12
13	U	102	BCL	C13-C15-C16-C17
13	S	101	BCL	C11-C10-C8-C9
13	Q	102	BCL	C11-C10-C8-C9
13	S	102	BCL	C6-C7-C8-C9
13	3	102	BCL	C14-C13-C15-C16
22	Q	104	CDL	C61-C62-C63-C64
23	M	419	LMT	C2-C3-C4-C5
22	K	103	CDL	C31-C32-C33-C34
20	M	418	PEF	C20-C21-C22-C23
14	L	302	BPH	C16-C17-C18-C20
13	F	102	BCL	C3-C5-C6-C7
13	W	101	BCL	C10-C11-C12-C13
13	5	102	BCL	C13-C15-C16-C17
22	H	302	CDL	C71-C72-C73-C74
19	G	101	CRT	C15-C16-C17-C19
19	U	103	CRT	C15-C16-C17-C19
14	M	404	BPH	C4C-C3C-CAC-CBC
13	5	101	BCL	C4C-C3C-CAC-CBC
19	9	102	CRT	C15-C16-C17-C19
22	H	304	CDL	OB9-CB7-OB8-CB6
12	1	105	PGV	C01-C02-C03-O11
22	Q	104	CDL	OA5-CA3-CA4-CA6
22	Y	102	CDL	OA5-CA3-CA4-CA6
12	A	105	PGV	C22-C23-C24-C25
13	7	101	BCL	C11-C10-C8-C7
13	Z	102	BCL	C11-C12-C13-C15
13	Q	102	BCL	C11-C10-C8-C7
13	U	101	BCL	C11-C10-C8-C7
13	D	102	BCL	C6-C7-C8-C10
13	1	101	BCL	C6-C7-C8-C10
13	A	101	BCL	C12-C13-C15-C16
13	U	102	BCL	C11-C10-C8-C7
13	U	102	BCL	C11-C12-C13-C15
13	M	402	BCL	C6-C7-C8-C10
13	5	101	BCL	C11-C10-C8-C7
13	Y	101	BCL	C6-C7-C8-C10
13	9	103	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
13	9	103	BCL	C11-C12-C13-C15
13	3	102	BCL	C6-C7-C8-C10
13	3	102	BCL	C11-C10-C8-C7
13	3	101	BCL	C11-C10-C8-C7
13	3	101	BCL	C12-C13-C15-C16
13	7	102	BCL	C11-C10-C8-C7
13	K	101	BCL	C11-C10-C8-C7
13	5	101	BCL	C16-C17-C18-C19
13	M	402	BCL	C5-C6-C7-C8
13	1	101	BCL	C16-C17-C18-C20
13	3	102	BCL	C15-C16-C17-C18
13	F	102	BCL	C13-C15-C16-C17
13	M	401	BCL	CAD-CBD-CGD-O2D
13	A	101	BCL	CAD-CBD-CGD-O2D
14	M	404	BPH	CAD-CBD-CGD-O2D
13	M	402	BCL	CAD-CBD-CGD-O2D
13	D	101	BCL	CAD-CBD-CGD-O2D
12	M	413	PGV	C13-C14-C15-C16
13	K	102	BCL	C10-C11-C12-C13
20	M	418	PEF	O5-C30-O3-C3
13	K	101	BCL	C4-C3-C5-C6
15	7	103	UQ8	C5-C4-O4-C4M
15	L	308	UQ8	C5-C4-O4-C4M
12	1	105	PGV	C19-C20-C21-C22
20	K	104	PEF	C1-C2-C3-O3
12	H	303	PGV	O03-C01-C02-C03
12	M	414	PGV	C02-C03-O11-P
22	K	103	CDL	CB3-CB4-CB6-OB8
12	1	105	PGV	O01-C02-C03-O11
12	M	414	PGV	O01-C02-C03-O11
13	S	102	BCL	C10-C11-C12-C13
13	5	101	BCL	C16-C17-C18-C20
13	7	102	BCL	C16-C17-C18-C19
21	V	102	LDA	C2-C1-N1-CM2
13	1	102	BCL	O1A-CGA-O2A-C1
13	F	101	BCL	O1A-CGA-O2A-C1
13	D	101	BCL	C5-C6-C7-C8
20	M	418	PEF	O2-C2-C3-O3
13	9	103	BCL	C8-C10-C11-C12
13	Z	102	BCL	O1A-CGA-O2A-C1
13	S	102	BCL	O1A-CGA-O2A-C1
22	Y	103	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
13	I	101	BCL	C11-C10-C8-C9
13	1	101	BCL	C6-C7-C8-C9
13	I	102	BCL	C6-C7-C8-C9
13	3	101	BCL	C6-C7-C8-C9
13	K	101	BCL	C11-C10-C8-C9
14	M	404	BPH	C8-C10-C11-C12
22	H	302	CDL	C76-C77-C78-C79
22	Y	102	CDL	C31-CA7-OA8-CA6
19	O	103	CRT	C29-C28-C30-C31
19	V	101	CRT	C5-C6-C7-C9
13	Z	102	BCL	C1A-C2A-CAA-CBA
13	A	103	BCL	C1A-C2A-CAA-CBA
13	3	102	BCL	C1A-C2A-CAA-CBA
13	7	102	BCL	C1A-C2A-CAA-CBA
13	M	401	BCL	C15-C16-C17-C18
13	7	102	BCL	C2-C1-O2A-CGA
21	V	102	LDA	C1-C2-C3-C4
12	L	305	PGV	C04-O12-P-O11
22	K	103	CDL	CB2-OB2-PB2-OB5
12	L	306	PGV	C25-C26-C27-C28
12	H	303	PGV	C02-C03-O11-P
12	L	306	PGV	C03-O11-P-O13
22	H	302	CDL	CA2-OA2-PA1-OA3
22	H	302	CDL	CA3-OA5-PA1-OA4
12	3	104	PGV	C04-O12-P-O14
12	M	414	PGV	C04-O12-P-O13
12	M	414	PGV	C04-O12-P-O14
22	Q	104	CDL	CB2-OB2-PB2-OB3
22	D	103	CDL	CB2-OB2-PB2-OB4
22	K	103	CDL	CB3-OB5-PB2-OB4
22	S	103	CDL	CA2-OA2-PA1-OA3
22	Y	102	CDL	CA3-OA5-PA1-OA4
22	Y	102	CDL	CB2-OB2-PB2-OB3
12	M	414	PGV	C01-C02-C03-O11
22	K	103	CDL	C51-C52-C53-C54
21	O	104	LDA	C2-C1-N1-O1
21	V	102	LDA	C2-C1-N1-O1
21	M	411	LDA	C2-C1-N1-O1
13	Y	101	BCL	C5-C6-C7-C8
22	Q	104	CDL	OA9-CA7-OA8-CA6
12	M	413	PGV	C12-C13-C14-C15
22	Q	104	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
13	K	102	BCL	C2C-C3C-CAC-CBC
13	I	102	BCL	C6-C7-C8-C10
13	U	102	BCL	C2C-C3C-CAC-CBC
13	M	402	BCL	C2C-C3C-CAC-CBC
13	M	402	BCL	C11-C12-C13-C15
12	M	413	PGV	O01-C02-C03-O11
13	3	101	BCL	C6-C7-C8-C10
13	F	101	BCL	C2C-C3C-CAC-CBC
13	K	101	BCL	C12-C13-C15-C16
13	U	102	BCL	C16-C17-C18-C19
11	C	508	LHG	C23-C24-C25-C26
22	Y	102	CDL	OA9-CA7-OA8-CA6
22	Q	104	CDL	OB6-CB4-CB6-OB8
22	S	103	CDL	OB6-CB4-CB6-OB8
13	W	101	BCL	C15-C16-C17-C18
13	5	102	BCL	C15-C16-C17-C18
14	M	404	BPH	C15-C16-C17-C18
22	H	302	CDL	C14-C15-C16-C17
12	1	105	PGV	C2-C3-C4-C5
13	Z	102	BCL	C11-C12-C13-C14
13	D	102	BCL	C6-C7-C8-C9
13	M	402	BCL	C11-C12-C13-C14
13	Y	101	BCL	C6-C7-C8-C9
13	9	103	BCL	C6-C7-C8-C9
13	3	102	BCL	C6-C7-C8-C9
13	1	102	BCL	C11-C10-C8-C9
13	K	101	BCL	C5-C6-C7-C8
19	0	101	CRT	C29-C28-C30-C31
22	Q	104	CDL	C32-C31-CA7-OA8
22	H	302	CDL	C74-C75-C76-C77
13	M	403	BCL	C13-C15-C16-C17
13	K	101	BCL	O1A-CGA-O2A-C1
20	M	418	PEF	C3-C2-O2-C10
22	Y	102	CDL	CA3-CA4-OA6-CA5
12	H	303	PGV	C01-C02-C03-O11
22	Q	104	CDL	OB5-CB3-CB4-CB6
12	M	413	PGV	C01-C02-C03-O11
13	Q	101	BCL	O1D-CGD-O2D-CED
12	3	104	PGV	C24-C25-C26-C27
12	H	303	PGV	C22-C23-C24-C25
12	A	105	PGV	C02-C03-O11-P
22	H	304	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
13	K	101	BCL	CBA-CGA-O2A-C1
13	D	101	BCL	C2-C3-C5-C6
12	1	105	PGV	C20-C19-O03-C01
13	M	403	BCL	CAA-CBA-CGA-O2A
12	L	305	PGV	C03-O11-P-O12
22	H	304	CDL	CB3-OB5-PB2-OB2
12	1	105	PGV	C03-O11-P-O12
12	1	105	PGV	C04-O12-P-O11
22	M	415	CDL	CA3-OA5-PA1-OA2
22	D	103	CDL	CA2-OA2-PA1-OA5
22	K	103	CDL	CA2-OA2-PA1-OA5
22	S	103	CDL	CB3-OB5-PB2-OB2
22	H	302	CDL	CB3-CB4-CB6-OB8
22	Y	102	CDL	CA3-CA4-CA6-OA8
13	S	101	BCL	C11-C10-C8-C7
13	S	102	BCL	C6-C7-C8-C10
13	A	101	BCL	C6-C7-C8-C10
22	H	304	CDL	C52-C53-C54-C55
13	I	102	BCL	C14-C13-C15-C16
13	Y	101	BCL	C11-C10-C8-C9
13	1	102	BCL	C14-C13-C15-C16
22	K	103	CDL	C57-C58-C59-C60
19	V	101	CRT	C15-C16-C17-C18
22	D	103	CDL	CB2-C1-CA2-OA2
21	M	411	LDA	N1-C1-C2-C3
13	1	101	BCL	O1A-CGA-O2A-C1
13	1	101	BCL	CBA-CGA-O2A-C1
13	A	101	BCL	CBA-CGA-O2A-C1
13	A	101	BCL	O1A-CGA-O2A-C1
13	S	102	BCL	C4-C3-C5-C6
12	1	105	PGV	O04-C19-O03-C01
13	A	101	BCL	C2-C1-O2A-CGA
13	K	101	BCL	C2-C1-O2A-CGA
13	M	402	BCL	C3-C5-C6-C7
13	L	301	BCL	C2A-CAA-CBA-CGA
13	M	401	BCL	C16-C17-C18-C19
13	5	101	BCL	C4-C3-C5-C6
13	1	101	BCL	C11-C10-C8-C9
13	5	102	BCL	C6-C7-C8-C9
12	M	414	PGV	O03-C01-C02-C03
14	L	302	BPH	O2A-C1-C2-C3
19	O	103	CRT	C34-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
13	K	101	BCL	C15-C16-C17-C18
22	K	103	CDL	CA3-CA4-OA6-CA5
22	K	103	CDL	CA6-CA4-OA6-CA5
13	O	101	BCL	C15-C16-C17-C18
13	1	102	BCL	C1A-C2A-CAA-CBA
13	3	101	BCL	C1A-C2A-CAA-CBA
13	K	102	BCL	C11-C10-C8-C7
13	I	101	BCL	C11-C10-C8-C7
13	M	402	BCL	C12-C13-C15-C16
13	3	102	BCL	C11-C12-C13-C15
13	7	102	BCL	C11-C12-C13-C15
12	M	413	PGV	C6-C7-C8-C9
12	A	105	PGV	O01-C02-C03-O11
12	M	414	PGV	C27-C28-C29-C30
22	H	302	CDL	C58-C59-C60-C61
13	Q	101	BCL	C3-C5-C6-C7
22	H	302	CDL	C15-C16-C17-C18
22	Q	104	CDL	C16-C17-C18-C19
13	5	102	BCL	C3-C5-C6-C7
13	K	102	BCL	C4-C3-C5-C6
13	3	101	BCL	C2-C1-O2A-CGA
23	F	103	LMT	O5B-C5B-C6B-O6B
13	7	101	BCL	O1A-CGA-O2A-C1
12	L	305	PGV	C29-C30-C31-C32
21	I	104	LDA	C1-C2-C3-C4
13	O	102	BCL	C4C-C3C-CAC-CBC
14	L	302	BPH	C4C-C3C-CAC-CBC
13	M	401	BCL	C13-C15-C16-C17
22	H	304	CDL	C14-C15-C16-C17
21	M	411	LDA	C1-C2-C3-C4
13	K	102	BCL	C15-C16-C17-C18
22	Y	102	CDL	OA5-CA3-CA4-OA6
13	F	101	BCL	O1D-CGD-O2D-CED
23	F	103	LMT	C6-C7-C8-C9
13	O	102	BCL	C15-C16-C17-C18
12	D	104	PGV	C01-C02-C03-O11
22	S	103	CDL	C72-C71-CB7-OB8
13	5	102	BCL	C4-C3-C5-C6
13	3	102	BCL	C12-C13-C15-C16
13	K	101	BCL	C2-C3-C5-C6
22	D	103	CDL	C32-C31-CA7-OA8
13	5	101	BCL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	L	306	PGV	C23-C24-C25-C26
12	L	305	PGV	C05-C04-O12-P
12	A	105	PGV	O03-C01-C02-O01
12	M	413	PGV	O03-C01-C02-O01
13	7	101	BCL	CBA-CGA-O2A-C1
13	Y	101	BCL	C4-C3-C5-C6
15	L	308	UQ8	C20-C19-C21-C22
13	F	101	BCL	C4-C3-C5-C6
22	K	103	CDL	C37-C38-C39-C40
13	3	101	BCL	CAA-CBA-CGA-O2A
13	Q	102	BCL	C6-C7-C8-C9
13	A	101	BCL	C6-C7-C8-C9
12	3	104	PGV	C1-C2-C3-C4
22	S	103	CDL	C71-C72-C73-C74
12	H	303	PGV	O01-C1-C2-C3
22	H	304	CDL	CA3-CA4-OA6-CA5
13	L	301	BCL	CAD-CBD-CGD-O2D
22	Y	102	CDL	CA6-CA4-OA6-CA5
13	O	102	BCL	C2-C1-O2A-CGA
21	M	411	LDA	C7-C8-C9-C10
19	V	101	CRT	C10-C11-C12-C14
19	V	101	CRT	C15-C16-C17-C19
19	2	101	CRT	C10-C11-C12-C14
19	O	103	CRT	C27-C28-C30-C31
19	Q	103	CRT	C5-C6-C7-C9
19	Q	103	CRT	C27-C28-C30-C31
15	L	309	UQ8	C5-C4-O4-C4M
15	7	103	UQ8	C9-C11-C12-C13
12	3	104	PGV	C11-C12-C13-C14
22	K	103	CDL	C12-C13-C14-C15
13	7	102	BCL	O2A-C1-C2-C3
22	K	103	CDL	C52-C51-CB5-OB6
12	L	305	PGV	C25-C26-C27-C28
13	K	102	BCL	C16-C17-C18-C19
13	3	102	BCL	C16-C17-C18-C19
13	M	402	BCL	CHA-CBD-CGD-O2D
13	M	403	BCL	CHA-CBD-CGD-O1D
12	A	105	PGV	C01-C02-C03-O11
12	L	305	PGV	C22-C23-C24-C25
12	L	306	PGV	O01-C1-C2-C3
19	0	101	CRT	C3-C1-C4-C5
19	2	101	CRT	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
13	D	101	BCL	C6-C7-C8-C10
13	O	101	BCL	C6-C7-C8-C10
13	3	102	BCL	C11-C12-C13-C14
13	5	101	BCL	C3-C5-C6-C7
21	J	102	LDA	C1-C2-C3-C4
13	O	101	BCL	C4-C3-C5-C6
13	5	101	BCL	C2-C3-C5-C6
19	O	103	CRT	C32-C33-C35-C36
19	1	103	CRT	C15-C16-C17-C19
13	0	102	BCL	CBA-CGA-O2A-C1
13	Z	102	BCL	C16-C17-C18-C19
12	H	303	PGV	O02-C1-C2-C3
23	F	103	LMT	C2B-C1B-O1B-C4'
22	K	103	CDL	C52-C51-CB5-OB7
12	L	306	PGV	O02-C1-C2-C3
13	3	101	BCL	CAA-CBA-CGA-O1A
13	9	103	BCL	C10-C11-C12-C13
22	H	304	CDL	CA2-OA2-PA1-OA3
22	H	304	CDL	CB3-OB5-PB2-OB3
12	H	303	PGV	C03-O11-P-O13
22	M	415	CDL	CA2-OA2-PA1-OA4
22	K	103	CDL	CA2-OA2-PA1-OA3
22	S	103	CDL	CB3-OB5-PB2-OB3
22	K	103	CDL	C33-C34-C35-C36
22	K	103	CDL	C53-C54-C55-C56
15	L	308	UQ8	C39-C41-C42-C43
13	3	101	BCL	C15-C16-C17-C18
22	Q	104	CDL	C71-C72-C73-C74
13	S	102	BCL	C2-C3-C5-C6
13	D	101	BCL	C6-C7-C8-C9
13	1	102	BCL	C6-C7-C8-C9
13	I	101	BCL	C10-C11-C12-C13
13	F	102	BCL	C8-C10-C11-C12
22	K	103	CDL	CA7-C31-C32-C33
13	Y	101	BCL	C10-C11-C12-C13
22	H	302	CDL	C11-C12-C13-C14
13	9	103	BCL	C4-C3-C5-C6
13	I	101	BCL	C15-C16-C17-C18
13	Z	102	BCL	C12-C13-C15-C16
13	K	102	BCL	C2-C3-C5-C6
13	5	102	BCL	C6-C7-C8-C10
13	5	102	BCL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
13	1	102	BCL	C6-C7-C8-C10
13	1	102	BCL	C11-C10-C8-C7
13	D	101	BCL	CAA-CBA-CGA-O2A
22	M	415	CDL	C32-C31-CA7-OA8
13	O	101	BCL	C5-C6-C7-C8
19	P	101	CRT	C15-C16-C17-C19
13	0	102	BCL	O1A-CGA-O2A-C1
13	U	102	BCL	CBA-CGA-O2A-C1
13	F	102	BCL	C15-C16-C17-C18
22	Q	104	CDL	C72-C71-CB7-OB8
13	D	101	BCL	CAA-CBA-CGA-O1A

There are no ring outliers.

90 monomers are involved in 285 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	K	104	PEF	1	0
12	A	105	PGV	5	0
13	7	101	BCL	3	0
12	L	305	PGV	4	0
19	6	101	CRT	2	0
13	O	102	BCL	4	0
23	F	103	LMT	5	0
15	M	417	UQ8	3	0
18	M	405	MQ8	5	0
12	L	306	PGV	4	0
13	S	101	BCL	5	0
22	H	304	CDL	3	0
21	O	104	LDA	1	0
15	7	103	UQ8	8	0
19	G	101	CRT	5	0
13	Z	102	BCL	7	0
22	H	302	CDL	3	0
13	0	102	BCL	8	0
12	3	104	PGV	3	0
19	Z	101	CRT	3	0
13	W	101	BCL	5	0
19	V	101	CRT	1	0
13	K	102	BCL	3	0
12	H	303	PGV	1	0
19	P	101	CRT	2	0
13	Q	102	BCL	4	0

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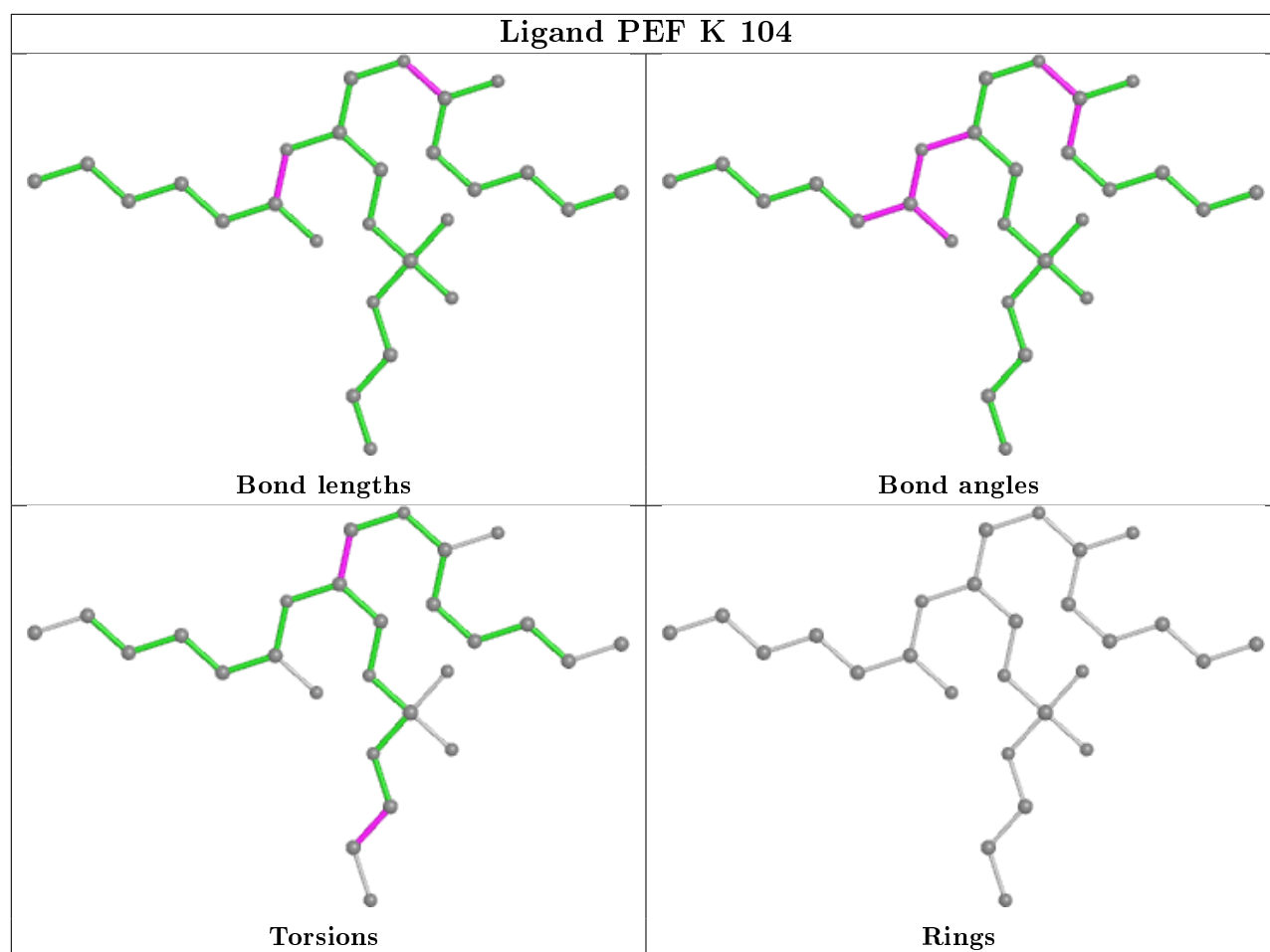
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	9	101	CRT	4	0
12	M	414	PGV	3	0
19	N	101	CRT	4	0
20	I	103	PEF	1	0
13	U	101	BCL	8	0
13	I	101	BCL	4	0
13	W	102	BCL	2	0
13	D	102	BCL	4	0
13	1	101	BCL	5	0
13	L	301	BCL	4	0
13	A	103	BCL	4	0
19	0	101	CRT	2	0
13	5	102	BCL	4	0
7	C	504	HEC	1	0
13	F	102	BCL	3	0
19	U	103	CRT	2	0
15	L	309	UQ8	1	0
13	M	401	BCL	6	0
21	I	104	LDA	6	0
12	D	104	PGV	2	0
13	Q	101	BCL	6	0
19	2	101	CRT	6	0
14	L	302	BPH	6	0
9	H	301	GOL	1	0
13	S	102	BCL	6	0
13	A	101	BCL	4	0
13	I	102	BCL	4	0
22	Q	104	CDL	3	0
14	M	404	BPH	6	0
19	J	101	CRT	3	0
13	U	102	BCL	4	0
13	M	402	BCL	2	0
13	5	101	BCL	10	0
23	M	419	LMT	3	0
19	O	103	CRT	2	0
19	M	406	CRT	4	0
19	A	104	CRT	3	0
13	Y	101	BCL	5	0
22	M	415	CDL	1	0
20	5	103	PEF	1	0
22	D	103	CDL	2	0
21	M	411	LDA	1	0

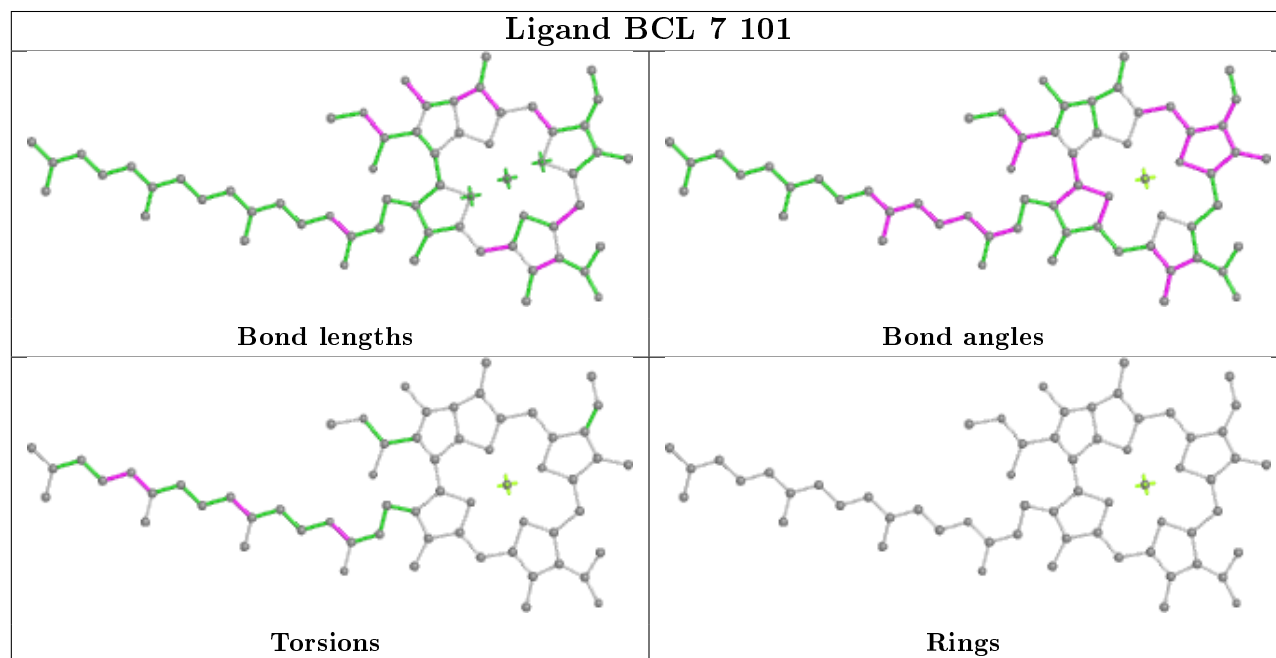
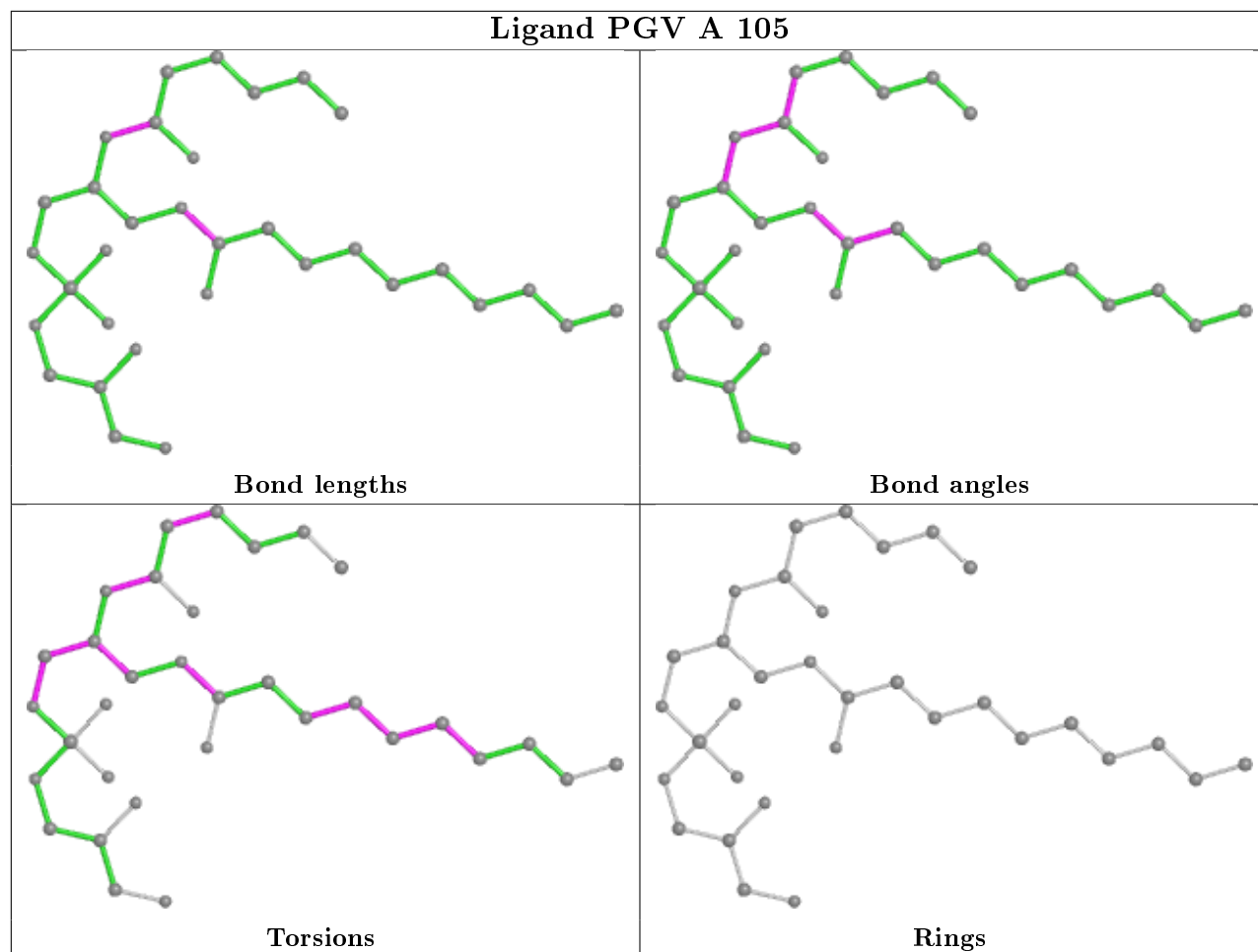
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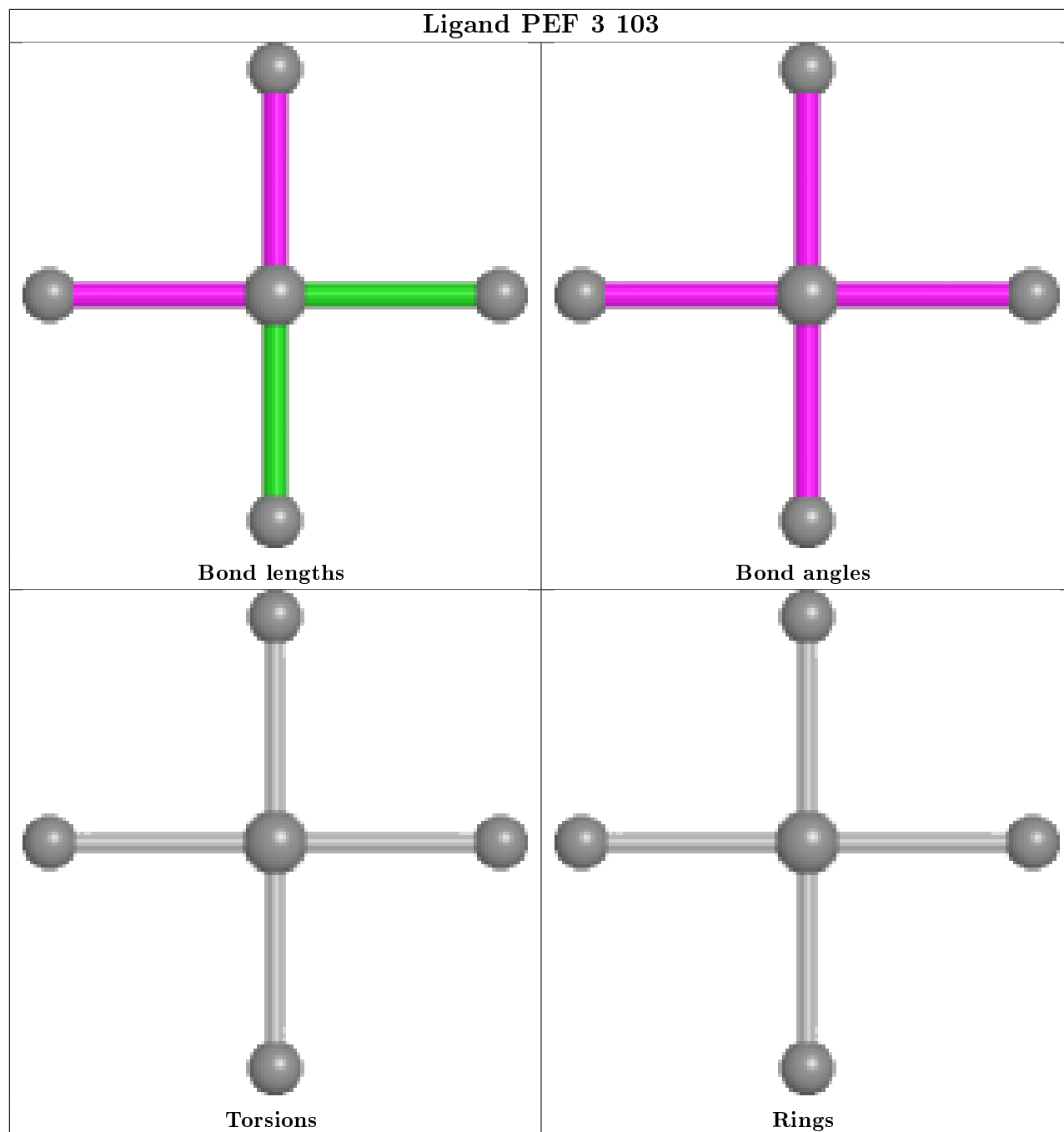
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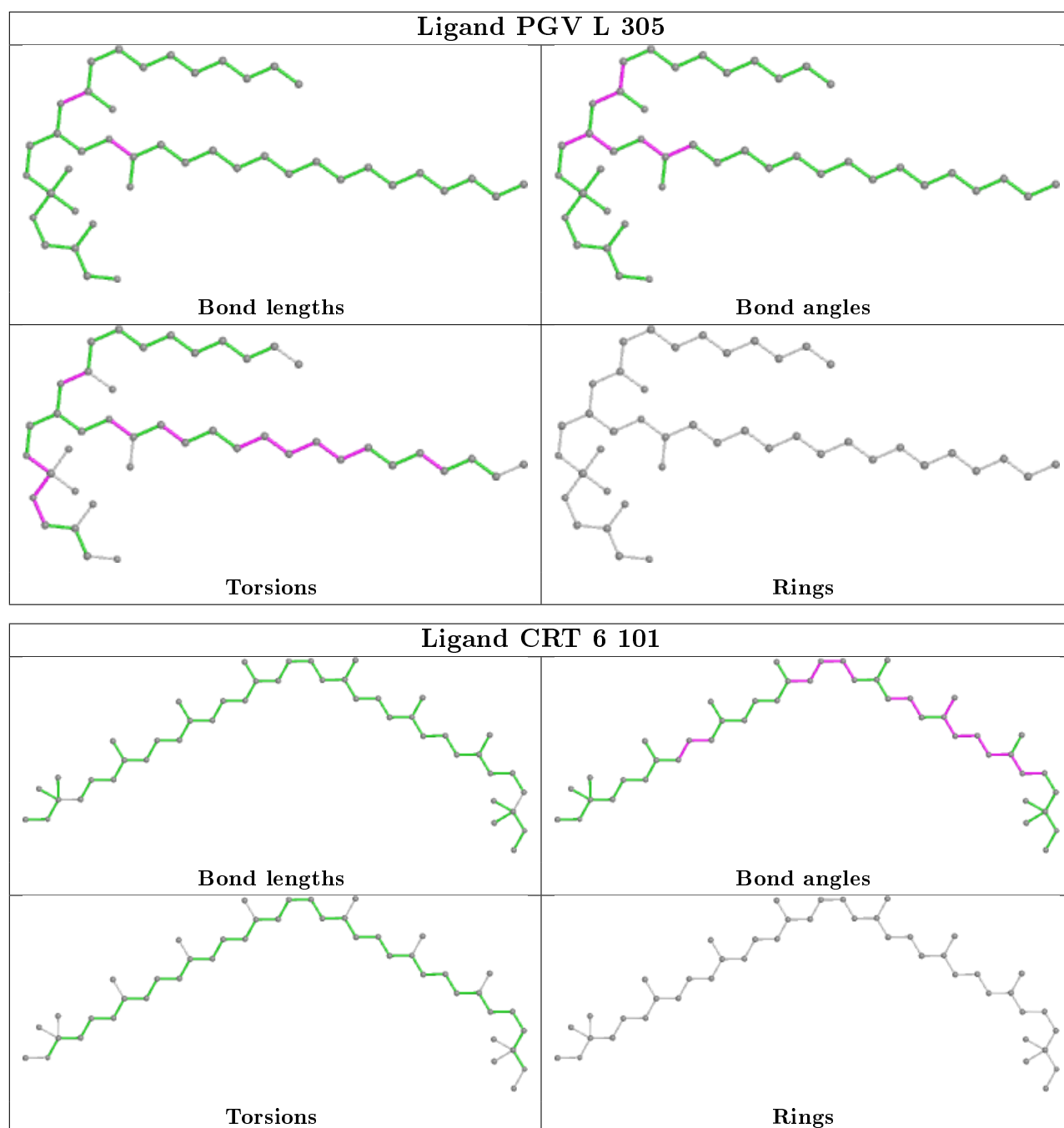
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	413	PGV	4	0
13	9	103	BCL	4	0
13	M	403	BCL	1	0
22	K	103	CDL	4	0
21	J	102	LDA	1	0
13	D	101	BCL	2	0
22	S	103	CDL	10	0
13	3	102	BCL	4	0
13	1	102	BCL	7	0
7	C	503	HEC	2	0
13	3	101	BCL	4	0
19	Q	103	CRT	2	0
15	L	303	UQ8	2	0
13	7	102	BCL	5	0
13	O	101	BCL	4	0
19	9	102	CRT	2	0
20	M	418	PEF	3	0
19	1	103	CRT	3	0
15	L	308	UQ8	7	0
13	F	101	BCL	2	0
13	K	101	BCL	2	0
22	Y	102	CDL	1	0

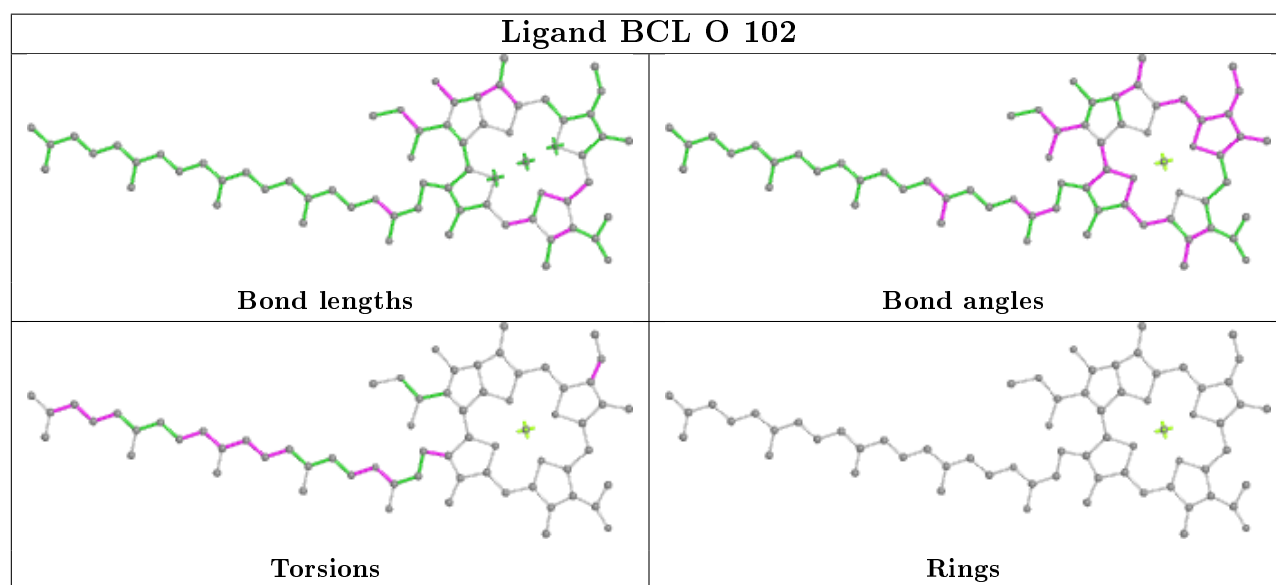
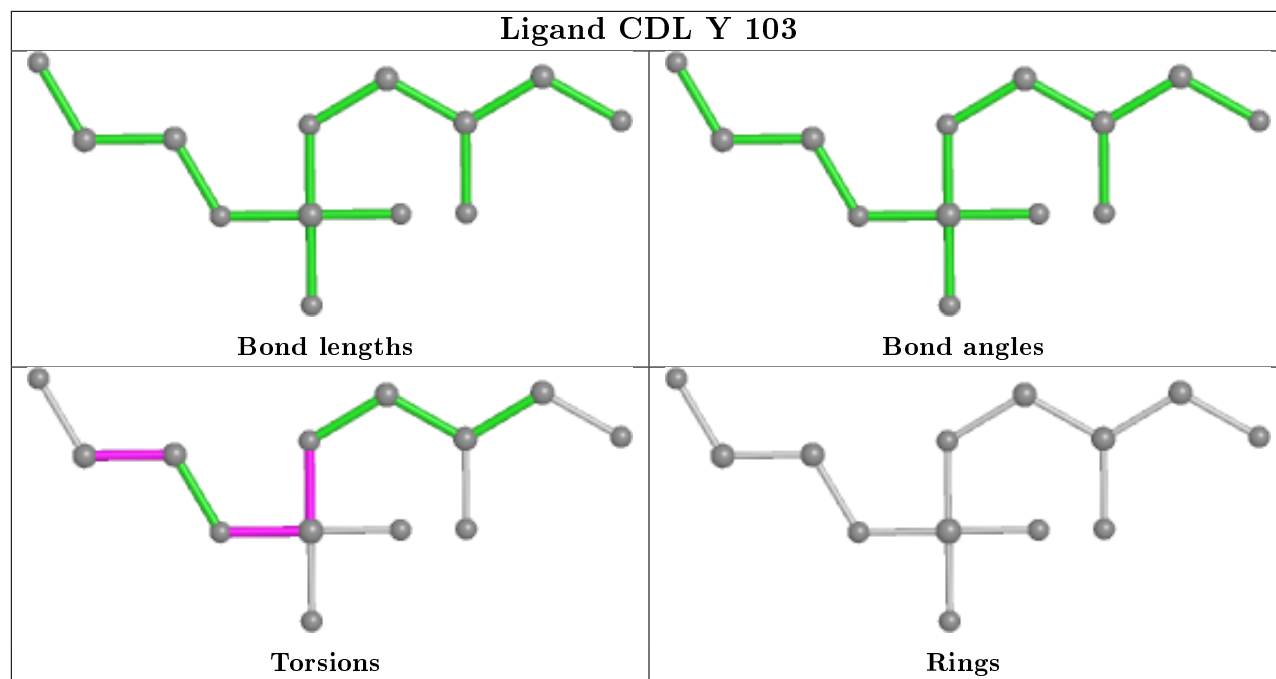
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

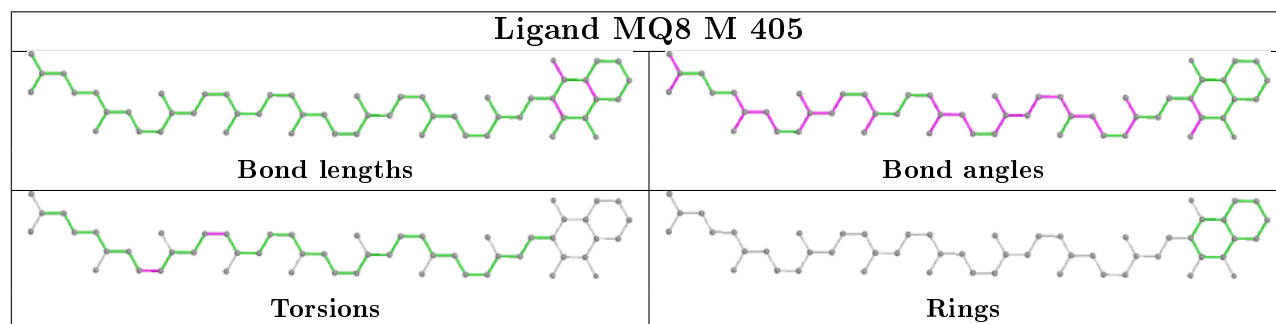
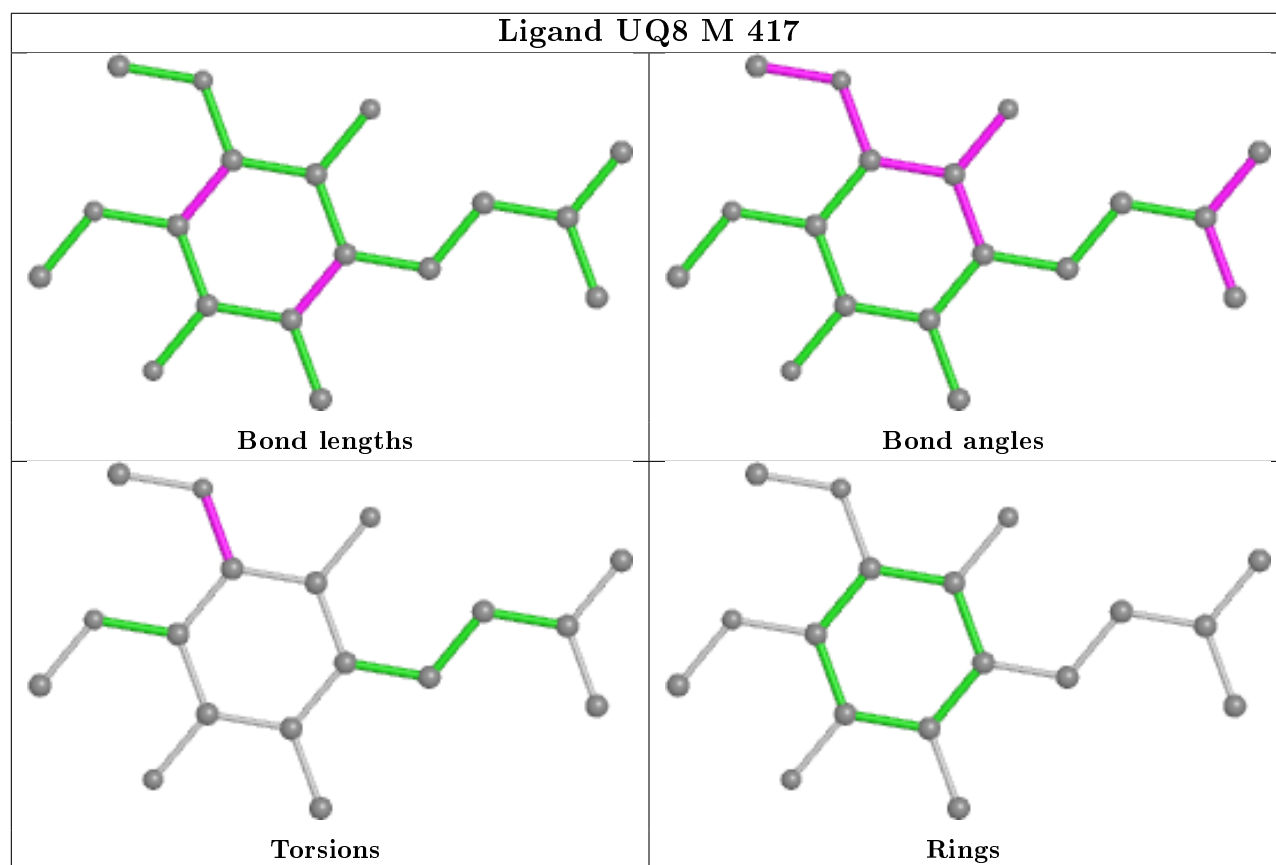
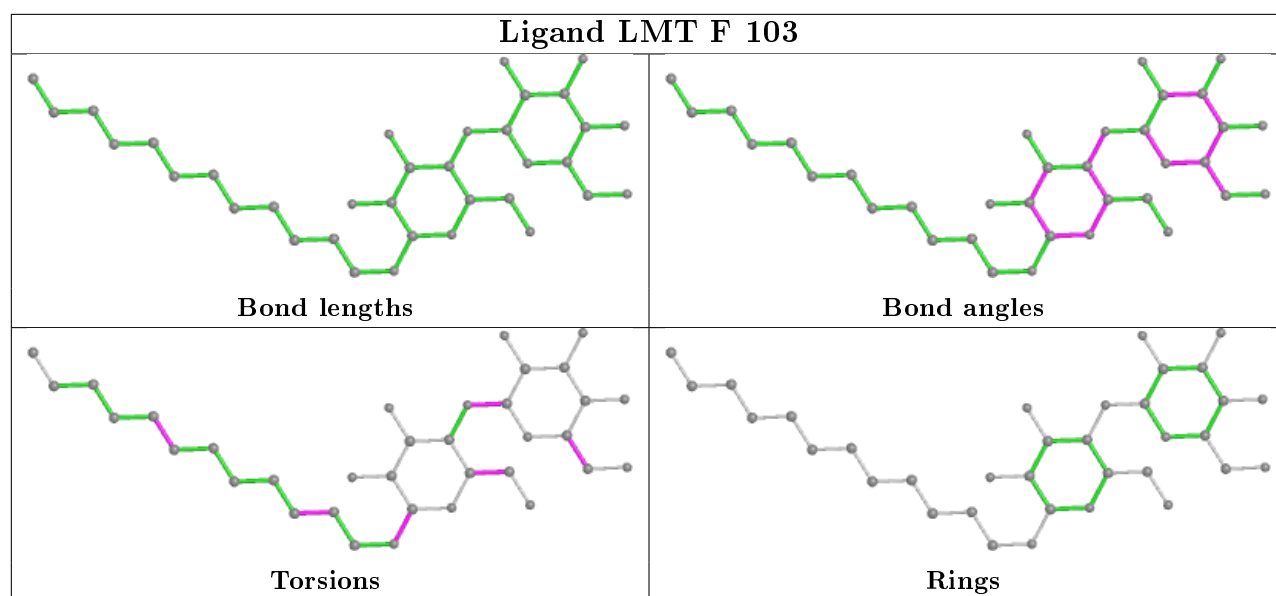


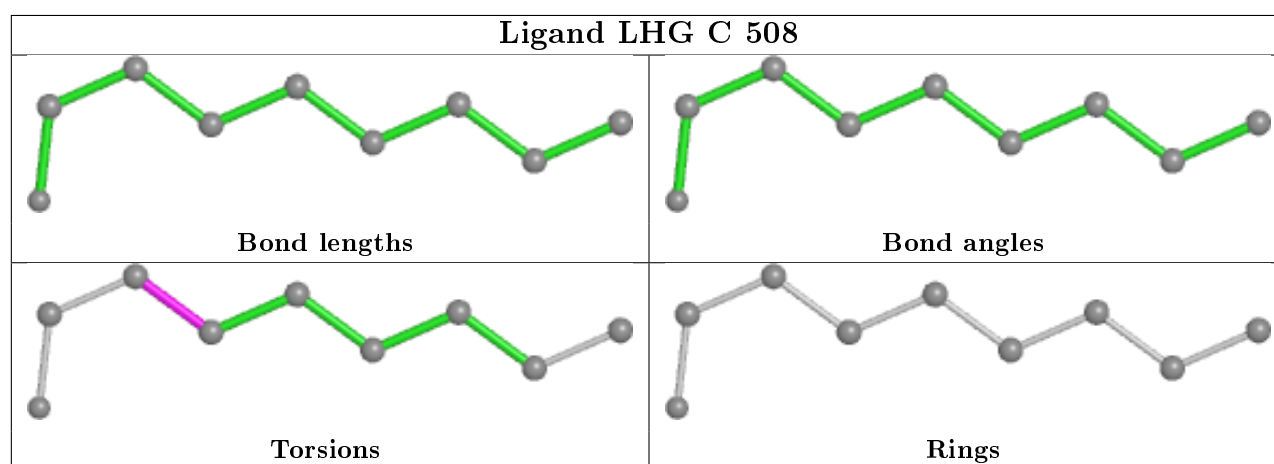
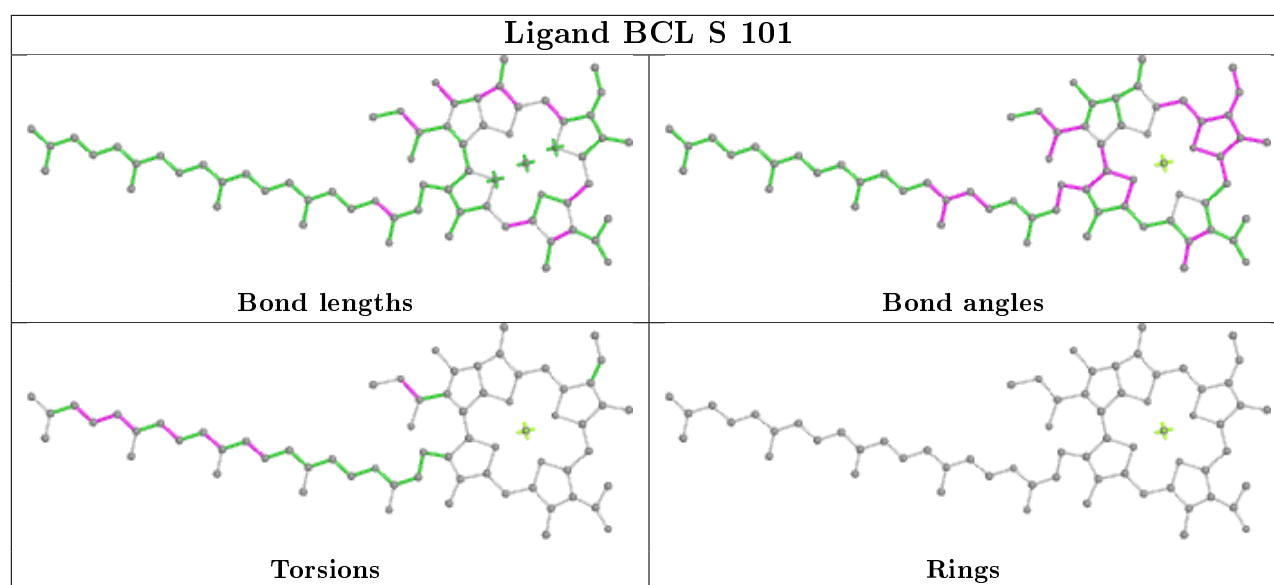
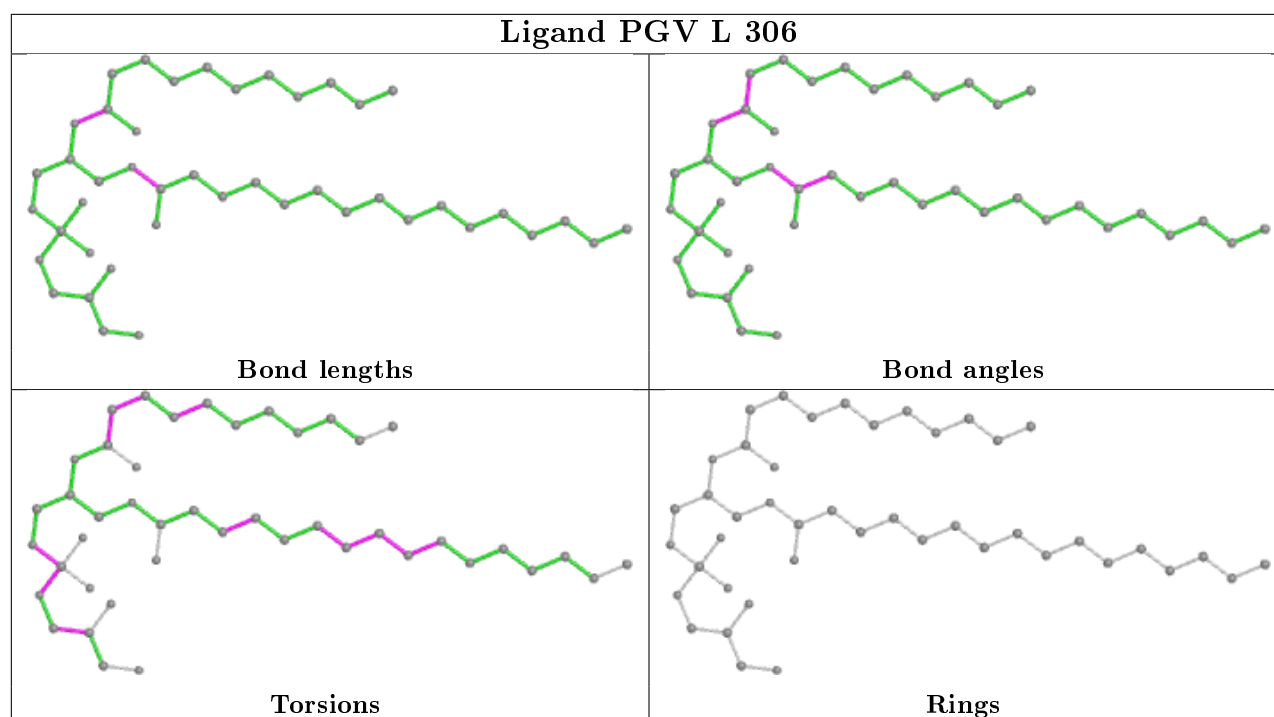


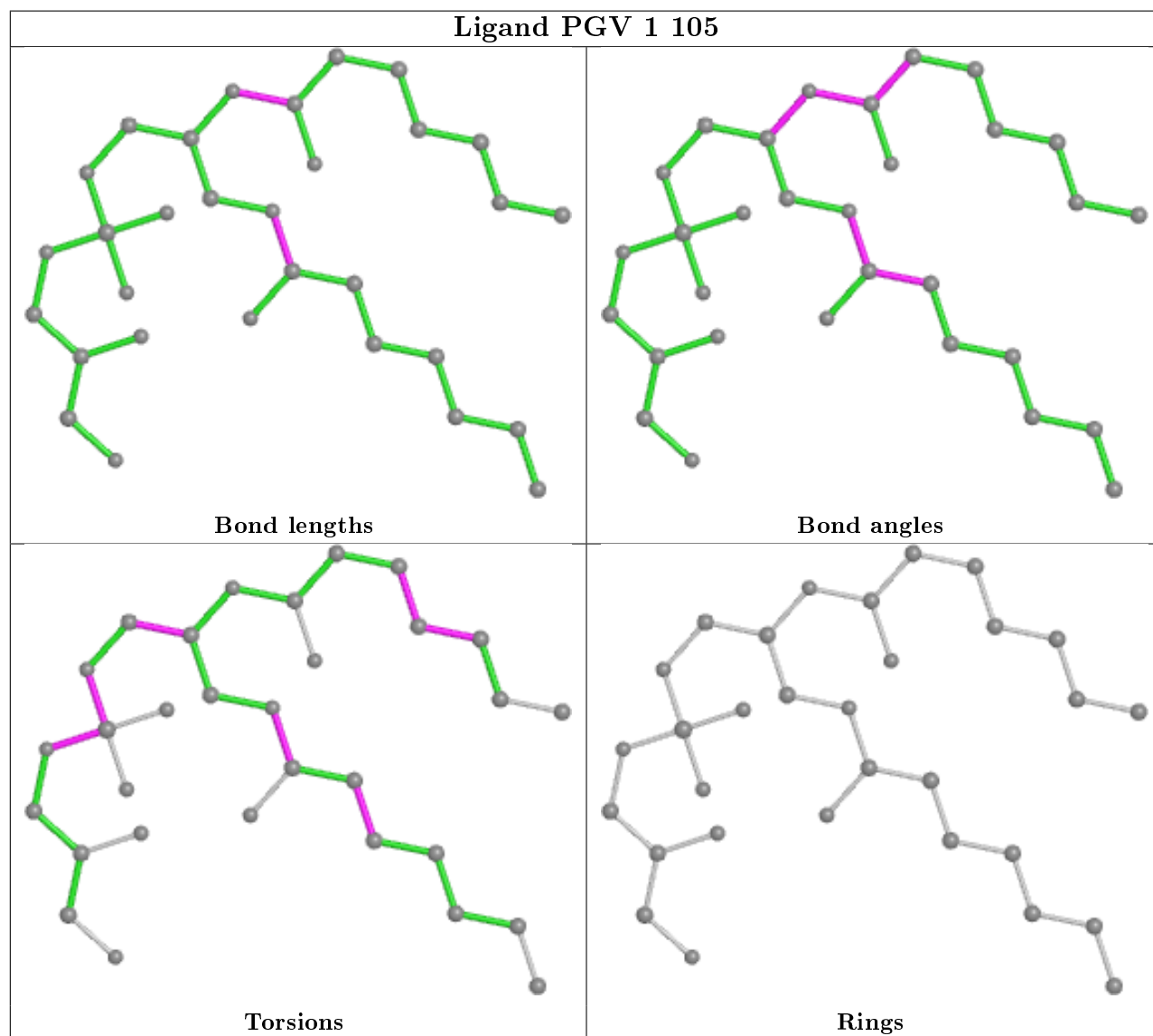
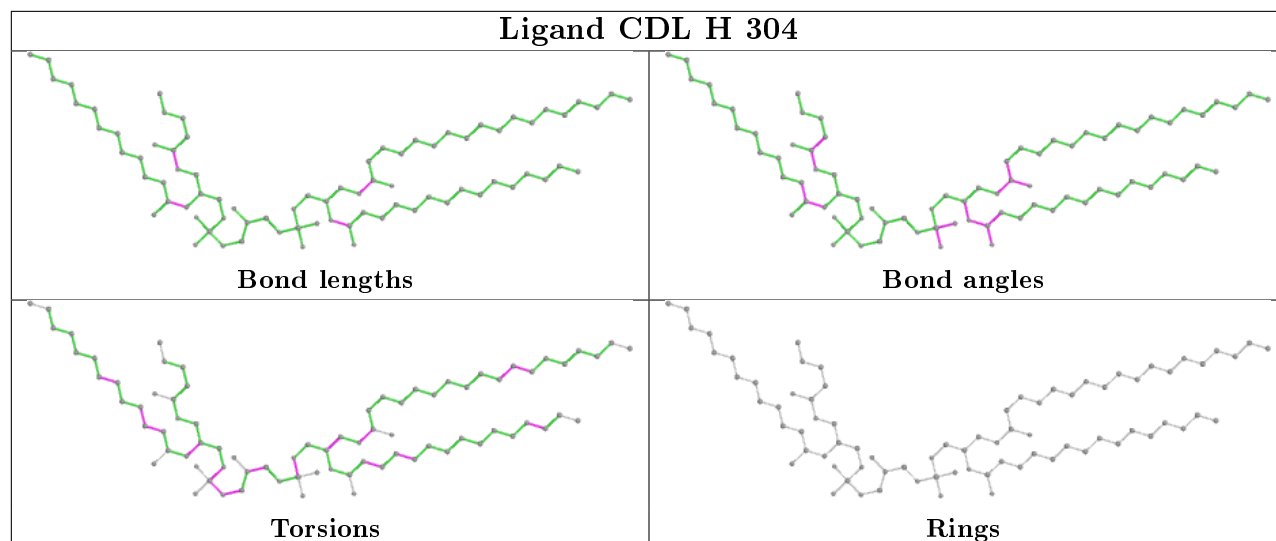


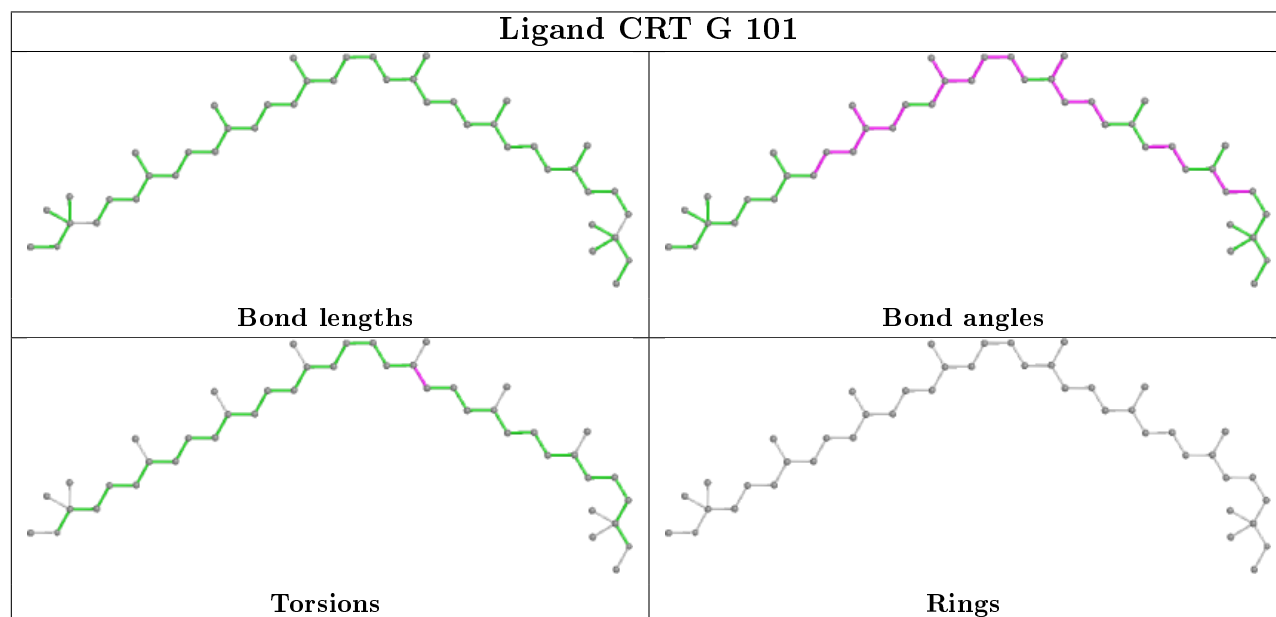
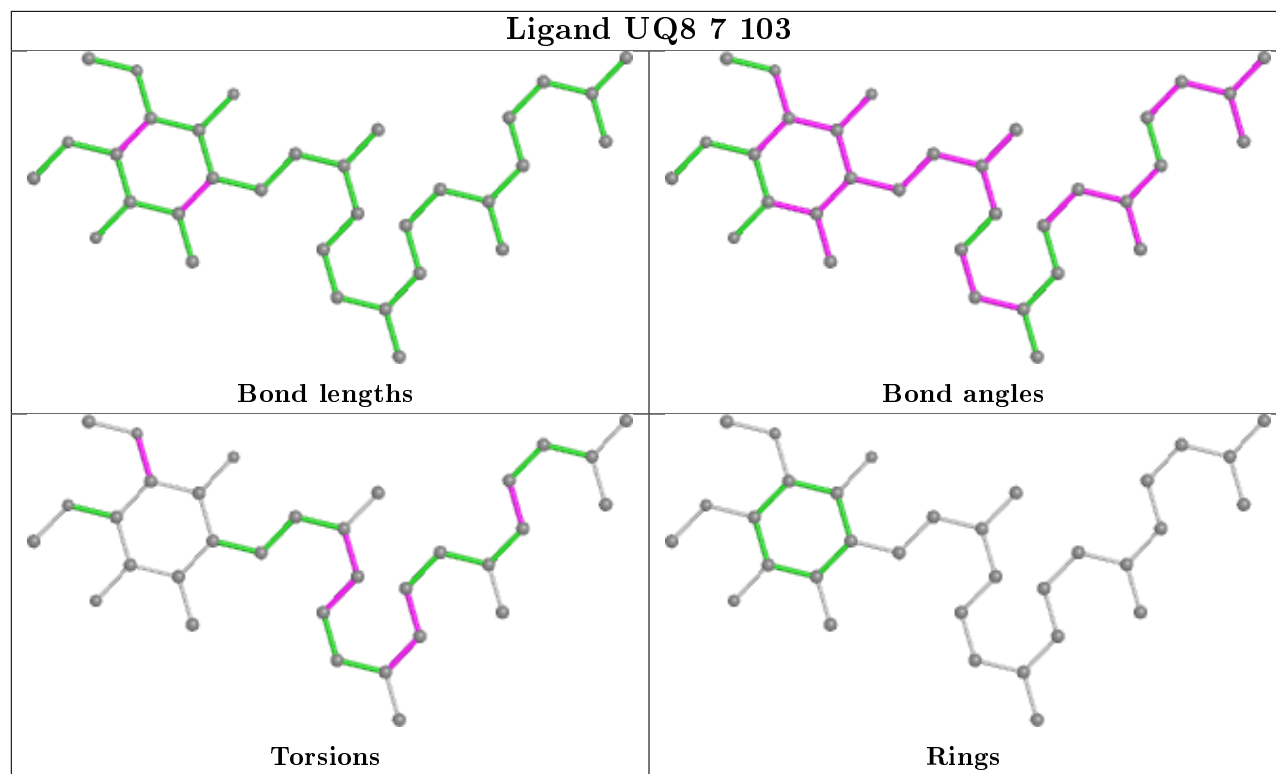




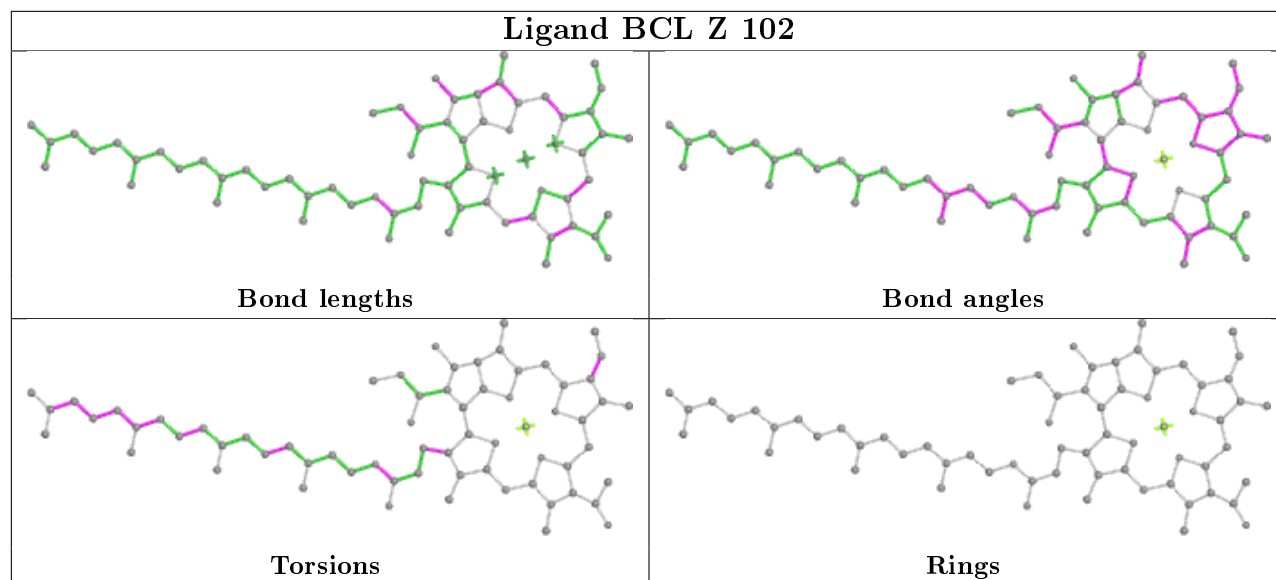




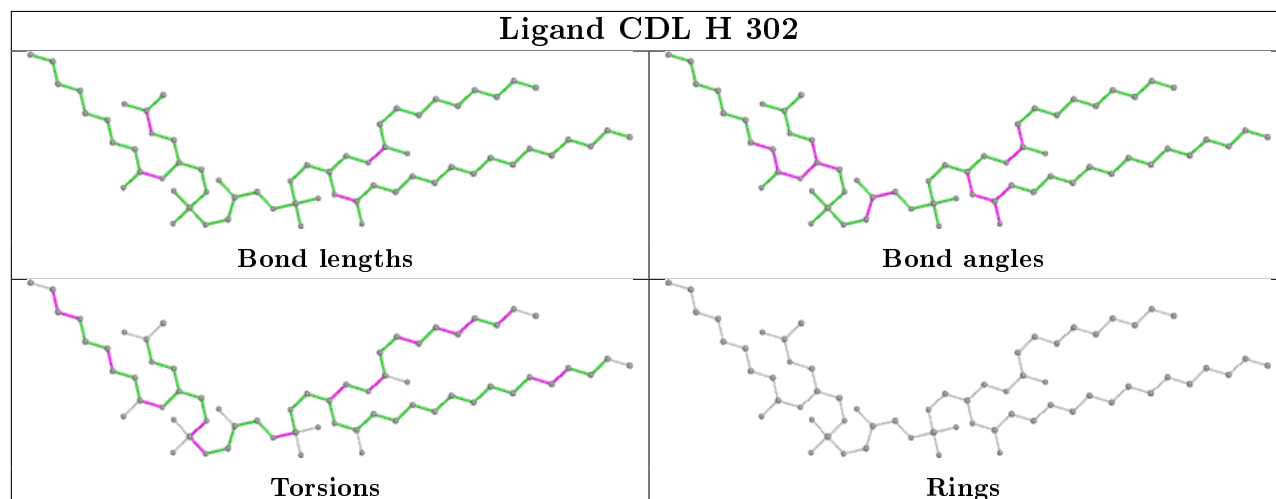




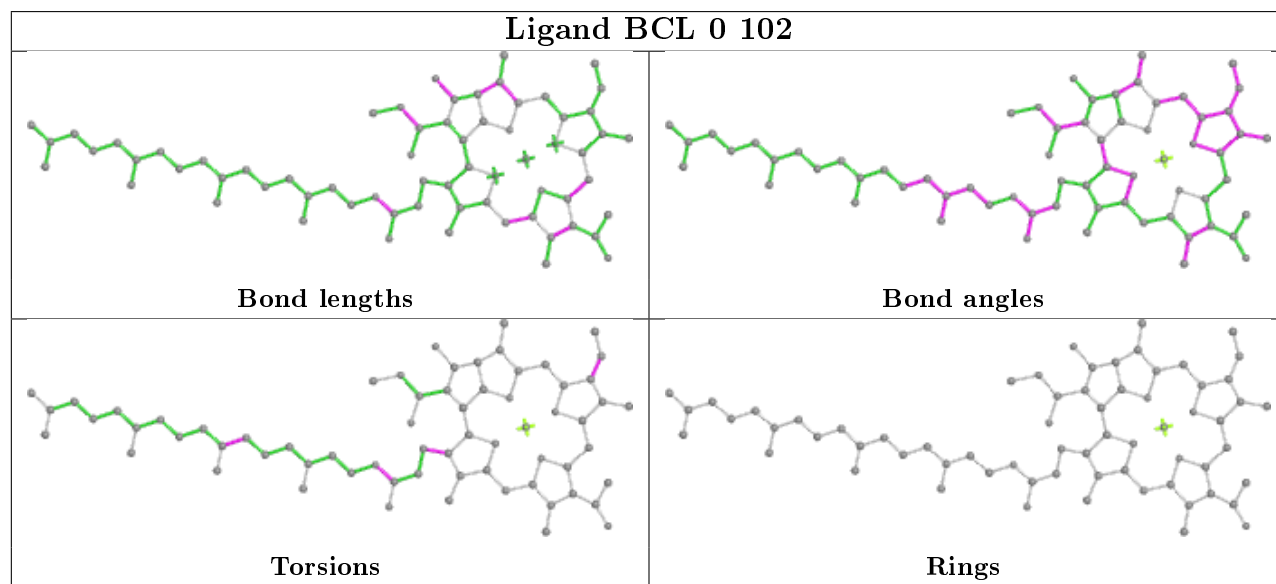
Ligand BCL Z 102

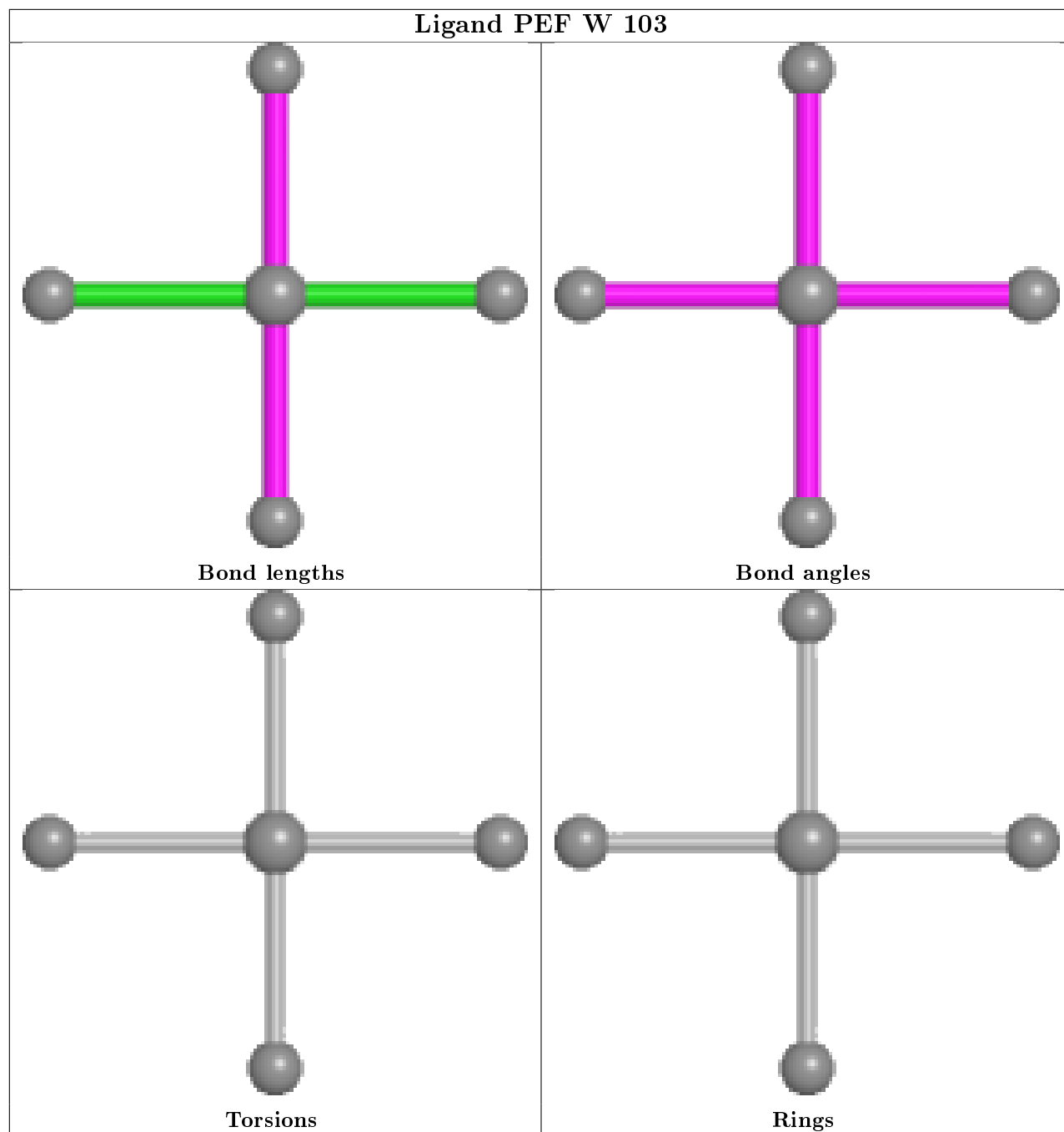


Ligand CDL H 302

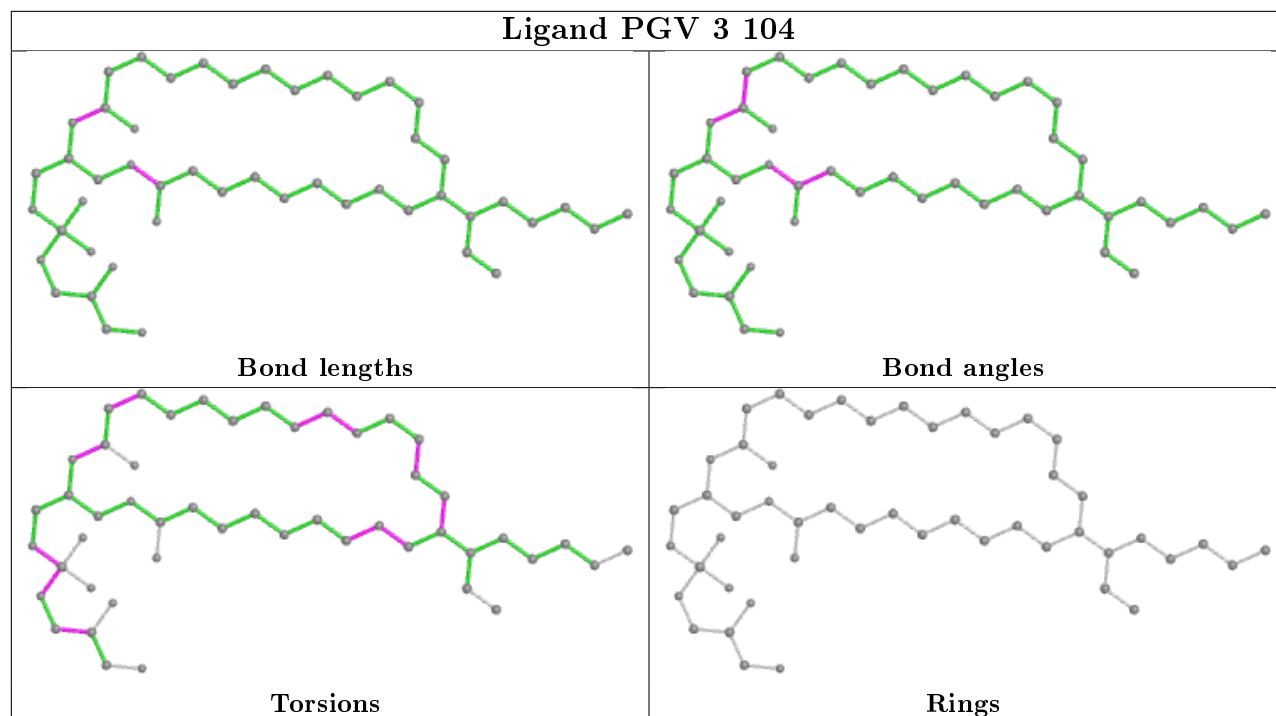


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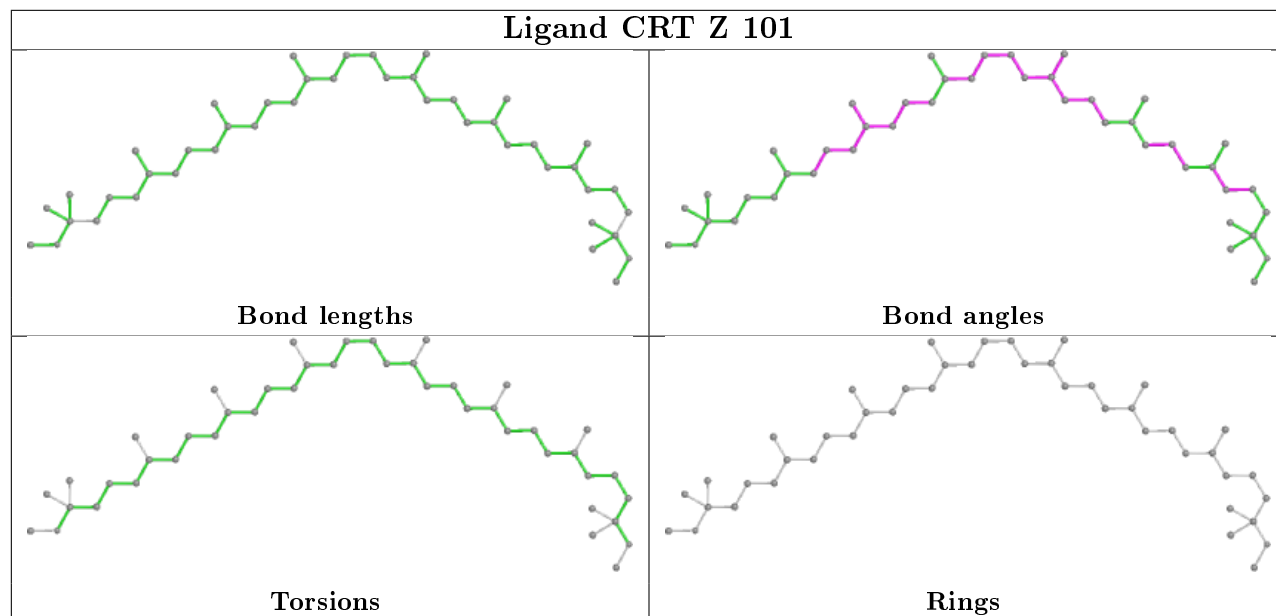


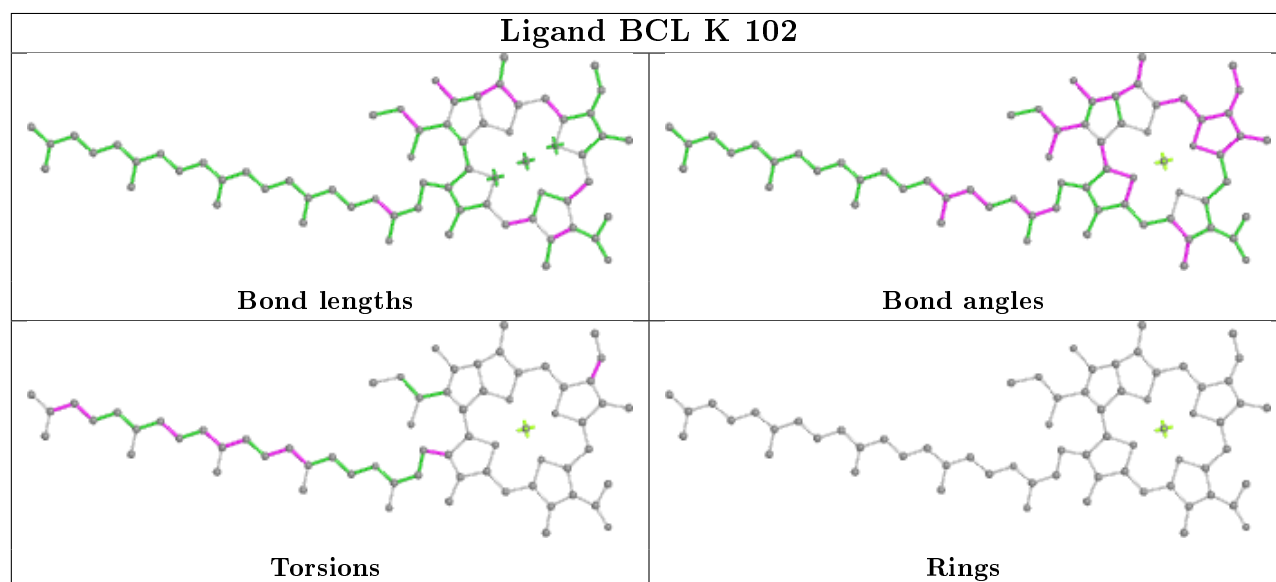
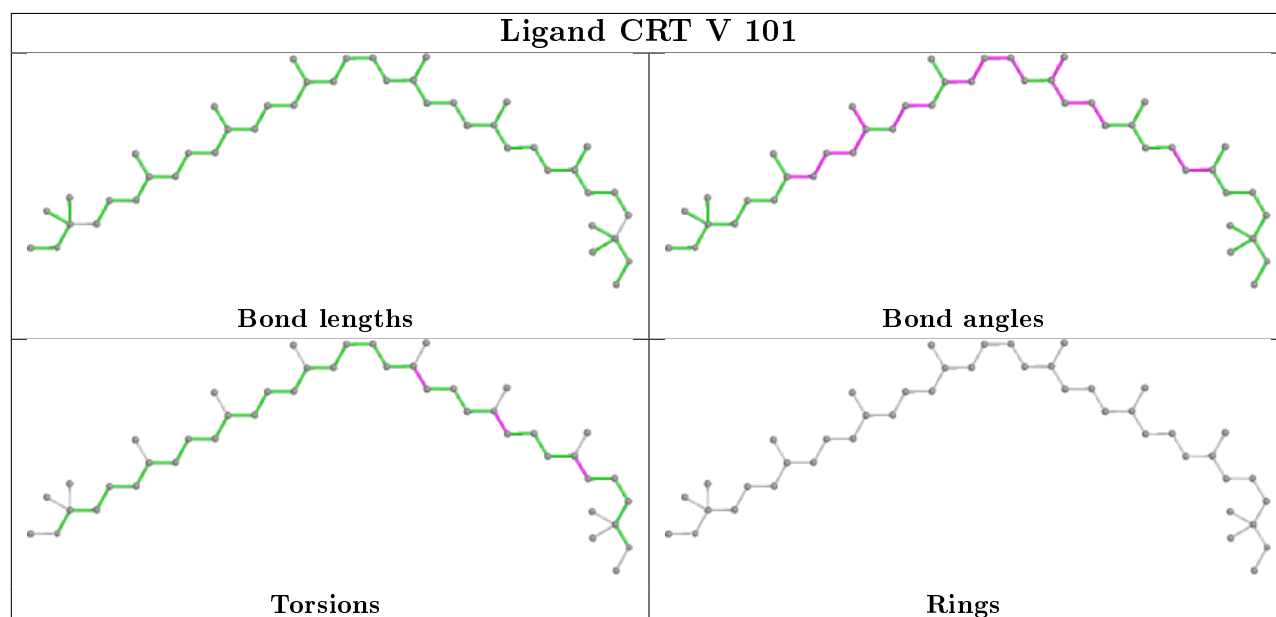
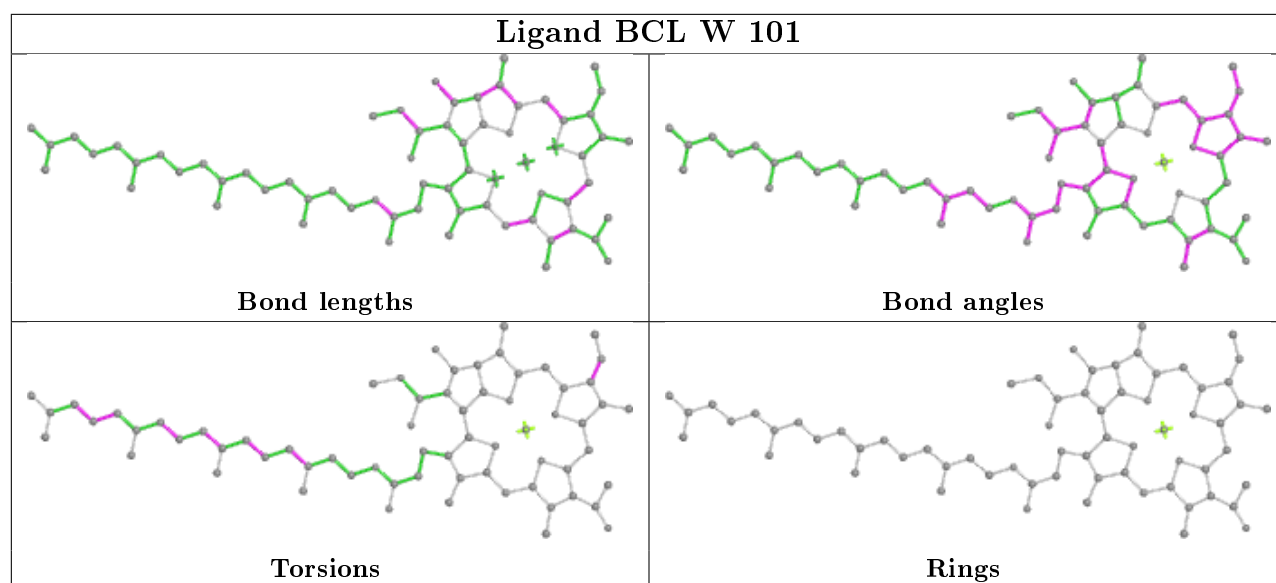


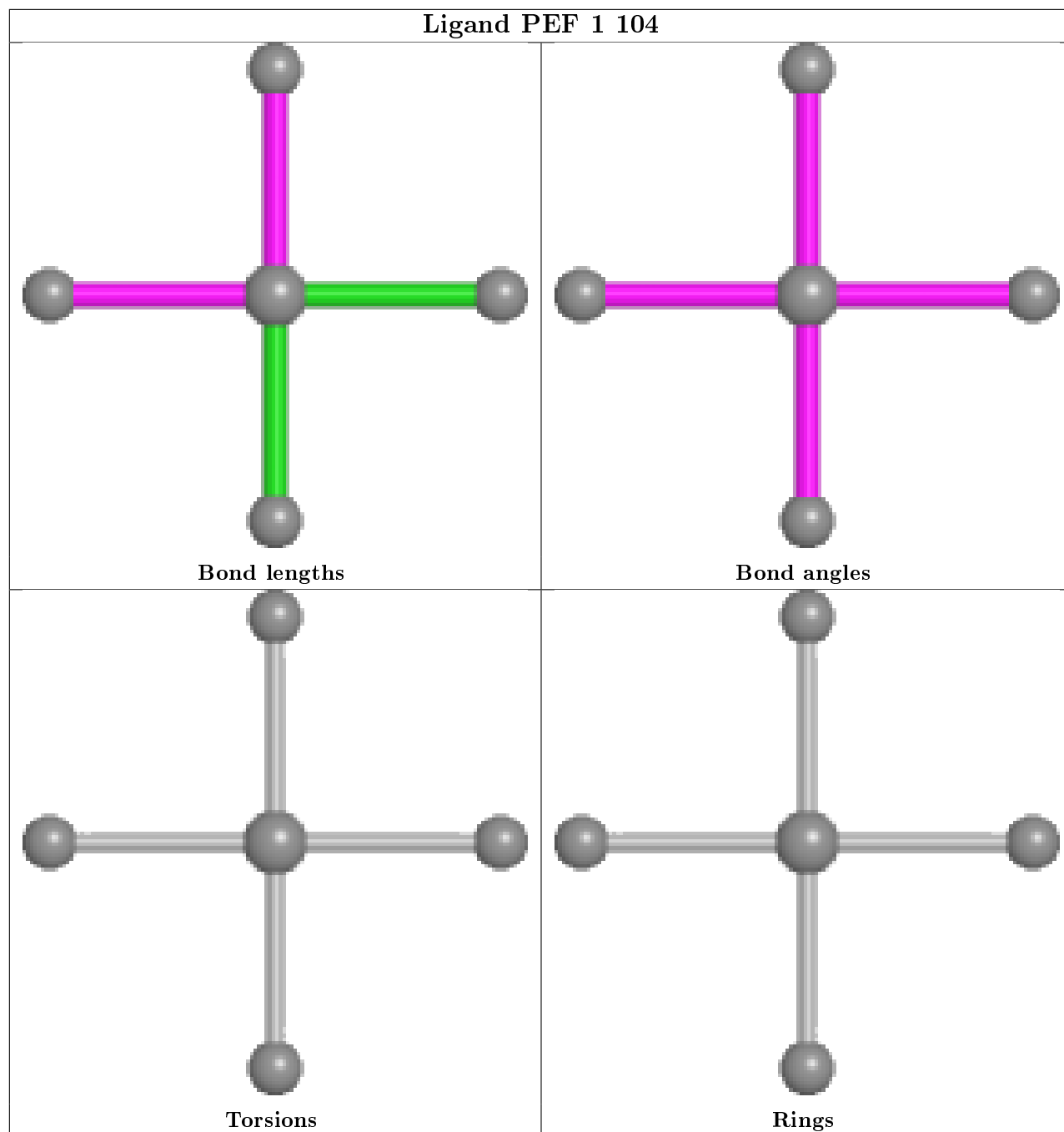
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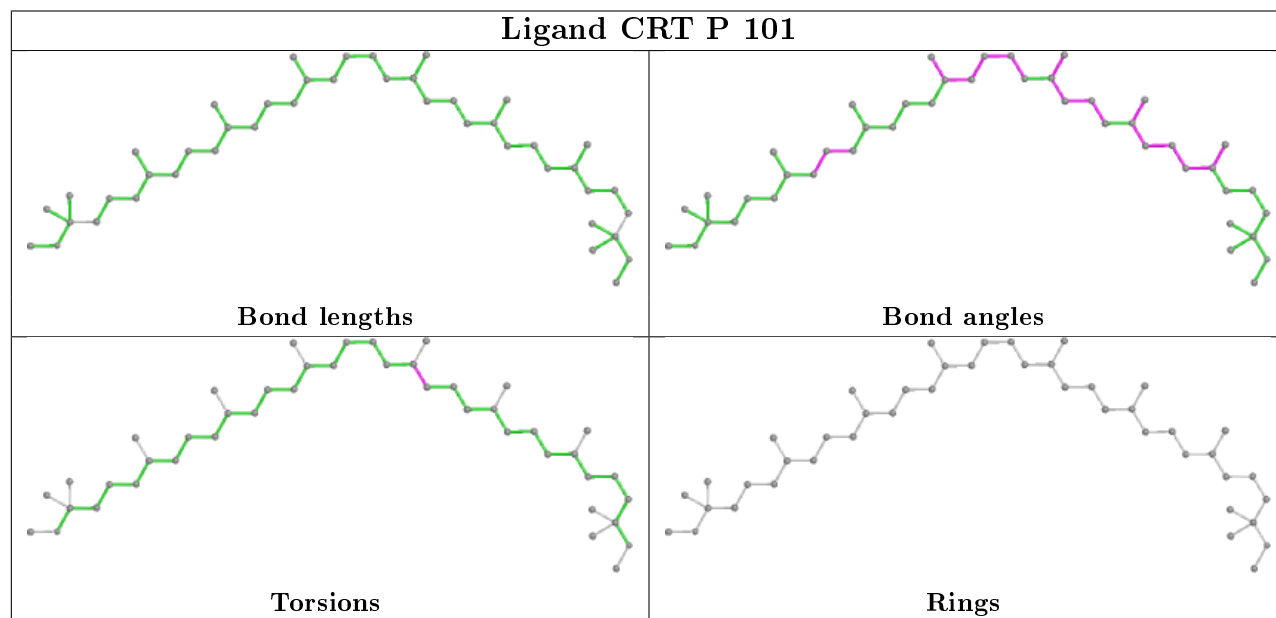
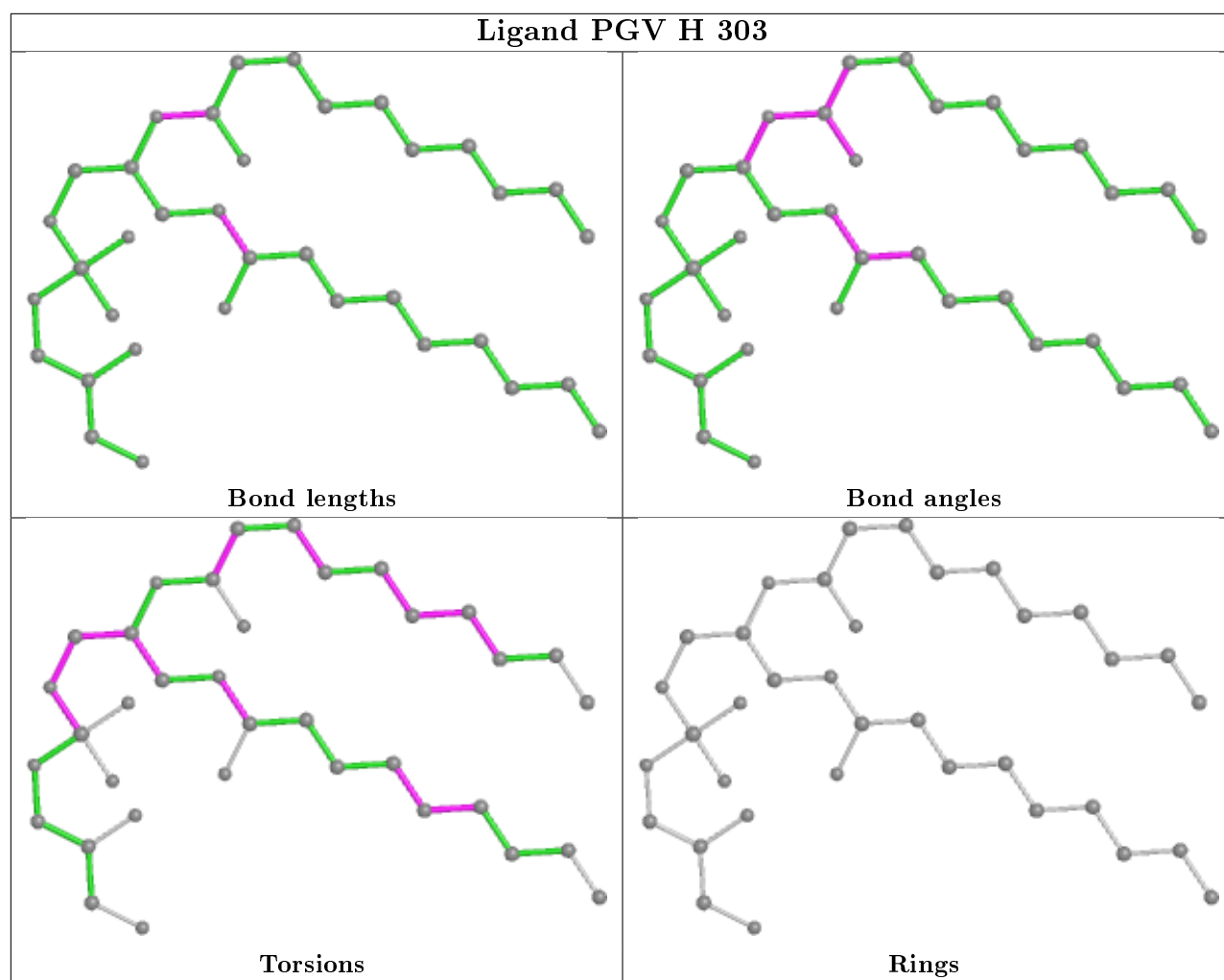


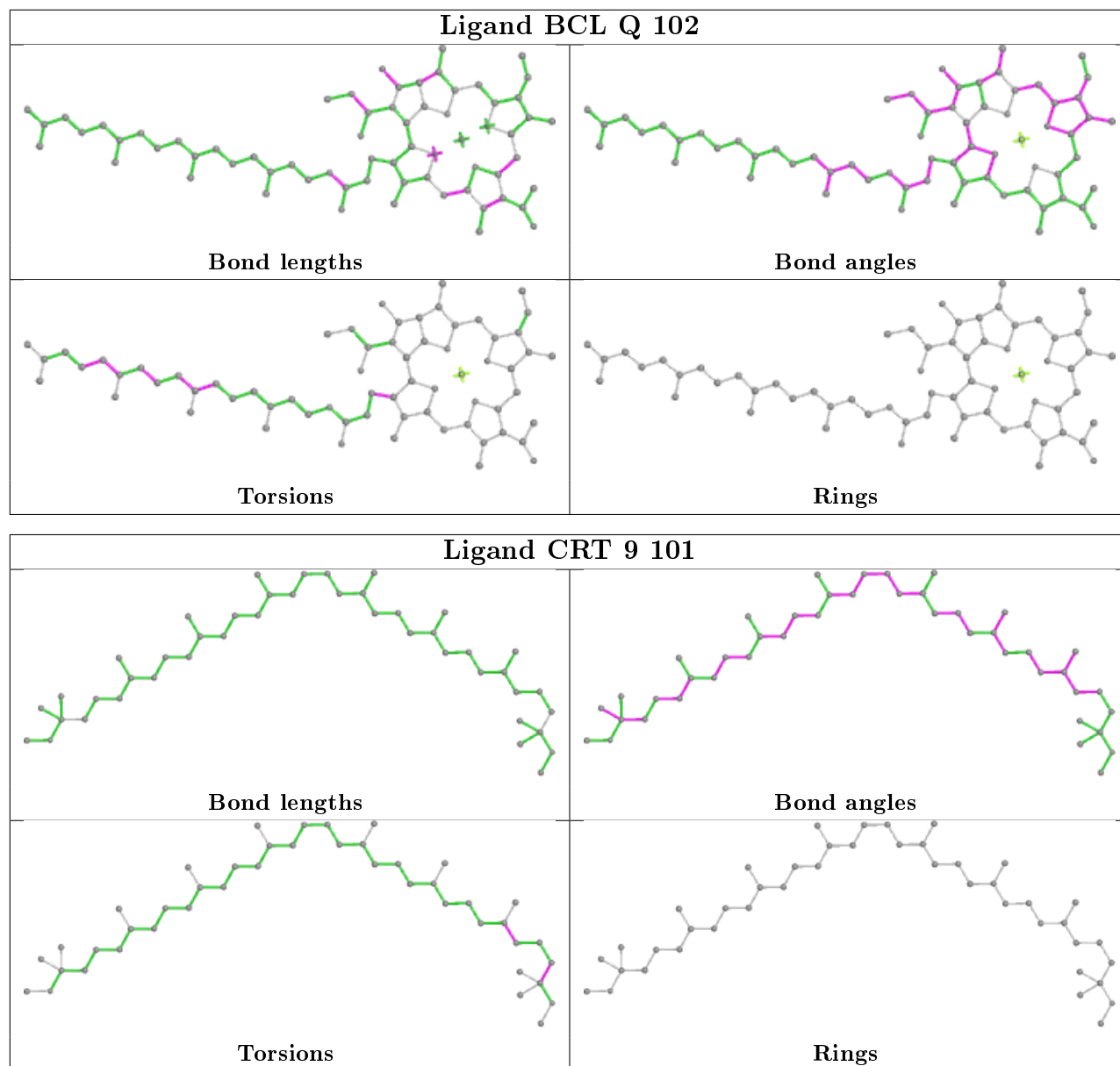
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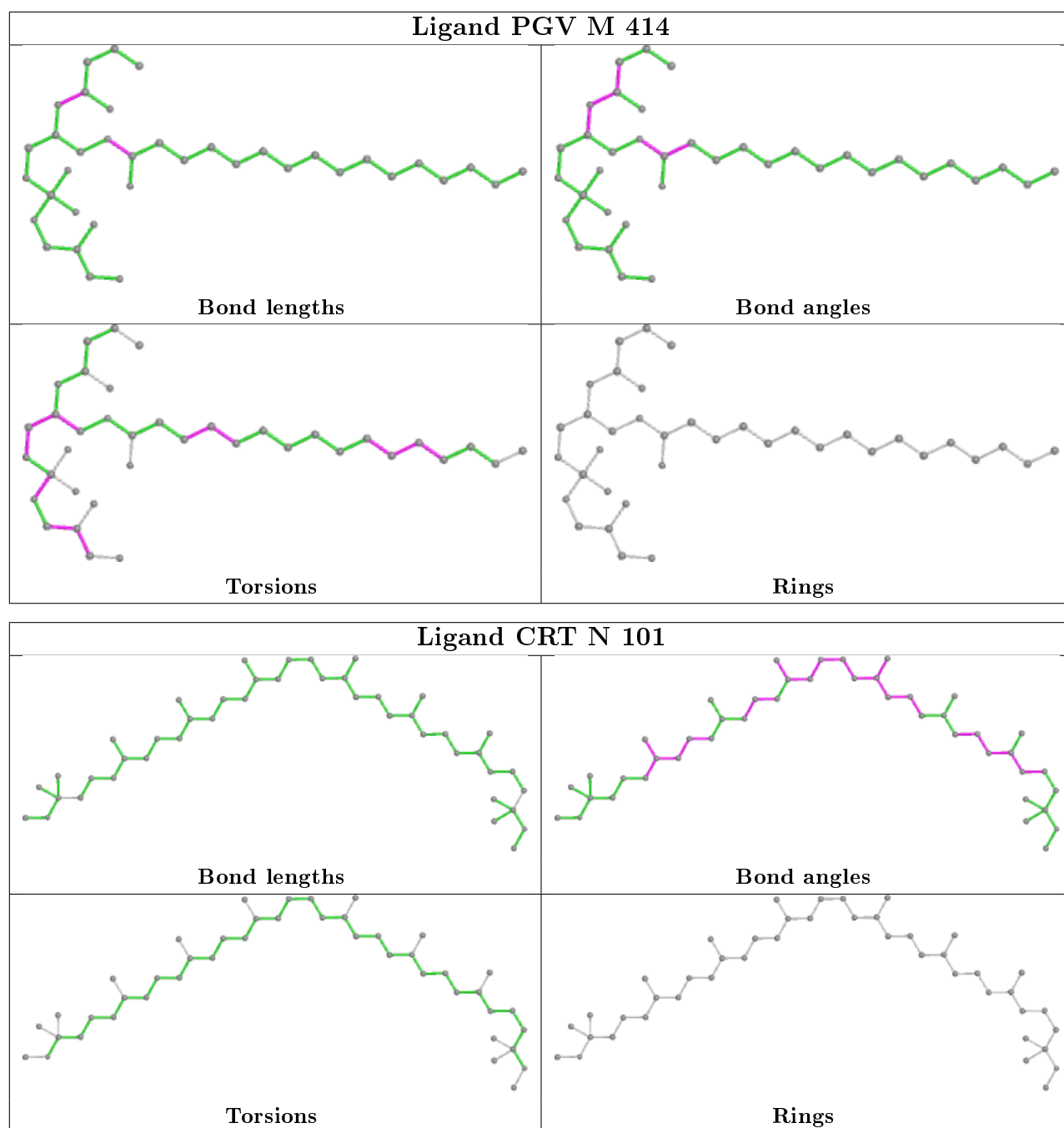


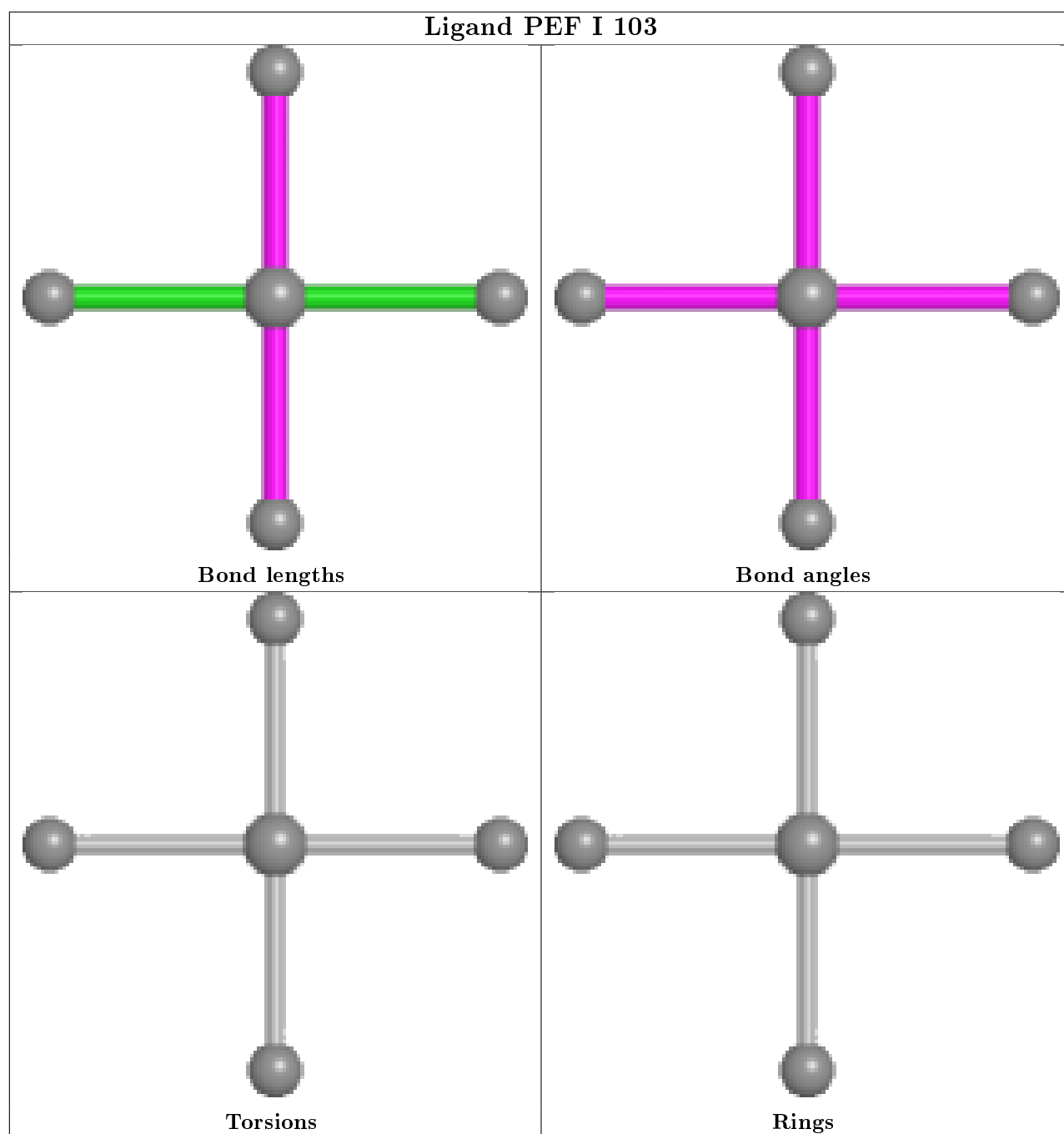




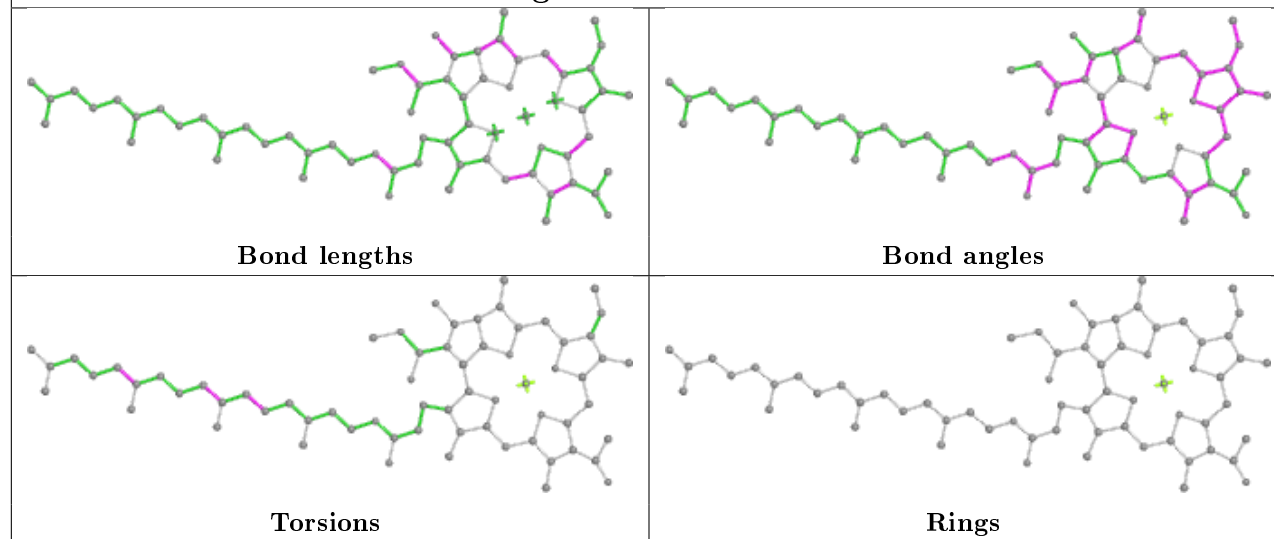




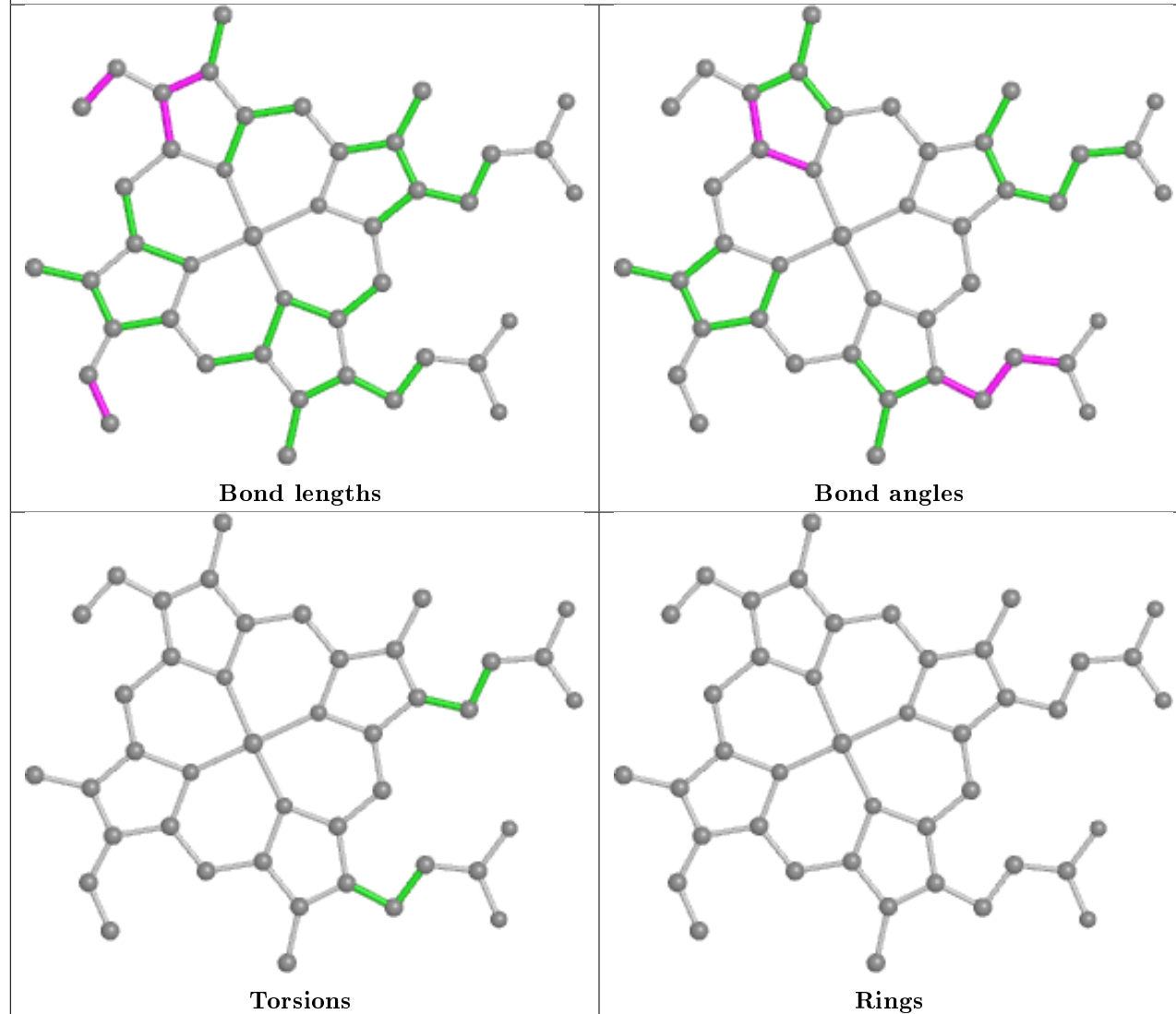


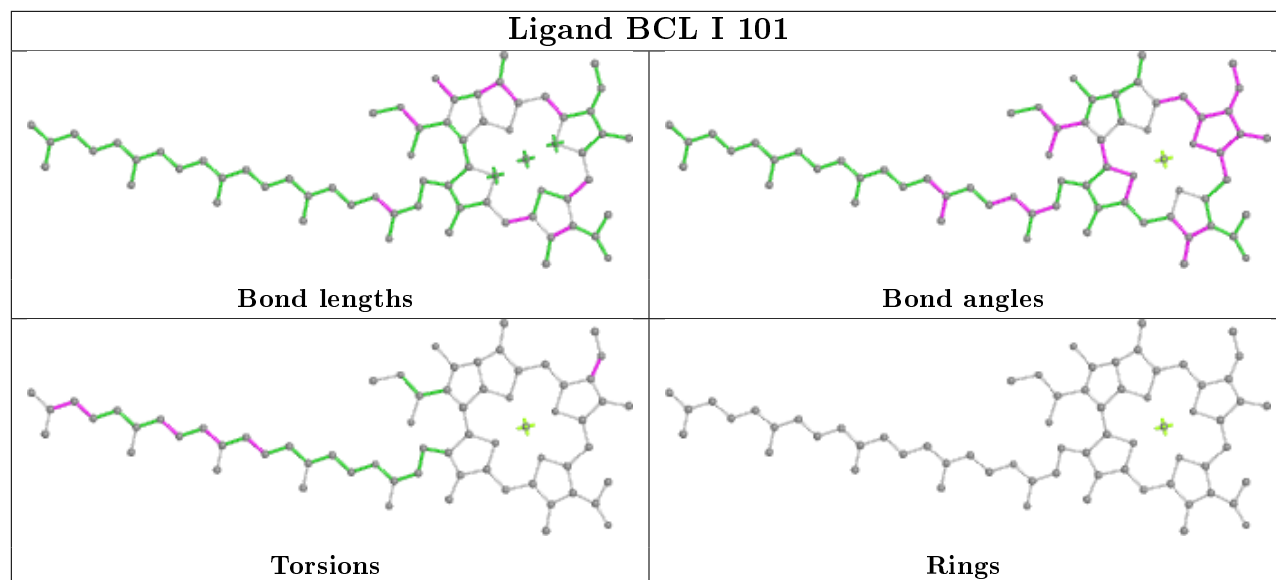
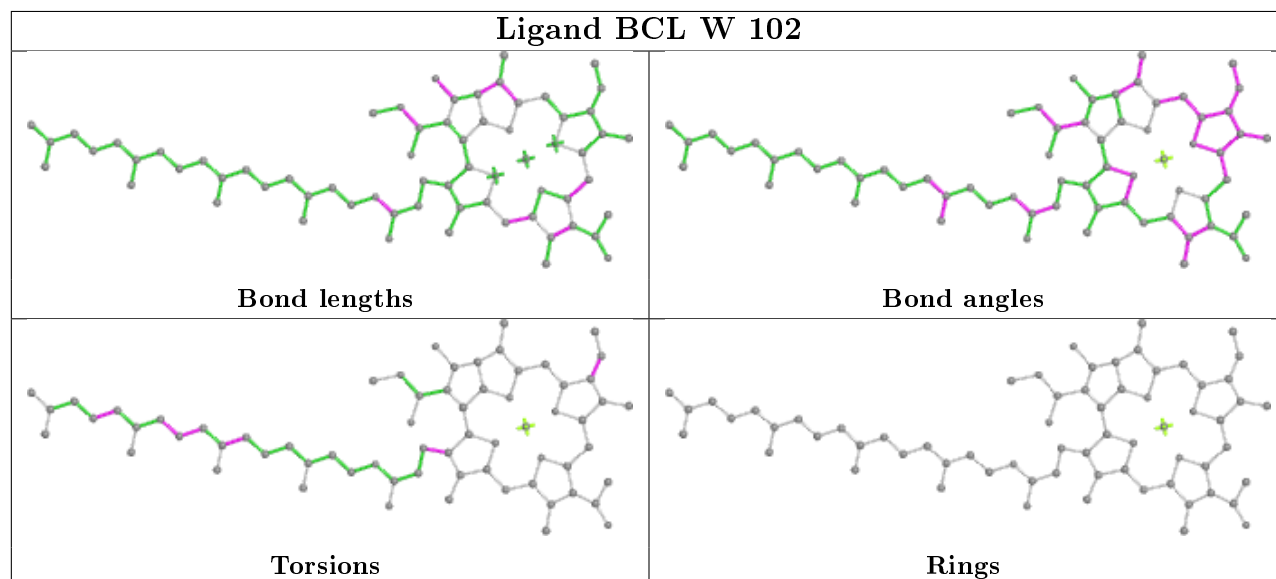
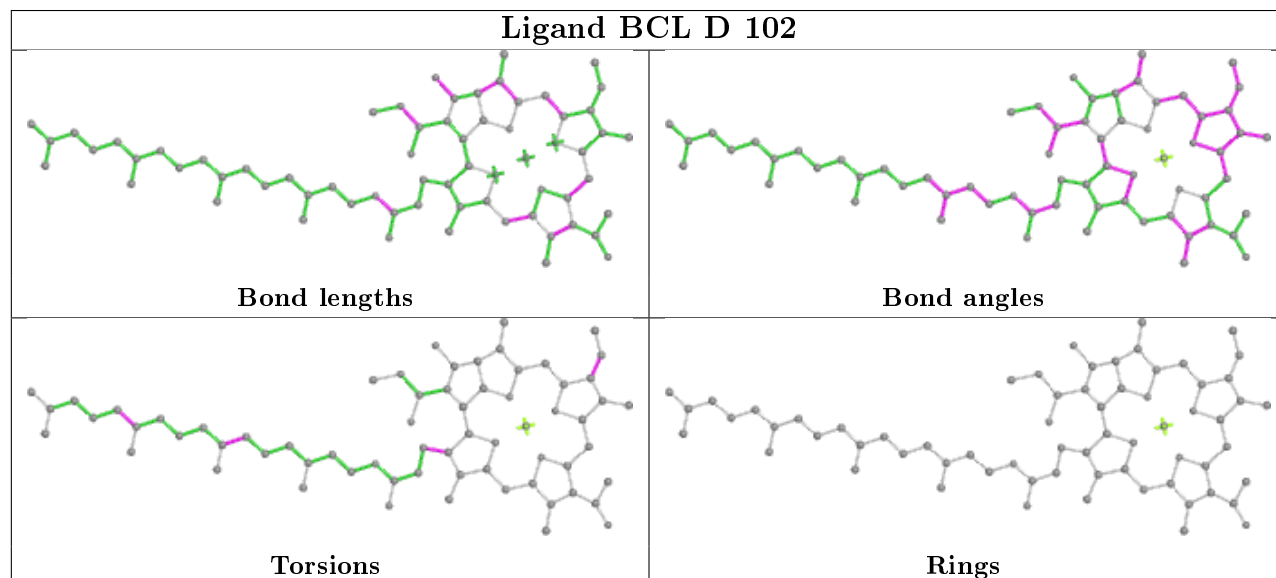


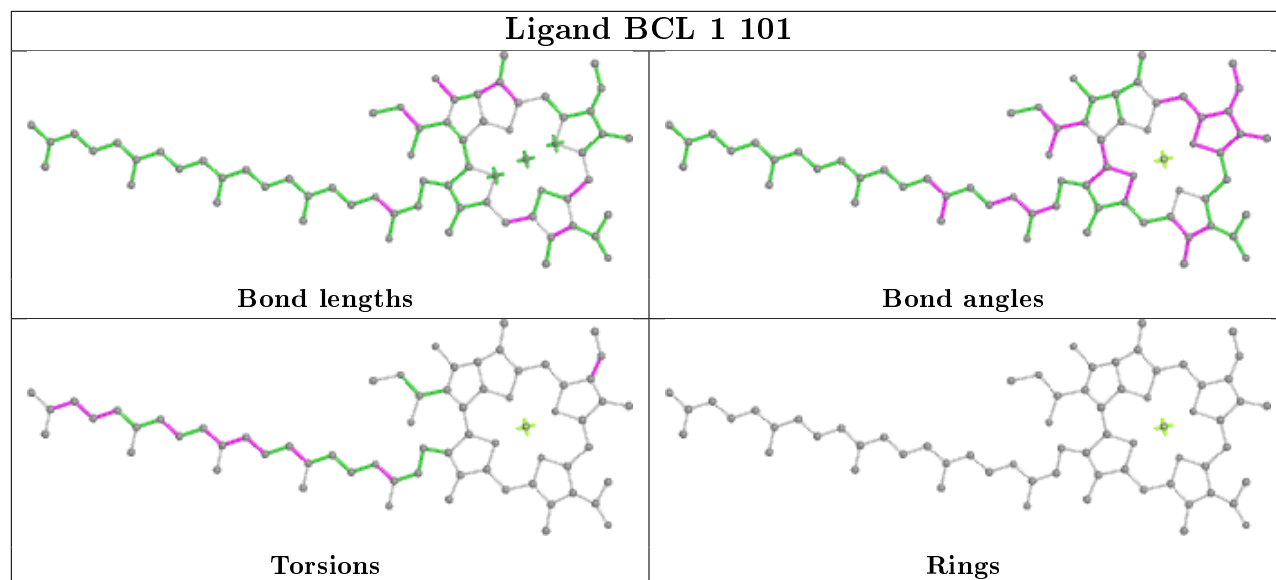
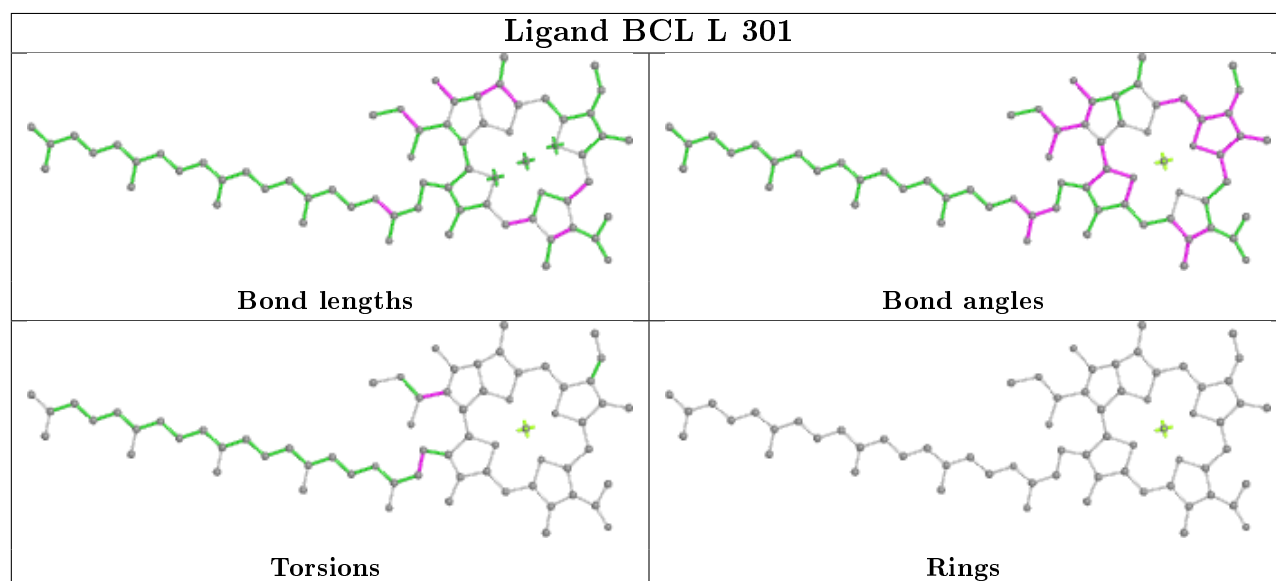
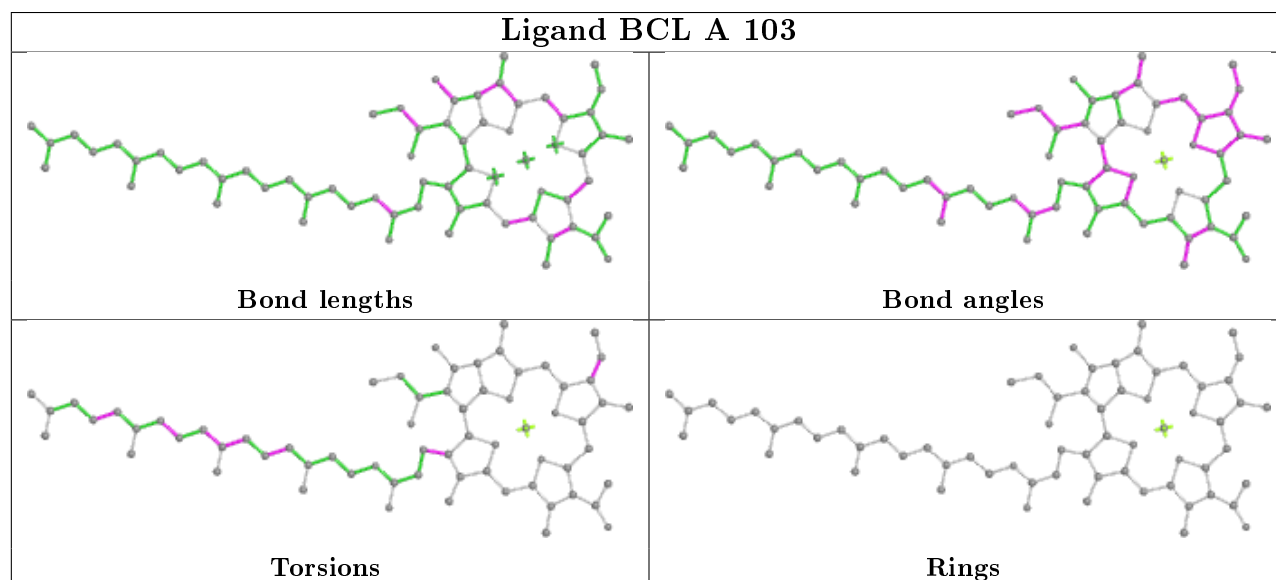
Ligand BCL U 101

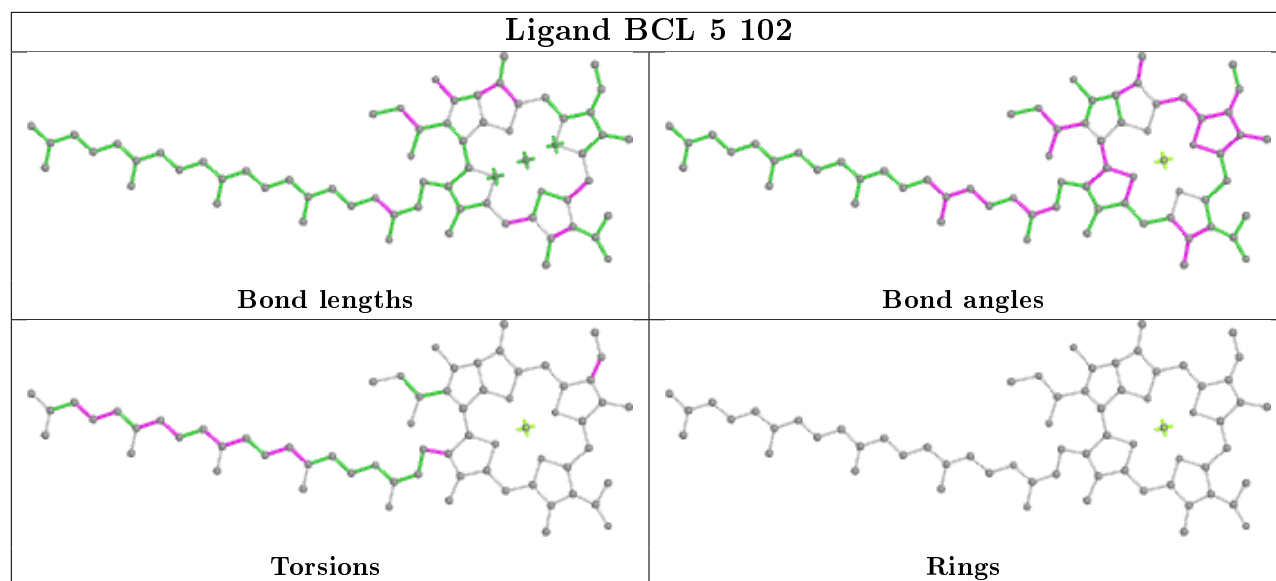
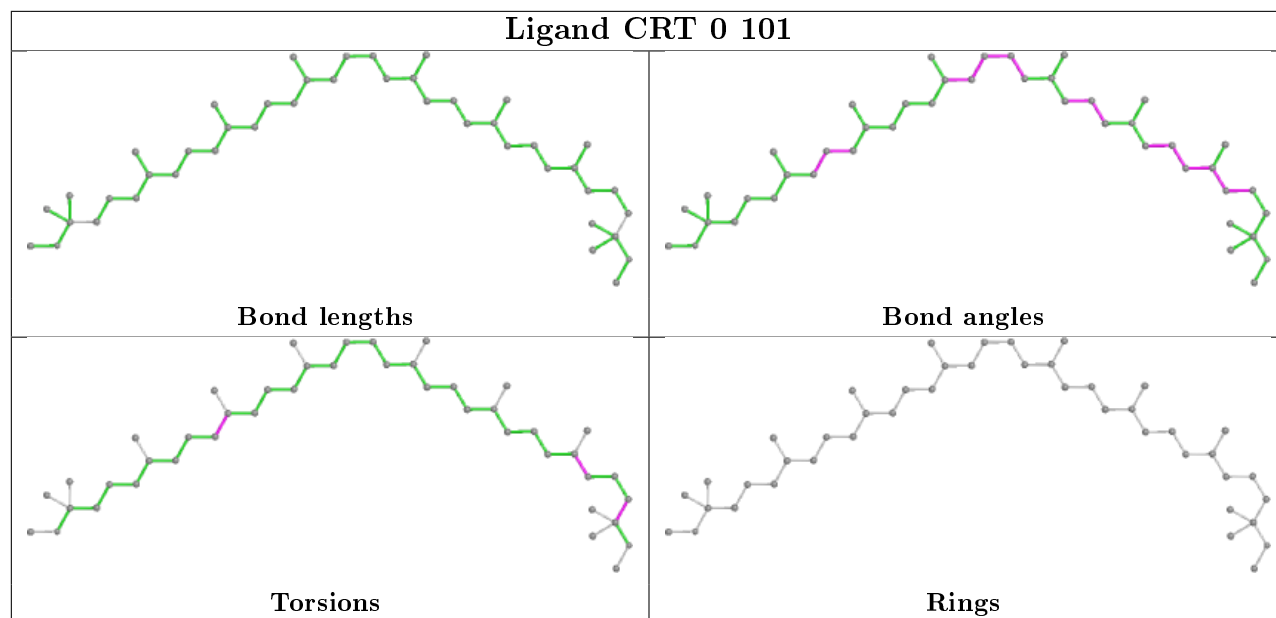


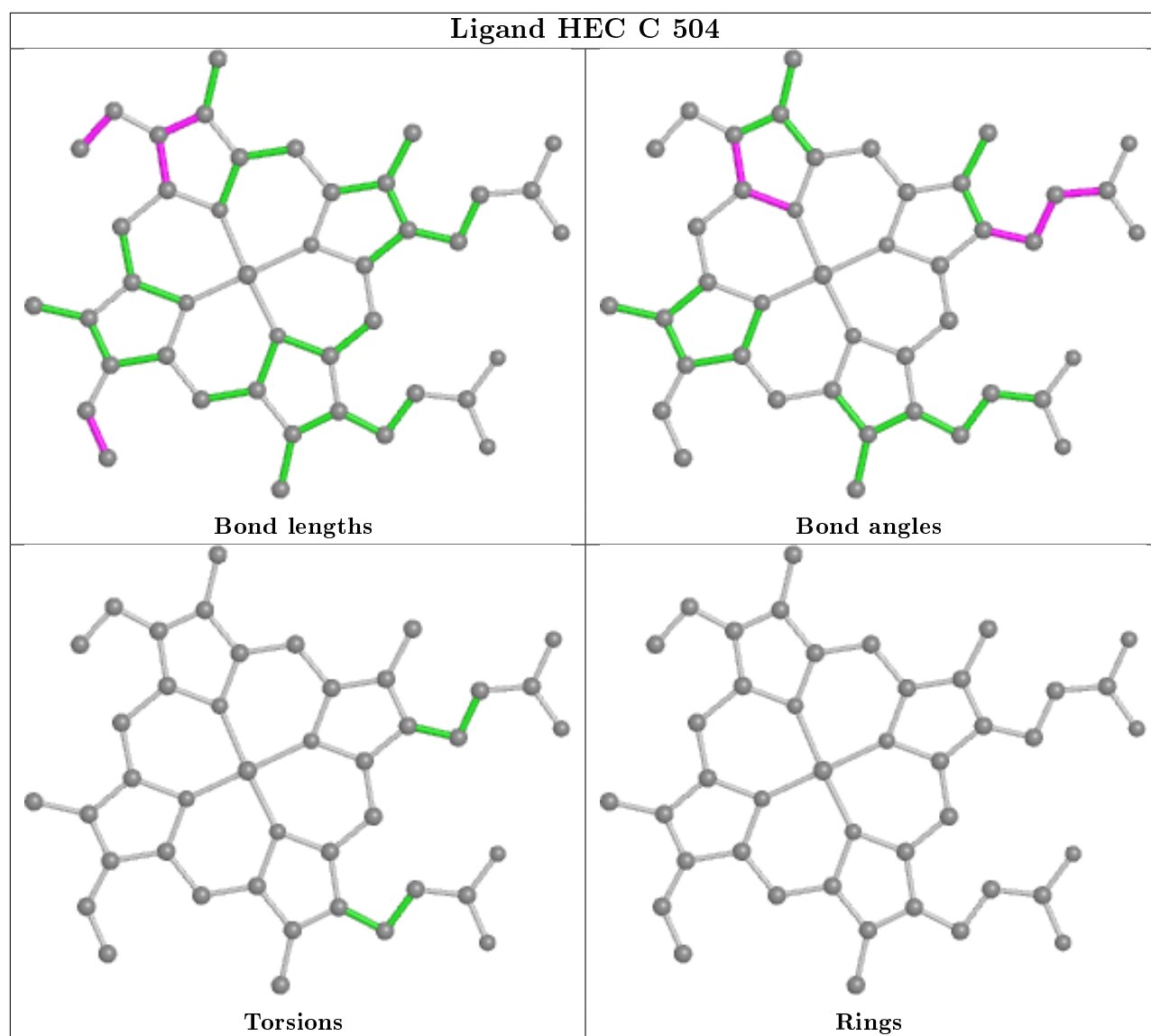
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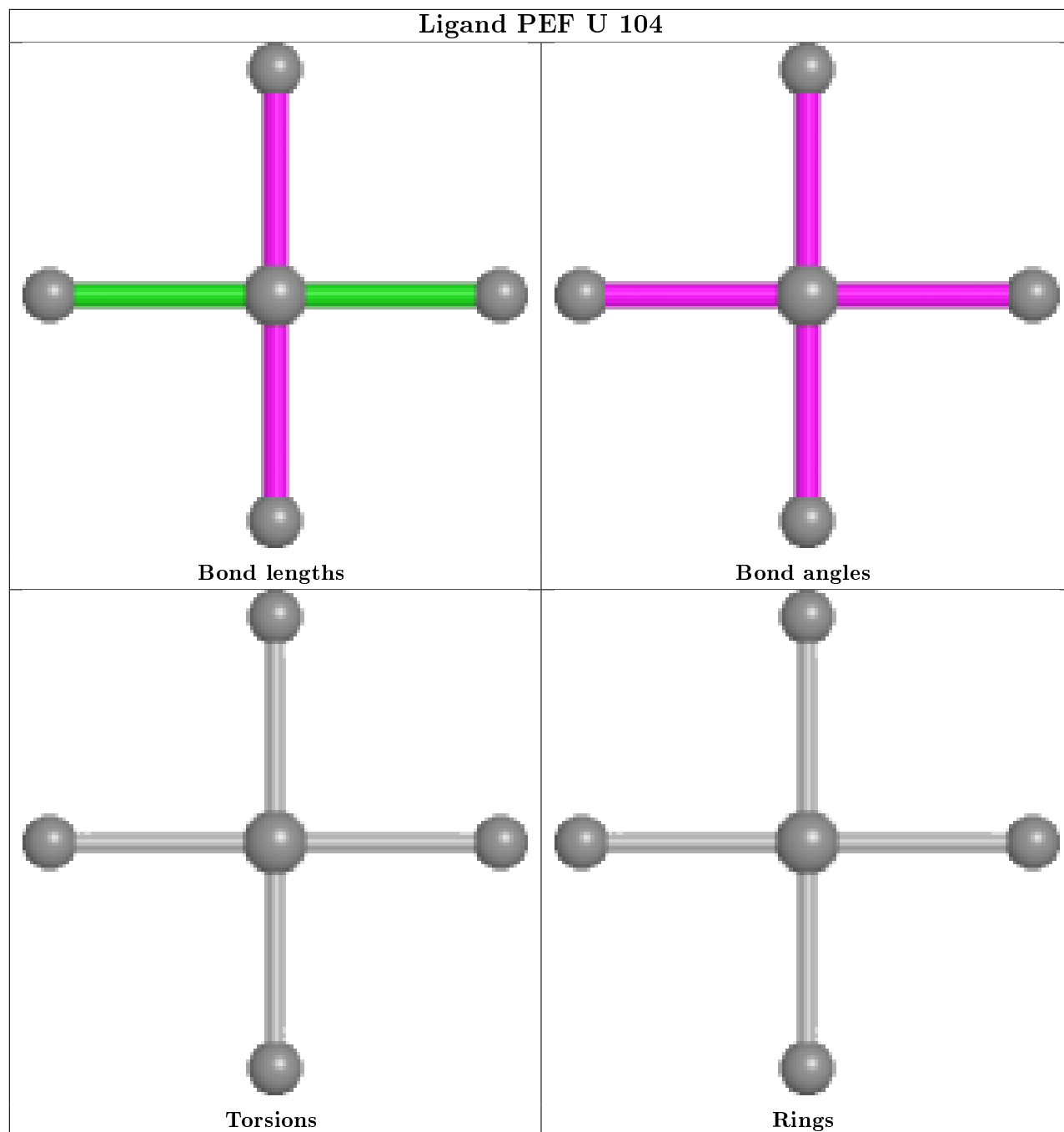


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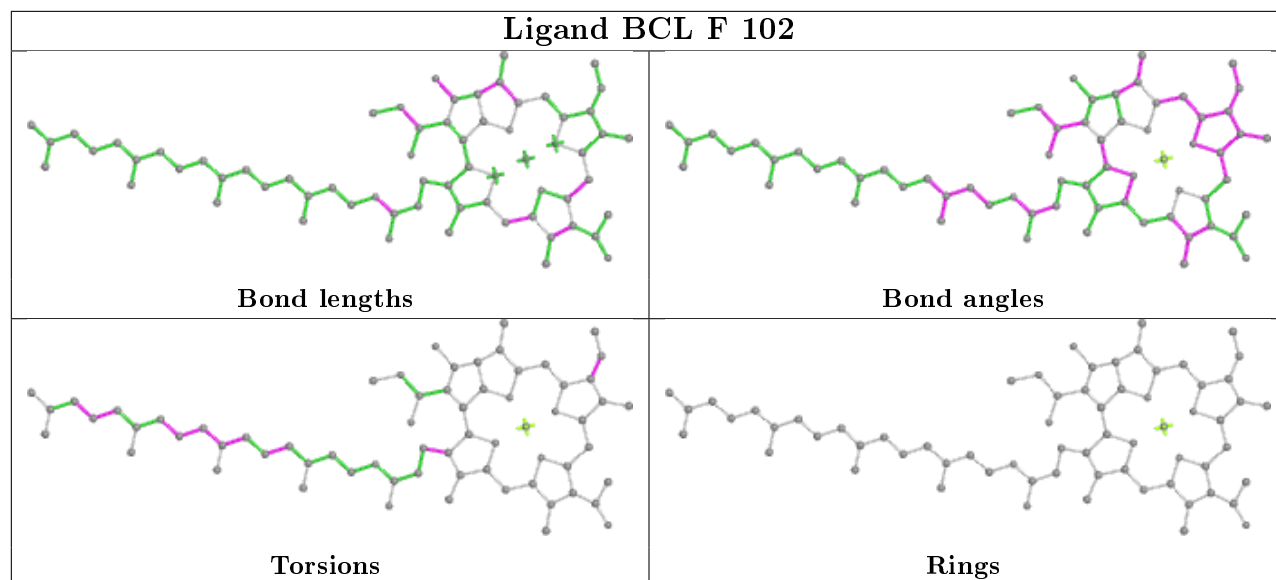
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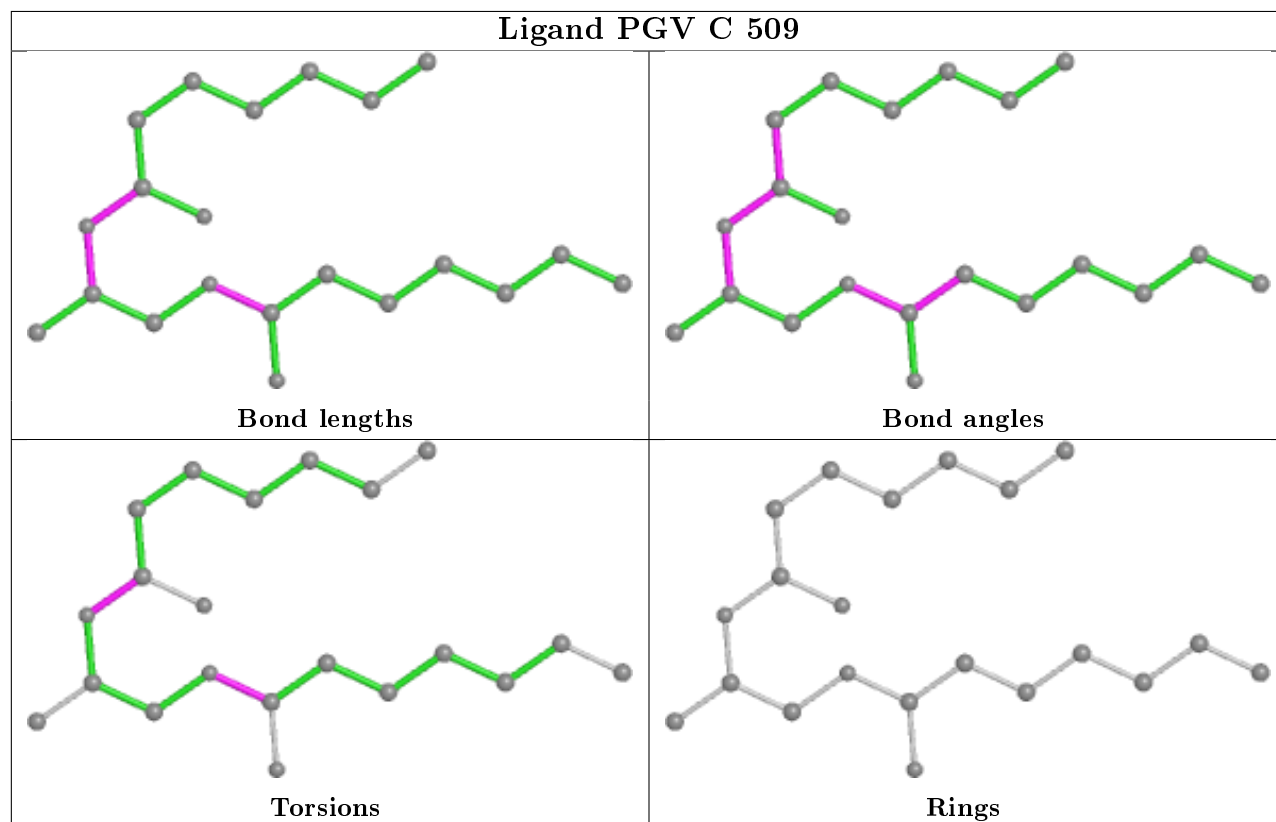


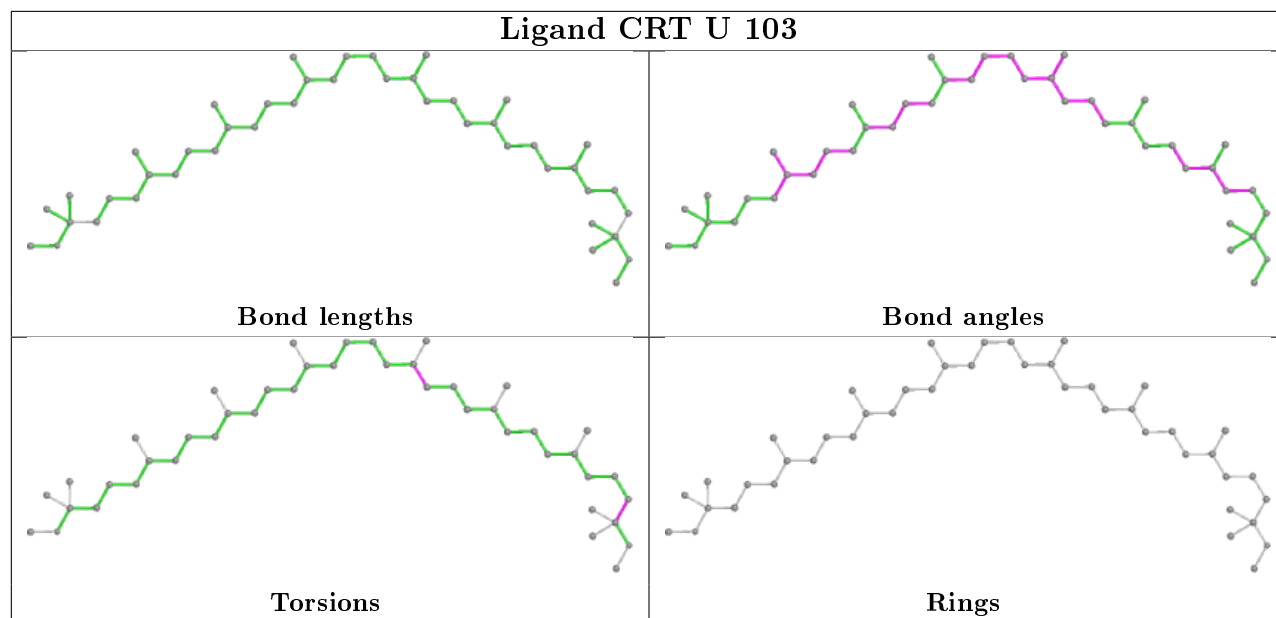


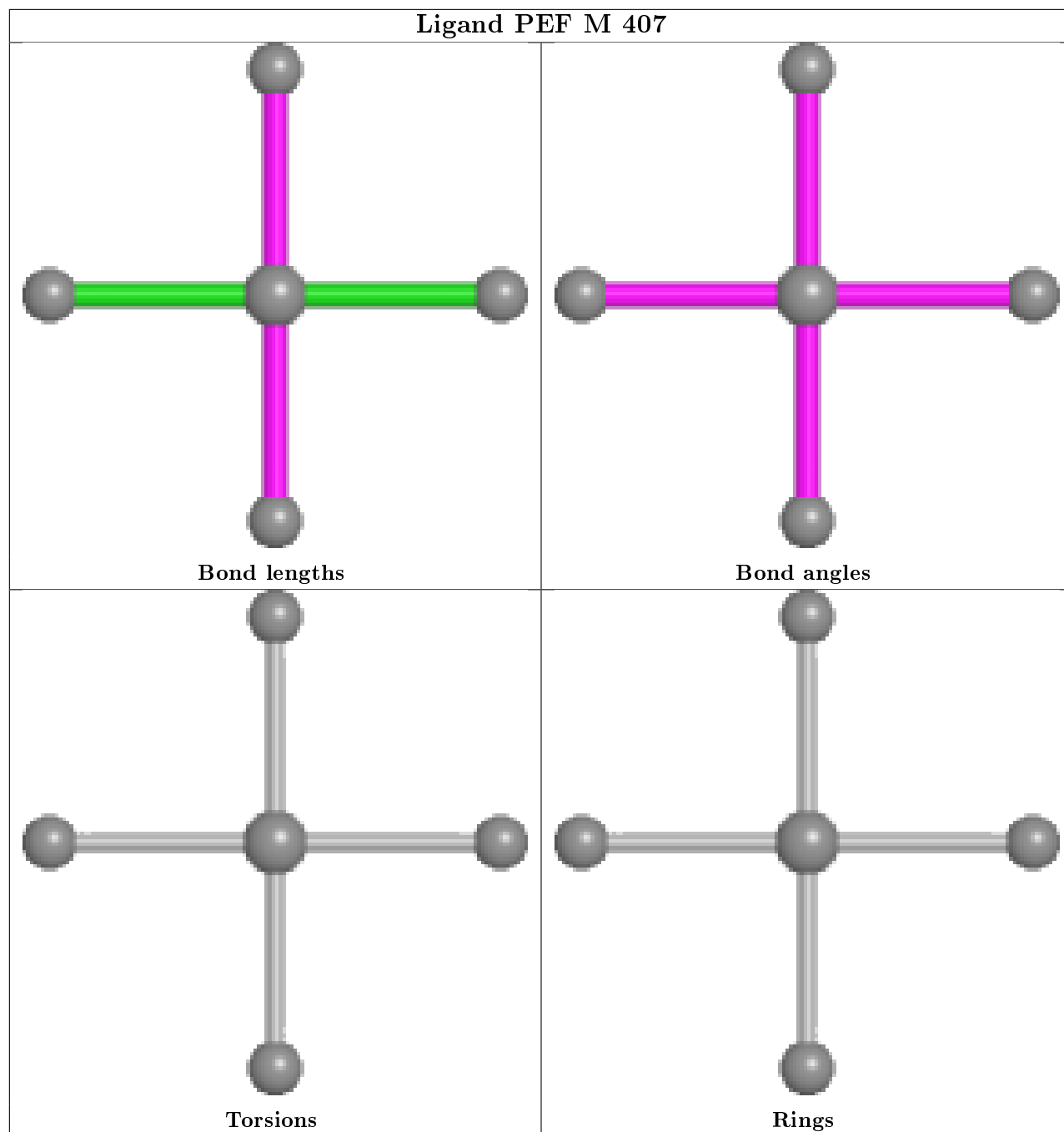
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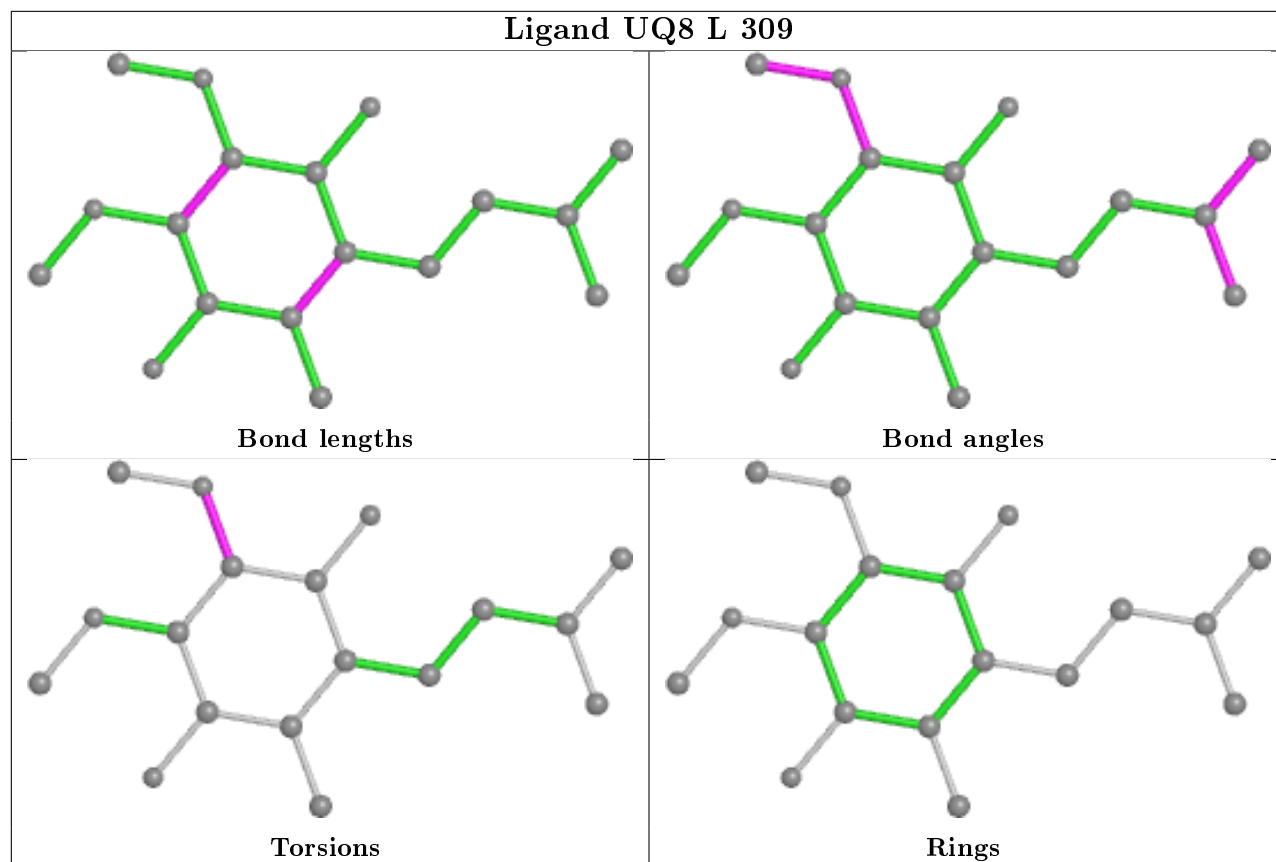
Ligand PGV C 509



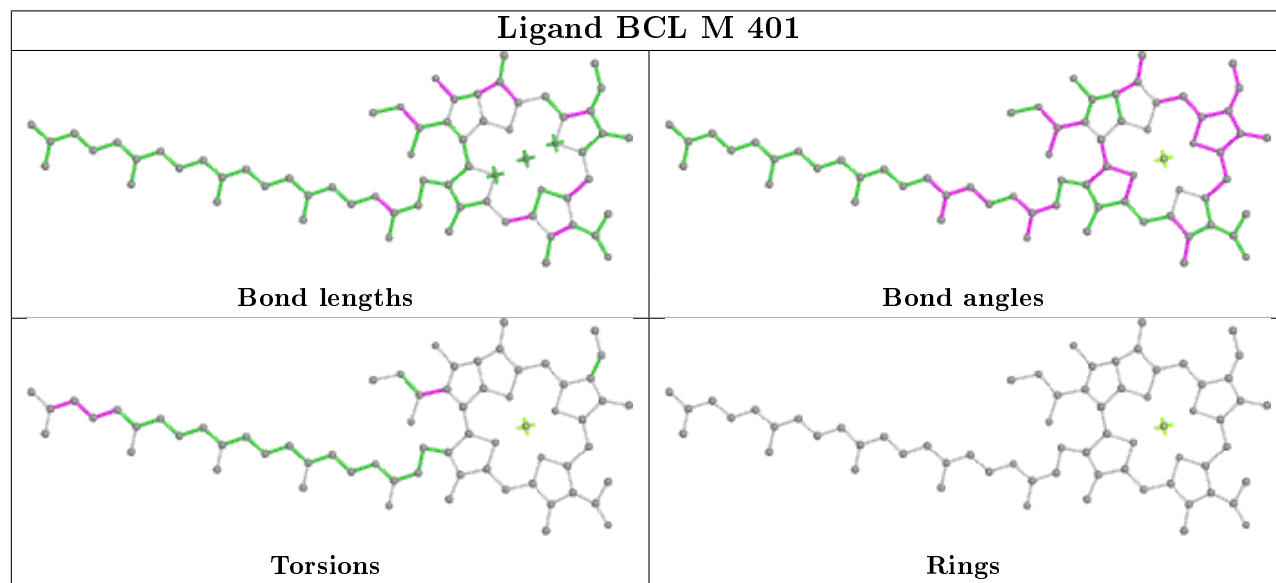


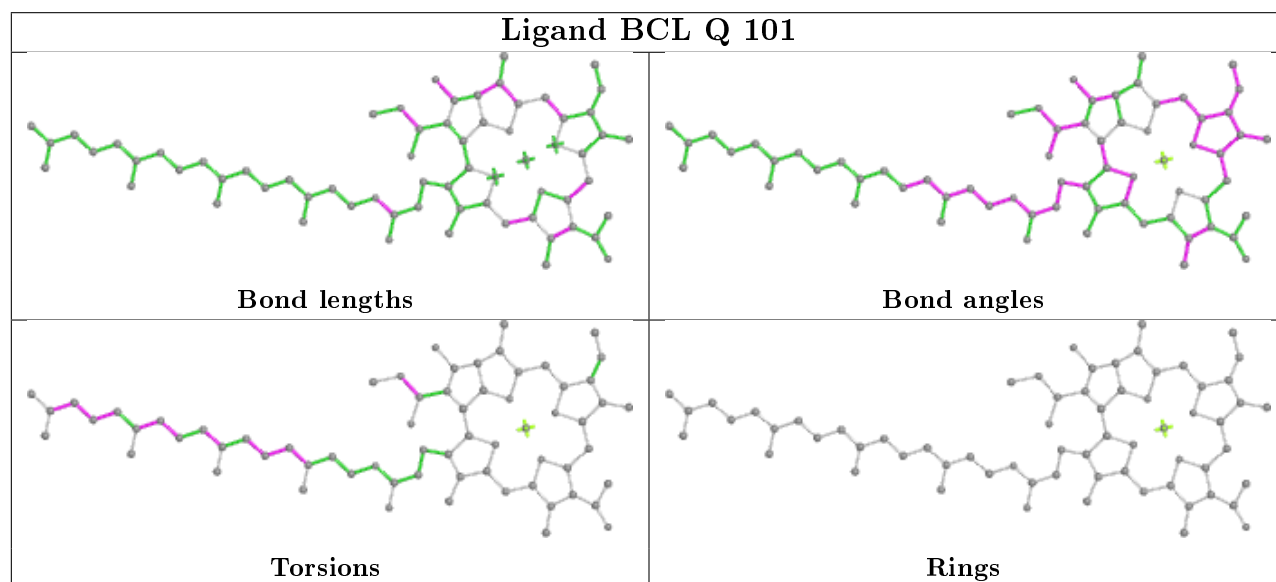
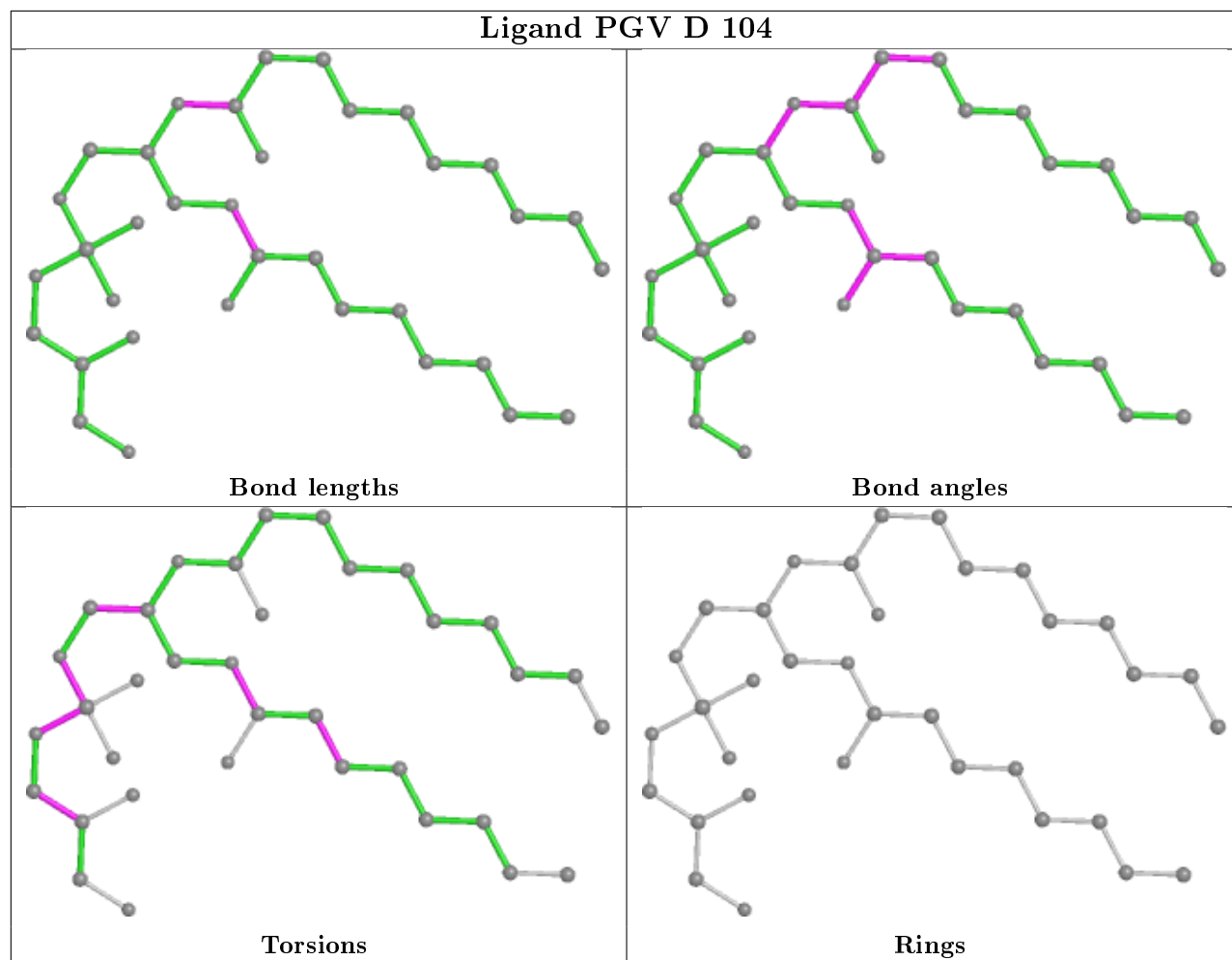


Ligand UQ8 L 309

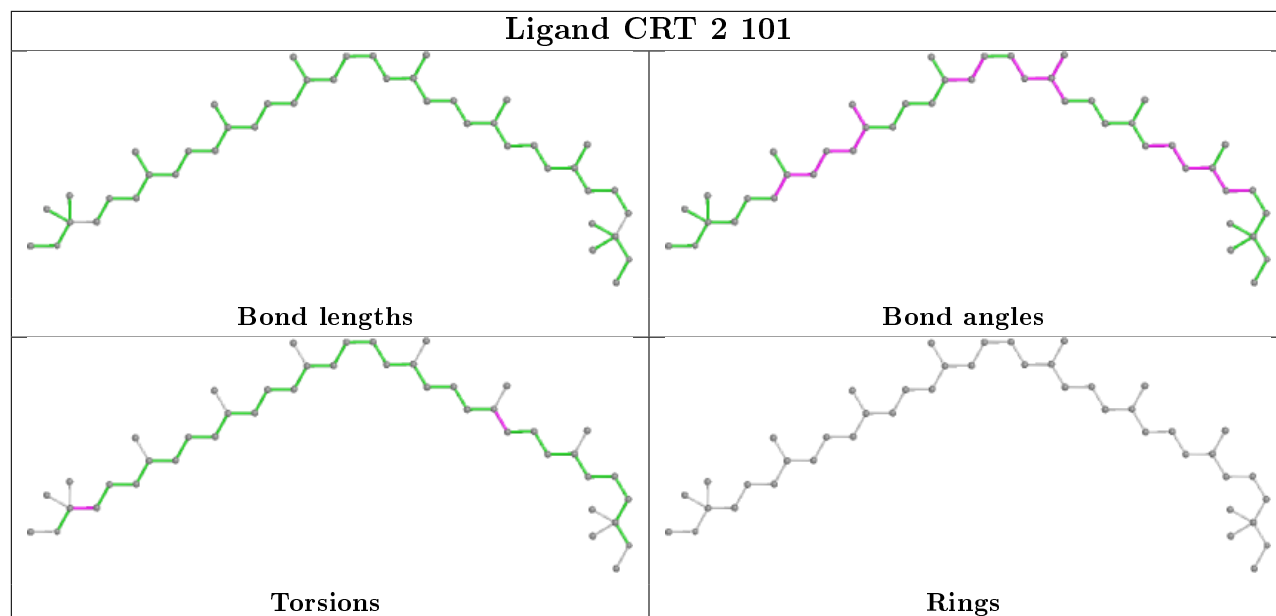


Ligand BCL M 401

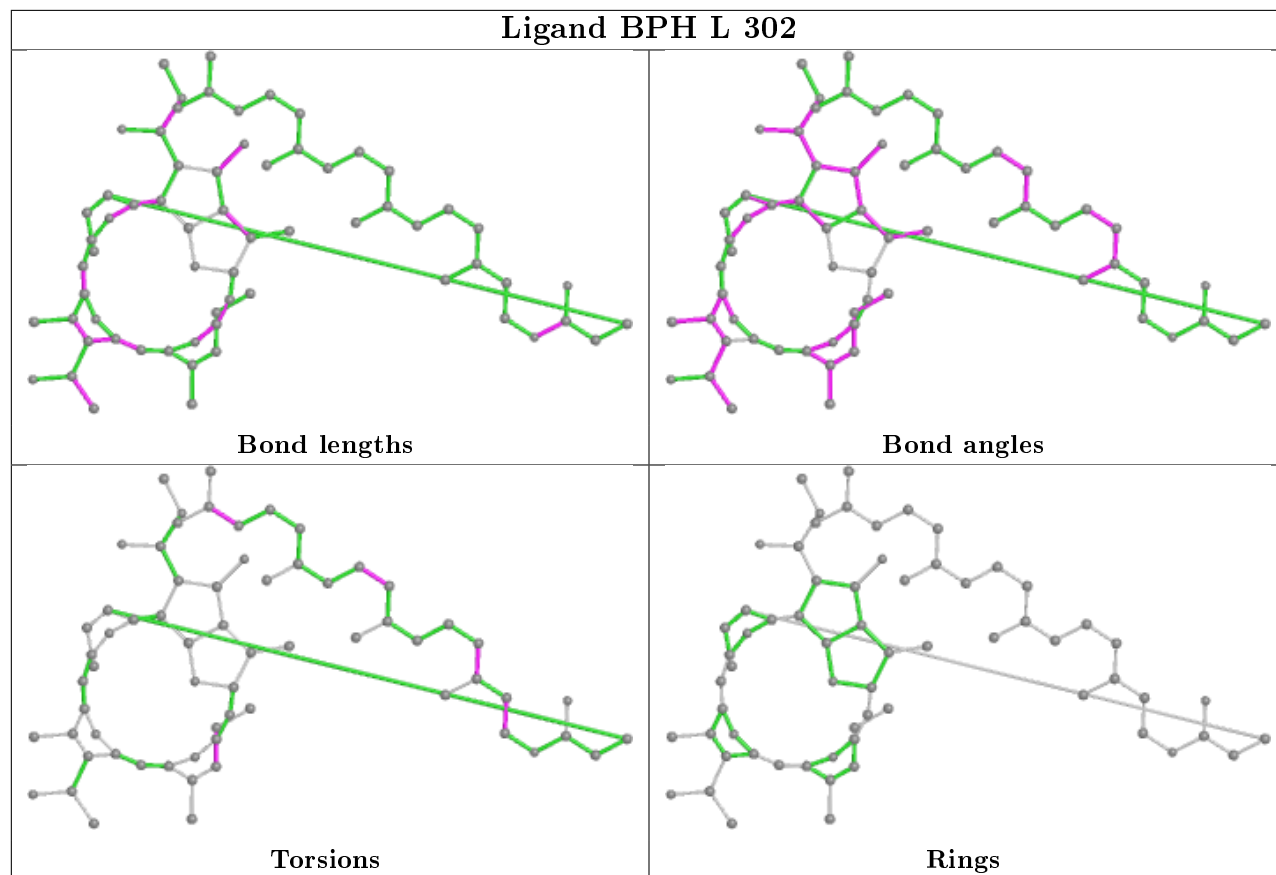


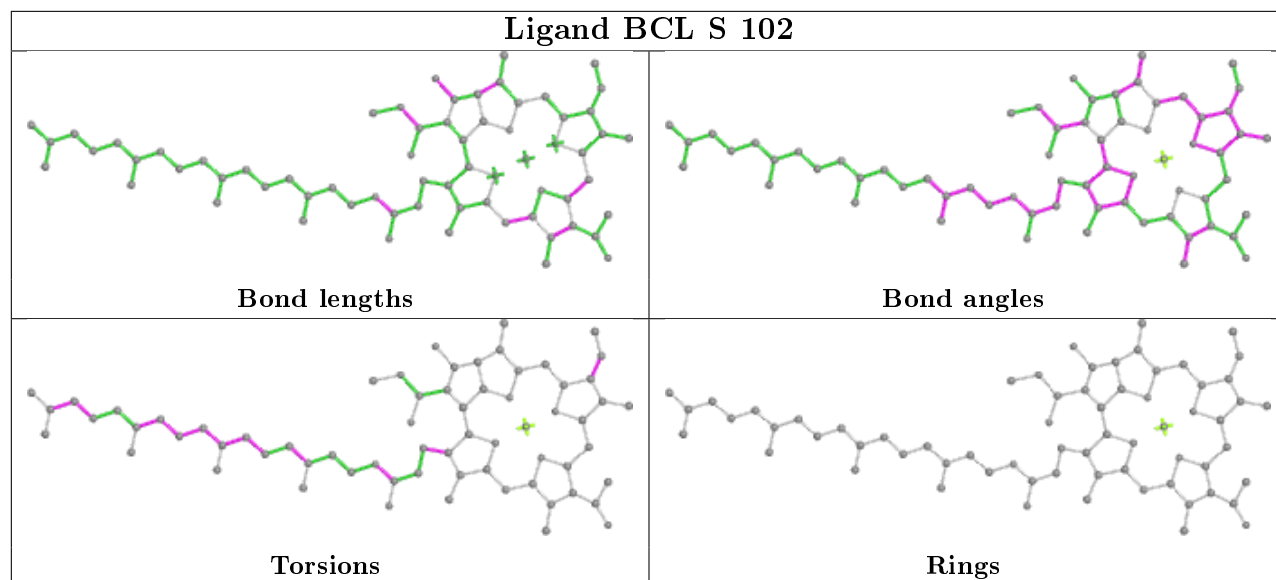
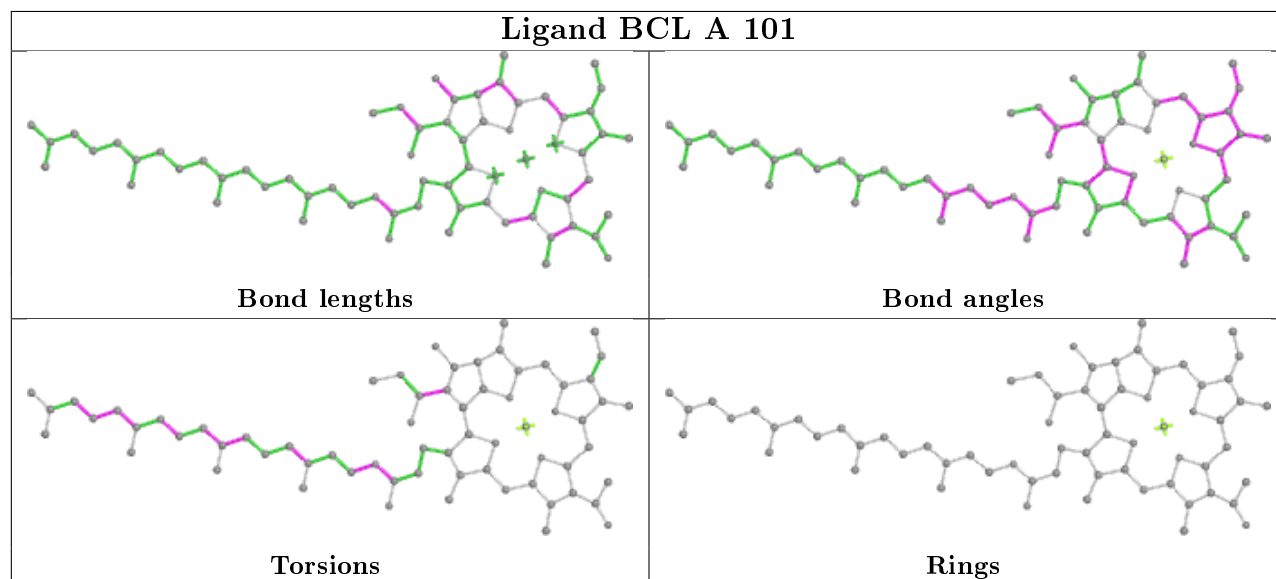
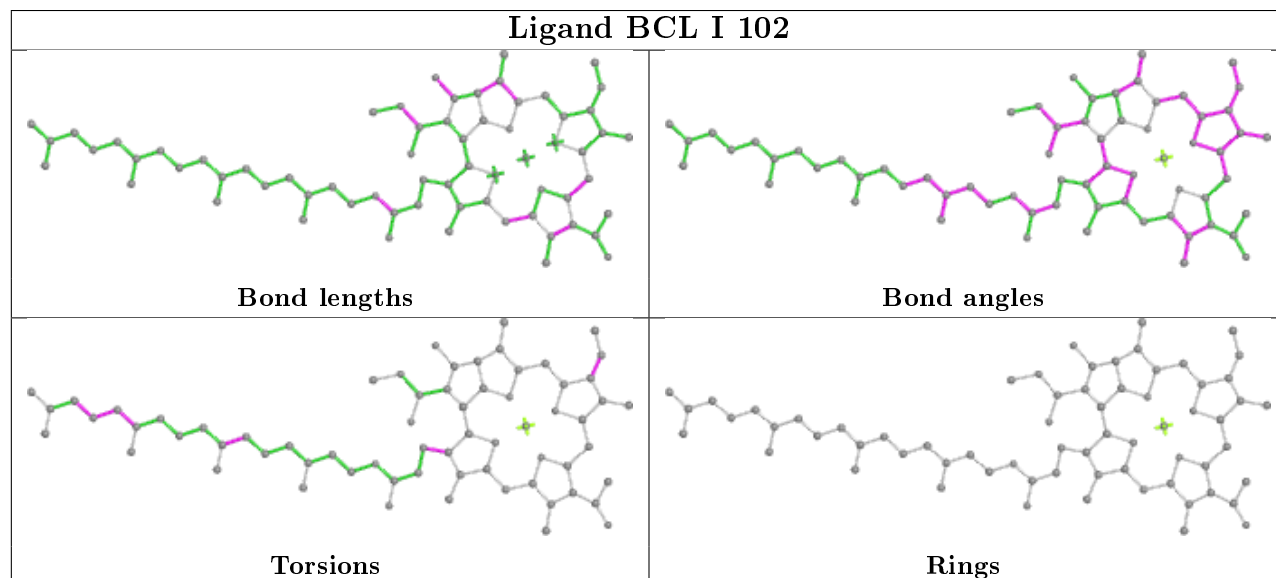


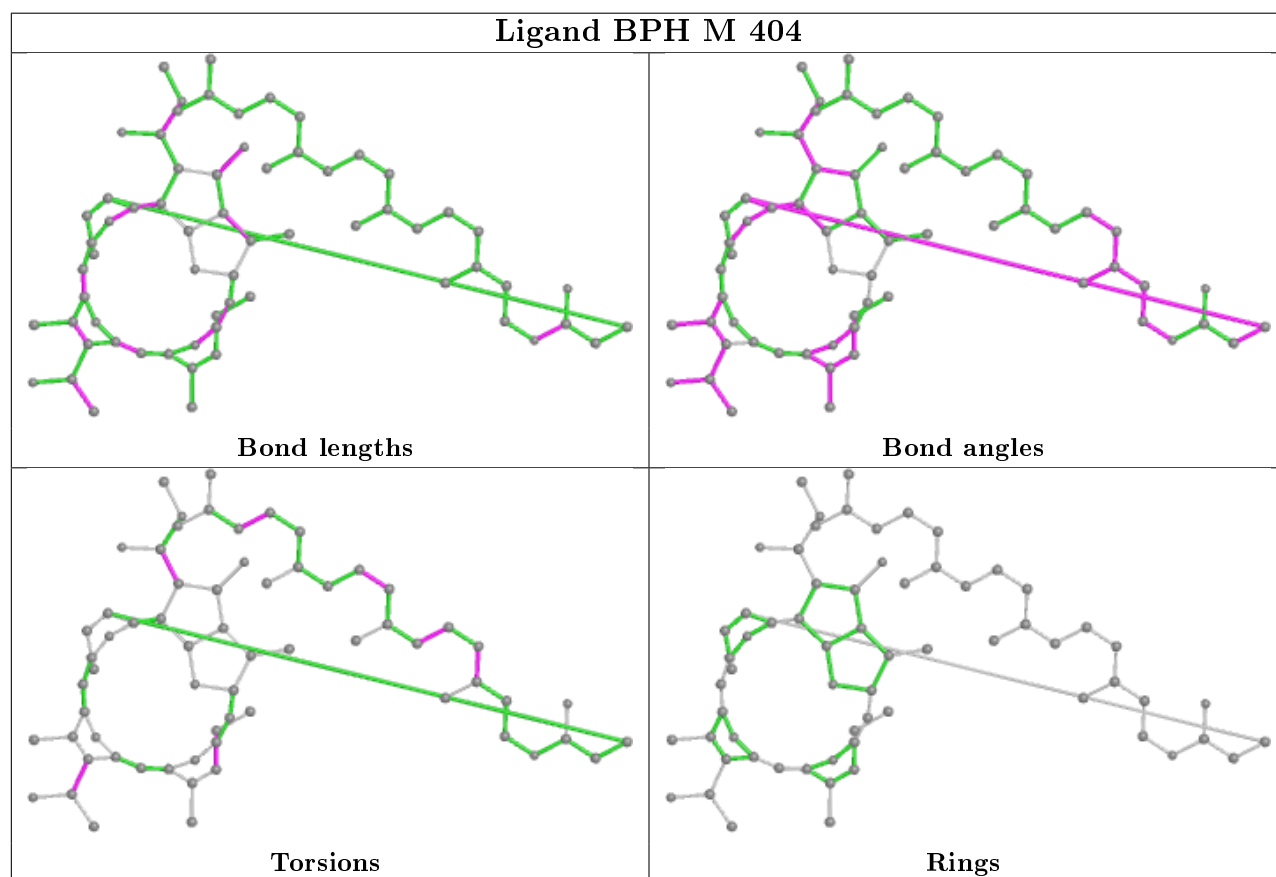
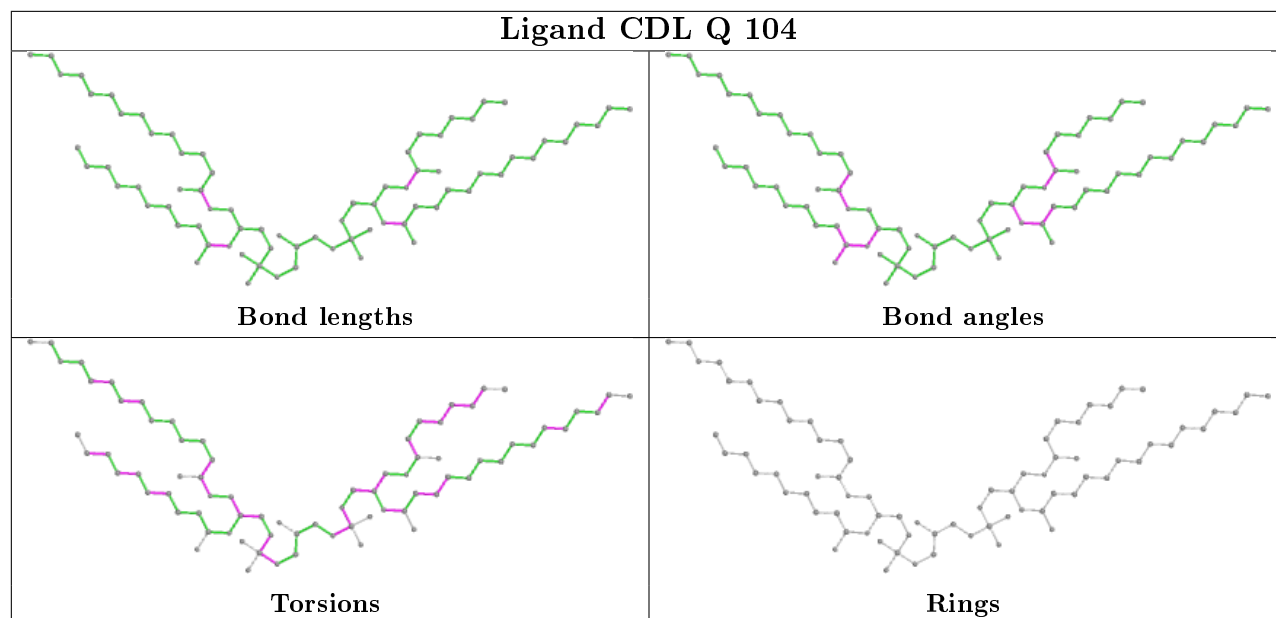
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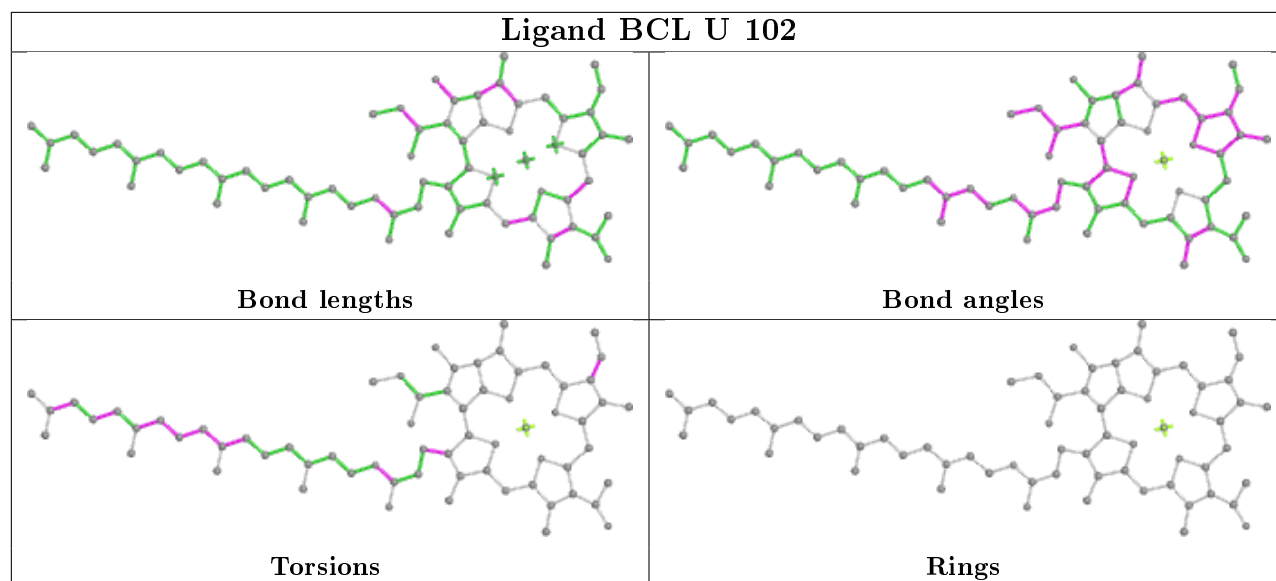
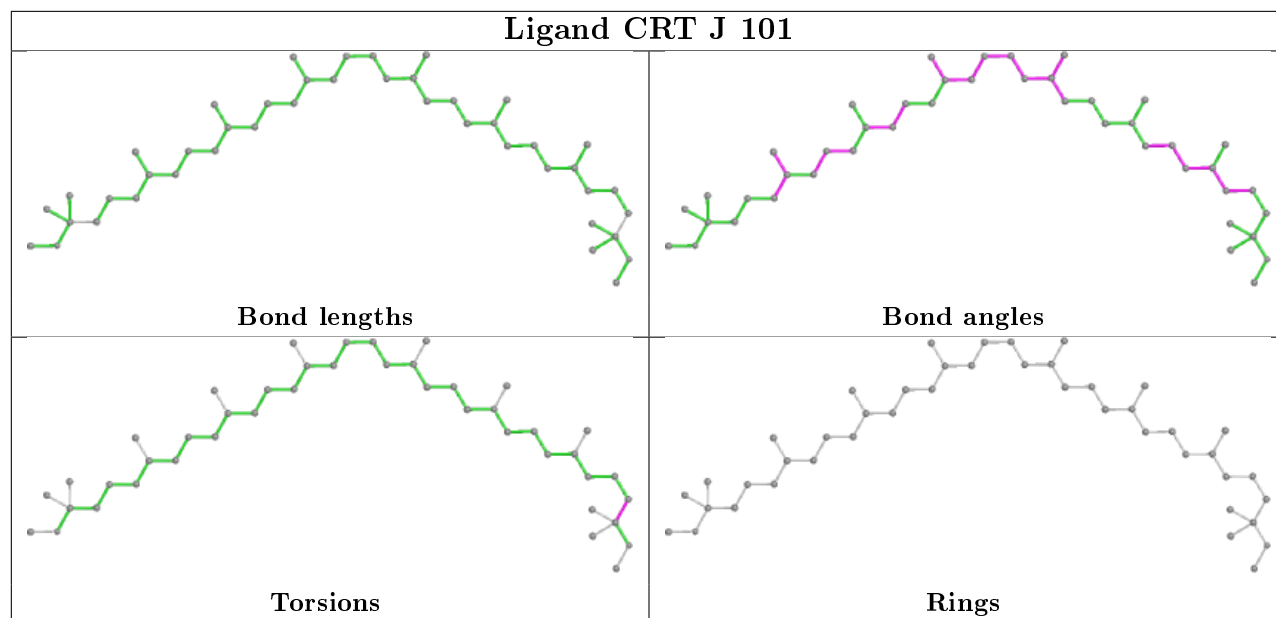


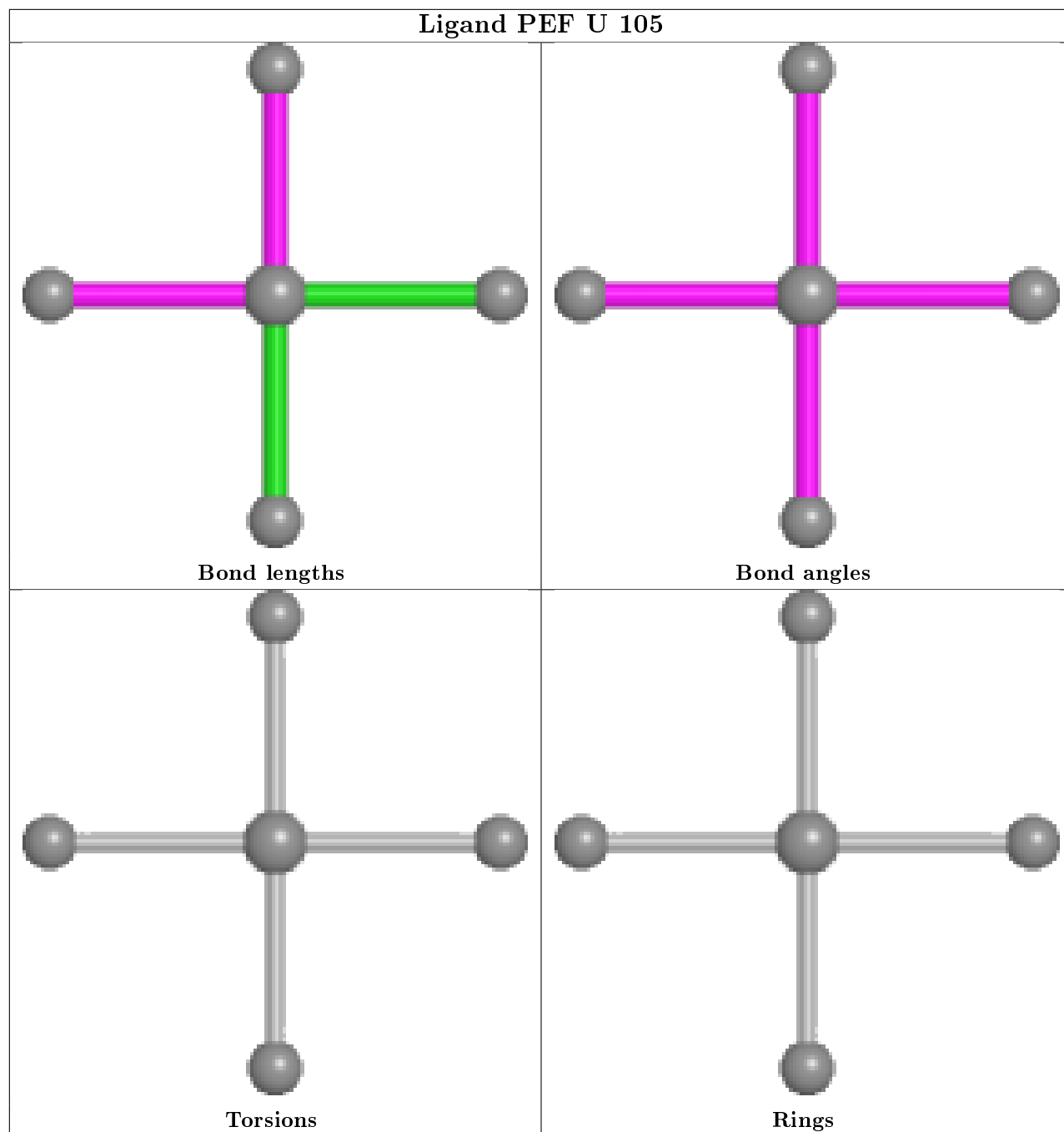
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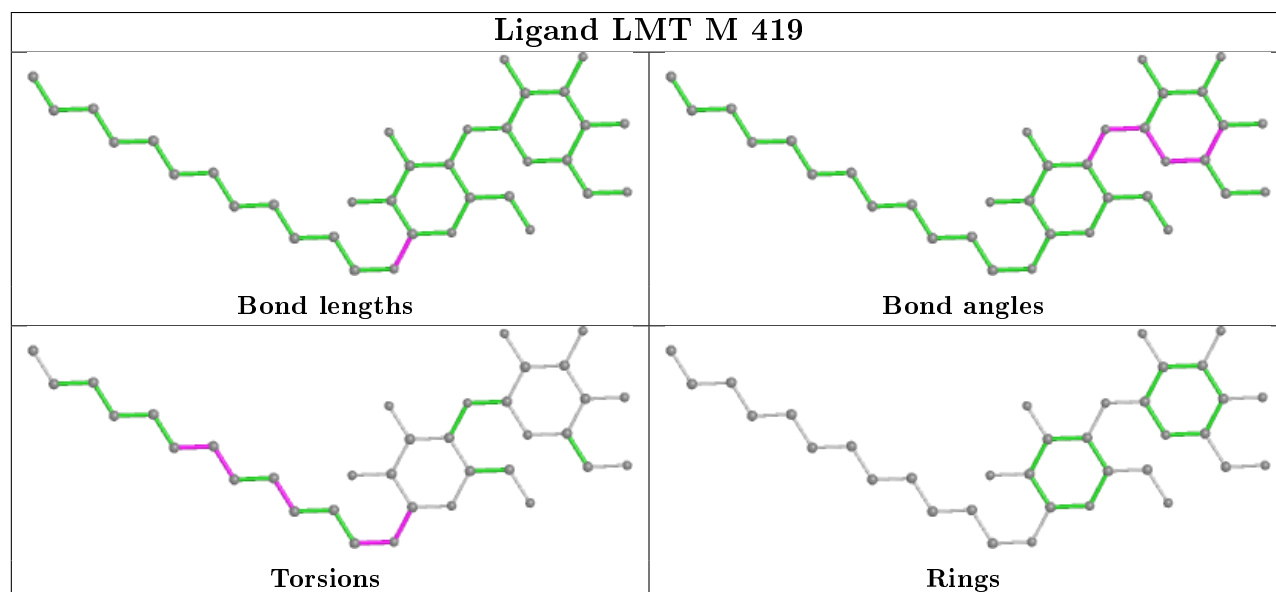
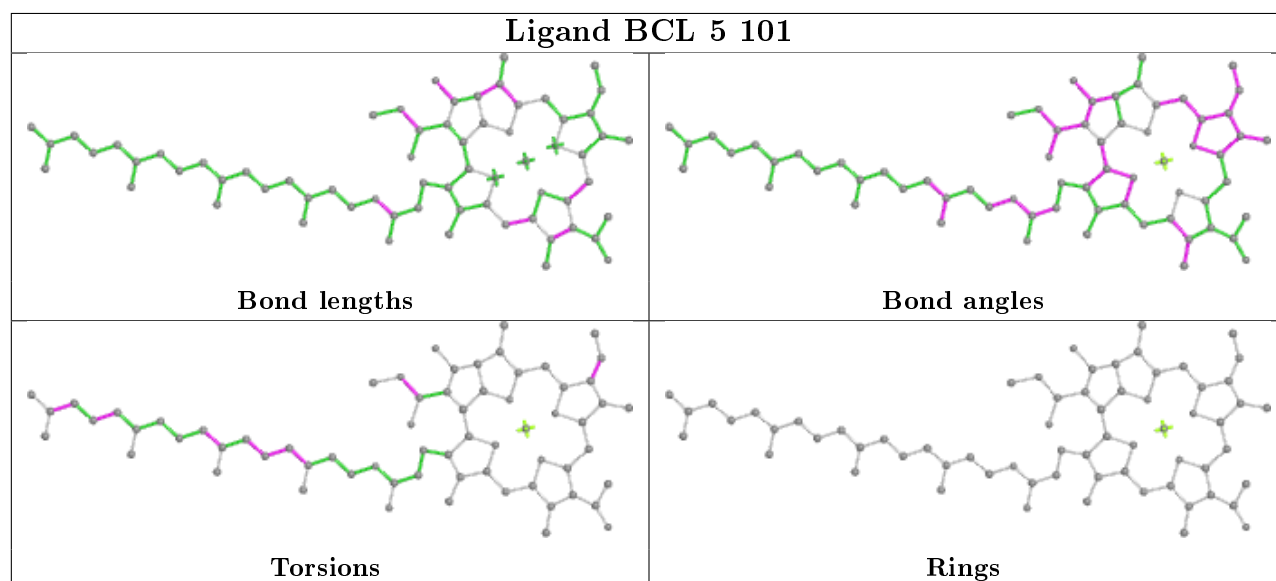
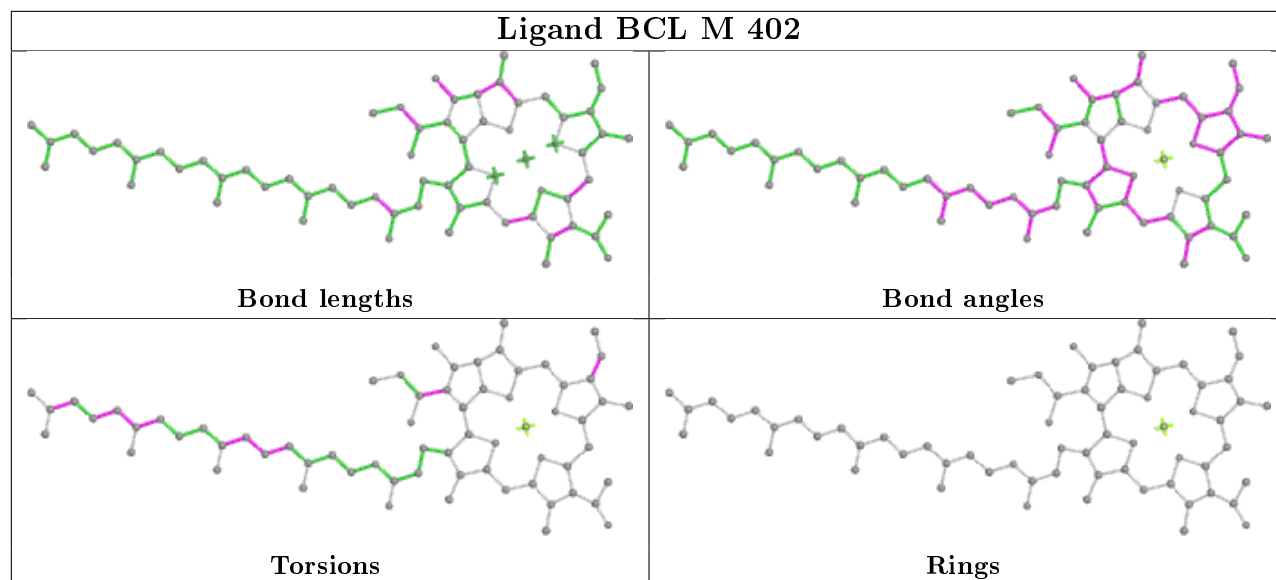


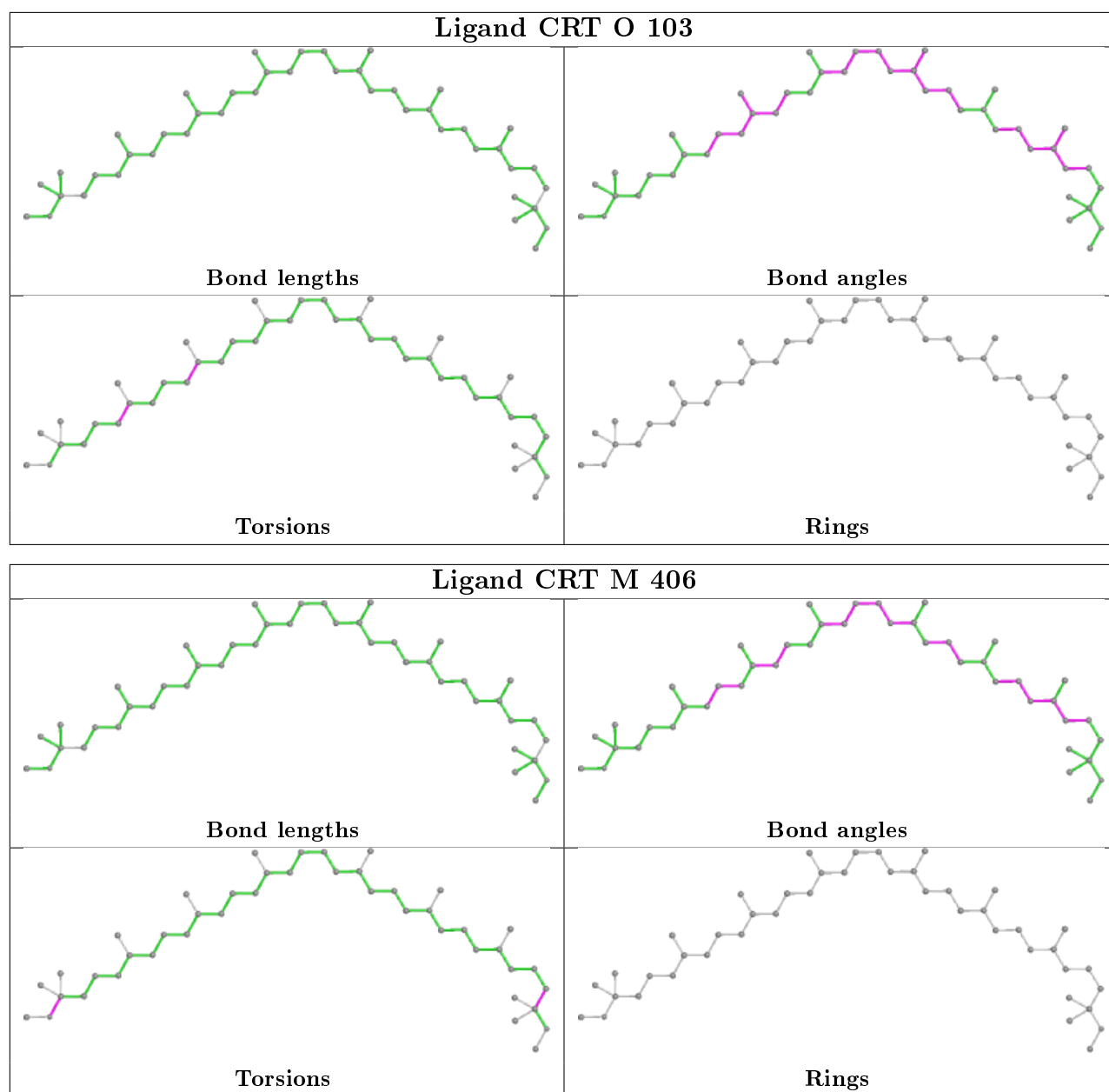
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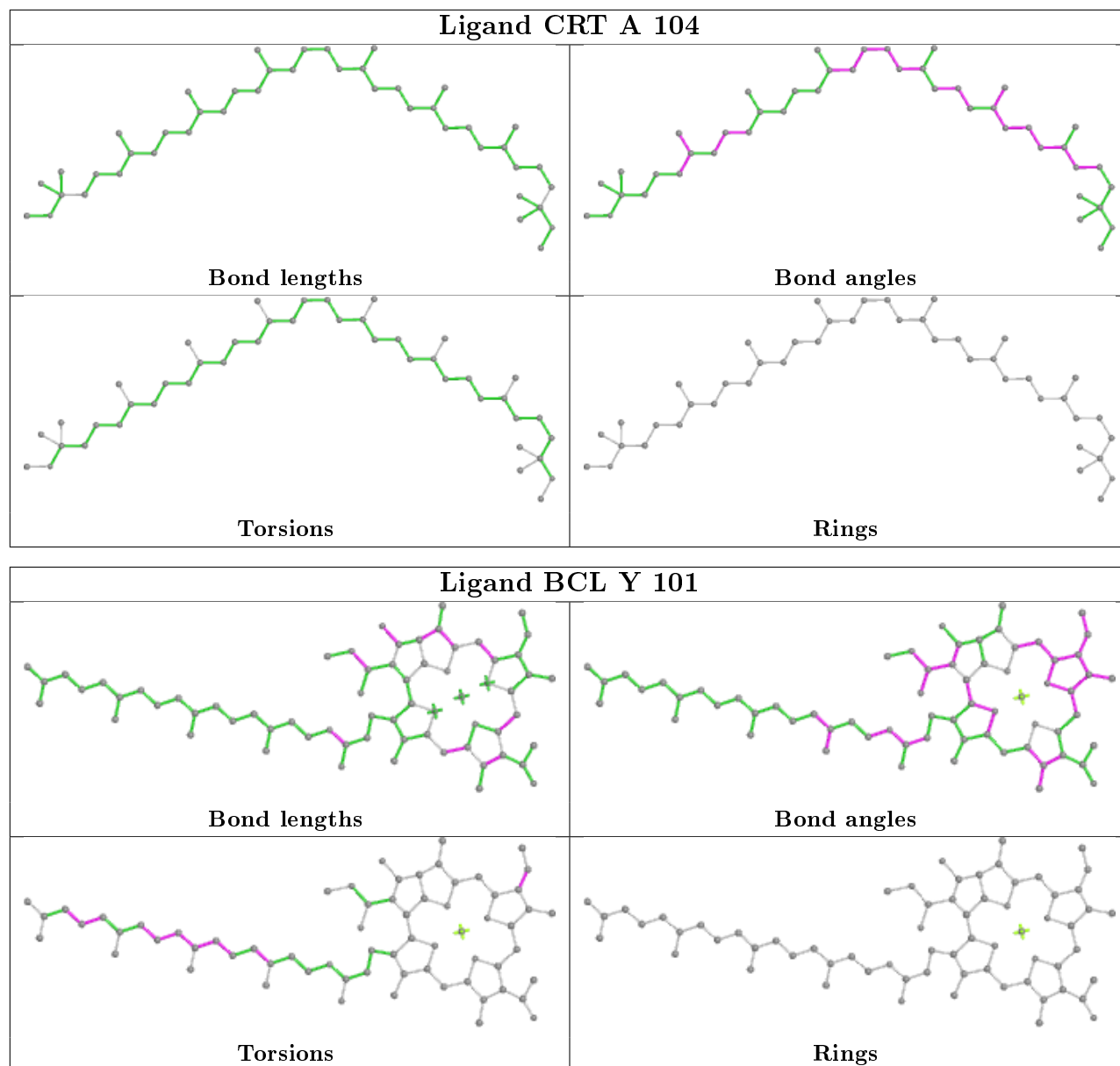


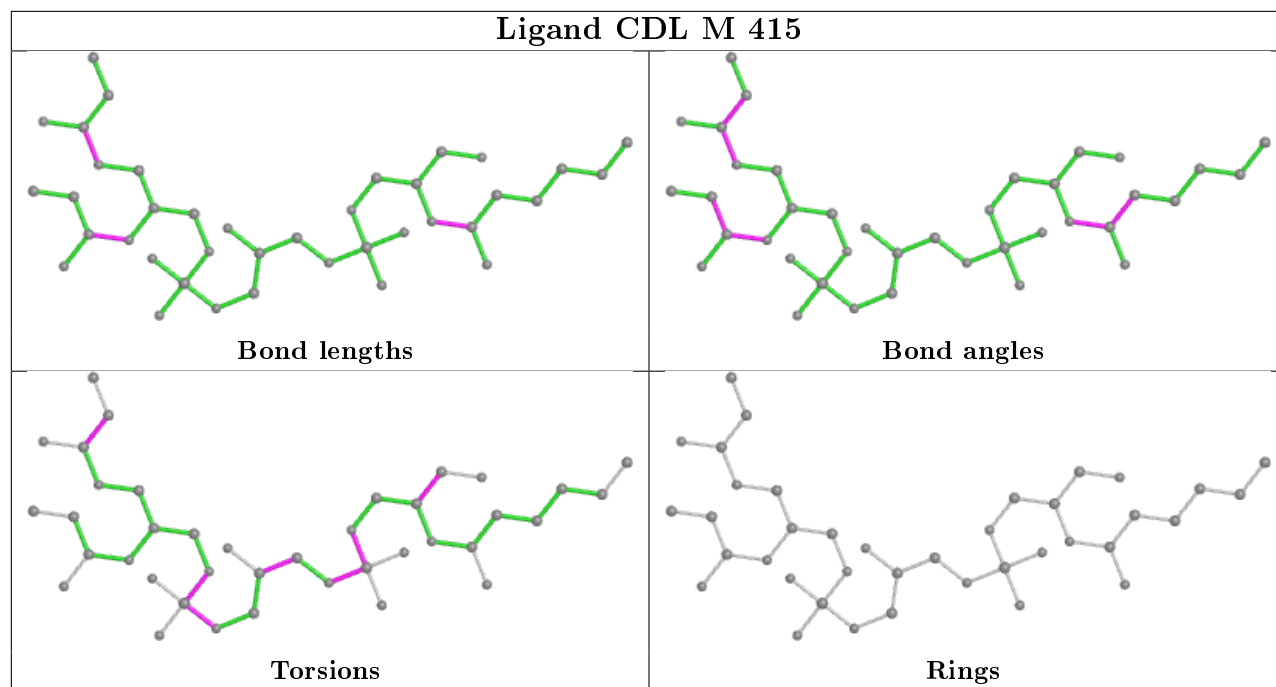




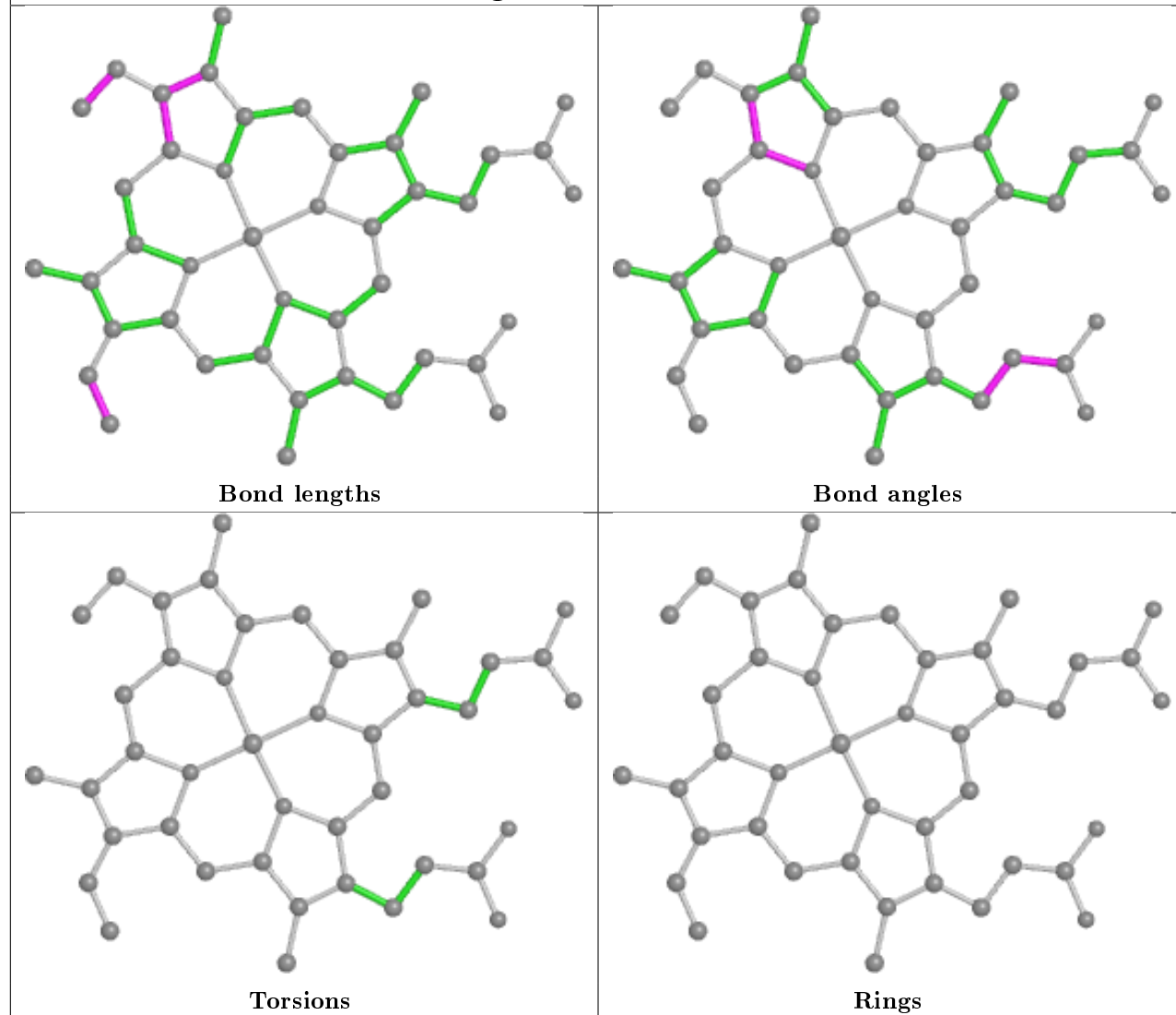


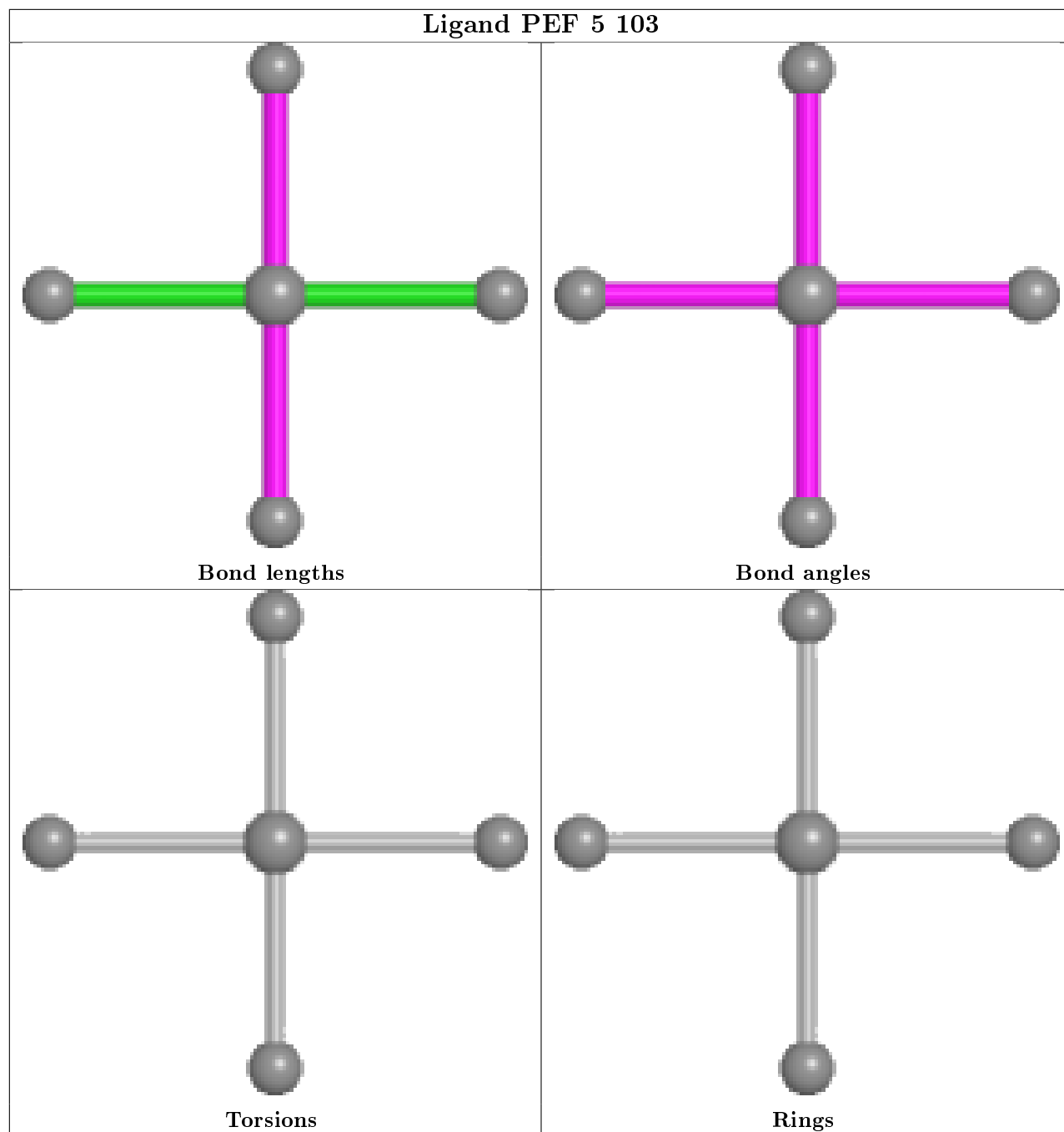


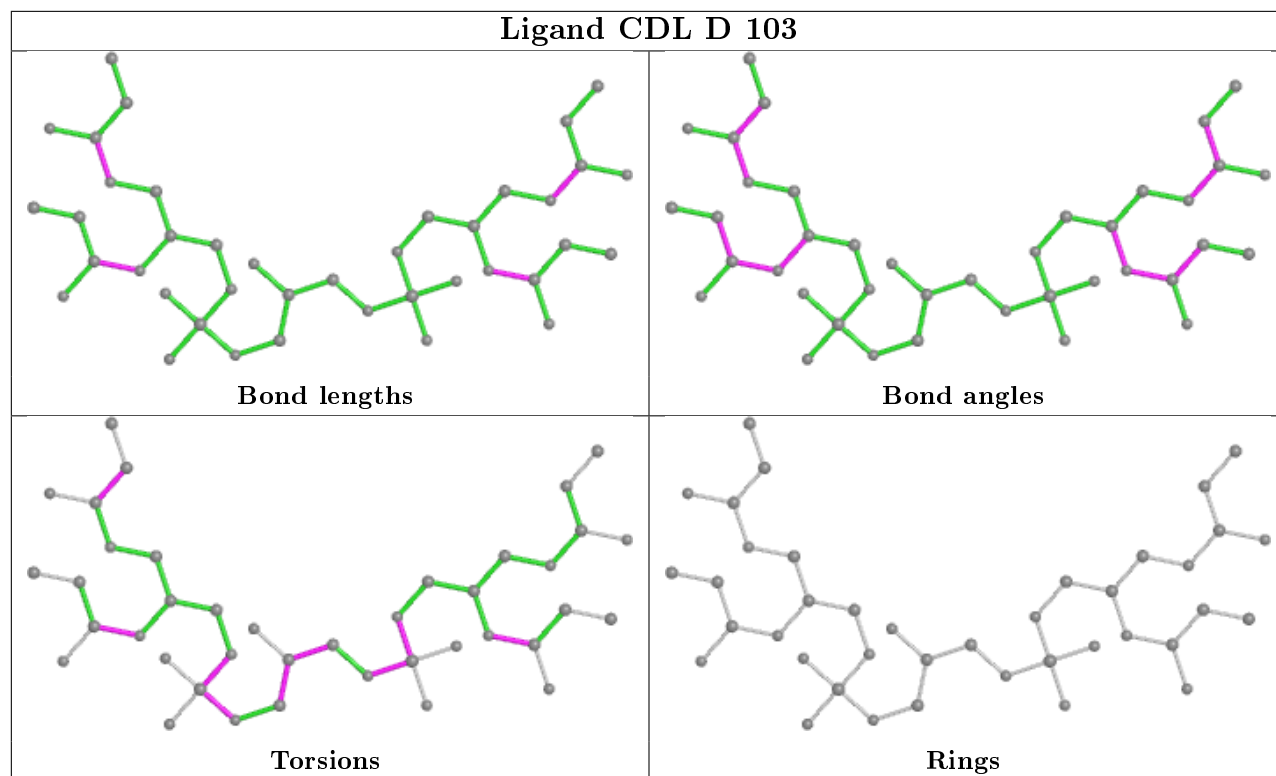


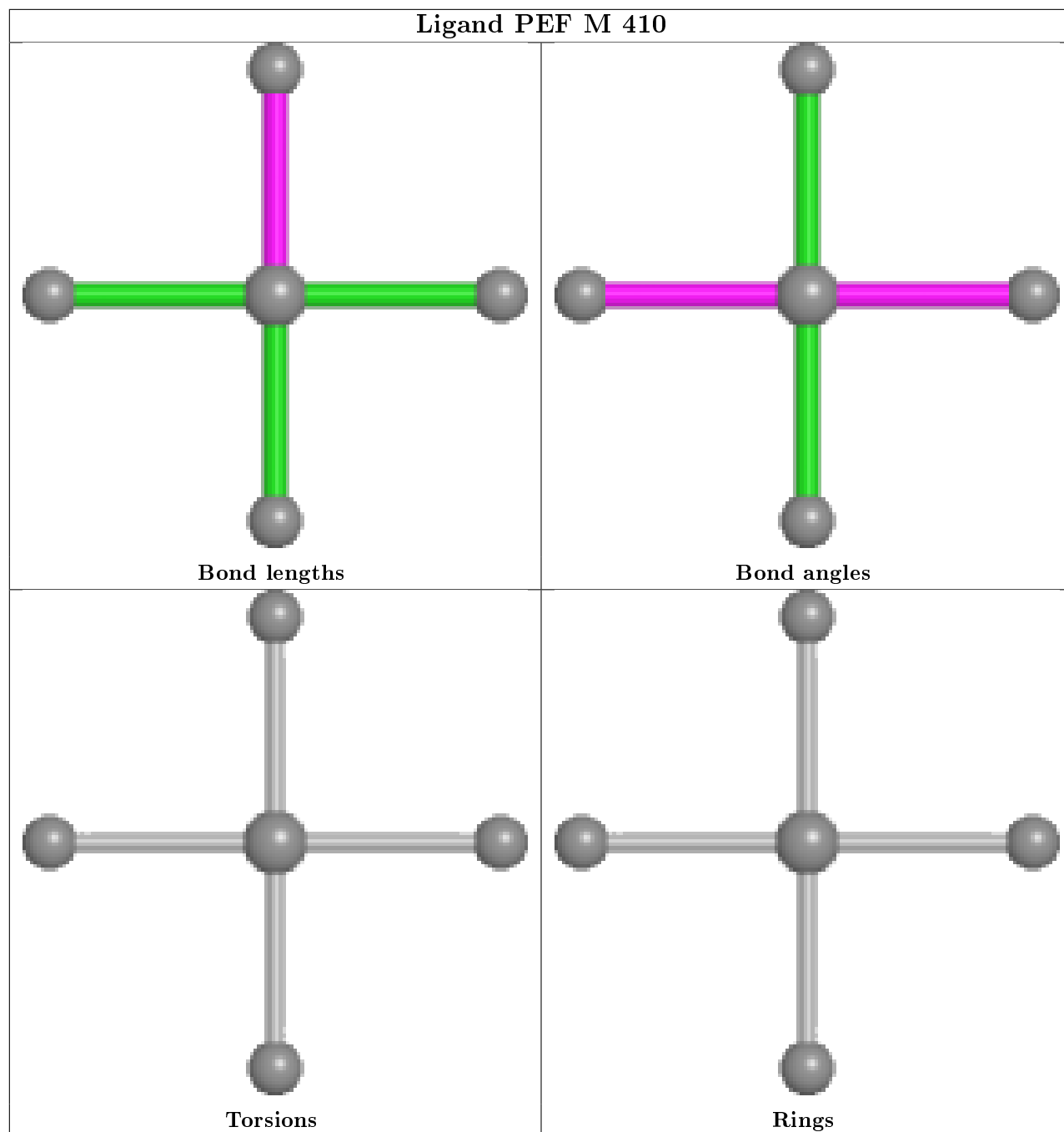


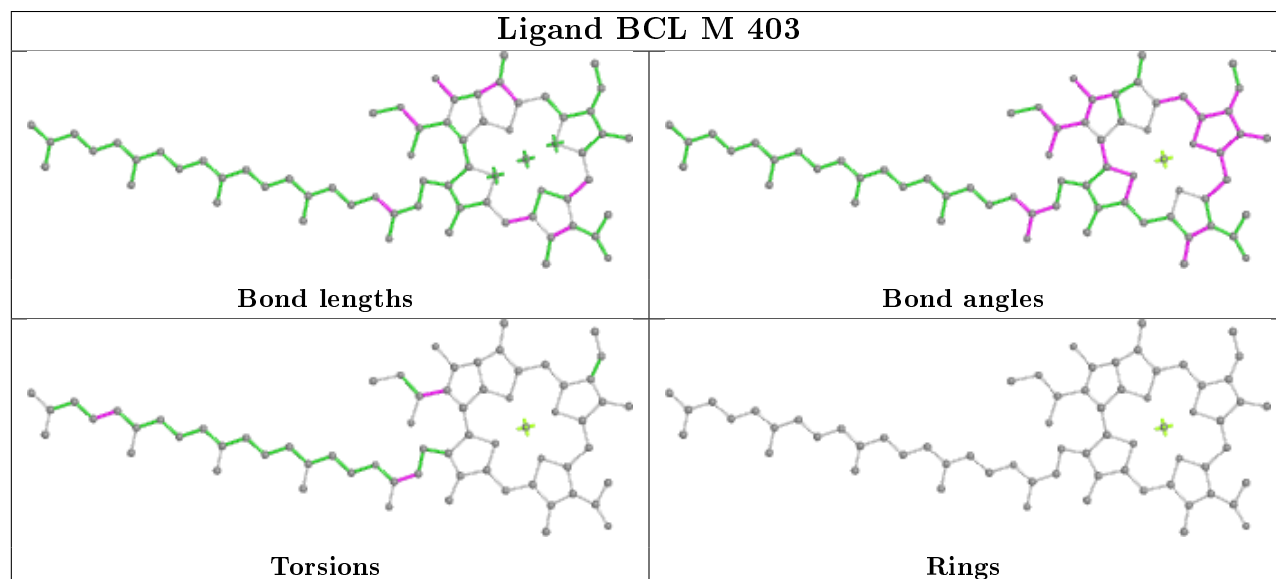
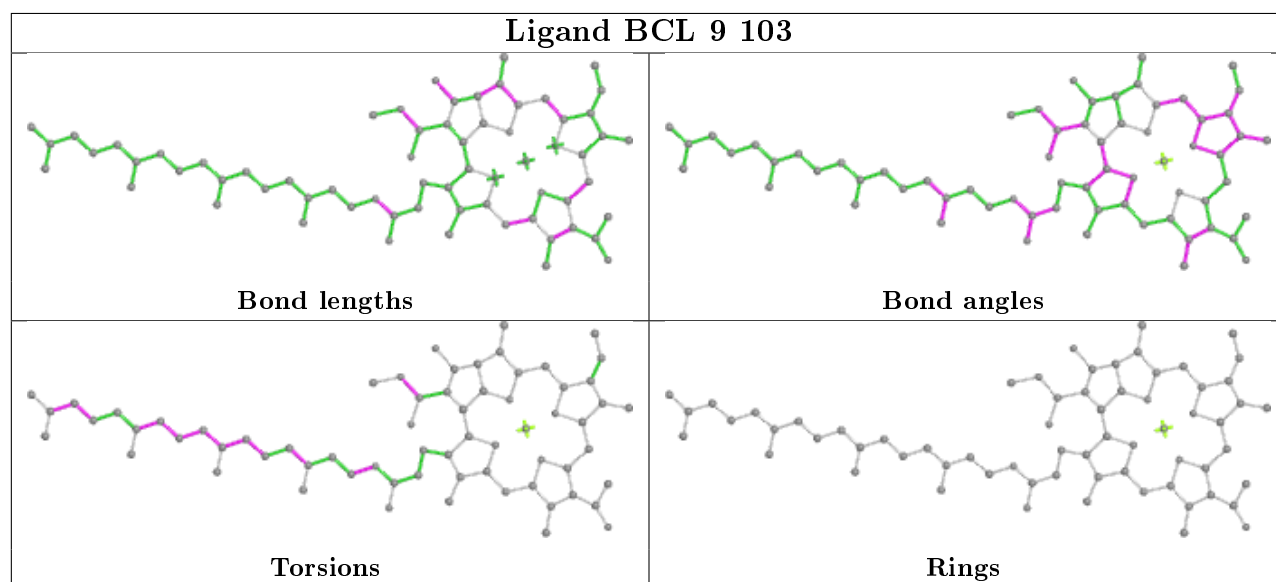
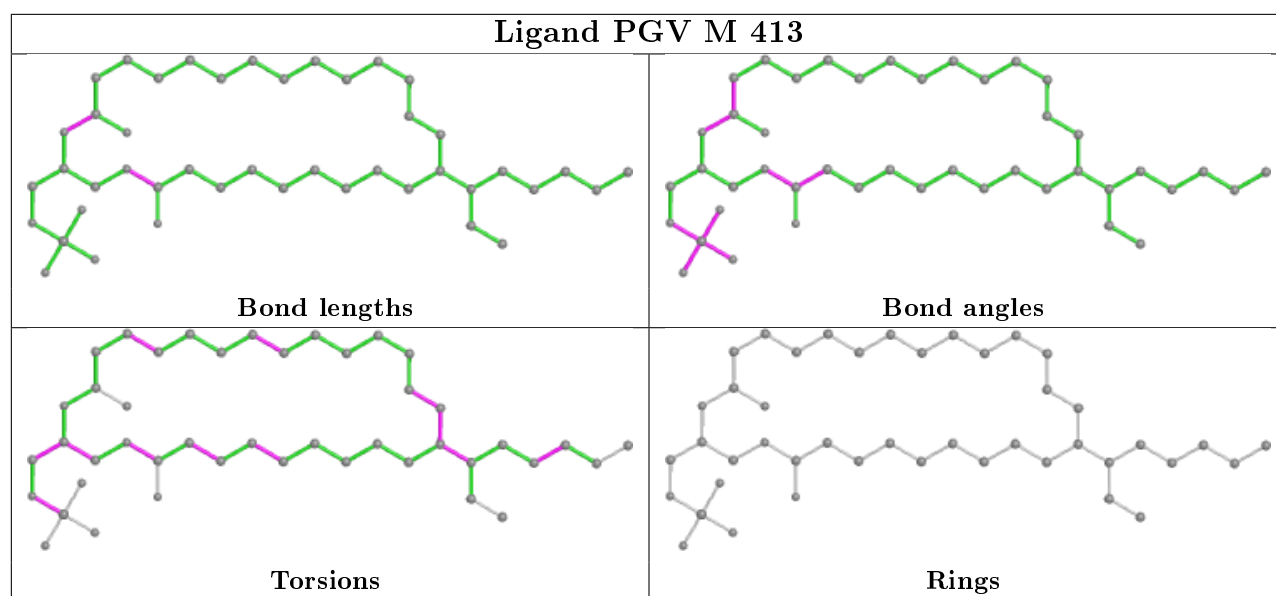
Ligand HEC C 502

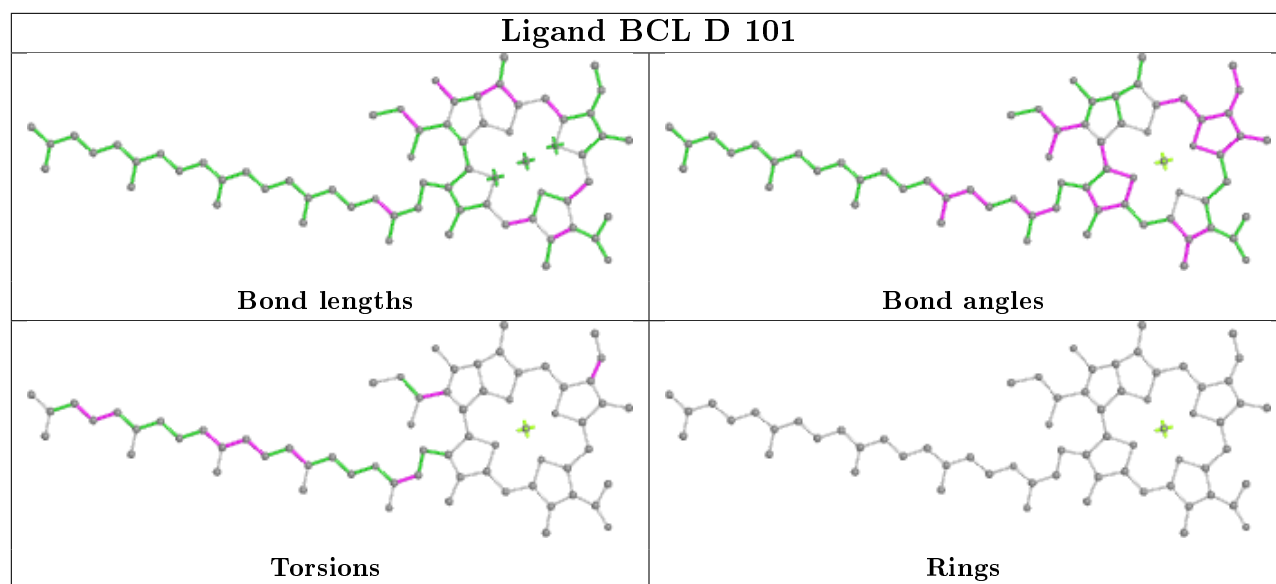
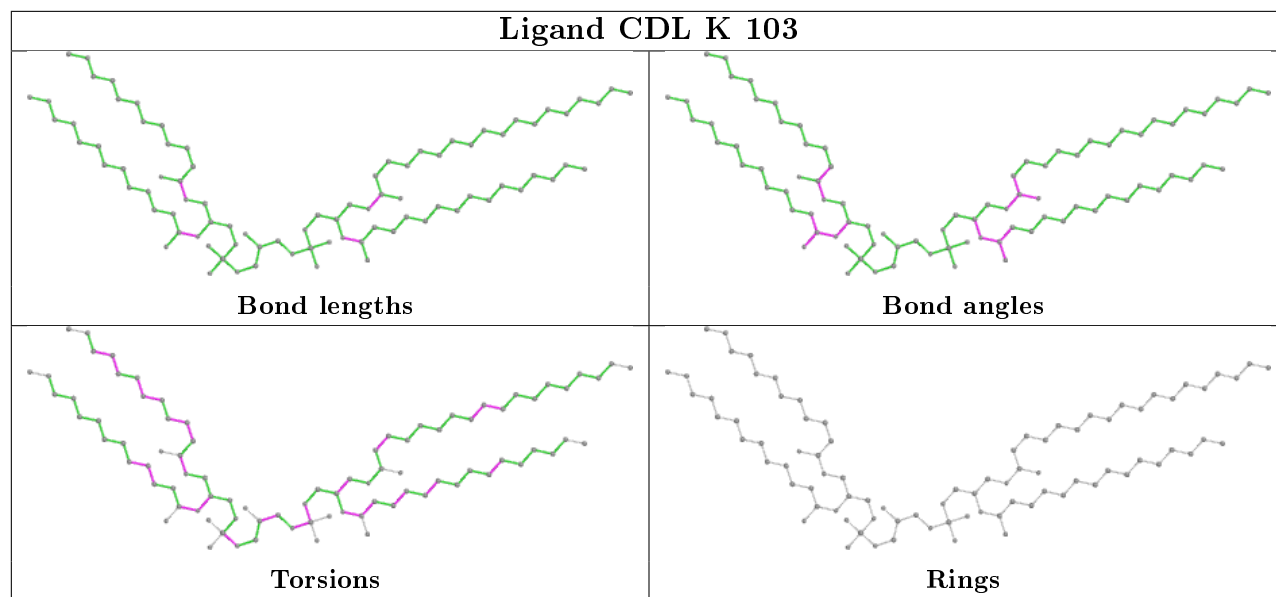


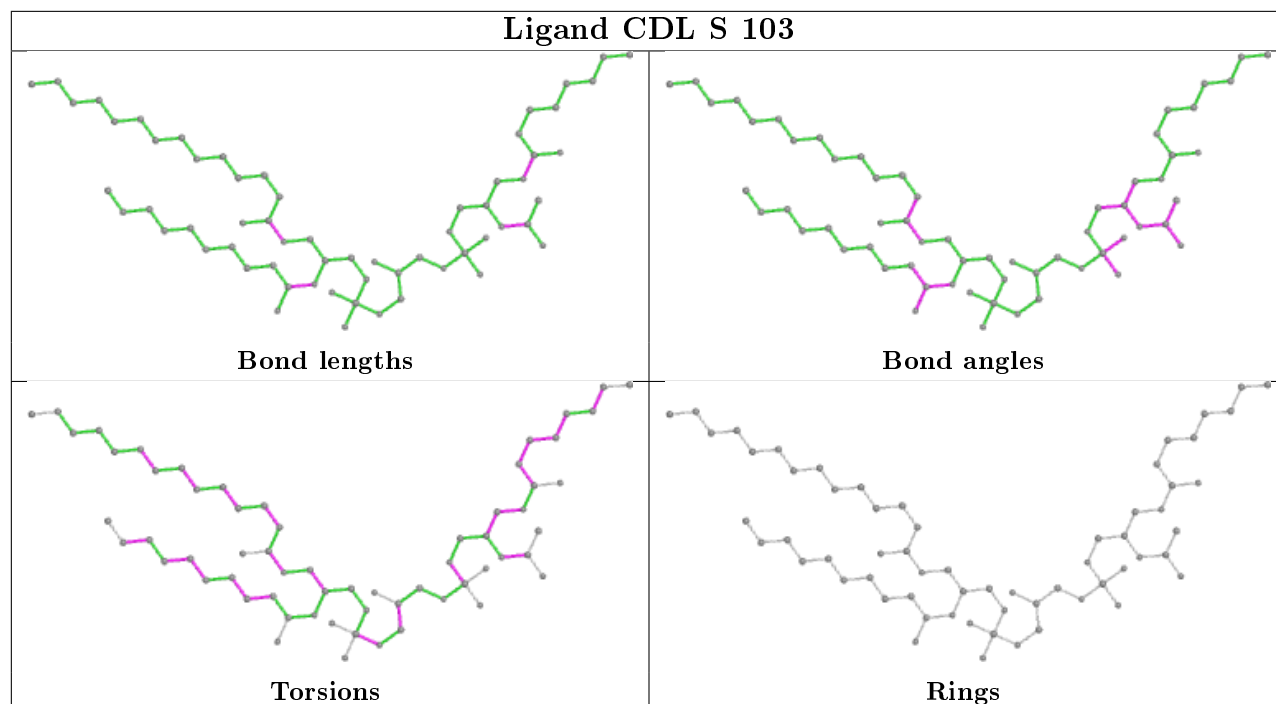
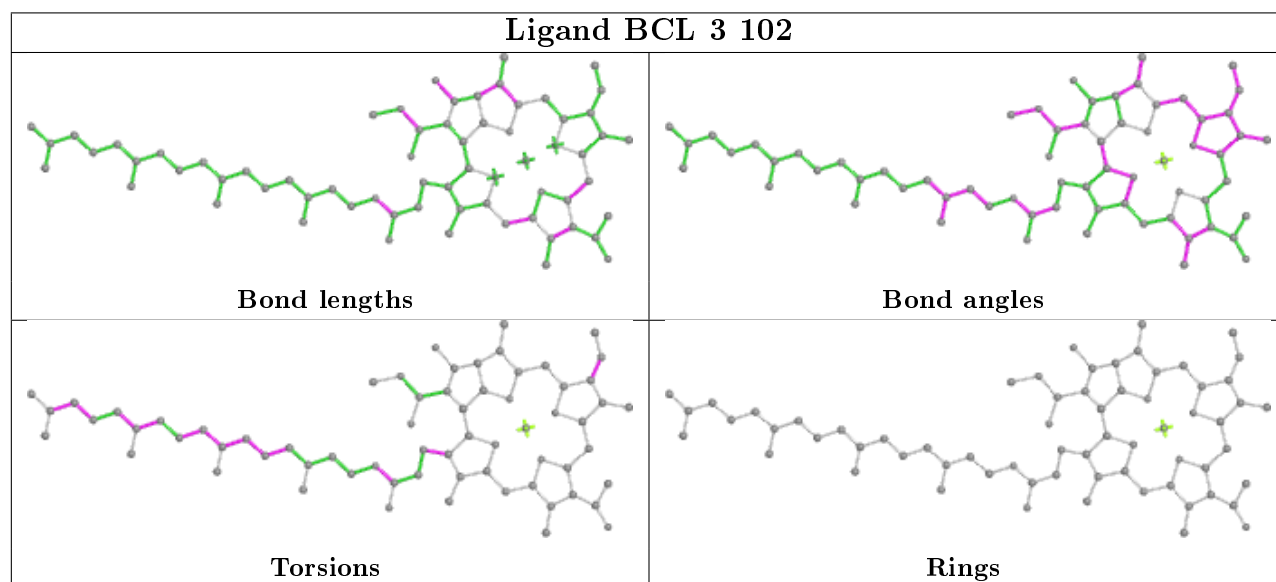




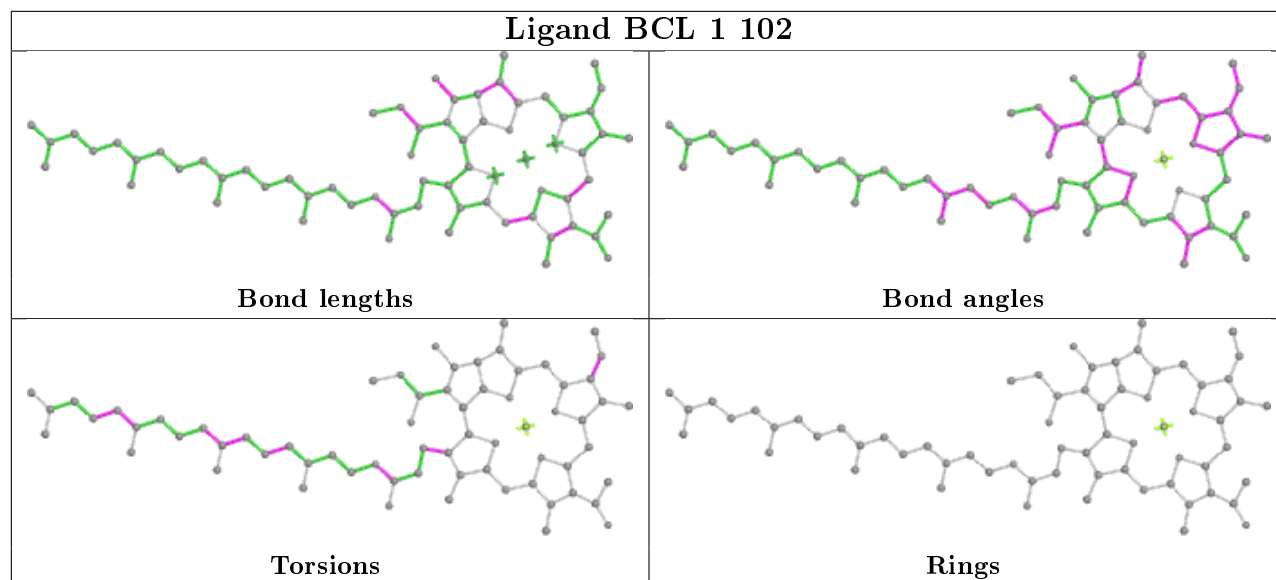




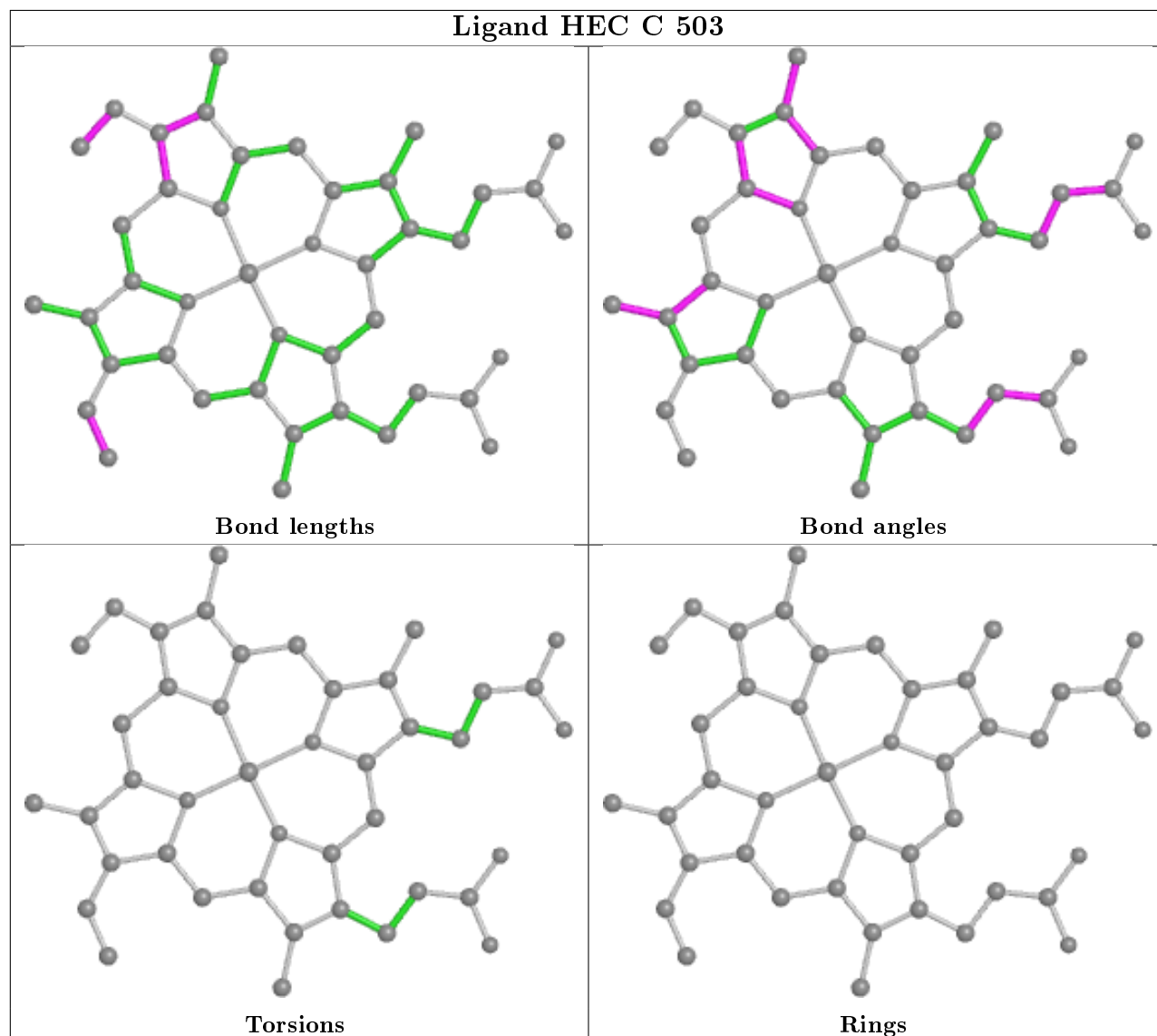


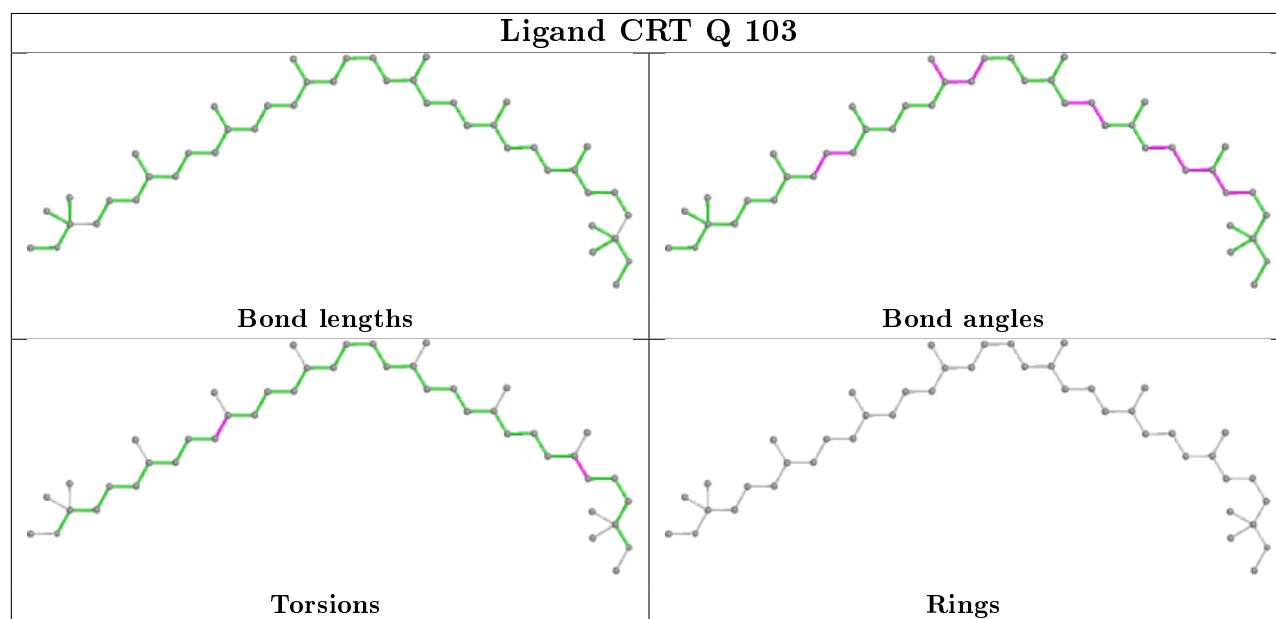
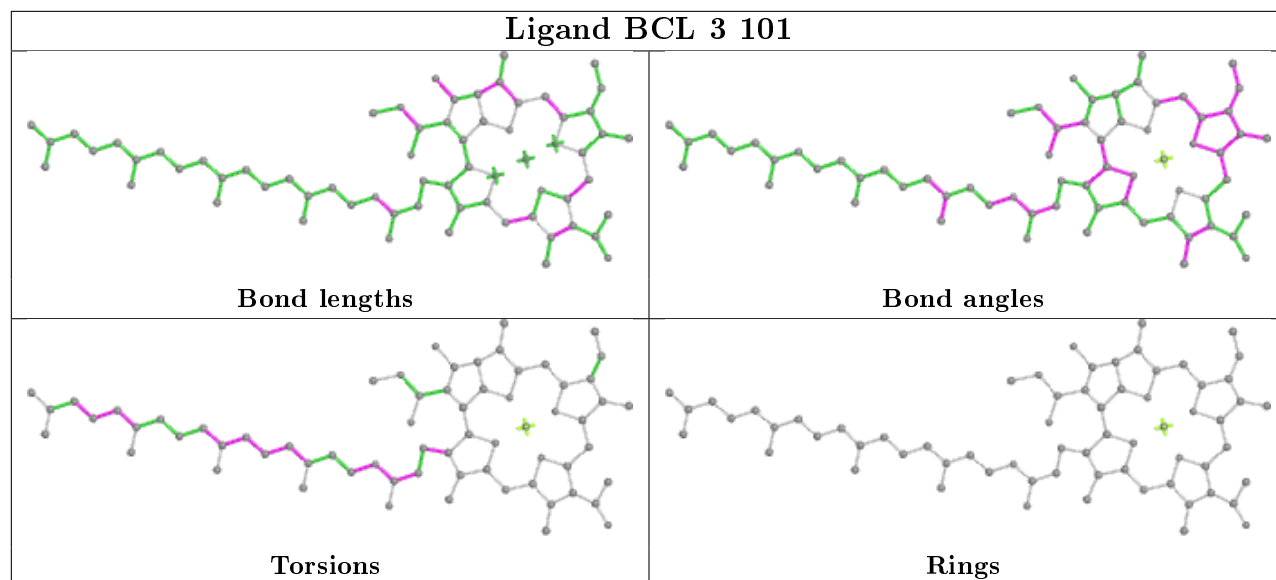
Ligand CDL S 103**Ligand BCL 3 102**

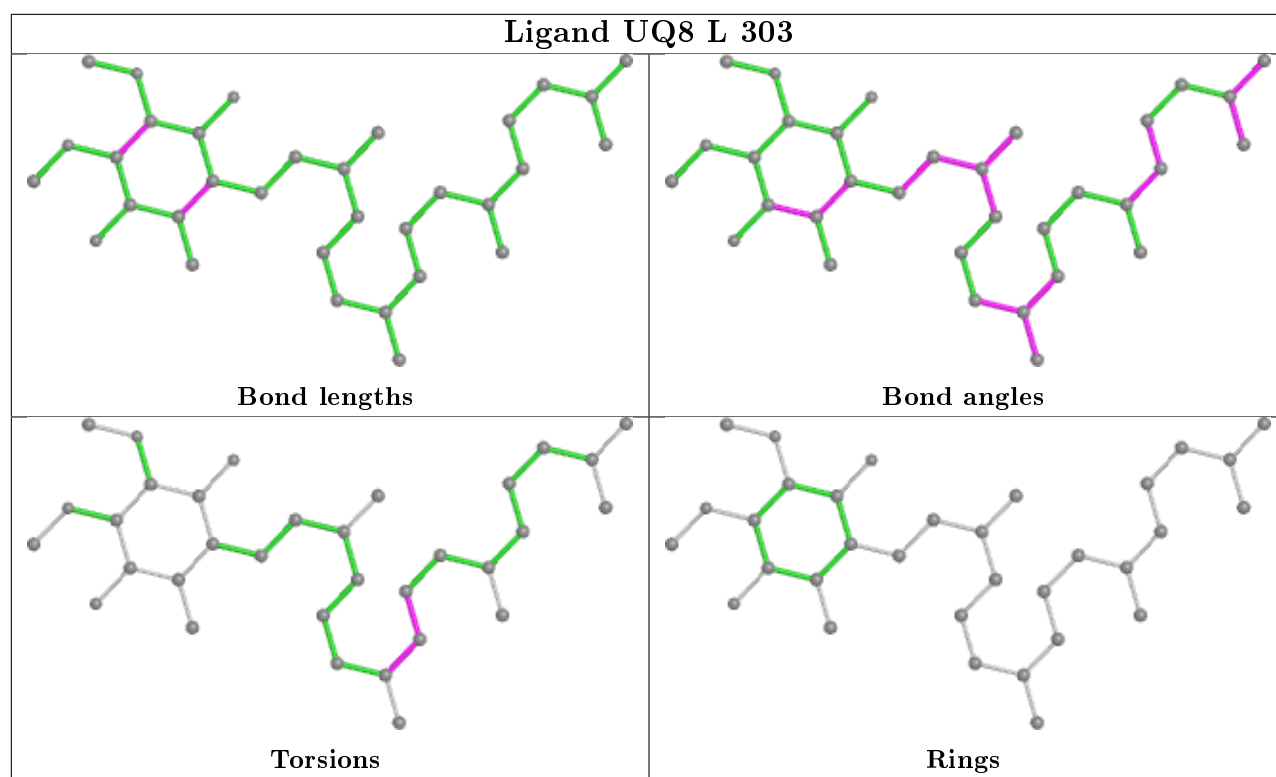
Ligand BCL 1 102

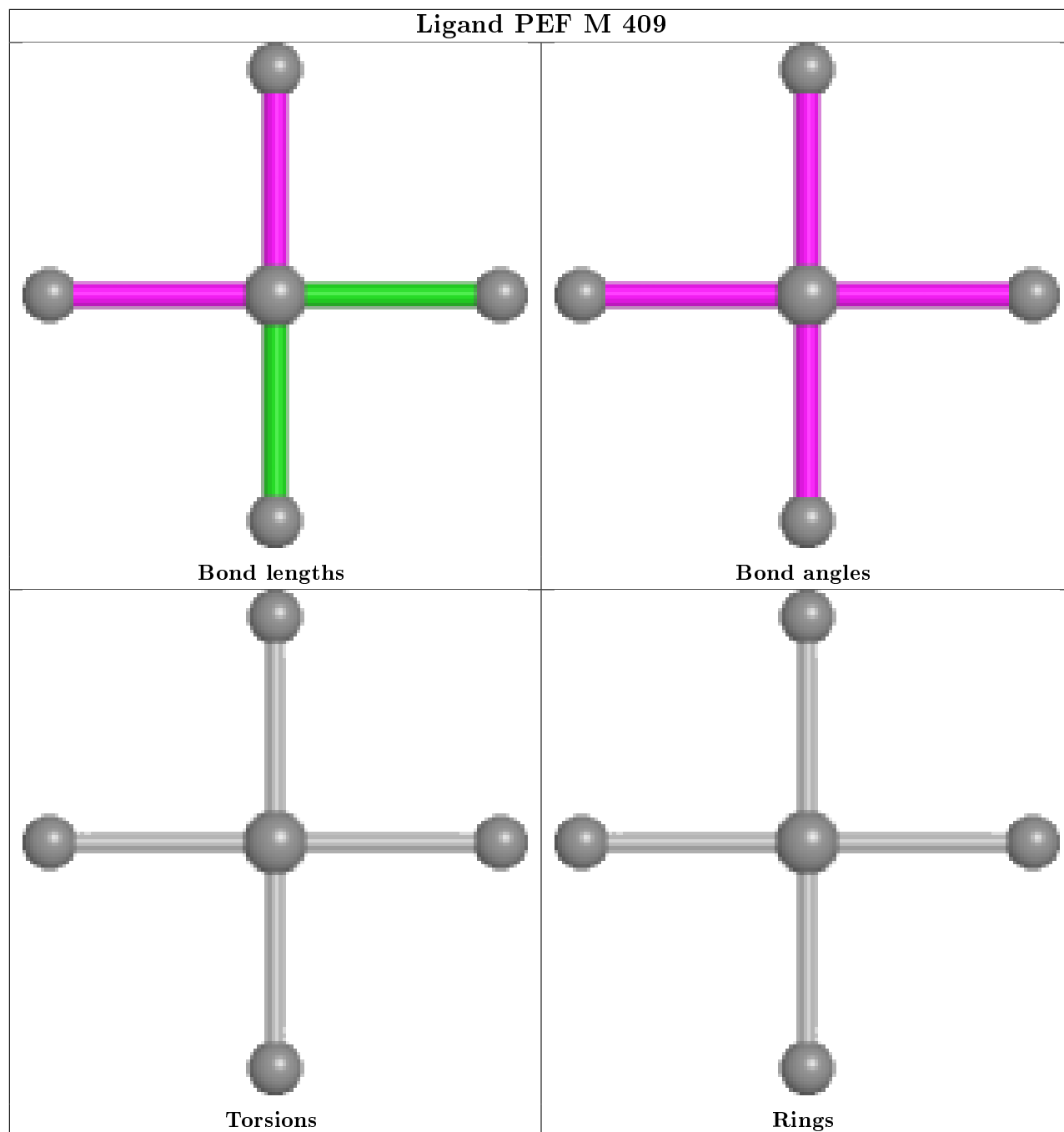


Ligand HEC C 503

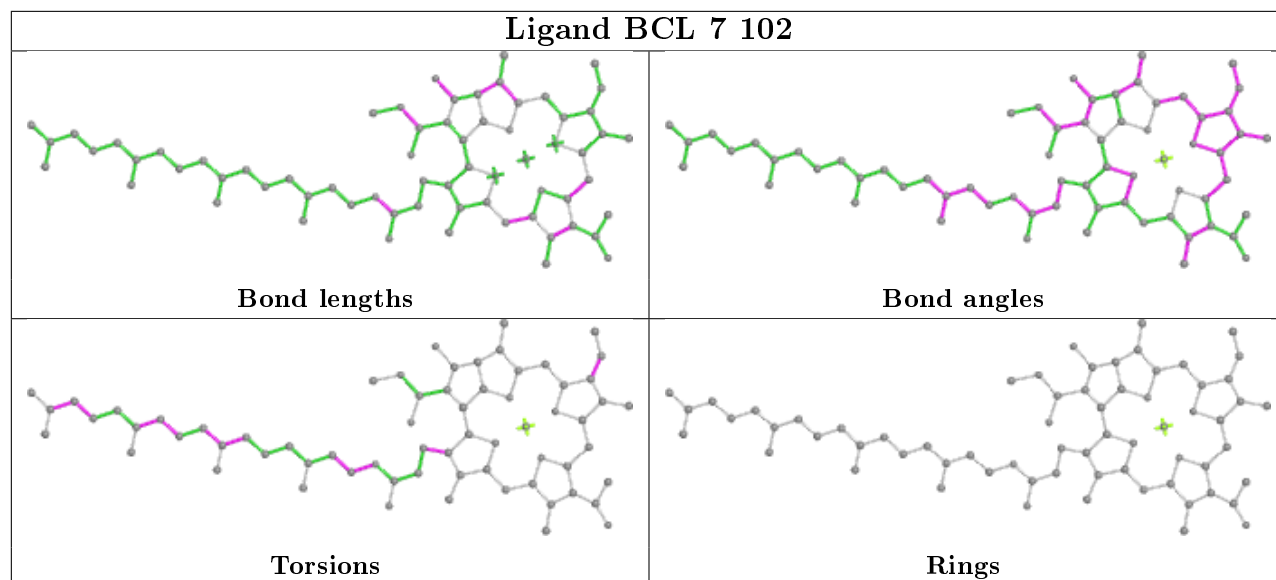




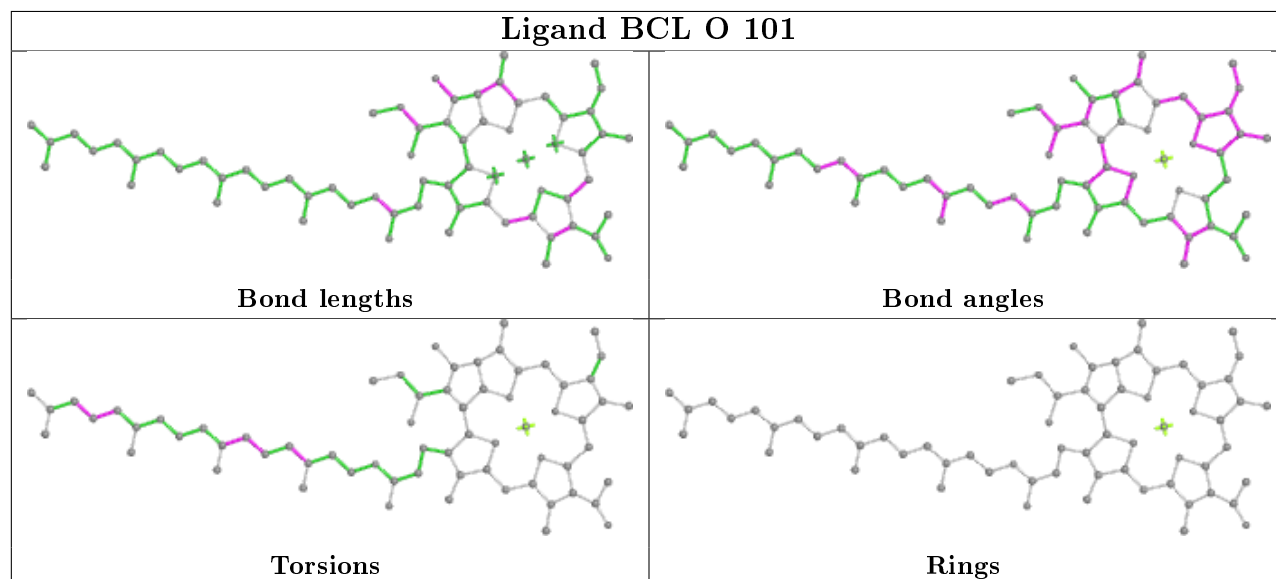




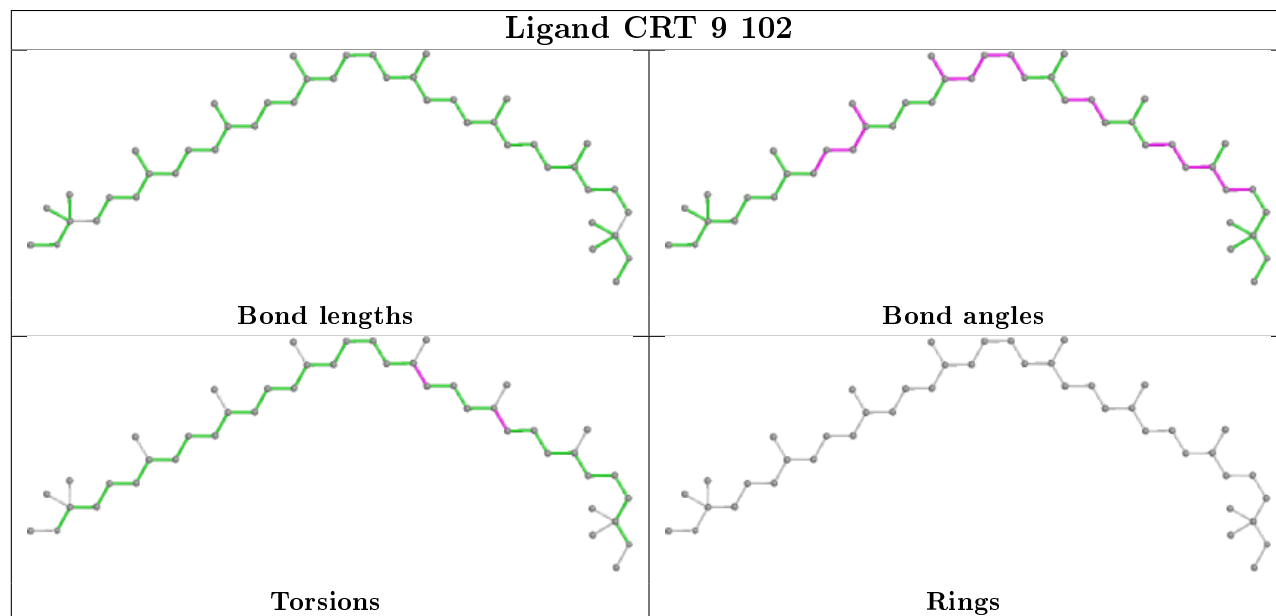
Ligand BCL 7 102

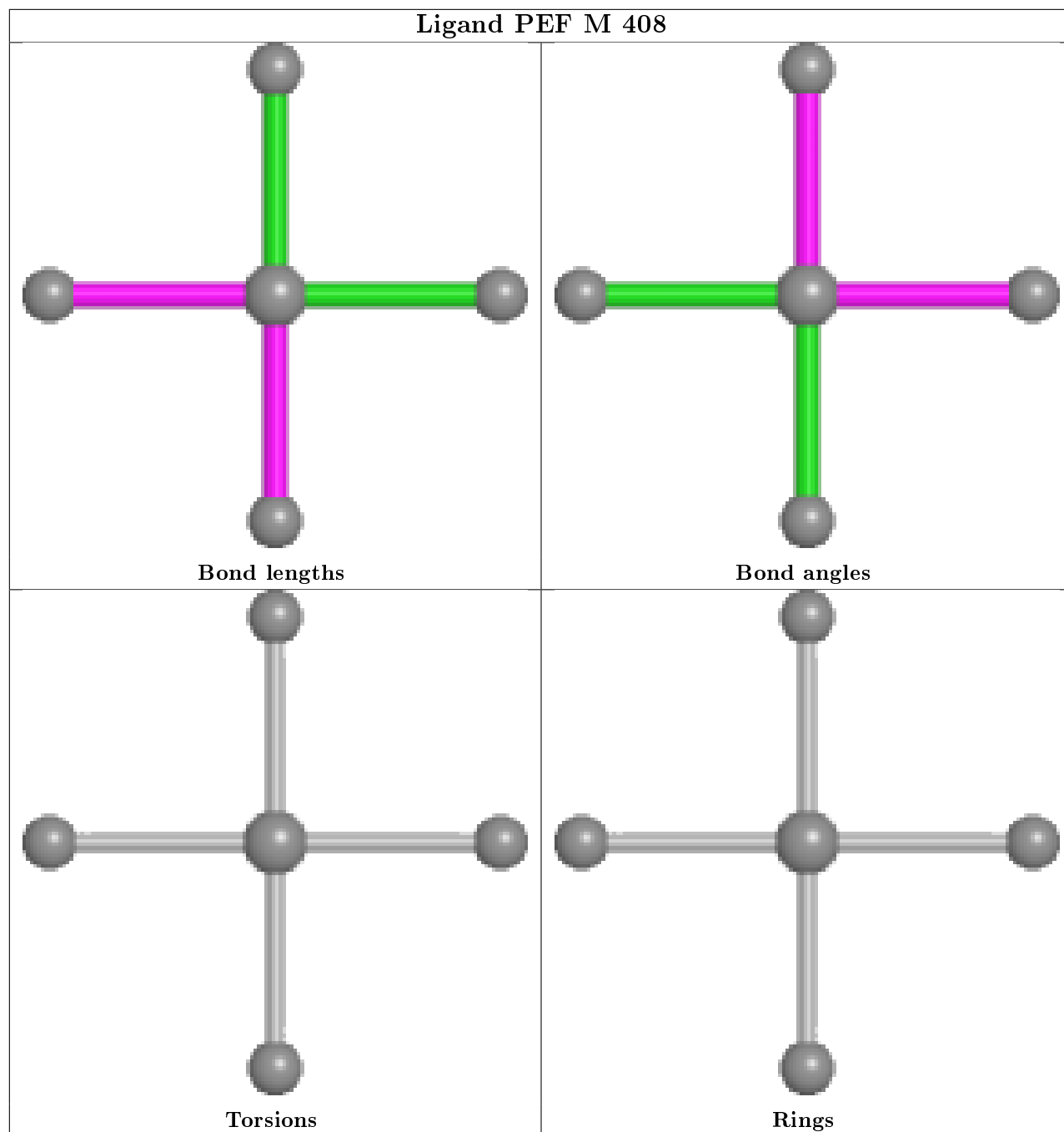


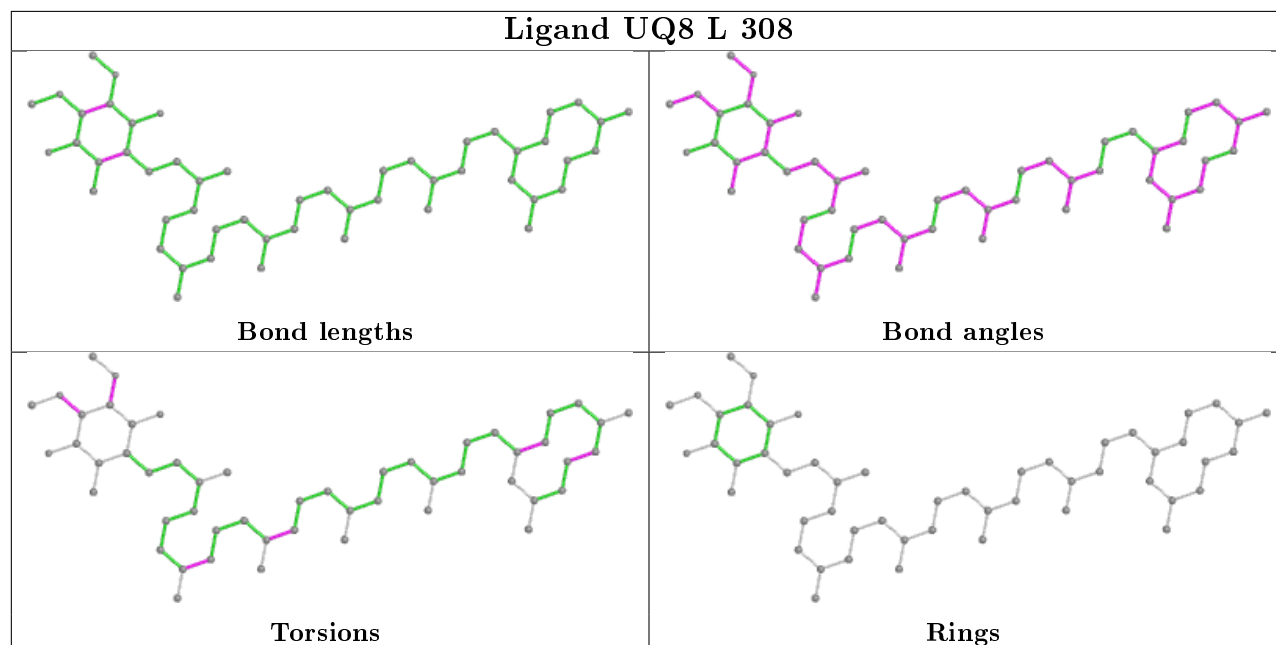
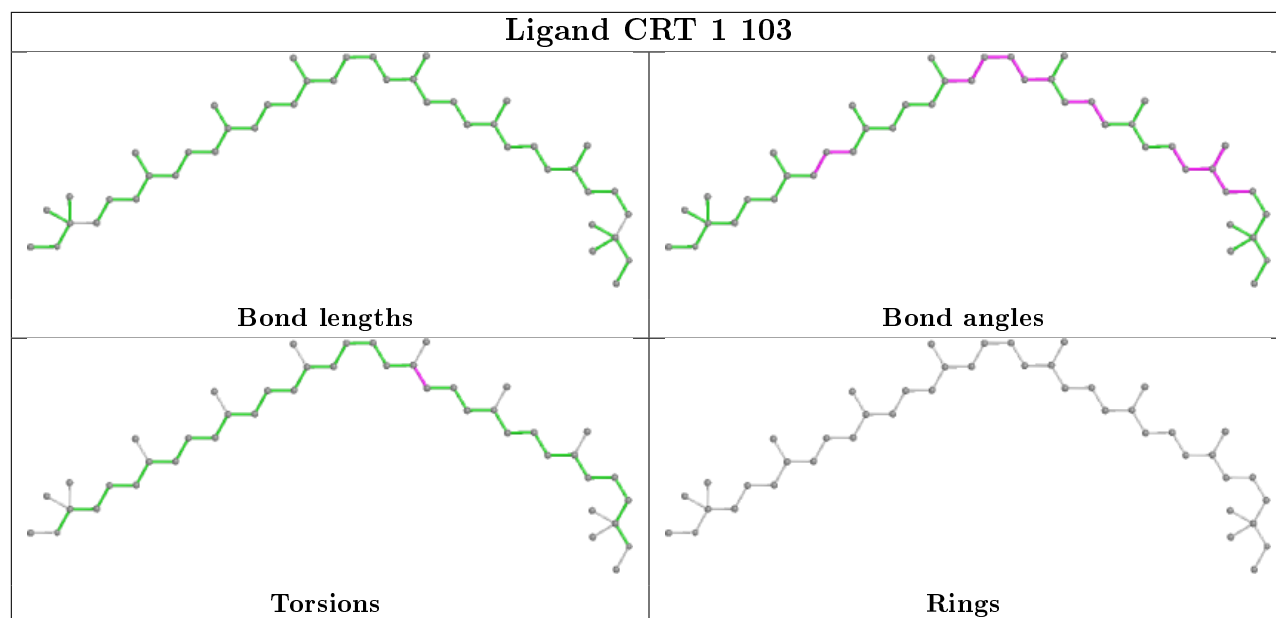
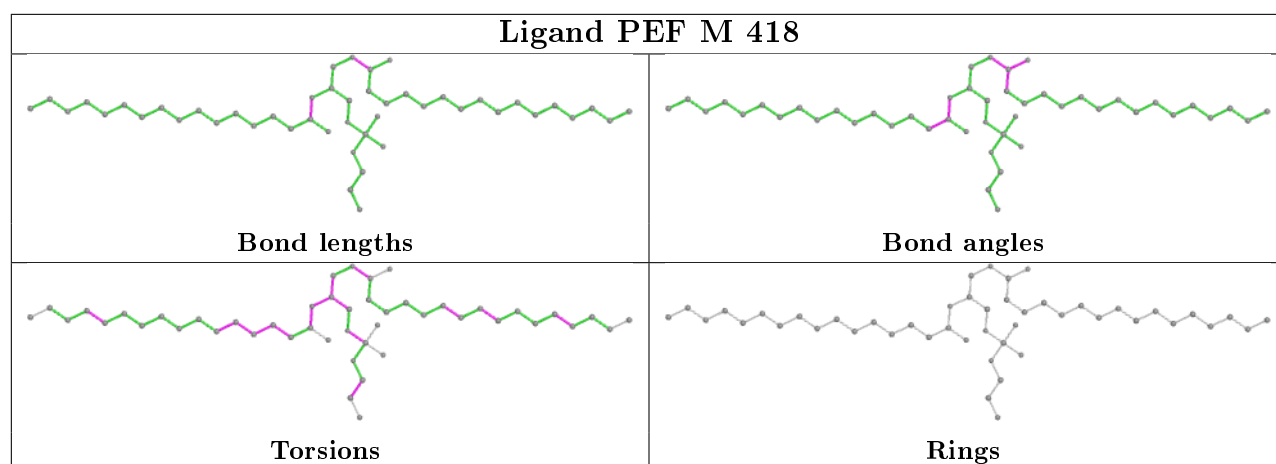
Ligand BCL O 101

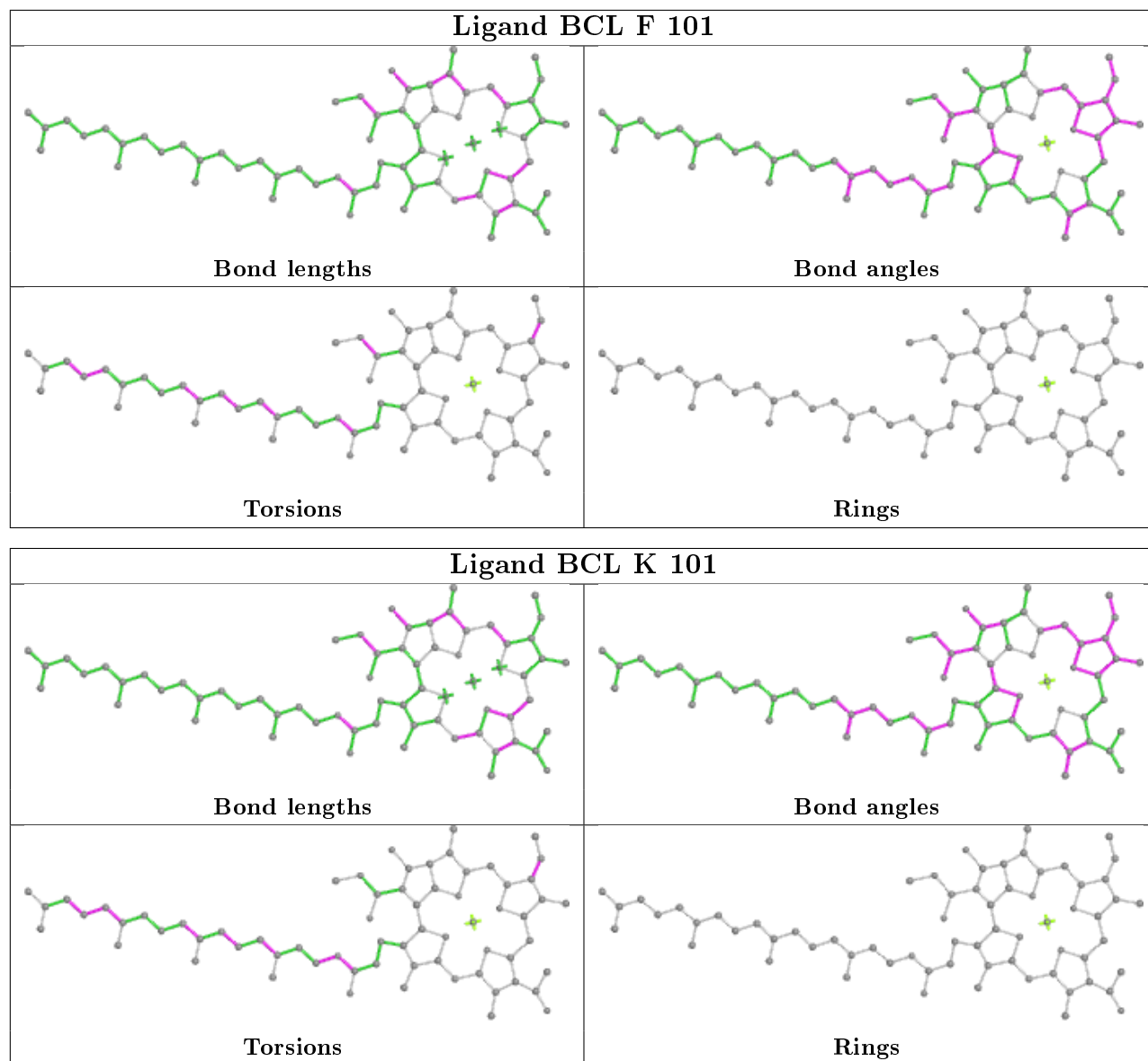


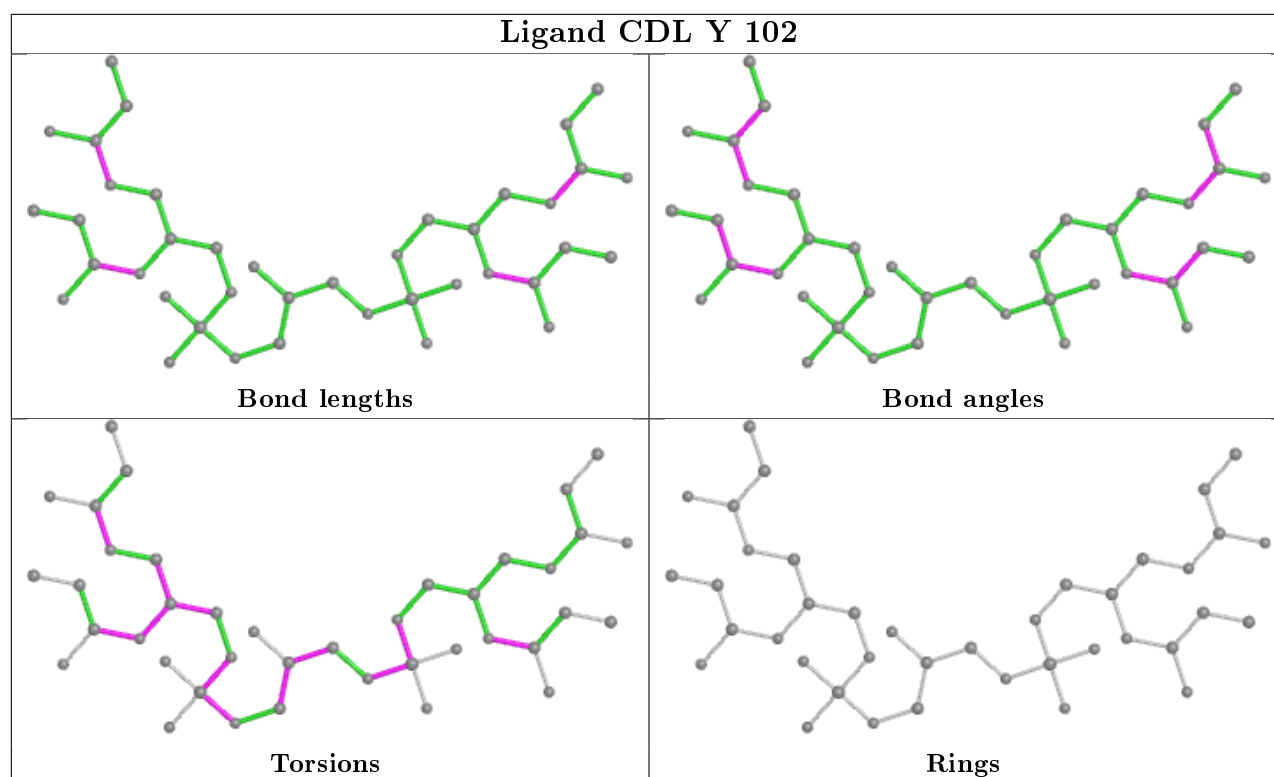
Ligand CRT 9 102











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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	311/404 (76%)	-0.07	8 (2%) 56 58	32, 48, 81, 113	0
2	L	280/281 (99%)	0.28	21 (7%) 14 15	31, 44, 59, 100	0
3	M	318/325 (97%)	0.28	10 (3%) 49 51	30, 42, 54, 85	0
4	H	255/259 (98%)	0.07	9 (3%) 44 47	41, 58, 87, 130	0
5	1	56/61 (91%)	0.85	11 (19%) 1 1	58, 75, 118, 138	0
5	3	56/61 (91%)	0.84	8 (14%) 2 2	59, 77, 106, 145	0
5	5	54/61 (88%)	1.01	8 (14%) 2 2	54, 70, 95, 114	0
5	7	57/61 (93%)	1.83	18 (31%) 0 0	54, 65, 127, 139	0
5	9	57/61 (93%)	1.15	12 (21%) 1 0	51, 64, 122, 153	0
5	A	54/61 (88%)	0.76	10 (18%) 1 1	55, 67, 98, 117	0
5	D	55/61 (90%)	0.55	5 (9%) 9 10	55, 69, 101, 136	0
5	F	55/61 (90%)	0.81	10 (18%) 1 1	55, 70, 126, 136	0
5	I	57/61 (93%)	0.60	8 (14%) 2 2	54, 70, 120, 150	0
5	K	57/61 (93%)	0.76	6 (10%) 6 7	50, 64, 109, 131	0
5	O	56/61 (91%)	0.79	9 (16%) 1 2	45, 58, 97, 133	0
5	Q	57/61 (93%)	0.69	10 (17%) 1 1	37, 49, 87, 143	0
5	S	56/61 (91%)	1.00	9 (16%) 1 2	40, 53, 109, 147	0
5	U	58/61 (95%)	1.19	13 (22%) 0 0	43, 56, 117, 144	0
5	W	56/61 (91%)	0.47	6 (10%) 6 6	47, 60, 98, 120	0
5	Y	57/61 (93%)	0.37	4 (7%) 16 18	51, 67, 113, 145	0
6	0	43/47 (91%)	1.04	11 (25%) 0 0	64, 74, 91, 116	0
6	2	41/47 (87%)	1.35	13 (31%) 0 0	68, 84, 105, 109	0
6	4	42/47 (89%)	1.27	11 (26%) 0 0	65, 80, 98, 107	0
6	6	42/47 (89%)	0.68	4 (9%) 8 9	63, 73, 92, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
6	8	41/47 (87%)	0.94	9 (21%) 0 0	65, 74, 96, 119	0
6	B	42/47 (89%)	0.85	8 (19%) 1 1	68, 80, 97, 108	0
6	E	38/47 (80%)	1.11	8 (21%) 1 0	69, 84, 113, 118	0
6	G	42/47 (89%)	1.74	17 (40%) 0 0	66, 88, 125, 148	0
6	J	42/47 (89%)	1.49	13 (30%) 0 0	64, 82, 107, 112	0
6	N	42/47 (89%)	0.70	5 (11%) 4 5	57, 75, 95, 102	0
6	P	42/47 (89%)	0.26	4 (9%) 8 9	49, 63, 84, 88	0
6	R	41/47 (87%)	0.47	5 (12%) 4 4	46, 58, 80, 82	0
6	T	43/47 (91%)	0.16	1 (2%) 60 63	49, 61, 82, 97	0
6	V	42/47 (89%)	0.66	5 (11%) 4 5	53, 72, 101, 116	0
6	X	41/47 (87%)	1.28	13 (31%) 0 0	60, 78, 103, 108	0
6	Z	40/47 (85%)	0.88	9 (22%) 0 0	63, 80, 101, 107	0
All	All	2726/2997 (90%)	0.57	331 (12%) 4 4	30, 60, 101, 153	0

All (331) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	3	58	LEU	11.3
5	U	6	ALA	9.6
5	7	58	LEU	9.5
5	9	58	LEU	7.6
5	7	8	LEU	7.5
5	S	4	MET	7.5
5	7	59	GLY	7.4
6	G	8	GLY	6.8
6	V	6	LEU	6.7
5	S	58	LEU	6.6
5	9	3	THR	6.6
5	1	5	ASN	6.4
6	E	9	LEU	6.4
5	O	4	MET	6.2
5	7	6	ALA	6.2
5	F	9	TYR	6.1
5	7	4	MET	6.1
5	K	58	LEU	6.0
6	G	9	LEU	5.7
6	E	10	THR	5.6
6	4	17	PHE	5.5

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Mol	Chain	Res	Type	RSRZ
5	7	57	ALA	5.5
6	G	12	ASP	5.5
4	H	5	ILE	5.5
5	1	6	ALA	5.4
5	5	6	ALA	5.4
6	G	5	SER	5.4
5	U	3	THR	5.3
6	G	10	THR	5.3
6	B	10	THR	5.1
5	Q	4	MET	5.1
5	1	4	MET	5.0
6	8	41	LEU	5.0
6	2	9	LEU	5.0
5	U	4	MET	5.0
5	9	4	MET	4.9
6	J	9	LEU	4.9
5	1	58	LEU	4.9
6	4	19	ALA	4.8
6	J	10	THR	4.7
5	7	3	THR	4.7
5	U	5	ASN	4.7
6	0	20	ILE	4.7
5	5	58	LEU	4.6
6	X	9	LEU	4.6
5	U	8	LEU	4.6
5	K	57	ALA	4.6
5	F	7	ASN	4.5
6	8	19	ALA	4.5
5	W	6	ALA	4.4
5	3	55	TYR	4.4
6	2	10	THR	4.3
6	Z	7	THR	4.2
6	X	12	ASP	4.2
6	J	20	ILE	4.1
5	7	7	ASN	4.1
6	G	14	ALA	4.1
6	R	19	ALA	4.1
6	6	5	SER	4.1
6	X	8	GLY	4.1
3	M	319	THR	4.1
5	A	9	TYR	4.0
5	S	8	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
6	V	26	TYR	4.0
2	L	42	PHE	3.9
5	5	53	VAL	3.9
6	J	14	ALA	3.9
6	B	9	LEU	3.9
5	D	13	LEU	3.9
5	W	9	TYR	3.9
6	J	26	TYR	3.8
5	I	6	ALA	3.8
5	Q	5	ASN	3.8
2	L	41	CYS	3.8
5	W	13	LEU	3.8
5	S	3	THR	3.8
2	L	38	VAL	3.8
5	3	53	VAL	3.7
5	A	26	ALA	3.7
6	X	26	TYR	3.7
4	H	52	ARG	3.7
5	I	9	TYR	3.6
2	L	48	LEU	3.6
6	V	5	SER	3.6
6	J	12	ASP	3.6
5	F	6	ALA	3.6
6	N	9	LEU	3.6
2	L	44	LEU	3.6
5	O	58	LEU	3.6
6	0	19	ALA	3.5
2	L	101	CYS	3.5
5	U	7	ASN	3.5
6	4	16	GLU	3.5
6	G	6	LEU	3.5
5	9	57	ALA	3.5
2	L	47	VAL	3.4
6	2	37	LEU	3.4
5	F	13	LEU	3.4
5	1	8	LEU	3.4
6	2	19	ALA	3.4
6	4	14	ALA	3.4
5	D	7	ASN	3.4
6	B	12	ASP	3.4
5	D	30	VAL	3.4
5	7	30	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
6	0	41	LEU	3.4
6	E	12	ASP	3.4
6	X	19	ALA	3.4
6	6	6	LEU	3.4
5	1	7	ASN	3.3
6	Z	40	TRP	3.3
5	Y	14	ILE	3.3
1	C	77	GLN	3.3
6	0	9	LEU	3.3
5	7	5	ASN	3.3
2	L	100	ILE	3.2
5	Y	3	THR	3.2
5	9	6	ALA	3.2
5	S	30[A]	VAL	3.2
5	7	33	LEU	3.2
5	D	29	ILE	3.2
5	F	11	ILE	3.2
5	7	14	ILE	3.2
6	B	14	ALA	3.1
5	U	34	LEU	3.1
6	E	37	LEU	3.1
6	J	6	LEU	3.1
6	J	15	LYS	3.1
6	J	23	GLN	3.1
6	2	11	ASP	3.1
2	L	49	LEU	3.1
5	3	9	TYR	3.1
5	A	58	LEU	3.1
5	Y	13	LEU	3.1
5	7	29	ILE	3.1
6	V	8	GLY	3.1
6	2	12	ASP	3.0
2	L	43	THR	3.0
5	S	34	LEU	3.0
6	G	17	PHE	3.0
6	E	41	LEU	3.0
6	2	6	LEU	3.0
6	8	6	LEU	3.0
6	8	37	LEU	3.0
5	A	29	ILE	3.0
6	X	10	THR	3.0
1	C	69	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
6	N	41	LEU	3.0
6	Z	12	ASP	3.0
6	8	12	ASP	3.0
6	J	16	GLU	2.9
6	P	9	LEU	2.9
6	X	6	LEU	2.9
6	Z	9	LEU	2.9
6	2	41	LEU	2.9
6	N	8	GLY	2.9
6	X	17	PHE	2.9
6	2	26	TYR	2.9
6	E	15	LYS	2.9
6	Z	20	ILE	2.9
6	X	15	LYS	2.9
5	U	35	ILE	2.9
6	G	15	LYS	2.9
5	3	54	SER	2.9
5	I	58	LEU	2.9
5	7	10	LYS	2.9
6	4	15	LYS	2.9
6	Z	26	TYR	2.8
6	G	11	ASP	2.8
5	Q	6	ALA	2.8
5	A	59	GLY	2.8
2	L	37	VAL	2.8
6	2	40	TRP	2.8
5	9	59	GLY	2.8
6	G	16	GLU	2.8
6	R	12	ASP	2.8
1	C	333	THR	2.8
5	F	5	ASN	2.8
5	5	7	ASN	2.8
6	Z	41	LEU	2.8
6	4	9	LEU	2.8
6	6	9	LEU	2.8
6	0	4	LYS	2.8
5	O	55	TYR	2.8
6	T	6	LEU	2.7
6	N	40	TRP	2.7
5	Y	6	ALA	2.7
5	F	10	LYS	2.7
5	F	53	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
5	Q	30	VAL	2.7
5	9	30	VAL	2.7
2	L	45	LEU	2.7
6	J	41	LEU	2.7
6	4	23	GLN	2.7
1	C	68	THR	2.7
5	9	7	ASN	2.7
1	C	66	ASP	2.7
5	Q	31	LEU	2.7
6	R	16	GLU	2.7
1	C	114	GLY	2.7
3	M	126	ILE	2.7
5	A	27	PHE	2.7
5	A	25	VAL	2.7
6	6	14	ALA	2.6
6	2	8	GLY	2.6
5	9	26	ALA	2.6
6	8	14	ALA	2.6
6	G	20	ILE	2.6
5	I	4	MET	2.6
3	M	62	PHE	2.6
2	L	40	PHE	2.6
6	G	7	THR	2.6
6	G	26	TYR	2.6
5	U	15	LEU	2.6
5	F	12	TRP	2.6
5	7	9	TYR	2.5
5	A	33	LEU	2.5
5	I	13	LEU	2.5
5	K	27	PHE	2.5
5	5	34	LEU	2.5
6	J	11	ASP	2.5
6	X	7	THR	2.5
5	1	51	ILE	2.5
6	8	16	GLU	2.5
5	Q	35	ILE	2.5
5	K	53	VAL	2.5
5	7	26	ALA	2.5
6	G	13	GLU	2.5
5	9	27	PHE	2.5
6	R	20	ILE	2.5
3	M	66	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
6	0	6	LEU	2.5
5	O	7	ASN	2.5
5	W	53	VAL	2.4
6	B	5	SER	2.4
5	I	34	LEU	2.4
5	3	8	LEU	2.4
5	7	31	LEU	2.4
5	U	32	GLY	2.4
5	3	57	ALA	2.4
6	0	14	ALA	2.4
5	9	14	ILE	2.4
2	L	2	ALA	2.4
6	X	20	ILE	2.4
5	O	30	VAL	2.4
3	M	55	LEU	2.4
5	O	31	LEU	2.4
5	D	9	TYR	2.4
5	1	14	ILE	2.4
5	A	30	VAL	2.4
5	5	33	LEU	2.4
6	G	41	LEU	2.4
6	X	14	ALA	2.4
5	W	5	ASN	2.4
6	E	11	ASP	2.3
3	M	59	LEU	2.3
6	B	46	LEU	2.3
6	V	9	LEU	2.3
4	H	22	PHE	2.3
4	H	48	ARG	2.3
5	U	10	LYS	2.3
6	B	37	LEU	2.3
6	Z	8	GLY	2.3
6	0	26	TYR	2.3
6	0	11	ASP	2.3
5	K	14	ILE	2.3
5	O	59	GLY	2.3
6	J	19	ALA	2.3
6	G	21	PHE	2.3
5	I	33	LEU	2.3
6	B	8	GLY	2.3
5	W	14	ILE	2.3
5	U	58	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
6	Z	37	LEU	2.3
4	H	205	LYS	2.2
6	R	9	LEU	2.2
6	P	8	GLY	2.2
6	8	10	THR	2.2
6	4	11	ASP	2.2
2	L	146	LEU	2.2
5	Q	8	LEU	2.2
5	1	17	PRO	2.2
2	L	105	ALA	2.2
5	3	7	ASN	2.2
6	E	40	TRP	2.2
6	4	13	GLU	2.2
5	Q	3	THR	2.2
6	0	23	GLN	2.2
4	H	50	GLY	2.2
5	O	53	VAL	2.2
5	Q	25	VAL	2.2
5	7	53	VAL	2.2
6	4	12	ASP	2.2
1	C	67	SER	2.2
5	U	33	LEU	2.2
5	1	12	TRP	2.2
2	L	39	GLY	2.2
6	P	26	TYR	2.2
5	S	27	PHE	2.2
6	N	12	ASP	2.2
5	5	30	VAL	2.2
2	L	50	ILE	2.1
4	H	26	LEU	2.1
3	M	130	TRP	2.1
4	H	11	ALA	2.1
5	O	57	ALA	2.1
6	4	26	TYR	2.1
6	2	15	LYS	2.1
6	P	37	LEU	2.1
5	9	9	TYR	2.1
1	C	70	PRO	2.1
5	K	30	VAL	2.1
3	M	124	LEU	2.1
5	5	18	ARG	2.1
5	1	9	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
4	H	24	PHE	2.1
2	L	103	ALA	2.1
2	L	111	LEU	2.1
6	8	9	LEU	2.1
6	2	42	TYR	2.0
5	I	14	ILE	2.0
5	S	33	LEU	2.0
6	X	23	GLN	2.0
6	0	5	SER	2.0
5	F	55	TYR	2.0
2	L	30	PHE	2.0
3	M	65	LEU	2.0
3	M	127	LEU	2.0
5	A	31	LEU	2.0
5	Q	7	ASN	2.0
5	S	31	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	PGV	3	104	51/51	0.48	0.39	76,101,155,158	0
16	UNL	P	102	12/-	0.62	0.23	67,74,82,82	0
21	LDA	M	411	14/16	0.64	0.30	65,82,109,113	0
20	PEF	M	407	5/47	0.64	0.15	161,162,163,165	0
20	PEF	3	103	5/47	0.67	0.18	136,137,138,142	0
16	UNL	J	103	12/-	0.68	0.20	74,79,93,94	0
12	PGV	C	509	21/51	0.69	0.27	81,101,108,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CDL	Y	102	40/100	0.69	0.25	114,129,148,149	0
19	CRT	1	103	44/44	0.70	0.21	58,78,96,99	0
21	LDA	O	104	14/16	0.71	0.31	61,75,110,112	0
20	PEF	U	105	5/47	0.72	0.15	156,156,159,160	0
22	CDL	S	103	62/100	0.73	0.23	73,116,153,162	0
23	LMT	M	419	35/35	0.73	0.23	64,99,112,121	0
22	CDL	Q	104	75/100	0.73	0.25	62,97,142,143	0
16	UNL	0	103	12/-	0.73	0.19	77,84,87,87	0
19	CRT	J	101	44/44	0.74	0.23	59,74,97,100	0
21	LDA	J	102	16/16	0.74	0.19	74,90,112,114	0
22	CDL	D	103	40/100	0.75	0.24	116,142,163,164	0
16	UNL	E	101	12/-	0.75	0.28	78,93,101,102	0
16	UNL	B	101	12/-	0.77	0.16	69,80,88,91	0
16	UNL	R	101	12/-	0.77	0.20	57,68,75,77	0
16	UNL	G	102	12/-	0.77	0.16	77,85,93,93	0
16	UNL	2	102	12/-	0.77	0.22	71,80,90,92	0
9	GOL	C	506	6/6	0.78	0.19	63,68,72,75	0
16	UNL	8	101	12/-	0.80	0.17	64,74,96,96	0
12	PGV	L	305	43/51	0.80	0.23	45,76,104,109	0
16	UNL	T	101	12/-	0.80	0.22	45,68,81,82	0
19	CRT	G	101	44/44	0.80	0.20	61,80,114,123	0
20	PEF	M	409	5/47	0.81	0.25	94,98,100,102	0
16	UNL	Z	103	12/-	0.81	0.17	68,80,92,95	0
21	LDA	V	102	16/16	0.81	0.20	60,77,119,122	0
16	UNL	X	101	12/-	0.81	0.14	68,76,82,85	0
12	PGV	1	105	31/51	0.82	0.18	83,102,125,129	0
19	CRT	U	103	44/44	0.82	0.18	48,72,91,96	0
16	UNL	6	102	12/-	0.82	0.23	76,81,91,93	0
15	UQ8	L	309	18/53	0.82	0.26	102,114,125,132	0
9	GOL	H	301	6/6	0.82	0.16	58,78,82,84	0
16	UNL	4	101	12/-	0.82	0.20	72,88,103,105	0
15	UQ8	L	308	53/53	0.82	0.31	60,90,99,104	0
20	PEF	5	103	5/47	0.82	0.15	126,127,129,131	0
19	CRT	9	101	44/44	0.82	0.19	53,68,100,105	0
12	PGV	L	306	44/51	0.83	0.22	53,75,98,108	0
10	SO4	M	412	5/5	0.83	0.14	125,126,126,130	0
15	UQ8	7	103	33/53	0.83	0.30	60,74,94,100	0
19	CRT	0	101	44/44	0.83	0.18	51,68,88,95	0
22	CDL	Y	103	13/100	0.84	0.17	107,120,124,128	0
20	PEF	K	104	27/47	0.84	0.28	63,85,92,97	0
22	CDL	K	103	86/100	0.84	0.31	56,92,114,120	0
23	LMT	F	103	35/35	0.84	0.18	61,78,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	PEF	1	104	5/47	0.84	0.15	119,119,121,121	0
19	CRT	2	101	44/44	0.85	0.18	67,78,94,99	0
20	PEF	U	104	5/47	0.85	0.18	113,115,116,118	0
16	UNL	M	416	9/-	0.86	0.44	58,64,73,75	0
19	CRT	6	101	44/44	0.86	0.17	48,69,84,87	0
10	SO4	L	304	5/5	0.86	0.26	136,137,138,138	0
19	CRT	A	104	44/44	0.87	0.18	62,74,97,101	0
22	CDL	H	302	64/100	0.87	0.29	75,89,107,113	0
20	PEF	W	103	5/47	0.87	0.11	146,148,148,149	0
12	PGV	D	104	35/51	0.88	0.19	55,72,100,113	0
12	PGV	M	414	37/51	0.88	0.17	60,83,116,121	0
12	PGV	M	413	46/51	0.89	0.16	52,74,89,94	0
12	PGV	A	105	33/51	0.89	0.22	60,93,108,109	0
16	UNL	L	307	12/-	0.89	0.21	79,88,96,96	0
19	CRT	9	102	44/44	0.90	0.17	51,67,94,105	0
20	PEF	M	408	5/47	0.90	0.09	56,67,83,95	0
19	CRT	Z	101	44/44	0.90	0.17	58,72,99,100	0
15	UQ8	M	417	18/53	0.90	0.27	61,74,96,102	0
19	CRT	V	101	44/44	0.90	0.15	41,62,85,87	0
19	CRT	O	103	44/44	0.90	0.16	37,51,75,82	0
10	SO4	C	507	5/5	0.90	0.15	113,114,117,120	0
19	CRT	N	101	44/44	0.90	0.14	50,67,86,94	0
19	CRT	Q	103	44/44	0.91	0.14	42,55,73,76	0
20	PEF	M	418	47/47	0.91	0.24	58,75,93,97	0
20	PEF	I	103	5/47	0.92	0.12	99,107,109,112	0
21	LDA	I	104	16/16	0.92	0.27	36,70,75,77	0
22	CDL	H	304	79/100	0.92	0.31	44,73,107,111	0
19	CRT	P	101	44/44	0.92	0.15	38,55,77,80	0
13	BCL	3	101	66/66	0.93	0.15	61,75,105,110	0
13	BCL	7	101	61/66	0.93	0.12	53,64,96,103	0
11	LHG	C	508	9/49	0.93	0.14	52,61,67,69	0
12	PGV	H	303	36/51	0.93	0.20	47,59,82,89	0
18	MQ8	M	405	53/53	0.93	0.24	36,53,116,123	0
13	BCL	1	102	66/66	0.93	0.14	49,70,97,104	0
13	BCL	L	301	66/66	0.94	0.11	27,34,43,70	0
13	BCL	Z	102	66/66	0.94	0.14	52,64,98,103	0
13	BCL	5	101	66/66	0.94	0.14	55,69,109,111	0
13	BCL	3	102	66/66	0.94	0.12	53,69,93,96	0
13	BCL	5	102	66/66	0.94	0.16	50,62,90,98	0
8	MG	C	505	1/1	0.94	0.11	36,36,36,36	0
14	BPH	L	302	65/65	0.94	0.17	29,40,54,59	0
13	BCL	9	103	66/66	0.94	0.13	54,63,103,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	BCL	7	102	66/66	0.94	0.14	53,63,95,102	0
13	BCL	K	102	66/66	0.95	0.14	47,58,98,102	0
13	BCL	F	102	66/66	0.95	0.14	55,70,107,113	0
15	UQ8	L	303	33/53	0.95	0.14	36,45,77,85	0
22	CDL	M	415	39/100	0.95	0.13	46,80,113,119	0
13	BCL	A	103	66/66	0.95	0.14	58,70,104,109	0
13	BCL	1	101	66/66	0.95	0.11	59,67,107,113	0
19	CRT	M	406	44/44	0.95	0.15	31,39,82,90	0
13	BCL	0	102	66/66	0.96	0.12	54,65,97,108	0
13	BCL	M	401	66/66	0.96	0.13	30,39,54,62	0
13	BCL	O	102	66/66	0.96	0.14	41,51,89,96	0
13	BCL	U	102	66/66	0.96	0.14	44,55,92,101	0
13	BCL	W	101	66/66	0.96	0.14	48,59,114,118	0
13	BCL	M	402	66/66	0.96	0.12	26,35,84,90	0
13	BCL	Q	101	66/66	0.96	0.13	40,48,94,99	0
13	BCL	Q	102	66/66	0.96	0.13	39,47,84,93	0
13	BCL	I	101	66/66	0.96	0.13	61,68,100,104	0
13	BCL	W	102	66/66	0.96	0.12	49,60,94,97	0
13	BCL	A	101	66/66	0.96	0.12	54,69,113,118	0
13	BCL	F	101	66/66	0.96	0.13	57,69,114,117	0
13	BCL	K	101	66/66	0.96	0.14	50,63,102,105	0
13	BCL	Y	101	66/66	0.96	0.12	49,60,110,113	0
13	BCL	D	101	66/66	0.96	0.12	55,70,117,121	0
13	BCL	I	102	66/66	0.96	0.13	51,65,93,95	0
13	BCL	D	102	66/66	0.96	0.12	57,69,91,92	0
13	BCL	O	101	66/66	0.97	0.12	44,54,102,112	0
14	BPH	M	404	65/65	0.97	0.13	29,38,111,115	0
13	BCL	S	102	66/66	0.97	0.12	40,48,90,96	0
13	BCL	U	101	66/66	0.97	0.12	42,53,101,104	0
13	BCL	M	403	66/66	0.97	0.11	27,34,45,54	0
13	BCL	S	101	66/66	0.97	0.13	38,49,96,110	0
7	HEC	C	504	43/43	0.98	0.09	34,40,47,54	0
7	HEC	C	502	43/43	0.98	0.09	39,46,52,55	0
20	PEF	M	410	5/47	0.98	0.11	40,45,52,54	0
7	HEC	C	503	43/43	0.98	0.09	29,35,42,46	0
24	CA	2	103	1/1	0.98	0.03	68,68,68,68	0
7	HEC	C	501	43/43	0.98	0.10	52,60,67,75	0
24	CA	4	102	1/1	0.98	0.07	68,68,68,68	0
24	CA	J	104	1/1	0.99	0.06	63,63,63,63	0
24	CA	6	103	1/1	0.99	0.04	67,67,67,67	0
24	CA	A	102	1/1	0.99	0.09	64,64,64,64	0
24	CA	N	102	1/1	0.99	0.07	56,56,56,56	0

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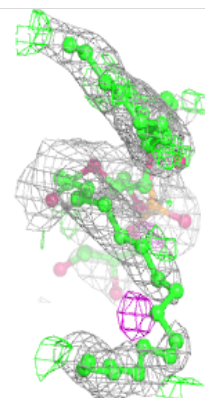
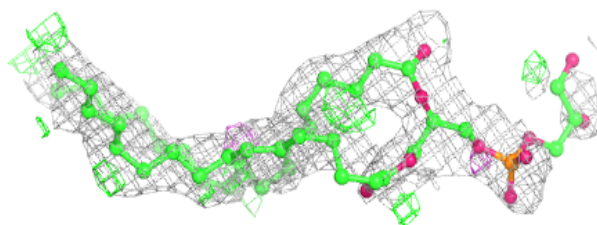
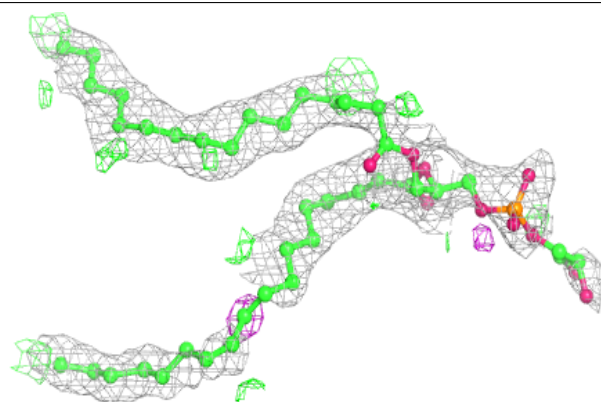
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CA	G	103	1/1	0.99	0.08	64,64,64,64	0
24	CA	X	102	1/1	0.99	0.05	60,60,60,60	0
24	CA	8	102	1/1	0.99	0.06	67,67,67,67	0
24	CA	V	103	1/1	0.99	0.09	52,52,52,52	0
24	CA	E	102	1/1	0.99	0.04	65,65,65,65	0
24	CA	Z	104	1/1	0.99	0.03	60,60,60,60	0
24	CA	B	102	1/1	0.99	0.04	64,64,64,64	0
24	CA	T	102	1/1	1.00	0.07	48,48,48,48	0
24	CA	R	102	1/1	1.00	0.10	44,44,44,44	0
17	FE	L	310	1/1	1.00	0.10	39,39,39,39	0
24	CA	P	103	1/1	1.00	0.11	47,47,47,47	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

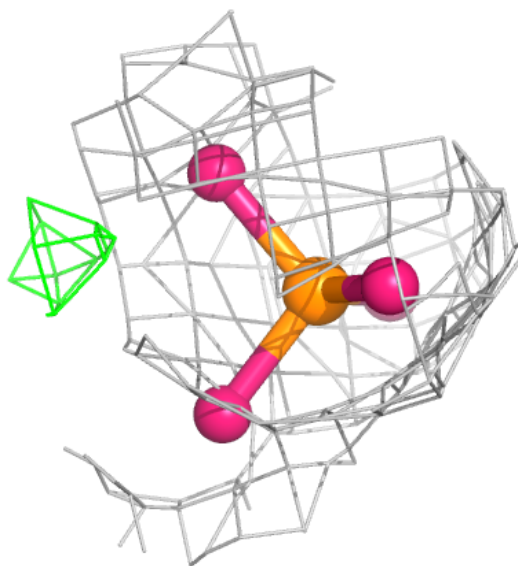
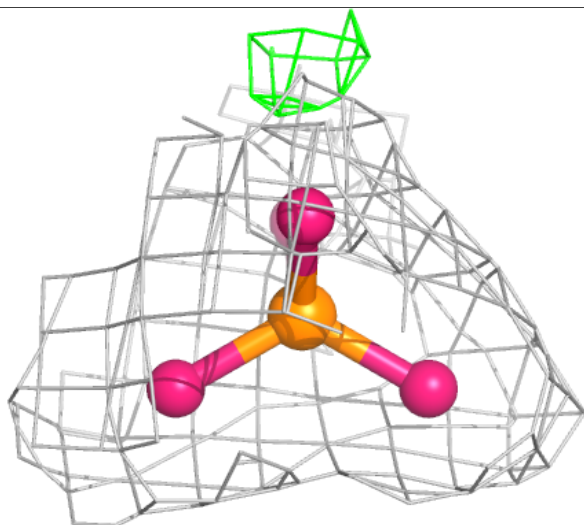
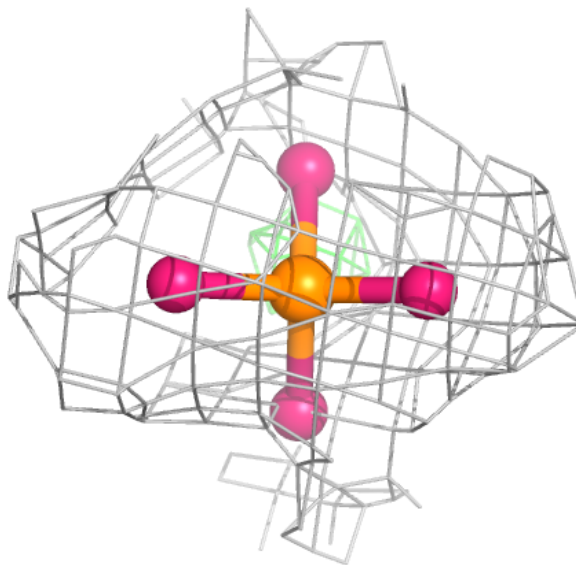
Electron density around PGV 3 104:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



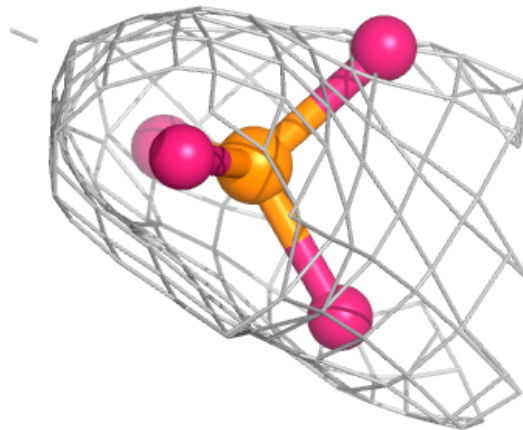
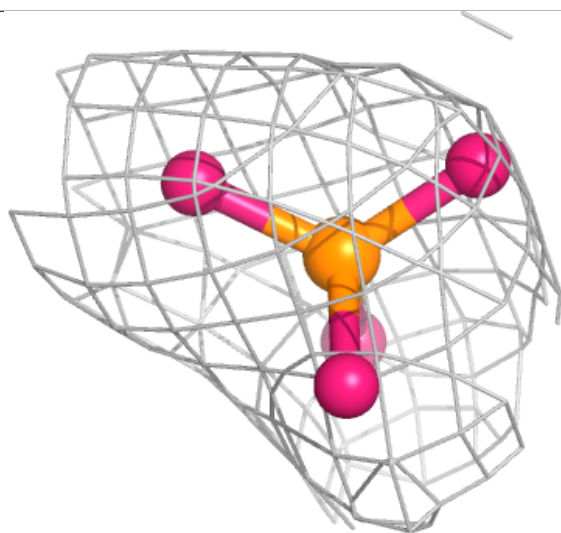
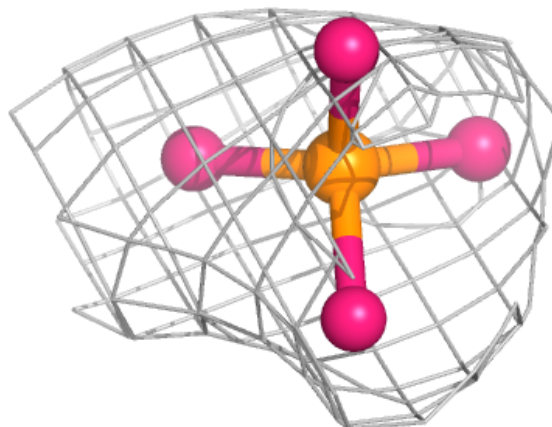
Electron density around PEF M 407:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



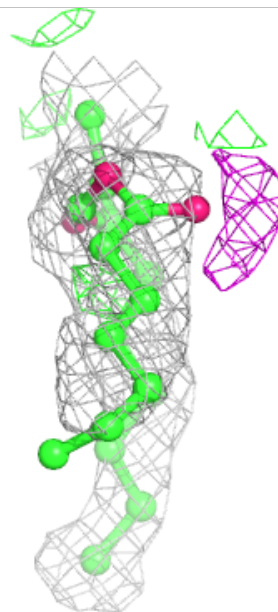
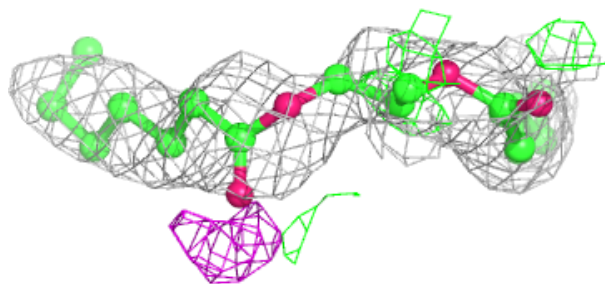
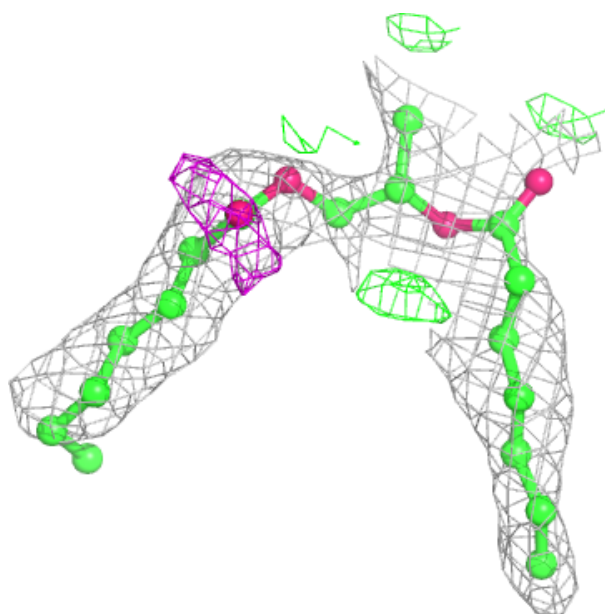
Electron density around PEF 3 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



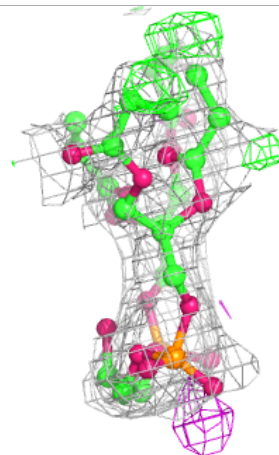
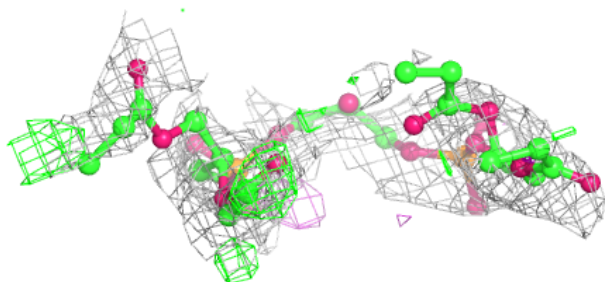
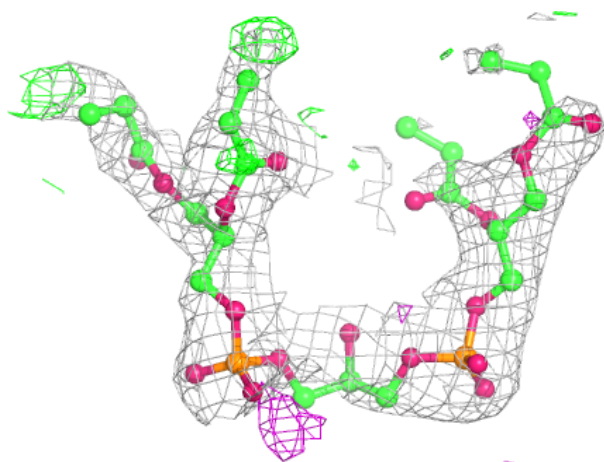
Electron density around PGV C 509:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



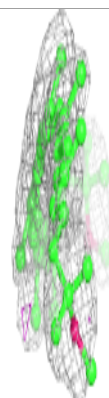
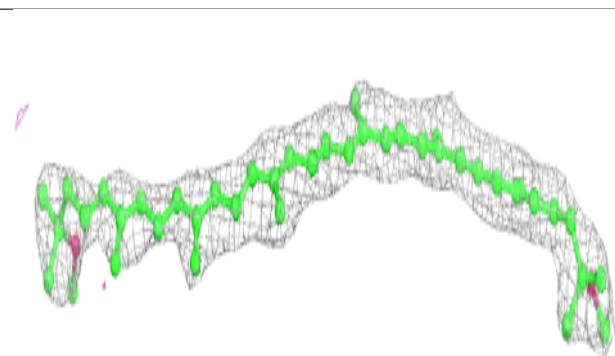
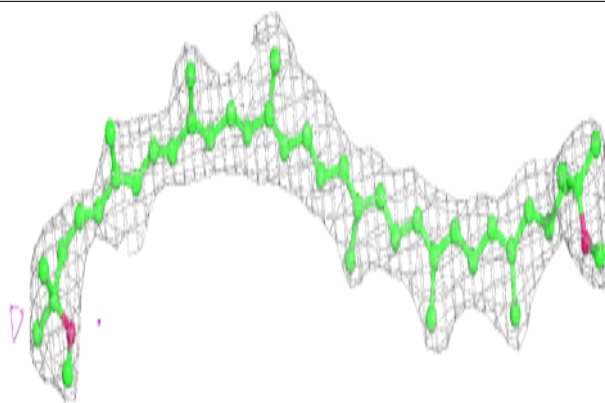
Electron density around CDL Y 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



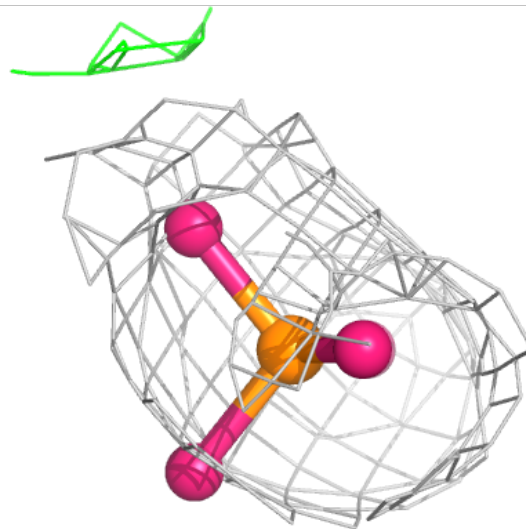
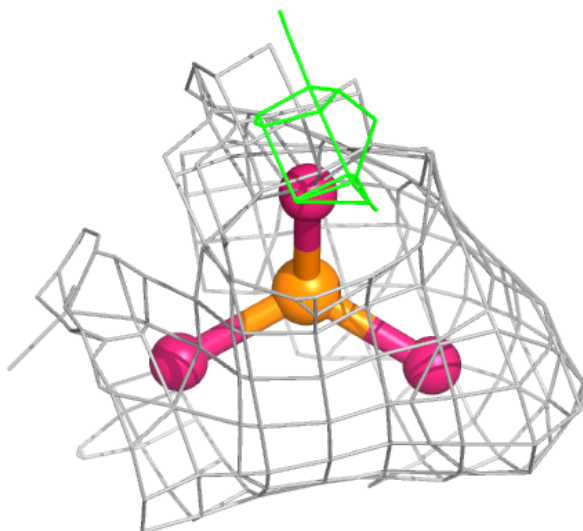
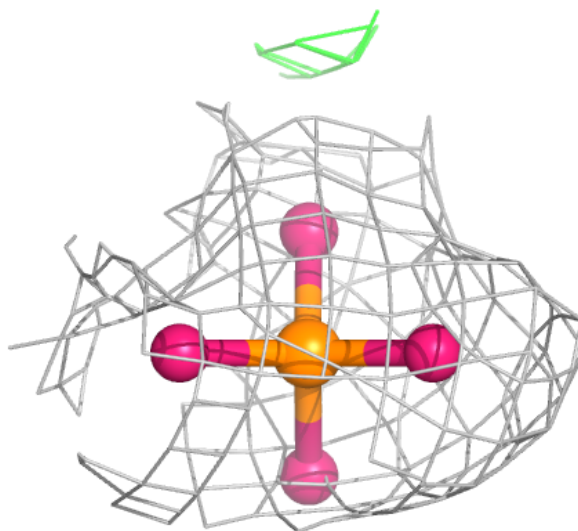
Electron density around CRT 1 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



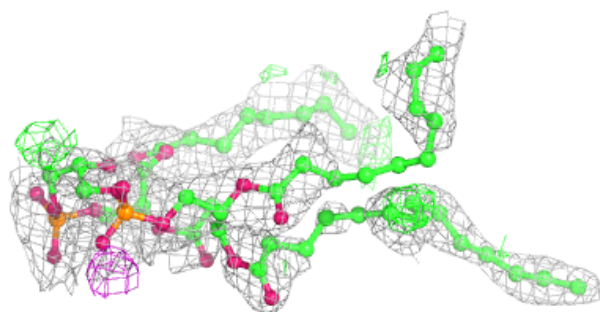
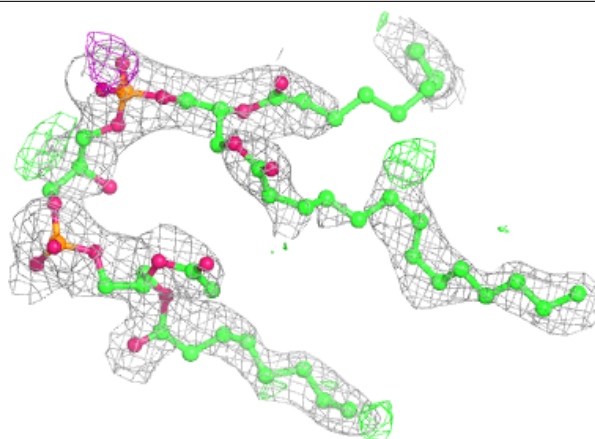
Electron density around PEF U 105:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

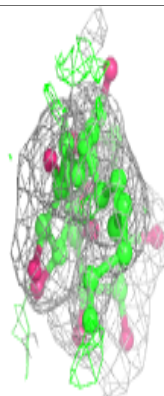
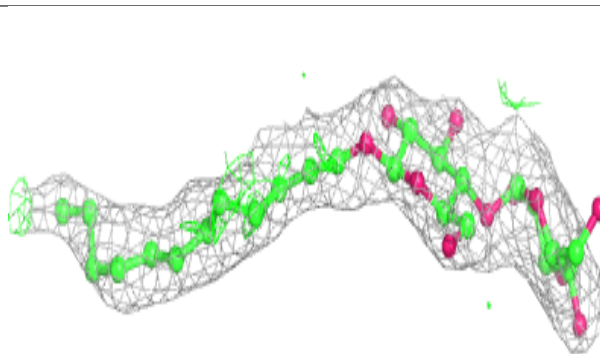
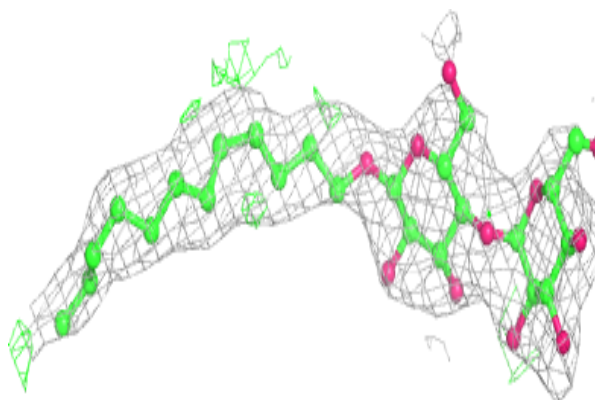


Electron density around CDL S 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

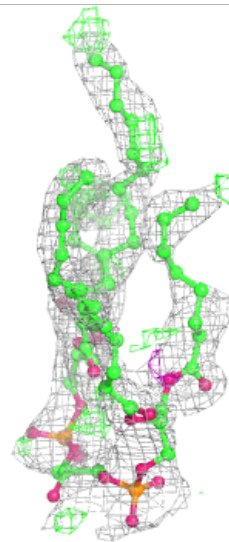
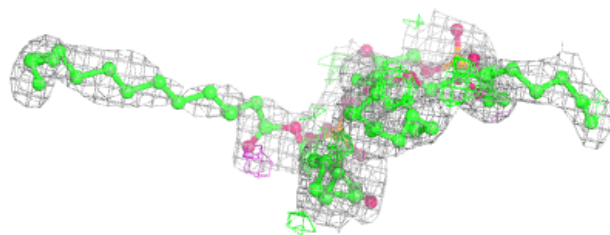
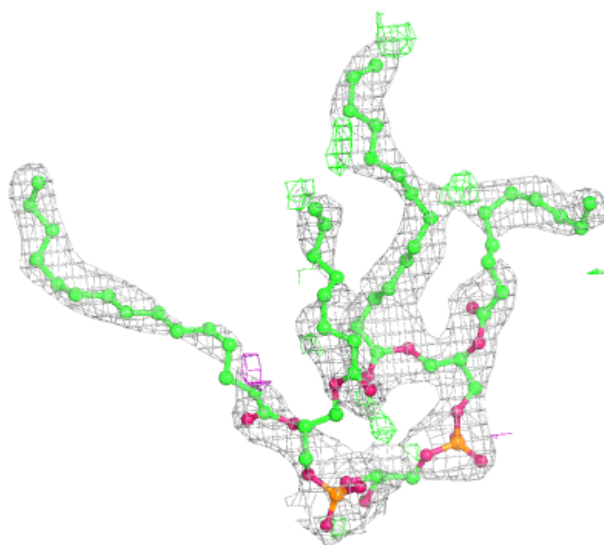
**Electron density around LMT M 419:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



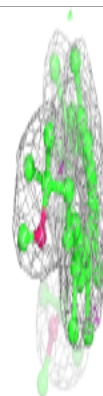
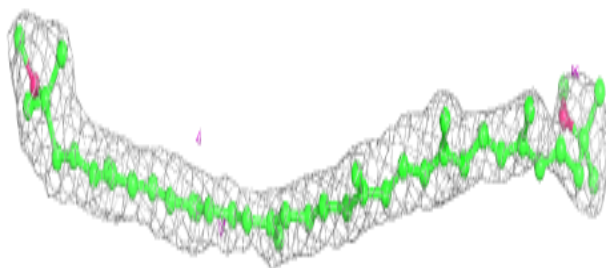
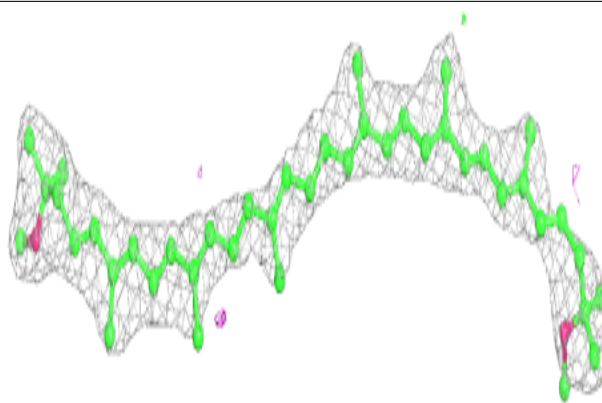
Electron density around CDL Q 104:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



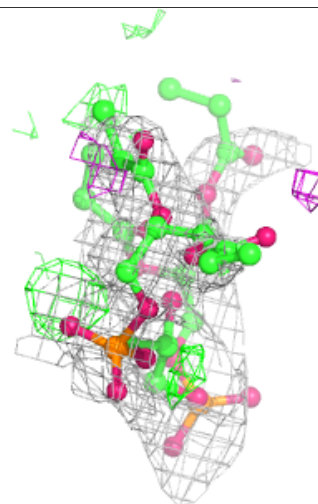
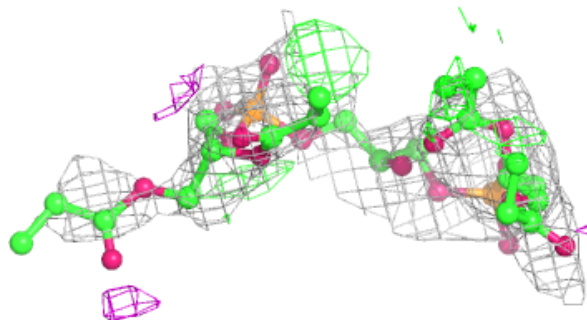
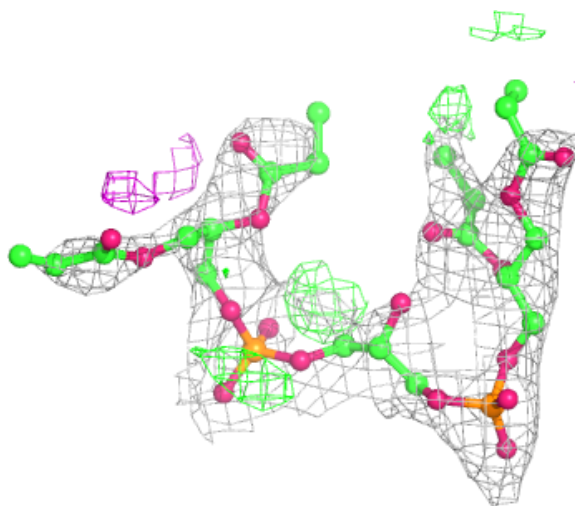
Electron density around CRT J 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



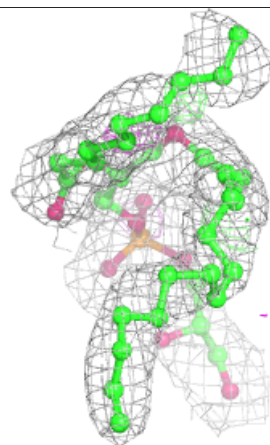
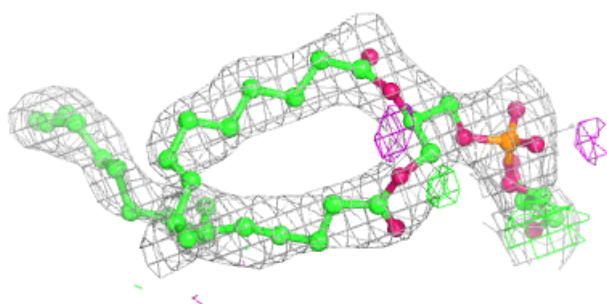
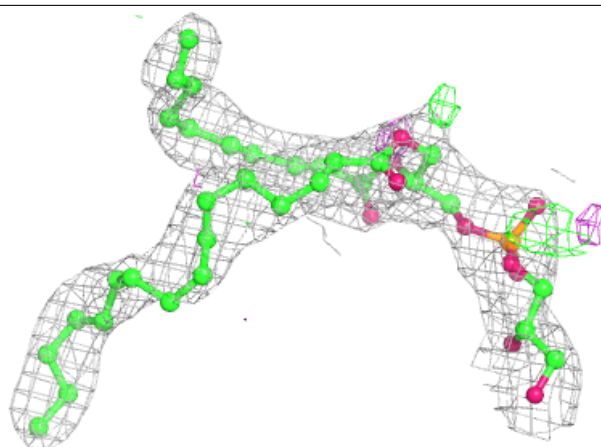
Electron density around CDL D 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

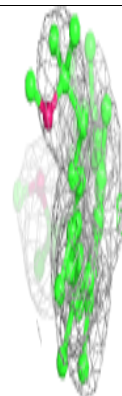
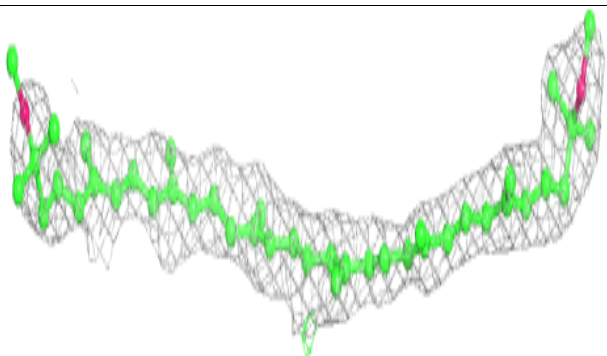
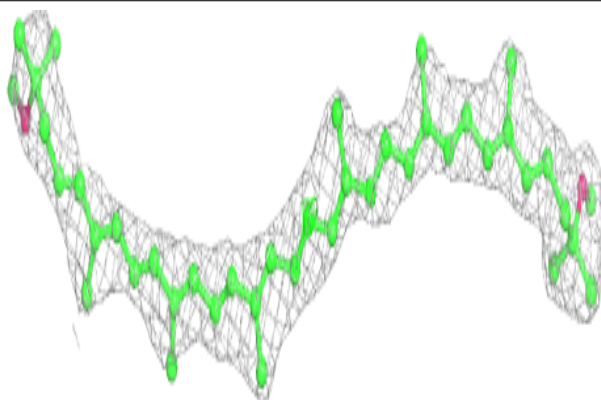


Electron density around PGV L 305:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

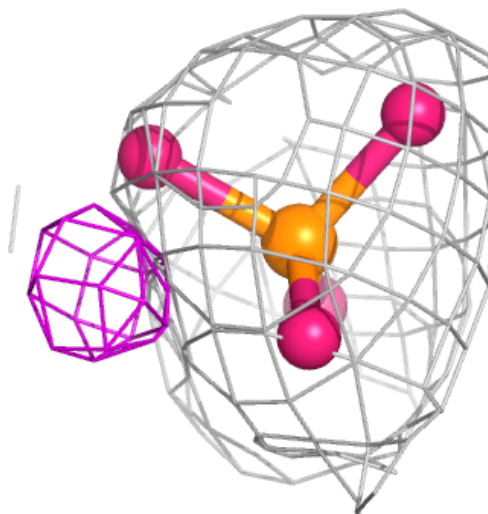
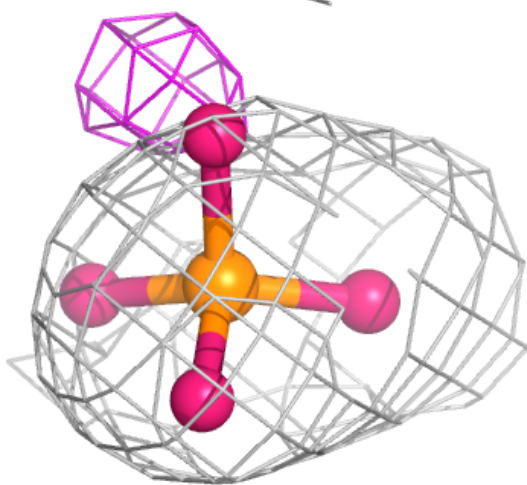
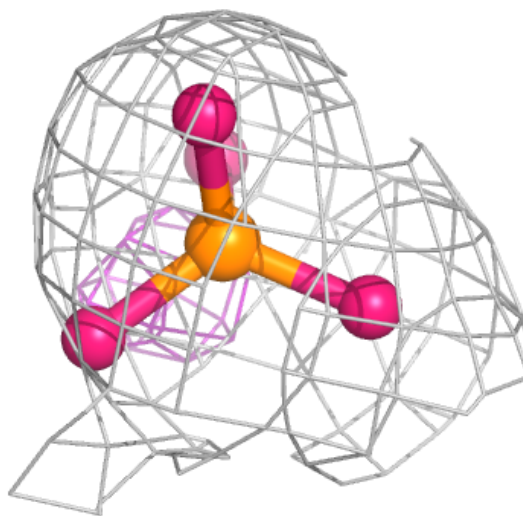
**Electron density around CRT G 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



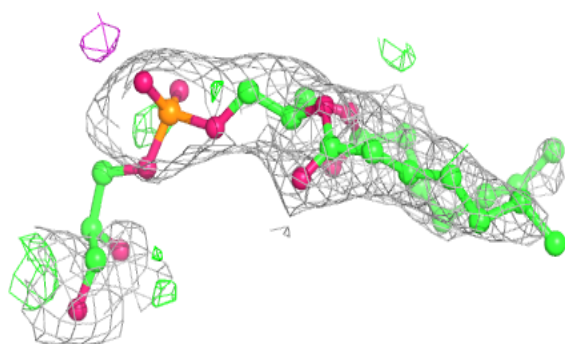
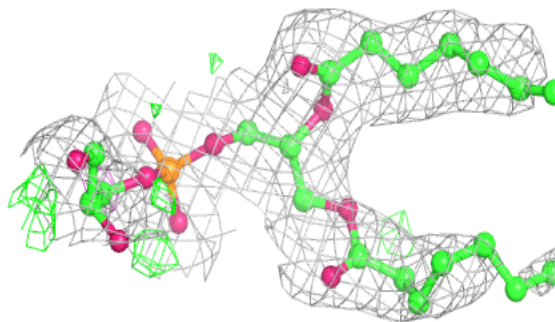
Electron density around PEF M 409:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

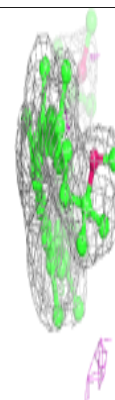
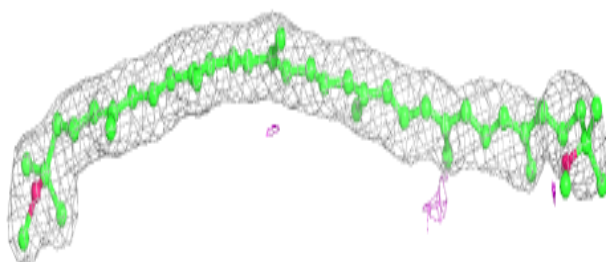
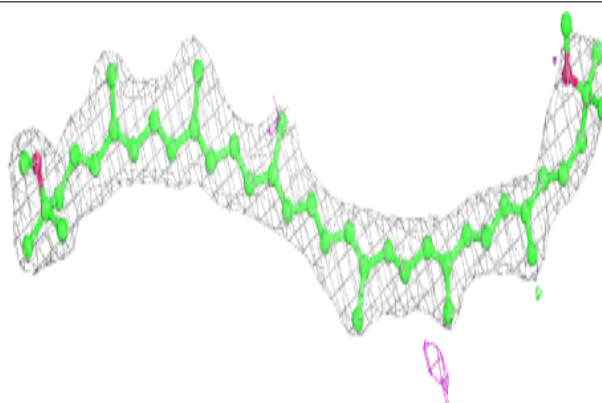


Electron density around PGV 1 105:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

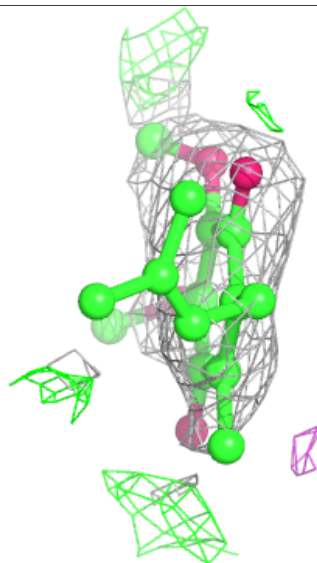
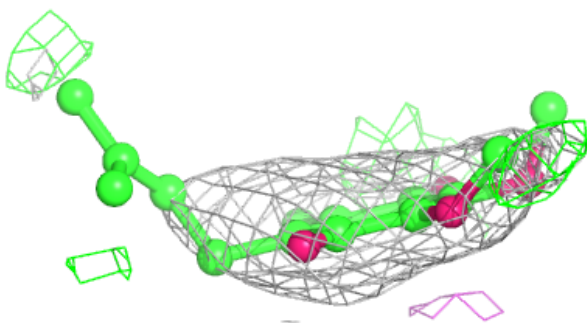
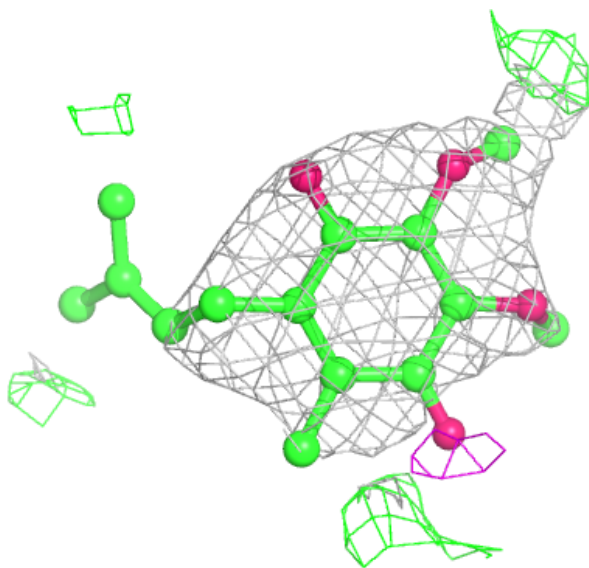
**Electron density around CRT U 103:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



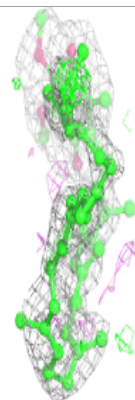
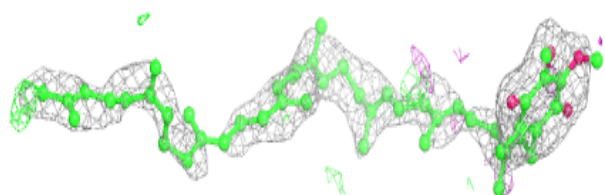
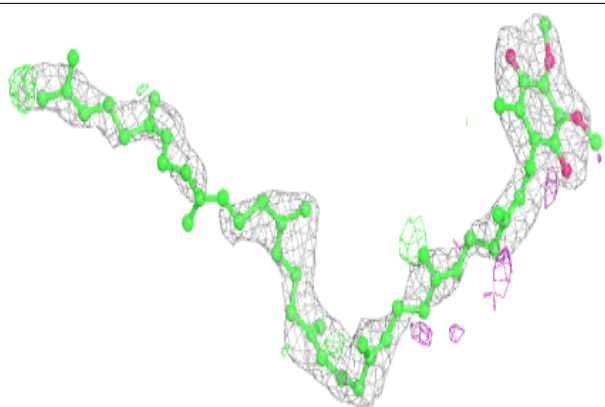
Electron density around UQ8 L 309:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



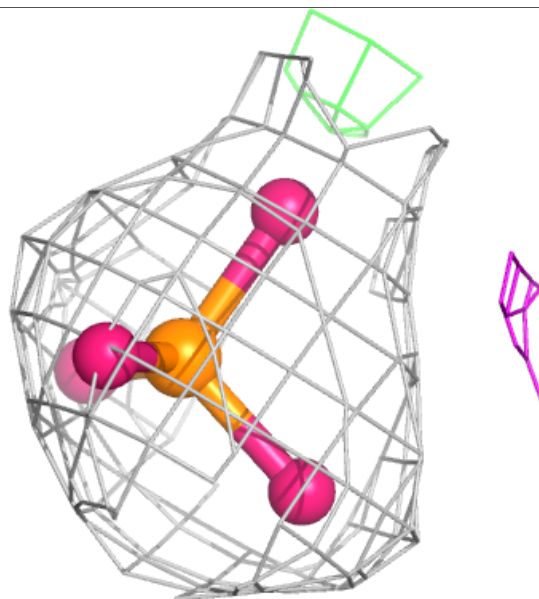
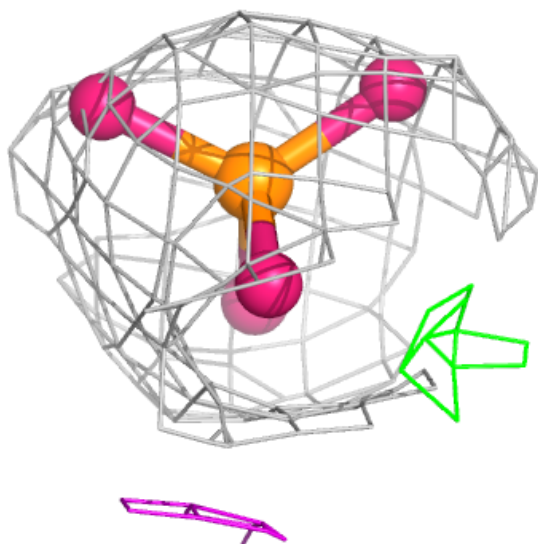
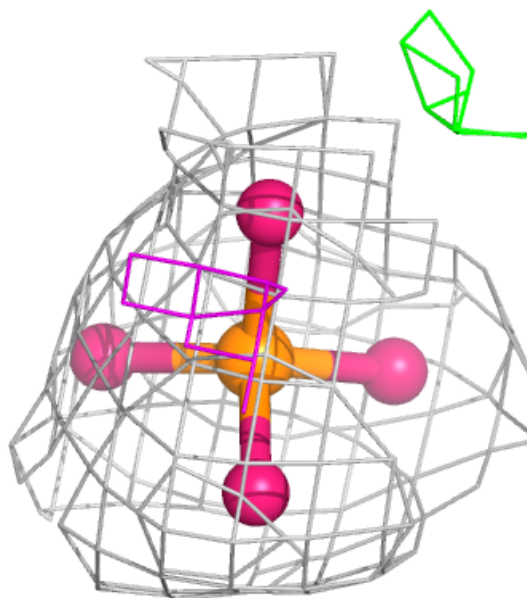
Electron density around UQ8 L 308:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



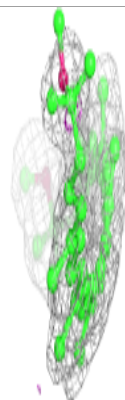
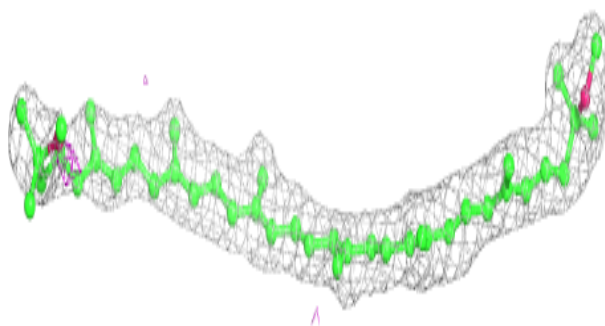
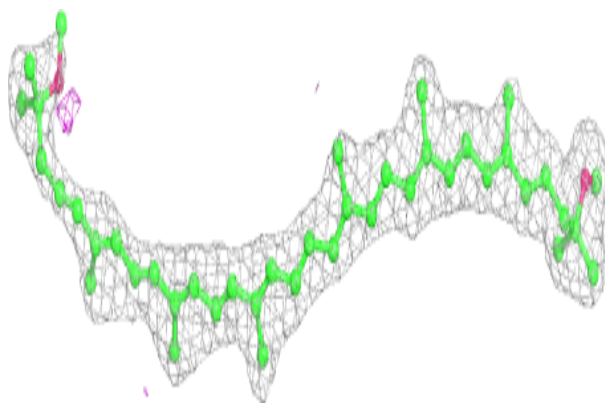
Electron density around PEF 5 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

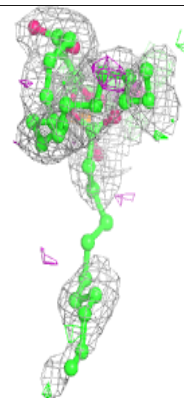
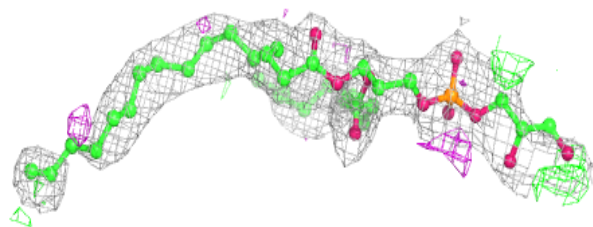
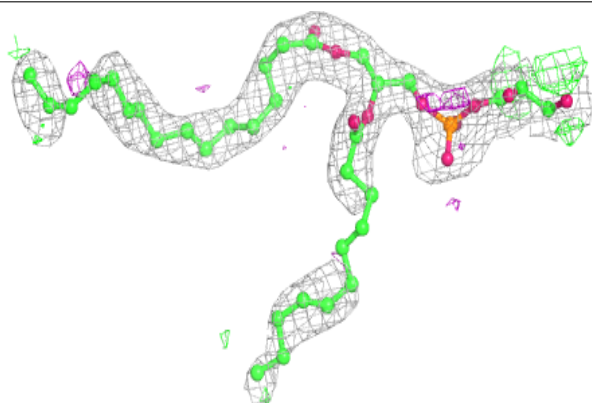


Electron density around CRT 9 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

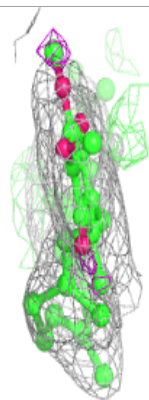
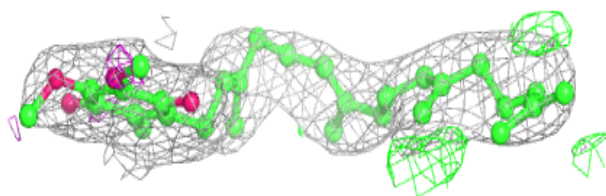
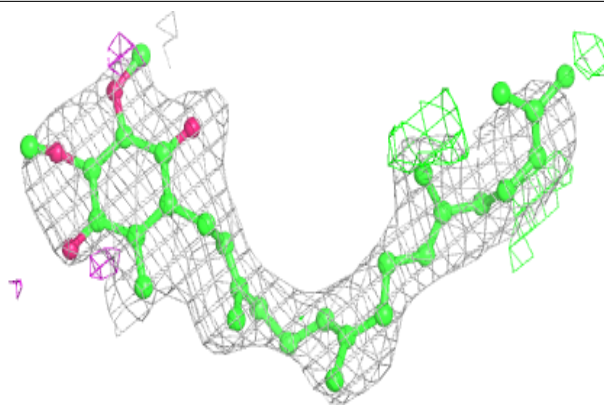
**Electron density around PGV L 306:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

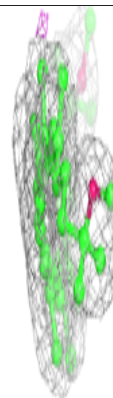
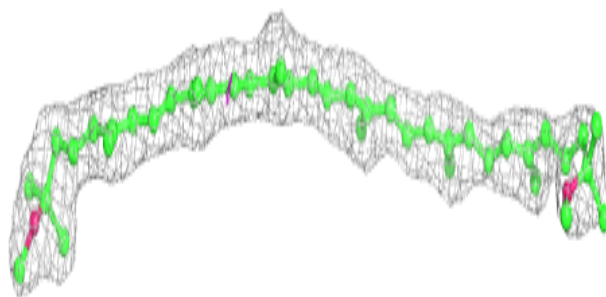
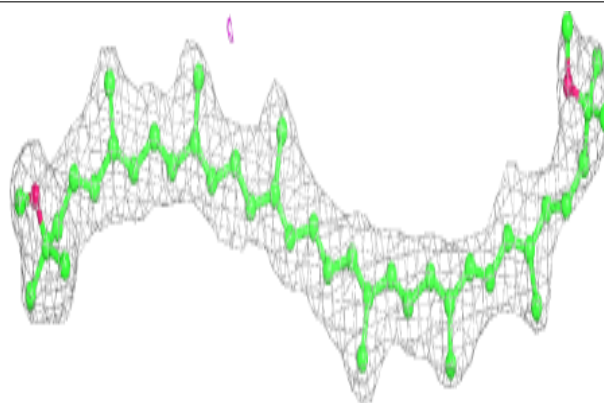


Electron density around UQ8 7 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

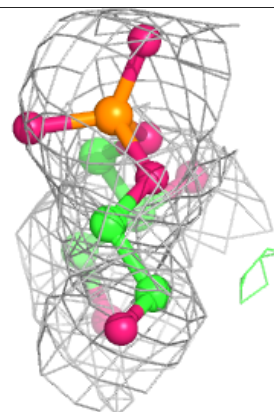
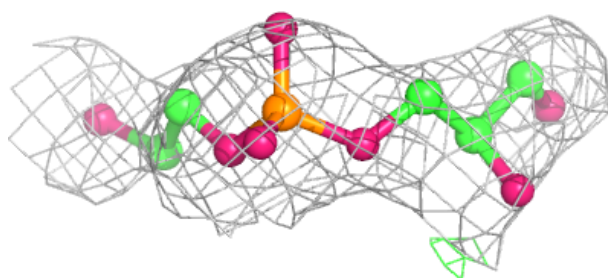
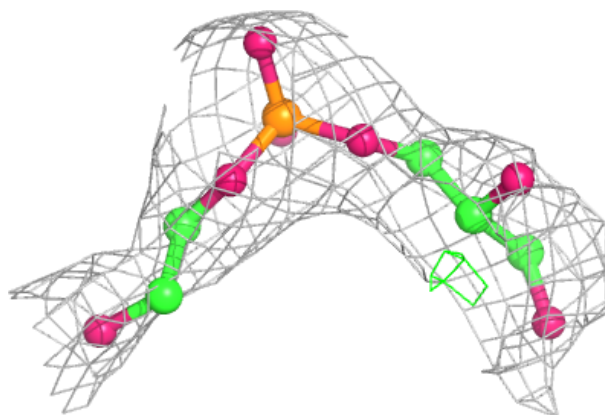
**Electron density around CRT 0 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

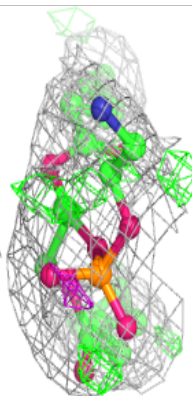
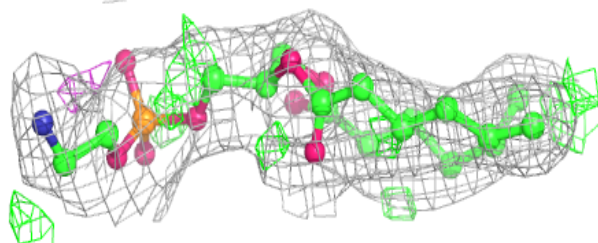
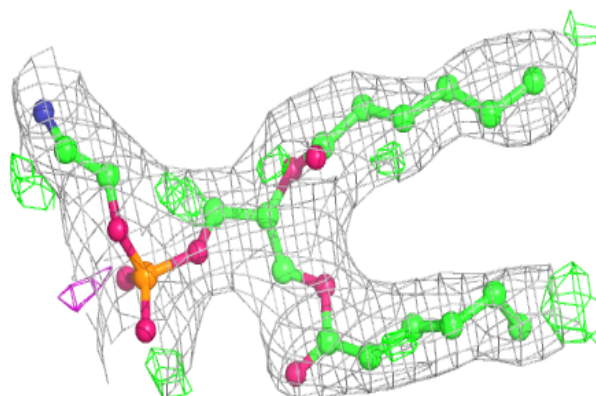


Electron density around CDL Y 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

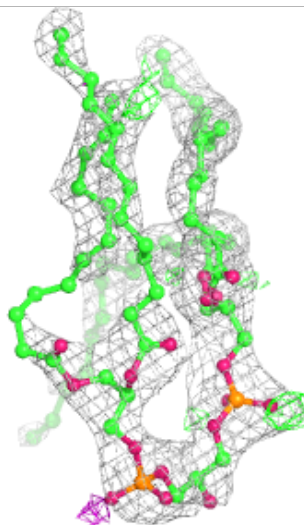
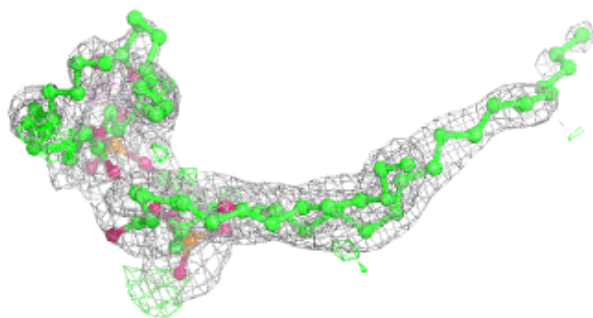
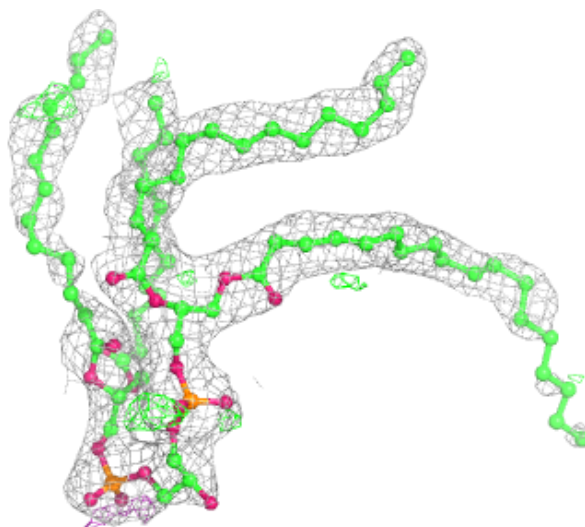
**Electron density around PEF K 104:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



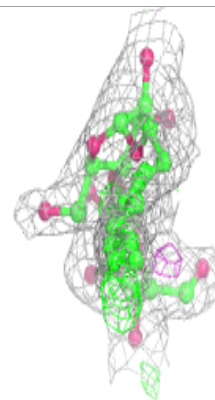
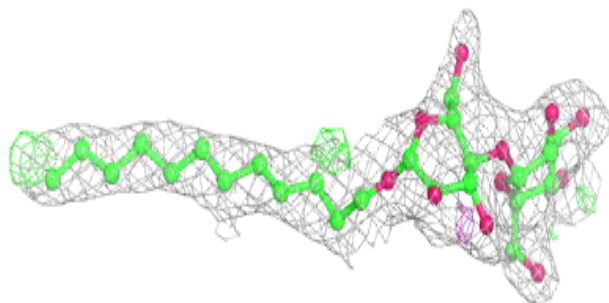
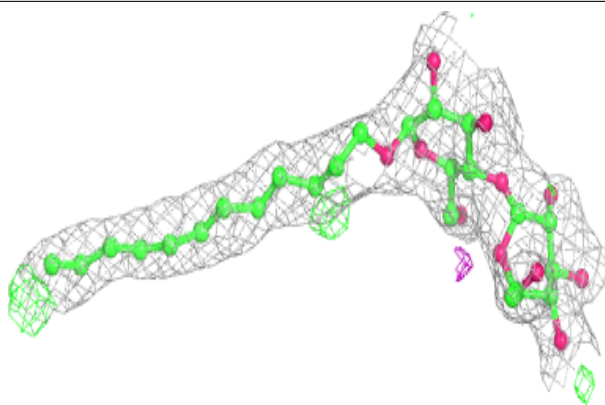
Electron density around CDL K 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



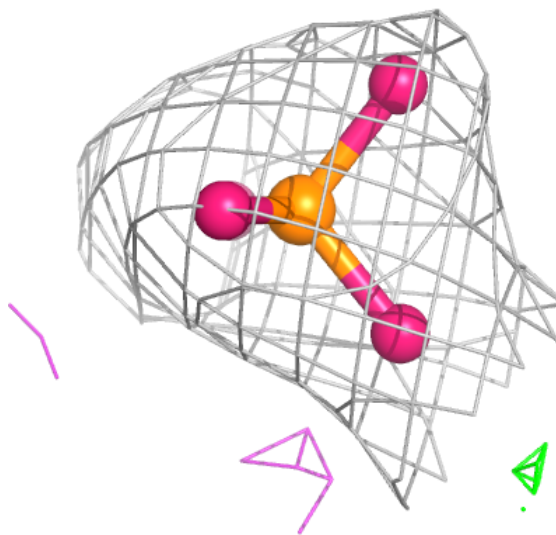
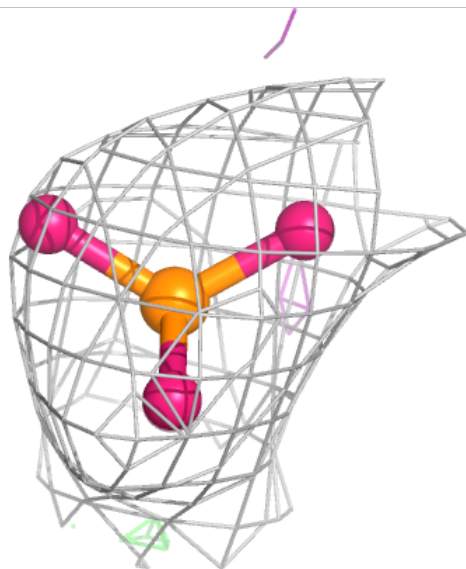
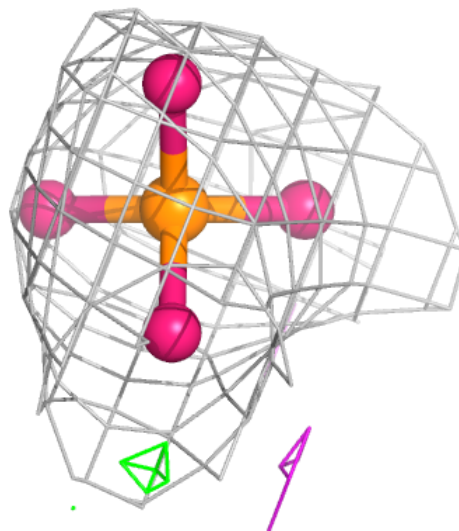
Electron density around LMT F 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



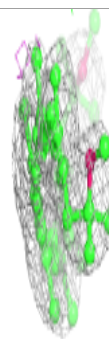
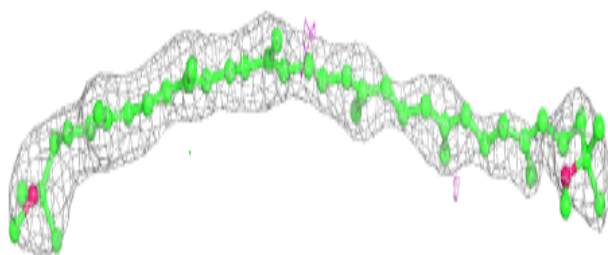
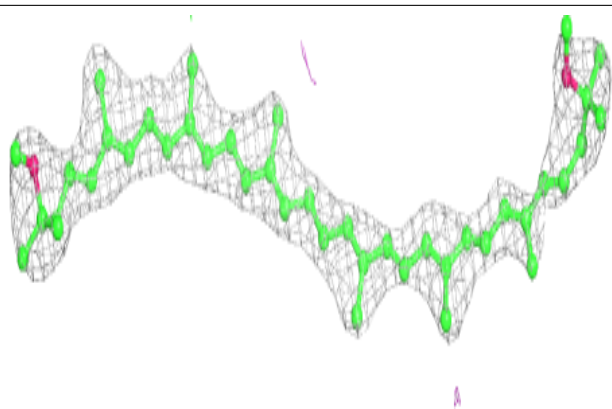
Electron density around PEF 1 104:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



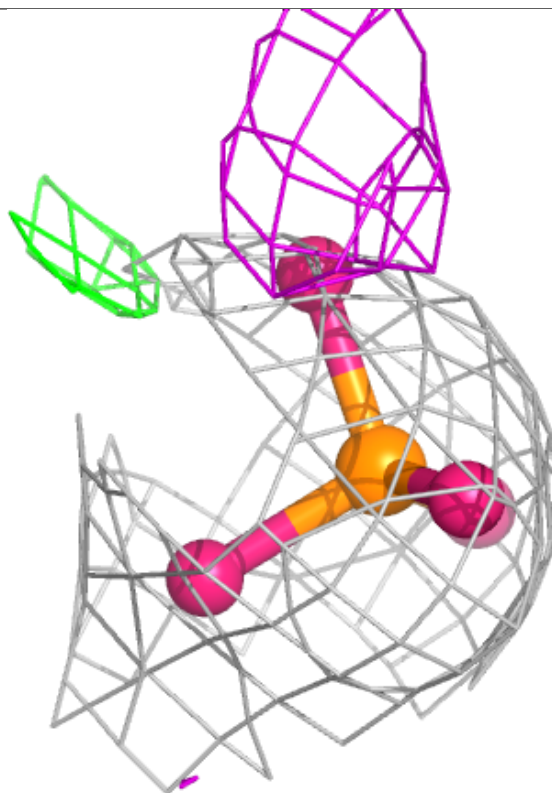
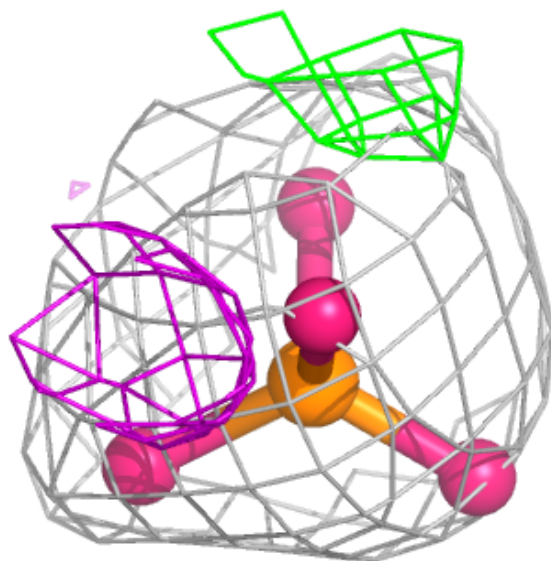
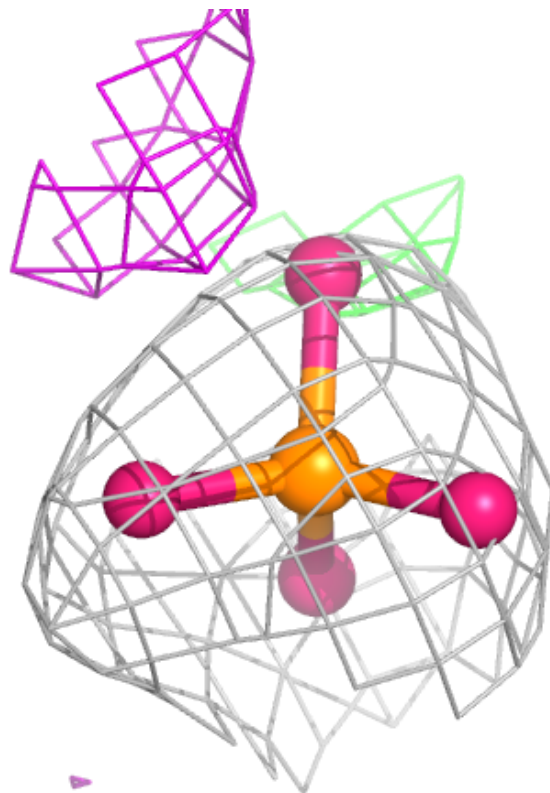
Electron density around CRT 2 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



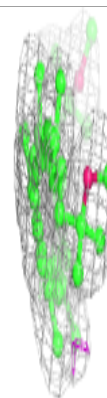
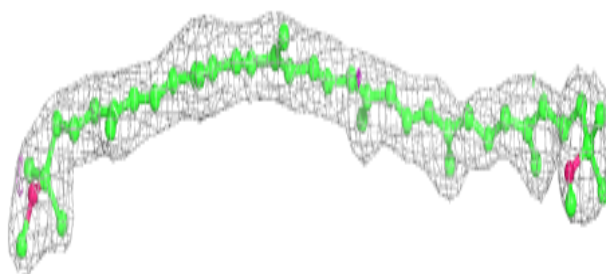
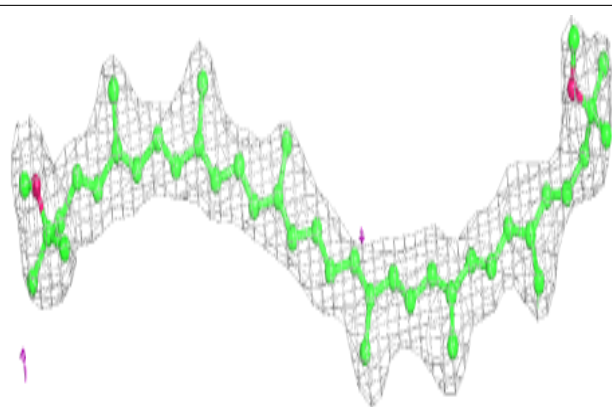
Electron density around PEF U 104:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

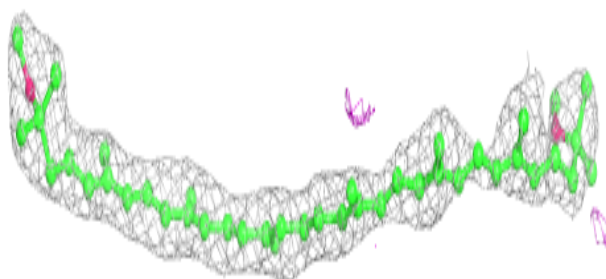
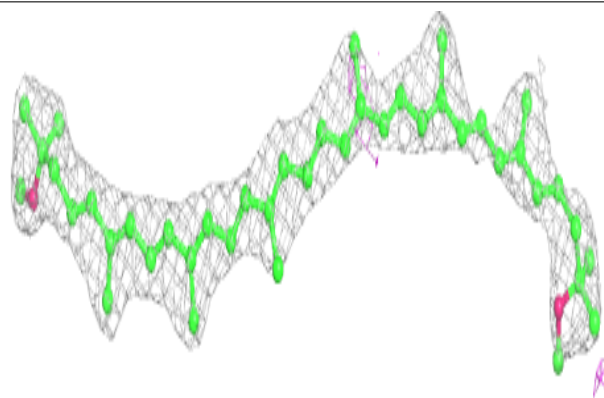


Electron density around CRT 6 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

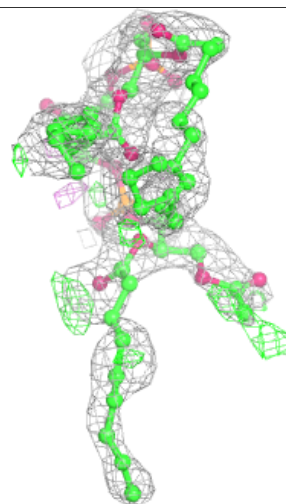
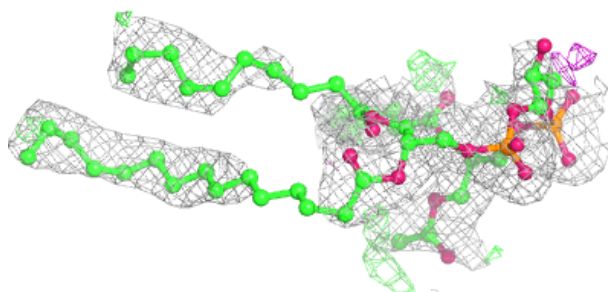
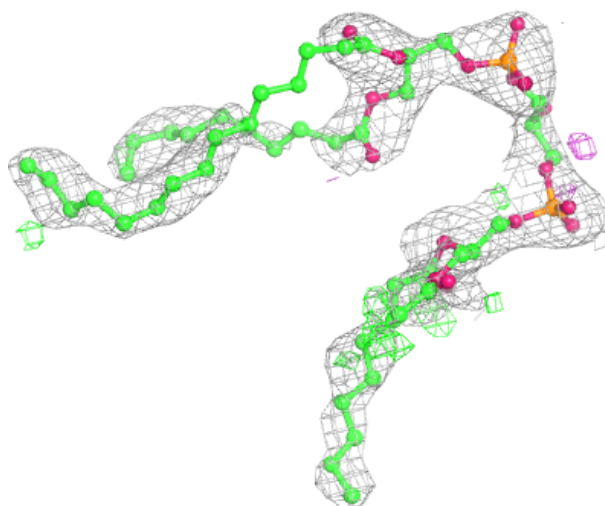
**Electron density around CRT A 104:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



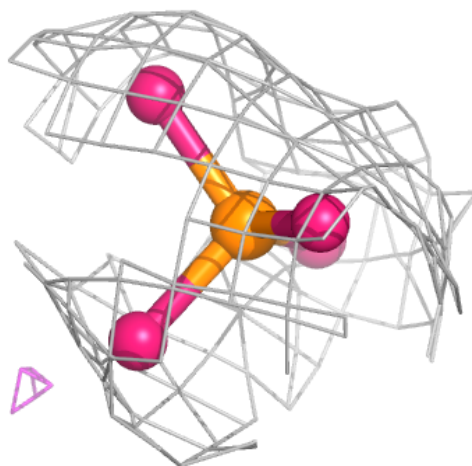
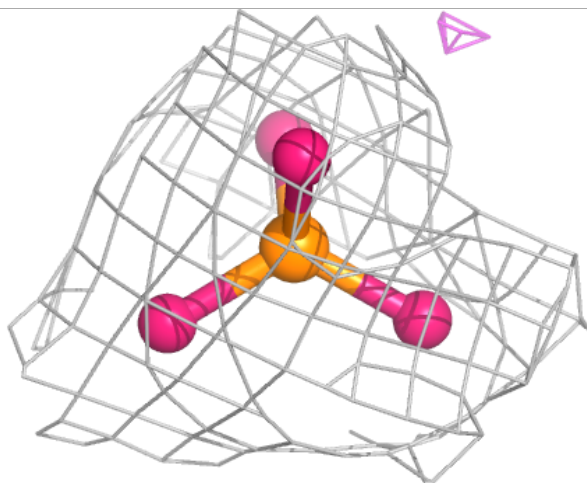
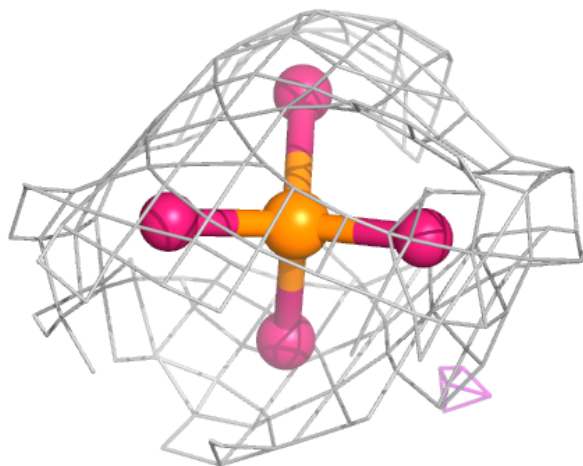
Electron density around CDL H 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



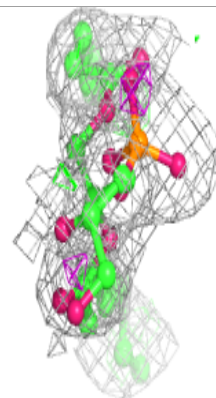
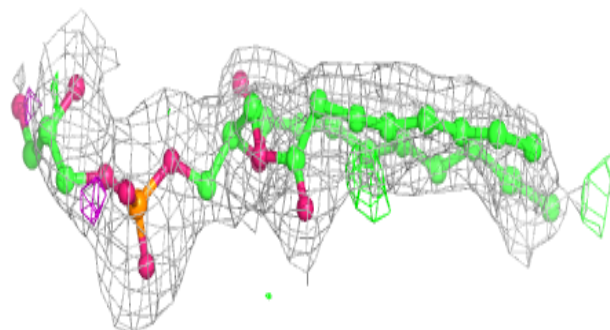
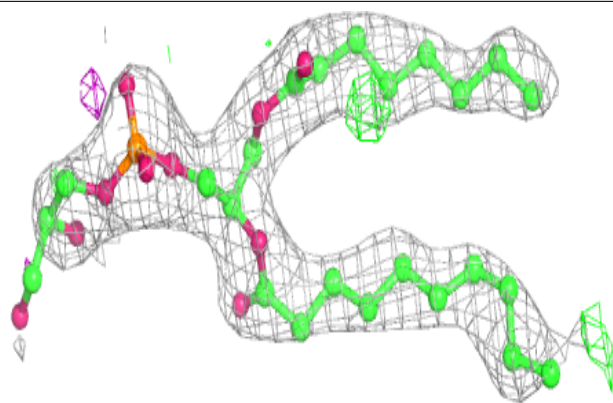
Electron density around PEF W 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

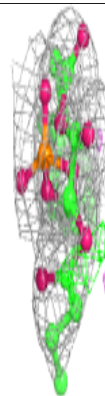
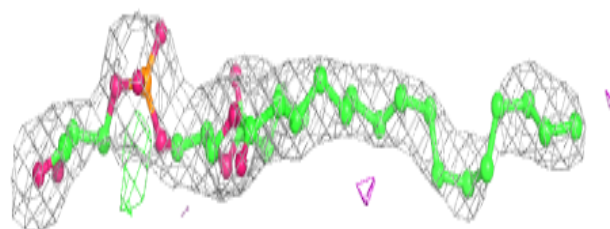
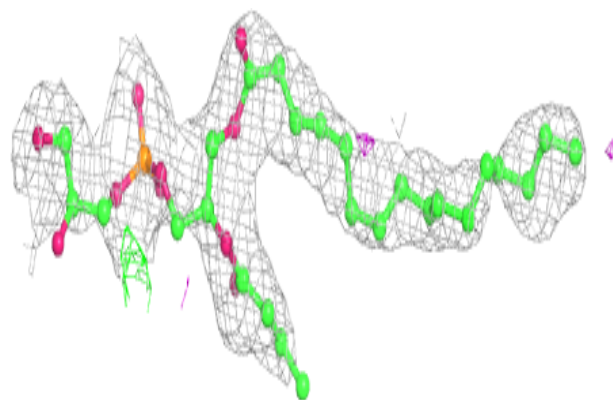


Electron density around PGV D 104:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

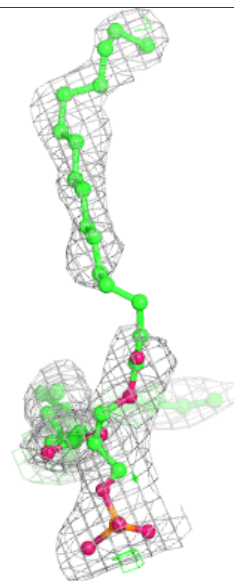
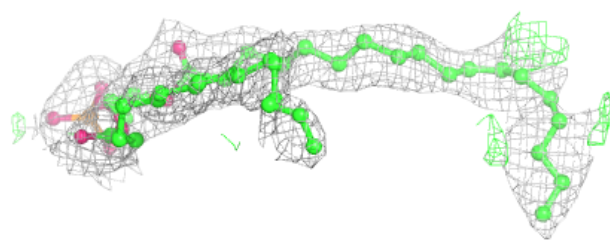
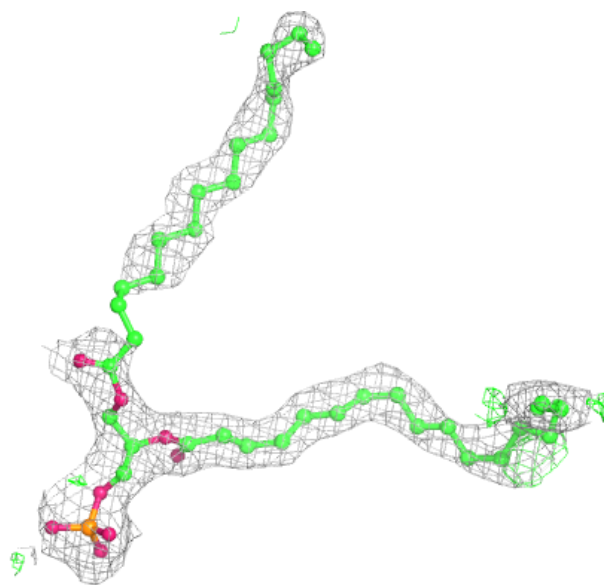
**Electron density around PGV M 414:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



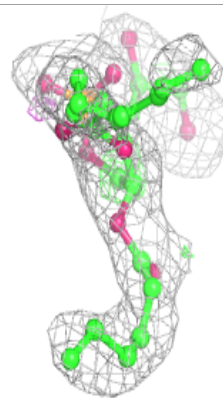
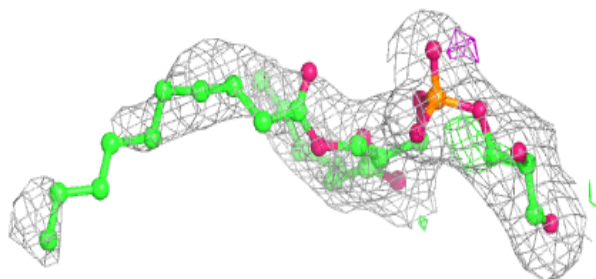
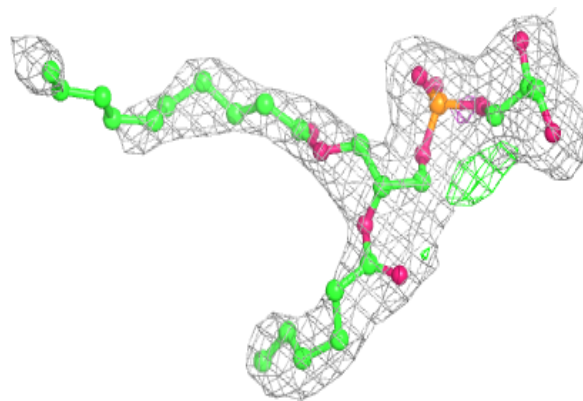
Electron density around PGV M 413:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

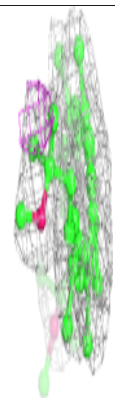
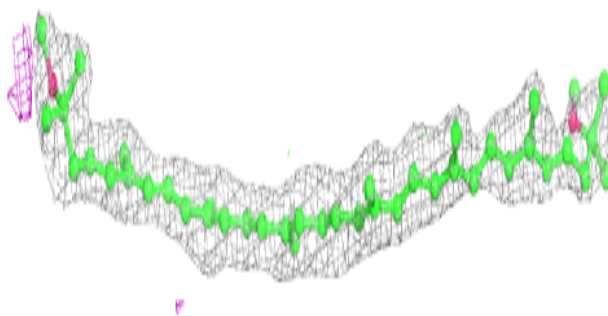
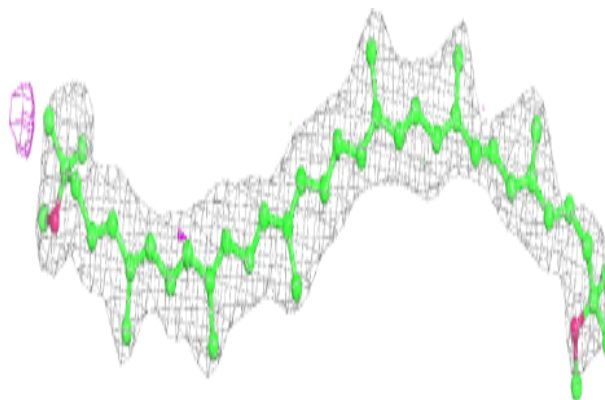


Electron density around PGV A 105:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

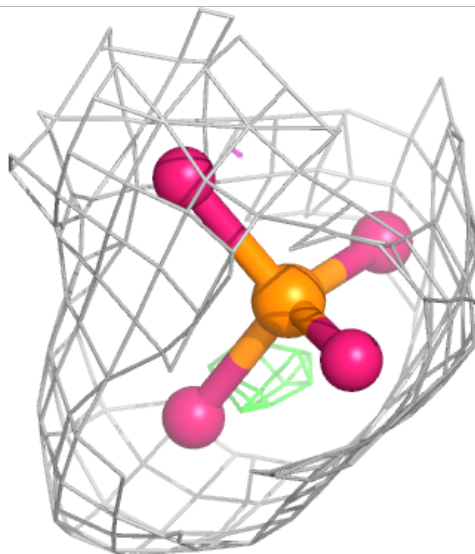
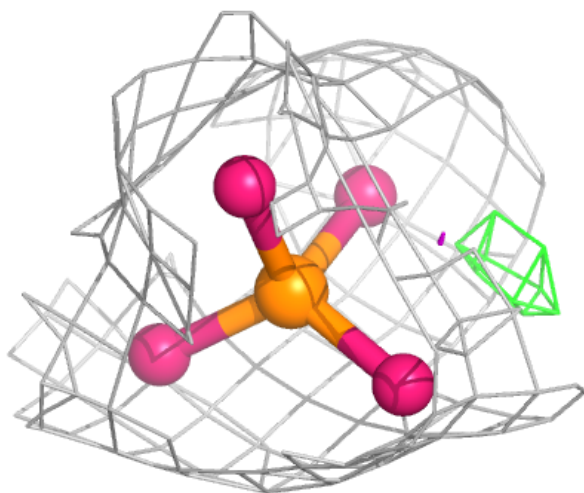
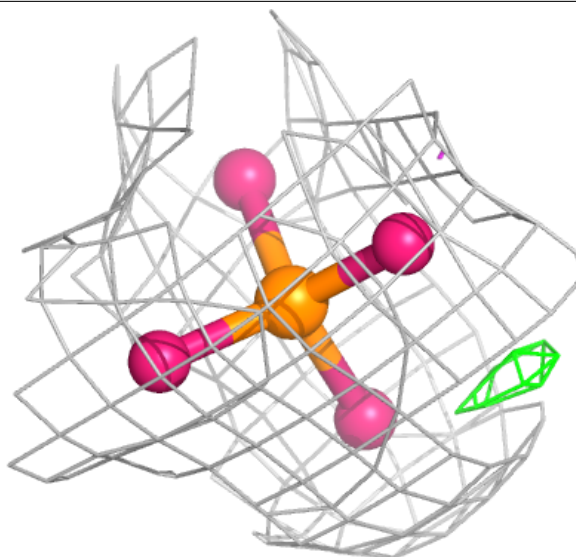
**Electron density around CRT 9 102:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



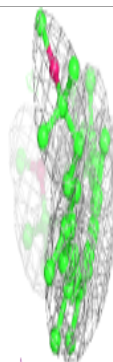
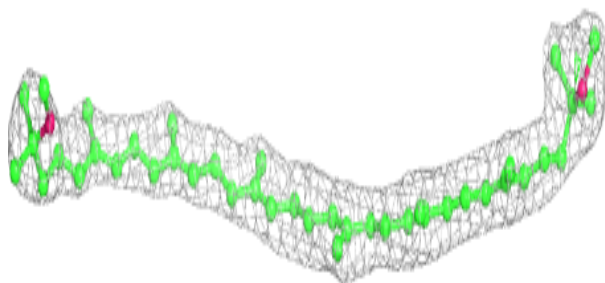
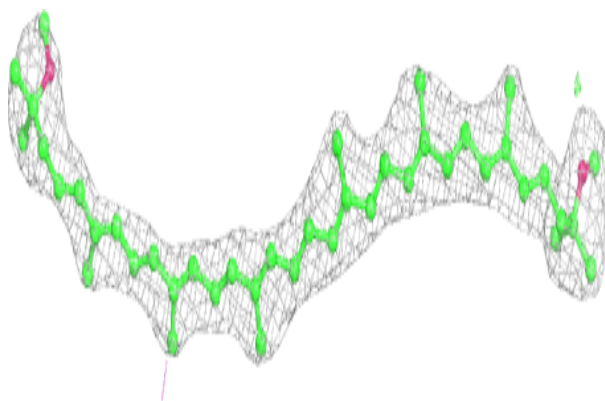
Electron density around PEF M 408:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

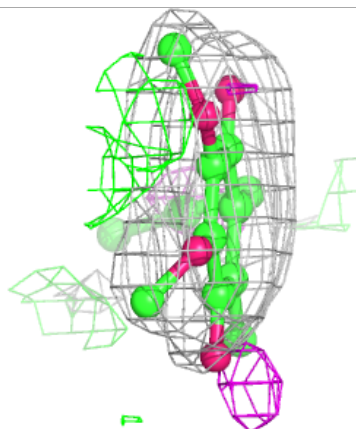
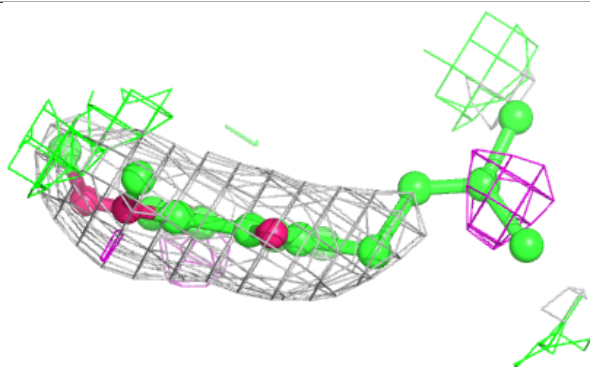
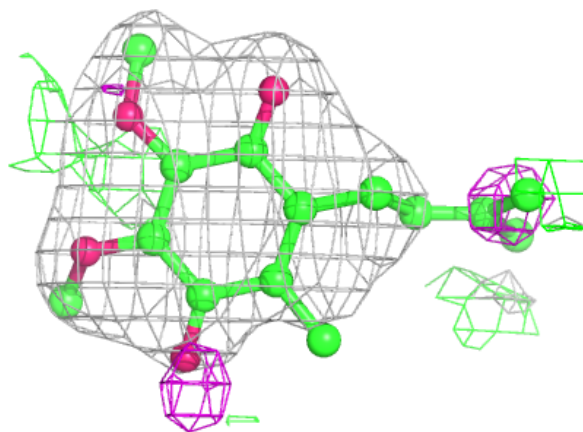


Electron density around CRT Z 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

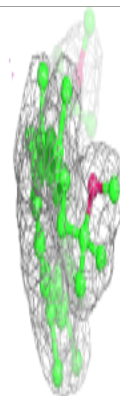
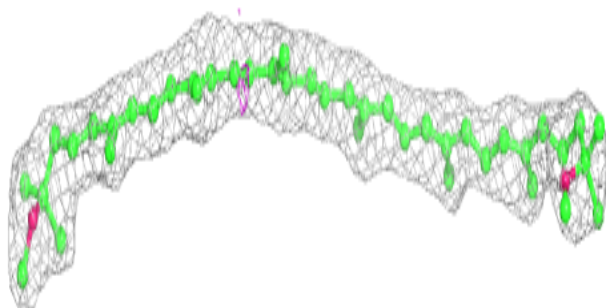
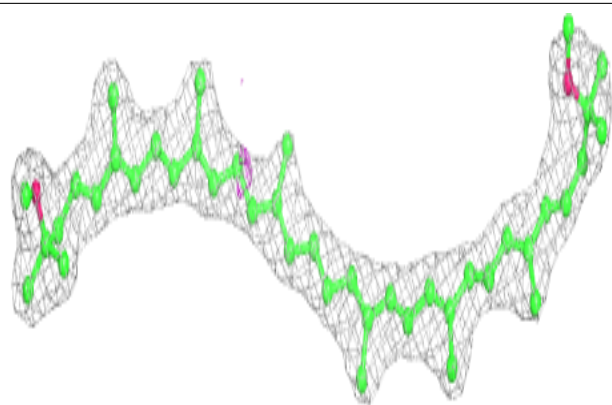
**Electron density around UQ8 M 417:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

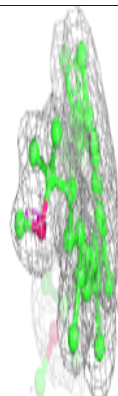
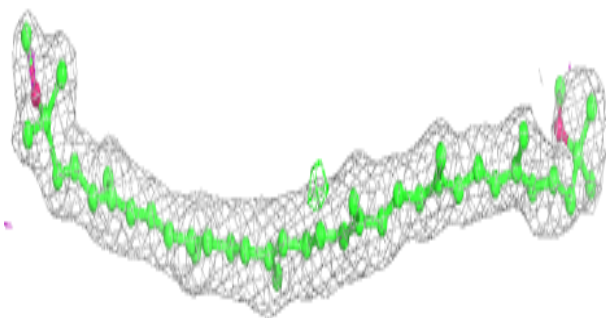
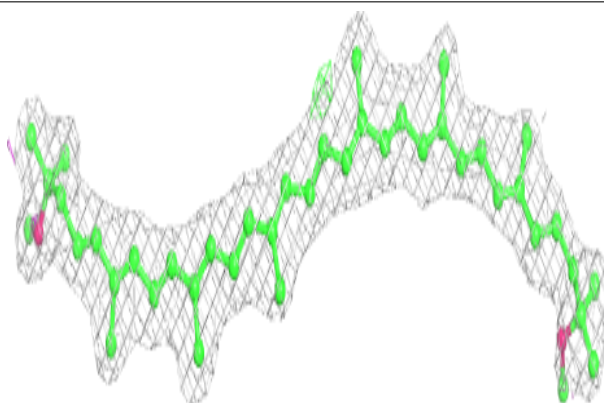


Electron density around CRT V 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

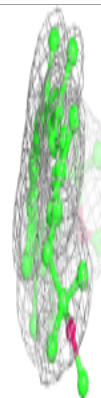
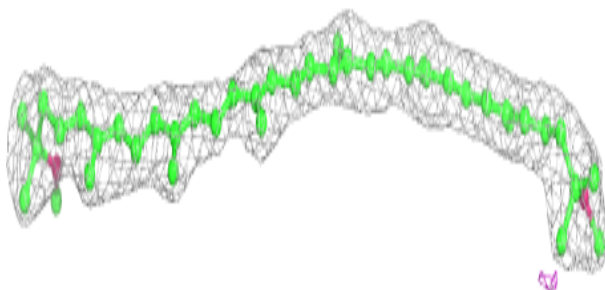
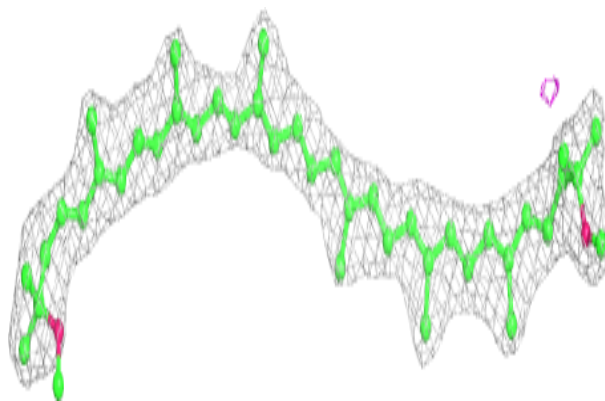
**Electron density around CRT O 103:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

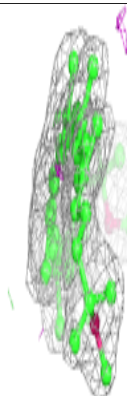
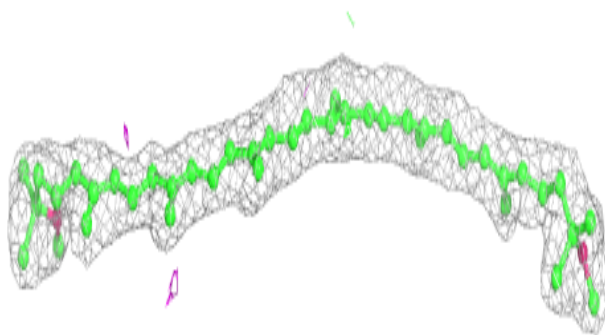
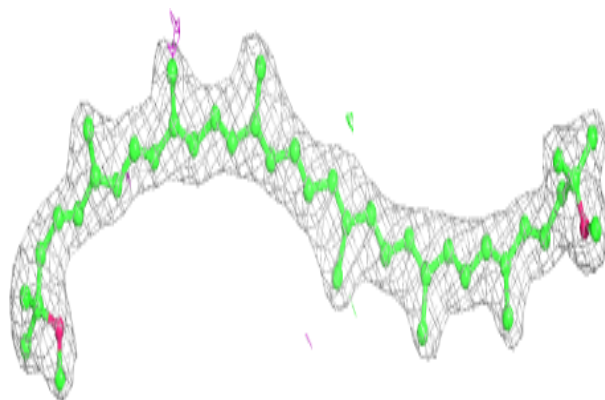


Electron density around CRT N 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

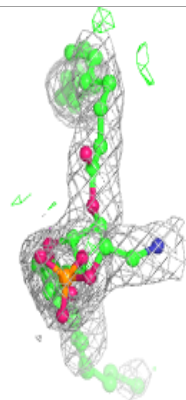
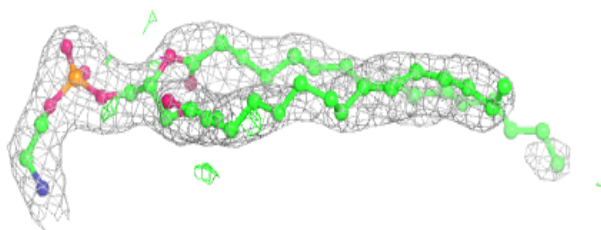
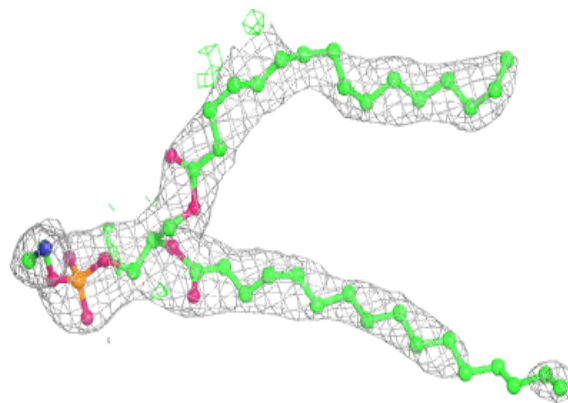
**Electron density around CRT Q 103:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



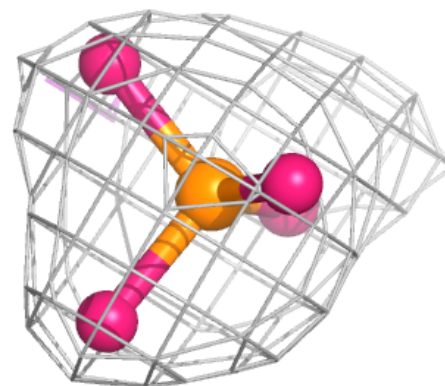
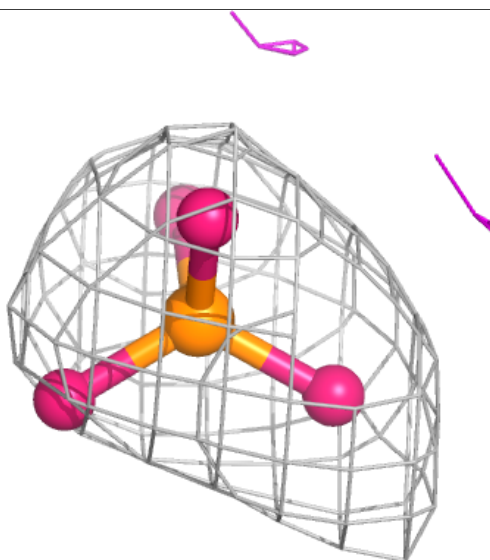
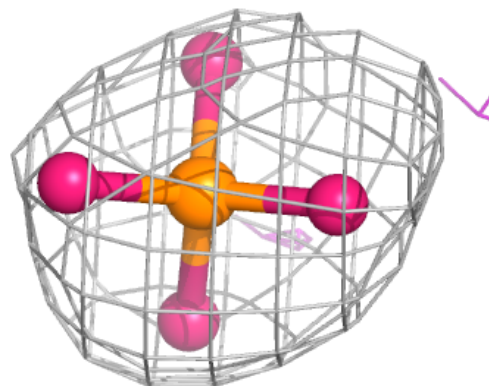
Electron density around PEF M 418:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



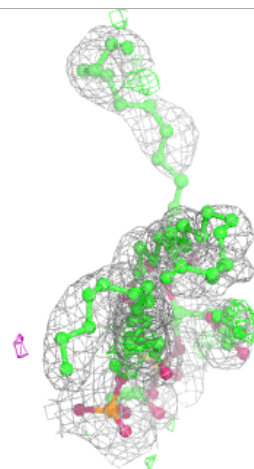
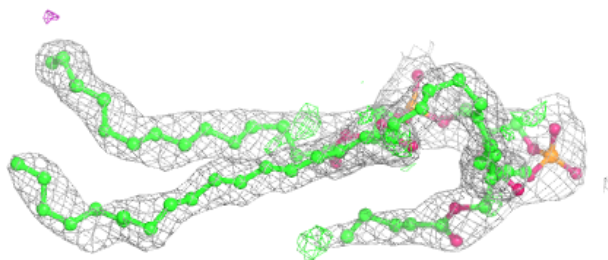
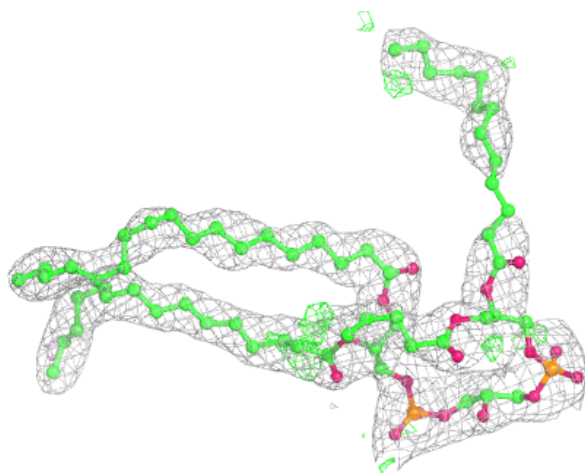
Electron density around PEF I 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



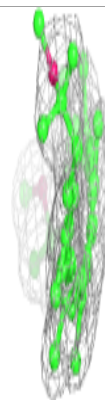
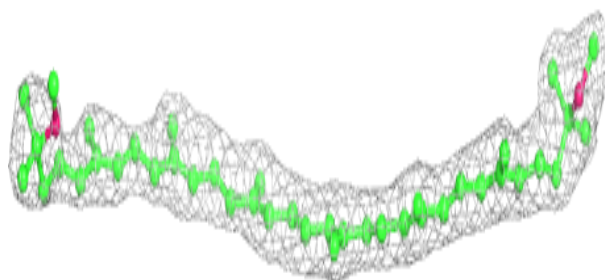
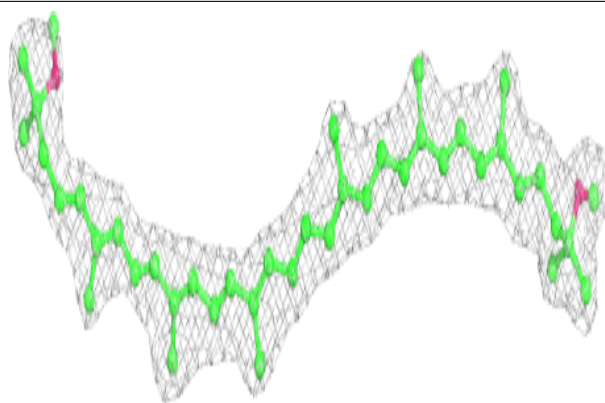
Electron density around CDL H 304:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

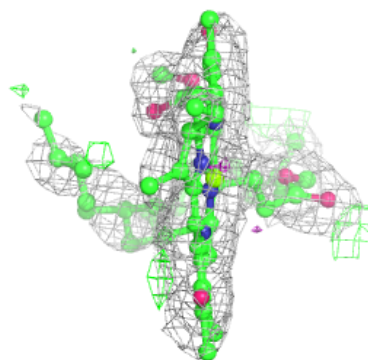
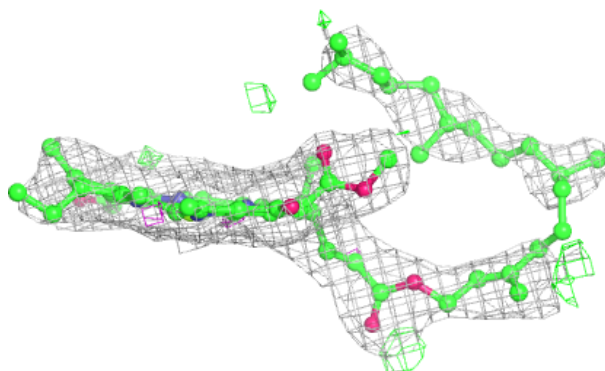
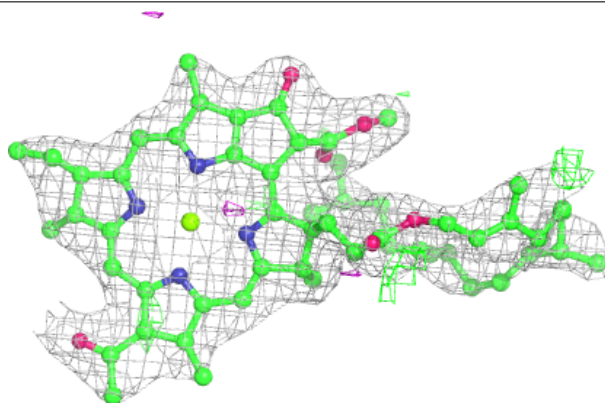


Electron density around CRT P 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

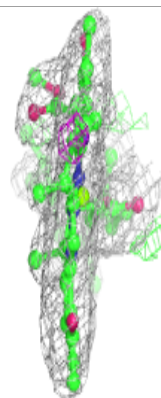
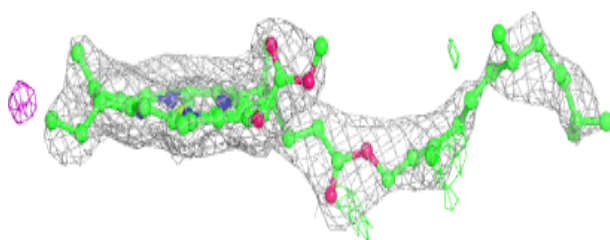
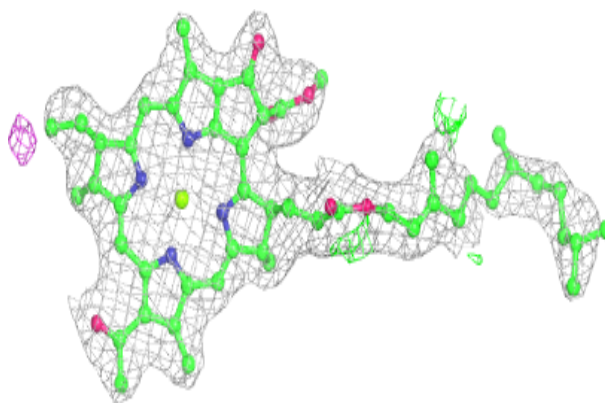
**Electron density around BCL 3 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

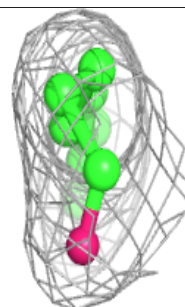
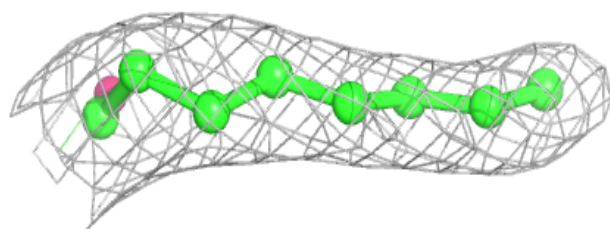
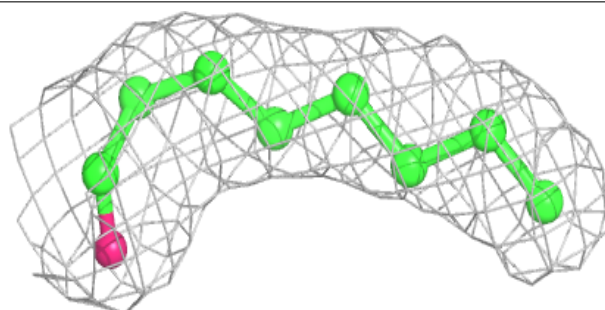


Electron density around BCL 7 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

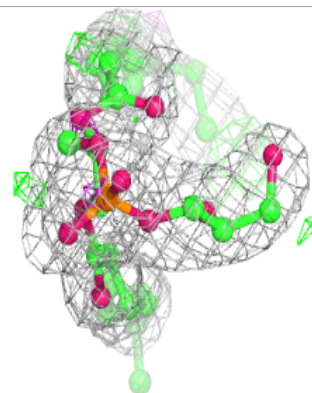
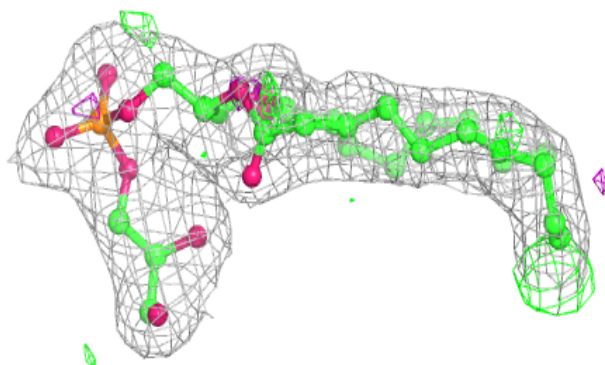
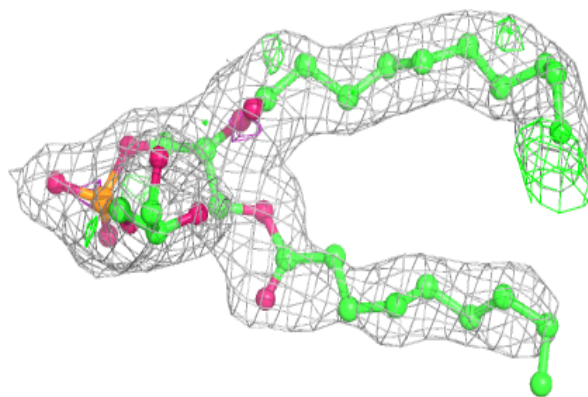
**Electron density around LHG C 508:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

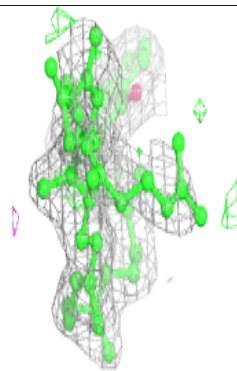
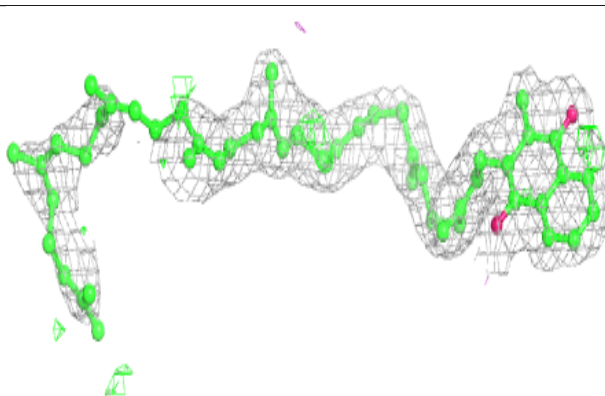
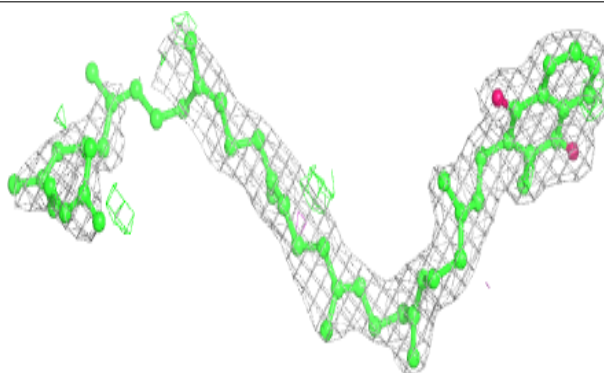


Electron density around PGV H 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

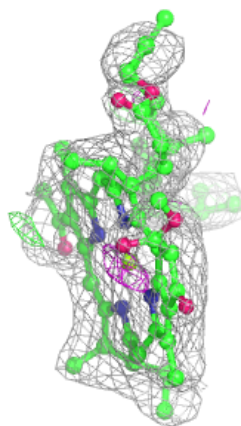
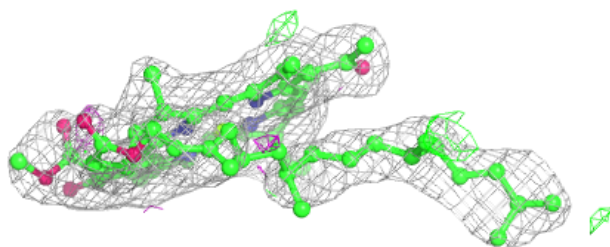
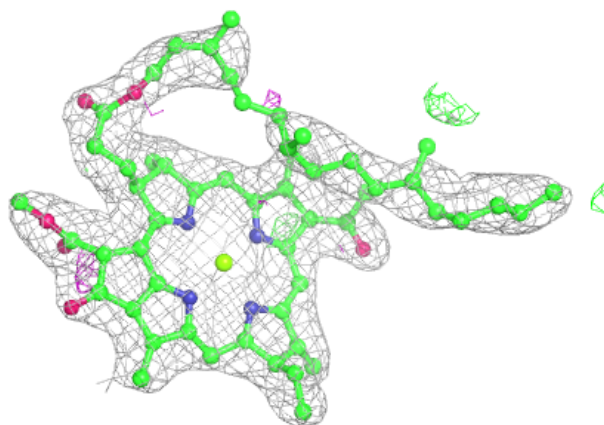
**Electron density around MQ8 M 405:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

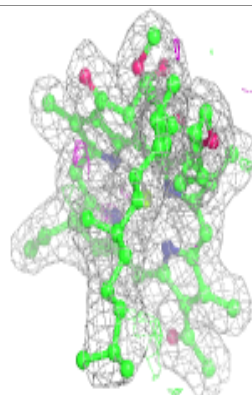
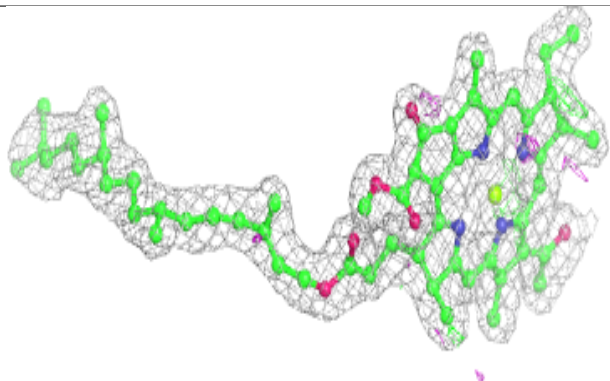
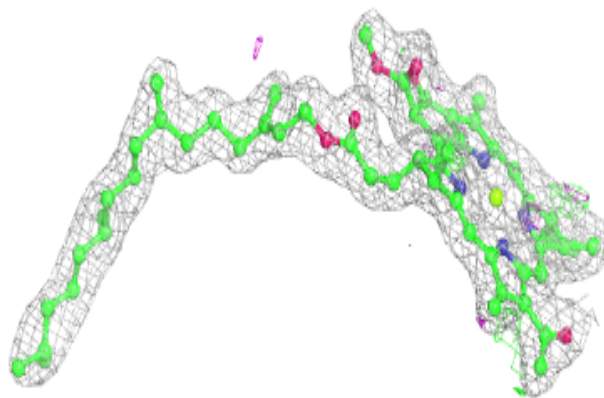


Electron density around BCL 1 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

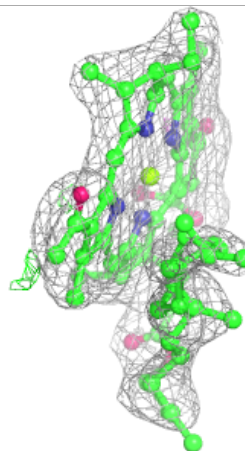
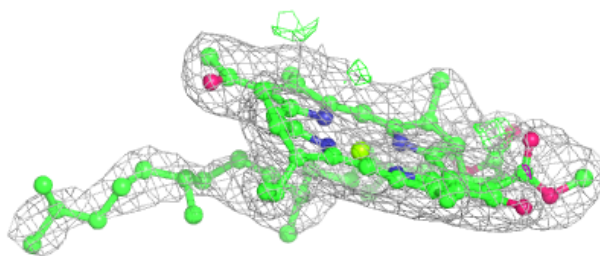
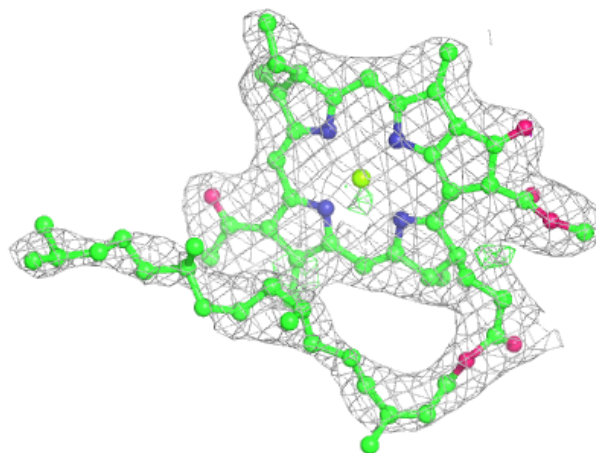
**Electron density around BCL L 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



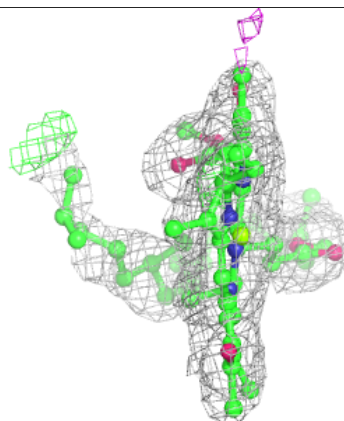
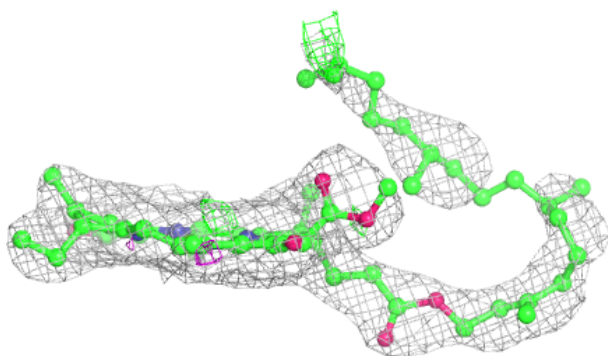
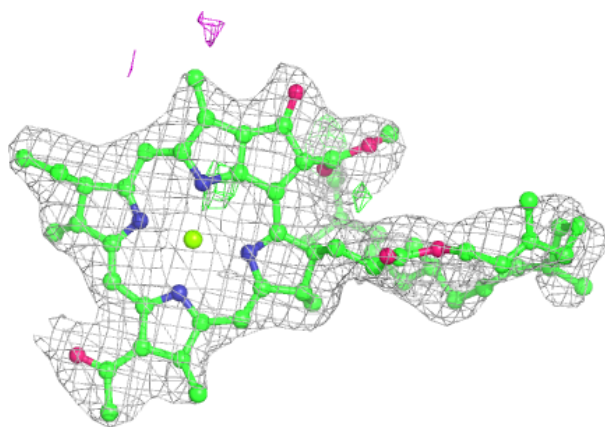
Electron density around BCL Z 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



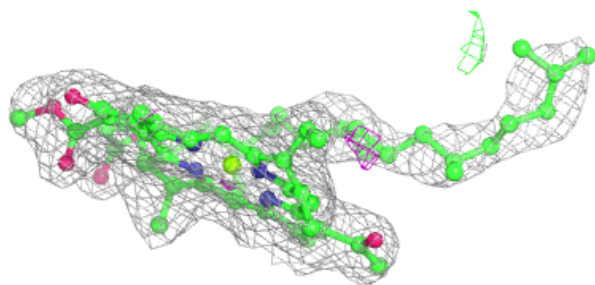
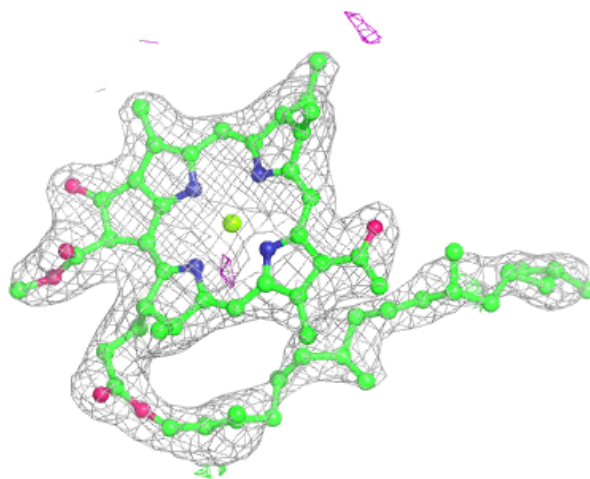
Electron density around BCL 5 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



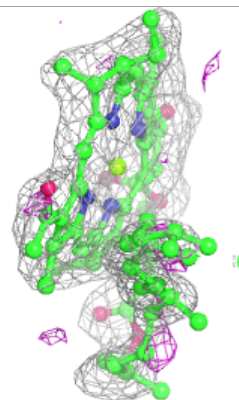
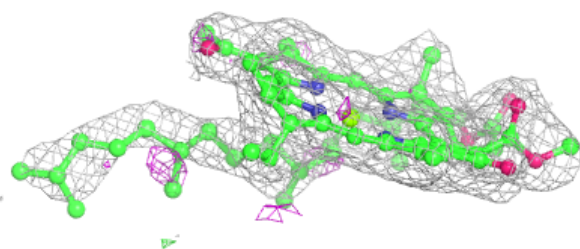
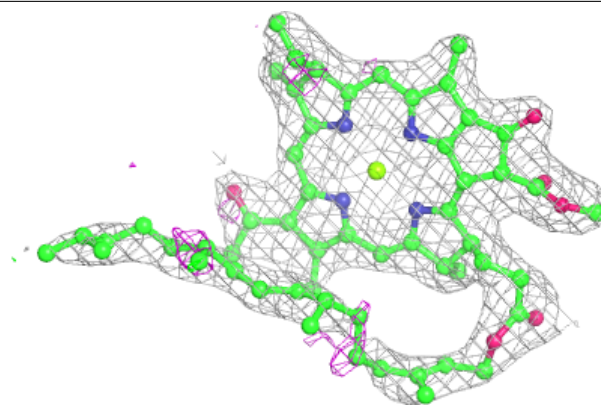
Electron density around BCL 3 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

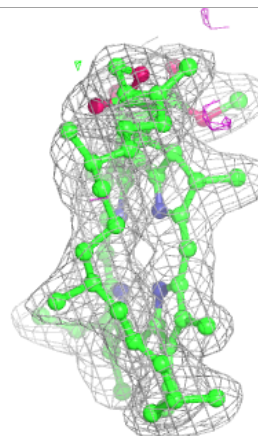
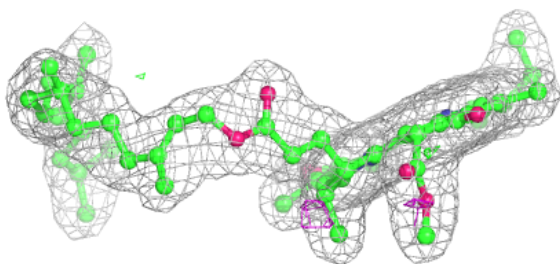
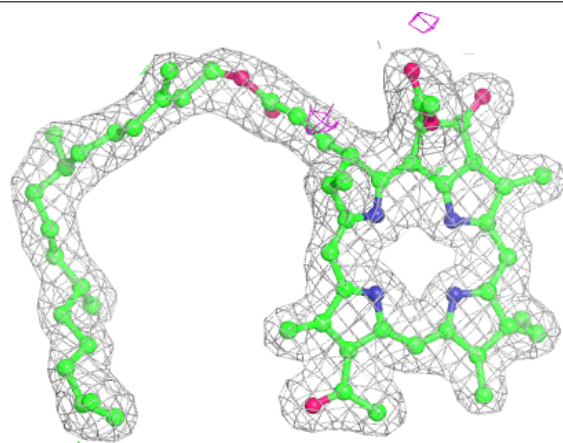


Electron density around BCL 5 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

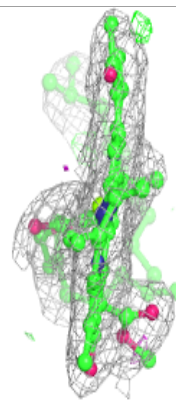
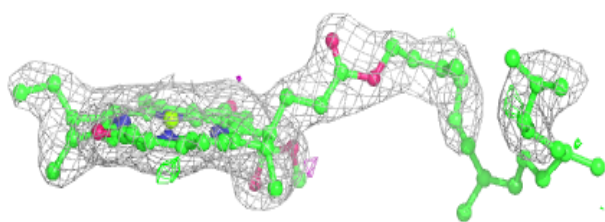
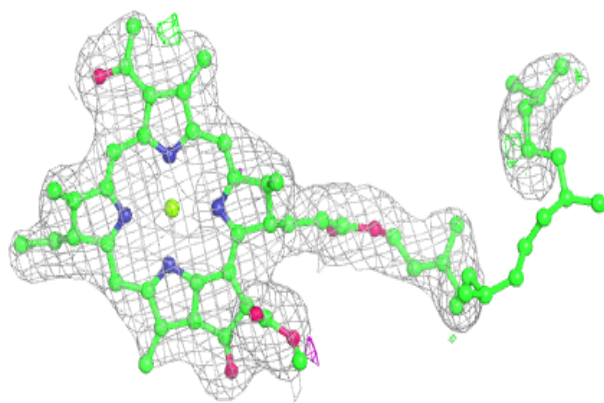
**Electron density around BPH L 302:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



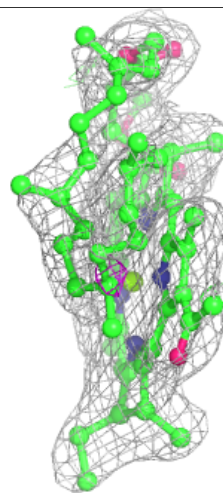
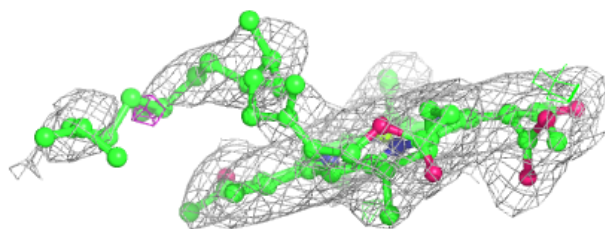
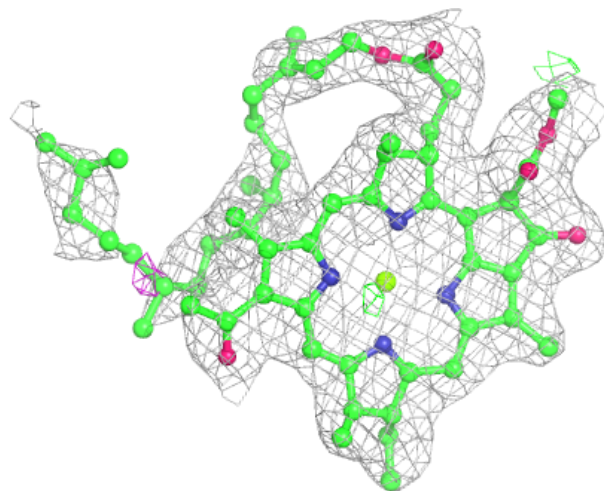
Electron density around BCL 9 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



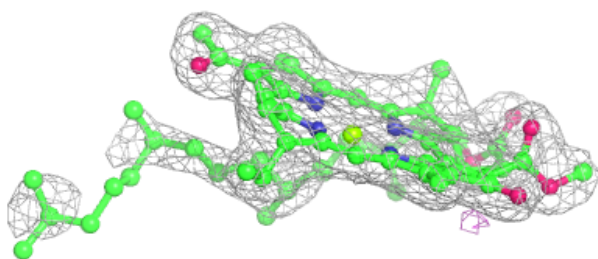
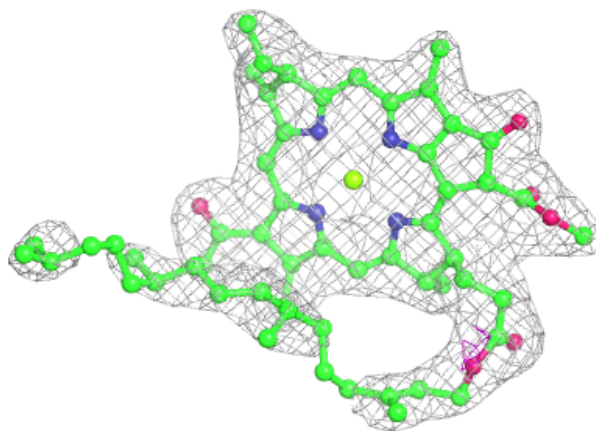
Electron density around BCL 7 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



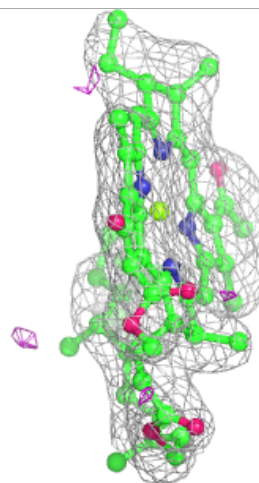
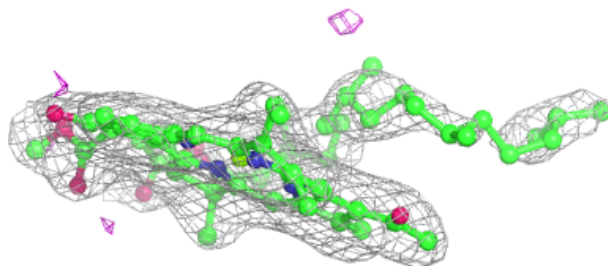
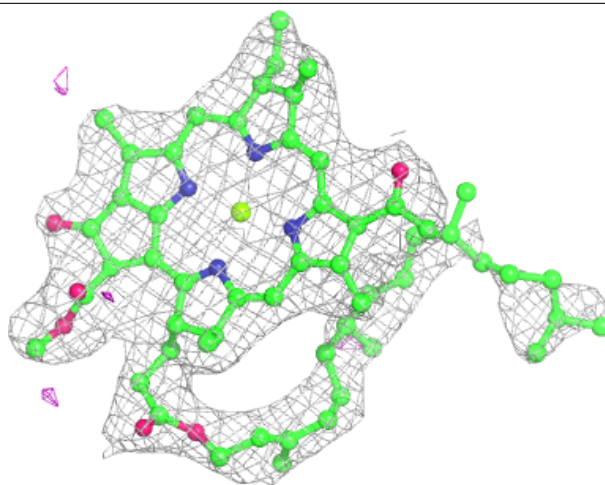
Electron density around BCL K 102:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



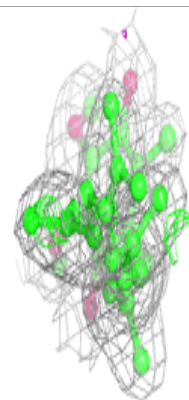
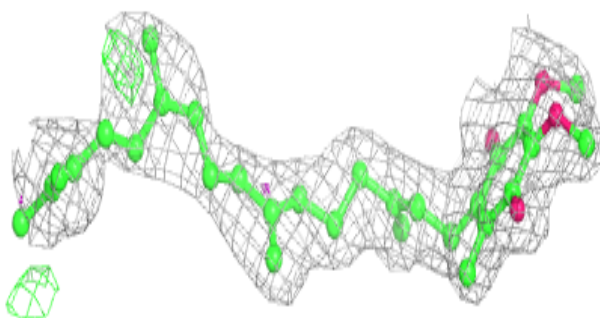
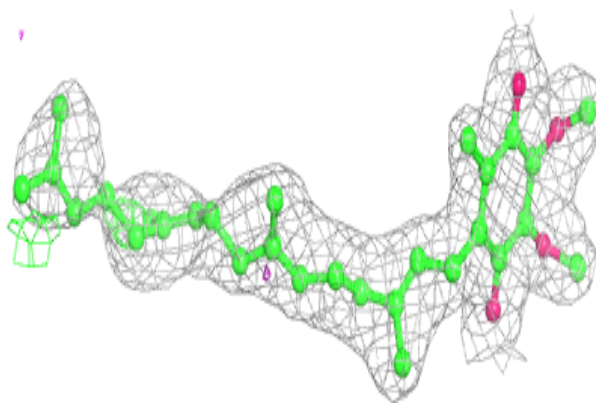
Electron density around BCL F 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

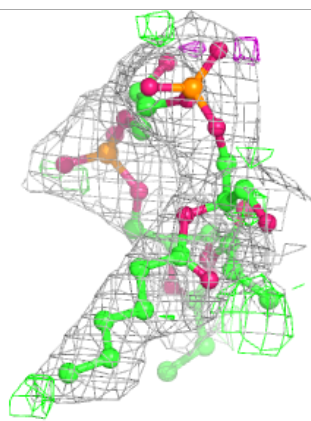
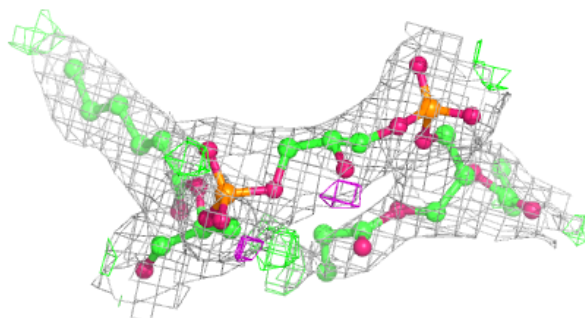
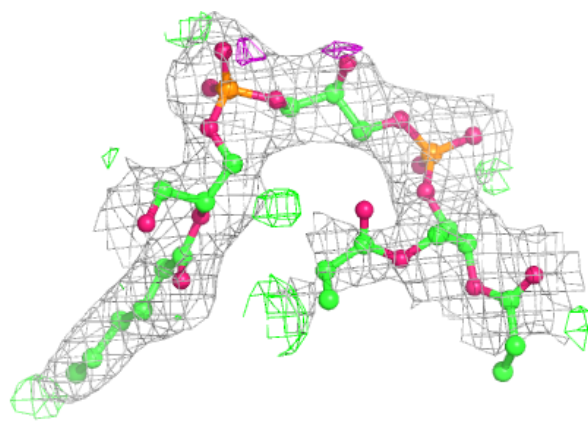


Electron density around UQ8 L 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

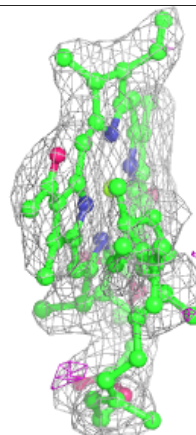
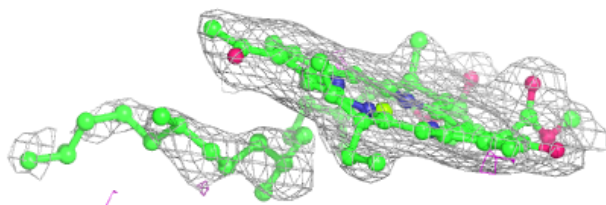
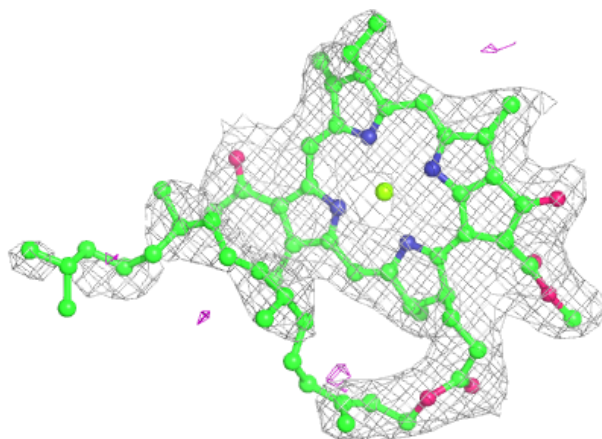
**Electron density around CDL M 415:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

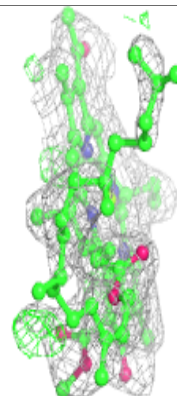
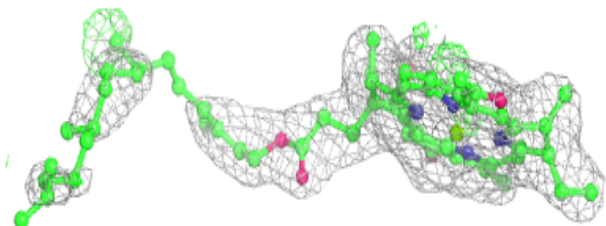
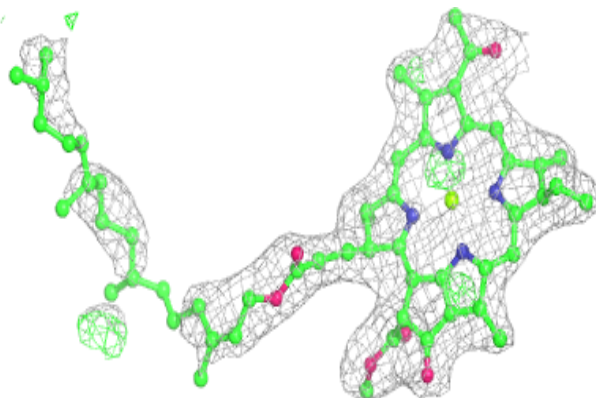


Electron density around BCL A 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

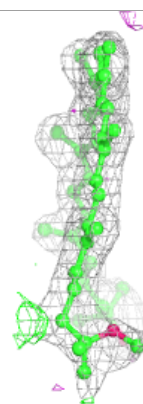
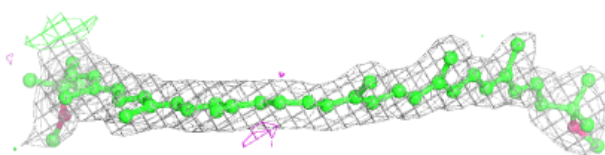
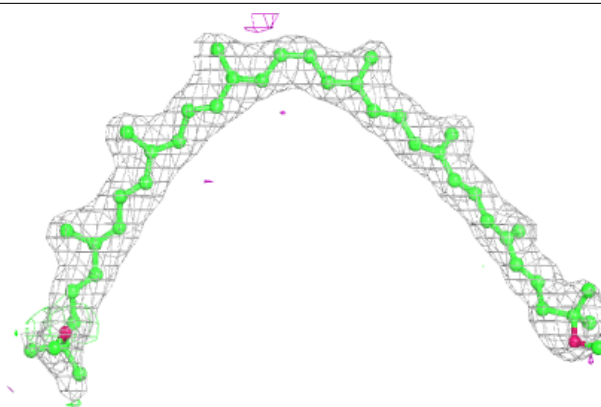
**Electron density around BCL 1 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



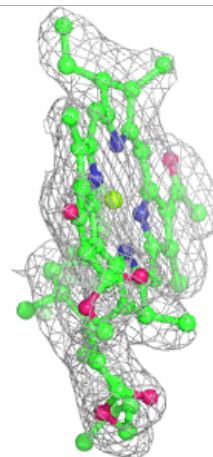
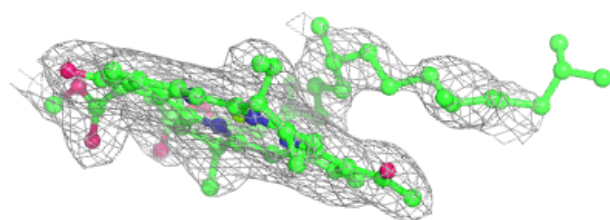
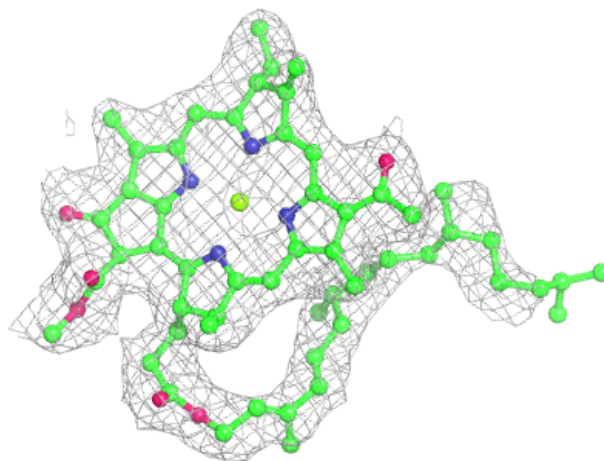
Electron density around CRT M 406:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



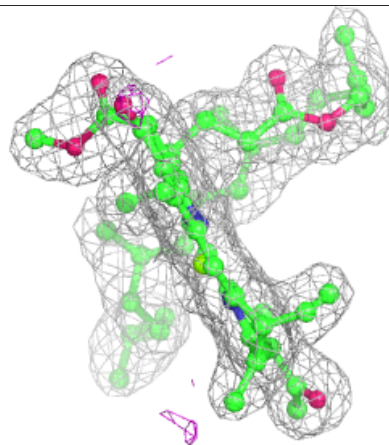
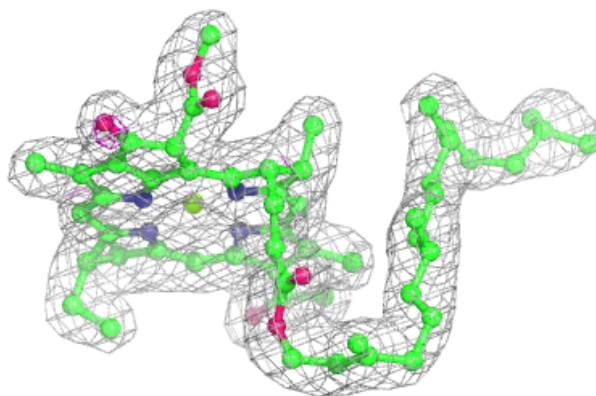
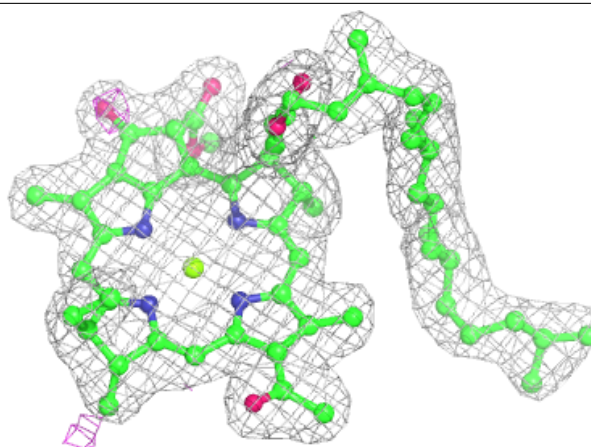
Electron density around BCL 0 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



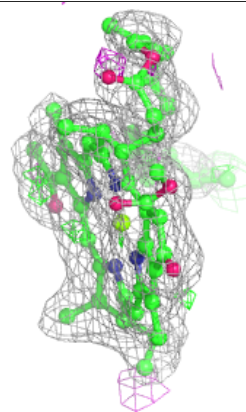
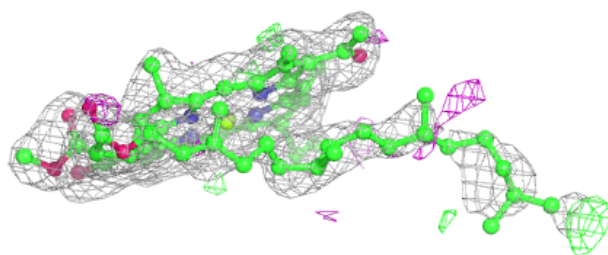
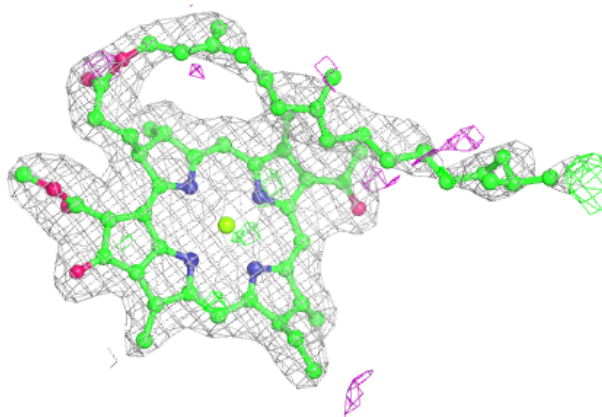
Electron density around BCL M 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



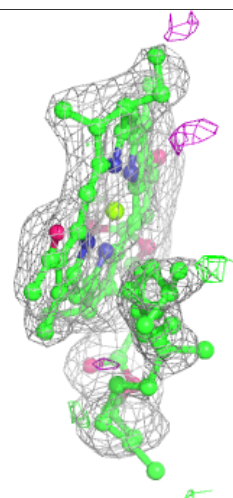
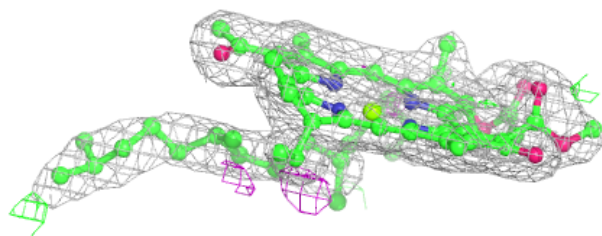
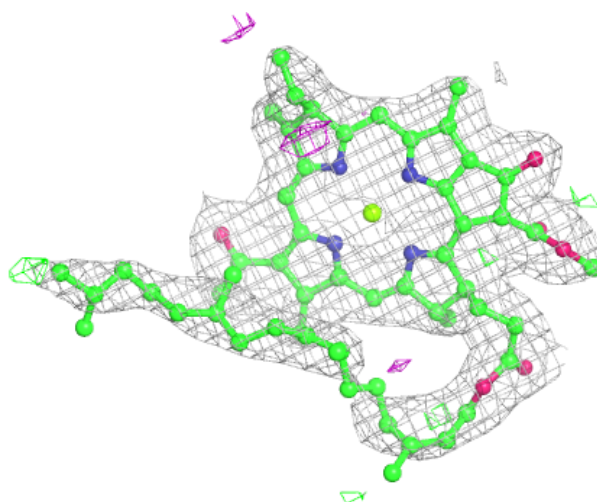
Electron density around BCL O 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



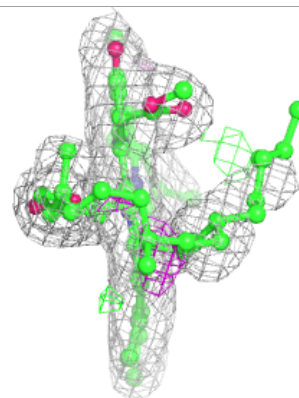
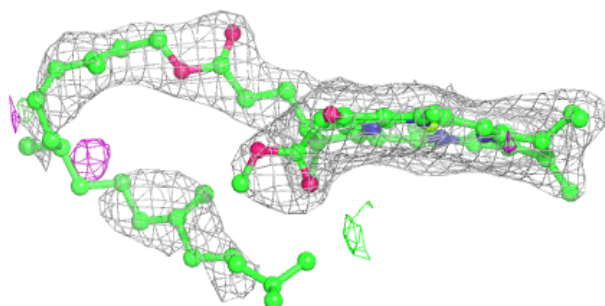
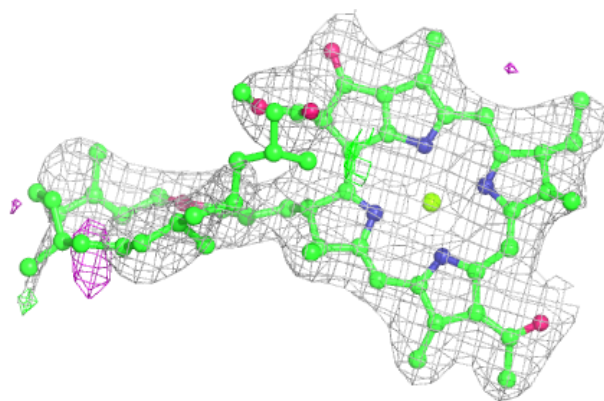
Electron density around BCL U 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



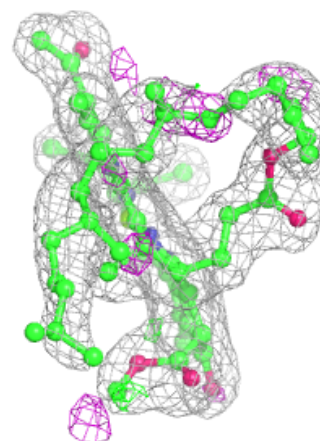
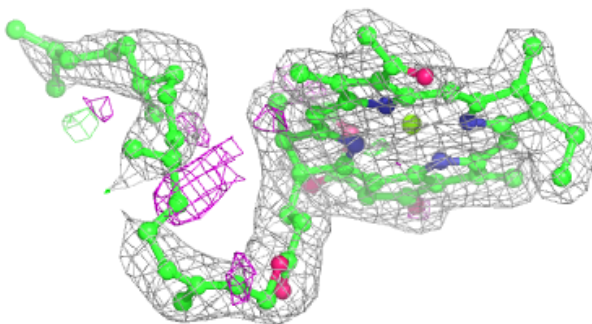
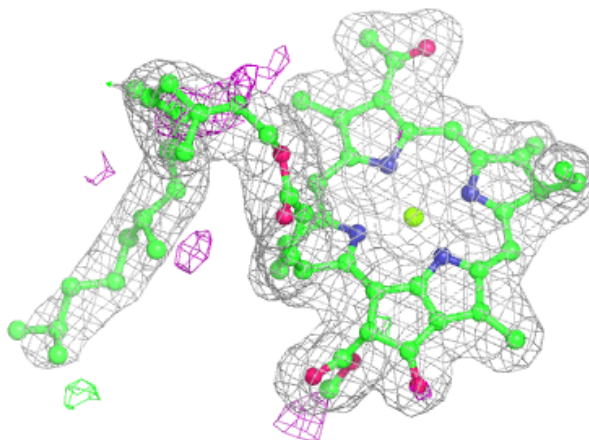
Electron density around BCL W 101:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



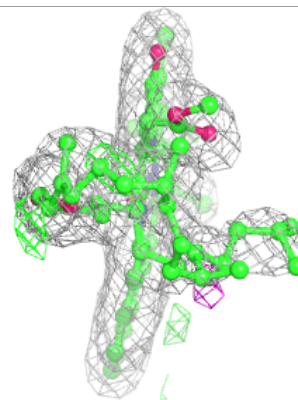
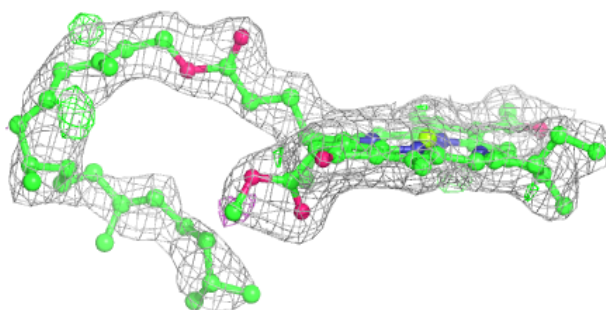
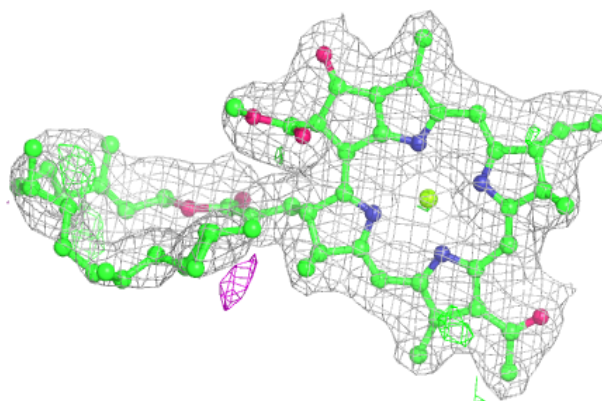
Electron density around BCL M 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

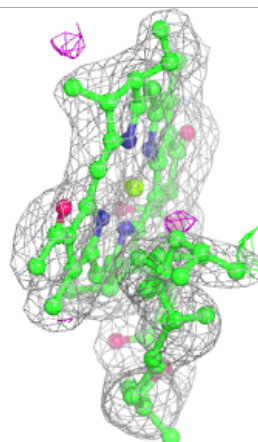
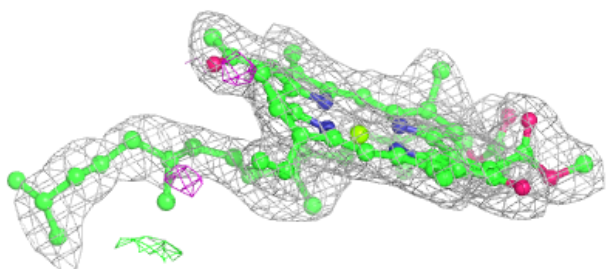
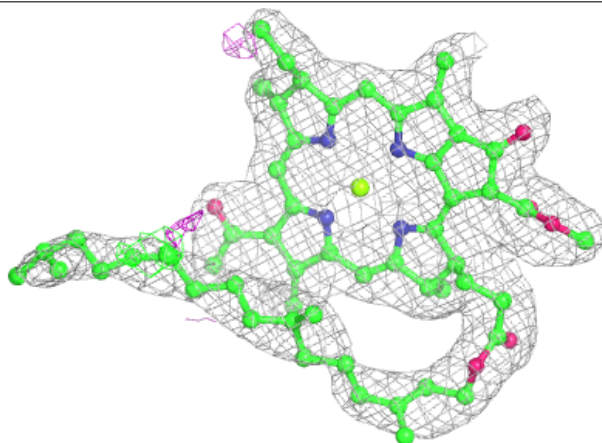


Electron density around BCL Q 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

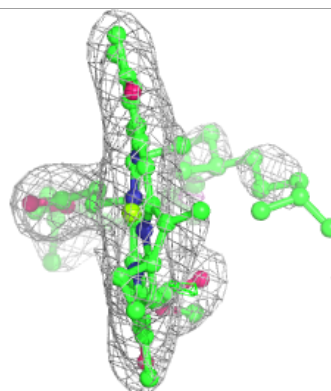
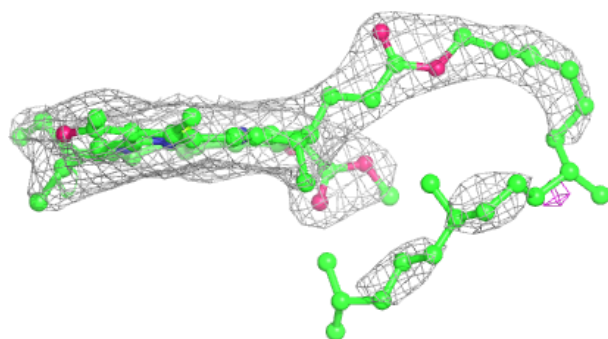
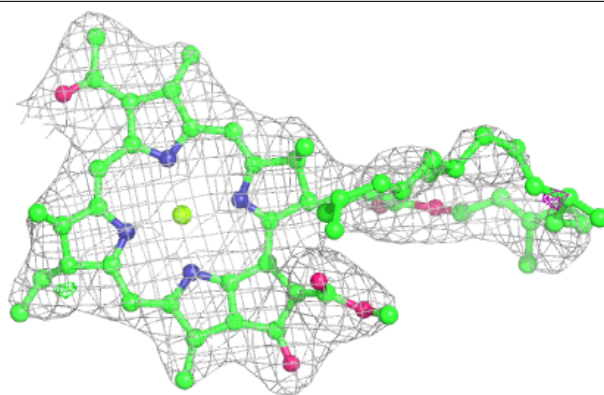
**Electron density around BCL Q 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

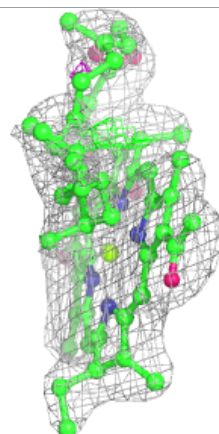
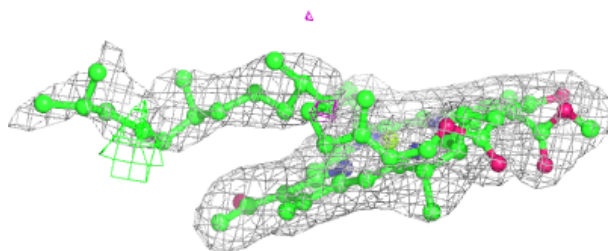
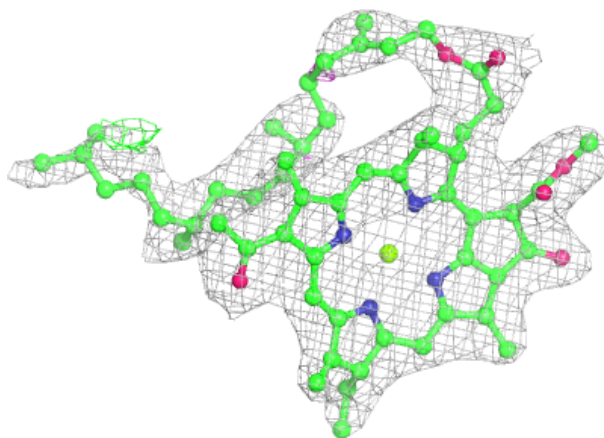


Electron density around BCL I 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

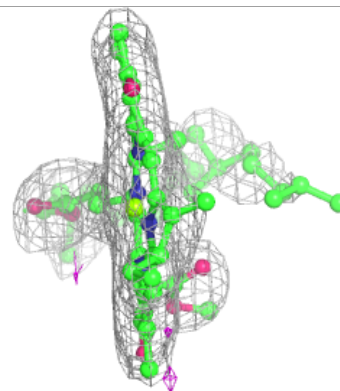
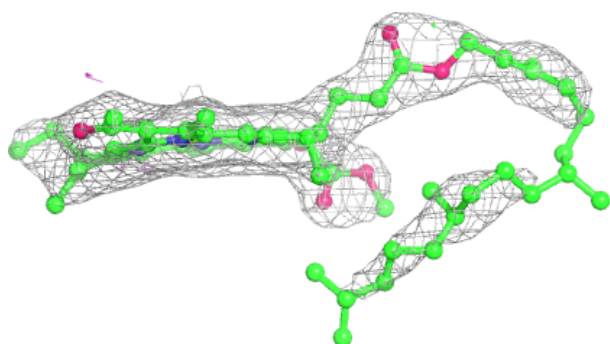
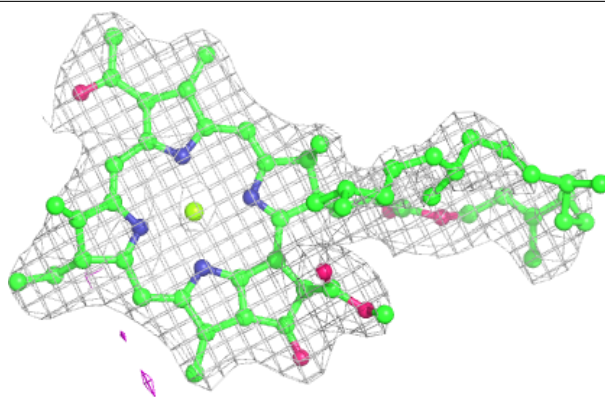
**Electron density around BCL W 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

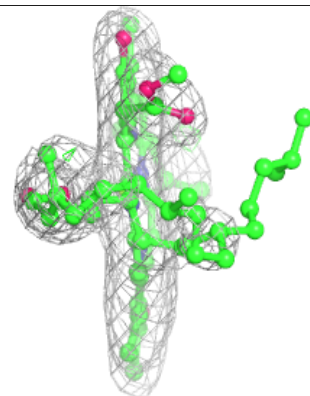
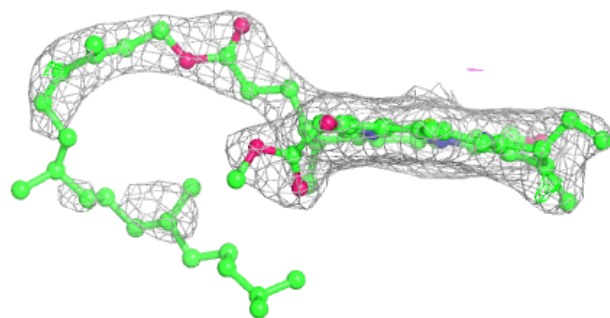
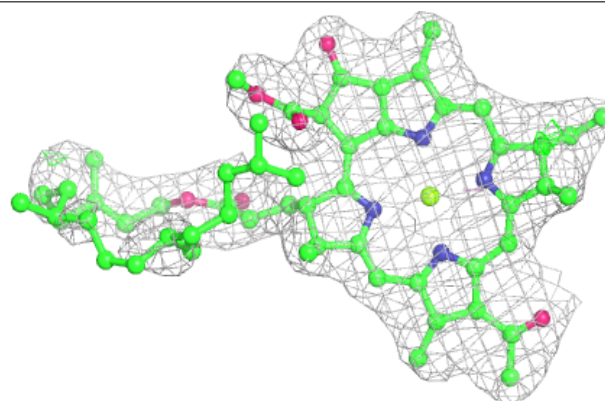


Electron density around BCL A 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

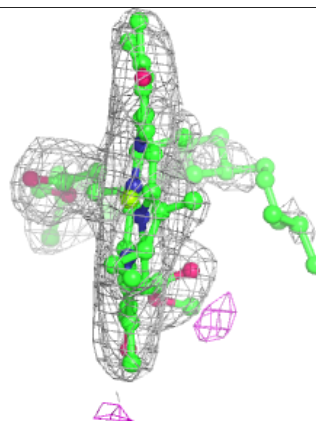
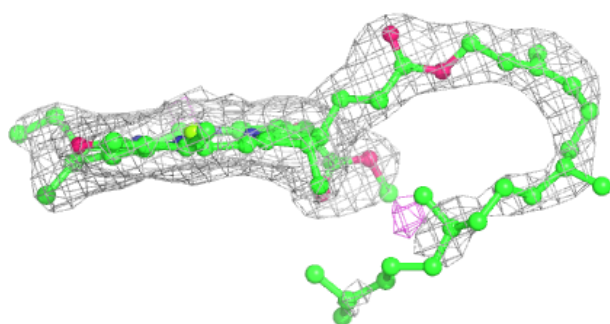
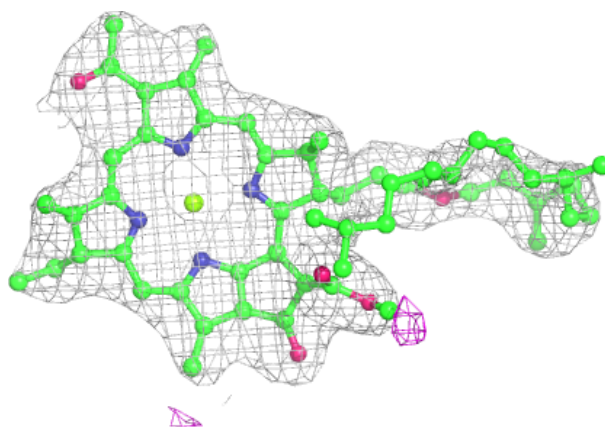
**Electron density around BCL F 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

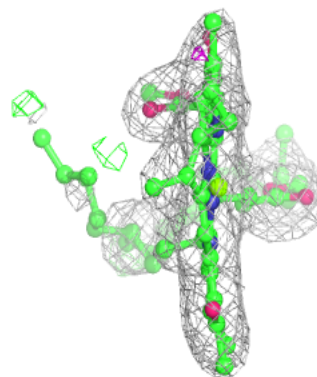
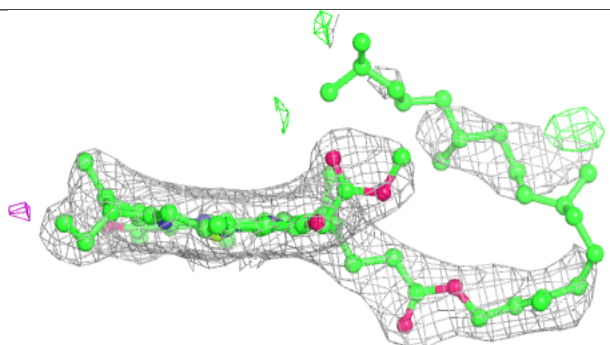
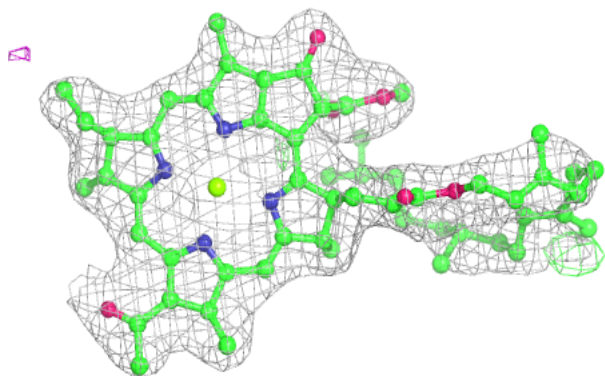


Electron density around BCL K 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

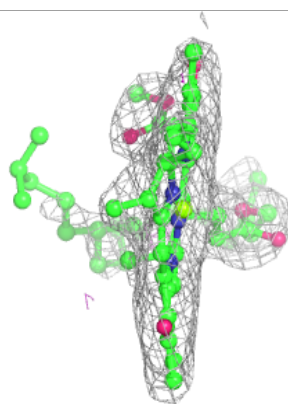
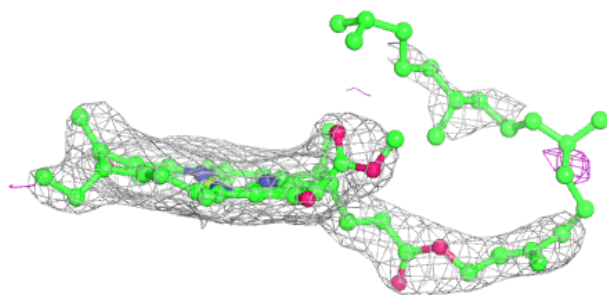
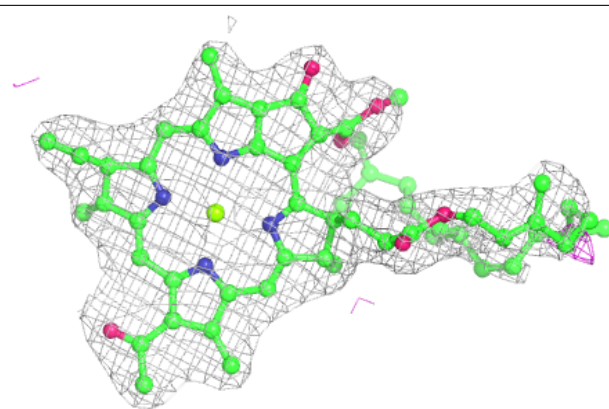
**Electron density around BCL Y 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

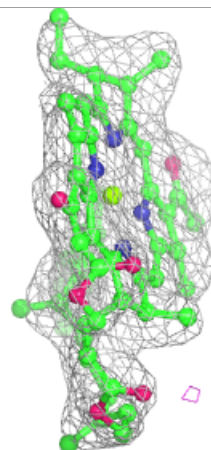
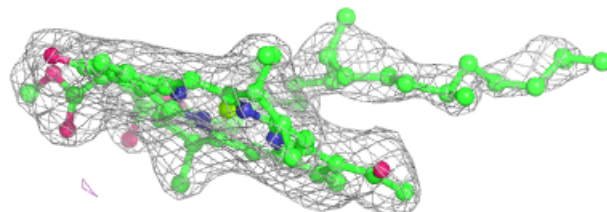
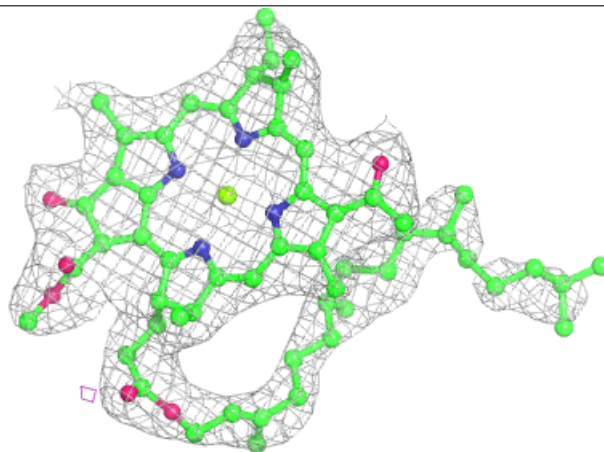


Electron density around BCL D 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

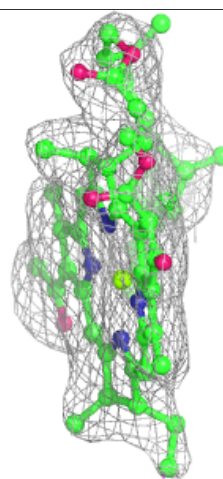
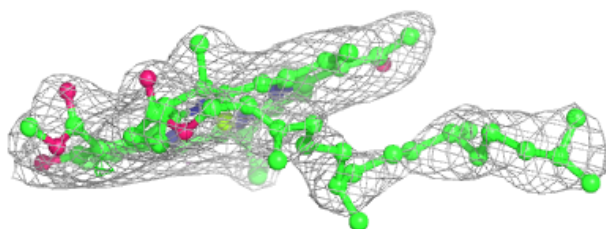
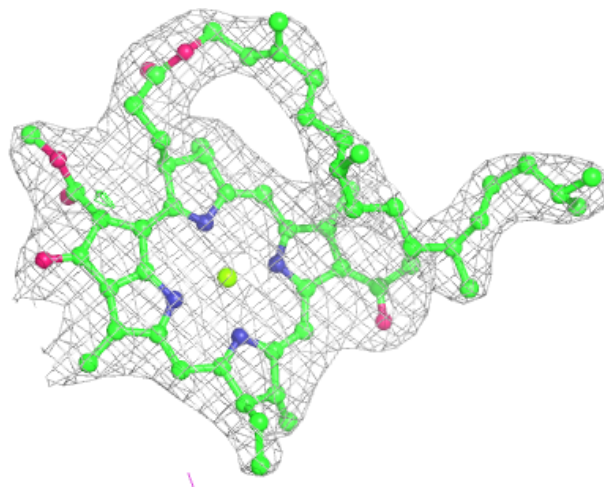
**Electron density around BCL I 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



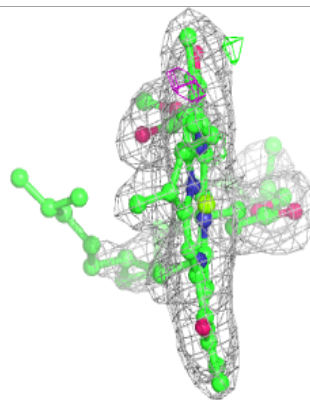
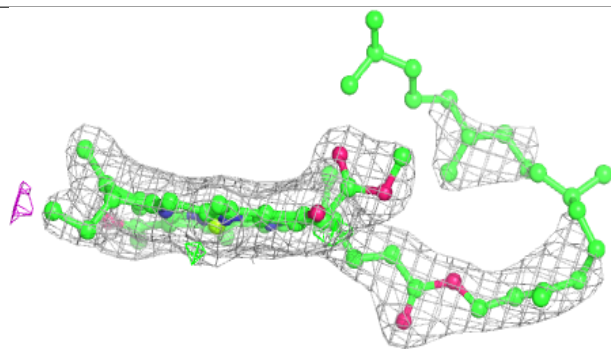
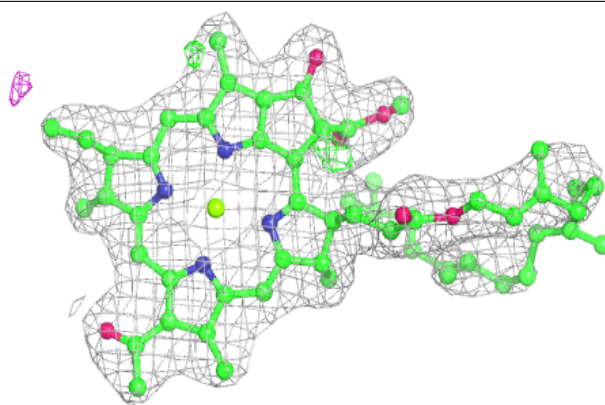
Electron density around BCL D 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

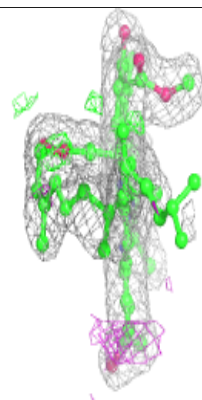
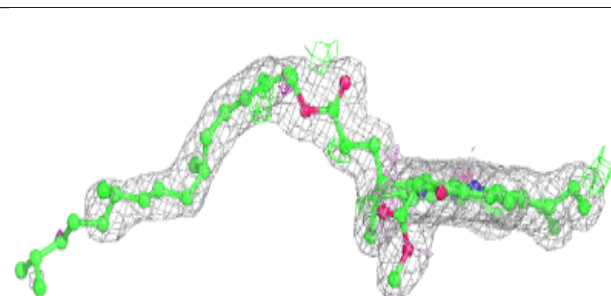
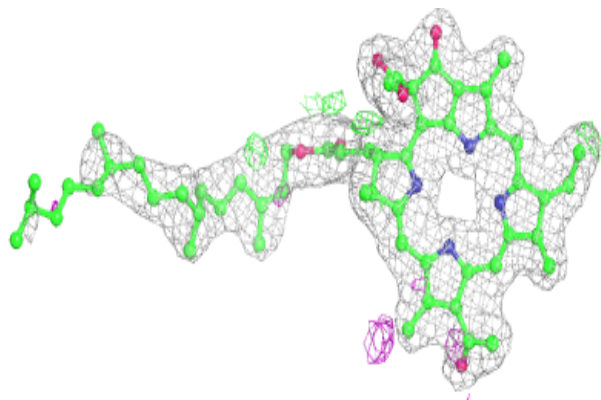


Electron density around BCL O 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

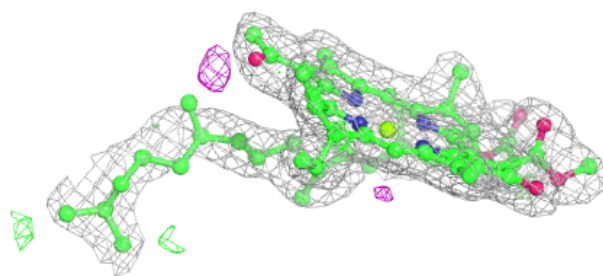
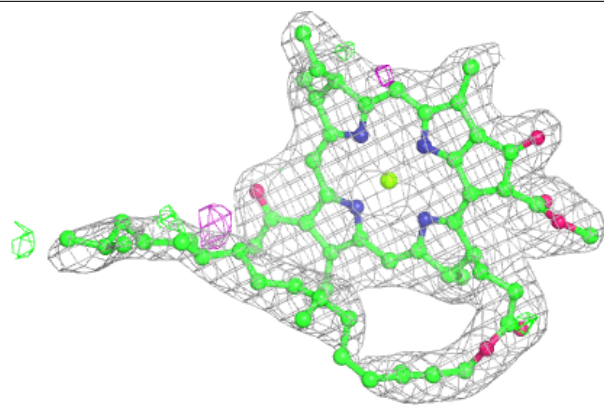
**Electron density around BPH M 404:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

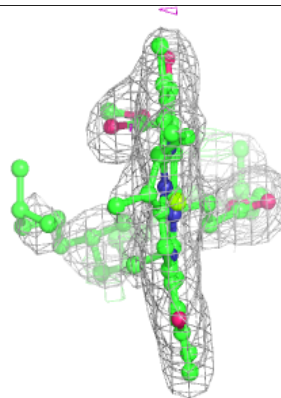
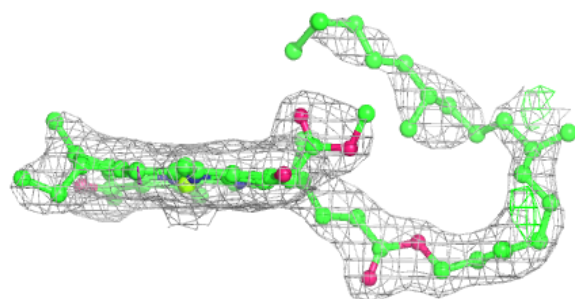
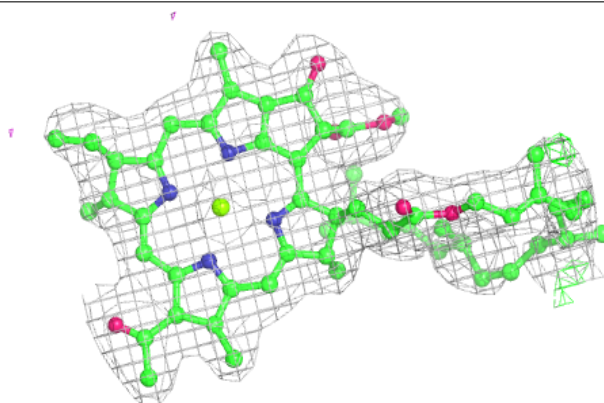


Electron density around BCL S 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

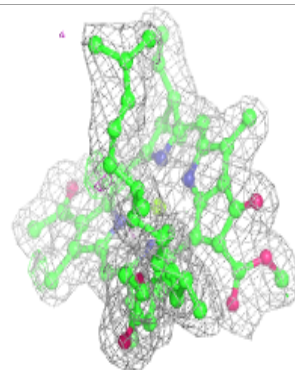
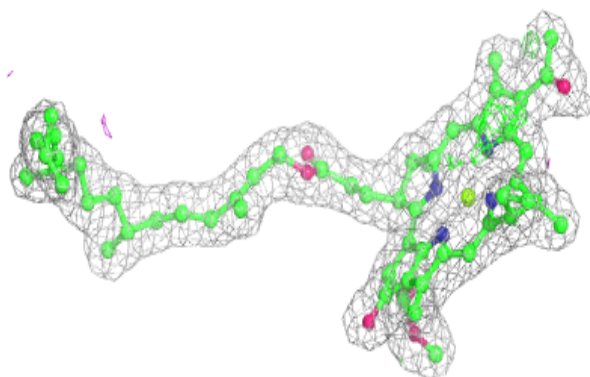
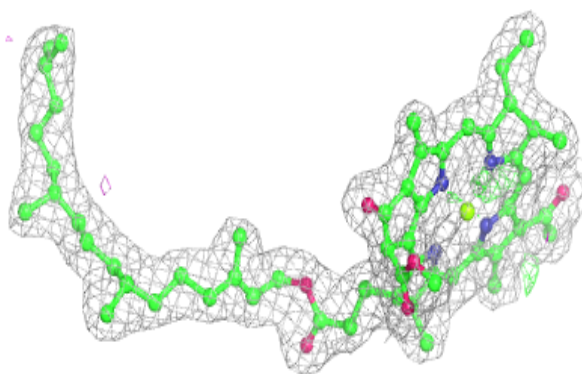
**Electron density around BCL U 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

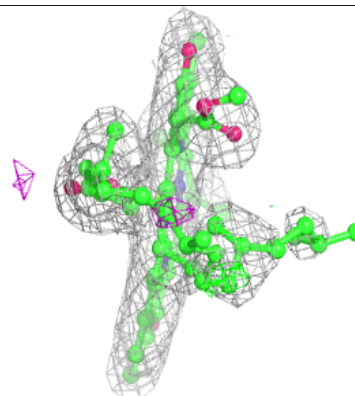
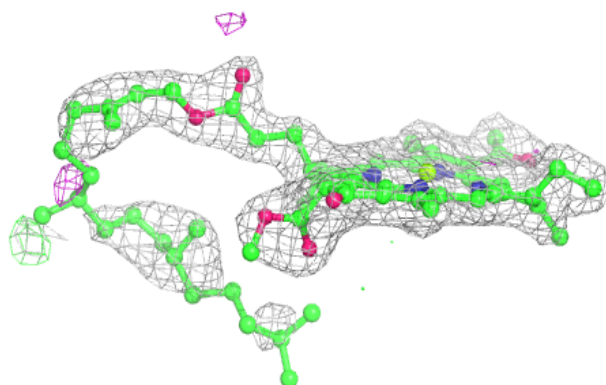
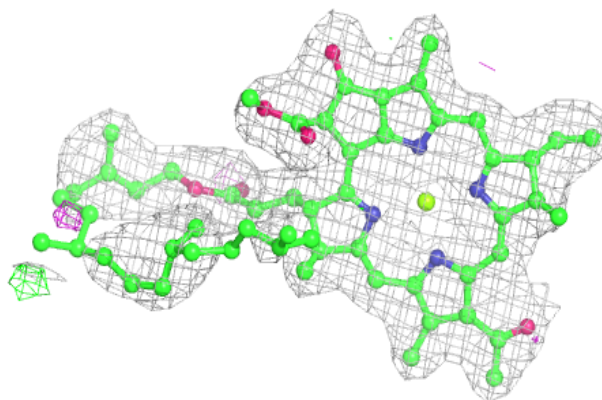


Electron density around BCL M 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

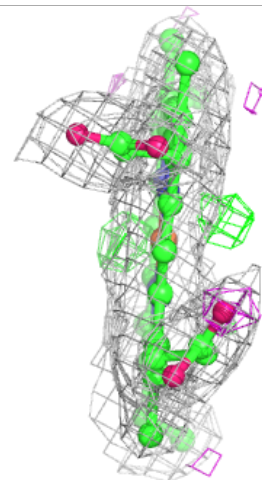
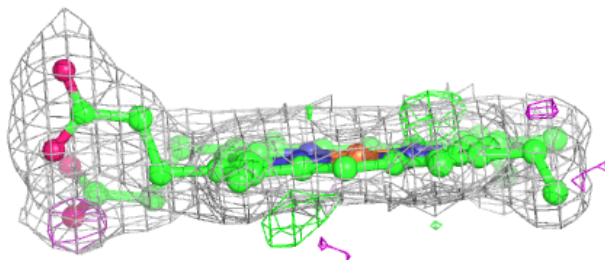
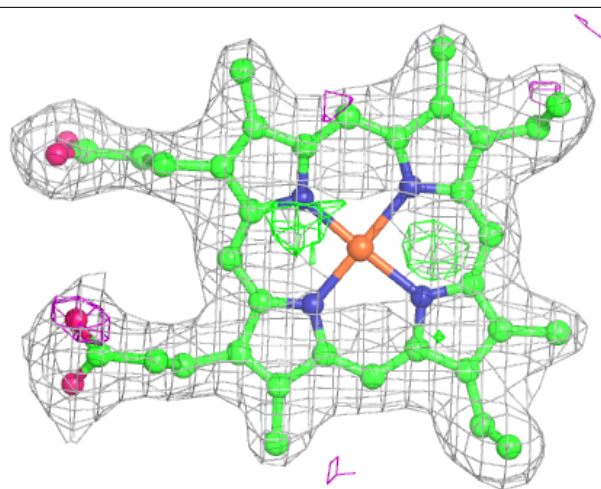
**Electron density around BCL S 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



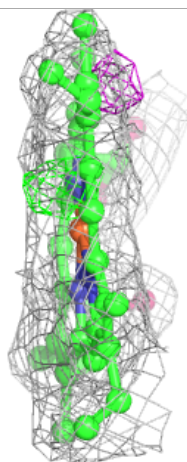
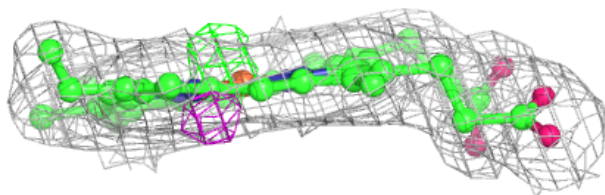
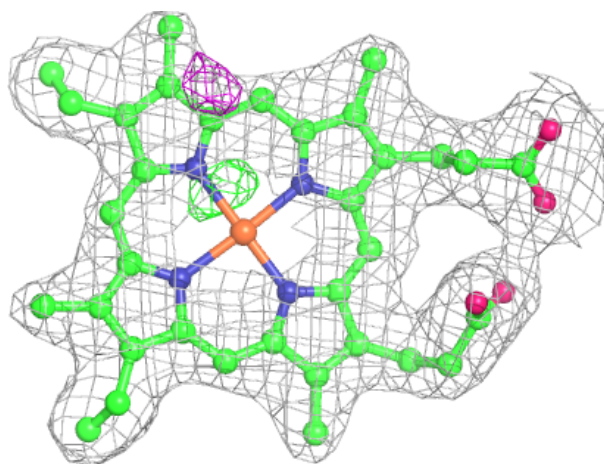
Electron density around HEC C 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



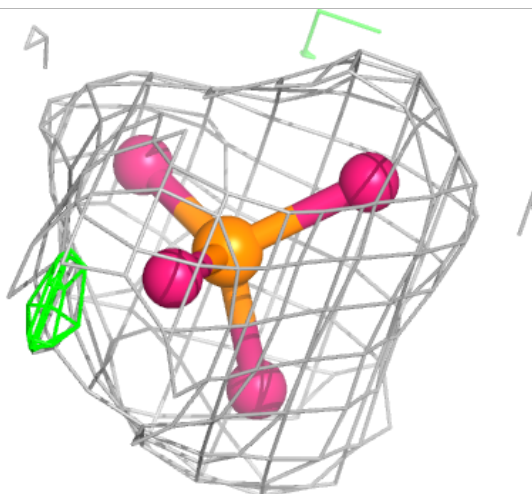
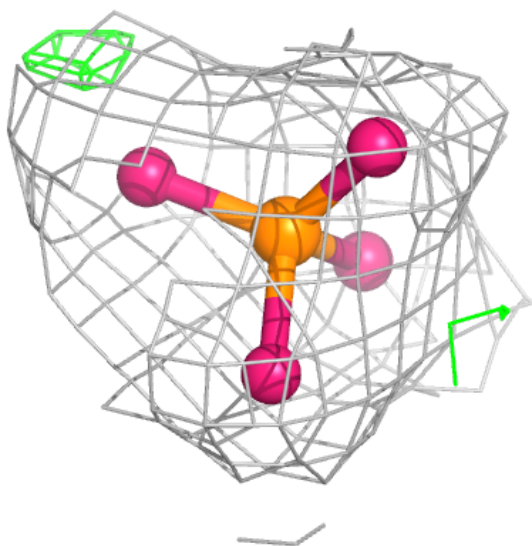
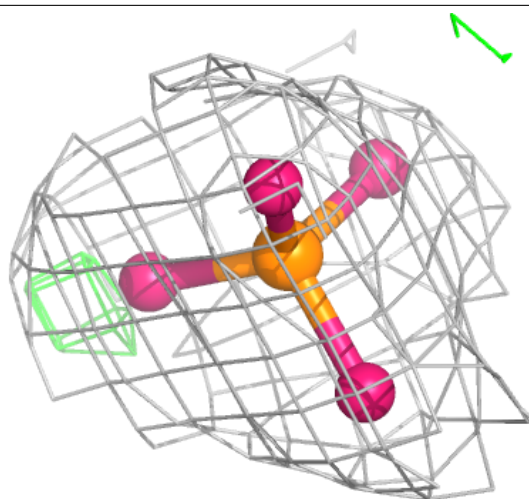
Electron density around HEC C 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



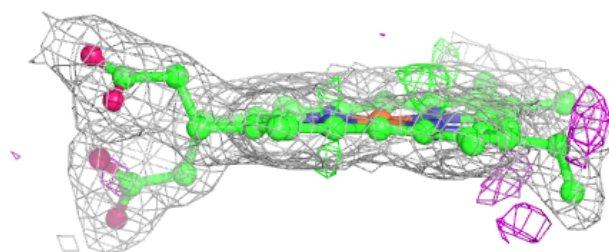
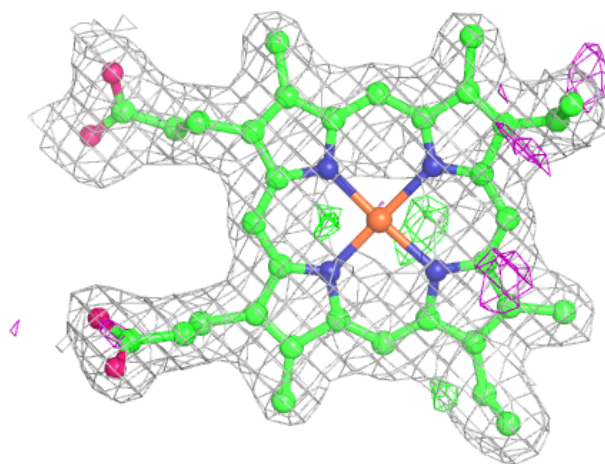
Electron density around PEF M 410:

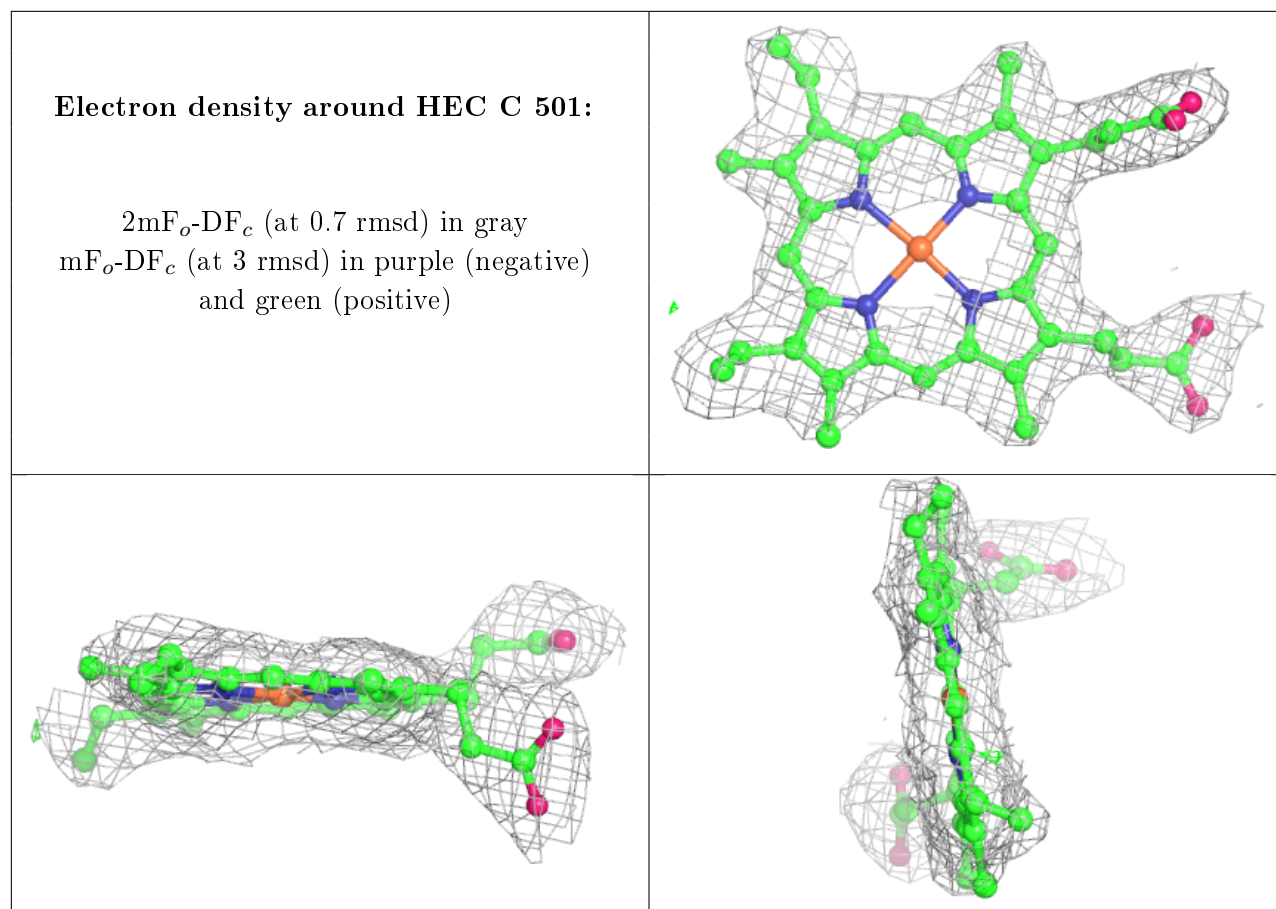
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC C 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.