



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 02:35 AM UTC

PDB ID : 5Y5S / pdb_00005y5s
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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

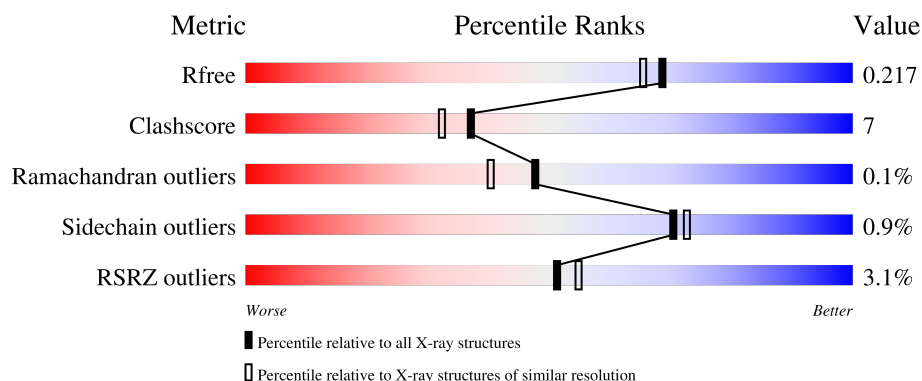
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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.



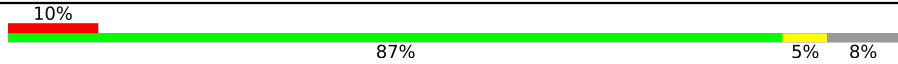
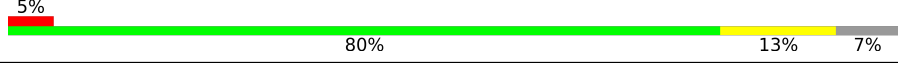
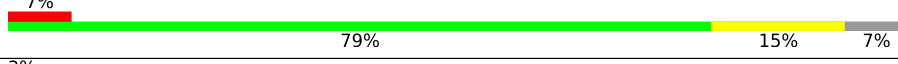
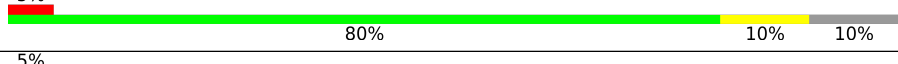
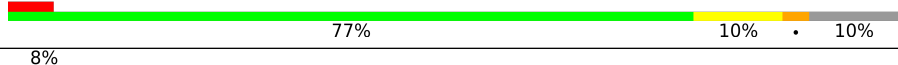
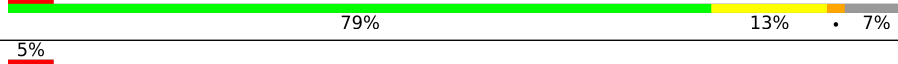
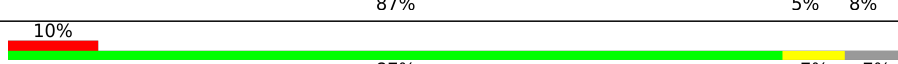
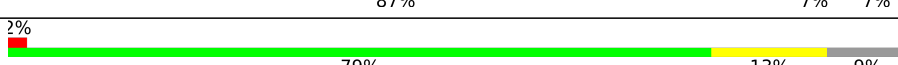
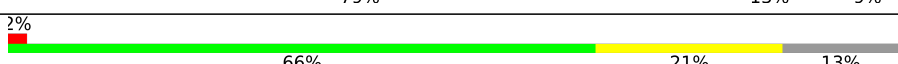
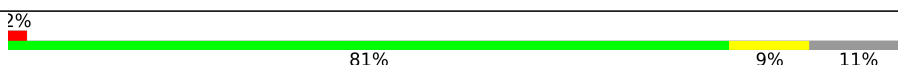
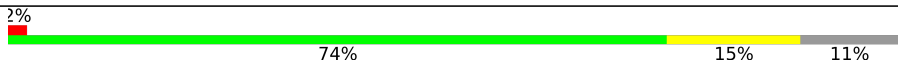
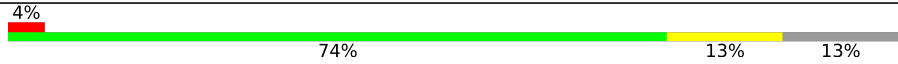
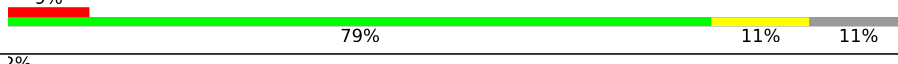
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 of 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	
2	L	281	
3	M	325	
4	H	259	
5	1	61	

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Mol	Chain	Length	Quality of chain
5	3	61	
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	

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Mol	Chain	Length	Quality of chain
6	P	47	
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	105	-	X	-	-
20	PEF	3	104	-	X	-	-
20	PEF	5	104	-	X	-	-
20	PEF	I	104	-	X	-	-
20	PEF	M	408	-	X	-	-
20	PEF	M	410	-	X	-	-
20	PEF	U	105	-	X	-	-
20	PEF	U	106	-	X	-	-
20	PEF	W	104	-	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.

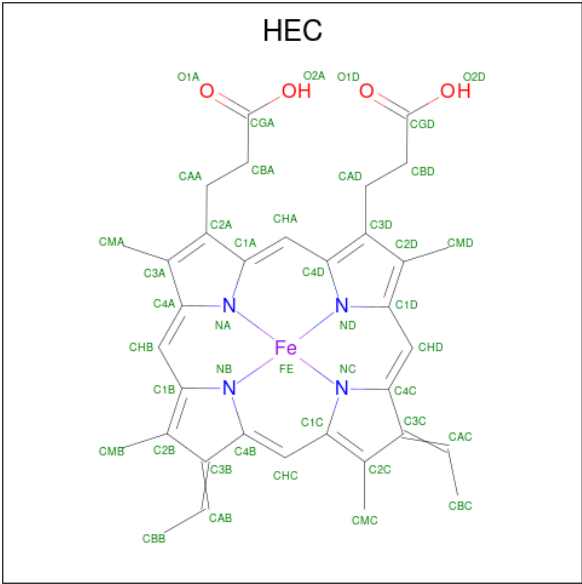
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	42	Total	C	N	O	S	0	0	0
			351	237	54	58	2			
6	E	38	Total	C	N	O	S	0	0	0
			326	222	50	52	2			
6	G	42	Total	C	N	O	S	0	0	0
			351	237	54	58	2			
6	J	42	Total	C	N	O	S	0	0	0
			351	237	54	58	2			
6	N	42	Total	C	N	O	S	0	0	0
			351	237	54	58	2			
6	P	42	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 (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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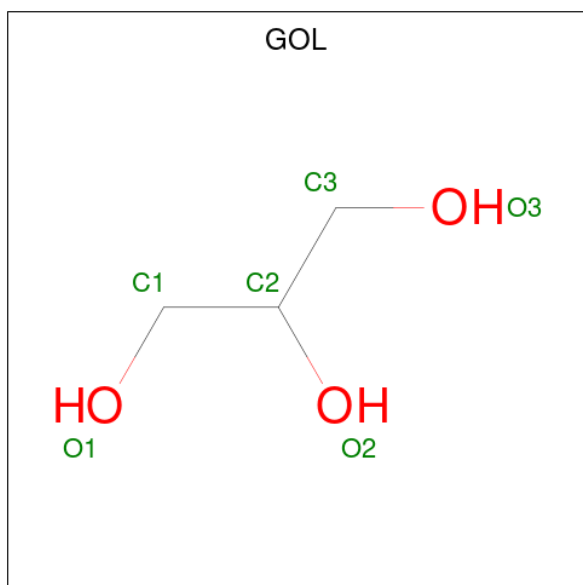
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
7	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

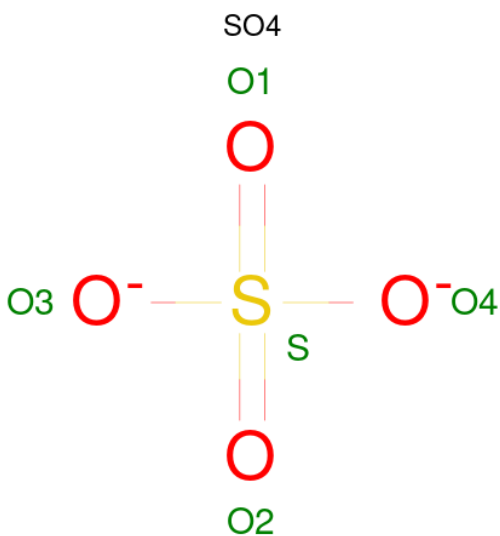
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Mg		
			1	1	0	0

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



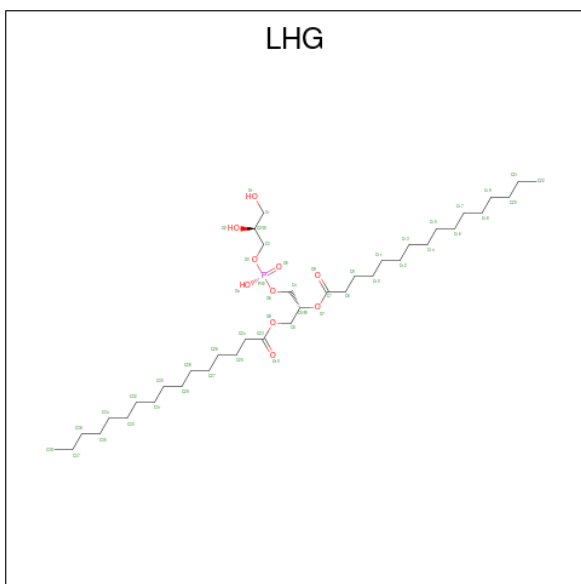
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O		
			6	3	3	0	0
9	H	1	Total	C	O		
			6	3	3	0	0

- Molecule 10 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



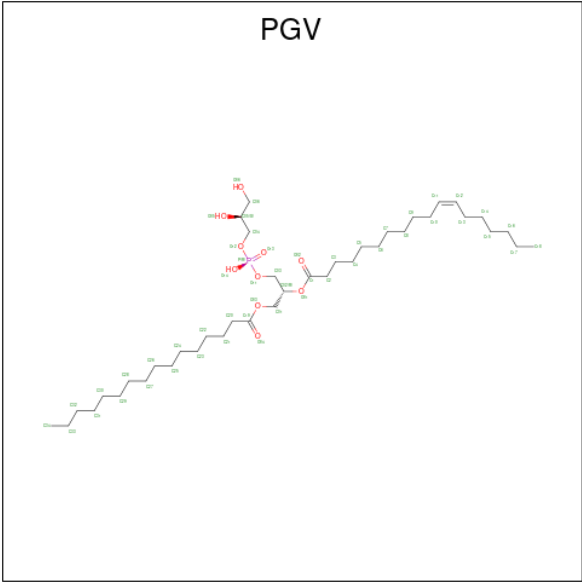
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total 5	O 4	S 1	0	0
10	L	1	Total 5	O 4	S 1	0	0
10	M	1	Total 5	O 4	S 1	0	0

- Molecule 11 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$).



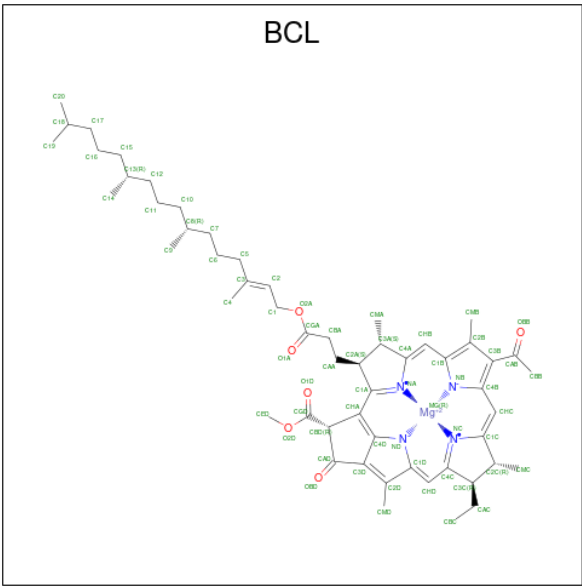
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O	0	0
			9	8	1		

- Molecule 12 is (1R)-2-{{[[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: 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 (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



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

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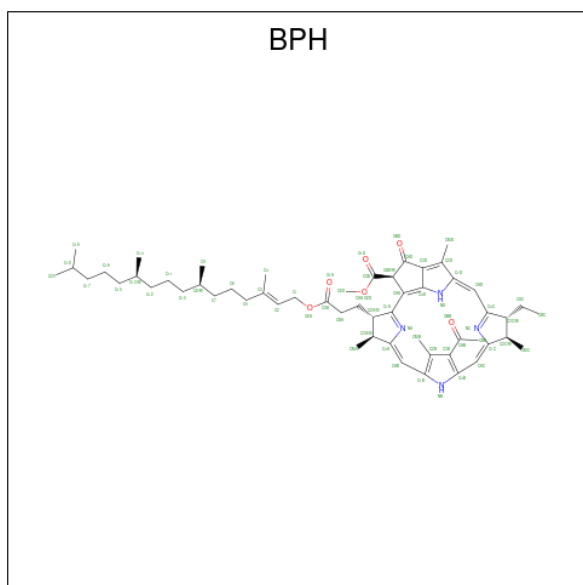
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	K	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	O	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	O	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	S	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	S	1	Total 66	C 55	Mg 1	N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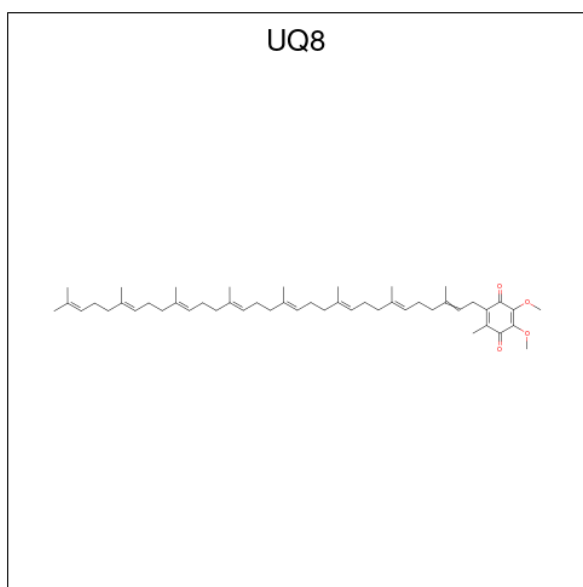
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	9	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
13	0	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 14 is BACTERIOPHEOPHYTIN A (CCD ID: 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 (CCD ID: 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 (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	L	1	Total	C	0	0
			12	12		
16	M	1	Total	C	0	0
			9	9		
16	B	1	Total	C	0	0
			12	12		
16	E	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	P	1	Total	C	0	0
			12	12		

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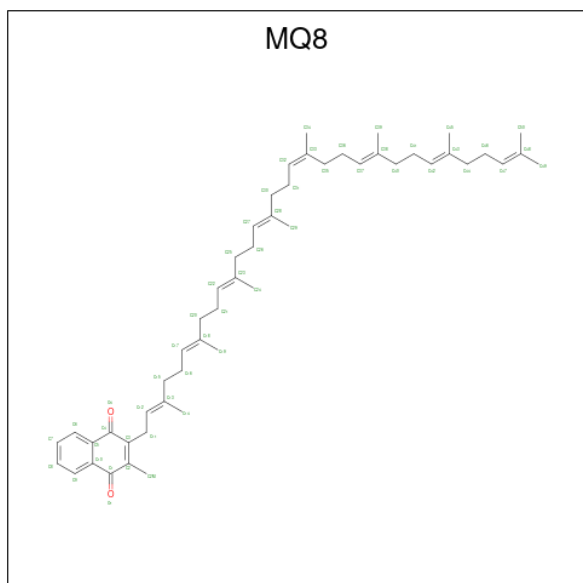
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	R	1	Total C 12 12	0	0
16	T	1	Total C 12 12	0	0
16	X	1	Total C 12 12	0	0
16	Z	1	Total C 12 12	0	0
16	2	1	Total C 12 12	0	0
16	4	1	Total C 12 12	0	0
16	6	1	Total C 12 12	0	0
16	8	1	Total C 12 12	0	0
16	0	1	Total C 12 12	0	0

- Molecule 17 is FE (III) ION (CCD ID: FE) (formula: Fe).

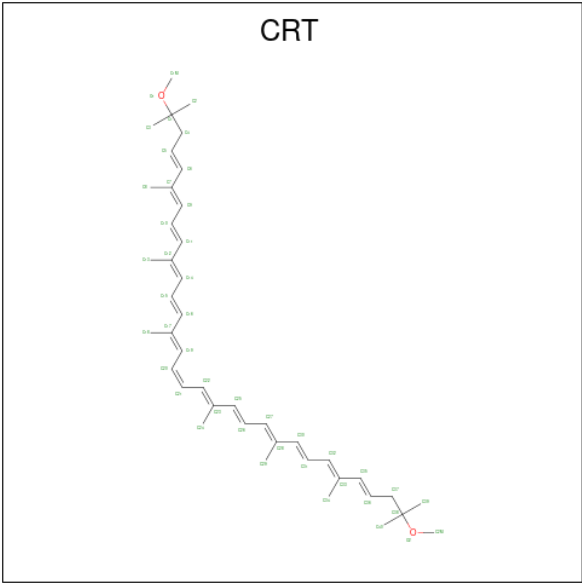
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	M	1	Total Fe 1 1	0	0

- Molecule 18 is MENAQUINONE 8 (CCD ID: MQ8) (formula: C₅₁H₇₂O₂).



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

- Molecule 19 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: C₄₂H₆₀O₂).



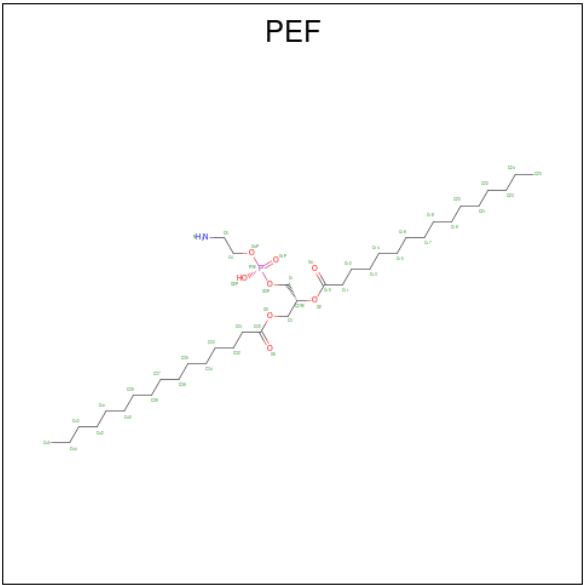
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	M	1	Total	C	O	0	0
			44	42	2		
19	A	1	Total	C	O	0	0
			44	42	2		
19	G	1	Total	C	O	0	0
			44	42	2		
19	J	1	Total	C	O	0	0
			44	42	2		
19	N	1	Total	C	O	0	0
			44	42	2		
19	O	1	Total	C	O	0	0
			44	42	2		
19	P	1	Total	C	O	0	0
			44	42	2		
19	Q	1	Total	C	O	0	0
			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 (CCD ID: PEF) (formula: C₃₇H₇₄NO₈P).



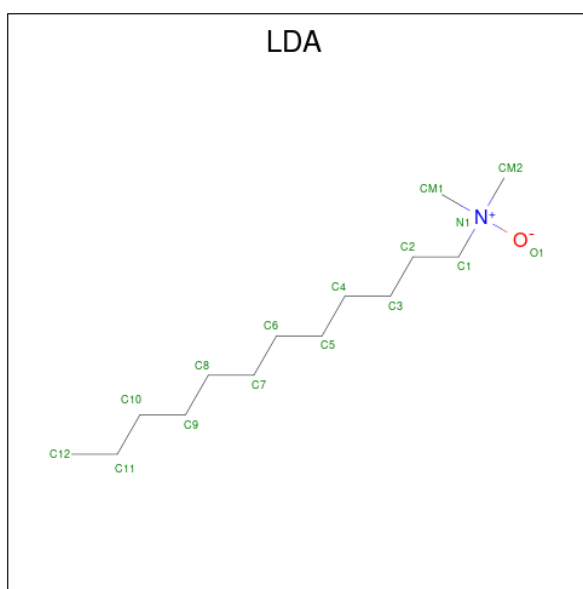
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	M	1	Total	O	P			0	0
			5	4	1				
20	M	1	Total	O	P			0	0
			5	4	1				
20	M	1	Total	O	P			0	0
			5	4	1				
20	M	1	Total	O	P			0	0
			5	4	1				
20	M	1	Total	C	N	O	P	0	0
			47	37	1	8	1		

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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 (CCD ID: LDA) (formula: C₁₄H₃₁NO).



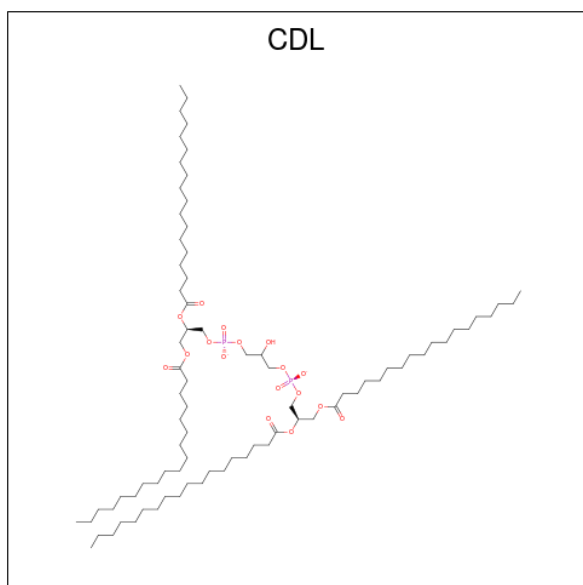
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	M	1	Total	C	N	O		
			14	12	1	1		
21	I	1	Total	C	N	O		
			16	14	1	1		
21	J	1	Total	C	N	O		
			16	14	1	1		

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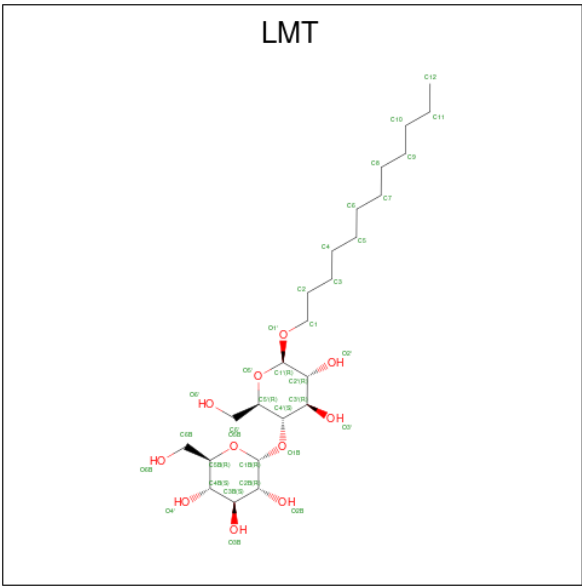
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	O	1	Total	C	N	O	0	0
			14	12	1	1		
21	V	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 22 is CARDIOLIPIN (CCD ID: 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 (CCD ID: 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 (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	1	Total	Ca	0	0
			1	1		
24	D	1	Total	Ca	0	0
			1	1		
24	F	1	Total	Ca	0	0
			1	1		
24	I	1	Total	Ca	0	0
			1	1		
24	K	1	Total	Ca	0	0
			1	1		
24	O	1	Total	Ca	0	0
			1	1		
24	Q	1	Total	Ca	0	0
			1	1		
24	S	1	Total	Ca	0	0
			1	1		
24	U	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	W	1	Total 1	Ca 1	0	0
24	Y	1	Total 1	Ca 1	0	0
24	1	1	Total 1	Ca 1	0	0
24	3	1	Total 1	Ca 1	0	0
24	5	1	Total 1	Ca 1	0	0
24	7	1	Total 1	Ca 1	0	0
24	9	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
25	J	4	Total 4	O 4	0	0

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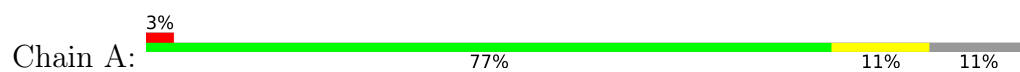
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	K	8	Total O 8 8	0	0
25	N	3	Total O 3 3	0	0
25	O	13	Total O 13 13	0	0
25	P	7	Total O 7 7	0	0
25	Q	18	Total O 18 18	0	0
25	R	9	Total O 9 9	0	0
25	S	12	Total O 12 12	0	0
25	T	11	Total O 11 11	0	0
25	U	15	Total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

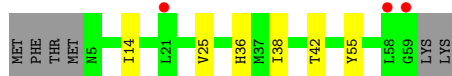
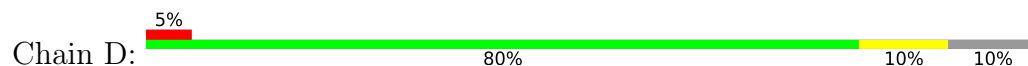
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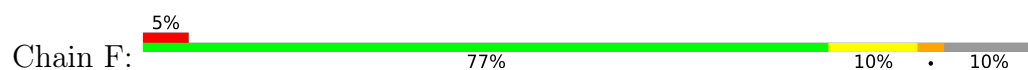
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	8	11	Total 11	O 11	0	0
25	9	13	Total 13	O 13	0	0
25	0	8	Total 8	O 8	0	0



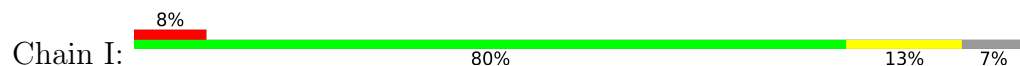
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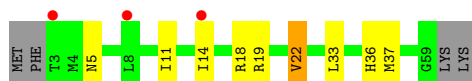
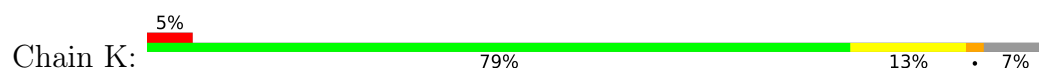
- Molecule 5: LH1 alpha polypeptide



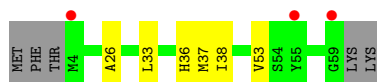
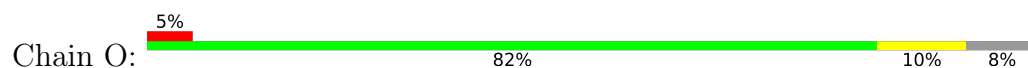
- Molecule 5: LH1 alpha polypeptide



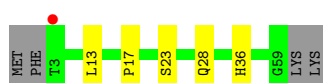
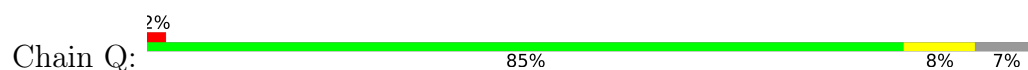
- Molecule 5: LH1 alpha polypeptide



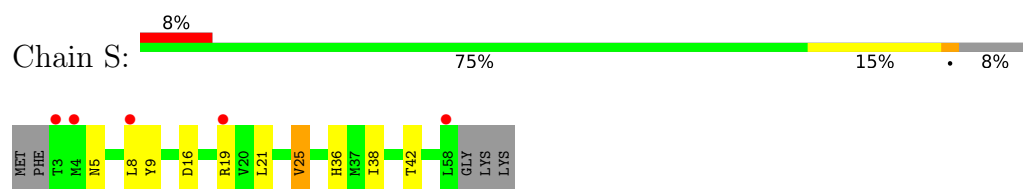
- Molecule 5: LH1 alpha polypeptide



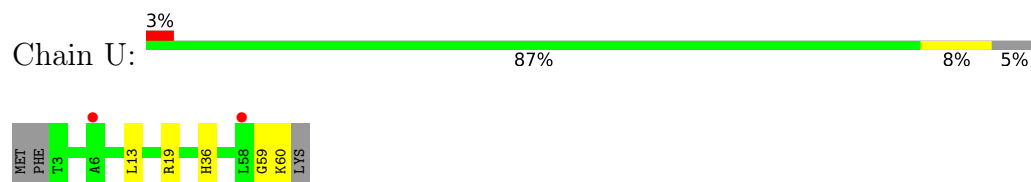
- Molecule 5: LH1 alpha polypeptide



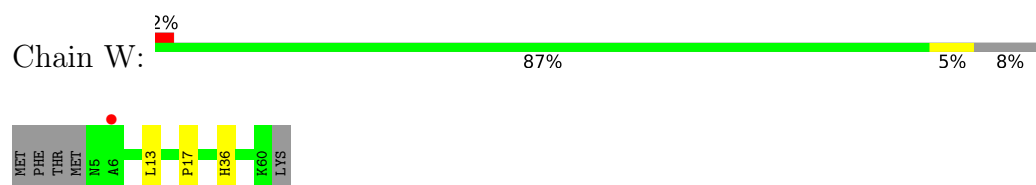
- Molecule 5: LH1 alpha polypeptide



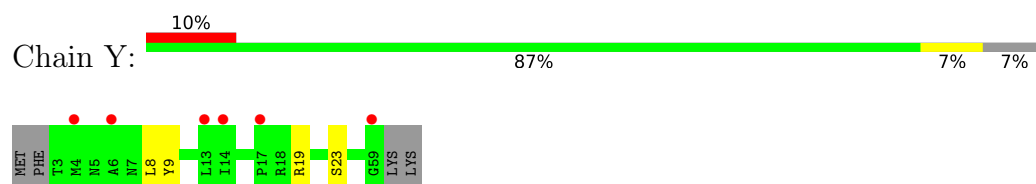
- Molecule 5: LH1 alpha polypeptide



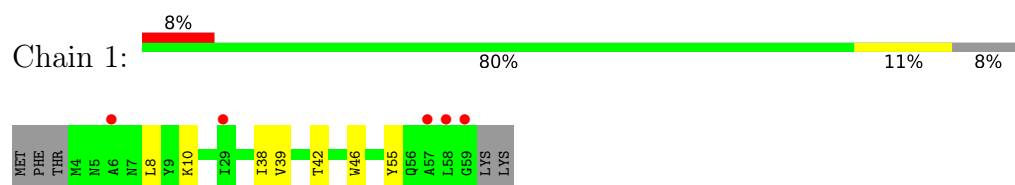
- Molecule 5: LH1 alpha polypeptide



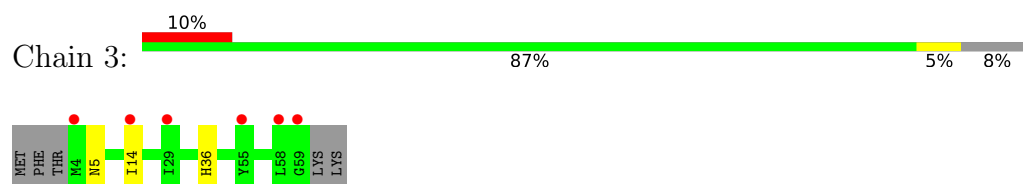
- Molecule 5: LH1 alpha polypeptide



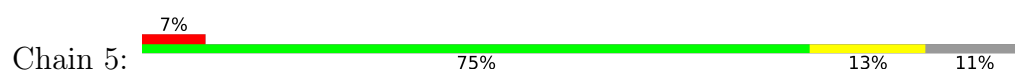
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide

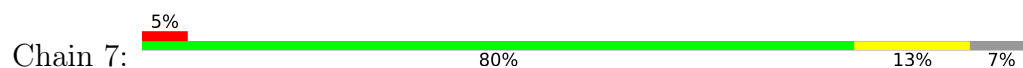


- Molecule 5: LH1 alpha polypeptide

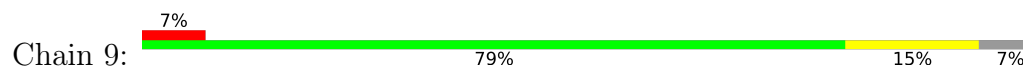




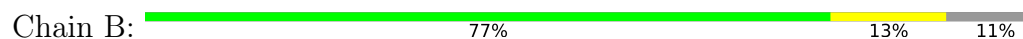
- Molecule 5: LH1 alpha polypeptide



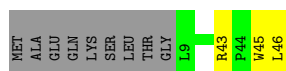
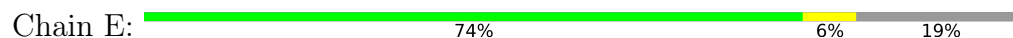
- Molecule 5: LH1 alpha polypeptide



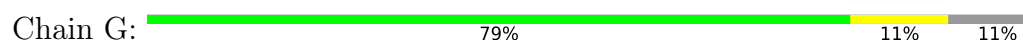
- Molecule 6: LH1 beta polypeptide



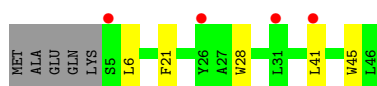
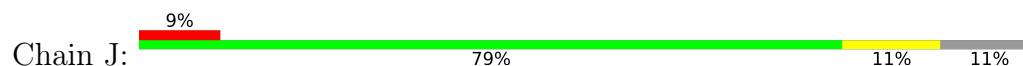
- Molecule 6: LH1 beta polypeptide



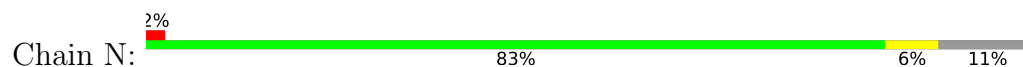
- Molecule 6: LH1 beta polypeptide

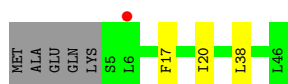


- Molecule 6: LH1 beta polypeptide

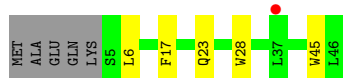
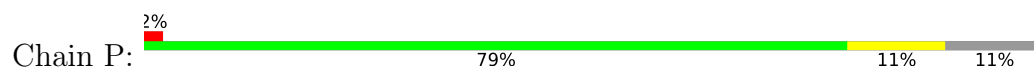


- Molecule 6: LH1 beta polypeptide

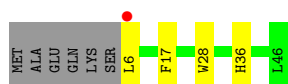
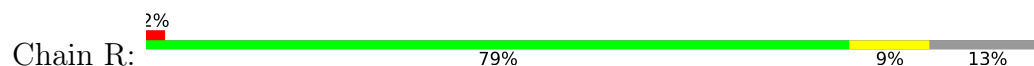




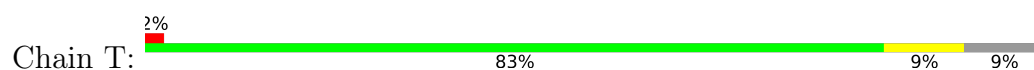
- Molecule 6: LH1 beta polypeptide



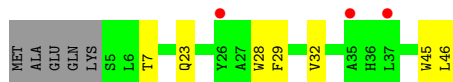
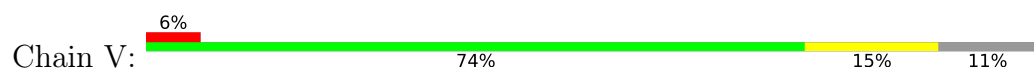
- Molecule 6: LH1 beta polypeptide



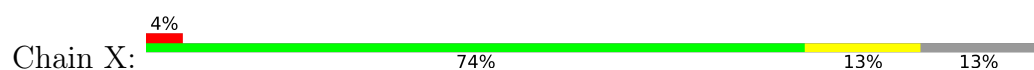
- Molecule 6: LH1 beta polypeptide



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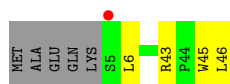
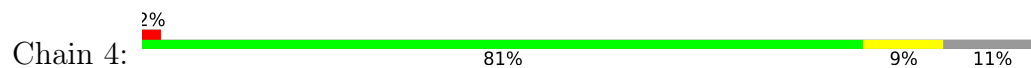
- Molecule 6: LH1 beta polypeptide



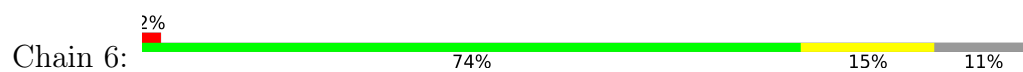
- Molecule 6: LH1 beta polypeptide



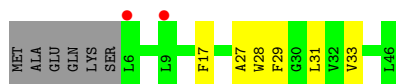
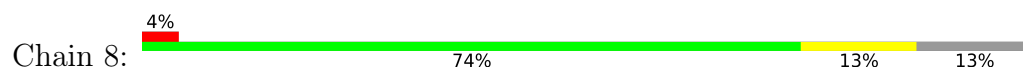
- Molecule 6: LH1 beta polypeptide



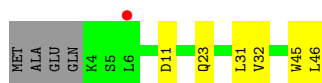
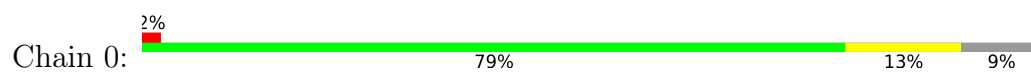
- Molecule 6: LH1 beta polypeptide



- 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 0.184 , 0.217	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 , 78.8	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	0.96	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

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	0.36	0/2487	0.52	0/3396
2	L	0.46	0/2326	0.56	0/3177
3	M	0.44	0/2658	0.56	0/3637
4	H	0.39	0/2034	0.50	0/2773
5	1	0.62	0/459	0.44	0/628
5	3	0.21	0/467	0.39	0/638
5	5	0.23	0/443	0.43	0/607
5	7	0.28	0/466	0.46	0/638
5	9	0.24	0/466	0.47	0/638
5	A	0.24	0/443	0.44	0/607
5	D	0.21	0/457	0.39	0/626
5	F	0.36	0/457	0.44	0/626
5	I	0.19	0/472	0.34	0/646
5	K	0.22	0/466	0.38	0/638
5	O	0.27	0/467	0.43	0/638
5	Q	0.41	0/466	0.48	0/638
5	S	0.34	0/483	0.51	0/661
5	U	0.28	0/475	0.42	0/649
5	W	0.24	0/460	0.43	0/629
5	Y	0.20	0/466	0.38	0/638
6	0	0.21	0/373	0.34	0/506
6	2	0.15	0/358	0.33	0/487
6	4	0.17	0/364	0.32	0/495
6	6	0.22	0/364	0.34	0/495
6	8	0.23	0/358	0.37	0/487
6	B	0.17	0/364	0.27	0/495
6	E	0.14	0/339	0.26	0/461
6	G	0.11	0/364	0.27	0/495
6	J	0.12	0/364	0.25	0/495
6	N	0.15	0/364	0.28	0/495
6	P	0.23	0/364	0.33	0/495

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	R	0.27	0/358	0.39	0/487
6	T	0.29	0/373	0.37	0/506
6	V	0.20	0/364	0.34	0/495
6	X	0.21	0/358	0.31	0/487
6	Z	0.13	0/350	0.27	0/476
All	All	0.33	0/22697	0.46	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	11	0
2	L	2236	0	2201	21	0
3	M	2555	0	2530	24	0
4	H	1976	0	1977	21	0
5	1	450	0	475	6	0
5	3	455	0	484	4	0
5	5	434	0	460	7	0
5	7	457	0	482	9	0
5	9	457	0	482	8	0
5	A	434	0	460	6	0
5	D	445	0	471	8	0
5	F	445	0	471	8	0
5	I	460	0	487	11	0
5	K	457	0	482	7	0
5	O	455	0	484	4	0
5	Q	457	0	482	7	0
5	S	468	0	501	11	0
5	U	466	0	495	4	0
5	W	451	0	479	3	0
5	Y	457	0	480	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	0	360	0	352	5	0
6	2	345	0	334	19	0
6	4	351	0	339	3	0
6	6	351	0	339	7	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	2	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	10	0
13	3	132	0	144	8	0
13	5	132	0	144	12	0
13	7	127	0	131	7	0
13	9	66	0	72	4	0
13	A	132	0	144	7	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	8	0
13	O	132	0	144	7	0
13	Q	132	0	144	11	0
13	S	132	0	144	10	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	6	0
14	L	65	0	74	5	0
14	M	65	0	74	7	0
15	7	33	0	39	10	0
15	L	104	0	128	10	0
15	M	18	0	15	4	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	M	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	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	N	44	0	60	3	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	2	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	1	1	0	0	0	0
24	3	1	0	0	0	0
24	5	1	0	0	0	0
24	7	1	0	0	0	0
24	9	1	0	0	0	0
24	A	1	0	0	0	0
24	D	1	0	0	0	0
24	F	1	0	0	0	0
24	I	1	0	0	0	0
24	K	1	0	0	0	0
24	O	1	0	0	0	0
24	Q	1	0	0	0	0
24	S	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	U	1	0	0	0	0
24	W	1	0	0	0	0
24	Y	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	3	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	0	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	385	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 (385) 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:104:CDL:OA4	1.88	1.20
6:2:9:LEU:HD21	6:2:14:ALA:N	1.54	1.19
22:S:104:CDL:C19	13:U:102:BCL:H51	1.83	1.08
5:S:19:ARG:NH1	22:S:104: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	0.91
14:L:302:BPH:HH C	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:105:LDA:HM21	1.46	0.79
23:M:420:LMT:H42	21:I:105:LDA:H42	1.65	0.78
19:1:104:CRT:H371	13:5:102:BCL:HMB2	1.64	0.78
6:2:9:LEU:HD23	6:2:10:THR:O	1.84	0.76
14:M:405:BPH:HBB3	14:M:405:BPH:HH C	1.69	0.75
22:S:104:CDL:C19	13:U:102:BCL:C5	2.65	0.74
13:D:103:BCL:H202	6:G:38:LEU:HD13	1.70	0.74
2:L:180:PRO:HA	2:L:183:MET:HE3	1.70	0.73
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
3:M:256:MET:HE3	18:M:406:MQ8:H142	1.74	0.70
13:1:103:BCL:H72	13:1:103:BCL:HMB2	1.75	0.68
6:2:9:LEU:HD22	6:2:14:ALA:CB	2.24	0.67
2:L:190:PHE:HB3	14:M:405:BPH:HBB2	1.76	0.67
22:Q:105:CDL:H142	22:Q:105:CDL:H362	1.76	0.66
4:H:121:LYS:HD2	4:H:234:TYR:HB3	1.78	0.66
19:6:101:CRT:H371	13:7:102:BCL:HMB2	1.78	0.65
19:J:101:CRT:H371	13:K:102:BCL:HMB2	1.78	0.64
13:Q:103:BCL:H51	13:S:102:BCL:H18	1.79	0.64
13:O:102:BCL:H72	13:O:102:BCL:HMB1	1.78	0.64
15:L:309:UQ8:H3M	13:M:403:BCL:H161	1.80	0.64
13:5:102:BCL:H172	6:6:31:LEU:HD21	1.80	0.63
2:L:206:VAL:HB	2:L:216:LYS:HB2	1.81	0.63
4:H:14:ILE:HG12	5:I:37:MET:HE2	1.82	0.62
5:A:18:ARG:HH22	12:A:105:PGV:H041	1.64	0.62
5:Y:23:SER:HB3	13:1:102:BCL:H172	1.80	0.62
5:3:14:ILE:HG22	6:4:6:LEU:HD23	1.81	0.61
19:V:101:CRT:H371	13:W:102:BCL:HMB2	1.83	0.60
14:L:302:BPH:HH C	14:L:302:BPH:CBB	2.30	0.60
4:H:258:LEU:O	5:5:19:ARG:HD2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:14:ILE:HD11	19:G:101:CRT:H23	1.84	0.59
6:Z:17:PHE:HA	19:Z:101:CRT:H6	1.84	0.59
13:Q:102:BCL:H43	6:R:28:TRP:CZ2	2.37	0.59
18:M:406:MQ8:H241	22:H:304:CDL:H772	1.84	0.59
5:W:36:HIS:CE1	13:W:103:BCL:HMD3	2.38	0.59
22:H:302:CDL:H551	22:H:302:CDL:H751	1.84	0.59
19:Q:104:CRT:H371	13:U:102:BCL:HMB2	1.84	0.59
5:D:36:HIS:CE1	13:D:103:BCL:HMD3	2.37	0.59
13:K:103:BCL:HMB2	13:K:103:BCL:H101	1.85	0.58
14:M:405:BPH:HBC3	14:M:405:BPH:HHD	1.85	0.58
6:2:9:LEU:CD2	6:2:13:GLU:HB2	2.33	0.58
21:M:412:LDA:H41	21:O:105: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:104:CDL:OB4	5:U:19:ARG:NH2	2.37	0.57
3:M:252:TRP:CE3	3:M:256:MET:HE2	2.40	0.57
4:H:44:ASP:H	12:A:105:PGV:H062	1.68	0.57
1:C:46:LYS:HD3	12:3:105:PGV:H062	1.87	0.57
5:7:26:ALA:HB3	15:7:104:UQ8:C4M	2.34	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:102:BCL:H42	1.88	0.56
19:A:104:CRT:H371	13:F:102:BCL:HMB2	1.88	0.56
5:F:36:HIS:CE1	13:F:103:BCL:HMD3	2.41	0.56
5:K:18:ARG:O	5:K:22:VAL:HG12	2.06	0.56
13:W:102:BCL:H172	13:W:102:BCL:HED3	1.88	0.55
5:Q:36:HIS:CE1	13:Q:103:BCL:HMD3	2.41	0.55
12:L:305:PGV:H81	12:D:105: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
3:M:69[A]:SER:OG	15:M:418:UQ8:H8	2.06	0.55
5:O:36:HIS:CE1	13:O:103:BCL:HMD3	2.41	0.54
5:I:36:HIS:CE1	13:I:103:BCL:HMD3	2.41	0.54
13:M:403:BCL:H72	14:M:405:BPH:HMB3	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	15:7:104:UQ8:H4MA	2.22	0.54
5:3:36:HIS:CE1	13:3:103:BCL:HMD3	2.43	0.54
4:H:60:ASP:HB2	22:D:104:CDL:HB22	1.89	0.53
5:1:39:VAL:HG21	13:1:103:BCL:HHD	1.90	0.53
6:2:9:LEU:CD2	6:2:14:ALA:CA	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:101:CRT:H35	13:3:102:BCL:HMB2	1.91	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
5:9:36:HIS:CE1	13:0:102:BCL:HMD3	2.44	0.52
13:Z:102:BCL:H142	13:Z:102:BCL:H102	1.91	0.52
5:7:5:ASN:ND2	6:0:23:GLN:OE1	2.38	0.52
6:G:17:PHE:HB2	19:G:101:CRT:H21A	1.92	0.52
5:I:41[A]:SER:HB2	21:I:105:LDA:H11	1.90	0.52
2:L:183:MET:HE1	2:L:272:TRP:CZ2	2.45	0.52
5:Q:28:GLN:CB	13:Q:102:BCL:H42	2.40	0.52
5:A:18:ARG:NH1	12:A:105:PGV:H012	2.25	0.52
5:I:41[B]:SER:HB3	21:I:105:LDA:H11	1.90	0.51
13:O:103:BCL:H121	6:P:45:TRP:HZ2	1.74	0.51
2:L:41:CYS:CB	15:7:104:UQ8:H1MA	2.40	0.51
13:Y:102:BCL:H172	13:Y:102:BCL:HED3	1.92	0.51
3:M:271:TRP:HZ2	20:M:419:PEF:H112	1.76	0.51
12:M:415:PGV:H05	5:S:19:ARG:NH2	2.25	0.51
6:N:17:PHE:HA	19:N:101:CRT:H6	1.92	0.51
6:G:17:PHE:HA	19:G:101:CRT:H6	1.93	0.51
13:S:103:BCL:H42	13:U:102:BCL:H151	1.91	0.51
6:2:9:LEU:HD21	6:2:14:ALA:CA	2.38	0.51
2:L:128:PHE:CE2	12:M:414:PGV:H51	2.45	0.51
13:5:102:BCL:H143	13:5:102:BCL:HBA1	1.93	0.51
1:C:144:HIS:HE1	7:C:504:HEC:NC	2.05	0.51
15:M:418:UQ8:H1MB	22:S:104:CDL:C43	2.40	0.51
5:S:5:ASN:ND2	6:V:23:GLN:OE1	2.44	0.51
1:C:158:GLY:O	25:C:601:HOH:O	2.19	0.50
2:L:186:ILE:HG12	13:L:301:BCL:HMB3	1.93	0.50
13:I:102:BCL:H43	6:J:28:TRP:CZ2	2.46	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
5:7:17:PRO:HB3	6:8:17:PHE:CE2	2.47	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
3:M:256:MET:CE	18:M:406:MQ8:H142	2.39	0.50
3:M:289:THR:HB	23:M:420:LMT:H12	1.93	0.50
2:L:270:GLU:OE2	25:L:401:HOH:O	2.20	0.49
5:F:46:TRP:CE3	13:F:102:BCL:HAC2	2.47	0.49
6:2:17:PHE:HA	19:2:101:CRT:H6	1.94	0.49
14:L:302:BPH:HBB2	3:M:210:TYR:HB3	1.93	0.49
12:3:105:PGV:H211	5:5:40:LEU:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:104:CRT:H292	13:S:102:BCL:H111	1.94	0.49
5:3:5:ASN:ND2	6:6:23:GLN:OE1	2.42	0.49
1:C:73:SER:HB2	1:C:83:LYS:HB3	1.94	0.49
2:L:190:PHE:HB3	14:M:405:BPH:CBB	2.42	0.49
5:9:29:ILE:HD11	13:9:104:BCL:H203	1.94	0.49
19:G:101:CRT:H371	13:I:102:BCL:HMB2	1.95	0.48
6:Z:45:TRP:CD1	6:Z:46:LEU:HG	2.47	0.48
3:M:173:LYS:NZ	25:M:504:HOH:O	2.37	0.48
2:L:196:LEU:HD11	3:M:269:ALA:HB1	1.94	0.48
4:H:17:TRP:CD1	23:F:104:LMT:H61	2.48	0.48
3:M:130:TRP:HZ3	22:K:104:CDL:H511	1.78	0.48
5:S:21:LEU:O	5:S:25:VAL:HG13	2.13	0.48
22:S:104:CDL:H721	22:S:104:CDL:C51	2.43	0.48
19:M:407: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
13:5:102:BCL:H51	13:5:102:BCL:H8	1.58	0.48
3:M:282:ILE:HG12	23:M:420:LMT:H101	1.96	0.48
5:7:26:ALA:HB3	15:7:104:UQ8:H4M	1.96	0.48
2:L:41:CYS:SG	15:7:104:UQ8:H1MA	2.54	0.48
4:H:20:TRP:NE1	12:H:303:PGV:H202	2.28	0.47
13:Y:102:BCL:H43	6:Z:28:TRP:CZ2	2.49	0.47
13:O:103:BCL:H93	13:O:103:BCL:H61	1.65	0.47
13:1:103:BCL:HMA3	13:3:102:BCL:HMB3	1.96	0.47
13:A:103:BCL:HAC2	6:B:45:TRP:CE3	2.49	0.47
5:5:18:ARG:NH1	20:5:104:PEF:O2P	2.42	0.47
6:Z:45:TRP:CE3	13:Z:102:BCL:HAC2	2.49	0.47
14:L:302:BPH:HBB1	3:M:210:TYR:CD2	2.50	0.47
3:M:7:ILE:HD12	12:M:414:PGV:H92	1.95	0.47
5:1:8:LEU:HD12	6:2:18:HIS:CE1	2.49	0.47
15:L:308:UQ8:H46A	6:6:21:PHE:CE1	2.50	0.47
13:D:102:BCL:H202	13:D:102:BCL:H162	1.79	0.47
6:4:43:ARG:HG3	5:5:55:TYR:CZ	2.49	0.47
13:5:103:BCL:H13	6:6:45:TRP:HZ2	1.79	0.47
20:M:419:PEF:H111	4:H:29:TYR:CE2	2.50	0.47
12:L:306:PGV:C11	15:L:308:UQ8:H26A	2.45	0.47
5:1:46:TRP:CE3	13:1:102:BCL:HAC2	2.50	0.47
13:9:104:BCL:H111	13:9:104:BCL:H72	1.51	0.47
15:7:104:UQ8:H17	15:7:104:UQ8:H13	1.70	0.47
1:C:71:LYS:NZ	1:C:84:ASP:O	2.44	0.46
5:F:37:MET:HB3	23:F:104:LMT:H42	1.97	0.46
13:Y:102:BCL:H91	13:Y:102:BCL:H112	1.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2:9:LEU:HD23	6:2:13:GLU:HB2	1.96	0.46
14:M:405:BPH:HBB3	14:M:405:BPH:CHC	2.43	0.46
13:W:102: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
5:5:38:ILE:O	5:5:42:THR:HG23	2.15	0.46
13:M:404:BCL:HAA2	13:M:404:BCL:HBD	1.96	0.46
6:B:45:TRP:CD1	6:B:46:LEU:HG	2.50	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
21:J:102:LDA:H81	6:N:38:LEU:HB3	1.97	0.46
12:3:105:PGV:H251	5:5:37:MET:HG3	1.98	0.46
19:P:101:CRT:H371	13:Q:102:BCL:HMB2	1.96	0.46
13:9:104:BCL:HHC	13:9:104:BCL:OBB	2.15	0.46
5:I:28:GLN:CB	13:I:102:BCL:H42	2.46	0.46
13:K:102:BCL:H51	13:K:102:BCL:H8	1.66	0.46
5:U:59:GLY:C	5:U:60:LYS:HD2	2.41	0.46
5:U:36:HIS:CE1	13:U:103:BCL:HMD1	2.50	0.46
15:M:418:UQ8:C1M	22:S:104:CDL:C43	2.94	0.46
5:K:33:LEU:O	5:K:37:MET:HG3	2.16	0.46
22:D:104:CDL:O1	22:D:104:CDL:OA7	2.33	0.46
13:S:103:BCL:H41	13:U:102:BCL:H203	1.97	0.46
13:W:102:BCL:H141	13:W:102:BCL:H161	1.73	0.46
19:1:104:CRT:H10	19:1:104:CRT:H81	1.85	0.46
12:M:415:PGV:H05	5:S:19:ARG:HH22	1.80	0.45
12:D:105:PGV:H05	23:F:104:LMT:H2B	1.97	0.45
13:Q:103:BCL:H91	6:R:36:HIS:CG	2.51	0.45
5:7:30:VAL:HG12	15:7:104:UQ8:H13	1.98	0.45
2:L:219:GLU:OE1	2:L:219:GLU:N	2.46	0.45
22:Q:105:CDL:H171	22:Q:105:CDL:H131	1.98	0.45
13:1:103:BCL:C2B	13:1:103:BCL:H101	2.46	0.45
15:7:104:UQ8:H7A	15:7:104:UQ8:H10	1.62	0.45
13:F:103:BCL:H152	13:F:103:BCL:H112	1.53	0.45
5:S:16:ASP:HB2	5:S:19:ARG:HH11	1.81	0.45
6:2:10:THR:OG1	6:2:13:GLU:HG3	2.16	0.45
13:5:102:BCL:H43	6:6:28:TRP:CZ2	2.51	0.45
5:9:9:TYR:OH	6:0:11:ASP:OD2	2.31	0.45
6:2:45:TRP:CD1	6:2:46:LEU:HG	2.52	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
5:1:38:ILE:O	5:1:42:THR:HG23	2.17	0.45
15:L:308:UQ8:H22	15:L:308:UQ8:H25	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:45:ARG:NH2	6:B:6:LEU:O	2.49	0.45
13:3:103:BCL:H42	13:5:102:BCL:H151	1.99	0.45
20:I:104:PEF:O3P	5:K:18:ARG:NH1	2.50	0.45
5:Q:23:SER:HB2	22:Q:105:CDL:H132	1.99	0.45
13:W:102:BCL:H62	13:W:102:BCL:H41	1.72	0.45
15:7:104:UQ8:H15	15:7:104:UQ8:H12	1.71	0.44
2:L:182:HIS:CE1	2:L:186:ILE:HD11	2.52	0.44
13:L:301:BCL:HMB1	13:L:301:BCL:HBB3	2.00	0.44
4:H:17:TRP:CG	23:F:104:LMT:H61	2.52	0.44
22:H:302:CDL:H521	5:D:25:VAL:HG11	1.99	0.44
6:6:17:PHE:HA	19:6:101:CRT:H6	1.98	0.44
13:7:102:BCL:H43	6:8:28:TRP:CZ2	2.52	0.44
19:9:102:CRT:H20	19:9:102:CRT:H181	1.89	0.44
13:S:102:BCL:H102	13:S:102:BCL:H13	1.65	0.44
19:J:101:CRT:H20	19:J:101:CRT:H181	1.81	0.44
5:5:14:ILE:HG22	6:6:6:LEU:HD12	2.00	0.44
13:I:103:BCL:HAC2	6:J:45:TRP:CE3	2.52	0.44
22:K:104:CDL:H521	22:K:104:CDL:H362	1.99	0.44
5:9:35:ILE:O	5:9:39:VAL:HG23	2.17	0.44
3:M:157:TYR:CZ	19:M:407:CRT:H293	2.53	0.44
5:A:21:LEU:HD12	5:A:21:LEU:HA	1.83	0.44
13:A:101:BCL:H102	13:A:101:BCL:H13	1.80	0.44
13:A:103:BCL:H112	13:A:103:BCL:H152	1.66	0.44
14:L:302:BPH:H202	13:M:402:BCL:C2B	2.47	0.44
5:S:9:TYR:CE1	6:T:15:LYS:HG3	2.52	0.44
13:L:301:BCL:CGA	13:M:402:BCL:HBC1	2.48	0.44
5:I:46:TRP:CD2	13:I:102:BCL:HAC2	2.53	0.44
5:1:10:LYS:HD3	19:1:104:CRT:H31A	1.99	0.44
5:K:19:ARG:HD3	22:K:104:CDL:OA5	2.17	0.44
19:Z:101:CRT:H20	19:Z:101:CRT:H181	1.86	0.44
6:0:45:TRP:CD1	6:0:46:LEU:HG	2.53	0.44
1:C:248:THR:HA	1:C:251:HIS:O	2.17	0.43
19:Q:104:CRT:H10	19:Q:104:CRT:H81	1.86	0.43
21:I:105:LDA:H61	20:K:105:PEF:H311	2.00	0.43
13:1:103: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
2:L:190:PHE:CD2	14:M:405:BPH:HBB1	2.53	0.43
15:L:303:UQ8:H20A	15:L:303:UQ8:H22A	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
12:M:414:PGV:H281	12:M:414:PGV:H312	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:G:101:CRT:H372	5:I:36:HIS:CG	2.54	0.43
13:S:103:BCL:H61	13:S:103:BCL:H93	1.69	0.43
1:C:280:ASN:OD1	1:C:304:ARG:HB2	2.19	0.43
5:F:58:LEU:HD23	5:F:58:LEU:H	1.78	0.43
5:S:38:ILE:O	5:S:42:THR:HG23	2.18	0.43
5:7:36:HIS:CE1	13:7:103:BCL:HMD1	2.54	0.43
5:9:36:HIS:CG	19:9:103:CRT:H372	2.54	0.43
7:C:504:HEC:HBC3	7:C:504:HEC:HMC3	1.99	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
13:5:102:BCL:H62	13:5:102:BCL:H41	1.79	0.43
3:M:203:MET:HB3	13:M:402:BCL:O1D	2.18	0.43
18:M:406:MQ8:H441	18:M:406:MQ8:H412	1.78	0.43
19:A:104:CRT:H20	19:A:104:CRT:H181	1.89	0.43
5:S:36:HIS:CE1	13:S:103:BCL:HMD3	2.53	0.43
13:5:102:BCL:H202	13:5:102:BCL:H162	1.80	0.43
5:D:36:HIS:CG	19:9:102:CRT:H372	2.54	0.43
13:U:103:BCL:H141	6:V:45:TRP:HZ2	1.84	0.43
13:1:102:BCL:H142	13:1:102:BCL:H111	1.73	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:H40A	15:L:308:UQ8:H42A	1.91	0.43
19:M:407:CRT:H21A	15:M:418:UQ8:H1MA	2.01	0.43
13:K:103:BCL:O1A	19:N:101:CRT:H27	2.18	0.43
13:L:301:BCL:HAA2	13:M:402:BCL:HAC2	2.01	0.43
13:A:103:BCL:OBB	13:A:103:BCL:HHC	2.19	0.43
2:L:229:VAL:O	12:M:415:PGV:H261	2.19	0.42
4:H:205:LYS:HD2	4:H:205:LYS:HA	1.80	0.42
5:F:17:PRO:HB3	6:G:17:PHE:CZ	2.54	0.42
5:I:5:ASN:OD1	5:I:6:ALA:N	2.52	0.42
19:U:104:CRT:H371	13:Y:102:BCL:HMB2	2.01	0.42
13:1:103:BCL:H52	13:1:103:BCL:H12	1.77	0.42
6:0:45:TRP:CE3	13:0:102:BCL:HAC2	2.54	0.42
12:L:306:PGV:H81	12:L:306:PGV:H52	1.68	0.42
3:M:271:TRP:CZ2	20:M:419:PEF:H112	2.53	0.42
5:K:11:ILE:HD12	5:K:14:ILE:HD12	2.01	0.42
5:Q:13:LEU:O	6:R:6:LEU:HA	2.19	0.42
5:Q:17:PRO:HB3	6:R:17:PHE:CZ	2.54	0.42
6:8:27:ALA:O	6:8:31:LEU:HD13	2.19	0.42
13:M:402:BCL:H13	13:M:402:BCL:H172	1.89	0.42
6:2:9:LEU:HD22	6:2:14:ALA:CA	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:101:BCL:H62	13:A:101:BCL:H41	1.69	0.42
5:Q:36:HIS:NE2	13:Q:103:BCL:HMD3	2.34	0.42
13:5:102:BCL:H141	13:5:102:BCL:H161	1.67	0.42
2:L:41:CYS:HB2	15:7:104:UQ8:H1MA	2.02	0.42
4:H:8:TYR:CE1	23:F:104:LMT:H5B	2.55	0.42
15:L:303:UQ8:H25	15:L:303:UQ8:H22	1.74	0.42
3:M:8:PHE:CE2	22:M:416:CDL:H312	2.55	0.42
22:H:304:CDL:H862	22:H:304:CDL:H592	2.00	0.42
6:B:21:PHE:HA	19:9:102:CRT:H14	2.00	0.42
13:F:103:BCL:OBB	13:F:103:BCL:HHC	2.20	0.42
6:P:17:PHE:HA	19:P:101:CRT:H6	2.01	0.42
13:Q:102:BCL:H203	13:Q:102:BCL:H162	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
4:H:121:LYS:HD2	4:H:234:TYR:CB	2.46	0.42
13:U:102:BCL:H92	13:U:102:BCL:H61	1.87	0.42
13:5:103:BCL:H162	13:5:103:BCL:H192	1.76	0.42
5:9:50:ASN:CG	5:9:54:SER:HB2	2.44	0.42
3:M:196:LEU:HD12	3:M:196:LEU:HA	1.74	0.42
4:H:43:SER:HB2	12:A:105:PGV:O06	2.20	0.42
4:H:100:LEU:HD11	9:H:301:GOL:H12	2.02	0.42
13:D:102:BCL:H41	13:D:102:BCL:H62	1.90	0.42
13:S:103:BCL:HHC	13:S:103:BCL:OBB	2.20	0.42
12:L:306:PGV:H302	12:M:414:PGV:H262	2.02	0.41
5:I:5:ASN:HD22	6:N:20:ILE:HA	1.85	0.41
5:S:19:ARG:NE	22:S:104:CDL:OA4	2.43	0.41
13:U:102:BCL:HED1	6:V:28:TRP:CZ3	2.55	0.41
13:U:103:BCL:H2	6:V:29:PHE:CE1	2.55	0.41
19:U:104:CRT:H14	6:X:21:PHE:HA	2.02	0.41
6:8:29:PHE:O	6:8:33:VAL:HG23	2.20	0.41
2:L:30:PHE:CD2	22:H:304:CDL:H142	2.55	0.41
6:J:21:PHE:CD2	19:J:101:CRT:H14	2.55	0.41
22:K:104:CDL:H711	5:O:26:ALA:HB3	2.02	0.41
13:U:103:BCL:H92	6:V:32:VAL:HG12	2.00	0.41
13:I:102:BCL:H62	13:I:102:BCL:H41	1.82	0.41
13:O:102:BCL:H62	13:O:102:BCL:H41	1.87	0.41
1:C:110:CYS:O	1:C:124:LYS:HB2	2.20	0.41
3:M:97:PRO:HD3	3:M:176:PRO:HB3	2.02	0.41
6:G:45:TRP:CD1	6:G:46:LEU:HG	2.56	0.41
13:I:103:BCL:H192	13:I:103:BCL:H161	1.84	0.41
19:O:104:CRT:H10	19:O:104:CRT:H81	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:102:BCL:H143	13:Q:102:BCL:H112	1.77	0.41
5:Y:19:ARG:HD3	22:Y:103:CDL:HA32	2.03	0.41
13:Z:102:BCL:H112	13:Z:102:BCL:HMB2	2.02	0.41
19:2:101:CRT:H20	19:2:101:CRT:H181	1.86	0.41
5:7:21:LEU:HD21	19:9:103:CRT:C14	2.49	0.41
2:L:49:LEU:HD21	5:9:37:MET:HE3	2.03	0.41
5:3:36:HIS:NE2	13:3:103:BCL:HMD3	2.35	0.41
2:L:73:ILE:HD13	12:L:305:PGV:H272	2.01	0.41
3:M:89:HIS:O	3:M:93:LEU:HG	2.20	0.41
18:M:406:MQ8:H401	18:M:406:MQ8:H362	1.82	0.41
4:H:44:ASP:HB2	12:A:105:PGV:H062	2.02	0.41
5:A:50:ASN:CG	5:A:54:SER:HB2	2.46	0.41
19:A:104:CRT:H26	19:A:104:CRT:H241	1.94	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
19:M:407:CRT:H10	19:M:407:CRT:H81	1.92	0.41
13:D:103:BCL:H151	13:D:103:BCL:H18	1.74	0.41
5:O:33:LEU:O	5:O:37[A]:MET:HG3	2.20	0.41
13:Q:103:BCL:HMB3	13:S:102:BCL:CHB	2.51	0.41
13:O:102:BCL:H8	13:O:102:BCL:H51	1.77	0.41
13:Y:102:BCL:H141	13:Y:102:BCL:H161	1.94	0.41
13:Z:102:BCL:H12	13:Z:102:BCL:H52	1.71	0.41
6:2:21:PHE:HA	19:2:101:CRT:H11	2.03	0.41
4:H:58:PHE:CD1	4:H:59:PRO:HA	2.56	0.41
22:H:302:CDL:H772	22:H:302:CDL:H742	1.95	0.41
22:S:104:CDL:C51	22:S:104:CDL:C72	2.99	0.41
6:Z:43:ARG:HG3	5:1:55:TYR:CZ	2.56	0.41
13:3:103:BCL:H93	13:3:103:BCL:H111	1.86	0.41
19:0:101:CRT:H27	13:0:102:BCL:O1A	2.21	0.41
12:L:305:PGV:H231	12:L:305:PGV:H52	2.03	0.41
12:L:306:PGV:C11	15:L:308:UQ8:H23	2.51	0.41
25:M:584:HOH:O	4:H:122:HIS:HE1	2.04	0.41
13:I:103:BCL:H111	13:I:103:BCL:H152	1.88	0.41
5:K:36:HIS:CE1	13:K:103:BCL:HMD1	2.56	0.41
13:U:102:BCL:H43	6:V:28:TRP:CZ2	2.56	0.41
13:Z:102:BCL:H141	13:Z:102:BCL:H162	1.73	0.41
13:5:103:BCL:H142	13:5:103:BCL:H111	1.80	0.41
13:0:102:BCL:HHC	13:0:102:BCL:OBB	2.21	0.41
13:S:103:BCL:H111	13:S:103:BCL:H91	1.78	0.40
13:3:102:BCL:H41	13:3:102:BCL:H62	1.79	0.40
5:7:35:ILE:HD12	13:7:103:BCL:O1D	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:7:103:BCL:H152	13:7:103:BCL:H112	1.54	0.40
5:D:36:HIS:NE2	13:D:103:BCL:HMD3	2.35	0.40
13:O:103:BCL:HHC	13:O:103:BCL:OBB	2.21	0.40
5:W:13:LEU:O	6:X:6:LEU:HB3	2.21	0.40
6:2:9:LEU:HD21	6:2:13:GLU:CB	2.51	0.40
19:2:101:CRT:H15	19:2:101:CRT:H131	1.98	0.40
5:9:29:ILE:HG13	13:9:104:BCL:H43	2.04	0.40
19:9:102:CRT:H36	19:9:102:CRT:H341	1.89	0.40
19:M:407:CRT:H26	19:M:407:CRT:H241	1.96	0.40
6:B:43:ARG:HG3	5:D:55:TYR:CE1	2.57	0.40
13:W:103:BCL:H121	13:W:103:BCL:H161	1.79	0.40
13:7:102:BCL:H61	13:7:102:BCL:H41	1.90	0.40
13:7:103:BCL:HED3	13:7:103:BCL:HBA2	2.04	0.40
25:H:431:HOH:O	21:I:105:LDA:HM13	2.21	0.40
13:A:101:BCL:HMB2	19:0:101:CRT:H371	2.03	0.40
13:O:102:BCL:H43	6:P:28:TRP:CZ2	2.56	0.40
19:2:101:CRT:C35	13:3:102: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 ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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
3	M	318/325 (98%)	311 (98%)	5 (2%)	2 (1%)	21	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
6	V	40/47 (85%)	40 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	48	40

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%)	257 (99%)	3 (1%)	63	63
2	L	229/229 (100%)	227 (99%)	2 (1%)	70	73
3	M	258/261 (99%)	257 (100%)	1 (0%)	84	87
4	H	211/211 (100%)	210 (100%)	1 (0%)	81	84
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%)	50	47
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%)	49 (96%)	2 (4%)	28	21
5	I	53/56 (95%)	53 (100%)	0	100	100
5	K	52/56 (93%)	51 (98%)	1 (2%)	50	47
5	O	52/56 (93%)	51 (98%)	1 (2%)	50	47
5	Q	52/56 (93%)	52 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	S	55/56 (98%)	53 (96%)	2 (4%)	31	23
5	U	53/56 (95%)	53 (100%)	0	100	100
5	W	51/56 (91%)	51 (100%)	0	100	100
5	Y	52/56 (93%)	51 (98%)	1 (2%)	50	47
6	0	36/39 (92%)	35 (97%)	1 (3%)	38	32
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%)	33 (94%)	2 (6%)	18	11
6	N	35/39 (90%)	35 (100%)	0	100	100
6	P	35/39 (90%)	34 (97%)	1 (3%)	37	31
6	R	34/39 (87%)	34 (100%)	0	100	100
6	T	36/39 (92%)	35 (97%)	1 (3%)	38	32
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%)	2318 (99%)	20 (1%)	70	73

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	163	LYS
1	C	212	ILE
1	C	333	THR
2	L	256	CYS
2	L	280	LEU
3	M	216	PHE
4	H	237	ASP
5	F	14	ILE
5	F	58	LEU
6	J	6	LEU

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Mol	Chain	Res	Type
6	J	41	LEU
5	K	22	VAL
5	O	53	VAL
6	P	6	LEU
5	S	8	LEU
5	S	25	VAL
6	T	31	LEU
5	Y	8	LEU
5	9	53	VAL
6	0	31	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	57	GLN
2	L	172	GLN
2	L	210	GLN
5	I	7	ASN
5	K	7	ASN
5	Y	50	ASN
5	1	7	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 144 ligands modelled in this entry, 18 are monoatomic and 16 are unknown - 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$
13	BCL	F	102	-	69,74,74	1.84	16 (23%)	79,115,115	2.17	24 (30%)
13	BCL	M	404	-	69,74,74	1.69	15 (21%)	79,115,115	1.94	18 (22%)
20	PEF	K	105	-	26,26,46	1.25	2 (7%)	29,31,51	1.47	4 (13%)
19	CRT	J	101	-	43,43,43	0.74	0	48,54,54	1.81	13 (27%)
9	GOL	H	301	-	5,5,5	0.91	0	5,5,5	1.02	0
15	UQ8	M	418	-	18,18,53	2.14	2 (11%)	24,25,67	1.50	5 (20%)
12	PGV	D	105	-	34,34,50	1.07	3 (8%)	37,40,56	1.22	5 (13%)
21	LDA	M	412	-	11,13,15	2.33	2 (18%)	12,15,17	0.48	0
13	BCL	3	103	-	69,74,74	1.83	15 (21%)	79,115,115	2.07	19 (24%)
12	PGV	M	415	-	36,36,50	1.08	2 (5%)	39,42,56	1.22	4 (10%)
20	PEF	U	105	-	4,4,46	2.62	2 (50%)	6,6,51	1.93	2 (33%)
20	PEF	U	106	-	4,4,46	2.74	2 (50%)	6,6,51	1.91	2 (33%)
21	LDA	I	105	-	13,15,15	2.18	2 (15%)	14,17,17	0.45	0
20	PEF	M	408	-	4,4,46	2.71	2 (50%)	6,6,51	1.89	2 (33%)
13	BCL	0	102	-	69,74,74	1.82	15 (21%)	79,115,115	2.13	22 (27%)
13	BCL	S	102	-	69,74,74	1.86	16 (23%)	79,115,115	2.18	23 (29%)
15	UQ8	L	309	-	18,18,53	2.14	2 (11%)	24,25,67	1.07	2 (8%)
7	HEC	C	502	1	46,50,50	1.71	8 (17%)	58,82,82	1.61	12 (20%)
12	PGV	H	303	-	35,35,50	1.11	2 (5%)	38,41,56	1.29	4 (10%)
13	BCL	3	102	-	69,74,74	1.80	17 (24%)	79,115,115	2.13	23 (29%)
22	CDL	Y	104	-	12,12,99	0.48	0	13,15,111	0.51	0
19	CRT	A	104	-	43,43,43	0.68	0	48,54,54	1.75	13 (27%)
10	SO4	C	507	-	4,4,4	0.24	0	6,6,6	0.13	0
18	MQ8	M	406	-	54,54,54	1.40	3 (5%)	67,69,69	1.48	15 (22%)
19	CRT	O	104	-	43,43,43	0.78	0	48,54,54	1.80	13 (27%)
20	PEF	3	104	-	4,4,46	2.71	2 (50%)	6,6,51	1.95	2 (33%)
22	CDL	S	104	-	61,61,99	1.11	5 (8%)	67,73,111	1.35	8 (11%)
13	BCL	O	103	-	69,74,74	1.78	14 (20%)	79,115,115	2.00	19 (24%)
15	UQ8	7	104	-	33,33,53	1.46	3 (9%)	42,43,67	2.12	16 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CRT	Z	101	-	43,43,43	0.65	0	48,54,54	2.00	14 (29%)
21	LDA	O	105	-	11,13,15	2.32	2 (18%)	12,15,17	0.47	0
19	CRT	6	101	-	43,43,43	0.72	0	48,54,54	1.77	11 (22%)
19	CRT	2	101	-	43,43,43	0.70	0	48,54,54	1.80	12 (25%)
20	PEF	W	104	-	4,4,46	2.73	2 (50%)	6,6,51	1.90	2 (33%)
12	PGV	M	414	-	45,45,50	1.06	2 (4%)	48,50,56	0.97	4 (8%)
19	CRT	Q	104	-	43,43,43	0.75	1 (2%)	48,54,54	1.83	8 (16%)
13	BCL	A	103	-	69,74,74	1.83	16 (23%)	79,115,115	2.08	20 (25%)
13	BCL	Z	102	-	69,74,74	1.80	15 (21%)	79,115,115	2.15	19 (24%)
21	LDA	V	102	-	13,15,15	2.15	2 (15%)	14,17,17	0.37	0
13	BCL	D	103	-	69,74,74	1.82	15 (21%)	79,115,115	2.13	18 (22%)
19	CRT	P	101	-	43,43,43	0.79	0	48,54,54	1.76	12 (25%)
13	BCL	5	103	-	69,74,74	1.79	16 (23%)	79,115,115	2.05	20 (25%)
22	CDL	Q	105	-	74,74,99	1.09	4 (5%)	80,86,111	1.15	8 (10%)
13	BCL	F	103	-	69,74,74	1.82	15 (21%)	79,115,115	2.10	19 (24%)
13	BCL	K	102	-	69,74,74	1.82	16 (23%)	79,115,115	2.19	23 (29%)
7	HEC	C	504	1	46,50,50	1.69	7 (15%)	58,82,82	1.70	11 (18%)
13	BCL	I	102	-	69,74,74	1.82	16 (23%)	79,115,115	2.20	22 (27%)
12	PGV	L	306	-	43,43,50	0.99	2 (4%)	46,49,56	1.14	3 (6%)
9	GOL	C	506	-	5,5,5	0.94	0	5,5,5	0.93	0
13	BCL	K	103	-	69,74,74	1.83	15 (21%)	79,115,115	2.14	19 (24%)
13	BCL	W	103	-	69,74,74	1.81	15 (21%)	79,115,115	2.04	18 (22%)
19	CRT	0	101	-	43,43,43	0.69	0	48,54,54	1.80	9 (18%)
19	CRT	M	407	-	43,43,43	0.87	0	48,54,54	1.77	11 (22%)
20	PEF	I	104	-	4,4,46	2.71	2 (50%)	6,6,51	1.88	2 (33%)
22	CDL	H	302	-	63,63,99	1.09	4 (6%)	69,75,111	1.35	9 (13%)
13	BCL	W	102	-	69,74,74	1.79	16 (23%)	79,115,115	2.35	24 (30%)
22	CDL	M	416	-	38,38,99	1.32	3 (7%)	43,49,111	1.20	3 (6%)
13	BCL	1	102	-	69,74,74	1.82	17 (24%)	79,115,115	2.21	23 (29%)
12	PGV	3	105	-	50,50,50	0.95	2 (4%)	53,56,56	0.93	3 (5%)
21	LDA	J	102	-	13,15,15	2.15	2 (15%)	14,17,17	0.44	0
10	SO4	M	413	-	4,4,4	0.24	0	6,6,6	0.11	0
11	LHG	C	508	-	7,8,48	0.34	0	6,7,54	0.43	0
13	BCL	U	103	-	69,74,74	1.85	15 (21%)	79,115,115	2.04	20 (25%)
19	CRT	1	104	-	43,43,43	0.70	0	48,54,54	1.71	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BCL	U	102	-	69,74,74	1.77	16 (23%)	79,115,115	2.12	23 (29%)
23	LMT	F	104	-	36,36,36	0.49	0	47,47,47	1.46	9 (19%)
13	BCL	Q	102	-	69,74,74	1.78	15 (21%)	79,115,115	2.12	26 (32%)
10	SO4	L	304	-	4,4,4	0.23	0	6,6,6	0.06	0
22	CDL	H	304	-	78,78,99	1.04	4 (5%)	84,90,111	1.16	8 (9%)
13	BCL	I	103	-	69,74,74	1.82	16 (23%)	79,115,115	2.06	21 (26%)
13	BCL	7	103	-	69,74,74	1.77	16 (23%)	79,115,115	1.97	20 (25%)
13	BCL	M	402	-	69,74,74	1.80	16 (23%)	79,115,115	2.03	25 (31%)
12	PGV	A	105	-	32,32,50	1.18	2 (6%)	35,38,56	1.20	3 (8%)
13	BCL	7	102	-	64,69,74	1.85	16 (25%)	73,109,115	2.26	22 (30%)
22	CDL	D	104	-	39,39,99	1.45	4 (10%)	45,51,111	1.32	7 (15%)
13	BCL	5	102	-	69,74,74	1.75	16 (23%)	79,115,115	2.20	24 (30%)
13	BCL	O	102	-	69,74,74	1.78	16 (23%)	79,115,115	2.25	24 (30%)
13	BCL	D	102	-	69,74,74	1.80	16 (23%)	79,115,115	2.23	21 (26%)
13	BCL	Y	102	-	69,74,74	1.80	16 (23%)	79,115,115	2.28	25 (31%)
20	PEF	M	419	-	46,46,46	0.96	2 (4%)	49,51,51	1.08	3 (6%)
20	PEF	M	409	-	4,4,46	1.90	2 (50%)	6,6,51	1.22	1 (16%)
14	BPH	M	405	-	59,70,70	2.51	13 (22%)	59,101,101	2.31	22 (37%)
13	BCL	S	103	-	69,74,74	1.78	15 (21%)	79,115,115	2.04	20 (25%)
19	CRT	9	102	-	43,43,43	0.72	0	48,54,54	1.88	15 (31%)
20	PEF	5	104	-	4,4,46	2.72	2 (50%)	6,6,51	1.86	2 (33%)
20	PEF	M	410	-	4,4,46	2.74	2 (50%)	6,6,51	1.91	2 (33%)
19	CRT	V	101	-	43,43,43	0.71	0	48,54,54	1.86	13 (27%)
22	CDL	K	104	-	85,85,99	1.00	4 (4%)	91,97,111	1.19	9 (9%)
22	CDL	Y	103	-	39,39,99	1.48	4 (10%)	45,51,111	1.22	4 (8%)
20	PEF	1	105	-	4,4,46	2.80	2 (50%)	6,6,51	1.88	2 (33%)
15	UQ8	L	303	-	33,33,53	1.67	2 (6%)	42,43,67	1.52	7 (16%)
19	CRT	U	104	-	43,43,43	0.71	0	48,54,54	1.95	14 (29%)
15	UQ8	L	308	-	53,53,53	1.23	2 (3%)	66,67,67	1.69	20 (30%)
14	BPH	L	302	-	59,70,70	2.46	14 (23%)	59,101,101	2.14	18 (30%)
20	PEF	M	411	-	4,4,46	2.46	1 (25%)	6,6,51	1.45	1 (16%)
13	BCL	L	301	-	69,74,74	1.74	14 (20%)	79,115,115	1.79	18 (22%)
7	HEC	C	501	1	46,50,50	1.68	9 (19%)	58,82,82	1.64	13 (22%)
7	HEC	C	503	1	46,50,50	1.68	10 (21%)	58,82,82	1.77	12 (20%)
12	PGV	1	106	-	30,30,50	1.21	2 (6%)	33,36,56	1.20	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BCL	9	104	-	69,74,74	1.78	15 (21%)	79,115,115	2.20	21 (26%)
23	LMT	M	420	-	36,36,36	0.47	1 (2%)	47,47,47	0.94	3 (6%)
12	PGV	C	509	-	20,20,50	1.45	3 (15%)	22,22,56	1.53	3 (13%)
19	CRT	G	101	-	43,43,43	0.69	0	48,54,54	1.83	13 (27%)
12	PGV	L	305	-	42,42,50	1.04	2 (4%)	45,48,56	1.27	3 (6%)
13	BCL	A	101	-	69,74,74	1.81	16 (23%)	79,115,115	2.16	24 (30%)
19	CRT	N	101	-	43,43,43	0.67	0	48,54,54	1.99	14 (29%)
13	BCL	Q	103	-	69,74,74	1.83	15 (21%)	79,115,115	2.04	19 (24%)
19	CRT	9	103	-	43,43,43	0.70	0	48,54,54	1.82	11 (22%)
13	BCL	1	103	-	69,74,74	1.82	15 (21%)	79,115,115	2.19	21 (26%)
13	BCL	M	403	-	69,74,74	1.78	14 (20%)	79,115,115	2.09	23 (29%)

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
13	BCL	F	102	-	-	13/41/137/137	-
13	BCL	M	404	-	-	4/41/137/137	-
20	PEF	K	105	-	-	3/30/30/50	-
19	CRT	J	101	-	-	1/51/51/51	-
9	GOL	H	301	-	-	0/4/4/4	-
15	UQ8	M	418	-	-	1/9/33/75	0/1/1/1
12	PGV	D	105	-	-	11/39/39/55	-
21	LDA	M	412	-	-	5/11/11/13	-
13	BCL	3	103	-	-	17/41/137/137	-
12	PGV	M	415	-	-	16/41/41/55	-
21	LDA	I	105	-	-	4/13/13/13	-
13	BCL	0	102	-	-	7/41/137/137	-
13	BCL	S	102	-	-	8/41/137/137	-
15	UQ8	L	309	-	-	1/9/33/75	0/1/1/1
7	HEC	C	502	1	-	8/14/54/54	-
12	PGV	H	303	-	-	16/40/40/55	-
13	BCL	3	102	-	-	18/41/137/137	-
22	CDL	Y	104	-	-	7/13/13/110	-
19	CRT	A	104	-	-	0/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	MQ8	M	406	-	-	2/47/67/67	0/2/2/2
19	CRT	O	104	-	-	4/51/51/51	-
22	CDL	S	104	-	-	28/71/71/110	-
13	BCL	O	103	-	-	16/41/137/137	-
15	UQ8	7	104	-	-	9/27/51/75	0/1/1/1
19	CRT	Z	101	-	-	0/51/51/51	-
21	LDA	O	105	-	-	8/11/11/13	-
19	CRT	6	101	-	-	0/51/51/51	-
19	CRT	2	101	-	-	2/51/51/51	-
12	PGV	M	414	-	-	16/47/47/55	-
19	CRT	Q	104	-	-	3/51/51/51	-
13	BCL	A	103	-	-	10/41/137/137	-
13	BCL	Z	102	-	-	15/41/137/137	-
21	LDA	V	102	-	-	5/13/13/13	-
13	BCL	D	103	-	-	7/41/137/137	-
19	CRT	P	101	-	-	0/51/51/51	-
13	BCL	5	103	-	-	13/41/137/137	-
22	CDL	Q	105	-	-	37/85/85/110	-
13	BCL	F	103	-	-	11/41/137/137	-
13	BCL	K	102	-	-	13/41/137/137	-
7	HEC	C	504	1	-	7/14/54/54	-
13	BCL	I	102	-	-	7/41/137/137	-
12	PGV	L	306	-	-	17/48/48/55	-
9	GOL	C	506	-	-	2/4/4/4	-
13	BCL	K	103	-	-	14/41/137/137	-
13	BCL	W	103	-	-	8/41/137/137	-
19	CRT	0	101	-	-	5/51/51/51	-
19	CRT	M	407	-	-	6/51/51/51	-
22	CDL	H	302	-	-	23/73/73/110	-
13	BCL	W	102	-	-	10/41/137/137	-
22	CDL	M	416	-	-	12/48/48/110	-
13	BCL	1	102	-	-	15/41/137/137	-
12	PGV	3	105	-	-	16/55/55/55	-
21	LDA	J	102	-	-	3/13/13/13	-
11	LHG	C	508	-	-	1/6/6/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCL	U	103	-	-	14/41/137/137	-
19	CRT	1	104	-	-	1/51/51/51	-
13	BCL	U	102	-	-	3/41/137/137	-
23	LMT	F	104	-	-	9/21/61/61	0/2/2/2
13	BCL	Q	102	-	-	15/41/137/137	-
22	CDL	H	304	-	-	20/89/89/110	-
13	BCL	I	103	-	-	10/41/137/137	-
13	BCL	7	103	-	-	13/41/137/137	-
13	BCL	M	402	-	-	3/41/137/137	-
12	PGV	A	105	-	-	13/37/37/55	-
13	BCL	7	102	-	-	6/35/131/137	-
22	CDL	D	104	-	-	17/50/50/110	-
13	BCL	5	102	-	-	11/41/137/137	-
13	BCL	O	102	-	-	5/41/137/137	-
13	BCL	D	102	-	-	10/41/137/137	-
13	BCL	Y	102	-	-	11/41/137/137	-
20	PEF	M	419	-	-	19/50/50/50	-
14	BPH	M	405	-	-	7/37/105/105	0/5/6/6
13	BCL	S	103	-	-	17/41/137/137	-
19	CRT	9	102	-	-	5/51/51/51	-
19	CRT	V	101	-	-	6/51/51/51	-
22	CDL	K	104	-	-	30/96/96/110	-
22	CDL	Y	103	-	-	24/50/50/110	-
15	UQ8	L	303	-	-	3/27/51/75	0/1/1/1
19	CRT	U	104	-	-	3/51/51/51	-
15	UQ8	L	308	-	-	10/51/75/75	0/1/1/1
14	BPH	L	302	-	-	6/37/105/105	0/5/6/6
13	BCL	L	301	-	-	1/41/137/137	-
7	HEC	C	501	1	-	6/14/54/54	-
7	HEC	C	503	1	-	4/14/54/54	-
12	PGV	1	106	-	-	8/35/35/55	-
13	BCL	9	104	-	-	16/41/137/137	-
23	LMT	M	420	-	-	6/21/61/61	0/2/2/2
12	PGV	C	509	-	-	4/21/21/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CRT	G	101	-	-	2/51/51/51	-
12	PGV	L	305	-	-	13/47/47/55	-
13	BCL	A	101	-	-	14/41/137/137	-
19	CRT	N	101	-	-	0/51/51/51	-
13	BCL	Q	103	-	-	9/41/137/137	-
19	CRT	9	103	-	-	4/51/51/51	-
13	BCL	1	103	-	-	12/41/137/137	-
13	BCL	M	403	-	-	13/41/137/137	-

All (724) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	405	BPH	C1B-C2B	9.32	1.49	1.39
14	M	405	BPH	C1D-C2D	9.00	1.49	1.39
14	L	302	BPH	C1B-C2B	8.87	1.49	1.39
15	L	303	UQ8	C6-C1	8.19	1.49	1.35
15	M	418	UQ8	C6-C1	7.90	1.49	1.35
15	L	309	UQ8	C6-C1	7.86	1.49	1.35
18	M	406	MQ8	C3-C2	7.62	1.48	1.35
14	L	302	BPH	C1D-C2D	7.47	1.47	1.39
15	L	308	UQ8	C6-C1	7.25	1.48	1.35
21	O	105	LDA	O1-N1	-6.82	1.25	1.42
21	M	412	LDA	O1-N1	-6.77	1.25	1.42
21	J	102	LDA	O1-N1	-6.77	1.25	1.42
21	V	102	LDA	O1-N1	-6.77	1.25	1.42
15	7	104	UQ8	C6-C1	6.67	1.47	1.35
21	I	105	LDA	O1-N1	-6.40	1.26	1.42
14	L	302	BPH	C3B-C4B	6.00	1.51	1.41
13	M	402	BCL	C3B-C4B	5.90	1.52	1.41
18	M	406	MQ8	C10-C5	5.55	1.49	1.40
14	M	405	BPH	C4D-CHA	5.39	1.47	1.39
13	S	102	BCL	C3B-C4B	5.36	1.51	1.41
14	L	302	BPH	C4D-CHA	5.35	1.47	1.39
14	M	405	BPH	C3B-C4B	5.25	1.49	1.41
13	U	103	BCL	C3B-C4B	5.24	1.51	1.41
13	K	103	BCL	O2D-CGD	5.23	1.46	1.33
14	L	302	BPH	C3D-C2D	5.19	1.48	1.39
13	U	103	BCL	O2D-CGD	5.14	1.45	1.33
13	M	403	BCL	C1D-ND	-5.10	1.31	1.37
13	1	103	BCL	O2D-CGD	5.09	1.45	1.33
13	7	103	BCL	O2D-CGD	5.07	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	103	BCL	O2D-CGD	5.05	1.45	1.33
13	1	102	BCL	O2D-CGD	5.04	1.45	1.33
14	M	405	BPH	O2D-CGD	5.01	1.45	1.33
13	W	103	BCL	O2D-CGD	5.00	1.45	1.33
13	3	102	BCL	O2D-CGD	5.00	1.45	1.33
14	L	302	BPH	C3B-C2B	4.99	1.48	1.39
13	F	103	BCL	O2D-CGD	4.99	1.45	1.33
13	A	101	BCL	C3B-C4B	4.98	1.51	1.41
13	0	102	BCL	O2D-CGD	4.91	1.45	1.33
13	3	103	BCL	O2D-CGD	4.91	1.45	1.33
13	I	102	BCL	O2D-CGD	4.90	1.45	1.33
13	Q	103	BCL	C3B-C4B	4.90	1.50	1.41
13	D	103	BCL	O2D-CGD	4.88	1.45	1.33
13	I	103	BCL	O2D-CGD	4.88	1.45	1.33
13	Q	102	BCL	C3B-C4B	4.86	1.50	1.41
20	1	105	PEF	P-O1P	4.82	1.61	1.50
13	W	103	BCL	C3B-C4B	4.80	1.50	1.41
13	L	301	BCL	C1D-ND	-4.80	1.31	1.37
13	D	103	BCL	C3B-C4B	4.79	1.50	1.41
13	F	102	BCL	O2D-CGD	4.78	1.45	1.33
13	5	102	BCL	O2D-CGD	4.77	1.44	1.33
13	5	103	BCL	C3B-C4B	4.76	1.50	1.41
13	Q	102	BCL	O2D-CGD	4.76	1.44	1.33
13	1	103	BCL	C3B-C4B	4.75	1.50	1.41
13	S	103	BCL	C3B-C4B	4.74	1.50	1.41
13	Z	102	BCL	O2D-CGD	4.71	1.44	1.33
13	S	103	BCL	O2D-CGD	4.71	1.44	1.33
13	7	102	BCL	C3B-C4B	4.71	1.50	1.41
13	K	103	BCL	C3B-C4B	4.71	1.50	1.41
13	A	101	BCL	O2D-CGD	4.70	1.44	1.33
13	O	103	BCL	C3B-C4B	4.70	1.50	1.41
20	U	106	PEF	P-O1P	4.70	1.61	1.50
13	D	102	BCL	O2D-CGD	4.69	1.44	1.33
20	W	104	PEF	P-O1P	4.69	1.61	1.50
20	M	410	PEF	P-O1P	4.69	1.61	1.50
13	O	102	BCL	C3B-C4B	4.68	1.50	1.41
20	3	104	PEF	P-O1P	4.68	1.61	1.50
13	S	103	BCL	CHC-C4B	4.68	1.49	1.39
20	M	408	PEF	P-O1P	4.67	1.61	1.50
13	7	102	BCL	O2D-CGD	4.67	1.44	1.33
13	0	102	BCL	C3B-C4B	4.66	1.50	1.41
13	3	103	BCL	C3B-C4B	4.66	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	W	102	BCL	O2D-CGD	4.66	1.44	1.33
13	1	102	BCL	C3B-C4B	4.64	1.50	1.41
13	F	102	BCL	C3B-C4B	4.64	1.50	1.41
20	5	104	PEF	P-O1P	4.64	1.61	1.50
13	7	103	BCL	C3B-C4B	4.64	1.50	1.41
13	D	102	BCL	C3B-C4B	4.63	1.50	1.41
13	I	103	BCL	C3B-C4B	4.63	1.50	1.41
7	C	504	HEC	CAC-C3C	4.63	1.50	1.35
13	O	102	BCL	O2D-CGD	4.62	1.44	1.33
20	I	104	PEF	P-O1P	4.62	1.61	1.50
13	Y	102	BCL	O2D-CGD	4.62	1.44	1.33
13	M	403	BCL	C3B-C4B	4.61	1.50	1.41
13	O	103	BCL	C1D-ND	-4.61	1.31	1.37
12	L	305	PGV	O01-C1	4.58	1.47	1.34
13	S	102	BCL	CHC-C4B	4.58	1.49	1.39
13	I	102	BCL	C3B-C4B	4.58	1.50	1.41
22	Q	105	CDL	OA8-CA7	4.57	1.46	1.33
13	3	102	BCL	C3B-C4B	4.57	1.50	1.41
13	Q	103	BCL	O2D-CGD	4.56	1.44	1.33
13	Z	102	BCL	C3B-C4B	4.56	1.50	1.41
22	M	416	CDL	OA8-CA7	4.55	1.46	1.33
13	K	102	BCL	O2D-CGD	4.55	1.44	1.33
13	5	103	BCL	O2D-CGD	4.55	1.44	1.33
13	U	102	BCL	C3B-C4B	4.55	1.50	1.41
13	L	301	BCL	C3B-C4B	4.54	1.50	1.41
7	C	503	HEC	CAC-C3C	4.54	1.49	1.35
20	M	411	PEF	P-O1P	4.54	1.61	1.50
13	M	404	BCL	C3B-C4B	4.52	1.50	1.41
13	M	403	BCL	CHC-C4B	4.51	1.49	1.39
13	O	103	BCL	O2D-CGD	4.51	1.44	1.33
12	M	414	PGV	O03-C19	4.51	1.46	1.33
13	9	104	BCL	C3B-C4B	4.51	1.50	1.41
22	H	304	CDL	OA6-CA5	4.51	1.47	1.34
13	5	102	BCL	C3B-C4B	4.50	1.50	1.41
12	H	303	PGV	O03-C19	4.50	1.46	1.33
21	I	105	LDA	C1-N1	-4.49	1.46	1.51
22	H	302	CDL	OA6-CA5	4.49	1.47	1.34
13	S	102	BCL	O2D-CGD	4.49	1.44	1.33
13	Q	103	BCL	CHB-C1B	4.48	1.49	1.39
13	M	403	BCL	CHB-C1B	4.48	1.49	1.39
13	L	301	BCL	O2D-CGD	4.48	1.44	1.33
13	K	102	BCL	C3B-C4B	4.47	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	9	104	BCL	CHC-C4B	4.47	1.49	1.39
13	S	102	BCL	OBD-CAD	4.46	1.30	1.22
7	C	504	HEC	CAB-C3B	4.46	1.49	1.35
13	1	103	BCL	O2A-CGA	4.45	1.46	1.33
13	U	103	BCL	CHC-C4B	4.45	1.49	1.39
13	A	103	BCL	C3B-C4B	4.44	1.49	1.41
13	K	103	BCL	CHC-C4B	4.44	1.49	1.39
13	U	102	BCL	O2D-CGD	4.43	1.44	1.33
13	O	102	BCL	O2A-CGA	4.43	1.46	1.33
13	M	402	BCL	O2A-CGA	4.43	1.46	1.33
13	Y	102	BCL	O2A-CGA	4.43	1.46	1.33
20	U	105	PEF	P-O1P	4.43	1.60	1.50
13	W	103	BCL	C1D-ND	-4.42	1.32	1.37
13	U	103	BCL	C1D-ND	-4.42	1.32	1.37
13	I	102	BCL	CHD-C1D	4.41	1.47	1.38
13	F	102	BCL	O2A-CGA	4.40	1.46	1.33
13	5	103	BCL	CHC-C4B	4.40	1.49	1.39
13	U	102	BCL	CHC-C4B	4.40	1.49	1.39
13	Y	102	BCL	C3B-C4B	4.39	1.49	1.41
13	Q	103	BCL	CHC-C4B	4.39	1.49	1.39
14	L	302	BPH	O2D-CGD	4.39	1.44	1.33
7	C	502	HEC	CAB-C3B	4.39	1.49	1.35
13	9	104	BCL	O2D-CGD	4.39	1.44	1.33
13	F	103	BCL	O2A-CGA	4.38	1.46	1.33
13	I	102	BCL	O2A-CGA	4.37	1.46	1.33
22	Y	103	CDL	OA8-CA7	4.37	1.46	1.33
13	O	103	BCL	CHC-C4B	4.37	1.49	1.39
13	Q	103	BCL	OBD-CAD	4.37	1.30	1.22
13	L	301	BCL	CHB-C1B	4.37	1.49	1.39
22	H	302	CDL	OB8-CB7	4.36	1.46	1.33
13	F	103	BCL	C3B-C4B	4.36	1.49	1.41
13	A	103	BCL	O2A-CGA	4.35	1.46	1.33
12	A	105	PGV	O03-C19	4.34	1.46	1.33
13	K	102	BCL	O2A-CGA	4.34	1.46	1.33
22	Q	105	CDL	OB8-CB7	4.34	1.46	1.33
22	H	304	CDL	OA8-CA7	4.34	1.46	1.33
13	M	402	BCL	O2D-CGD	4.33	1.43	1.33
12	1	106	PGV	O03-C19	4.32	1.46	1.33
13	3	102	BCL	O2A-CGA	4.32	1.45	1.33
22	Y	103	CDL	OB8-CB7	4.32	1.45	1.33
20	M	419	PEF	O3-C30	4.32	1.45	1.33
13	1	102	BCL	O2A-CGA	4.32	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	104	CDL	OB8-CB7	4.32	1.45	1.33
13	7	102	BCL	O2A-CGA	4.31	1.45	1.33
22	Y	103	CDL	OB6-CB5	4.31	1.46	1.34
13	M	404	BCL	CHC-C4B	4.31	1.49	1.39
13	W	102	BCL	C3B-C4B	4.30	1.49	1.41
13	Q	103	BCL	CHD-C1D	4.30	1.46	1.38
13	F	103	BCL	C1D-ND	-4.30	1.32	1.37
13	W	103	BCL	O2A-CGA	4.30	1.45	1.33
13	5	102	BCL	O2A-CGA	4.30	1.45	1.33
13	I	103	BCL	CHC-C4B	4.29	1.49	1.39
13	I	103	BCL	O2A-CGA	4.29	1.45	1.33
7	C	501	HEC	CAC-C3C	4.29	1.48	1.35
13	1	102	BCL	CHD-C1D	4.29	1.46	1.38
13	S	102	BCL	O2A-CGA	4.29	1.45	1.33
13	Q	102	BCL	CHC-C4B	4.29	1.49	1.39
13	3	103	BCL	O2A-CGA	4.29	1.45	1.33
12	1	106	PGV	O01-C1	4.29	1.46	1.34
13	O	103	BCL	O2A-CGA	4.28	1.45	1.33
12	3	105	PGV	O01-C1	4.28	1.46	1.34
22	Y	103	CDL	OA6-CA5	4.28	1.46	1.34
12	L	306	PGV	O03-C19	4.28	1.45	1.33
13	Z	102	BCL	O2A-CGA	4.27	1.45	1.33
13	I	103	BCL	C1D-ND	-4.27	1.32	1.37
13	3	103	BCL	CHC-C4B	4.26	1.49	1.39
22	D	104	CDL	OB8-CB7	4.26	1.45	1.33
13	3	103	BCL	OBD-CAD	4.25	1.29	1.22
13	A	101	BCL	CHD-C1D	4.25	1.46	1.38
22	D	104	CDL	OA6-CA5	4.24	1.46	1.34
22	K	104	CDL	OA6-CA5	4.24	1.46	1.34
13	A	103	BCL	C1D-ND	-4.24	1.32	1.37
13	3	102	BCL	CHD-C1D	4.24	1.46	1.38
13	D	102	BCL	O2A-CGA	4.23	1.45	1.33
22	D	104	CDL	OA8-CA7	4.23	1.45	1.33
13	K	103	BCL	O2A-CGA	4.22	1.45	1.33
12	3	105	PGV	O03-C19	4.22	1.45	1.33
13	0	102	BCL	O2A-CGA	4.22	1.45	1.33
12	L	305	PGV	O03-C19	4.21	1.45	1.33
7	C	502	HEC	CAC-C3C	4.20	1.48	1.35
14	M	405	BPH	CHA-CBD	-4.20	1.46	1.51
13	A	101	BCL	O2A-CGA	4.19	1.45	1.33
13	W	103	BCL	CHC-C4B	4.18	1.48	1.39
13	K	102	BCL	CHC-C4B	4.18	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	M	416	CDL	OA6-CA5	4.18	1.46	1.34
22	D	104	CDL	OB6-CB5	4.17	1.46	1.34
13	W	102	BCL	O2A-CGA	4.17	1.45	1.33
13	U	102	BCL	O2A-CGA	4.17	1.45	1.33
13	K	103	BCL	C1D-ND	-4.17	1.32	1.37
22	Q	105	CDL	OB6-CB5	4.17	1.46	1.34
12	M	415	PGV	O01-C1	4.17	1.46	1.34
13	S	102	BCL	CHD-C1D	4.16	1.46	1.38
13	D	103	BCL	CHD-C1D	4.16	1.46	1.38
7	C	501	HEC	CBB-CAB	-4.16	1.34	1.49
12	A	105	PGV	O01-C1	4.16	1.46	1.34
12	C	509	PGV	O03-C19	4.16	1.45	1.33
14	M	405	BPH	C3D-C2D	4.15	1.46	1.39
13	W	102	BCL	CHD-C1D	4.15	1.46	1.38
13	Q	102	BCL	CHD-C1D	4.15	1.46	1.38
12	L	306	PGV	O01-C1	4.14	1.46	1.34
13	F	102	BCL	CHD-C1D	4.14	1.46	1.38
13	D	103	BCL	CHC-C4B	4.14	1.48	1.39
13	0	102	BCL	CHD-C1D	4.13	1.46	1.38
12	M	414	PGV	O01-C1	4.13	1.46	1.34
22	K	104	CDL	OA8-CA7	4.13	1.45	1.33
20	K	105	PEF	O3-C30	4.12	1.45	1.33
13	M	402	BCL	CHC-C4B	4.12	1.48	1.39
20	M	419	PEF	O2-C10	4.12	1.45	1.34
13	M	403	BCL	O2A-CGA	4.12	1.45	1.33
14	M	405	BPH	C3B-C2B	4.12	1.46	1.39
7	C	502	HEC	CBC-CAC	-4.12	1.34	1.49
13	7	102	BCL	CHC-C4B	4.11	1.48	1.39
22	Q	105	CDL	OA6-CA5	4.11	1.45	1.34
13	D	103	BCL	C1D-ND	-4.11	1.32	1.37
13	0	102	BCL	CHC-C4B	4.11	1.48	1.39
13	5	102	BCL	CHD-C1D	4.10	1.46	1.38
12	M	415	PGV	O03-C19	4.10	1.45	1.33
22	H	304	CDL	OB8-CB7	4.10	1.45	1.33
13	Y	102	BCL	CHD-C1D	4.10	1.46	1.38
13	1	102	BCL	CHC-C4B	4.10	1.48	1.39
13	O	102	BCL	CHC-C4B	4.09	1.48	1.39
13	U	103	BCL	O2A-CGA	4.09	1.45	1.33
13	Q	102	BCL	O2A-CGA	4.09	1.45	1.33
7	C	502	HEC	CBB-CAB	-4.09	1.34	1.49
13	M	404	BCL	CHB-C1B	4.09	1.48	1.39
13	M	404	BCL	O2D-CGD	4.08	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Q	103	BCL	O2A-CGA	4.08	1.45	1.33
13	Y	102	BCL	CHC-C4B	4.08	1.48	1.39
22	M	416	CDL	OB6-CB5	4.08	1.45	1.34
13	3	103	BCL	CHB-C1B	4.07	1.48	1.39
13	A	101	BCL	CHC-C4B	4.07	1.48	1.39
13	D	103	BCL	O2A-CGA	4.07	1.45	1.33
13	S	103	BCL	OBD-CAD	4.06	1.29	1.22
13	3	103	BCL	C1D-ND	-4.06	1.32	1.37
13	9	104	BCL	C1D-ND	-4.05	1.32	1.37
13	1	103	BCL	CHC-C4B	4.05	1.48	1.39
13	5	103	BCL	CHB-C1B	4.05	1.48	1.39
13	7	103	BCL	CHB-C1B	4.05	1.48	1.39
13	7	102	BCL	CHD-C1D	4.04	1.46	1.38
13	W	102	BCL	CHB-C1B	4.04	1.48	1.39
13	D	102	BCL	CHD-C1D	4.04	1.46	1.38
13	7	103	BCL	OBD-CAD	4.03	1.29	1.22
7	C	501	HEC	CAB-C3B	4.03	1.48	1.35
13	Z	102	BCL	CHD-C1D	4.03	1.46	1.38
13	9	104	BCL	O2A-CGA	4.03	1.45	1.33
13	1	102	BCL	OBD-CAD	4.02	1.29	1.22
13	K	102	BCL	CHD-C1D	4.02	1.46	1.38
13	A	103	BCL	CHD-C1D	4.00	1.46	1.38
13	O	102	BCL	CHD-C1D	4.00	1.46	1.38
7	C	501	HEC	CBC-CAC	-4.00	1.34	1.49
13	5	103	BCL	O2A-CGA	4.00	1.45	1.33
13	L	301	BCL	CHC-C4B	4.00	1.48	1.39
12	H	303	PGV	O01-C1	4.00	1.45	1.34
22	H	304	CDL	OB6-CB5	4.00	1.45	1.34
13	0	102	BCL	C1D-ND	-4.00	1.32	1.37
13	W	103	BCL	CHB-C1B	3.99	1.48	1.39
22	K	104	CDL	OB6-CB5	3.99	1.45	1.34
20	K	105	PEF	O2-C10	3.99	1.45	1.34
13	1	103	BCL	CHB-C1B	3.99	1.48	1.39
7	C	504	HEC	CBB-CAB	-3.98	1.34	1.49
13	Z	102	BCL	CHC-C4B	3.98	1.48	1.39
13	O	102	BCL	CHB-C1B	3.98	1.48	1.39
22	S	104	CDL	OB6-CB5	3.98	1.44	1.35
13	F	102	BCL	CHC-C4B	3.98	1.48	1.39
12	C	509	PGV	O01-C1	3.98	1.45	1.34
13	U	102	BCL	C1D-ND	-3.97	1.32	1.37
13	0	102	BCL	OBD-CAD	3.97	1.29	1.22
13	O	103	BCL	CHB-C1B	3.97	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	102	BCL	CHC-C4B	3.96	1.48	1.39
13	W	102	BCL	C1D-ND	-3.96	1.32	1.37
13	I	103	BCL	CHB-C1B	3.96	1.48	1.39
13	S	102	BCL	CHB-C1B	3.96	1.48	1.39
7	C	504	HEC	CBC-CAC	-3.95	1.34	1.49
12	D	105	PGV	O03-C19	3.95	1.44	1.33
13	S	103	BCL	CHB-C1B	3.94	1.48	1.39
22	H	302	CDL	OB6-CB5	3.94	1.45	1.34
13	Q	103	BCL	C1D-ND	-3.94	1.32	1.37
13	1	103	BCL	CHD-C1D	3.94	1.46	1.38
13	F	102	BCL	OBD-CAD	3.93	1.29	1.22
13	7	103	BCL	O2A-CGA	3.93	1.44	1.33
7	C	503	HEC	CBC-CAC	-3.93	1.35	1.49
13	1	103	BCL	C1D-ND	-3.93	1.32	1.37
13	A	103	BCL	OBD-CAD	3.92	1.29	1.22
13	U	103	BCL	CHB-C1B	3.92	1.48	1.39
13	9	104	BCL	CHD-C1D	3.92	1.46	1.38
13	W	102	BCL	CHC-C4B	3.91	1.48	1.39
13	K	103	BCL	CHD-C1D	3.91	1.46	1.38
13	F	102	BCL	C1D-ND	-3.91	1.32	1.37
13	9	104	BCL	OBD-CAD	3.91	1.29	1.22
13	D	102	BCL	C1D-ND	-3.91	1.32	1.37
13	A	103	BCL	CHC-C4B	3.91	1.48	1.39
13	K	102	BCL	OBD-CAD	3.90	1.29	1.22
13	5	102	BCL	CHC-C4B	3.90	1.48	1.39
13	F	103	BCL	CHC-C4B	3.89	1.48	1.39
13	A	103	BCL	CHB-C1B	3.88	1.48	1.39
13	F	103	BCL	CHB-C1B	3.87	1.48	1.39
13	K	103	BCL	CHB-C1B	3.87	1.48	1.39
13	Y	102	BCL	C1D-ND	-3.87	1.32	1.37
13	A	101	BCL	C1D-ND	-3.86	1.32	1.37
13	L	301	BCL	OBD-CAD	3.86	1.29	1.22
13	M	402	BCL	CHB-C1B	3.85	1.48	1.39
13	7	103	BCL	C1D-ND	-3.85	1.32	1.37
13	K	102	BCL	CHB-C1B	3.85	1.48	1.39
13	F	103	BCL	CHD-C1D	3.85	1.45	1.38
13	U	103	BCL	CHD-C1D	3.85	1.45	1.38
14	L	302	BPH	O2A-CGA	3.84	1.44	1.33
13	A	101	BCL	OBD-CAD	3.84	1.29	1.22
13	3	102	BCL	CHB-C1B	3.84	1.48	1.39
22	S	104	CDL	OB8-CB7	3.84	1.44	1.33
13	M	403	BCL	CHD-C1D	3.84	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Q	102	BCL	C1D-ND	-3.84	1.32	1.37
13	I	102	BCL	CHC-C4B	3.83	1.48	1.39
13	S	103	BCL	CHD-C1D	3.83	1.45	1.38
22	S	104	CDL	OA8-CA7	3.82	1.44	1.33
13	F	103	BCL	OBD-CAD	3.82	1.29	1.22
13	S	103	BCL	O2A-CGA	3.82	1.44	1.33
13	5	102	BCL	CHB-C1B	3.81	1.48	1.39
13	7	102	BCL	CHB-C1B	3.80	1.47	1.39
13	S	103	BCL	C1D-ND	-3.79	1.32	1.37
15	L	308	UQ8	C4-C3	3.78	1.50	1.36
13	1	103	BCL	OBD-CAD	3.76	1.29	1.22
13	5	103	BCL	C1D-ND	-3.76	1.32	1.37
13	I	103	BCL	CHD-C1D	3.76	1.45	1.38
13	1	102	BCL	CHB-C1B	3.75	1.47	1.39
14	L	302	BPH	OBD-CAD	3.74	1.27	1.22
13	7	102	BCL	OBD-CAD	3.74	1.28	1.22
13	L	301	BCL	CHD-C1D	3.74	1.45	1.38
15	L	309	UQ8	C4-C3	3.74	1.49	1.36
13	9	104	BCL	CHB-C1B	3.73	1.47	1.39
13	W	103	BCL	OBD-CAD	3.73	1.28	1.22
13	7	103	BCL	CHC-C4B	3.73	1.47	1.39
13	5	103	BCL	OBD-CAD	3.73	1.28	1.22
13	S	102	BCL	C3D-C2D	3.72	1.49	1.39
7	C	503	HEC	CAB-C3B	3.71	1.47	1.35
13	F	102	BCL	CHB-C1B	3.70	1.47	1.39
21	J	102	LDA	C1-N1	-3.70	1.47	1.51
13	Z	102	BCL	CHB-C1B	3.69	1.47	1.39
14	M	405	BPH	OBD-CAD	3.69	1.27	1.22
13	D	102	BCL	CHB-C1B	3.69	1.47	1.39
13	0	102	BCL	CHB-C1B	3.68	1.47	1.39
13	M	404	BCL	O2A-CGA	3.68	1.44	1.33
13	O	103	BCL	OBD-CAD	3.68	1.28	1.22
13	3	103	BCL	CHD-C1D	3.68	1.45	1.38
13	Z	102	BCL	C1D-ND	-3.68	1.33	1.37
13	I	102	BCL	CHB-C1B	3.68	1.47	1.39
13	D	103	BCL	CHB-C1B	3.67	1.47	1.39
13	Y	102	BCL	OBD-CAD	3.67	1.28	1.22
12	D	105	PGV	O01-C1	3.67	1.44	1.34
13	D	102	BCL	OBD-CAD	3.67	1.28	1.22
13	M	402	BCL	C1D-ND	-3.66	1.33	1.37
15	M	418	UQ8	C4-C3	3.66	1.49	1.36
13	5	103	BCL	CHD-C1D	3.66	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F	103	BCL	C3D-C2D	3.66	1.49	1.39
13	Z	102	BCL	OBD-CAD	3.66	1.28	1.22
13	3	102	BCL	CHC-C4B	3.66	1.47	1.39
13	K	102	BCL	C1D-ND	-3.65	1.33	1.37
13	5	103	BCL	C3D-C2D	3.65	1.49	1.39
13	D	103	BCL	OBD-CAD	3.65	1.28	1.22
13	S	102	BCL	C1D-ND	-3.65	1.33	1.37
14	M	405	BPH	O2A-CGA	3.65	1.44	1.33
15	L	303	UQ8	C4-C3	3.65	1.49	1.36
21	M	412	LDA	C1-N1	-3.64	1.47	1.51
13	3	102	BCL	OBD-CAD	3.63	1.28	1.22
13	U	103	BCL	OBD-CAD	3.63	1.28	1.22
13	O	102	BCL	C1D-ND	-3.63	1.33	1.37
13	7	103	BCL	CHD-C1D	3.63	1.45	1.38
13	O	103	BCL	C4B-NB	-3.63	1.33	1.37
13	I	103	BCL	OBD-CAD	3.63	1.28	1.22
13	Z	102	BCL	C3D-C2D	3.62	1.48	1.39
13	U	102	BCL	CHB-C1B	3.62	1.47	1.39
13	A	101	BCL	C3D-C2D	3.62	1.48	1.39
13	Y	102	BCL	CHB-C1B	3.61	1.47	1.39
13	M	404	BCL	CHD-C1D	3.60	1.45	1.38
21	V	102	LDA	C1-N1	-3.59	1.47	1.51
13	U	102	BCL	OBD-CAD	3.58	1.28	1.22
13	L	301	BCL	O2A-CGA	3.58	1.43	1.33
13	9	104	BCL	C3D-C2D	3.58	1.48	1.39
13	U	102	BCL	CHD-C1D	3.58	1.45	1.38
13	M	402	BCL	CHD-C1D	3.57	1.45	1.38
13	3	103	BCL	C3D-C2D	3.57	1.48	1.39
13	D	103	BCL	C3D-C2D	3.55	1.48	1.39
13	I	102	BCL	OBD-CAD	3.55	1.28	1.22
13	D	102	BCL	C3D-C2D	3.55	1.48	1.39
13	O	102	BCL	C3D-C2D	3.55	1.48	1.39
13	3	102	BCL	C1D-ND	-3.54	1.33	1.37
13	K	103	BCL	OBD-CAD	3.54	1.28	1.22
13	0	102	BCL	C3D-C2D	3.53	1.48	1.39
13	5	102	BCL	C1D-ND	-3.53	1.33	1.37
13	U	102	BCL	C3D-C2D	3.52	1.48	1.39
13	I	102	BCL	C3D-C2D	3.51	1.48	1.39
13	I	102	BCL	C1D-ND	-3.51	1.33	1.37
13	W	102	BCL	OBD-CAD	3.51	1.28	1.22
13	W	103	BCL	C3D-C2D	3.50	1.48	1.39
13	Q	102	BCL	CHB-C1B	3.50	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	402	BCL	C3D-C2D	3.49	1.48	1.39
13	Q	102	BCL	C3D-C2D	3.48	1.48	1.39
13	A	101	BCL	CHB-C1B	3.48	1.47	1.39
13	M	402	BCL	OBD-CAD	3.48	1.28	1.22
13	K	102	BCL	C4B-NB	-3.47	1.33	1.37
13	W	102	BCL	C3D-C2D	3.46	1.48	1.39
13	1	102	BCL	C1D-ND	-3.46	1.33	1.37
21	O	105	LDA	C1-N1	-3.45	1.47	1.51
13	F	102	BCL	C3D-C2D	3.45	1.48	1.39
13	I	103	BCL	C3D-C2D	3.45	1.48	1.39
14	M	405	BPH	CBD-CGD	-3.44	1.48	1.52
13	K	103	BCL	C3D-C2D	3.44	1.48	1.39
13	S	103	BCL	C3D-C2D	3.44	1.48	1.39
13	O	103	BCL	CHD-C1D	3.42	1.45	1.38
13	U	103	BCL	C3D-C2D	3.42	1.48	1.39
13	Y	102	BCL	C3D-C2D	3.42	1.48	1.39
15	7	104	UQ8	C4-C3	3.41	1.48	1.36
13	F	102	BCL	C4B-NB	-3.41	1.33	1.37
13	M	403	BCL	O2D-CGD	3.40	1.41	1.33
13	M	403	BCL	C1B-NB	-3.37	1.33	1.37
13	W	103	BCL	CHD-C1D	3.37	1.45	1.38
13	K	102	BCL	C3D-C2D	3.34	1.48	1.39
13	1	102	BCL	C3D-C2D	3.34	1.48	1.39
13	Q	103	BCL	C3D-C2D	3.34	1.48	1.39
13	Y	102	BCL	C1B-NB	-3.33	1.33	1.37
13	A	103	BCL	C3D-C2D	3.33	1.48	1.39
13	7	103	BCL	C3D-C2D	3.31	1.48	1.39
13	1	103	BCL	C3D-C2D	3.29	1.48	1.39
13	3	102	BCL	C3D-C2D	3.29	1.48	1.39
13	7	102	BCL	C3D-C2D	3.27	1.47	1.39
13	F	103	BCL	C4B-NB	-3.25	1.33	1.37
13	7	102	BCL	C1D-ND	-3.25	1.33	1.37
13	O	103	BCL	C3D-C2D	3.25	1.47	1.39
13	A	103	BCL	C1B-NB	-3.23	1.33	1.37
13	W	102	BCL	C1B-NB	-3.20	1.33	1.37
7	C	503	HEC	CBB-CAB	-3.19	1.37	1.49
13	5	102	BCL	C3D-C2D	3.19	1.47	1.39
13	5	102	BCL	OBD-CAD	3.19	1.28	1.22
13	M	404	BCL	OBD-CAD	3.18	1.28	1.22
13	M	404	BCL	C1D-ND	-3.17	1.33	1.37
13	Z	102	BCL	C4B-NB	-3.17	1.33	1.37
13	D	103	BCL	C1B-NB	-3.16	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	I	102	BCL	C4B-NB	-3.15	1.33	1.37
13	O	102	BCL	OBD-CAD	3.12	1.27	1.22
13	5	102	BCL	C1B-C2B	3.12	1.50	1.43
13	U	102	BCL	CHD-C4C	3.11	1.47	1.39
14	L	302	BPH	C4B-NB	-3.10	1.33	1.38
13	Z	102	BCL	C1B-NB	-3.09	1.33	1.37
13	M	402	BCL	C1B-C2B	3.09	1.50	1.43
13	K	103	BCL	C4B-NB	-3.09	1.33	1.37
13	S	102	BCL	CHD-C4C	3.07	1.47	1.39
13	M	404	BCL	C3D-C2D	3.06	1.47	1.39
13	U	102	BCL	C1B-NB	-3.05	1.33	1.37
13	F	103	BCL	C1B-NB	-3.04	1.33	1.37
13	Q	102	BCL	C1B-NB	-3.04	1.33	1.37
13	D	102	BCL	C4B-NB	-3.04	1.33	1.37
13	7	103	BCL	C1B-C2B	3.04	1.50	1.43
13	K	102	BCL	C1B-NB	-3.03	1.33	1.37
13	I	102	BCL	C1B-NB	-3.03	1.33	1.37
13	A	101	BCL	CHD-C4C	3.03	1.47	1.39
13	M	403	BCL	OBD-CAD	3.03	1.27	1.22
13	3	102	BCL	C1B-C2B	3.02	1.50	1.43
13	I	103	BCL	C4B-NB	-3.02	1.33	1.37
13	O	102	BCL	C1B-NB	-3.01	1.33	1.37
13	F	102	BCL	C1B-NB	-3.01	1.33	1.37
22	S	104	CDL	OA6-CA5	3.00	1.42	1.34
13	3	102	BCL	CHD-C4C	3.00	1.47	1.39
13	Q	102	BCL	OBD-CAD	3.00	1.27	1.22
13	5	102	BCL	C1B-NB	-2.99	1.33	1.37
13	0	102	BCL	C4B-NB	-2.98	1.33	1.37
13	7	102	BCL	C1B-NB	-2.97	1.34	1.37
13	Y	102	BCL	C4B-NB	-2.97	1.34	1.37
13	Q	103	BCL	C1B-C2B	2.95	1.50	1.43
13	I	103	BCL	C1B-NB	-2.94	1.34	1.37
13	9	104	BCL	C4B-NB	-2.94	1.34	1.37
13	F	102	BCL	CHD-C4C	2.94	1.47	1.39
13	W	102	BCL	C4B-NB	-2.94	1.34	1.37
13	1	103	BCL	C1B-NB	-2.94	1.34	1.37
13	L	301	BCL	C3D-C2D	2.93	1.47	1.39
13	W	102	BCL	CHD-C4C	2.93	1.47	1.39
13	5	103	BCL	C1B-NB	-2.93	1.34	1.37
13	7	102	BCL	CHD-C4C	2.91	1.47	1.39
13	3	103	BCL	C1B-NB	-2.89	1.34	1.37
13	D	103	BCL	C4B-NB	-2.89	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	I	102	BCL	CHD-C4C	2.88	1.47	1.39
13	D	102	BCL	CHD-C4C	2.88	1.47	1.39
13	5	103	BCL	C4D-CHA	2.88	1.48	1.38
13	1	102	BCL	C1B-NB	-2.87	1.34	1.37
13	A	103	BCL	C4B-NB	-2.87	1.34	1.37
13	0	102	BCL	C1B-NB	-2.87	1.34	1.37
13	7	102	BCL	C1B-C2B	2.87	1.49	1.43
13	A	103	BCL	CHD-C4C	2.86	1.47	1.39
13	Y	102	BCL	CHD-C4C	2.86	1.47	1.39
13	O	102	BCL	C4B-NB	-2.85	1.34	1.37
13	3	103	BCL	C4B-NB	-2.84	1.34	1.37
13	D	103	BCL	CHD-C4C	2.84	1.47	1.39
13	M	403	BCL	C3D-C2D	2.83	1.46	1.39
13	U	103	BCL	C1B-NB	-2.83	1.34	1.37
13	Q	103	BCL	C1B-NB	-2.82	1.34	1.37
13	D	102	BCL	C1B-NB	-2.81	1.34	1.37
13	W	103	BCL	C1B-NB	-2.81	1.34	1.37
14	L	302	BPH	CHA-CBD	-2.80	1.48	1.51
13	K	102	BCL	CHD-C4C	2.79	1.47	1.39
13	Q	102	BCL	CHD-C4C	2.79	1.47	1.39
13	9	104	BCL	CHD-C4C	2.78	1.47	1.39
14	L	302	BPH	C1D-ND	-2.78	1.33	1.38
13	Z	102	BCL	CHD-C4C	2.77	1.47	1.39
7	C	501	HEC	C1B-NB	-2.77	1.34	1.39
7	C	503	HEC	C1D-ND	-2.77	1.34	1.39
13	1	103	BCL	C4D-CHA	2.77	1.47	1.38
13	K	103	BCL	CHD-C4C	2.77	1.47	1.39
13	Q	102	BCL	C4B-NB	-2.76	1.34	1.37
13	1	102	BCL	C1B-C2B	2.76	1.49	1.43
13	O	102	BCL	CHD-C4C	2.76	1.47	1.39
13	S	102	BCL	C4B-NB	-2.76	1.34	1.37
13	3	102	BCL	C1B-NB	-2.75	1.34	1.37
13	K	103	BCL	C4D-CHA	2.75	1.47	1.38
13	W	103	BCL	C4B-NB	-2.75	1.34	1.37
13	1	103	BCL	C4B-NB	-2.75	1.34	1.37
13	9	104	BCL	C1B-C2B	2.75	1.49	1.43
13	5	103	BCL	C1B-C2B	2.74	1.49	1.43
13	L	301	BCL	C1B-C2B	2.73	1.49	1.43
13	3	102	BCL	C4B-NB	-2.73	1.34	1.37
13	S	103	BCL	C1B-NB	-2.73	1.34	1.37
13	U	103	BCL	C1B-C2B	2.73	1.49	1.43
13	L	301	BCL	CHD-C4C	2.73	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	K	103	BCL	C1B-C2B	2.71	1.49	1.43
13	Z	102	BCL	C1B-C2B	2.70	1.49	1.43
13	7	103	BCL	C4B-NB	-2.69	1.34	1.37
13	F	103	BCL	C4D-CHA	2.69	1.47	1.38
13	F	102	BCL	C1B-C2B	2.68	1.49	1.43
13	1	102	BCL	CHD-C4C	2.68	1.46	1.39
7	C	502	HEC	C1D-ND	-2.68	1.34	1.39
13	I	103	BCL	C1B-C2B	2.67	1.49	1.43
13	W	103	BCL	C1B-C2B	2.67	1.49	1.43
13	I	103	BCL	CHD-C4C	2.67	1.46	1.39
13	K	102	BCL	C4D-CHA	2.67	1.47	1.38
13	D	103	BCL	C4D-CHA	2.67	1.47	1.38
13	K	103	BCL	C1B-NB	-2.67	1.34	1.37
13	I	102	BCL	C4D-CHA	2.67	1.47	1.38
13	U	103	BCL	C4D-CHA	2.66	1.47	1.38
13	M	402	BCL	CHD-C4C	2.66	1.46	1.39
7	C	504	HEC	C1B-NB	-2.66	1.34	1.39
13	1	103	BCL	C1B-C2B	2.66	1.49	1.43
13	S	103	BCL	C1B-C2B	2.65	1.49	1.43
13	D	102	BCL	C4D-CHA	2.64	1.47	1.38
13	U	103	BCL	C4B-NB	-2.64	1.34	1.37
13	D	102	BCL	C1B-C2B	2.64	1.49	1.43
13	K	102	BCL	C1B-C2B	2.63	1.49	1.43
13	0	102	BCL	C4D-CHA	2.63	1.47	1.38
14	L	302	BPH	CBD-CGD	-2.63	1.49	1.52
13	I	102	BCL	C1B-C2B	2.63	1.49	1.43
13	F	103	BCL	C1B-C2B	2.62	1.49	1.43
7	C	502	HEC	C1B-NB	-2.62	1.34	1.39
13	0	102	BCL	CHD-C4C	2.62	1.46	1.39
13	3	103	BCL	C4D-CHA	2.62	1.47	1.38
13	A	101	BCL	C1B-NB	-2.62	1.34	1.37
13	3	103	BCL	CHD-C4C	2.62	1.46	1.39
13	U	103	BCL	CHD-C4C	2.61	1.46	1.39
14	M	405	BPH	C1D-ND	-2.61	1.33	1.38
13	7	103	BCL	CHD-C4C	2.60	1.46	1.39
13	F	103	BCL	CHD-C4C	2.60	1.46	1.39
13	5	103	BCL	CHD-C4C	2.60	1.46	1.39
13	0	102	BCL	C1B-C2B	2.60	1.49	1.43
13	A	103	BCL	C1B-C2B	2.60	1.49	1.43
13	A	103	BCL	C4D-CHA	2.60	1.47	1.38
13	7	102	BCL	C4B-NB	-2.60	1.34	1.37
13	S	103	BCL	CHD-C4C	2.57	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	7	103	BCL	C4D-CHA	2.57	1.47	1.38
13	F	102	BCL	C4D-CHA	2.56	1.47	1.38
13	O	102	BCL	C4D-CHA	2.56	1.47	1.38
13	D	103	BCL	C1B-C2B	2.56	1.49	1.43
13	Q	102	BCL	C4D-CHA	2.56	1.47	1.38
13	W	103	BCL	CHD-C4C	2.56	1.46	1.39
13	Z	102	BCL	C4D-CHA	2.55	1.47	1.38
13	S	102	BCL	C1B-NB	-2.55	1.34	1.37
13	1	102	BCL	C4B-NB	-2.55	1.34	1.37
13	A	101	BCL	C1B-C2B	2.55	1.49	1.43
13	A	101	BCL	C4B-NB	-2.55	1.34	1.37
13	5	102	BCL	CHD-C4C	2.54	1.46	1.39
7	C	503	HEC	C1B-NB	-2.54	1.34	1.39
22	H	302	CDL	OA8-CA7	2.53	1.45	1.33
20	M	409	PEF	P-O4P	2.53	1.62	1.54
7	C	501	HEC	C1D-ND	-2.53	1.34	1.39
13	W	102	BCL	C4D-CHA	2.53	1.47	1.38
13	L	301	BCL	C1B-NB	-2.53	1.34	1.37
13	Y	102	BCL	C4D-CHA	2.52	1.47	1.38
13	Q	103	BCL	C4D-CHA	2.51	1.47	1.38
13	M	404	BCL	C3B-C2B	2.51	1.51	1.42
13	3	102	BCL	C4D-CHA	2.50	1.47	1.38
13	7	102	BCL	C4D-CHA	2.50	1.47	1.38
7	C	501	HEC	C4D-ND	-2.49	1.34	1.39
20	M	409	PEF	P-O3P	2.48	1.61	1.54
13	S	102	BCL	C4D-CHA	2.48	1.46	1.38
13	W	103	BCL	C4D-CHA	2.48	1.46	1.38
13	M	402	BCL	C4D-CHA	2.47	1.46	1.38
13	I	103	BCL	C4D-CHA	2.47	1.46	1.38
13	A	101	BCL	C4D-CHA	2.47	1.46	1.38
13	5	102	BCL	C4D-CHA	2.47	1.46	1.38
13	Q	103	BCL	MG-NA	2.46	2.12	2.06
13	1	103	BCL	CHD-C4C	2.46	1.46	1.39
13	O	103	BCL	CHD-C4C	2.45	1.46	1.39
13	5	102	BCL	C4B-NB	-2.45	1.34	1.37
13	1	102	BCL	C4D-CHA	2.45	1.46	1.38
13	5	103	BCL	C4B-NB	-2.44	1.34	1.37
13	9	104	BCL	C4D-CHA	2.44	1.46	1.38
13	W	102	BCL	C1B-C2B	2.44	1.48	1.43
13	M	404	BCL	C1B-C2B	2.42	1.48	1.43
20	1	105	PEF	P-O3P	2.41	1.61	1.54
13	3	103	BCL	C1B-C2B	2.41	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	I	104	PEF	P-O4P	2.40	1.61	1.54
13	U	102	BCL	C4D-CHA	2.40	1.46	1.38
13	S	103	BCL	C4B-NB	-2.40	1.34	1.37
14	M	405	BPH	C4B-NB	-2.39	1.34	1.38
13	Q	102	BCL	C3D-C4D	-2.37	1.38	1.44
13	A	101	BCL	C3B-C2B	2.37	1.50	1.42
20	U	105	PEF	P-O4P	2.37	1.61	1.54
20	U	106	PEF	P-O3P	2.36	1.61	1.54
13	S	103	BCL	C4D-CHA	2.36	1.46	1.38
7	C	503	HEC	C4B-NB	-2.36	1.35	1.39
13	U	102	BCL	C3B-C2B	2.36	1.50	1.42
20	5	104	PEF	P-O4P	2.35	1.61	1.54
20	W	104	PEF	P-O4P	2.35	1.61	1.54
20	M	408	PEF	P-O4P	2.34	1.61	1.54
20	M	410	PEF	P-O3P	2.34	1.61	1.54
13	M	403	BCL	CHD-C4C	2.33	1.45	1.39
13	9	104	BCL	C1B-NB	-2.32	1.34	1.37
12	C	509	PGV	O01-C02	-2.32	1.43	1.47
13	Q	103	BCL	CHD-C4C	2.31	1.45	1.39
13	1	103	BCL	C3B-C2B	2.31	1.50	1.42
13	O	103	BCL	C1B-C2B	2.31	1.48	1.43
13	U	102	BCL	C4B-NB	-2.30	1.34	1.37
13	M	403	BCL	C1B-C2B	2.30	1.48	1.43
20	3	104	PEF	P-O3P	2.30	1.61	1.54
13	Y	102	BCL	C1B-C2B	2.30	1.48	1.43
7	C	503	HEC	C4D-ND	-2.30	1.35	1.39
13	I	103	BCL	C3B-C2B	2.29	1.50	1.42
13	M	404	BCL	C3D-C4D	-2.27	1.39	1.44
13	S	102	BCL	C3B-C2B	2.27	1.50	1.42
13	O	102	BCL	C1B-C2B	2.27	1.48	1.43
13	M	402	BCL	C1B-NB	-2.27	1.34	1.37
13	5	103	BCL	C3B-C2B	2.27	1.50	1.42
13	L	301	BCL	C3D-C4D	-2.27	1.39	1.44
13	O	103	BCL	C4D-CHA	2.26	1.46	1.38
7	C	501	HEC	C4B-NB	-2.26	1.35	1.39
13	U	103	BCL	C3B-C2B	2.26	1.50	1.42
13	K	102	BCL	C3B-C2B	2.25	1.50	1.42
13	O	103	BCL	C1B-NB	-2.25	1.34	1.37
13	O	102	BCL	C3B-C2B	2.25	1.50	1.42
13	Z	102	BCL	C3B-C2B	2.23	1.50	1.42
13	I	102	BCL	C3D-C4D	-2.23	1.39	1.44
13	D	102	BCL	C3D-C4D	-2.23	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	404	BCL	CHD-C4C	2.23	1.45	1.39
13	D	102	BCL	C3B-C2B	2.23	1.50	1.42
13	M	403	BCL	C1D-C2D	2.22	1.49	1.45
7	C	504	HEC	C1D-ND	-2.22	1.35	1.39
7	C	502	HEC	C4D-ND	-2.22	1.35	1.39
13	Q	102	BCL	C3B-C2B	2.22	1.50	1.42
7	C	502	HEC	C4B-NB	-2.21	1.35	1.39
13	1	102	BCL	C3B-C2B	2.21	1.50	1.42
13	7	103	BCL	C3B-C2B	2.20	1.50	1.42
13	U	102	BCL	C1B-C2B	2.20	1.48	1.43
13	5	102	BCL	C3D-C4D	-2.20	1.39	1.44
13	S	102	BCL	C1B-C2B	2.20	1.48	1.43
13	3	102	BCL	C3D-C4D	-2.20	1.39	1.44
13	W	103	BCL	C3B-C2B	2.20	1.50	1.42
13	Y	102	BCL	C3B-C2B	2.19	1.50	1.42
13	7	102	BCL	C3D-C4D	-2.19	1.39	1.44
13	F	102	BCL	C3D-C4D	-2.19	1.39	1.44
13	3	102	BCL	C3B-C2B	2.18	1.50	1.42
13	W	102	BCL	C3D-C4D	-2.18	1.39	1.44
13	F	103	BCL	C3B-C2B	2.17	1.50	1.42
7	C	504	HEC	C4B-NB	-2.17	1.35	1.39
13	S	103	BCL	C3B-C2B	2.16	1.50	1.42
13	9	104	BCL	C3B-C2B	2.16	1.50	1.42
13	W	102	BCL	C3B-C2B	2.16	1.50	1.42
13	M	403	BCL	C4D-CHA	2.16	1.45	1.38
13	3	103	BCL	C3B-C2B	2.16	1.50	1.42
13	F	102	BCL	C3B-C2B	2.16	1.49	1.42
13	7	102	BCL	C3B-C2B	2.14	1.49	1.42
13	M	404	BCL	C4D-CHA	2.14	1.45	1.38
13	U	102	BCL	C3D-C4D	-2.14	1.39	1.44
13	5	103	BCL	C3D-C4D	-2.14	1.39	1.44
13	I	102	BCL	C3B-C2B	2.13	1.49	1.42
13	K	102	BCL	C3D-C4D	-2.13	1.39	1.44
13	L	301	BCL	C4D-CHA	2.12	1.45	1.38
13	A	101	BCL	C3D-C4D	-2.12	1.39	1.44
13	5	102	BCL	C3B-C2B	2.12	1.49	1.42
13	7	103	BCL	C1B-NB	-2.12	1.35	1.37
22	S	104	CDL	OA6-CA4	-2.12	1.41	1.46
13	D	103	BCL	C3B-C2B	2.10	1.49	1.42
7	C	503	HEC	C1D-C2D	2.10	1.48	1.43
13	K	103	BCL	C3B-C2B	2.10	1.49	1.42
13	M	402	BCL	C4B-NB	-2.10	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	402	BCL	C3B-C2B	2.10	1.49	1.42
13	M	404	BCL	C1B-NB	-2.10	1.35	1.37
23	M	420	LMT	O1'-C1'	2.09	1.43	1.40
13	Q	103	BCL	C3B-C2B	2.09	1.49	1.42
19	Q	104	CRT	C37-C36	2.09	1.53	1.50
13	0	102	BCL	C3B-C2B	2.08	1.49	1.42
18	M	406	MQ8	O4-C4	2.07	1.27	1.23
13	Y	102	BCL	C3D-C4D	-2.05	1.39	1.44
13	A	103	BCL	C3B-C2B	2.05	1.49	1.42
14	L	302	BPH	C1B-NB	-2.04	1.34	1.38
13	1	102	BCL	C3D-C4D	-2.04	1.39	1.44
12	D	105	PGV	O01-C02	-2.04	1.41	1.46
13	S	102	BCL	C3D-C4D	-2.04	1.39	1.44
7	C	501	HEC	C4A-C3A	-2.04	1.41	1.45
13	7	103	BCL	C3D-C4D	-2.04	1.39	1.44
15	7	104	UQ8	O4-C4M	-2.03	1.40	1.45
7	C	503	HEC	C1C-NC	-2.03	1.35	1.39
13	1	102	BCL	C1D-C2D	2.03	1.49	1.45
13	3	102	BCL	C1D-C2D	2.03	1.49	1.45
13	M	402	BCL	C3C-C4C	-2.03	1.49	1.51
13	I	103	BCL	C3D-C4D	-2.03	1.39	1.44
13	O	102	BCL	C3D-C4D	-2.01	1.39	1.44
13	A	103	BCL	C3D-C4D	-2.01	1.39	1.44

All (1261) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	N	101	CRT	C37-C36-C35	-7.89	113.83	124.91
13	W	102	BCL	O2D-CGD-CBD	7.67	124.63	111.23
13	M	403	BCL	C4A-NA-C1A	-7.63	103.20	106.68
19	U	104	CRT	C37-C36-C35	-7.62	114.20	124.91
13	A	101	BCL	C4A-NA-C1A	-7.50	103.26	106.68
19	M	407	CRT	C37-C36-C35	-7.35	114.59	124.91
13	O	102	BCL	C4A-NA-C1A	-7.33	103.34	106.68
13	W	102	BCL	C4A-NA-C1A	-7.24	103.38	106.68
13	U	102	BCL	O2D-CGD-CBD	7.15	123.73	111.23
19	0	101	CRT	C37-C36-C35	-7.15	114.87	124.91
13	S	103	BCL	C4A-NA-C1A	-7.15	103.42	106.68
13	D	102	BCL	C4A-NA-C1A	-7.15	103.42	106.68
14	M	405	BPH	O2D-CGD-CBD	7.02	118.66	110.95
13	S	102	BCL	O2D-CGD-CBD	6.94	123.36	111.23
13	W	102	BCL	CAC-C3C-C4C	6.85	127.80	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	103	BCL	C4A-NA-C1A	-6.76	103.60	106.68
13	A	103	BCL	C4A-NA-C1A	-6.74	103.60	106.68
13	9	104	BCL	C4A-NA-C1A	-6.71	103.62	106.68
13	Q	102	BCL	O2D-CGD-CBD	6.67	122.88	111.23
19	Q	104	CRT	C37-C36-C35	-6.63	115.61	124.91
13	9	104	BCL	O2D-CGD-CBD	6.56	122.70	111.23
13	M	402	BCL	C4A-NA-C1A	-6.55	103.69	106.68
13	Q	103	BCL	C4A-NA-C1A	-6.42	103.75	106.68
13	1	102	BCL	C4A-NA-C1A	-6.42	103.75	106.68
13	Y	102	BCL	O2D-CGD-CBD	6.41	122.44	111.23
13	Y	102	BCL	C4A-NA-C1A	-6.40	103.76	106.68
13	Z	102	BCL	C4A-NA-C1A	-6.39	103.76	106.68
13	7	102	BCL	O2D-CGD-CBD	6.35	122.34	111.23
13	1	103	BCL	C1C-NC-C4C	-6.35	103.78	106.68
13	F	102	BCL	C4A-NA-C1A	-6.33	103.79	106.68
7	C	503	HEC	CBB-CAB-C3B	-6.33	114.79	127.43
13	5	102	BCL	O2D-CGD-CBD	6.28	122.21	111.23
19	O	104	CRT	C37-C36-C35	-6.27	116.10	124.91
13	W	102	BCL	CMC-C2C-C1C	6.27	128.63	111.77
14	L	302	BPH	C2B-C1B-NB	6.26	113.95	109.43
13	W	103	BCL	C1C-NC-C4C	-6.21	103.85	106.68
13	0	102	BCL	CMC-C2C-C1C	6.21	128.46	111.77
13	3	102	BCL	O2D-CGD-CBD	6.18	122.04	111.23
13	1	103	BCL	CMC-C2C-C1C	6.18	128.37	111.77
13	K	103	BCL	C4A-NA-C1A	-6.15	103.87	106.68
13	I	102	BCL	CMC-C2C-C1C	6.13	128.24	111.77
13	D	103	BCL	CAC-C3C-C4C	6.11	126.15	112.58
13	O	102	BCL	O2D-CGD-CBD	6.11	121.92	111.23
19	2	101	CRT	C37-C36-C35	-6.10	116.34	124.91
13	K	102	BCL	C4A-NA-C1A	-6.10	103.90	106.68
13	F	102	BCL	CMC-C2C-C1C	6.10	128.16	111.77
13	1	103	BCL	CAC-C3C-C4C	6.10	126.12	112.58
13	Q	102	BCL	C4A-NA-C1A	-6.09	103.90	106.68
13	K	103	BCL	CMC-C2C-C1C	6.09	128.13	111.77
13	5	103	BCL	CMC-C2C-C1C	6.08	128.12	111.77
13	F	102	BCL	CAC-C3C-C4C	6.08	126.08	112.58
13	O	103	BCL	C4A-NA-C1A	-6.08	103.91	106.68
13	A	101	BCL	O2D-CGD-CBD	6.07	121.84	111.23
13	M	403	BCL	CAC-C3C-C4C	6.06	126.03	112.58
19	P	101	CRT	C37-C36-C35	-6.06	116.40	124.91
13	O	102	BCL	CMC-C2C-C1C	6.05	128.03	111.77
13	I	102	BCL	C4A-NA-C1A	-6.05	103.92	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	7	103	BCL	CAC-C3C-C4C	6.02	125.94	112.58
13	3	102	BCL	C4A-NA-C1A	-6.00	103.94	106.68
13	D	102	BCL	CAC-C3C-C4C	5.99	125.88	112.58
13	D	103	BCL	CMC-C2C-C1C	5.98	127.84	111.77
13	3	103	BCL	CMC-C2C-C1C	5.97	127.82	111.77
13	0	102	BCL	C1C-NC-C4C	-5.97	103.96	106.68
13	1	102	BCL	CMC-C2C-C1C	5.97	127.81	111.77
13	F	103	BCL	CMC-C2C-C1C	5.96	127.79	111.77
13	A	103	BCL	CMC-C2C-C1C	5.95	127.76	111.77
13	Y	102	BCL	CAC-C3C-C4C	5.95	125.78	112.58
13	5	102	BCL	CMC-C2C-C1C	5.92	127.69	111.77
7	C	504	HEC	CBB-CAB-C3B	-5.92	115.59	127.43
19	9	103	CRT	C37-C36-C35	-5.92	116.60	124.91
13	Y	102	BCL	CMC-C2C-C1C	5.92	127.69	111.77
13	F	103	BCL	CAC-C3C-C4C	5.91	125.69	112.58
19	9	102	CRT	C37-C36-C35	-5.84	116.71	124.91
13	Z	102	BCL	CMC-C2C-C1C	5.84	127.46	111.77
13	K	102	BCL	O2D-CGD-CBD	5.83	121.42	111.23
13	D	102	BCL	CMC-C2C-C1C	5.82	127.42	111.77
13	A	103	BCL	CAC-C3C-C4C	5.82	125.50	112.58
13	U	102	BCL	C4A-NA-C1A	-5.81	104.03	106.68
13	S	102	BCL	CAC-C3C-C4C	5.80	125.47	112.58
13	7	102	BCL	C4A-NA-C1A	-5.79	104.04	106.68
13	I	102	BCL	CAC-C3C-C4C	5.78	125.41	112.58
13	K	103	BCL	CAC-C3C-C4C	5.77	125.38	112.58
13	Z	102	BCL	CAC-C3C-C4C	5.77	125.38	112.58
19	J	101	CRT	C37-C36-C35	-5.76	116.82	124.91
13	U	103	BCL	C1C-NC-C4C	-5.76	104.05	106.68
13	1	102	BCL	CAC-C3C-C4C	5.74	125.32	112.58
19	Z	101	CRT	C21-C22-C23	-5.74	119.23	127.28
13	3	103	BCL	C4A-NA-C1A	-5.72	104.07	106.68
13	1	103	BCL	C1D-CHD-C4C	-5.71	112.86	126.62
13	I	103	BCL	CMC-C2C-C1C	5.69	127.05	111.77
19	V	101	CRT	C37-C36-C35	-5.69	116.93	124.91
13	I	103	BCL	C4A-NA-C1A	-5.68	104.09	106.68
13	A	101	BCL	CMC-C2C-C1C	5.64	126.94	111.77
13	K	102	BCL	CAC-C3C-C4C	5.61	125.03	112.58
13	K	102	BCL	CMC-C2C-C1C	5.61	126.84	111.77
13	5	102	BCL	CAC-C3C-C4C	5.60	125.00	112.58
13	W	103	BCL	CMC-C2C-C1C	5.57	126.75	111.77
13	5	102	BCL	C4A-NA-C1A	-5.55	104.15	106.68
13	Z	102	BCL	C1C-NC-C4C	-5.50	104.17	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	I	103	BCL	CAC-C3C-C4C	5.50	124.78	112.58
13	9	104	BCL	CMC-C2C-C1C	5.48	126.49	111.77
13	K	103	BCL	C2B-C1B-NB	5.46	115.99	110.33
13	O	102	BCL	C1C-NC-C4C	-5.46	104.19	106.68
13	1	102	BCL	O2D-CGD-CBD	5.46	120.77	111.23
13	Y	102	BCL	C2B-C1B-NB	5.46	115.98	110.33
13	9	104	BCL	C1C-NC-C4C	-5.45	104.19	106.68
14	L	302	BPH	CMC-C2C-C1C	5.44	126.34	114.61
13	W	103	BCL	C4A-NA-C1A	-5.42	104.20	106.68
13	3	103	BCL	CAC-C3C-C4C	5.42	124.62	112.58
13	S	103	BCL	CMC-C2C-C1C	5.42	126.33	111.77
7	C	501	HEC	CHC-C4B-NB	5.41	130.34	124.45
19	6	101	CRT	C37-C36-C35	-5.40	117.33	124.91
13	M	402	BCL	C2B-C1B-NB	5.39	115.91	110.33
13	0	102	BCL	CAC-C3C-C4C	5.36	124.49	112.58
13	0	102	BCL	C4A-NA-C1A	-5.35	104.24	106.68
13	3	103	BCL	C1D-CHD-C4C	-5.35	113.71	126.62
13	7	103	BCL	CMC-C2C-C1C	5.32	126.07	111.77
13	W	103	BCL	CAC-C3C-C4C	5.31	124.37	112.58
13	3	102	BCL	CAC-C3C-C4C	5.31	124.36	112.58
13	3	102	BCL	CMC-C2C-C1C	5.30	126.02	111.77
13	F	102	BCL	O2D-CGD-CBD	5.30	120.50	111.23
13	Q	102	BCL	C2B-C1B-NB	5.29	115.81	110.33
13	U	103	BCL	C4A-NA-C1A	-5.27	104.28	106.68
13	D	103	BCL	C2B-C1B-NB	5.27	115.79	110.33
13	1	103	BCL	C4A-NA-C1A	-5.26	104.28	106.68
13	U	103	BCL	CAC-C3C-C4C	5.25	124.23	112.58
13	S	102	BCL	C4A-NA-C1A	-5.25	104.29	106.68
13	I	102	BCL	O2D-CGD-CBD	5.24	120.39	111.23
13	5	103	BCL	C4A-NA-C1A	-5.23	104.29	106.68
15	L	303	UQ8	C15-C14-C16	5.21	124.28	115.23
13	D	102	BCL	O2D-CGD-CBD	5.21	120.33	111.23
13	O	103	BCL	CAC-C3C-C4C	5.19	124.11	112.58
13	7	102	BCL	CAC-C3C-C4C	5.16	124.04	112.58
13	Q	103	BCL	C3C-C4C-CHD	-5.16	112.51	123.39
13	F	103	BCL	C1C-NC-C4C	-5.16	104.33	106.68
13	7	103	BCL	C1C-NC-C4C	-5.15	104.33	106.68
13	7	102	BCL	CMC-C2C-C1C	5.15	125.62	111.77
13	U	103	BCL	CMC-C2C-C1C	5.15	125.61	111.77
14	M	405	BPH	C4D-CHA-CBD	-5.14	105.99	108.45
13	F	102	BCL	C1C-NC-C4C	-5.14	104.33	106.68
13	5	103	BCL	C1C-NC-C4C	-5.13	104.34	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Z	102	BCL	C2B-C1B-NB	5.13	115.65	110.33
13	F	103	BCL	C2B-C1B-NB	5.13	115.64	110.33
13	S	102	BCL	C2B-C1B-NB	5.10	115.62	110.33
13	D	102	BCL	C1C-NC-C4C	-5.08	104.36	106.68
19	Z	101	CRT	C37-C36-C35	-5.07	117.79	124.91
13	K	102	BCL	C1C-NC-C4C	-5.07	104.37	106.68
13	S	103	BCL	C1C-NC-C4C	-5.06	104.37	106.68
13	0	102	BCL	C2B-C1B-NB	5.05	115.57	110.33
15	7	104	UQ8	C1M-C1-C6	-5.05	116.15	124.45
13	I	102	BCL	C2B-C1B-NB	5.05	115.56	110.33
13	A	101	BCL	CAC-C3C-C4C	5.03	123.75	112.58
13	I	102	BCL	C1C-NC-C4C	-5.03	104.39	106.68
19	G	101	CRT	C37-C36-C35	-5.02	117.86	124.91
13	1	102	BCL	C2B-C1B-NB	5.01	115.52	110.33
13	5	103	BCL	CAC-C3C-C4C	5.00	123.68	112.58
13	K	103	BCL	C1D-CHD-C4C	-5.00	114.57	126.62
13	S	102	BCL	CMC-C2C-C1C	4.99	125.19	111.77
13	O	103	BCL	C2B-C1B-NB	4.97	115.48	110.33
13	M	404	BCL	C4A-NA-C1A	-4.96	104.42	106.68
13	M	403	BCL	CMC-C2C-C1C	4.94	125.05	111.77
22	S	104	CDL	OB6-CB5-C51	4.94	119.89	111.09
13	K	103	BCL	C1C-NC-C4C	-4.93	104.43	106.68
13	F	103	BCL	O2D-CGD-CBD	4.92	119.84	111.23
13	F	103	BCL	C4A-NA-C1A	-4.92	104.44	106.68
13	Z	102	BCL	C1D-CHD-C4C	-4.90	114.81	126.62
13	5	102	BCL	C1C-NC-C4C	-4.89	104.45	106.68
15	7	104	UQ8	C6-C1-C2	4.89	123.03	119.17
22	H	302	CDL	OA6-CA5-C11	4.88	122.03	111.48
13	U	102	BCL	CMC-C2C-C1C	4.87	124.87	111.77
13	L	301	BCL	C3C-C4C-CHD	-4.87	113.12	123.39
13	K	102	BCL	C2B-C1B-NB	4.87	115.37	110.33
12	L	305	PGV	O01-C1-C2	4.83	121.94	111.48
13	O	103	BCL	CMC-C2C-C1C	4.83	124.74	111.77
13	W	102	BCL	O2D-CGD-O1D	-4.82	114.46	123.85
13	1	103	BCL	O2D-CGD-CBD	4.80	119.63	111.23
13	S	103	BCL	CAC-C3C-C4C	4.80	123.25	112.58
7	C	501	HEC	CBB-CAB-C3B	-4.80	117.83	127.43
19	N	101	CRT	C21-C22-C23	-4.80	120.55	127.28
13	I	103	BCL	C2B-C1B-NB	4.78	115.28	110.33
14	L	302	BPH	O2D-CGD-CBD	4.77	116.19	110.95
13	I	103	BCL	C1D-CHD-C4C	-4.77	115.11	126.62
13	7	102	BCL	C2B-C1B-NB	4.77	115.27	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	W	103	BCL	C1D-CHD-C4C	-4.76	115.13	126.62
13	U	102	BCL	C2B-C1B-NB	4.76	115.27	110.33
19	G	101	CRT	C4-C5-C6	-4.75	118.24	124.91
19	V	101	CRT	C21-C22-C23	-4.75	120.61	127.28
13	A	103	BCL	C2B-C1B-NB	4.74	115.24	110.33
13	5	103	BCL	C2B-C1B-NB	4.73	115.23	110.33
14	M	405	BPH	C1-C2-C3	-4.73	118.45	126.20
13	O	102	BCL	CAC-C3C-C4C	4.73	123.07	112.58
13	M	402	BCL	C1D-CHD-C4C	-4.72	115.24	126.62
13	F	103	BCL	C1D-CHD-C4C	-4.72	115.24	126.62
13	M	402	BCL	CMC-C2C-C1C	4.70	124.41	111.77
13	1	102	BCL	C1C-NC-C4C	-4.70	104.53	106.68
19	1	104	CRT	C37-C36-C35	-4.69	118.33	124.91
13	O	102	BCL	C2B-C1B-NB	4.69	115.19	110.33
20	K	105	PEF	O2-C10-C11	4.67	121.59	111.48
22	S	104	CDL	CB4-OB6-CB5	-4.67	109.59	117.85
13	9	104	BCL	C2B-C1B-NB	4.66	115.16	110.33
13	D	102	BCL	C1D-CHD-C4C	-4.66	115.39	126.62
13	3	103	BCL	C1C-NC-C4C	-4.65	104.56	106.68
13	L	301	BCL	O2D-CGD-CBD	4.65	119.36	111.23
14	M	405	BPH	C2B-C1B-NB	4.65	112.79	109.43
13	Q	103	BCL	C1C-NC-C4C	-4.64	104.56	106.68
13	0	102	BCL	C1D-CHD-C4C	-4.62	115.47	126.62
19	Q	104	CRT	C21-C22-C23	-4.62	120.80	127.28
13	Q	103	BCL	C1D-CHD-C4C	-4.60	115.52	126.62
19	A	104	CRT	C37-C36-C35	-4.60	118.45	124.91
13	Q	102	BCL	CMC-C2C-C1C	4.60	124.14	111.77
19	9	102	CRT	C21-C22-C23	-4.59	120.83	127.28
13	M	404	BCL	C1D-CHD-C4C	-4.59	115.55	126.62
13	W	103	BCL	C3C-C4C-CHD	-4.59	113.72	123.39
13	A	101	BCL	C2B-C1B-NB	4.58	115.07	110.33
22	H	304	CDL	OB6-CB5-C51	4.57	121.38	111.48
13	K	102	BCL	C1D-CHD-C4C	-4.57	115.59	126.62
13	L	301	BCL	C4A-NA-C1A	-4.57	104.59	106.68
13	1	102	BCL	CHD-C1D-ND	-4.57	118.37	124.80
13	9	104	BCL	C3C-C4C-CHD	-4.57	113.76	123.39
19	J	101	CRT	C21-C22-C23	-4.56	120.89	127.28
12	M	415	PGV	O01-C1-C2	4.54	121.31	111.48
13	S	103	BCL	C3C-C4C-CHD	-4.53	113.83	123.39
13	Y	102	BCL	C1C-NC-C4C	-4.53	104.61	106.68
13	U	102	BCL	C3C-C4C-CHD	-4.53	113.84	123.39
13	I	102	BCL	C1D-CHD-C4C	-4.52	115.72	126.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	102	BCL	C1D-CHD-C4C	-4.51	115.74	126.62
13	D	103	BCL	C1D-CHD-C4C	-4.51	115.75	126.62
13	3	102	BCL	C2B-C1B-NB	4.50	115.00	110.33
13	Y	102	BCL	C1D-CHD-C4C	-4.50	115.76	126.62
13	F	102	BCL	C2B-C1B-NB	4.50	114.99	110.33
13	M	404	BCL	CAC-C3C-C4C	4.50	122.56	112.58
13	Q	103	BCL	CMC-C2C-C1C	4.49	123.84	111.77
13	3	103	BCL	C2B-C1B-NB	4.49	114.98	110.33
19	6	101	CRT	C5-C6-C7	-4.49	119.11	125.89
13	1	103	BCL	C2B-C1B-NB	4.47	114.97	110.33
13	M	403	BCL	C3C-C4C-CHD	-4.47	113.97	123.39
19	9	103	CRT	C21-C22-C23	-4.46	121.02	127.28
13	D	102	BCL	C2B-C1B-NB	4.45	114.94	110.33
13	A	103	BCL	C1C-NC-C4C	-4.45	104.65	106.68
13	D	103	BCL	C1C-NC-C4C	-4.44	104.65	106.68
13	S	103	BCL	C1D-CHD-C4C	-4.44	115.92	126.62
13	9	104	BCL	C1D-CHD-C4C	-4.44	115.92	126.62
13	7	102	BCL	C3C-C4C-CHD	-4.43	114.04	123.39
13	U	103	BCL	C2B-C1B-NB	4.43	114.92	110.33
13	W	102	BCL	C1C-NC-C4C	-4.42	104.66	106.68
13	7	102	BCL	C1D-CHD-C4C	-4.41	115.98	126.62
12	H	303	PGV	O01-C1-C2	4.40	121.00	111.48
13	U	102	BCL	O2D-CGD-O1D	-4.38	115.32	123.85
13	7	103	BCL	C2B-C1B-NB	4.38	114.87	110.33
12	L	306	PGV	O01-C1-C2	4.38	120.95	111.48
22	K	104	CDL	OA6-CA5-C11	4.38	120.95	111.48
13	U	102	BCL	C1C-NC-C4C	-4.38	104.68	106.68
13	I	103	BCL	O2D-CGD-CBD	4.37	118.87	111.23
22	K	104	CDL	OB6-CB5-C51	4.35	120.89	111.48
13	5	102	BCL	C1D-CHD-C4C	-4.35	116.13	126.62
13	7	102	BCL	C1C-NC-C4C	-4.35	104.70	106.68
13	M	404	BCL	O2D-CGD-CBD	4.34	118.83	111.23
13	7	103	BCL	C1D-CHD-C4C	-4.34	116.15	126.62
19	G	101	CRT	C21-C22-C23	-4.34	121.19	127.28
13	U	103	BCL	C1D-CHD-C4C	-4.34	116.16	126.62
19	A	104	CRT	C21-C22-C23	-4.33	121.20	127.28
13	Z	102	BCL	O2D-CGD-CBD	4.32	118.78	111.23
13	W	103	BCL	C2B-C1B-NB	4.31	114.80	110.33
23	F	104	LMT	C1'-O5'-C5'	4.31	122.14	113.72
13	F	103	BCL	C3C-C4C-CHD	-4.31	114.31	123.39
7	C	503	HEC	CHC-C4B-NB	4.29	129.12	124.45
13	L	301	BCL	C2B-C1B-NB	4.28	114.77	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	K	103	BCL	O2D-CGD-CBD	4.28	118.71	111.23
13	O	102	BCL	C3C-C4C-CHD	-4.27	114.40	123.39
13	F	102	BCL	C1D-CHD-C4C	-4.26	116.33	126.62
13	9	104	BCL	CAC-C3C-C4C	4.26	122.04	112.58
13	O	103	BCL	C3C-C4C-CHD	-4.26	114.42	123.39
13	Q	103	BCL	O2D-CGD-CBD	4.25	118.66	111.23
13	O	103	BCL	C1D-CHD-C4C	-4.25	116.38	126.62
13	S	103	BCL	C2B-C1B-NB	4.25	114.73	110.33
7	C	502	HEC	CHC-C4B-NB	4.24	129.07	124.45
13	5	103	BCL	C3C-C4C-CHD	-4.23	114.47	123.39
13	Q	103	BCL	C2B-C1B-NB	4.23	114.71	110.33
15	7	104	UQ8	C7-C8-C9	-4.23	119.55	126.83
22	H	302	CDL	OB6-CB5-C51	4.22	120.60	111.48
13	U	102	BCL	C1D-CHD-C4C	-4.22	116.45	126.62
7	C	504	HEC	CHC-C4B-NB	4.19	129.02	124.45
13	U	103	BCL	C3C-C4C-CHD	-4.19	114.56	123.39
13	A	101	BCL	C1D-CHD-C4C	-4.19	116.52	126.62
13	1	102	BCL	C1D-CHD-C4C	-4.18	116.54	126.62
13	M	403	BCL	C2B-C1B-NB	4.17	114.65	110.33
13	S	102	BCL	C3C-C4C-CHD	-4.16	114.61	123.39
22	Q	105	CDL	OA6-CA5-C11	4.16	120.48	111.48
13	A	103	BCL	C1D-CHD-C4C	-4.15	116.61	126.62
13	W	102	BCL	C2B-C1B-NB	4.14	114.62	110.33
13	5	102	BCL	C2B-C1B-NB	4.13	114.61	110.33
13	5	103	BCL	C1D-CHD-C4C	-4.11	116.70	126.62
22	Q	105	CDL	OB6-CB5-C51	4.10	120.34	111.48
13	Q	102	BCL	C3C-C4C-CHD	-4.06	114.83	123.39
13	M	404	BCL	C2C-C3C-C4C	-4.05	95.27	101.34
13	I	103	BCL	C1C-NC-C4C	-4.05	104.83	106.68
7	C	504	HEC	CBC-CAC-C3C	-4.04	119.36	127.43
13	U	102	BCL	CAC-C3C-C4C	4.03	121.54	112.58
19	P	101	CRT	C21-C22-C23	-4.02	121.63	127.28
13	Y	102	BCL	CHD-C1D-ND	-4.02	119.15	124.80
13	A	101	BCL	C3C-C4C-CHD	-4.01	114.93	123.39
7	C	502	HEC	CBB-CAB-C3B	-4.01	119.42	127.43
13	M	402	BCL	C2C-C3C-C4C	-4.01	95.34	101.34
12	1	106	PGV	O01-C1-C2	4.01	120.15	111.48
13	9	104	BCL	O2D-CGD-O1D	-4.00	116.06	123.85
13	K	103	BCL	C3C-C4C-CHD	-3.97	115.02	123.39
13	M	402	BCL	C3C-C4C-CHD	-3.94	115.08	123.39
20	3	104	PEF	O4P-P-O2P	3.94	120.18	107.91
13	M	402	BCL	CAC-C3C-C4C	3.94	121.33	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	5	103	BCL	O2D-CGD-CBD	3.93	118.11	111.23
13	D	103	BCL	O2D-CGD-CBD	3.93	118.10	111.23
20	U	105	PEF	O3P-P-O2P	3.92	120.11	107.91
13	W	102	BCL	C3C-C4C-CHD	-3.92	115.13	123.39
20	U	106	PEF	O4P-P-O2P	3.91	120.08	107.91
13	3	102	BCL	CHD-C1D-ND	-3.91	119.31	124.80
19	V	101	CRT	C4-C5-C6	-3.90	119.43	124.91
13	O	103	BCL	O2D-CGD-CBD	3.89	118.03	111.23
13	S	102	BCL	C1D-CHD-C4C	-3.89	117.24	126.62
7	C	503	HEC	CBC-CAC-C3C	-3.88	119.67	127.43
13	M	404	BCL	O2D-CGD-O1D	-3.88	116.29	123.85
13	3	103	BCL	C3C-C4C-CHD	-3.88	115.21	123.39
14	L	302	BPH	C4D-CHA-CBD	-3.88	106.60	108.45
14	L	302	BPH	C4A-C3A-C2A	-3.88	99.15	102.84
13	M	404	BCL	C1C-NC-C4C	-3.88	104.91	106.68
20	I	104	PEF	O3P-P-O2P	3.87	119.96	107.91
13	D	103	BCL	C3C-C4C-CHD	-3.87	115.24	123.39
14	M	405	BPH	C4A-C3A-C2A	-3.86	99.16	102.84
20	1	105	PEF	O4P-P-O2P	3.86	119.91	107.91
20	W	104	PEF	O3P-P-O2P	3.85	119.89	107.91
13	A	103	BCL	C3C-C4C-CHD	-3.84	115.29	123.39
20	M	408	PEF	O3P-P-O2P	3.84	119.85	107.91
19	Z	101	CRT	C4-C5-C6	-3.83	119.54	124.91
13	3	102	BCL	C1D-CHD-C4C	-3.81	117.42	126.62
13	M	404	BCL	C3C-C4C-CHD	-3.81	115.35	123.39
19	6	101	CRT	C21-C22-C23	-3.81	121.94	127.28
13	5	102	BCL	O2D-CGD-O1D	-3.80	116.44	123.85
15	7	104	UQ8	C7-C6-C1	-3.80	118.37	124.89
20	M	410	PEF	O4P-P-O2P	3.80	119.73	107.91
13	I	103	BCL	C3C-C4C-CHD	-3.79	115.40	123.39
20	5	104	PEF	O3P-P-O2P	3.78	119.67	107.91
14	M	405	BPH	C4-C3-C5	3.78	121.78	115.23
13	F	102	BCL	C3C-C4C-CHD	-3.77	115.44	123.39
13	K	102	BCL	C3C-C4C-CHD	-3.76	115.46	123.39
22	H	304	CDL	OA6-CA5-C11	3.73	119.55	111.48
13	3	102	BCL	C3C-C4C-CHD	-3.73	115.53	123.39
13	D	102	BCL	CHD-C1D-ND	-3.73	119.56	124.80
13	Q	102	BCL	CMD-C2D-C1D	3.72	131.29	124.73
13	W	102	BCL	C1D-CHD-C4C	-3.72	117.64	126.62
13	0	102	BCL	O2D-CGD-CBD	3.71	117.72	111.23
13	M	404	BCL	CMD-C2D-C1D	3.71	131.26	124.73
7	C	502	HEC	CHA-C1A-NA	3.70	128.48	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	I	102	BCL	C1D-ND-C4D	3.69	108.90	106.31
13	W	103	BCL	O2D-CGD-CBD	3.69	117.68	111.23
13	S	102	BCL	O2D-CGD-O1D	-3.69	116.67	123.85
19	0	101	CRT	C4-C5-C6	-3.69	119.74	124.91
14	L	302	BPH	OBD-CAD-C3D	-3.68	122.15	127.89
22	M	416	CDL	OB6-CB5-C51	3.67	119.42	111.48
13	L	301	BCL	CAC-C3C-C4C	3.67	120.73	112.58
13	7	102	BCL	CHD-C1D-ND	-3.66	119.65	124.80
13	Y	102	BCL	C3C-C4C-CHD	-3.65	115.69	123.39
19	1	104	CRT	C21-C22-C23	-3.65	122.15	127.28
12	3	105	PGV	O01-C1-C2	3.65	119.37	111.48
20	M	419	PEF	O2-C10-C11	3.64	119.36	111.48
13	0	102	BCL	C3C-C4C-CHD	-3.64	115.72	123.39
13	3	103	BCL	C1-C2-C3	-3.63	120.25	126.20
12	H	303	PGV	C02-O01-C1	-3.63	109.12	117.80
13	5	102	BCL	C1D-ND-C4D	3.62	108.85	106.31
13	7	103	BCL	O2D-CGD-CBD	3.62	117.56	111.23
19	2	101	CRT	C21-C22-C23	-3.62	122.20	127.28
13	W	102	BCL	C1-C2-C3	-3.62	120.26	126.20
13	3	103	BCL	O2D-CGD-CBD	3.62	117.55	111.23
19	U	104	CRT	C21-C22-C23	-3.61	122.21	127.28
12	A	105	PGV	O01-C1-C2	3.61	119.29	111.48
12	C	509	PGV	C02-O01-C1	-3.59	112.61	117.78
14	M	405	BPH	C1A-C2A-C3A	-3.59	99.43	102.84
13	D	102	BCL	C3C-C4C-CHD	-3.58	115.84	123.39
13	A	101	BCL	C1C-NC-C4C	-3.58	105.05	106.68
13	5	102	BCL	CHD-C1D-ND	-3.58	119.77	124.80
12	C	509	PGV	O01-C1-C2	3.58	119.22	111.48
13	S	103	BCL	C1-C2-C3	-3.57	120.35	126.20
13	O	103	BCL	C1C-NC-C4C	-3.57	105.05	106.68
14	M	405	BPH	CMA-C3A-C4A	-3.57	106.93	114.61
13	L	301	BCL	C1D-CHD-C4C	-3.56	118.02	126.62
14	M	405	BPH	C2D-C1D-ND	3.56	112.01	109.43
14	M	405	BPH	CMC-C2C-C3C	3.56	127.89	114.13
13	M	404	BCL	C2B-C1B-NB	3.56	114.02	110.33
13	A	103	BCL	CBC-CAC-C3C	-3.55	105.88	113.41
19	2	101	CRT	C4-C5-C6	-3.55	119.93	124.91
12	L	305	PGV	C03-C02-C01	-3.54	103.53	111.78
13	5	102	BCL	C3C-C4C-CHD	-3.54	115.93	123.39
13	M	402	BCL	O2D-CGD-CBD	3.54	117.41	111.23
13	A	101	BCL	O2D-CGD-O1D	-3.53	116.97	123.85
13	M	404	BCL	CMC-C2C-C1C	3.52	121.22	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	3	102	BCL	C1C-NC-C4C	-3.51	105.08	106.68
13	7	103	BCL	C3C-C4C-CHD	-3.51	116.00	123.39
22	S	104	CDL	OA6-CA5-C11	3.50	119.06	111.48
13	7	102	BCL	CMD-C2D-C1D	3.50	130.89	124.73
13	M	402	BCL	C1C-NC-C4C	-3.49	105.09	106.68
13	Q	103	BCL	C4-C3-C5	3.48	121.28	115.23
13	Q	103	BCL	CAC-C3C-C4C	3.47	120.30	112.58
13	A	103	BCL	O2D-CGD-CBD	3.47	117.29	111.23
13	U	103	BCL	O2D-CGD-CBD	3.46	117.28	111.23
19	O	104	CRT	C5-C6-C7	-3.45	120.68	125.89
22	K	104	CDL	OB8-CB7-C71	3.44	122.33	111.83
19	Q	104	CRT	C10-C9-C7	-3.44	122.45	127.28
13	S	102	BCL	CMD-C2D-C1D	3.43	130.77	124.73
13	Q	102	BCL	CAC-C3C-C4C	3.43	120.19	112.58
13	M	403	BCL	C1D-CHD-C4C	-3.43	118.36	126.62
22	M	416	CDL	OA8-CA7-C31	3.42	121.55	111.15
13	3	102	BCL	CMC-C2C-C3C	3.42	127.22	113.98
13	O	102	BCL	C1-O2A-CGA	3.42	124.94	116.65
13	Y	102	BCL	O2D-CGD-O1D	-3.42	117.19	123.85
19	9	103	CRT	C10-C9-C7	-3.40	122.50	127.28
13	Y	102	BCL	CBC-CAC-C3C	-3.40	106.20	113.41
13	Q	102	BCL	CMC-C2C-C3C	3.39	127.10	113.98
13	M	403	BCL	C1C-NC-C4C	-3.39	105.13	106.68
12	D	105	PGV	C02-O01-C1	-3.39	109.69	117.80
13	I	102	BCL	CBC-CAC-C3C	-3.38	106.24	113.41
19	0	101	CRT	C21-C22-C23	-3.38	122.53	127.28
20	K	105	PEF	C2-O2-C10	-3.38	109.70	117.80
13	O	102	BCL	O2D-CGD-O1D	-3.38	117.27	123.85
14	M	405	BPH	C3D-C4D-ND	3.37	112.03	107.71
19	M	407	CRT	C26-C27-C28	-3.36	122.57	127.28
13	7	102	BCL	C1-C2-C3	-3.35	120.71	126.20
13	I	102	BCL	CMC-C2C-C3C	3.32	126.84	113.98
20	M	419	PEF	O3-C30-C31	3.32	121.95	111.83
22	K	104	CDL	CB4-OB6-CB5	-3.32	109.86	117.80
13	3	102	BCL	O2D-CGD-O1D	-3.31	117.40	123.85
22	H	302	CDL	CB4-OB6-CB5	-3.31	109.86	117.80
19	9	103	CRT	C4-C5-C6	-3.31	120.27	124.91
15	7	104	UQ8	C12-C13-C14	-3.30	120.06	127.62
13	A	103	BCL	C4-C3-C5	3.30	120.96	115.23
13	Q	102	BCL	C1D-CHD-C4C	-3.30	118.67	126.62
13	U	103	BCL	C2C-C3C-C4C	-3.29	96.41	101.34
13	Q	103	BCL	C1-C2-C3	-3.28	120.82	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	104	CRT	C10-C9-C7	-3.28	122.68	127.28
13	Z	102	BCL	C1-C2-C3	-3.27	120.83	126.20
14	M	405	BPH	CMC-C2C-C1C	3.27	121.65	114.61
19	A	104	CRT	C5-C6-C7	-3.26	120.97	125.89
15	7	104	UQ8	C17-C18-C19	-3.25	120.17	127.62
13	5	102	BCL	C1-O2A-CGA	3.25	124.52	116.65
13	5	103	BCL	O2D-CGD-O1D	-3.25	117.52	123.85
13	1	102	BCL	C3C-C4C-CHD	-3.25	116.54	123.39
19	Z	101	CRT	C20-C19-C17	-3.25	122.72	127.28
13	1	103	BCL	CBC-CAC-C3C	-3.25	106.53	113.41
19	J	101	CRT	C20-C19-C17	-3.24	122.73	127.28
23	F	104	LMT	C4B-C3B-C2B	-3.24	105.14	110.83
19	P	101	CRT	C4-C5-C6	-3.23	120.38	124.91
14	L	302	BPH	CBC-CAC-C3C	-3.23	107.42	113.78
13	D	102	BCL	CMC-C2C-C3C	3.23	126.46	113.98
13	K	102	BCL	CHD-C1D-ND	-3.22	120.27	124.80
13	I	102	BCL	C3C-C4C-CHD	-3.21	116.62	123.39
13	D	102	BCL	C1D-ND-C4D	3.21	108.56	106.31
13	S	102	BCL	CMC-C2C-C3C	3.20	126.36	113.98
13	A	101	BCL	CMC-C2C-C3C	3.20	126.35	113.98
19	O	104	CRT	C21-C20-C19	-3.19	116.99	123.52
13	K	102	BCL	CMC-C2C-C3C	3.19	126.32	113.98
19	M	407	CRT	C14-C15-C16	-3.18	113.97	123.20
13	Y	102	BCL	C1D-ND-C4D	3.18	108.55	106.31
13	L	301	BCL	CMC-C2C-C3C	3.17	126.25	113.98
13	F	103	BCL	CBC-CAC-C3C	-3.17	106.69	113.41
13	0	102	BCL	O2A-CGA-CBA	3.17	121.49	111.83
18	M	406	MQ8	C29-C28-C30	3.16	120.71	115.23
13	M	403	BCL	C1-C2-C3	-3.15	121.03	126.20
19	M	407	CRT	C4-C5-C6	-3.15	120.48	124.91
7	C	503	HEC	CHD-C4C-NC	3.15	127.89	124.45
13	K	102	BCL	CBC-CAC-C3C	-3.15	106.73	113.41
13	Z	102	BCL	CMC-C2C-C3C	3.15	126.16	113.98
22	H	302	CDL	OB8-CB7-C71	3.14	121.41	111.83
13	S	102	BCL	CBA-CAA-C2A	-3.14	104.46	113.79
13	Q	102	BCL	O2D-CGD-O1D	-3.13	117.75	123.85
19	1	104	CRT	C5-C6-C7	-3.13	121.16	125.89
13	M	403	BCL	C2A-C1A-CHA	-3.13	118.43	123.87
19	V	101	CRT	C21-C20-C19	-3.13	117.12	123.52
13	D	102	BCL	C4-C3-C5	3.12	120.64	115.23
19	1	104	CRT	C4-C5-C6	-3.12	120.54	124.91
19	J	101	CRT	C32-C31-C30	-3.11	114.19	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	308	UQ8	C22-C23-C24	-3.10	120.53	127.62
19	P	101	CRT	C10-C9-C7	-3.10	122.94	127.28
7	C	501	HEC	CHA-C1A-NA	3.09	127.82	124.45
19	Q	104	CRT	C5-C6-C7	-3.09	121.22	125.89
22	Y	103	CDL	OA8-CA7-C31	3.09	120.54	111.15
13	3	102	BCL	C3B-C4B-NB	3.09	113.84	109.76
15	L	308	UQ8	O5-C5-C6	-3.09	115.81	121.79
13	S	103	BCL	O2D-CGD-CBD	3.09	116.63	111.23
13	O	102	BCL	CMC-C2C-C3C	3.09	125.93	113.98
19	Z	101	CRT	C21-C20-C19	-3.09	117.20	123.52
7	C	504	HEC	CHA-C1A-NA	3.09	127.81	124.45
13	I	103	BCL	CMC-C2C-C3C	3.08	125.90	113.98
13	I	102	BCL	C1-O2A-CGA	3.07	124.09	116.65
13	M	402	BCL	O2A-CGA-CBA	3.07	121.21	111.83
13	1	102	BCL	CMC-C2C-C3C	3.07	125.85	113.98
13	U	103	BCL	CED-O2D-CGD	3.06	122.86	115.92
13	Q	102	BCL	CBA-CAA-C2A	-3.06	104.69	113.79
19	Z	101	CRT	C32-C31-C30	-3.05	114.36	123.20
15	L	308	UQ8	C27-C28-C29	-3.05	120.64	127.62
23	F	104	LMT	O5'-C1'-C2'	3.05	116.63	110.37
13	F	102	BCL	CMC-C2C-C3C	3.04	125.75	113.98
13	S	102	BCL	CBC-CAC-C3C	-3.04	106.96	113.41
12	L	306	PGV	O03-C19-C20	3.03	121.09	111.83
13	W	103	BCL	CMC-C2C-C3C	3.03	125.71	113.98
14	L	302	BPH	C3D-C4D-ND	3.03	111.59	107.71
13	9	104	BCL	C4-C3-C5	3.03	120.48	115.23
19	9	102	CRT	C10-C9-C7	-3.03	123.03	127.28
19	9	103	CRT	C5-C6-C7	-3.02	121.32	125.89
13	5	102	BCL	CMC-C2C-C3C	3.02	125.67	113.98
19	Q	104	CRT	C14-C15-C16	-3.02	114.44	123.20
13	5	103	BCL	C4-C3-C5	3.02	120.47	115.23
13	K	103	BCL	CBC-CAC-C3C	-3.02	107.00	113.41
22	H	302	CDL	CA6-CA4-CA3	-3.02	104.74	111.78
13	K	102	BCL	O2D-CGD-O1D	-3.02	117.97	123.85
22	Q	105	CDL	CA4-OA6-CA5	-3.02	110.57	117.80
13	Z	102	BCL	C3C-C4C-CHD	-3.02	117.03	123.39
19	9	102	CRT	C20-C19-C17	-3.01	123.05	127.28
19	V	101	CRT	C10-C9-C7	-3.01	123.06	127.28
14	M	405	BPH	C6-C5-C3	-3.01	106.14	113.47
13	1	102	BCL	CBC-CAC-C3C	-3.00	107.04	113.41
13	M	403	BCL	C1-O2A-CGA	3.00	123.92	116.65
19	N	101	CRT	C34-C33-C35	3.00	122.67	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	N	101	CRT	C4-C5-C6	-3.00	120.70	124.91
13	D	102	BCL	O2D-CGD-O1D	-3.00	118.01	123.85
13	S	103	BCL	C4-C3-C5	3.00	120.43	115.23
19	9	102	CRT	C21-C20-C19	-3.00	117.39	123.52
7	C	503	HEC	CHA-C1A-NA	2.99	127.71	124.45
13	7	102	BCL	CMC-C2C-C3C	2.99	125.54	113.98
13	9	104	BCL	CMC-C2C-C3C	2.98	125.49	113.98
14	L	302	BPH	C2D-C1D-ND	2.97	111.58	109.43
13	M	402	BCL	CMC-C2C-C3C	2.97	125.45	113.98
13	M	403	BCL	CHD-C1D-ND	-2.96	120.63	124.80
13	Z	102	BCL	C1D-ND-C4D	2.96	108.39	106.31
18	M	406	MQ8	C26-C27-C28	-2.96	120.84	127.62
19	6	101	CRT	C14-C15-C16	-2.96	114.63	123.20
15	L	308	UQ8	C35-C34-C36	2.95	120.36	115.23
13	I	103	BCL	CBC-CAC-C3C	-2.95	107.15	113.41
13	D	103	BCL	CBC-CAC-C3C	-2.95	107.15	113.41
13	L	301	BCL	O2D-CGD-O1D	-2.95	118.10	123.85
13	U	103	BCL	CMC-C2C-C3C	2.95	125.39	113.98
13	U	103	BCL	C4-C3-C5	2.95	120.34	115.23
19	6	101	CRT	C4-C5-C6	-2.95	120.78	124.91
13	1	103	BCL	C2C-C3C-C4C	-2.94	96.93	101.34
19	Z	101	CRT	C5-C6-C7	-2.94	121.45	125.89
13	D	103	BCL	CMC-C2C-C3C	2.94	125.34	113.98
7	C	504	HEC	CHA-C4D-ND	2.94	129.19	123.86
19	J	101	CRT	C5-C6-C7	-2.94	121.45	125.89
13	Y	102	BCL	CMC-C2C-C3C	2.94	125.33	113.98
19	U	104	CRT	C32-C31-C30	-2.93	114.70	123.20
13	A	103	BCL	CMC-C2C-C3C	2.93	125.32	113.98
22	H	304	CDL	CB4-OB6-CB5	-2.93	110.79	117.80
22	Y	103	CDL	OB8-CB7-C71	2.93	120.03	111.15
13	I	103	BCL	O2D-CGD-O1D	-2.93	118.15	123.85
19	U	104	CRT	C4-C5-C6	-2.92	120.81	124.91
13	D	103	BCL	C4-C3-C5	2.92	120.30	115.23
7	C	502	HEC	CBC-CAC-C3C	-2.92	121.60	127.43
14	M	405	BPH	CBA-CAA-C2A	-2.92	105.19	113.78
13	5	103	BCL	C3D-C2D-C1D	-2.91	101.86	105.83
13	0	102	BCL	C4-C3-C5	2.91	120.28	115.23
13	Q	103	BCL	C2C-C3C-C4C	-2.91	96.98	101.34
13	Z	102	BCL	CBC-CAC-C3C	-2.91	107.24	113.41
13	W	103	BCL	C4-C3-C5	2.91	120.28	115.23
19	V	101	CRT	C14-C15-C16	-2.91	114.78	123.20
18	M	406	MQ8	C24-C23-C25	2.90	120.27	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	F	104	LMT	C1'-C2'-C3'	2.90	116.12	110.01
13	3	103	BCL	C1D-ND-C4D	2.90	108.35	106.31
7	C	502	HEC	CHD-C4C-NC	2.90	127.61	124.45
13	Q	102	BCL	C6-C5-C3	-2.90	106.40	113.47
13	S	102	BCL	C1C-NC-C4C	-2.90	105.36	106.68
20	M	411	PEF	O3P-P-O2P	2.89	116.91	107.91
13	W	102	BCL	CMD-C2D-C1D	2.89	129.82	124.73
13	Y	102	BCL	C1-O2A-CGA	2.89	123.64	116.65
13	F	103	BCL	CMC-C2C-C3C	2.89	125.14	113.98
13	M	404	BCL	O2A-CGA-CBA	2.89	120.64	111.83
13	7	103	BCL	C4A-NA-C1A	-2.88	105.36	106.68
12	A	105	PGV	O03-C19-C20	2.88	120.61	111.83
19	U	104	CRT	C18-C17-C16	2.88	122.49	118.09
13	0	102	BCL	C6-C5-C3	-2.88	106.46	113.47
13	W	102	BCL	C4-C3-C5	2.87	120.22	115.23
19	G	101	CRT	C14-C15-C16	-2.87	114.88	123.20
13	F	103	BCL	O2D-CGD-O1D	-2.87	118.26	123.85
13	W	102	BCL	CMC-C2C-C3C	2.87	125.08	113.98
19	9	102	CRT	C4-C5-C6	-2.87	120.89	124.91
14	L	302	BPH	CMA-C3A-C4A	-2.87	108.43	114.61
7	C	504	HEC	C4B-NB-C1B	2.87	110.50	105.82
12	M	414	PGV	O12-P-O11	-2.87	99.19	106.67
13	0	102	BCL	CMC-C2C-C3C	2.86	125.06	113.98
19	M	407	CRT	C32-C31-C30	-2.86	114.90	123.20
15	7	104	UQ8	O5-C5-C6	-2.86	116.25	121.79
13	D	102	BCL	CBC-CAC-C3C	-2.86	107.34	113.41
13	K	103	BCL	C4-C3-C5	2.86	120.19	115.23
13	M	402	BCL	CBC-CAC-C3C	-2.86	107.36	113.41
13	3	102	BCL	CMD-C2D-C1D	2.86	129.76	124.73
22	D	104	CDL	OA8-CA7-C31	2.85	119.81	111.15
19	1	104	CRT	C20-C19-C17	-2.85	123.28	127.28
15	L	303	UQ8	C16-C14-C13	-2.85	114.76	121.17
13	O	103	BCL	CBC-CAC-C3C	-2.85	107.37	113.41
13	I	102	BCL	CHD-C1D-ND	-2.85	120.79	124.80
22	H	304	CDL	OB8-CB7-C71	2.85	120.53	111.83
13	7	103	BCL	C3B-C4B-NB	2.85	113.52	109.76
15	7	104	UQ8	O4-C4-C3	-2.85	112.86	123.64
13	7	103	BCL	C4-C3-C5	2.85	120.17	115.23
13	K	102	BCL	C1D-ND-C4D	2.85	108.31	106.31
15	7	104	UQ8	C20-C19-C21	2.85	120.17	115.23
19	2	101	CRT	C32-C31-C30	-2.84	114.96	123.20
15	M	418	UQ8	C7-C6-C1	-2.84	120.02	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	501	HEC	CHD-C1D-ND	2.84	129.01	123.86
22	S	104	CDL	CB6-CB4-CB3	-2.84	105.16	111.78
14	L	302	BPH	O2D-CGD-O1D	-2.84	118.32	123.85
13	I	102	BCL	O2D-CGD-O1D	-2.84	118.32	123.85
19	2	101	CRT	C20-C19-C17	-2.84	123.30	127.28
7	C	502	HEC	C4B-NB-C1B	2.84	110.45	105.82
13	5	103	BCL	C2D-C1D-ND	2.83	112.93	110.13
13	F	103	BCL	C4-C3-C5	2.83	120.14	115.23
15	L	308	UQ8	C10-C9-C11	2.83	120.14	115.23
13	3	103	BCL	CMC-C2C-C3C	2.82	124.88	113.98
13	Q	102	BCL	C3D-C2D-C1D	-2.82	101.99	105.83
13	M	402	BCL	C1-C2-C3	-2.81	121.59	126.20
13	F	102	BCL	C1-O2A-CGA	2.81	123.45	116.65
13	1	103	BCL	CMC-C2C-C3C	2.81	124.83	113.98
15	7	104	UQ8	C7-C6-C5	2.80	121.77	118.52
13	1	102	BCL	C4-C3-C5	2.80	120.09	115.23
19	6	101	CRT	C10-C9-C7	-2.80	123.35	127.28
19	P	101	CRT	C32-C31-C30	-2.80	115.09	123.20
22	K	104	CDL	OA8-CA7-C31	2.80	120.36	111.83
18	M	406	MQ8	C41-C42-C43	-2.80	121.22	127.62
12	C	509	PGV	O03-C19-C20	2.79	120.35	111.83
19	J	101	CRT	C18-C17-C16	2.79	122.35	118.09
13	Q	103	BCL	CMC-C2C-C3C	2.79	124.77	113.98
13	3	102	BCL	C4-C3-C5	2.78	120.06	115.23
19	N	101	CRT	C5-C6-C7	-2.78	121.69	125.89
12	H	303	PGV	O03-C19-C20	2.78	120.32	111.83
13	K	103	BCL	C2C-C3C-C4C	-2.78	97.17	101.34
12	1	106	PGV	O03-C19-C20	2.78	120.31	111.83
13	S	102	BCL	C4-C3-C5	2.78	120.06	115.23
12	D	105	PGV	O03-C19-O04	-2.78	116.68	123.63
7	C	502	HEC	CHB-C1B-NB	2.78	128.90	123.86
19	P	101	CRT	C14-C15-C16	-2.78	115.15	123.20
19	O	104	CRT	C26-C27-C28	-2.78	123.38	127.28
15	L	308	UQ8	C7-C8-C9	-2.78	122.05	126.83
13	Z	102	BCL	C2C-C3C-C4C	-2.77	97.18	101.34
19	N	101	CRT	C21-C20-C19	-2.77	117.85	123.52
22	D	104	CDL	OB8-CB7-C71	2.77	119.55	111.15
19	A	104	CRT	C14-C15-C16	-2.77	115.18	123.20
19	9	102	CRT	C32-C31-C30	-2.77	115.18	123.20
13	U	102	BCL	CMC-C2C-C3C	2.77	124.68	113.98
14	M	405	BPH	O1D-CGD-CBD	-2.76	120.53	124.72
13	5	103	BCL	CMC-C2C-C3C	2.76	124.67	113.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	101	CRT	C9-C10-C11	-2.76	115.19	123.20
14	L	302	BPH	C1A-C2A-C3A	-2.76	100.21	102.84
13	O	103	BCL	C2A-C1A-CHA	-2.76	119.08	123.87
12	D	105	PGV	O03-C19-C20	2.76	120.25	111.83
13	7	102	BCL	O2D-CGD-O1D	-2.76	118.48	123.85
13	S	102	BCL	C1-C2-C3	-2.76	121.68	126.20
12	D	105	PGV	O01-C1-C2	2.75	117.44	111.48
15	7	104	UQ8	C22-C23-C24	-2.75	118.49	127.64
14	L	302	BPH	CMC-C2C-C3C	2.75	124.73	114.13
19	U	104	CRT	C20-C19-C17	-2.74	123.43	127.28
22	Q	105	CDL	OB8-CB7-C71	2.74	120.19	111.83
13	F	102	BCL	O2D-CGD-O1D	-2.74	118.52	123.85
13	3	103	BCL	CHD-C1D-ND	-2.74	120.95	124.80
13	O	103	BCL	C4-C3-C5	2.74	119.98	115.23
19	A	104	CRT	C32-C31-C30	-2.74	115.27	123.20
13	K	103	BCL	CMC-C2C-C3C	2.74	124.56	113.98
13	Z	102	BCL	C3B-C4B-NB	2.74	113.37	109.76
13	7	102	BCL	O1D-CGD-CBD	-2.74	119.12	124.52
13	3	102	BCL	C2A-C1A-CHA	-2.73	119.12	123.87
15	L	308	UQ8	C1M-C1-C6	-2.73	119.96	124.45
19	M	407	CRT	C5-C6-C7	-2.73	121.76	125.89
13	D	102	BCL	O2A-CGA-CBA	2.73	120.17	111.83
12	A	105	PGV	C02-O01-C1	-2.73	111.25	117.80
19	9	103	CRT	C21-C20-C19	-2.73	117.93	123.52
13	A	103	BCL	C3B-C4B-NB	2.73	113.36	109.76
19	0	101	CRT	C32-C31-C30	-2.73	115.30	123.20
13	M	403	BCL	CBC-CAC-C3C	-2.73	107.63	113.41
22	D	104	CDL	OA6-CA5-C11	2.73	120.94	110.93
13	7	103	BCL	CMC-C2C-C3C	2.72	124.52	113.98
13	F	102	BCL	CMD-C2D-C1D	2.72	129.53	124.73
19	U	104	CRT	C14-C15-C16	-2.72	115.31	123.20
13	5	102	BCL	CBC-CAC-C3C	-2.72	107.64	113.41
15	L	308	UQ8	C15-C14-C16	2.72	119.95	115.23
13	1	102	BCL	O2D-CGD-O1D	-2.72	118.56	123.85
7	C	503	HEC	C4B-NB-C1B	2.72	110.25	105.82
15	M	418	UQ8	C10-C9-C11	2.72	120.84	114.59
12	M	415	PGV	C02-O01-C1	-2.71	111.30	117.80
14	L	302	BPH	C6-C5-C3	-2.71	106.86	113.47
13	Q	103	BCL	O2A-CGA-CBA	2.70	120.08	111.83
13	Q	103	BCL	C2D-C1D-ND	2.70	112.80	110.13
19	Z	101	CRT	C29-C28-C30	2.70	122.21	118.09
13	7	103	BCL	C4D-CHA-C1A	-2.70	118.03	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	S	102	BCL	C3D-C2D-C1D	-2.69	102.16	105.83
19	A	104	CRT	C20-C19-C17	-2.69	123.51	127.28
14	L	302	BPH	C4-C3-C5	2.69	119.89	115.23
13	9	104	BCL	CMD-C2D-C1D	2.69	129.46	124.73
19	U	104	CRT	C10-C9-C7	-2.68	123.51	127.28
13	1	103	BCL	C3C-C4C-CHD	-2.68	117.73	123.39
12	3	105	PGV	O03-C19-C20	2.68	120.01	111.83
13	I	103	BCL	C6-C5-C3	-2.68	106.94	113.47
13	L	301	BCL	CMC-C2C-C1C	2.68	118.97	111.77
15	L	308	UQ8	C17-C18-C19	-2.68	121.50	127.62
13	5	102	BCL	CHA-C4D-ND	2.67	138.07	132.55
13	1	103	BCL	C1D-ND-C4D	2.67	108.19	106.31
13	5	103	BCL	C1-C2-C3	-2.67	121.83	126.20
13	7	103	BCL	CBC-CAC-C3C	-2.67	107.75	113.41
19	G	101	CRT	C9-C10-C11	-2.66	115.48	123.20
13	I	102	BCL	CMD-C2D-C1D	2.66	129.42	124.73
13	A	101	BCL	C4-C3-C5	2.66	119.84	115.23
13	W	102	BCL	CBC-CAC-C3C	-2.65	107.78	113.41
13	M	402	BCL	C2D-C1D-ND	2.65	112.75	110.13
13	A	101	BCL	CMD-C2D-C1D	2.65	129.40	124.73
13	Q	102	BCL	O1D-CGD-CBD	-2.65	119.30	124.52
7	C	503	HEC	CHB-C1B-NB	2.64	128.66	123.86
13	W	102	BCL	CHA-C4D-ND	2.64	138.00	132.55
7	C	501	HEC	CAD-CBD-CGD	2.64	120.67	113.67
22	D	104	CDL	CB4-OB6-CB5	-2.64	111.47	117.80
22	D	104	CDL	OB6-CB5-C51	2.64	120.63	110.93
19	O	104	CRT	C32-C31-C30	-2.64	115.55	123.20
13	Q	102	BCL	C1C-NC-C4C	-2.64	105.47	106.68
22	S	104	CDL	OA8-CA7-C31	2.64	119.88	111.83
13	D	102	BCL	C1-C2-C3	-2.63	121.88	126.20
13	U	102	BCL	CGD-CBD-CAD	-2.63	102.33	110.85
13	0	102	BCL	CBC-CAC-C3C	-2.63	107.83	113.41
12	L	305	PGV	O03-C19-C20	2.63	119.85	111.83
13	M	403	BCL	C3D-C2D-C1D	-2.63	102.24	105.83
13	O	102	BCL	C3D-C2D-C1D	-2.63	102.25	105.83
13	K	102	BCL	O2A-CGA-CBA	2.62	119.83	111.83
13	I	103	BCL	O2A-CGA-CBA	2.62	119.81	111.83
19	M	407	CRT	C20-C19-C17	-2.61	123.61	127.28
19	0	101	CRT	C10-C9-C7	-2.61	123.61	127.28
13	1	103	BCL	O2D-CGD-O1D	-2.61	118.77	123.85
13	F	102	BCL	C4-C3-C5	2.61	119.75	115.23
12	H	303	PGV	O01-C1-O02	-2.60	117.61	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	308	UQ8	C20-C19-C21	2.60	119.75	115.23
19	9	103	CRT	C14-C15-C16	-2.60	115.66	123.20
19	9	102	CRT	C14-C15-C16	-2.60	115.68	123.20
13	1	103	BCL	O2A-CGA-CBA	2.59	119.75	111.83
23	F	104	LMT	C1B-O5B-C5B	2.59	118.78	113.72
22	H	304	CDL	OA8-CA7-C31	2.59	119.74	111.83
13	D	103	BCL	O2A-CGA-CBA	2.59	119.74	111.83
19	6	101	CRT	C13-C12-C11	2.59	122.05	118.09
13	O	103	BCL	O2D-CGD-O1D	-2.59	118.81	123.85
13	Z	102	BCL	O2D-CGD-O1D	-2.59	118.81	123.85
23	M	420	LMT	C1B-O1B-C4'	-2.59	111.84	117.98
13	S	102	BCL	CHC-C1C-NC	2.59	128.13	124.40
7	C	504	HEC	CHB-C1B-NB	2.59	128.55	123.86
19	1	104	CRT	C21-C20-C19	-2.59	118.23	123.52
14	M	405	BPH	OBB-CAB-C3B	2.59	124.31	119.99
19	O	104	CRT	C14-C15-C16	-2.58	115.71	123.20
13	W	103	BCL	CBC-CAC-C3C	-2.58	107.93	113.41
20	M	409	PEF	O2P-P-O1P	2.58	120.08	110.95
19	G	101	CRT	C21-C20-C19	-2.58	118.24	123.52
13	1	103	BCL	C1-C2-C3	-2.58	121.97	126.20
19	O	104	CRT	C21-C22-C23	-2.58	123.66	127.28
13	I	102	BCL	CHA-C4D-ND	2.58	137.87	132.55
13	O	103	BCL	CMC-C2C-C3C	2.58	123.96	113.98
13	I	102	BCL	C3B-C4B-NB	2.58	113.16	109.76
13	9	104	BCL	O2A-CGA-O1A	-2.58	117.18	123.63
13	U	102	BCL	C2A-C1A-CHA	-2.57	119.40	123.87
18	M	406	MQ8	C36-C37-C38	-2.57	121.73	127.62
12	M	414	PGV	O03-C19-C20	2.57	119.68	111.83
23	F	104	LMT	O5'-C5'-C4'	2.57	115.04	109.72
19	A	104	CRT	C10-C9-C7	-2.57	123.67	127.28
13	M	403	BCL	O2D-CGD-O1D	-2.57	118.85	123.85
13	7	103	BCL	CHB-C1B-NB	-2.57	120.19	124.05
13	F	102	BCL	CBC-CAC-C3C	-2.56	107.98	113.41
7	C	504	HEC	CHD-C1D-ND	2.56	128.50	123.86
13	A	101	BCL	C1-C2-C3	-2.56	122.01	126.20
19	2	101	CRT	C9-C10-C11	-2.55	115.80	123.20
13	W	102	BCL	O2A-CGA-CBA	2.55	119.62	111.83
19	V	101	CRT	C29-C28-C30	2.55	121.99	118.09
13	K	103	BCL	O2A-CGA-CBA	2.55	119.61	111.83
19	Q	104	CRT	C32-C31-C30	-2.55	115.81	123.20
19	A	104	CRT	C4-C5-C6	-2.55	121.34	124.91
20	M	410	PEF	O3P-P-O1P	-2.55	101.95	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	U	104	CRT	C21-C20-C19	-2.54	118.31	123.52
7	C	502	HEC	CHA-C4D-ND	2.54	128.47	123.86
13	O	102	BCL	CMD-C2D-C1D	2.54	129.21	124.73
19	9	103	CRT	C32-C31-C30	-2.54	115.84	123.20
13	Q	102	BCL	C1-O2A-CGA	2.54	122.80	116.65
13	Z	102	BCL	C4-C3-C5	2.54	119.63	115.23
19	U	104	CRT	C5-C6-C7	-2.54	122.06	125.89
13	L	301	BCL	O2A-CGA-O1A	-2.53	117.29	123.63
13	I	103	BCL	C4-C3-C5	2.53	119.63	115.23
13	0	102	BCL	C3B-C4B-NB	2.53	113.10	109.76
20	K	105	PEF	O3-C30-C31	2.53	119.55	111.83
19	6	101	CRT	C21-C20-C19	-2.53	118.34	123.52
13	M	404	BCL	O2A-CGA-O1A	-2.53	117.30	123.63
15	M	418	UQ8	C4M-O4-C4	2.53	125.36	116.47
13	0	102	BCL	C1-C2-C3	-2.53	122.06	126.20
13	0	102	BCL	C1D-ND-C4D	2.53	108.08	106.31
13	A	103	BCL	O2A-CGA-CBA	2.53	119.53	111.83
13	Q	102	BCL	C1-C2-C3	-2.52	122.06	126.20
13	3	103	BCL	CBC-CAC-C3C	-2.52	108.06	113.41
19	0	101	CRT	C9-C10-C11	-2.52	115.89	123.20
19	O	104	CRT	C29-C28-C30	2.52	121.94	118.09
13	Q	102	BCL	CHD-C1D-ND	-2.52	121.26	124.80
13	D	103	BCL	C3B-C4B-NB	2.52	113.08	109.76
19	G	101	CRT	C32-C31-C30	-2.52	115.91	123.20
19	9	102	CRT	C13-C12-C11	2.51	121.93	118.09
13	O	102	BCL	CHA-C4D-ND	2.51	137.73	132.55
19	2	101	CRT	C18-C17-C16	2.51	121.93	118.09
15	7	104	UQ8	O4-C4-C5	2.51	125.11	116.64
13	D	103	BCL	C1-C2-C3	-2.51	122.08	126.20
13	1	103	BCL	CHD-C1D-ND	-2.51	121.27	124.80
19	Q	104	CRT	C4-C5-C6	-2.51	121.39	124.91
13	1	102	BCL	C3B-C4B-NB	2.50	113.06	109.76
7	C	504	HEC	O2A-CGA-CBA	2.50	121.90	114.00
7	C	503	HEC	CHA-C4D-ND	2.50	128.39	123.86
18	M	406	MQ8	C50-C48-C49	2.50	120.34	114.59
7	C	501	HEC	CHD-C4C-NC	2.50	127.17	124.45
13	S	103	BCL	C2C-C3C-C4C	-2.50	97.60	101.34
12	M	414	PGV	O14-P-O13	2.50	120.56	110.83
15	L	308	UQ8	C12-C13-C14	-2.49	121.91	127.62
13	M	404	BCL	CHA-C1A-NA	-2.49	120.75	126.39
13	M	403	BCL	C3A-C2A-C1A	-2.49	97.61	101.34
13	5	102	BCL	C3B-C4B-NB	2.49	113.04	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	405	BPH	C4C-C3C-C2C	-2.48	100.48	102.84
15	L	308	UQ8	C3M-O3-C3	2.48	125.20	116.47
20	3	104	PEF	O3P-P-O1P	-2.48	102.17	110.95
13	1	102	BCL	C2A-C1A-CHA	-2.48	119.57	123.87
13	1	102	BCL	C1D-ND-C4D	2.47	108.05	106.31
18	M	406	MQ8	C39-C38-C40	2.47	119.52	115.23
7	C	501	HEC	CHA-C4D-ND	2.47	128.35	123.86
13	K	103	BCL	C1-C2-C3	-2.47	122.14	126.20
19	9	102	CRT	C5-C6-C7	-2.47	122.16	125.89
19	6	101	CRT	C9-C10-C11	-2.47	116.04	123.20
13	M	403	BCL	O2A-CGA-CBA	2.47	119.37	111.83
19	6	101	CRT	C32-C31-C30	-2.47	116.04	123.20
13	Z	102	BCL	O2A-CGA-CBA	2.47	119.35	111.83
13	5	102	BCL	O2A-CGA-CBA	2.46	119.35	111.83
13	M	404	BCL	CHD-C1D-ND	-2.46	121.34	124.80
22	Q	105	CDL	OA6-CA5-OA7	-2.46	117.95	123.70
19	Q	104	CRT	C9-C10-C11	-2.46	116.07	123.20
13	W	102	BCL	C2A-C1A-CHA	-2.46	119.60	123.87
13	W	103	BCL	O2A-CGA-CBA	2.46	119.33	111.83
13	S	103	BCL	CMC-C2C-C3C	2.46	123.48	113.98
13	M	402	BCL	O2A-CGA-O1A	-2.46	117.48	123.63
13	1	102	BCL	O2A-CGA-CBA	2.46	119.32	111.83
13	7	102	BCL	C1-O2A-CGA	2.45	122.59	116.65
13	U	103	BCL	C2D-C1D-ND	2.45	112.55	110.13
19	P	101	CRT	C13-C12-C11	2.45	121.83	118.09
13	L	301	BCL	C1C-NC-C4C	-2.45	105.56	106.68
20	K	105	PEF	O2-C10-O4	-2.45	117.98	123.70
13	Q	103	BCL	C2A-C1A-CHA	-2.45	119.62	123.87
13	S	103	BCL	C3D-C2D-C1D	-2.45	102.49	105.83
22	Y	103	CDL	OA6-CA5-C11	2.45	119.91	110.93
13	F	102	BCL	O2A-CGA-CBA	2.44	119.29	111.83
19	U	104	CRT	C34-C33-C35	2.44	121.82	118.09
13	U	102	BCL	O2A-CGA-CBA	2.44	119.28	111.83
13	3	103	BCL	C4-C3-C5	2.44	119.46	115.23
13	M	403	BCL	C2D-C1D-ND	2.44	112.54	110.13
22	Y	103	CDL	OB6-CB5-C51	2.44	119.89	110.93
13	F	103	BCL	C3B-C4B-NB	2.44	112.97	109.76
19	2	101	CRT	C5-C6-C7	-2.43	122.22	125.89
12	M	415	PGV	O03-C19-C20	2.43	119.24	111.83
13	Y	102	BCL	CHA-C1A-NA	-2.43	120.89	126.39
13	M	403	BCL	CMD-C2D-C1D	2.43	129.00	124.73
13	Y	102	BCL	CMD-C2D-C1D	2.42	129.00	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	7	102	BCL	CHA-C4D-ND	2.42	137.55	132.55
19	A	104	CRT	C21-C20-C19	-2.42	118.56	123.52
13	U	102	BCL	C3D-C2D-C1D	-2.42	102.53	105.83
15	L	308	UQ8	C7-C6-C1	-2.42	120.74	124.89
19	1	104	CRT	C32-C31-C30	-2.42	116.19	123.20
15	L	303	UQ8	C10-C9-C11	2.42	119.42	115.23
19	N	101	CRT	C9-C10-C11	-2.42	116.20	123.20
19	O	104	CRT	C10-C9-C7	-2.41	123.90	127.28
23	F	104	LMT	O1B-C4'-C5'	-2.41	103.15	109.48
22	M	416	CDL	OA6-CA5-C11	2.41	119.78	110.93
19	1	104	CRT	C14-C15-C16	-2.41	116.22	123.20
19	O	104	CRT	C9-C10-C11	-2.41	116.22	123.20
19	Z	101	CRT	C14-C15-C16	-2.40	116.23	123.20
13	I	102	BCL	CHA-C1A-NA	-2.40	120.95	126.39
18	M	406	MQ8	C45-C43-C44	2.40	119.40	115.23
13	Q	103	BCL	CED-O2D-CGD	2.40	121.36	115.92
13	1	102	BCL	CMD-C2D-C1D	2.40	128.96	124.73
22	K	104	CDL	CA4-OA6-CA5	-2.40	112.05	117.80
13	9	104	BCL	C3D-C2D-C1D	-2.40	102.56	105.83
19	9	102	CRT	C36-C35-C33	-2.40	122.27	125.89
22	H	304	CDL	OB6-CB5-OB7	-2.40	118.10	123.70
13	K	102	BCL	CHA-C4D-ND	2.40	137.50	132.55
13	L	301	BCL	C2D-C1D-ND	2.39	112.49	110.13
15	7	104	UQ8	O5-C5-C4	2.39	126.08	121.03
19	G	101	CRT	C18-C17-C16	2.39	121.73	118.09
13	A	101	BCL	O2A-CGA-CBA	2.38	119.11	111.83
13	F	102	BCL	C1D-ND-C4D	2.38	107.98	106.31
19	O	104	CRT	C20-C19-C17	-2.38	123.94	127.28
13	U	103	BCL	CAA-CBA-CGA	-2.38	106.45	113.21
15	L	308	UQ8	C25-C24-C26	2.38	119.36	115.23
13	F	102	BCL	CHD-C1D-ND	-2.38	121.45	124.80
13	M	404	BCL	C3D-C2D-C1D	-2.38	102.59	105.83
13	U	102	BCL	CMD-C2D-C1D	2.38	128.91	124.73
13	7	103	BCL	C3D-C2D-C1D	-2.38	102.59	105.83
13	U	102	BCL	CHB-C1B-C2B	-2.38	120.53	127.43
13	D	102	BCL	CHA-C1A-NA	-2.37	121.02	126.39
13	O	102	BCL	C4-C3-C5	2.37	119.35	115.23
14	L	302	BPH	OBD-CAD-CBD	2.37	129.31	125.82
13	F	103	BCL	C1-C2-C3	-2.37	122.31	126.20
13	S	102	BCL	O1D-CGD-CBD	-2.37	119.84	124.52
13	K	102	BCL	CMD-C2D-C1D	2.37	128.90	124.73
20	W	104	PEF	O4P-P-O1P	-2.37	102.58	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	0	101	CRT	C5-C6-C7	-2.37	122.31	125.89
13	Q	102	BCL	CHA-C4D-ND	2.36	137.43	132.55
13	U	102	BCL	C1-O2A-CGA	2.36	122.37	116.65
15	L	309	UQ8	C10-C9-C11	2.36	120.03	114.59
13	A	101	BCL	CHA-C1A-NA	-2.36	121.05	126.39
13	O	103	BCL	CMB-C2B-C3B	2.36	133.11	125.67
13	3	102	BCL	CBC-CAC-C3C	-2.36	108.41	113.41
13	I	103	BCL	C2A-C1A-CHA	-2.36	119.78	123.87
14	M	405	BPH	O2A-C1-C2	-2.35	99.05	108.11
13	O	103	BCL	C2D-C1D-ND	2.35	112.45	110.13
20	M	408	PEF	O4P-P-O1P	-2.35	102.63	110.95
13	U	103	BCL	C3B-C4B-NB	2.35	112.86	109.76
13	Q	103	BCL	C3B-C4B-NB	2.35	112.86	109.76
13	3	102	BCL	C1-O2A-CGA	2.35	122.33	116.65
13	L	301	BCL	O2A-CGA-CBA	2.34	118.98	111.83
13	A	101	BCL	C1-O2A-CGA	2.34	122.32	116.65
19	2	101	CRT	C29-C28-C30	2.34	121.67	118.09
7	C	501	HEC	C4B-NB-C1B	2.34	109.64	105.82
13	3	102	BCL	C1D-ND-C4D	2.34	107.95	106.31
13	F	102	BCL	C3B-C4B-NB	2.34	112.85	109.76
13	K	102	BCL	C4-C3-C5	2.34	119.29	115.23
22	Q	105	CDL	CB4-OB6-CB5	-2.34	112.20	117.80
14	M	405	BPH	CGD-CBD-CAD	-2.34	103.28	110.85
13	Q	102	BCL	C1D-ND-C4D	2.33	107.95	106.31
13	5	103	BCL	O2A-CGA-CBA	2.33	118.95	111.83
19	U	104	CRT	C26-C27-C28	-2.33	124.01	127.28
13	O	103	BCL	C3D-C2D-C1D	-2.33	102.65	105.83
13	3	102	BCL	CHA-C4D-ND	2.33	137.36	132.55
13	K	102	BCL	CHA-C1A-NA	-2.33	121.11	126.39
19	N	101	CRT	C32-C31-C30	-2.33	116.45	123.20
20	U	106	PEF	O3P-P-O1P	-2.33	102.72	110.95
7	C	501	HEC	CHB-C1B-NB	2.33	128.08	123.86
13	W	102	BCL	C3B-C4B-NB	2.33	112.83	109.76
13	M	403	BCL	C4-C3-C5	2.32	119.26	115.23
22	H	304	CDL	OB4-PB2-OB3	2.32	123.26	112.44
13	M	402	BCL	CHA-C4D-ND	2.32	137.34	132.55
13	Z	102	BCL	CHA-C1A-NA	-2.32	121.13	126.39
13	9	104	BCL	C2A-C1A-CHA	-2.32	119.84	123.87
13	Y	102	BCL	C3B-C4B-NB	2.32	112.82	109.76
18	M	406	MQ8	C11-C3-C2	-2.32	120.91	124.89
13	U	102	BCL	CHA-C4D-ND	2.32	137.34	132.55
19	N	101	CRT	C27-C26-C25	-2.32	116.47	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	V	101	CRT	C27-C26-C25	-2.32	116.48	123.20
19	Z	101	CRT	C27-C26-C25	-2.32	116.48	123.20
19	Z	101	CRT	C18-C17-C16	2.32	121.62	118.09
19	P	101	CRT	C21-C20-C19	-2.32	118.78	123.52
22	K	104	CDL	OB6-CB5-OB7	-2.31	118.30	123.70
15	L	308	UQ8	C30-C29-C31	2.31	119.24	115.23
13	3	103	BCL	O2A-CGA-CBA	2.31	118.88	111.83
7	C	502	HEC	CHD-C1D-ND	2.31	128.05	123.86
13	9	104	BCL	O2A-CGA-CBA	2.31	118.87	111.83
13	1	103	BCL	C4-C3-C5	2.31	119.23	115.23
23	F	104	LMT	O5B-C5B-C6B	2.30	112.15	106.44
13	M	402	BCL	C2A-C1A-CHA	-2.30	119.87	123.87
13	O	103	BCL	O2A-CGA-CBA	2.30	118.86	111.83
19	A	104	CRT	C9-C10-C11	-2.30	116.53	123.20
12	M	414	PGV	O01-C1-C2	2.30	116.46	111.48
13	5	103	BCL	C3B-C4B-NB	2.30	112.80	109.76
13	W	102	BCL	C1D-ND-C4D	2.30	107.93	106.31
13	7	103	BCL	CHC-C4B-C3B	-2.30	122.60	131.72
13	Y	102	BCL	CHA-C4D-ND	2.30	137.28	132.55
19	9	103	CRT	C9-C10-C11	-2.30	116.55	123.20
22	S	104	CDL	OB4-PB2-OB3	2.29	123.12	112.44
13	M	402	BCL	C3D-C2D-C1D	-2.29	102.70	105.83
20	U	105	PEF	O4P-P-O1P	-2.29	102.84	110.95
19	J	101	CRT	C21-C20-C19	-2.29	118.83	123.52
13	O	102	BCL	C2A-C1A-CHA	-2.29	119.89	123.87
13	O	102	BCL	CHA-C1A-NA	-2.29	121.21	126.39
13	F	102	BCL	C1-C2-C3	-2.29	122.45	126.20
7	C	504	HEC	O2D-CGD-CBD	2.29	121.22	114.00
13	M	403	BCL	CHC-C4B-C3B	-2.29	122.64	131.72
13	5	102	BCL	C4-C3-C5	2.28	119.19	115.23
18	M	406	MQ8	C34-C33-C35	2.28	119.19	115.23
19	N	101	CRT	C18-C17-C16	2.28	121.58	118.09
13	1	102	BCL	C2C-C3C-C4C	-2.28	97.92	101.34
13	K	102	BCL	C1-C2-C3	-2.28	122.46	126.20
19	N	101	CRT	C14-C15-C16	-2.28	116.59	123.20
13	1	102	BCL	C1-O2A-CGA	2.28	122.17	116.65
13	S	103	BCL	C1-O2A-CGA	2.28	122.17	116.65
22	H	302	CDL	OB6-CB5-OB7	-2.28	118.38	123.70
13	L	301	BCL	CMD-C2D-C1D	2.28	128.74	124.73
19	M	407	CRT	C10-C9-C7	-2.28	124.08	127.28
19	Z	101	CRT	C26-C27-C28	-2.28	124.09	127.28
13	F	103	BCL	CHA-C1A-NA	-2.28	121.24	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	105	PEF	O3P-P-O1P	-2.27	102.92	110.95
13	A	101	BCL	C2A-C1A-CHA	-2.27	119.93	123.87
13	F	102	BCL	CHA-C4D-ND	2.27	137.23	132.55
22	S	104	CDL	OA6-CA5-OA7	-2.26	118.41	123.70
20	5	104	PEF	O4P-P-O1P	-2.26	102.95	110.95
19	2	101	CRT	C35-C33-C32	-2.26	115.45	119.01
13	L	301	BCL	C2A-C1A-CHA	-2.26	119.94	123.87
13	7	103	BCL	C1-C2-C3	-2.26	122.50	126.20
13	F	102	BCL	CHA-C1A-NA	-2.26	121.28	126.39
18	M	406	MQ8	C2M-C2-C3	-2.26	120.74	124.45
13	K	103	BCL	O2D-CGD-O1D	-2.26	119.45	123.85
19	J	101	CRT	C34-C33-C35	2.26	121.54	118.09
13	U	103	BCL	O2A-CGA-CBA	2.26	118.72	111.83
13	W	102	BCL	CHD-C1D-ND	-2.26	121.63	124.80
13	5	103	BCL	C4D-CHA-C1A	-2.26	118.55	121.24
13	U	103	BCL	C1-C2-C3	-2.26	122.50	126.20
13	F	103	BCL	O2A-CGA-CBA	2.25	118.71	111.83
13	7	102	BCL	C2A-C1A-CHA	-2.25	119.95	123.87
22	K	104	CDL	OB8-CB7-OB9	-2.25	117.99	123.63
19	0	101	CRT	C14-C15-C16	-2.25	116.67	123.20
13	3	102	BCL	CHC-C1C-NC	2.25	127.65	124.40
13	5	102	BCL	CMD-C2D-C1D	2.25	128.69	124.73
13	5	103	BCL	C2A-C1A-CHA	-2.25	119.96	123.87
13	A	101	BCL	CHD-C1D-ND	-2.25	121.63	124.80
22	D	104	CDL	CA4-OA6-CA5	-2.25	112.41	117.80
13	Q	102	BCL	O2A-CGA-CBA	2.25	118.69	111.83
20	I	104	PEF	O4P-P-O1P	-2.24	103.01	110.95
19	M	407	CRT	C9-C10-C11	-2.24	116.70	123.20
13	5	102	BCL	CHA-C1A-NA	-2.24	121.31	126.39
13	A	101	BCL	CBC-CAC-C3C	-2.24	108.66	113.41
13	Y	102	BCL	O2A-CGA-CBA	2.24	118.67	111.83
15	L	303	UQ8	C6-C1-C2	2.24	120.94	119.17
13	I	102	BCL	O2A-CGA-CBA	2.24	118.66	111.83
13	D	102	BCL	CHA-C4D-ND	2.24	137.16	132.55
22	H	302	CDL	CA4-OA6-CA5	-2.24	112.44	117.80
13	W	103	BCL	C2D-C1D-ND	2.23	112.34	110.13
13	U	102	BCL	CHA-C1A-NA	-2.23	121.33	126.39
19	U	104	CRT	C27-C26-C25	-2.23	116.73	123.20
15	7	104	UQ8	C10-C9-C11	2.23	119.10	115.23
13	1	102	BCL	CHB-C1B-C2B	-2.23	120.96	127.43
22	Q	105	CDL	OA8-CA7-C31	2.23	118.63	111.83
15	L	303	UQ8	C25-C24-C26	2.23	119.72	114.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	3	103	BCL	CHA-C1A-NA	-2.23	121.35	126.39
13	K	103	BCL	CHA-C4D-ND	2.23	137.14	132.55
13	I	103	BCL	C1-C2-C3	-2.22	122.55	126.20
18	M	406	MQ8	C14-C13-C15	2.22	119.09	115.23
19	V	101	CRT	C18-C17-C16	2.22	121.48	118.09
13	0	102	BCL	O2A-CGA-O1A	-2.22	118.07	123.63
13	I	103	BCL	CHD-C1D-ND	-2.22	121.67	124.80
13	5	103	BCL	C2C-C3C-C4C	-2.22	98.01	101.34
13	S	103	BCL	C2A-C3A-C4A	-2.22	98.28	101.87
13	1	103	BCL	C3B-C4B-NB	2.22	112.69	109.76
19	N	101	CRT	C10-C9-C7	-2.22	124.17	127.28
7	C	503	HEC	CAD-CBD-CGD	2.22	119.55	113.67
19	V	101	CRT	C31-C32-C33	-2.22	124.17	127.28
13	O	103	BCL	CHB-C1B-C2B	-2.22	120.99	127.43
13	L	301	BCL	C3D-C2D-C1D	-2.22	102.81	105.83
14	L	302	BPH	C1C-C2C-C3C	-2.22	100.73	102.84
13	7	103	BCL	C2D-C1D-ND	2.21	112.32	110.13
13	W	103	BCL	C2C-C3C-C4C	-2.21	98.02	101.34
13	3	102	BCL	O2A-CGA-CBA	2.21	118.57	111.83
19	V	101	CRT	C32-C31-C30	-2.21	116.80	123.20
13	A	101	BCL	O2A-CGA-O1A	-2.21	118.10	123.63
19	J	101	CRT	C10-C9-C7	-2.21	124.18	127.28
13	D	102	BCL	CMD-C2D-C1D	2.21	128.62	124.73
13	7	103	BCL	O2A-CGA-CBA	2.21	118.56	111.83
13	A	103	BCL	CED-O2D-CGD	2.21	120.92	115.92
13	U	102	BCL	O2A-CGA-O1A	-2.20	118.11	123.63
13	O	102	BCL	C1D-ND-C4D	2.20	107.86	106.31
13	O	102	BCL	CHB-C1B-C2B	-2.20	121.04	127.43
13	S	103	BCL	C2A-C1A-CHA	-2.20	120.06	123.87
23	F	104	LMT	C3B-C4B-C5B	-2.20	106.25	110.23
19	9	102	CRT	C26-C27-C28	-2.19	124.20	127.28
13	Q	103	BCL	C3D-C2D-C1D	-2.19	102.84	105.83
13	9	104	BCL	CHC-C4B-C3B	-2.19	123.01	131.72
13	F	103	BCL	CHC-C1C-NC	2.19	127.56	124.40
13	9	104	BCL	CHA-C4D-ND	2.19	137.06	132.55
22	S	104	CDL	OB6-CB5-OB7	-2.19	118.77	122.99
19	N	101	CRT	C20-C19-C17	-2.19	124.21	127.28
14	L	302	BPH	C11-C10-C8	-2.19	108.70	115.97
19	9	102	CRT	C27-C26-C25	-2.19	116.86	123.20
18	M	406	MQ8	C21-C20-C18	-2.19	105.94	113.19
13	U	103	BCL	C3D-C2D-C1D	-2.19	102.85	105.83
13	U	103	BCL	O2D-CGD-O1D	-2.18	119.59	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	M	406	MQ8	C16-C17-C18	-2.18	122.62	127.62
13	K	103	BCL	CHA-C1A-NA	-2.18	121.45	126.39
15	L	308	UQ8	C42-C43-C44	-2.18	120.37	127.64
22	K	104	CDL	OA6-CA5-OA7	-2.18	118.61	123.70
13	K	102	BCL	CHB-C1B-C2B	-2.18	121.10	127.43
13	W	102	BCL	O2A-CGA-O1A	-2.18	118.18	123.63
19	P	101	CRT	C9-C10-C11	-2.18	116.89	123.20
13	9	104	BCL	C2D-C1D-ND	2.18	112.28	110.13
13	M	403	BCL	O2A-CGA-O1A	-2.18	118.18	123.63
19	O	104	CRT	C18-C17-C16	2.18	121.41	118.09
15	L	303	UQ8	C22-C21-C19	-2.17	105.98	113.19
23	M	420	LMT	O5B-C5B-C4B	2.17	113.61	109.70
13	U	102	BCL	CHC-C1C-NC	2.17	127.53	124.40
13	S	102	BCL	C2D-C1D-ND	2.17	112.27	110.13
13	9	104	BCL	CHA-C1A-NA	-2.17	121.48	126.39
19	P	101	CRT	C18-C17-C16	2.17	121.40	118.09
13	D	103	BCL	CHA-C1A-NA	-2.17	121.48	126.39
19	J	101	CRT	C26-C27-C28	-2.17	124.24	127.28
7	C	503	HEC	CHD-C1D-ND	2.17	127.79	123.86
13	Y	102	BCL	C4-C3-C5	2.16	118.98	115.23
13	S	102	BCL	CHA-C4D-ND	2.16	137.01	132.55
13	M	402	BCL	C3B-C4B-NB	2.16	112.61	109.76
19	J	101	CRT	C9-C10-C11	-2.16	116.94	123.20
13	D	103	BCL	CHC-C1C-NC	2.16	127.52	124.40
13	F	102	BCL	C2A-C1A-CHA	-2.16	120.12	123.87
19	A	104	CRT	C13-C12-C11	2.16	121.38	118.09
19	N	101	CRT	C35-C33-C32	-2.15	115.62	119.01
13	U	102	BCL	CBC-CAC-C3C	-2.15	108.84	113.41
13	Y	102	BCL	CGD-CBD-CAD	-2.15	103.88	110.85
13	A	101	BCL	CHC-C1C-NC	2.15	127.50	124.40
13	0	102	BCL	CHA-C1A-NA	-2.15	121.52	126.39
14	M	405	BPH	CBC-CAC-C3C	-2.15	109.55	113.78
13	F	103	BCL	C3D-C2D-C1D	-2.15	102.90	105.83
19	G	101	CRT	C26-C27-C28	-2.15	124.26	127.28
13	Y	102	BCL	CHB-C1B-C2B	-2.15	121.20	127.43
13	Q	102	BCL	CHC-C1C-NC	2.14	127.50	124.40
13	7	102	BCL	C4-C3-C5	2.14	118.95	115.23
13	5	102	BCL	OBD-CAD-C3D	-2.14	123.41	128.42
15	L	308	UQ8	C37-C38-C39	-2.14	122.72	127.62
13	A	103	BCL	C2A-C1A-CHA	-2.14	120.15	123.87
13	W	103	BCL	C1-C2-C3	-2.14	122.69	126.20
15	M	418	UQ8	O5-C5-C6	-2.14	117.65	121.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	P	101	CRT	C27-C26-C25	-2.14	117.00	123.20
13	O	102	BCL	CGD-CBD-CAD	-2.14	103.92	110.85
13	A	103	BCL	C3D-C2D-C1D	-2.14	102.91	105.83
23	M	420	LMT	C1B-O5B-C5B	2.14	117.89	113.72
15	L	308	UQ8	C8-C7-C6	-2.14	106.82	112.08
13	Y	102	BCL	C1-C2-C3	-2.14	122.70	126.20
13	1	103	BCL	CHA-C4D-ND	2.14	136.95	132.55
13	7	102	BCL	O2A-CGA-CBA	2.13	118.34	111.83
13	M	403	BCL	CMC-C2C-C3C	2.13	122.22	113.98
13	Q	103	BCL	CAA-CBA-CGA	-2.13	107.16	113.21
13	Q	102	BCL	CHB-C1B-C2B	-2.13	121.24	127.43
19	G	101	CRT	C29-C28-C30	2.13	121.34	118.09
13	W	103	BCL	C3B-C4B-NB	2.13	112.57	109.76
13	Y	102	BCL	O1D-CGD-CBD	-2.13	120.32	124.52
14	M	405	BPH	C4-C3-C2	-2.13	118.16	123.63
13	Q	102	BCL	CBC-CAC-C3C	-2.13	108.90	113.41
19	G	101	CRT	C5-C6-C7	-2.13	122.68	125.89
7	C	502	HEC	C4C-NC-C1C	2.13	109.29	105.82
13	9	104	BCL	C1-C2-C3	-2.12	122.72	126.20
13	7	103	BCL	CAA-CBA-CGA	-2.12	107.18	113.21
7	C	501	HEC	CBC-CAC-C3C	-2.12	123.20	127.43
13	Z	102	BCL	CHA-C4D-ND	2.12	136.92	132.55
13	S	103	BCL	CAA-CBA-CGA	-2.12	107.19	113.21
7	C	503	HEC	O2D-CGD-CBD	2.12	120.69	114.00
14	M	405	BPH	CBB-CAB-C3B	-2.12	114.00	120.34
7	C	504	HEC	CHD-C1D-C2D	-2.12	121.28	127.43
22	H	304	CDL	OB8-CB7-OB9	-2.11	118.34	123.63
13	1	102	BCL	CHA-C4D-ND	2.11	136.91	132.55
13	M	402	BCL	CMD-C2D-C1D	2.11	128.45	124.73
13	A	103	BCL	CHA-C1A-NA	-2.11	121.61	126.39
13	K	102	BCL	C3B-C4B-NB	2.11	112.54	109.76
18	M	406	MQ8	C21-C22-C23	-2.11	122.80	127.62
13	W	102	BCL	CHA-C1A-NA	-2.11	121.62	126.39
13	I	102	BCL	CHC-C1C-NC	2.10	127.44	124.40
13	Q	102	BCL	CHA-C1A-NA	-2.10	121.63	126.39
19	9	103	CRT	C29-C28-C30	2.10	121.30	118.09
7	C	502	HEC	CHB-C1B-C2B	-2.10	121.32	127.43
15	7	104	UQ8	C25-C24-C26	2.10	119.42	114.59
13	3	102	BCL	CHC-C4B-C3B	-2.10	123.38	131.72
13	I	103	BCL	CHC-C1C-NC	2.10	127.43	124.40
13	F	103	BCL	C2D-C1D-ND	2.10	112.20	110.13
13	O	102	BCL	CBC-CAC-C3C	-2.10	108.96	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	7	102	BCL	CHA-C1A-NA	-2.10	121.64	126.39
20	M	419	PEF	O3-C30-O5	-2.10	118.38	123.63
13	3	103	BCL	C2C-C3C-C4C	-2.10	98.20	101.34
13	U	102	BCL	CMB-C2B-C3B	2.10	132.29	125.67
7	C	503	HEC	C2A-C1A-NA	-2.10	108.30	110.32
13	M	404	BCL	CHA-C4D-ND	2.10	136.88	132.55
13	M	402	BCL	CHB-C1B-C2B	-2.10	121.34	127.43
19	U	104	CRT	C35-C33-C32	-2.09	115.71	119.01
13	O	102	BCL	CMB-C2B-C3B	2.09	132.27	125.67
13	5	102	BCL	C1-C2-C3	-2.09	122.77	126.20
13	I	103	BCL	C3B-C4B-NB	2.09	112.52	109.76
13	S	102	BCL	CHD-C1D-ND	-2.09	121.86	124.80
13	L	301	BCL	CHD-C1D-ND	-2.09	121.87	124.80
13	M	402	BCL	CHA-C1A-NA	-2.09	121.67	126.39
15	L	303	UQ8	C7-C8-C9	-2.09	123.24	126.83
13	U	103	BCL	C2A-C1A-CHA	-2.09	120.25	123.87
19	O	104	CRT	C27-C26-C25	-2.08	117.16	123.20
13	Y	102	BCL	CHC-C1C-NC	2.08	127.41	124.40
13	I	103	BCL	CHA-C1A-NA	-2.08	121.67	126.39
13	7	102	BCL	C3B-C4B-NB	2.08	112.51	109.76
13	M	404	BCL	CAA-C2A-C3A	-2.08	107.37	113.00
13	A	101	BCL	CHA-C4D-ND	2.08	136.84	132.55
13	3	103	BCL	C1-O2A-CGA	2.08	121.69	116.65
13	D	102	BCL	CHB-C1B-C2B	-2.08	121.39	127.43
7	C	501	HEC	C2A-C1A-NA	-2.08	108.32	110.32
19	1	104	CRT	C27-C26-C25	-2.08	117.18	123.20
19	G	101	CRT	C24-C23-C25	2.08	121.26	118.09
7	C	502	HEC	O2D-CGD-CBD	2.08	120.56	114.00
22	H	302	CDL	C12-C11-CA5	-2.07	106.09	113.69
13	A	101	BCL	C1D-ND-C4D	2.07	107.77	106.31
15	L	308	UQ8	C4M-O4-C4	2.07	123.76	116.47
13	A	103	BCL	C1-C2-C3	-2.07	122.80	126.20
13	0	102	BCL	C2C-C3C-C4C	-2.07	98.23	101.34
19	9	103	CRT	C24-C23-C22	-2.07	119.46	122.82
13	0	102	BCL	CHB-C1B-C2B	-2.07	121.41	127.43
13	D	103	BCL	O2D-CGD-O1D	-2.07	119.82	123.85
13	1	103	BCL	CHC-C4B-C3B	-2.07	123.49	131.72
19	A	104	CRT	C34-C33-C35	2.07	121.25	118.09
19	0	101	CRT	C21-C20-C19	-2.07	119.29	123.52
13	K	103	BCL	C3B-C2B-C1B	-2.07	99.79	106.40
13	1	102	BCL	CHD-C1D-C2D	-2.07	121.19	125.49
13	O	102	BCL	C3B-C4B-NB	2.06	112.48	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	M	407	CRT	C21-C22-C23	-2.06	124.38	127.28
13	O	102	BCL	C11-C10-C8	-2.06	109.11	115.97
13	I	103	BCL	C1D-ND-C4D	2.06	107.76	106.31
12	1	106	PGV	C02-O01-C1	-2.06	112.87	117.80
19	A	104	CRT	C27-C26-C25	-2.06	117.23	123.20
13	L	301	BCL	CHC-C1C-NC	2.06	127.37	124.40
19	V	101	CRT	C9-C10-C11	-2.05	117.25	123.20
12	M	415	PGV	O01-C1-O02	-2.05	118.90	123.70
15	L	308	UQ8	C40-C39-C41	2.05	118.79	115.23
13	0	102	BCL	C3D-C2D-C1D	-2.05	103.03	105.83
13	K	102	BCL	C1-O2A-CGA	2.05	121.62	116.65
19	J	101	CRT	C14-C15-C16	-2.05	117.26	123.20
13	5	103	BCL	CHA-C1A-NA	-2.05	121.76	126.39
13	5	102	BCL	CHD-C1D-C2D	-2.05	121.23	125.49
13	5	102	BCL	C2A-C1A-CHA	-2.05	120.32	123.87
13	W	103	BCL	C3D-C2D-C1D	-2.04	103.04	105.83
22	Q	105	CDL	OB6-CB5-OB7	-2.04	118.93	123.70
19	J	101	CRT	C18-C17-C19	-2.04	119.50	122.82
13	W	102	BCL	CGD-CBD-CAD	-2.04	104.23	110.85
15	L	309	UQ8	C4M-O4-C4	2.04	123.65	116.47
19	2	101	CRT	C10-C9-C7	-2.04	124.42	127.28
19	6	101	CRT	C34-C33-C35	2.04	121.20	118.09
13	S	102	BCL	C2A-C1A-CHA	-2.04	120.33	123.87
12	3	105	PGV	C02-O01-C1	-2.04	112.92	117.80
13	O	103	BCL	CHA-C4D-ND	2.04	136.75	132.55
13	W	103	BCL	CHC-C1C-NC	2.04	127.34	124.40
13	I	102	BCL	CHB-C1B-C2B	-2.04	121.52	127.43
13	D	102	BCL	C2A-C3A-C4A	-2.04	98.58	101.87
15	7	104	UQ8	C22-C21-C19	-2.03	106.44	113.19
12	D	105	PGV	C3-C2-C1	-2.03	106.24	113.69
13	7	102	BCL	C3D-C2D-C1D	-2.03	103.06	105.83
13	M	402	BCL	O2D-CGD-O1D	-2.03	119.89	123.85
13	Q	102	BCL	CMB-C2B-C3B	2.03	132.08	125.67
13	3	103	BCL	CED-O2D-CGD	2.03	120.53	115.92
13	A	103	BCL	CHC-C4B-C3B	-2.03	123.65	131.72
13	K	103	BCL	C3D-C2D-C1D	-2.03	103.06	105.83
19	1	104	CRT	C34-C33-C35	2.03	121.19	118.09
7	C	501	HEC	CHD-C1D-C2D	-2.03	121.53	127.43
12	L	306	PGV	O01-C1-O02	-2.03	118.96	123.70
19	M	407	CRT	C20-C21-C22	2.03	127.67	123.52
13	F	102	BCL	CHC-C1C-NC	2.03	127.33	124.40
19	9	102	CRT	C18-C17-C16	2.03	121.19	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	103	BCL	CHA-C4D-ND	2.03	136.73	132.55
13	S	103	BCL	CMD-C2D-C1D	2.03	128.30	124.73
13	O	102	BCL	CHA-C4D-ND	2.02	136.73	132.55
13	K	102	BCL	O1D-CGD-CBD	-2.02	120.53	124.52
13	A	103	BCL	CMD-C2D-C1D	2.02	128.29	124.73
13	S	102	BCL	CHB-C1B-C2B	-2.02	121.56	127.43
13	1	103	BCL	CHA-C1A-NA	-2.02	121.81	126.39
13	F	102	BCL	C3D-C2D-C1D	-2.02	103.07	105.83
13	I	102	BCL	C4-C3-C5	2.02	118.73	115.23
13	3	102	BCL	O1D-CGD-CBD	-2.02	120.54	124.52
19	V	101	CRT	C34-C33-C35	2.02	121.17	118.09
13	S	103	BCL	C4-C3-C2	-2.02	118.45	123.63
13	A	101	BCL	CHB-C1B-C2B	-2.01	121.58	127.43
13	M	403	BCL	CHA-C4D-ND	2.01	136.70	132.55
19	Z	101	CRT	C34-C33-C35	2.01	121.16	118.09
7	C	501	HEC	CHB-C1B-C2B	-2.01	121.59	127.43
19	P	101	CRT	C34-C33-C35	2.01	121.16	118.09
13	S	103	BCL	CHA-C1A-NA	-2.01	121.84	126.39
19	2	101	CRT	C21-C20-C19	-2.01	119.41	123.52
13	M	402	BCL	C4-C3-C5	2.01	118.71	115.23
22	D	104	CDL	OA6-CA5-OA7	-2.01	119.02	123.70
22	H	302	CDL	CB2-C1-CA2	-2.00	106.88	112.65
13	M	402	BCL	CHC-C4B-C3B	-2.00	123.76	131.72
19	9	102	CRT	C9-C10-C11	-2.00	117.40	123.20
15	M	418	UQ8	O4-C4-C5	2.00	123.39	116.64
13	W	102	BCL	CHC-C4B-C3B	-2.00	123.77	131.72
19	G	101	CRT	C10-C9-C7	-2.00	124.47	127.28
12	1	106	PGV	O03-C19-O04	-2.00	118.62	123.63

There are no chirality outliers.

All (888) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	501	HEC	C2B-C3B-CAB-CBB
7	C	501	HEC	C4B-C3B-CAB-CBB
7	C	501	HEC	C2C-C3C-CAC-CBC
7	C	501	HEC	C4C-C3C-CAC-CBC
7	C	502	HEC	C2B-C3B-CAB-CBB
7	C	502	HEC	C4B-C3B-CAB-CBB
7	C	502	HEC	C2C-C3C-CAC-CBC
7	C	502	HEC	C4C-C3C-CAC-CBC
7	C	503	HEC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
7	C	503	HEC	C4B-C3B-CAB-CBB
7	C	503	HEC	C2C-C3C-CAC-CBC
7	C	503	HEC	C4C-C3C-CAC-CBC
7	C	504	HEC	C2B-C3B-CAB-CBB
7	C	504	HEC	C4B-C3B-CAB-CBB
7	C	504	HEC	C2C-C3C-CAC-CBC
7	C	504	HEC	C4C-C3C-CAC-CBC
12	C	509	PGV	C2-C1-O01-C02
12	L	305	PGV	C04-O12-P-O13
12	L	306	PGV	C03-O11-P-O12
12	L	306	PGV	C03-O11-P-O14
12	L	306	PGV	C04-O12-P-O11
12	L	306	PGV	C04-O12-P-O13
12	L	306	PGV	C04-O12-P-O14
12	L	306	PGV	O12-C04-C05-C06
12	M	414	PGV	C03-O11-P-O12
12	M	414	PGV	C03-O11-P-O13
12	M	414	PGV	C03-O11-P-O14
12	M	415	PGV	C04-C05-C06-O06
12	H	303	PGV	O03-C01-C02-O01
12	D	105	PGV	C03-O11-P-O12
12	D	105	PGV	C03-O11-P-O13
12	D	105	PGV	C03-O11-P-O14
12	D	105	PGV	C04-O12-P-O11
12	D	105	PGV	C04-O12-P-O14
12	D	105	PGV	O12-C04-C05-O05
12	D	105	PGV	O04-C19-O03-C01
12	D	105	PGV	C20-C19-O03-C01
12	1	106	PGV	C04-O12-P-O13
12	3	105	PGV	C03-O11-P-O12
12	3	105	PGV	C03-O11-P-O13
12	3	105	PGV	C03-O11-P-O14
12	3	105	PGV	C04-O12-P-O11
12	3	105	PGV	C04-O12-P-O14
13	M	403	BCL	C4C-C3C-CAC-CBC
13	M	403	BCL	C6-C7-C8-C9
13	M	404	BCL	CAD-CBD-CGD-O1D
13	M	404	BCL	CAD-CBD-CGD-O2D
13	A	101	BCL	C14-C13-C15-C16
13	A	103	BCL	C4C-C3C-CAC-CBC
13	D	102	BCL	C4C-C3C-CAC-CBC
13	D	103	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
13	F	102	BCL	C4C-C3C-CAC-CBC
13	F	103	BCL	C1A-C2A-CAA-CBA
13	F	103	BCL	C4C-C3C-CAC-CBC
13	I	102	BCL	C4C-C3C-CAC-CBC
13	I	103	BCL	C1A-C2A-CAA-CBA
13	I	103	BCL	C2C-C3C-CAC-CBC
13	I	103	BCL	C4C-C3C-CAC-CBC
13	K	102	BCL	C4C-C3C-CAC-CBC
13	K	103	BCL	C4C-C3C-CAC-CBC
13	Q	102	BCL	C4-C3-C5-C6
13	Q	103	BCL	C1A-C2A-CAA-CBA
13	S	103	BCL	C4C-C3C-CAC-CBC
13	U	103	BCL	C1A-C2A-CAA-CBA
13	U	103	BCL	C4C-C3C-CAC-CBC
13	U	103	BCL	C11-C10-C8-C9
13	W	102	BCL	C2C-C3C-CAC-CBC
13	W	102	BCL	C4C-C3C-CAC-CBC
13	W	103	BCL	C1A-C2A-CAA-CBA
13	W	103	BCL	C3A-C2A-CAA-CBA
13	W	103	BCL	C4C-C3C-CAC-CBC
13	Y	102	BCL	C2C-C3C-CAC-CBC
13	Y	102	BCL	C4C-C3C-CAC-CBC
13	Z	102	BCL	C2C-C3C-CAC-CBC
13	Z	102	BCL	C4C-C3C-CAC-CBC
13	1	102	BCL	C2C-C3C-CAC-CBC
13	1	102	BCL	C4C-C3C-CAC-CBC
13	1	103	BCL	C2C-C3C-CAC-CBC
13	1	103	BCL	C4C-C3C-CAC-CBC
13	3	102	BCL	C4-C3-C5-C6
13	3	103	BCL	C4C-C3C-CAC-CBC
13	5	103	BCL	C1A-C2A-CAA-CBA
13	5	103	BCL	C4C-C3C-CAC-CBC
13	5	103	BCL	C11-C12-C13-C14
13	7	102	BCL	C4-C3-C5-C6
13	7	103	BCL	C4C-C3C-CAC-CBC
13	7	103	BCL	C11-C10-C8-C9
13	0	102	BCL	C1A-C2A-CAA-CBA
13	0	102	BCL	C2C-C3C-CAC-CBC
13	0	102	BCL	C4C-C3C-CAC-CBC
14	M	405	BPH	C2C-C3C-CAC-CBC
15	L	308	UQ8	C35-C34-C36-C37
19	M	407	CRT	O1-C1-C4-C5

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Mol	Chain	Res	Type	Atoms
19	M	407	CRT	C2-C1-C4-C5
19	M	407	CRT	C39-C38-O2-C2M
19	9	103	CRT	C10-C11-C12-C14
20	M	419	PEF	O4P-C4-C5-N
20	M	419	PEF	C1-O3P-P-O2P
20	M	419	PEF	C1-O3P-P-O4P
20	K	105	PEF	O4P-C4-C5-N
21	M	412	LDA	C2-C1-N1-CM1
21	M	412	LDA	C2-C1-N1-CM2
21	O	105	LDA	C2-C1-N1-CM1
21	O	105	LDA	C2-C1-N1-CM2
21	O	105	LDA	N1-C1-C2-C3
21	V	102	LDA	C2-C1-N1-CM1
21	V	102	LDA	N1-C1-C2-C3
22	M	416	CDL	O1-C1-CB2-OB2
22	M	416	CDL	CA2-OA2-PA1-OA3
22	M	416	CDL	CB2-OB2-PB2-OB3
22	M	416	CDL	CB2-OB2-PB2-OB4
22	M	416	CDL	CB2-OB2-PB2-OB5
22	M	416	CDL	CB3-OB5-PB2-OB2
22	M	416	CDL	CB3-OB5-PB2-OB3
22	M	416	CDL	CB3-OB5-PB2-OB4
22	M	416	CDL	OB6-CB4-CB6-OB8
22	H	302	CDL	CA2-OA2-PA1-OA4
22	H	302	CDL	CA2-OA2-PA1-OA5
22	H	302	CDL	CA3-OA5-PA1-OA2
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
22	H	304	CDL	O1-C1-CB2-OB2
22	H	304	CDL	CA2-OA2-PA1-OA4
22	H	304	CDL	CA3-OA5-PA1-OA2
22	H	304	CDL	CA3-OA5-PA1-OA3
22	D	104	CDL	CA2-OA2-PA1-OA3
22	D	104	CDL	CA3-OA5-PA1-OA2
22	D	104	CDL	CA3-OA5-PA1-OA3
22	D	104	CDL	CA3-OA5-PA1-OA4
22	D	104	CDL	CB2-OB2-PB2-OB3
22	D	104	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
22	D	104	CDL	CB3-OB5-PB2-OB2
22	D	104	CDL	CB3-OB5-PB2-OB4
22	K	104	CDL	CB3-OB5-PB2-OB2
22	K	104	CDL	CB3-OB5-PB2-OB4
22	K	104	CDL	OB7-CB5-OB6-CB4
22	K	104	CDL	C51-CB5-OB6-CB4
22	Q	105	CDL	CA2-OA2-PA1-OA3
22	Q	105	CDL	CA2-OA2-PA1-OA5
22	Q	105	CDL	CA3-OA5-PA1-OA2
22	Q	105	CDL	CA3-OA5-PA1-OA3
22	Q	105	CDL	CB2-OB2-PB2-OB5
22	Q	105	CDL	CB3-OB5-PB2-OB2
22	Q	105	CDL	CB3-OB5-PB2-OB3
22	Q	105	CDL	CB3-OB5-PB2-OB4
22	S	104	CDL	CA2-OA2-PA1-OA5
22	S	104	CDL	OA9-CA7-OA8-CA6
22	S	104	CDL	C31-CA7-OA8-CA6
22	S	104	CDL	OB7-CB5-OB6-CB4
22	Y	103	CDL	CA2-C1-CB2-OB2
22	Y	103	CDL	CA2-OA2-PA1-OA3
22	Y	103	CDL	CA3-OA5-PA1-OA2
22	Y	103	CDL	CA3-OA5-PA1-OA3
22	Y	103	CDL	CB2-OB2-PB2-OB5
22	Y	103	CDL	CB3-OB5-PB2-OB2
22	Y	103	CDL	CB3-OB5-PB2-OB4
22	Y	104	CDL	CB2-OB2-PB2-OB3
22	Y	104	CDL	CB2-OB2-PB2-OB4
22	Y	104	CDL	CB2-OB2-PB2-OB5
22	Y	104	CDL	CB3-OB5-PB2-OB2
22	Y	104	CDL	CB3-OB5-PB2-OB3
22	Y	104	CDL	CB3-OB5-PB2-OB4
23	M	420	LMT	O5'-C1'-O1'-C1
23	F	104	LMT	C2'-C1'-O1'-C1
23	F	104	LMT	O5'-C1'-O1'-C1
22	S	104	CDL	C51-CB5-OB6-CB4
12	C	509	PGV	O04-C19-O03-C01
12	C	509	PGV	C20-C19-O03-C01
12	C	509	PGV	O02-C1-O01-C02
12	3	105	PGV	O02-C1-O01-C02
13	W	102	BCL	C4-C3-C5-C6
15	L	303	UQ8	C15-C14-C16-C17
15	L	308	UQ8	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
15	7	104	UQ8	C12-C11-C9-C10
13	Q	102	BCL	C2-C3-C5-C6
13	W	102	BCL	C2-C3-C5-C6
13	3	102	BCL	C2-C3-C5-C6
13	7	102	BCL	C2-C3-C5-C6
15	L	303	UQ8	C13-C14-C16-C17
15	L	308	UQ8	C33-C34-C36-C37
15	L	308	UQ8	C13-C14-C16-C17
15	7	104	UQ8	C12-C11-C9-C8
13	3	102	BCL	C3-C5-C6-C7
12	L	306	PGV	O12-C04-C05-O05
22	Y	103	CDL	O1-C1-CA2-OA2
22	Y	103	CDL	O1-C1-CB2-OB2
12	3	105	PGV	C2-C1-O01-C02
23	F	104	LMT	C4'-C5'-C6'-O6'
22	S	104	CDL	CB4-CB6-OB8-CB7
13	A	101	BCL	C4-C3-C5-C6
13	1	102	BCL	C4-C3-C5-C6
13	1	102	BCL	C2-C3-C5-C6
15	7	104	UQ8	C19-C21-C22-C23
18	M	406	MQ8	C33-C35-C36-C37
18	M	406	MQ8	C38-C40-C41-C42
13	S	102	BCL	CBD-CGD-O2D-CED
13	9	104	BCL	CBD-CGD-O2D-CED
22	S	104	CDL	C36-C37-C38-C39
12	3	105	PGV	O12-C04-C05-C06
22	H	304	CDL	CA2-C1-CB2-OB2
12	M	414	PGV	C20-C19-O03-C01
13	O	103	BCL	CBA-CGA-O2A-C1
22	K	104	CDL	C31-CA7-OA8-CA6
14	M	405	BPH	C4-C3-C5-C6
13	A	101	BCL	C2-C3-C5-C6
14	M	405	BPH	C2-C3-C5-C6
13	O	103	BCL	C3-C5-C6-C7
13	1	103	BCL	C3-C5-C6-C7
13	M	403	BCL	C14-C13-C15-C16
13	A	103	BCL	C6-C7-C8-C9
13	F	103	BCL	C6-C7-C8-C9
13	F	103	BCL	C11-C10-C8-C9
13	K	102	BCL	C14-C13-C15-C16
13	K	103	BCL	C6-C7-C8-C9
13	K	103	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
13	O	103	BCL	C6-C7-C8-C9
13	O	103	BCL	C11-C10-C8-C9
13	Q	102	BCL	C11-C12-C13-C14
13	Q	103	BCL	C14-C13-C15-C16
13	S	102	BCL	C14-C13-C15-C16
13	S	103	BCL	C11-C10-C8-C9
13	U	103	BCL	C11-C12-C13-C14
13	W	103	BCL	C6-C7-C8-C9
13	Z	102	BCL	C14-C13-C15-C16
13	3	102	BCL	C14-C13-C15-C16
13	3	103	BCL	C11-C10-C8-C9
13	7	103	BCL	C6-C7-C8-C9
23	M	420	LMT	C2'-C1'-O1'-C1
22	K	104	CDL	O1-C1-CB2-OB2
22	S	104	CDL	O1-C1-CA2-OA2
19	V	101	CRT	C5-C6-C7-C8
19	9	102	CRT	C5-C6-C7-C8
19	9	103	CRT	C10-C11-C12-C13
19	0	101	CRT	C5-C6-C7-C8
22	K	104	CDL	OA9-CA7-OA8-CA6
12	L	305	PGV	C20-C19-O03-C01
13	3	103	BCL	C8-C10-C11-C12
13	O	103	BCL	C8-C10-C11-C12
13	Q	102	BCL	C5-C6-C7-C8
13	5	102	BCL	C5-C6-C7-C8
23	F	104	LMT	O5'-C5'-C6'-O6'
9	C	506	GOL	O1-C1-C2-O2
13	9	104	BCL	C11-C10-C8-C7
13	1	102	BCL	C5-C6-C7-C8
13	3	102	BCL	C5-C6-C7-C8
22	Q	105	CDL	CB5-C51-C52-C53
15	L	303	UQ8	C14-C16-C17-C18
15	7	104	UQ8	C14-C16-C17-C18
13	W	103	BCL	C8-C10-C11-C12
15	L	308	UQ8	C3-C4-O4-C4M
15	7	104	UQ8	C3-C4-O4-C4M
22	K	104	CDL	CB7-C71-C72-C73
12	A	105	PGV	C2-C1-O01-C02
13	O	103	BCL	C5-C6-C7-C8
13	D	102	BCL	C13-C15-C16-C17
13	F	102	BCL	C15-C16-C17-C18
22	S	104	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	S	104	CDL	CA7-C31-C32-C33
12	M	414	PGV	O04-C19-O03-C01
13	I	102	BCL	C5-C6-C7-C8
13	O	102	BCL	C13-C15-C16-C17
13	Y	102	BCL	C8-C10-C11-C12
13	1	102	BCL	C13-C15-C16-C17
12	3	105	PGV	O12-C04-C05-O05
22	D	104	CDL	O1-C1-CB2-OB2
20	M	419	PEF	C10-C11-C12-C13
13	A	101	BCL	C13-C15-C16-C17
13	S	103	BCL	C5-C6-C7-C8
13	7	102	BCL	C8-C10-C11-C12
14	M	405	BPH	C5-C6-C7-C8
12	A	105	PGV	C20-C19-O03-C01
13	Q	102	BCL	CBD-CGD-O2D-CED
13	O	103	BCL	O1A-CGA-O2A-C1
12	A	105	PGV	O02-C1-O01-C02
12	D	105	PGV	O12-C04-C05-C06
22	M	416	CDL	CA2-C1-CB2-OB2
22	D	104	CDL	CA2-C1-CB2-OB2
22	K	104	CDL	CA2-C1-CB2-OB2
22	Y	103	CDL	CB2-C1-CA2-OA2
13	S	102	BCL	C5-C6-C7-C8
13	Y	102	BCL	C13-C15-C16-C17
13	Z	102	BCL	C8-C10-C11-C12
13	1	102	BCL	C15-C16-C17-C18
13	5	102	BCL	C13-C15-C16-C17
22	S	104	CDL	CB7-C71-C72-C73
13	U	102	BCL	C5-C6-C7-C8
13	W	102	BCL	C13-C15-C16-C17
13	W	103	BCL	C13-C15-C16-C17
13	Z	102	BCL	C13-C15-C16-C17
13	Z	102	BCL	C15-C16-C17-C18
13	A	103	BCL	C13-C15-C16-C17
13	I	103	BCL	C15-C16-C17-C18
13	Q	103	BCL	C13-C15-C16-C17
22	K	104	CDL	C11-CA5-OA6-CA4
21	I	105	LDA	C4-C5-C6-C7
22	S	104	CDL	C34-C35-C36-C37
22	K	104	CDL	OA7-CA5-OA6-CA4
12	M	415	PGV	O12-C04-C05-O05
12	L	305	PGV	O04-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
12	A	105	PGV	C1-C2-C3-C4
19	G	101	CRT	C15-C16-C17-C18
19	U	104	CRT	C15-C16-C17-C18
19	9	103	CRT	C15-C16-C17-C18
13	Q	102	BCL	C10-C11-C12-C13
13	Q	103	BCL	C10-C11-C12-C13
9	C	506	GOL	O1-C1-C2-C3
13	Q	102	BCL	C16-C17-C18-C19
13	9	104	BCL	C16-C17-C18-C19
14	L	302	BPH	C16-C17-C18-C19
23	F	104	LMT	C1-C2-C3-C4
13	F	102	BCL	C13-C15-C16-C17
13	O	103	BCL	C16-C17-C18-C20
13	S	103	BCL	C16-C17-C18-C19
13	9	104	BCL	C16-C17-C18-C20
13	1	103	BCL	C13-C15-C16-C17
22	Q	105	CDL	C37-C38-C39-C40
12	1	106	PGV	C3-C4-C5-C6
21	I	105	LDA	C6-C7-C8-C9
22	H	302	CDL	C73-C74-C75-C76
13	U	103	BCL	C8-C10-C11-C12
21	O	105	LDA	C3-C4-C5-C6
13	F	103	BCL	C10-C11-C12-C13
13	Q	102	BCL	C15-C16-C17-C18
13	7	103	BCL	C10-C11-C12-C13
12	L	305	PGV	C2-C1-O01-C02
22	Y	103	CDL	C51-CB5-OB6-CB4
12	H	303	PGV	C6-C7-C8-C9
21	J	102	LDA	C4-C5-C6-C7
22	Q	105	CDL	C12-C13-C14-C15
22	H	304	CDL	CA5-C11-C12-C13
13	3	103	BCL	CBA-CGA-O2A-C1
13	1	102	BCL	C10-C11-C12-C13
12	M	414	PGV	C2-C3-C4-C5
21	I	105	LDA	C2-C3-C4-C5
12	A	105	PGV	O04-C19-O03-C01
13	K	103	BCL	C3-C5-C6-C7
13	A	103	BCL	C3A-C2A-CAA-CBA
13	D	103	BCL	C3A-C2A-CAA-CBA
13	F	103	BCL	C3A-C2A-CAA-CBA
13	I	103	BCL	C3A-C2A-CAA-CBA
13	K	103	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	O	103	BCL	C3A-C2A-CAA-CBA
13	Q	103	BCL	C3A-C2A-CAA-CBA
13	S	103	BCL	C3A-C2A-CAA-CBA
13	U	103	BCL	C3A-C2A-CAA-CBA
13	Z	102	BCL	C3A-C2A-CAA-CBA
13	1	103	BCL	C3A-C2A-CAA-CBA
13	3	103	BCL	C3A-C2A-CAA-CBA
13	5	103	BCL	C3A-C2A-CAA-CBA
13	7	103	BCL	C3A-C2A-CAA-CBA
13	0	102	BCL	C3A-C2A-CAA-CBA
12	M	414	PGV	C30-C31-C32-C33
12	M	415	PGV	C29-C30-C31-C32
13	F	102	BCL	C5-C6-C7-C8
12	M	414	PGV	C19-C20-C21-C22
13	I	102	BCL	C16-C17-C18-C19
22	Q	105	CDL	C14-C15-C16-C17
20	M	419	PEF	C11-C12-C13-C14
22	H	304	CDL	C11-C12-C13-C14
22	Q	105	CDL	C72-C73-C74-C75
22	H	302	CDL	C59-C60-C61-C62
12	L	306	PGV	C1-C2-C3-C4
12	L	305	PGV	C23-C24-C25-C26
12	H	303	PGV	C2-C3-C4-C5
20	M	419	PEF	C36-C37-C38-C39
15	L	308	UQ8	C4-C3-O3-C3M
15	M	418	UQ8	C3-C4-O4-C4M
22	H	304	CDL	C79-C80-C81-C82
22	S	104	CDL	C13-C14-C15-C16
13	S	103	BCL	C16-C17-C18-C20
12	M	415	PGV	C21-C22-C23-C24
13	F	102	BCL	CBD-CGD-O2D-CED
22	D	104	CDL	C11-CA5-OA6-CA4
22	Q	105	CDL	C51-CB5-OB6-CB4
22	Y	103	CDL	C11-CA5-OA6-CA4
22	S	104	CDL	C16-C17-C18-C19
13	Z	102	BCL	C3-C5-C6-C7
12	M	414	PGV	C14-C15-C16-C17
21	O	105	LDA	C2-C3-C4-C5
22	Q	105	CDL	C51-C52-C53-C54
12	L	305	PGV	O02-C1-O01-C02
22	Y	103	CDL	OB7-CB5-OB6-CB4
22	K	104	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	Q	105	CDL	C73-C74-C75-C76
22	S	104	CDL	C32-C33-C34-C35
13	S	103	BCL	C15-C16-C17-C18
13	3	102	BCL	C13-C15-C16-C17
13	3	103	BCL	C5-C6-C7-C8
12	L	305	PGV	C26-C27-C28-C29
21	O	105	LDA	C1-C2-C3-C4
13	A	103	BCL	C11-C10-C8-C9
13	5	103	BCL	C11-C10-C8-C9
12	M	414	PGV	C21-C22-C23-C24
21	J	102	LDA	C5-C6-C7-C8
12	L	306	PGV	C20-C21-C22-C23
12	H	303	PGV	C4-C5-C6-C7
13	U	103	BCL	C10-C11-C12-C13
13	O	103	BCL	C16-C17-C18-C19
13	Q	102	BCL	C16-C17-C18-C20
12	L	305	PGV	C19-C20-C21-C22
13	9	104	BCL	C5-C6-C7-C8
13	3	103	BCL	O1A-CGA-O2A-C1
19	9	102	CRT	C5-C6-C7-C9
19	0	101	CRT	C5-C6-C7-C9
22	S	104	CDL	C72-C73-C74-C75
13	K	102	BCL	C13-C15-C16-C17
20	M	419	PEF	C12-C13-C14-C15
13	A	103	BCL	C3-C5-C6-C7
13	W	102	BCL	C5-C6-C7-C8
13	M	403	BCL	C16-C17-C18-C19
13	3	103	BCL	C3-C5-C6-C7
22	H	304	CDL	OB6-CB4-CB6-OB8
22	Q	105	CDL	C35-C36-C37-C38
12	L	306	PGV	C3-C4-C5-C6
12	L	305	PGV	C24-C25-C26-C27
23	F	104	LMT	O5B-C1B-O1B-C4'
13	O	103	BCL	C13-C15-C16-C17
22	Q	105	CDL	C58-C59-C60-C61
23	M	420	LMT	C4-C5-C6-C7
12	H	303	PGV	C20-C19-O03-C01
20	M	419	PEF	C11-C10-O2-C2
12	M	415	PGV	C28-C29-C30-C31
12	A	105	PGV	C20-C21-C22-C23
12	M	415	PGV	O05-C05-C06-O06
22	S	104	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
13	D	103	BCL	C1A-C2A-CAA-CBA
13	K	103	BCL	C1A-C2A-CAA-CBA
13	O	103	BCL	C1A-C2A-CAA-CBA
13	S	103	BCL	C1A-C2A-CAA-CBA
13	S	102	BCL	C15-C16-C17-C18
22	H	304	CDL	C78-C79-C80-C81
12	3	105	PGV	C11-C10-C9-C8
22	Q	105	CDL	OB7-CB5-OB6-CB4
13	A	103	BCL	C6-C7-C8-C10
13	D	103	BCL	C12-C13-C15-C16
13	F	102	BCL	C11-C10-C8-C7
13	F	103	BCL	C6-C7-C8-C10
13	K	103	BCL	C6-C7-C8-C10
13	O	103	BCL	C6-C7-C8-C10
13	A	103	BCL	C2C-C3C-CAC-CBC
13	I	102	BCL	C2C-C3C-CAC-CBC
19	M	407	CRT	C3-C1-C4-C5
19	J	101	CRT	C2-C1-C4-C5
19	9	102	CRT	C2-C1-C4-C5
19	9	102	CRT	C3-C1-C4-C5
19	0	101	CRT	C2-C1-C4-C5
22	H	302	CDL	C71-CB7-OB8-CB6
14	L	302	BPH	C2-C3-C5-C6
22	D	104	CDL	C51-CB5-OB6-CB4
13	F	102	BCL	C11-C10-C8-C9
13	3	102	BCL	C11-C10-C8-C9
13	5	102	BCL	C11-C10-C8-C9
22	H	304	CDL	C71-CB7-OB8-CB6
13	W	103	BCL	C10-C11-C12-C13
22	D	104	CDL	OA7-CA5-OA6-CA4
22	Y	103	CDL	OA7-CA5-OA6-CA4
22	S	104	CDL	CA3-CA4-CA6-OA8
22	K	104	CDL	C77-C78-C79-C80
13	Y	102	BCL	C15-C16-C17-C18
13	3	102	BCL	CBA-CGA-O2A-C1
12	L	306	PGV	C26-C27-C28-C29
13	M	403	BCL	C13-C15-C16-C17
13	A	101	BCL	C10-C11-C12-C13
12	3	105	PGV	C25-C26-C27-C28
12	H	303	PGV	C21-C22-C23-C24
12	A	105	PGV	C23-C24-C25-C26
14	L	302	BPH	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	K	104	CDL	C76-C77-C78-C79
12	H	303	PGV	O01-C02-C03-O11
22	Q	105	CDL	OB5-CB3-CB4-OB6
13	D	102	BCL	C4-C3-C5-C6
14	L	302	BPH	C4-C3-C5-C6
12	3	105	PGV	C13-C14-C15-C16
13	M	403	BCL	C16-C17-C18-C20
20	M	419	PEF	C40-C41-C42-C43
22	Y	103	CDL	OA6-CA4-CA6-OA8
22	S	104	CDL	C74-C75-C76-C77
13	F	102	BCL	CBA-CGA-O2A-C1
13	S	103	BCL	CBA-CGA-O2A-C1
20	M	419	PEF	C31-C30-O3-C3
21	O	105	LDA	C7-C8-C9-C10
19	M	407	CRT	C40-C38-O2-C2M
12	3	105	PGV	C7-C8-C9-C10
13	A	103	BCL	C10-C11-C12-C13
13	S	102	BCL	C10-C11-C12-C13
13	1	102	BCL	C16-C17-C18-C19
13	1	103	BCL	CBA-CGA-O2A-C1
13	D	103	BCL	C14-C13-C15-C16
13	Q	103	BCL	C11-C10-C8-C9
13	U	102	BCL	C14-C13-C15-C16
13	9	104	BCL	C11-C10-C8-C9
13	9	104	BCL	C11-C12-C13-C14
13	0	102	BCL	C6-C7-C8-C9
13	Q	102	BCL	C13-C15-C16-C17
13	I	102	BCL	C16-C17-C18-C20
23	M	420	LMT	C5-C6-C7-C8
20	M	419	PEF	O3P-C1-C2-C3
13	M	403	BCL	C6-C7-C8-C10
13	A	101	BCL	C12-C13-C15-C16
13	D	103	BCL	C6-C7-C8-C10
13	I	103	BCL	C12-C13-C15-C16
13	K	102	BCL	C11-C10-C8-C7
13	Q	103	BCL	C11-C10-C8-C7
13	U	103	BCL	C11-C10-C8-C7
13	U	103	BCL	C11-C12-C13-C15
13	1	102	BCL	C6-C7-C8-C10
13	1	103	BCL	C12-C13-C15-C16
13	3	102	BCL	C11-C10-C8-C7
13	3	103	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
13	3	103	BCL	C11-C10-C8-C7
13	5	102	BCL	C11-C10-C8-C7
13	7	103	BCL	C11-C10-C8-C7
13	9	104	BCL	C11-C12-C13-C15
22	H	304	CDL	CB5-C51-C52-C53
22	S	104	CDL	C11-C12-C13-C14
13	A	101	BCL	C15-C16-C17-C18
13	S	102	BCL	C13-C15-C16-C17
12	H	303	PGV	O04-C19-O03-C01
13	3	102	BCL	O1A-CGA-O2A-C1
22	H	302	CDL	OB9-CB7-OB8-CB6
13	9	104	BCL	C15-C16-C17-C18
13	Z	102	BCL	CBA-CGA-O2A-C1
13	7	103	BCL	C15-C16-C17-C18
19	Q	104	CRT	C5-C6-C7-C8
19	V	101	CRT	C10-C11-C12-C13
22	H	304	CDL	CB3-CB4-CB6-OB8
22	Q	105	CDL	CA3-CA4-CA6-OA8
22	S	104	CDL	CB3-CB4-CB6-OB8
12	A	105	PGV	C21-C22-C23-C24
13	I	103	BCL	C13-C15-C16-C17
22	M	416	CDL	CB3-CB4-CB6-OB8
20	M	419	PEF	O4-C10-O2-C2
20	M	419	PEF	O3P-C1-C2-O2
22	Q	105	CDL	OA5-CA3-CA4-OA6
13	S	102	BCL	O1D-CGD-O2D-CED
22	Q	105	CDL	C74-C75-C76-C77
12	M	415	PGV	C20-C21-C22-C23
20	M	419	PEF	C13-C14-C15-C16
22	H	304	CDL	C60-C61-C62-C63
22	K	104	CDL	C36-C37-C38-C39
13	5	103	BCL	C10-C11-C12-C13
13	5	102	BCL	C16-C17-C18-C19
22	Q	105	CDL	OA6-CA4-CA6-OA8
22	S	104	CDL	OA6-CA4-CA6-OA8
13	F	103	BCL	C3-C5-C6-C7
12	D	105	PGV	C19-C20-C21-C22
22	H	304	CDL	OB9-CB7-OB8-CB6
13	9	104	BCL	O1D-CGD-O2D-CED
13	1	102	BCL	C16-C17-C18-C20
13	D	102	BCL	C15-C16-C17-C18
13	I	103	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
13	K	102	BCL	C11-C10-C8-C9
13	1	102	BCL	C6-C7-C8-C9
13	3	102	BCL	C6-C7-C8-C9
13	3	103	BCL	C14-C13-C15-C16
12	L	306	PGV	C24-C25-C26-C27
12	H	303	PGV	C5-C6-C7-C8
22	K	104	CDL	C34-C35-C36-C37
14	L	302	BPH	C16-C17-C18-C20
13	5	102	BCL	C4C-C3C-CAC-CBC
13	U	103	BCL	C13-C15-C16-C17
15	7	104	UQ8	C13-C14-C16-C17
13	S	103	BCL	C8-C10-C11-C12
20	M	419	PEF	O5-C30-O3-C3
12	M	415	PGV	O12-C04-C05-C06
22	S	104	CDL	CB2-C1-CA2-OA2
20	M	419	PEF	C34-C35-C36-C37
22	K	104	CDL	C31-C32-C33-C34
13	5	103	BCL	C13-C15-C16-C17
12	1	106	PGV	C01-C02-C03-O11
22	Q	105	CDL	OA5-CA3-CA4-CA6
23	M	420	LMT	C2-C3-C4-C5
13	W	102	BCL	C10-C11-C12-C13
19	2	101	CRT	C10-C11-C12-C13
13	M	403	BCL	C11-C12-C13-C15
13	I	103	BCL	C6-C7-C8-C10
13	Y	102	BCL	C6-C7-C8-C10
13	Z	102	BCL	C11-C12-C13-C15
13	3	102	BCL	C6-C7-C8-C10
13	3	102	BCL	C12-C13-C15-C16
13	7	103	BCL	C6-C7-C8-C10
13	9	104	BCL	C6-C7-C8-C10
20	M	419	PEF	C20-C21-C22-C23
19	G	101	CRT	C15-C16-C17-C19
19	U	104	CRT	C15-C16-C17-C19
19	9	103	CRT	C15-C16-C17-C19
22	H	302	CDL	C71-C72-C73-C74
13	F	102	BCL	O1A-CGA-O2A-C1
13	1	103	BCL	O1A-CGA-O2A-C1
22	D	104	CDL	OB7-CB5-OB6-CB4
13	K	102	BCL	C4-C3-C5-C6
22	Q	105	CDL	C61-C62-C63-C64
13	S	103	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	A	105	PGV	C22-C23-C24-C25
13	D	102	BCL	C5-C6-C7-C8
12	M	415	PGV	O01-C02-C03-O11
12	1	106	PGV	O01-C02-C03-O11
12	H	303	PGV	O03-C01-C02-C03
22	Q	105	CDL	CB3-CB4-CB6-OB8
13	Z	102	BCL	O1A-CGA-O2A-C1
13	M	403	BCL	C5-C6-C7-C8
15	7	104	UQ8	C15-C14-C16-C17
12	M	414	PGV	C13-C14-C15-C16
22	Y	104	CDL	O1-C1-CB2-OB2
13	3	103	BCL	C15-C16-C17-C18
20	M	419	PEF	O2-C2-C3-O3
13	M	403	BCL	C11-C12-C13-C14
13	D	103	BCL	C6-C7-C8-C9
13	S	103	BCL	C6-C7-C8-C9
13	Y	102	BCL	C6-C7-C8-C9
22	Y	103	CDL	C31-CA7-OA8-CA6
13	F	103	BCL	C13-C15-C16-C17
19	9	102	CRT	O1-C1-C4-C5
13	K	103	BCL	C10-C11-C12-C13
13	5	102	BCL	C16-C17-C18-C20
13	7	103	BCL	C16-C17-C18-C19
13	M	402	BCL	C15-C16-C17-C18
21	V	102	LDA	C2-C1-N1-CM2
13	S	103	BCL	C10-C11-C12-C13
22	H	302	CDL	C76-C77-C78-C79
13	A	103	BCL	C1A-C2A-CAA-CBA
13	Z	102	BCL	C1A-C2A-CAA-CBA
13	3	103	BCL	C1A-C2A-CAA-CBA
13	7	103	BCL	C1A-C2A-CAA-CBA
12	1	106	PGV	C19-C20-C21-C22
15	L	308	UQ8	C5-C4-O4-C4M
15	7	104	UQ8	C5-C4-O4-C4M
13	9	104	BCL	C8-C10-C11-C12
19	V	101	CRT	C5-C6-C7-C9
12	M	414	PGV	C12-C13-C14-C15
22	Q	105	CDL	OA9-CA7-OA8-CA6
12	M	415	PGV	C01-C02-C03-O11
22	Y	103	CDL	OA5-CA3-CA4-CA6
12	L	306	PGV	C25-C26-C27-C28
13	D	102	BCL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
13	K	102	BCL	C12-C13-C15-C16
14	M	405	BPH	C8-C10-C11-C12
13	M	403	BCL	C2C-C3C-CAC-CBC
13	F	102	BCL	C2C-C3C-CAC-CBC
13	K	103	BCL	C2C-C3C-CAC-CBC
13	U	103	BCL	C2C-C3C-CAC-CBC
22	Q	105	CDL	C31-CA7-OA8-CA6
12	M	415	PGV	C02-C03-O11-P
13	Y	102	BCL	C5-C6-C7-C8
22	Y	103	CDL	OA9-CA7-OA8-CA6
12	M	414	PGV	O01-C02-C03-O11
13	D	102	BCL	C11-C10-C8-C9
13	Z	102	BCL	C11-C12-C13-C14
13	3	103	BCL	C6-C7-C8-C9
13	9	104	BCL	C6-C7-C8-C9
22	K	104	CDL	C51-C52-C53-C54
21	M	412	LDA	C2-C1-N1-O1
21	O	105	LDA	C2-C1-N1-O1
21	V	102	LDA	C2-C1-N1-O1
22	Q	105	CDL	OB6-CB4-CB6-OB8
22	S	104	CDL	OB6-CB4-CB6-OB8
20	K	105	PEF	C1-C2-C3-O3
22	K	104	CDL	CB3-CB4-CB6-OB8
21	V	102	LDA	C1-C2-C3-C4
13	M	404	BCL	C13-C15-C16-C17
12	L	306	PGV	C03-O11-P-O13
12	M	415	PGV	C04-O12-P-O11
12	M	415	PGV	C04-O12-P-O13
12	M	415	PGV	C04-O12-P-O14
12	H	303	PGV	C03-O11-P-O13
22	M	416	CDL	CA2-OA2-PA1-OA5
22	H	302	CDL	CA2-OA2-PA1-OA3
22	H	302	CDL	CA3-OA5-PA1-OA4
22	H	304	CDL	CB3-OB5-PB2-OB3
22	D	104	CDL	CB2-OB2-PB2-OB4
22	K	104	CDL	CA2-OA2-PA1-OA3
22	Q	105	CDL	CB2-OB2-PB2-OB3
22	S	104	CDL	CA2-OA2-PA1-OA3
22	S	104	CDL	CB3-OB5-PB2-OB3
22	Y	103	CDL	CA3-OA5-PA1-OA4
22	Y	103	CDL	CB2-OB2-PB2-OB3
13	K	102	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
13	D	102	BCL	C2-C3-C5-C6
12	H	303	PGV	C02-C03-O11-P
19	O	104	CRT	C29-C28-C30-C31
13	U	103	BCL	C16-C17-C18-C19
22	H	302	CDL	C14-C15-C16-C17
13	K	102	BCL	O1A-CGA-O2A-C1
12	1	106	PGV	C2-C3-C4-C5
22	H	302	CDL	C74-C75-C76-C77
20	M	419	PEF	C3-C2-O2-C10
22	Y	103	CDL	CA3-CA4-OA6-CA5
13	W	102	BCL	C15-C16-C17-C18
13	5	103	BCL	C15-C16-C17-C18
14	M	405	BPH	C15-C16-C17-C18
12	M	414	PGV	C01-C02-C03-O11
12	H	303	PGV	C01-C02-C03-O11
22	Q	105	CDL	OB5-CB3-CB4-CB6
13	I	103	BCL	C14-C13-C15-C16
13	Q	102	BCL	C11-C10-C8-C9
13	1	103	BCL	C11-C10-C8-C9
13	1	103	BCL	C14-C13-C15-C16
13	A	101	BCL	C6-C7-C8-C10
13	Q	102	BCL	C11-C10-C8-C7
13	Q	103	BCL	C12-C13-C15-C16
13	K	102	BCL	CBA-CGA-O2A-C1
22	Q	105	CDL	C32-C31-CA7-OA8
12	1	106	PGV	C20-C19-O03-C01
12	H	303	PGV	C22-C23-C24-C25
12	3	105	PGV	C24-C25-C26-C27
22	Y	103	CDL	CA3-CA4-CA6-OA8
13	M	404	BCL	CAA-CBA-CGA-O2A
19	0	101	CRT	C29-C28-C30-C31
13	Q	102	BCL	O1D-CGD-O2D-CED
13	M	403	BCL	C3-C5-C6-C7
13	S	103	BCL	C4-C3-C5-C6
23	M	420	LMT	C2-C1-O1'-C1'
13	W	102	BCL	C11-C10-C8-C9
13	Y	102	BCL	C11-C10-C8-C9
13	A	101	BCL	CBA-CGA-O2A-C1
13	1	102	BCL	CBA-CGA-O2A-C1
13	1	102	BCL	O1A-CGA-O2A-C1
13	5	102	BCL	C4-C3-C5-C6
13	A	101	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	H	304	CDL	C52-C53-C54-C55
22	K	104	CDL	C57-C58-C59-C60
13	S	102	BCL	C12-C13-C15-C16
13	W	103	BCL	C6-C7-C8-C10
13	7	103	BCL	C11-C12-C13-C15
12	1	106	PGV	O04-C19-O03-C01
19	V	101	CRT	C15-C16-C17-C18
22	D	104	CDL	CB2-C1-CA2-OA2
22	H	302	CDL	CB3-CB4-CB6-OB8
13	5	103	BCL	C3-C5-C6-C7
13	U	103	BCL	C6-C7-C8-C9
13	1	102	BCL	C11-C10-C8-C9
13	5	103	BCL	C6-C7-C8-C9
13	M	402	BCL	C16-C17-C18-C19
22	K	104	CDL	CA3-CA4-OA6-CA5
22	K	104	CDL	CA6-CA4-OA6-CA5
13	K	103	BCL	C4-C3-C5-C6
13	L	301	BCL	C2A-CAA-CBA-CGA
13	1	103	BCL	C1A-C2A-CAA-CBA
13	3	102	BCL	C1A-C2A-CAA-CBA
7	C	501	HEC	CAA-CBA-CGA-O2A
12	A	105	PGV	O01-C02-C03-O11
7	C	501	HEC	CAA-CBA-CGA-O1A
12	A	105	PGV	C02-C03-O11-P
22	H	304	CDL	C1-CA2-OA2-PA1
7	C	502	HEC	CAA-CBA-CGA-O2A
7	C	502	HEC	CAD-CBD-CGD-O1D
12	M	414	PGV	C6-C7-C8-C9
13	K	102	BCL	C15-C16-C17-C18
13	M	403	BCL	C12-C13-C15-C16
13	K	103	BCL	C11-C10-C8-C7
13	Q	102	BCL	C11-C12-C13-C15
13	W	102	BCL	C11-C10-C8-C7
13	3	103	BCL	C11-C12-C13-C15
13	O	102	BCL	C15-C16-C17-C18
19	U	104	CRT	C2-C1-C4-C5
19	0	101	CRT	C3-C1-C4-C5
7	C	502	HEC	CAA-CBA-CGA-O1A
7	C	504	HEC	CAD-CBD-CGD-O1D
19	O	104	CRT	C34-C33-C35-C36
13	5	103	BCL	C4-C3-C5-C6
12	M	415	PGV	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
13	K	102	BCL	C2-C3-C5-C6
23	F	104	LMT	O5B-C5B-C6B-O6B
22	H	302	CDL	C58-C59-C60-C61
13	F	102	BCL	C4-C3-C5-C6
15	L	308	UQ8	C20-C19-C21-C22
13	Q	102	BCL	C3-C5-C6-C7
13	M	402	BCL	C13-C15-C16-C17
13	K	103	BCL	C15-C16-C17-C18
22	H	302	CDL	C15-C16-C17-C18
12	M	415	PGV	O03-C01-C02-C03
22	Q	105	CDL	C16-C17-C18-C19
7	C	502	HEC	CAD-CBD-CGD-O2D
13	O	103	BCL	C4C-C3C-CAC-CBC
21	I	105	LDA	C1-C2-C3-C4
22	Y	103	CDL	OA5-CA3-CA4-OA6
13	Y	102	BCL	C4-C3-C5-C6
7	C	504	HEC	CAD-CBD-CGD-O2D
13	O	103	BCL	C15-C16-C17-C18
13	7	102	BCL	O1A-CGA-O2A-C1
22	H	304	CDL	C14-C15-C16-C17
12	D	105	PGV	C01-C02-C03-O11
12	M	414	PGV	O03-C01-C02-O01
12	A	105	PGV	O03-C01-C02-O01
12	L	305	PGV	C29-C30-C31-C32
13	A	101	BCL	C11-C10-C8-C9
13	S	103	BCL	C11-C12-C13-C14
22	S	104	CDL	C72-C71-CB7-OB8
13	K	102	BCL	C2-C1-O2A-CGA
13	9	104	BCL	C2-C1-O2A-CGA
23	F	104	LMT	C6-C7-C8-C9
22	K	104	CDL	C37-C38-C39-C40
12	L	306	PGV	C23-C24-C25-C26
22	H	304	CDL	CA3-CA4-OA6-CA5
22	Y	103	CDL	CA6-CA4-OA6-CA5
12	3	105	PGV	C11-C12-C13-C14
15	L	309	UQ8	C5-C4-O4-C4M
21	M	412	LDA	C1-C2-C3-C4
13	5	102	BCL	C3-C5-C6-C7
13	5	102	BCL	C2-C3-C5-C6
13	7	102	BCL	CBA-CGA-O2A-C1
23	F	104	LMT	C2B-C1B-O1B-C4'
12	L	305	PGV	C05-C04-O12-P

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Mol	Chain	Res	Type	Atoms
13	F	102	BCL	O1D-CGD-O2D-CED
22	S	104	CDL	C71-C72-C73-C74
13	O	102	BCL	C4-C3-C5-C6
13	5	102	BCL	CBD-CGD-O2D-CED
13	A	101	BCL	C6-C7-C8-C9
13	U	102	BCL	C11-C10-C8-C9
12	L	305	PGV	C25-C26-C27-C28
21	M	412	LDA	C7-C8-C9-C10
12	A	105	PGV	C01-C02-C03-O11
22	K	104	CDL	C12-C13-C14-C15
13	3	102	BCL	CAA-CBA-CGA-O2A
13	K	103	BCL	C16-C17-C18-C19
13	3	103	BCL	C16-C17-C18-C19
13	S	103	BCL	C2-C3-C5-C6
13	A	101	BCL	C11-C10-C8-C7
13	D	102	BCL	C6-C7-C8-C10
13	O	102	BCL	C6-C7-C8-C10
13	S	103	BCL	C11-C12-C13-C15
13	U	103	BCL	C6-C7-C8-C10
12	L	305	PGV	C22-C23-C24-C25
12	H	303	PGV	O01-C1-C2-C3
13	A	101	BCL	C2-C1-O2A-CGA
12	3	105	PGV	C1-C2-C3-C4
11	C	508	LHG	C23-C24-C25-C26
13	K	103	BCL	C2-C3-C5-C6
7	C	504	HEC	CAA-CBA-CGA-O2A
13	Q	103	BCL	C6-C7-C8-C9
13	7	102	BCL	C11-C10-C8-C9
15	7	104	UQ8	C9-C11-C12-C13
13	9	104	BCL	C4-C3-C5-C6
12	L	306	PGV	O01-C1-C2-C3
22	K	104	CDL	C52-C51-CB5-OB6
13	5	103	BCL	C2-C3-C5-C6
19	O	104	CRT	C27-C28-C30-C31
19	Q	104	CRT	C5-C6-C7-C9
19	Q	104	CRT	C27-C28-C30-C31
19	V	101	CRT	C10-C11-C12-C14
19	V	101	CRT	C15-C16-C17-C19
19	2	101	CRT	C10-C11-C12-C14
13	Z	102	BCL	C16-C17-C18-C19
13	3	102	BCL	C2-C1-O2A-CGA
13	7	103	BCL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
13	Z	102	BCL	C12-C13-C15-C16
13	1	103	BCL	C6-C7-C8-C10
13	5	103	BCL	C11-C12-C13-C15
13	F	102	BCL	C2-C3-C5-C6
13	9	104	BCL	C10-C11-C12-C13
14	L	302	BPH	O2A-C1-C2-C3
13	3	102	BCL	C15-C16-C17-C18
22	Q	105	CDL	C71-C72-C73-C74
22	D	104	CDL	C32-C31-CA7-OA8
13	I	102	BCL	C10-C11-C12-C13
21	J	102	LDA	C1-C2-C3-C4
22	K	104	CDL	C53-C54-C55-C56
22	K	104	CDL	C33-C34-C35-C36
13	Y	102	BCL	C10-C11-C12-C13
12	H	303	PGV	O02-C1-C2-C3
13	0	102	BCL	CBA-CGA-O2A-C1
13	3	103	BCL	C11-C12-C13-C14
13	F	103	BCL	C8-C10-C11-C12
22	K	104	CDL	C52-C51-CB5-OB7
19	M	407	CRT	C35-C36-C37-C38
13	7	103	BCL	C3-C5-C6-C7
13	O	102	BCL	C5-C6-C7-C8
19	O	104	CRT	C32-C33-C35-C36
19	1	104	CRT	C15-C16-C17-C19
13	F	103	BCL	C15-C16-C17-C18
13	I	102	BCL	C15-C16-C17-C18
12	L	306	PGV	O02-C1-C2-C3
13	3	102	BCL	CAA-CBA-CGA-O1A
15	L	308	UQ8	C39-C41-C42-C43
15	L	308	UQ8	C18-C19-C21-C22
14	M	405	BPH	CAD-CBD-CGD-O2D
22	Q	105	CDL	C72-C71-CB7-OB8
13	0	102	BCL	O1A-CGA-O2A-C1
13	O	103	BCL	C2-C1-O2A-CGA
22	H	302	CDL	C11-C12-C13-C14
22	Q	105	CDL	C59-C60-C61-C62
20	K	105	PEF	O3-C30-C31-C32
13	D	102	BCL	CAA-CBA-CGA-O2A
22	K	104	CDL	CA7-C31-C32-C33

There are no ring outliers.

90 monomers are involved in 279 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	F	102	BCL	2	0
13	M	404	BCL	1	0
20	K	105	PEF	1	0
19	J	101	CRT	3	0
9	H	301	GOL	1	0
15	M	418	UQ8	4	0
12	D	105	PGV	2	0
21	M	412	LDA	1	0
13	3	103	BCL	4	0
12	M	415	PGV	3	0
21	I	105	LDA	6	0
13	0	102	BCL	8	0
13	S	102	BCL	4	0
15	L	309	UQ8	1	0
12	H	303	PGV	1	0
13	3	102	BCL	4	0
19	A	104	CRT	3	0
18	M	406	MQ8	5	0
19	O	104	CRT	2	0
22	S	104	CDL	10	0
13	O	103	BCL	4	0
15	7	104	UQ8	10	0
19	Z	101	CRT	2	0
21	O	105	LDA	1	0
19	6	101	CRT	2	0
19	2	101	CRT	6	0
12	M	414	PGV	4	0
19	Q	104	CRT	2	0
13	A	103	BCL	3	0
13	Z	102	BCL	6	0
13	D	103	BCL	4	0
19	P	101	CRT	2	0
13	5	103	BCL	3	0
22	Q	105	CDL	3	0
13	F	103	BCL	3	0
13	K	102	BCL	2	0
7	C	504	HEC	2	0
13	I	102	BCL	4	0
12	L	306	PGV	4	0
13	K	103	BCL	3	0
13	W	103	BCL	2	0
19	0	101	CRT	2	0
19	M	407	CRT	5	0

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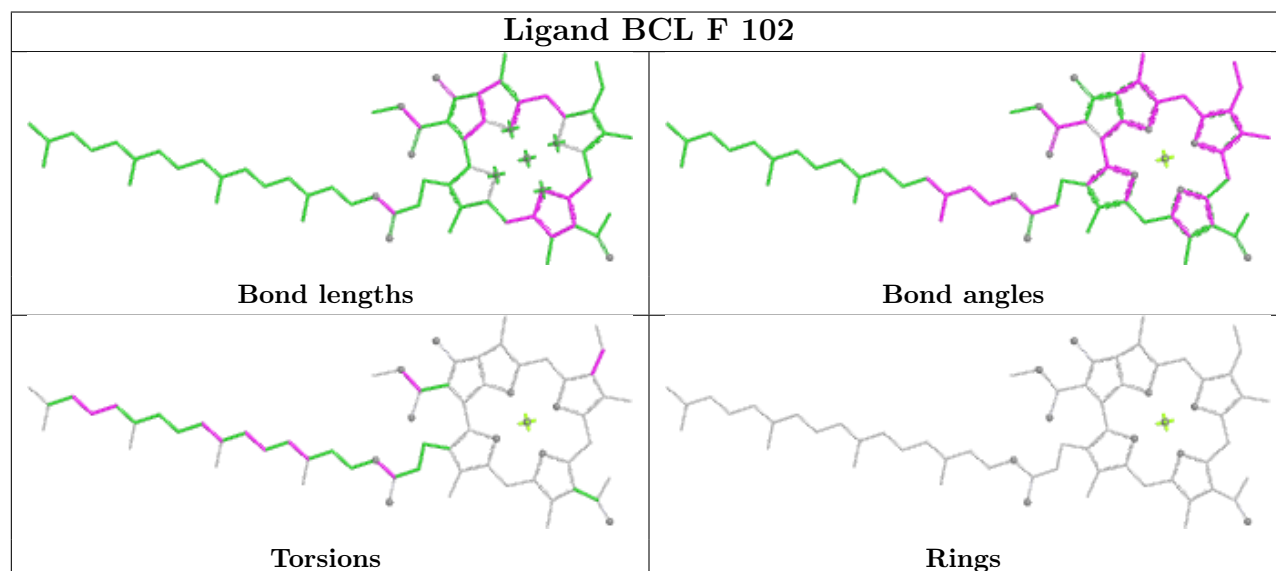
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	I	104	PEF	1	0
22	H	302	CDL	3	0
13	W	102	BCL	5	0
22	M	416	CDL	1	0
13	1	102	BCL	4	0
12	3	105	PGV	3	0
21	J	102	LDA	1	0
13	U	103	BCL	4	0
19	1	104	CRT	3	0
13	U	102	BCL	8	0
23	F	104	LMT	5	0
13	Q	102	BCL	6	0
22	H	304	CDL	3	0
13	I	103	BCL	4	0
13	7	103	BCL	4	0
13	M	402	BCL	5	0
12	A	105	PGV	5	0
13	7	102	BCL	3	0
22	D	104	CDL	2	0
13	5	102	BCL	9	0
13	O	102	BCL	3	0
13	D	102	BCL	2	0
13	Y	102	BCL	5	0
20	M	419	PEF	3	0
14	M	405	BPH	7	0
13	S	103	BCL	6	0
19	9	102	CRT	4	0
20	5	104	PEF	1	0
19	V	101	CRT	1	0
22	K	104	CDL	4	0
22	Y	103	CDL	1	0
15	L	303	UQ8	2	0
19	U	104	CRT	2	0
15	L	308	UQ8	7	0
14	L	302	BPH	5	0
13	L	301	BCL	4	0
7	C	503	HEC	1	0
13	9	104	BCL	4	0
23	M	420	LMT	3	0
19	G	101	CRT	5	0
12	L	305	PGV	4	0
13	A	101	BCL	4	0

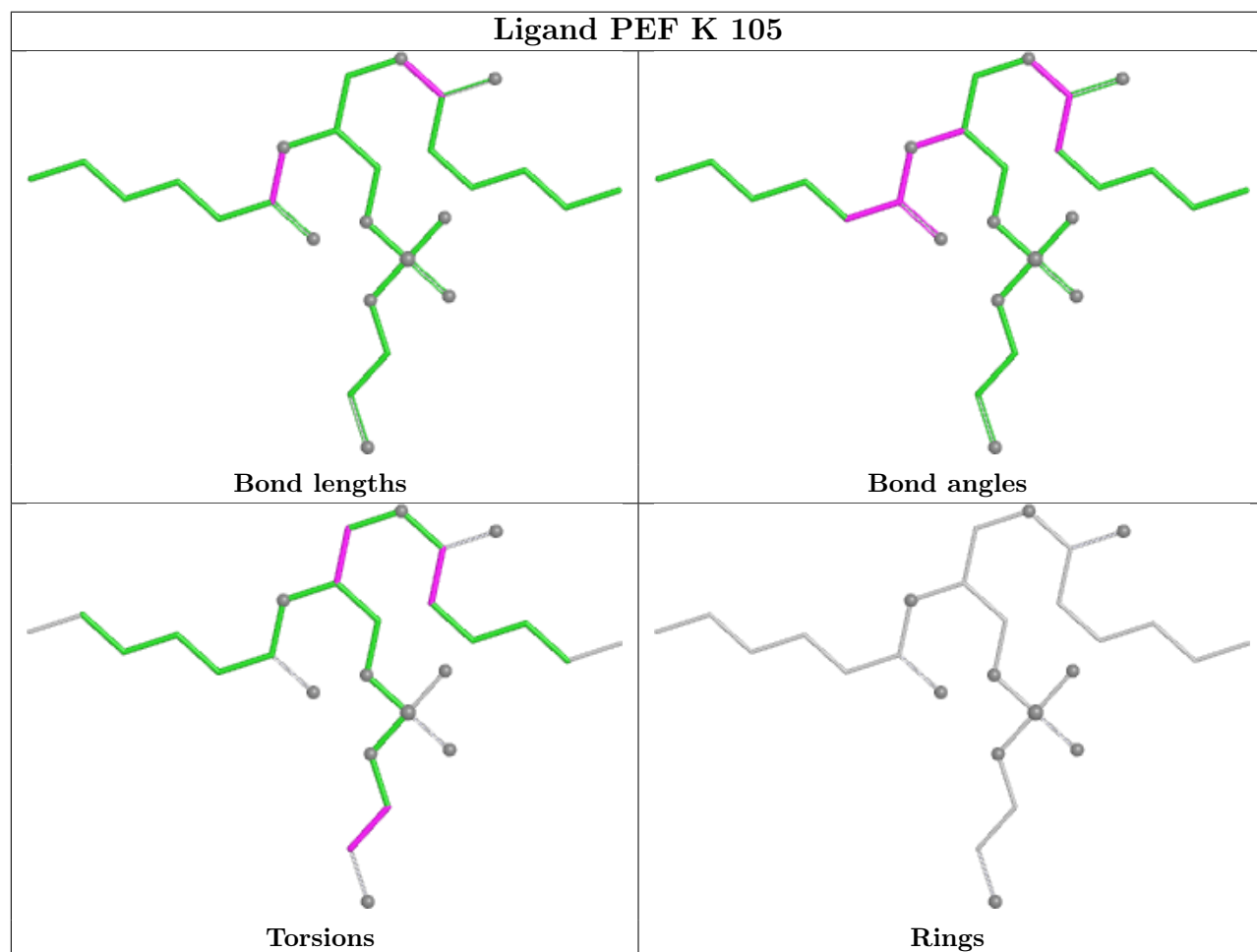
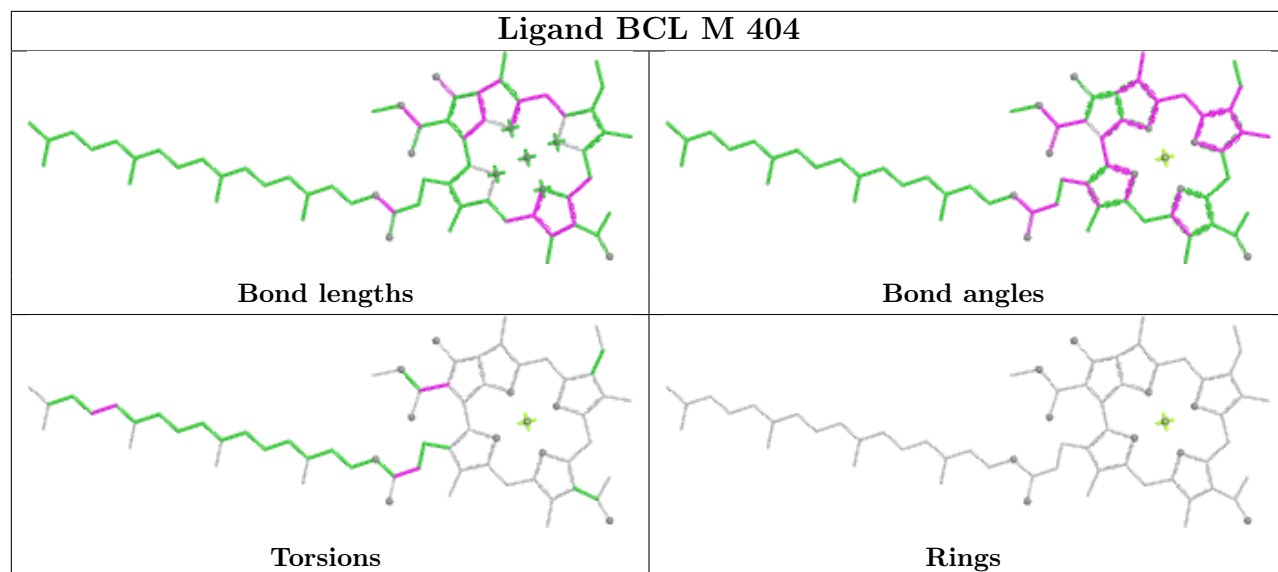
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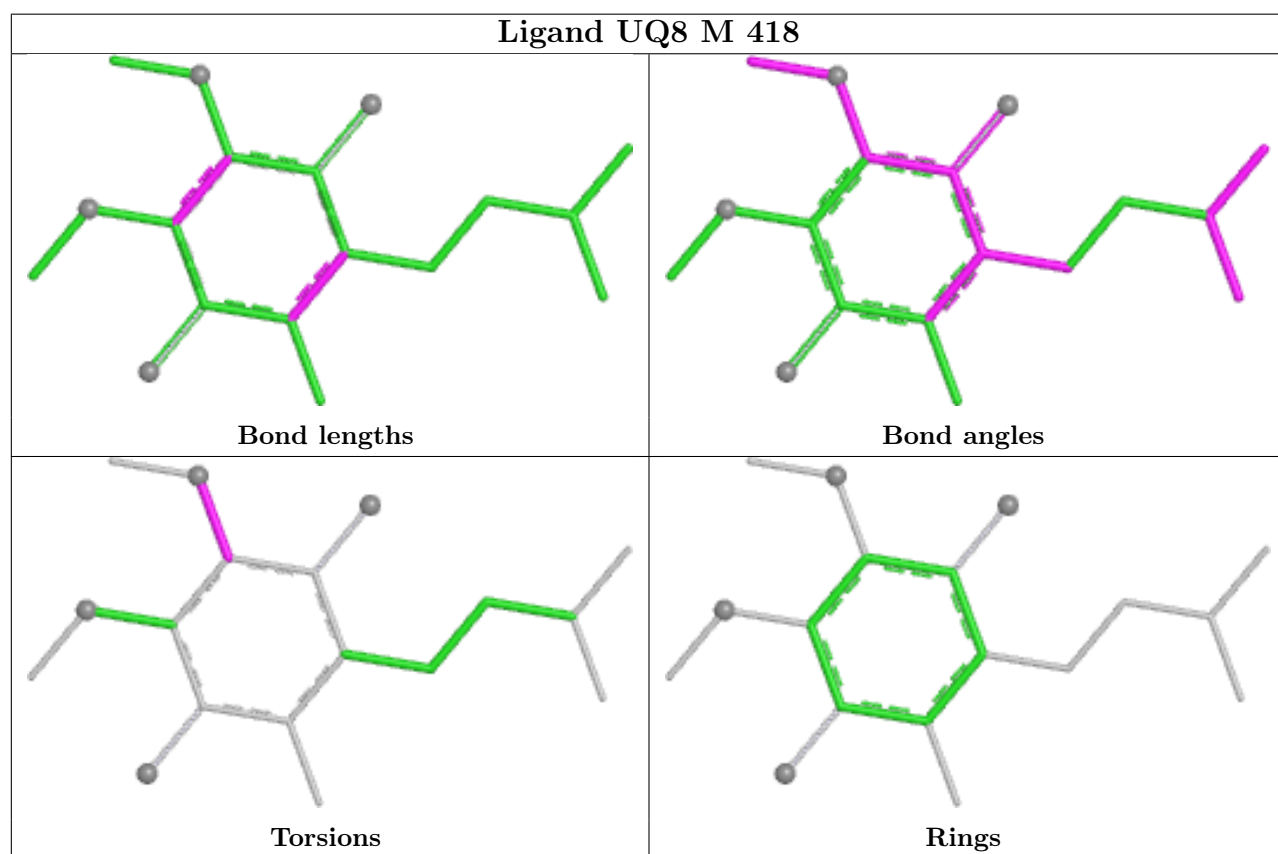
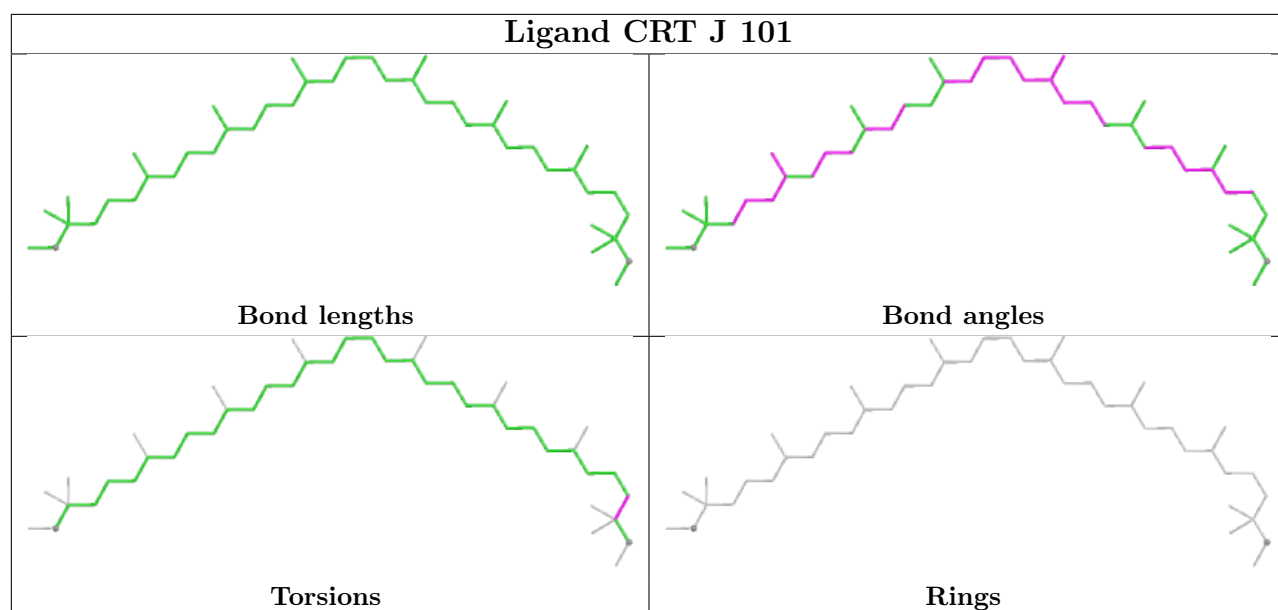
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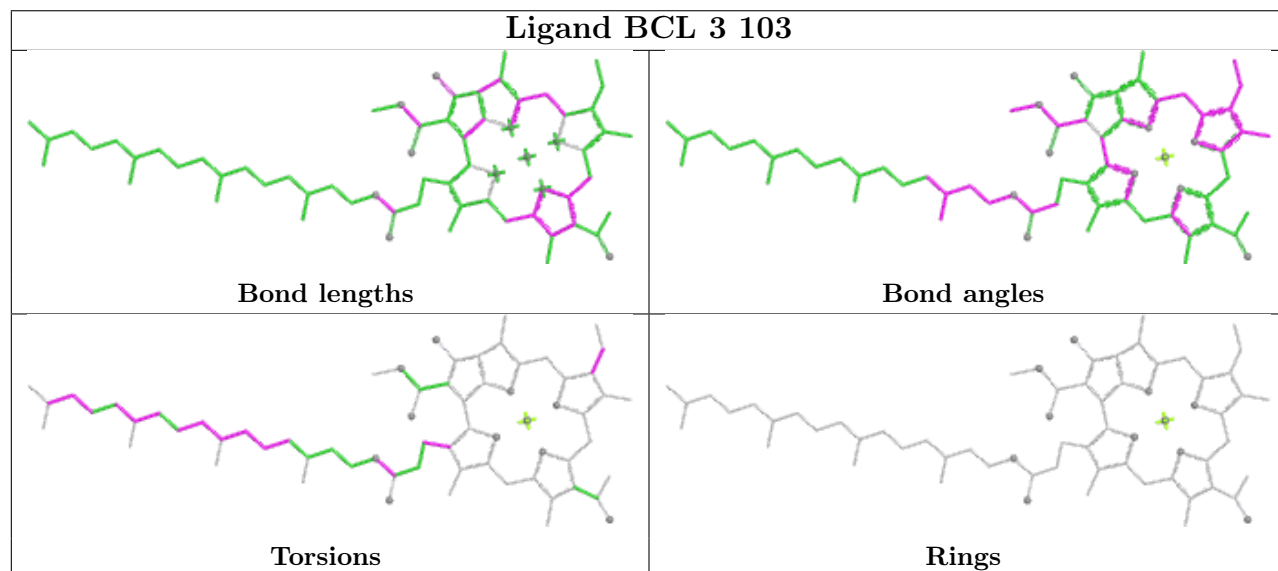
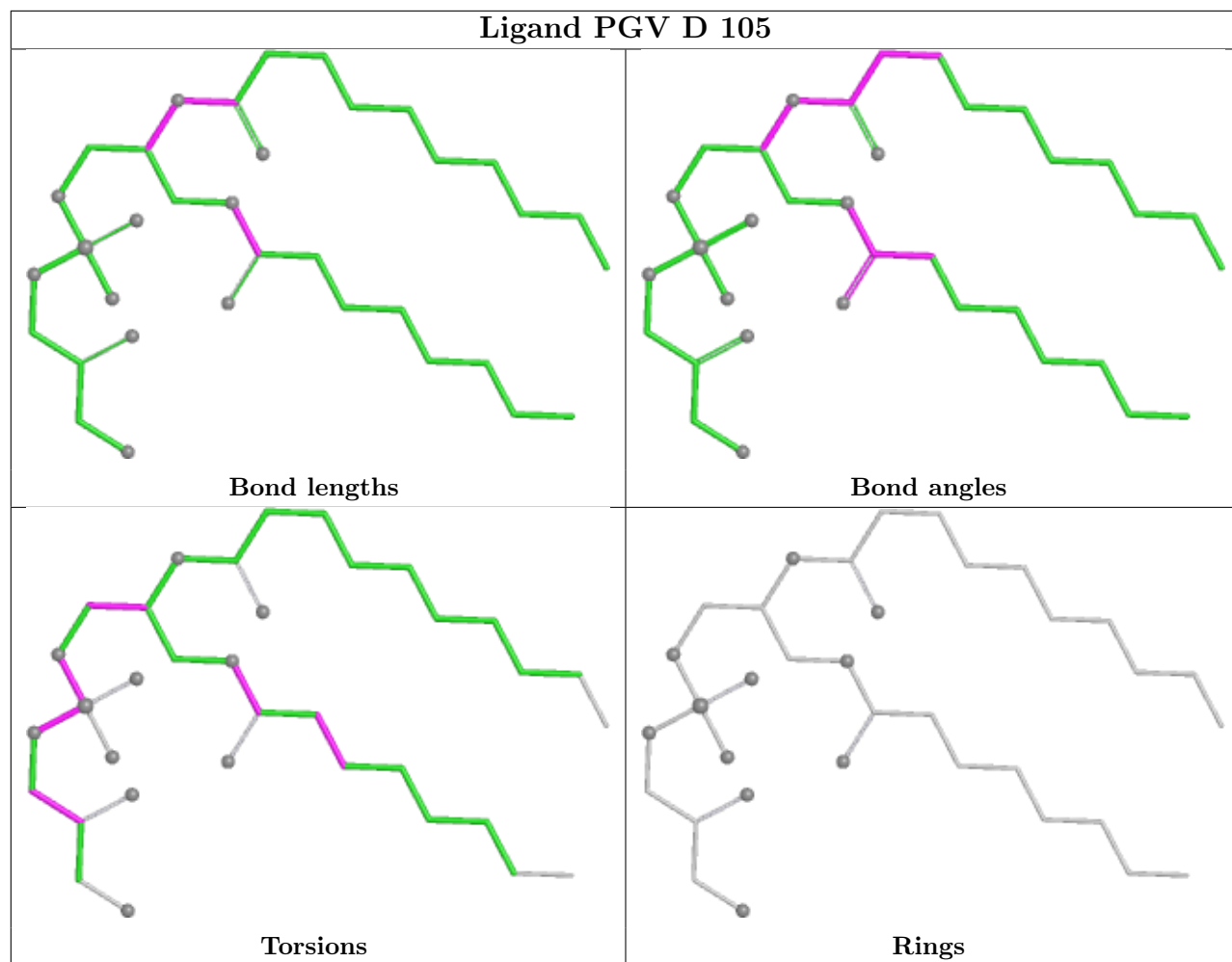
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	N	101	CRT	3	0
13	Q	103	BCL	5	0
19	9	103	CRT	2	0
13	1	103	BCL	6	0
13	M	403	BCL	2	0

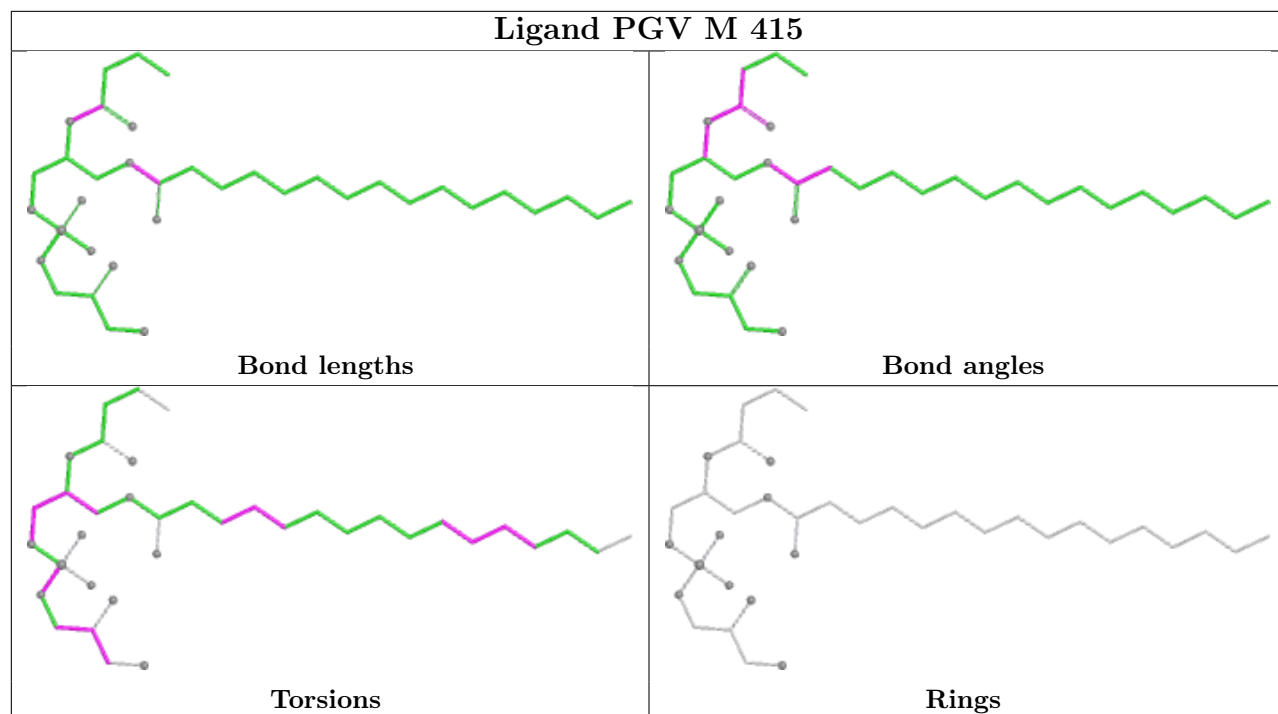
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

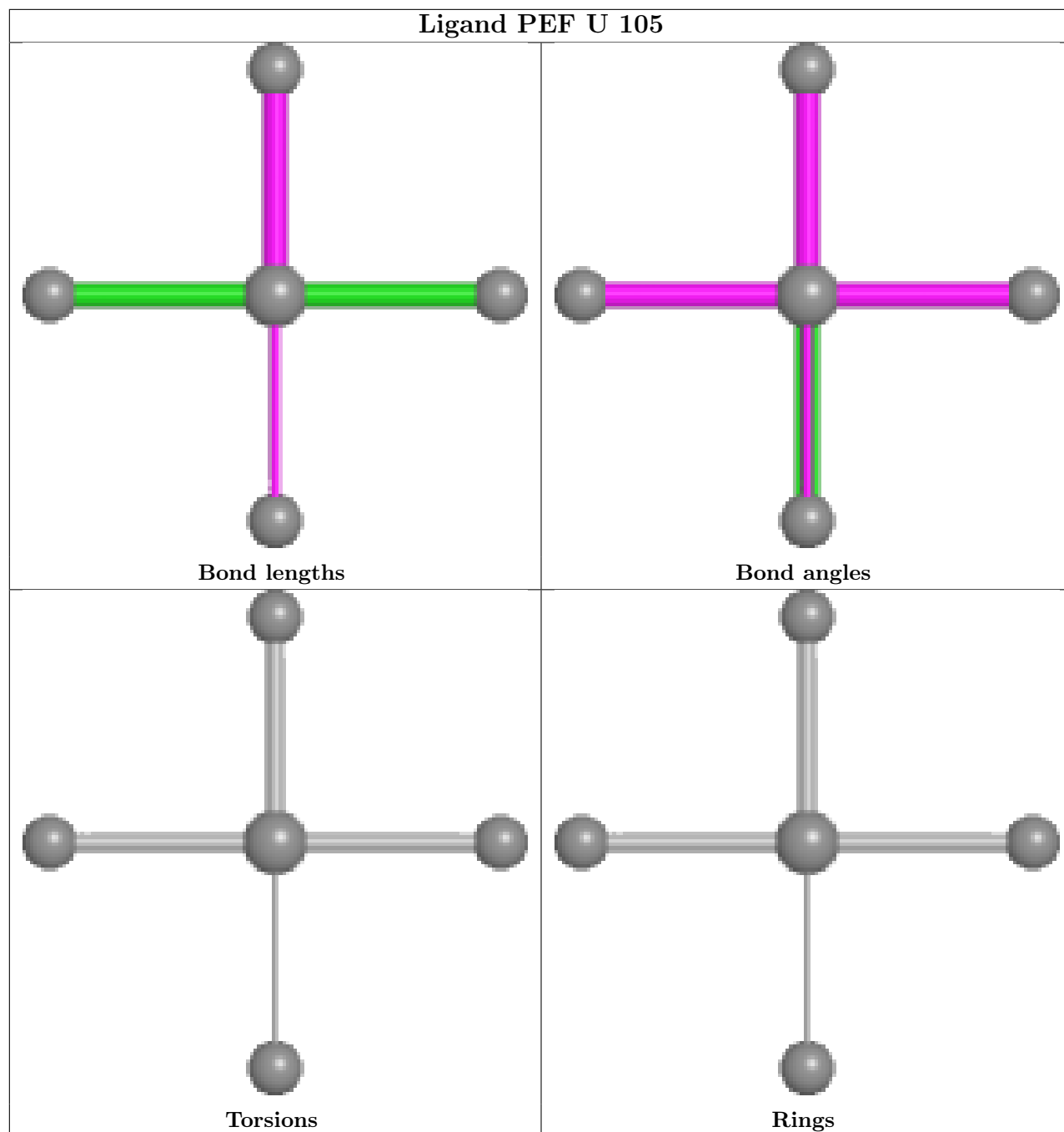


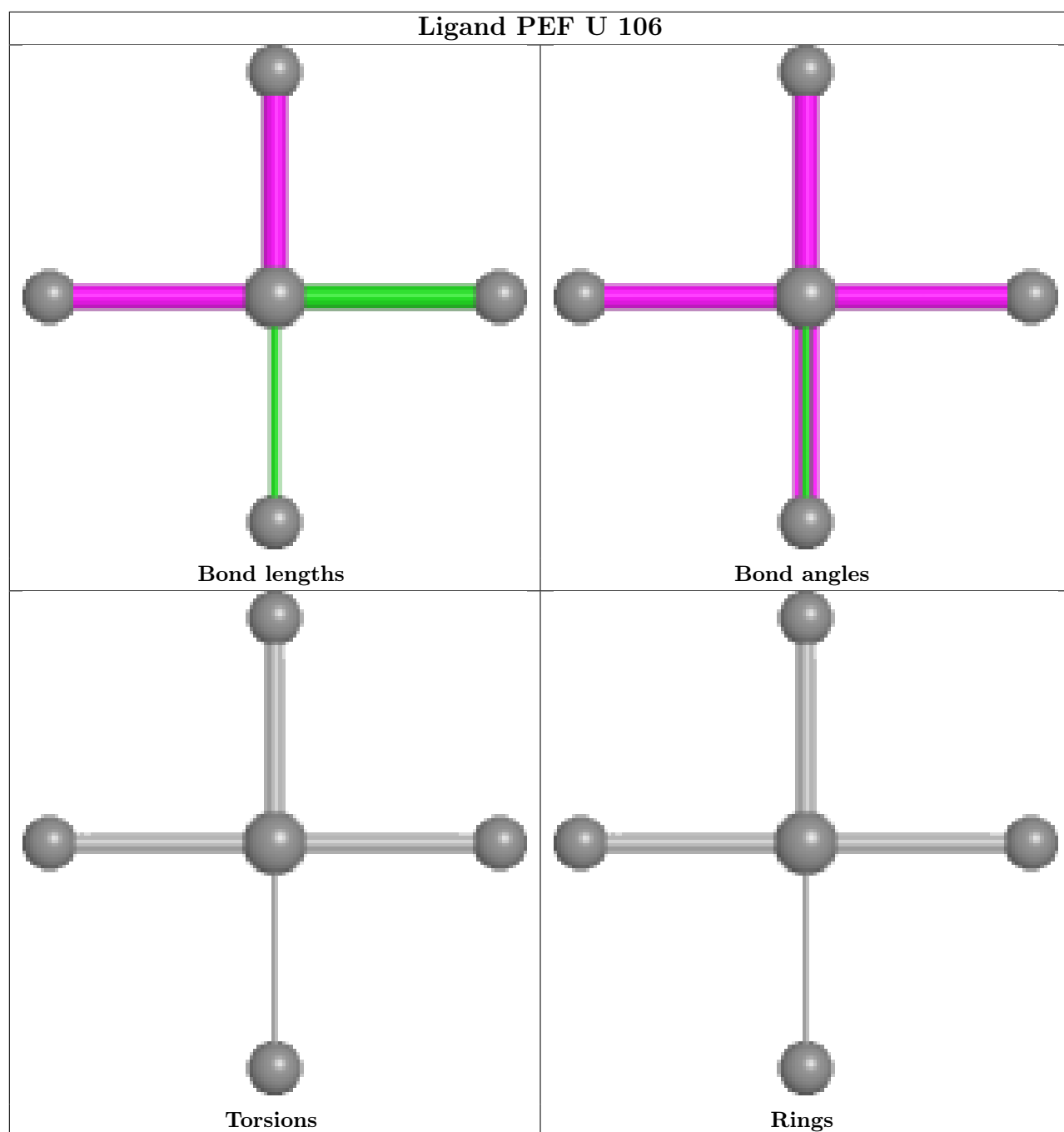


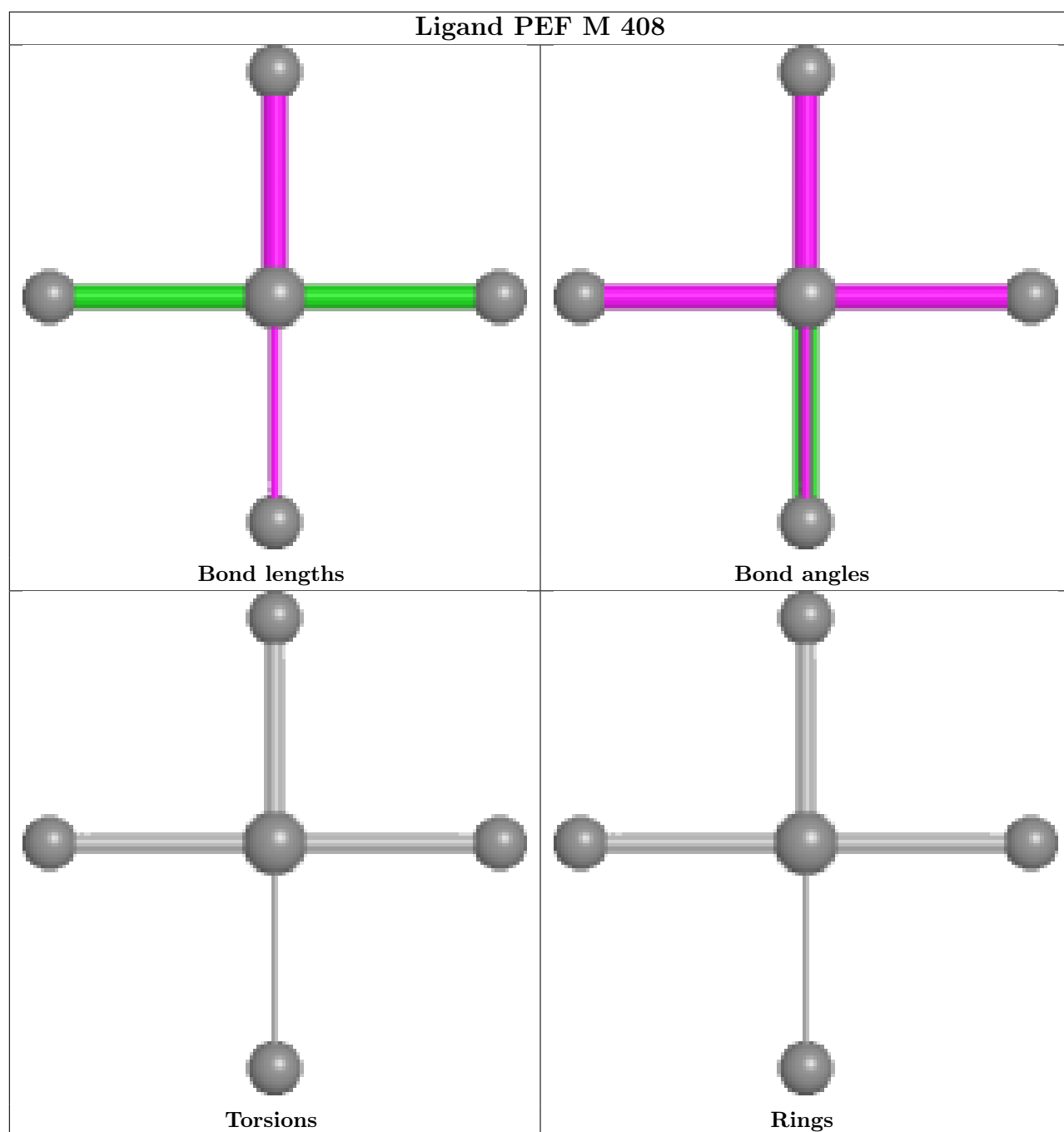


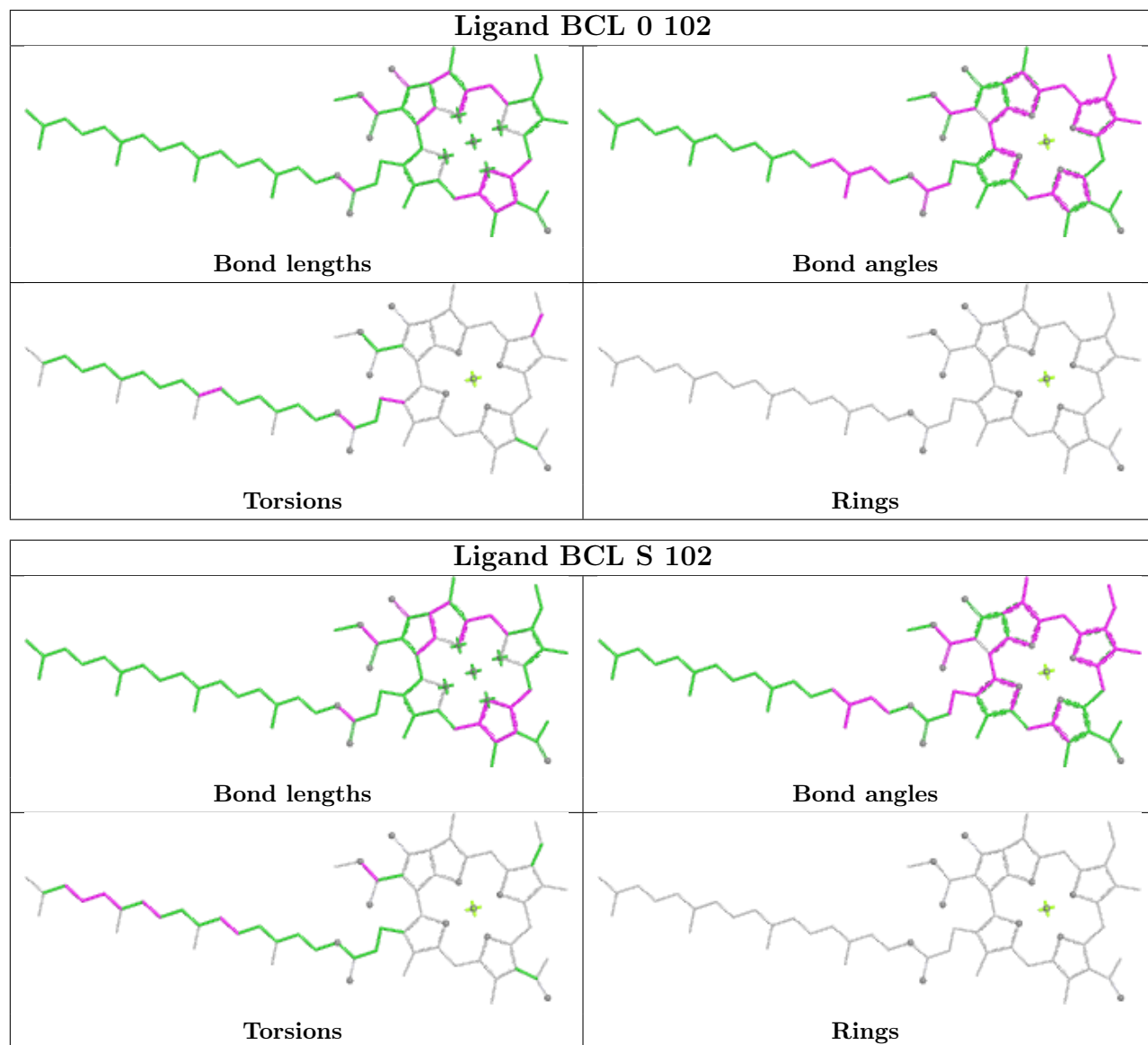


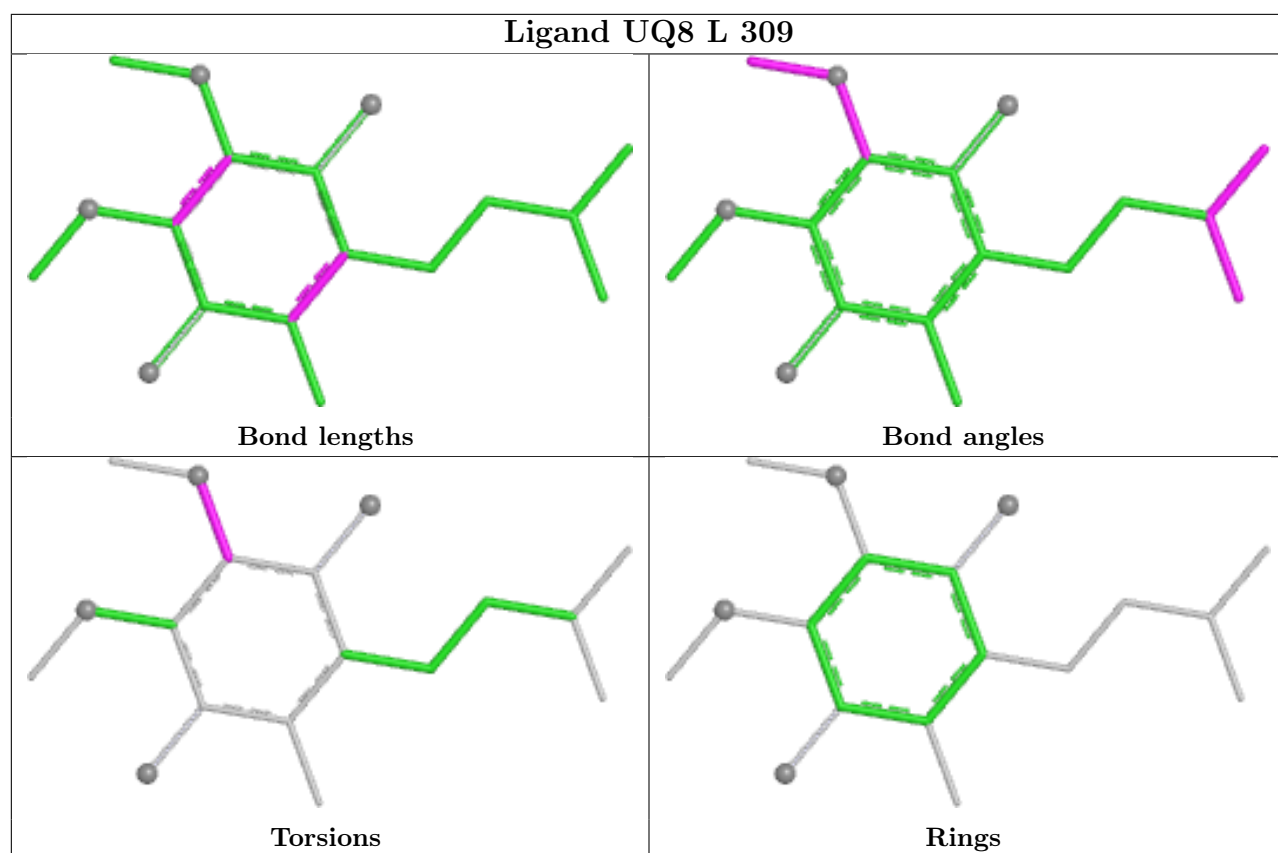




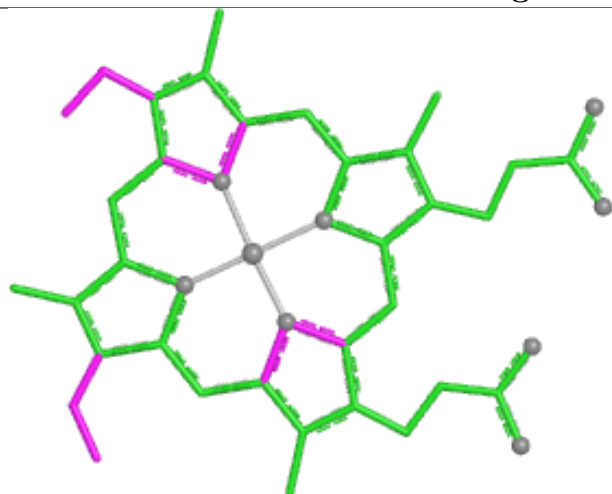




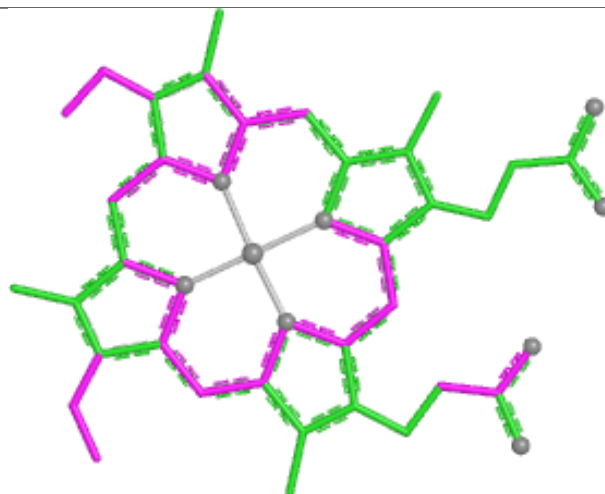




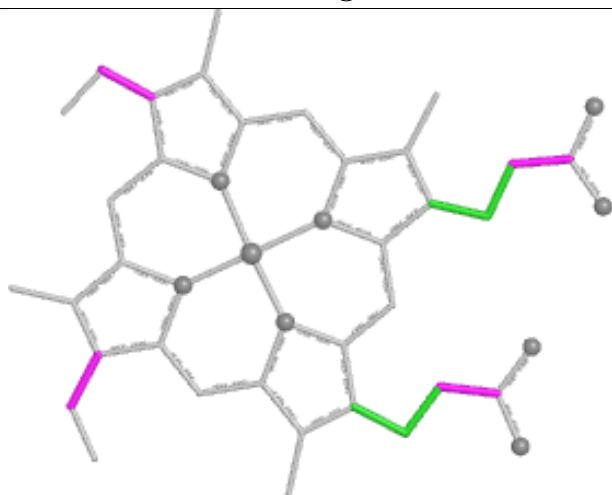
Ligand HEC C 502



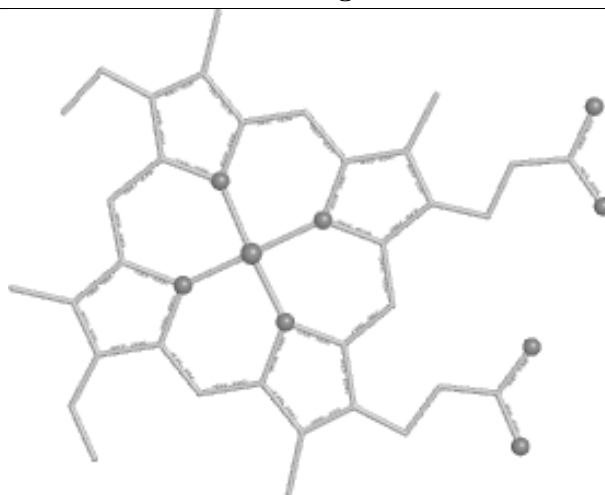
Bond lengths



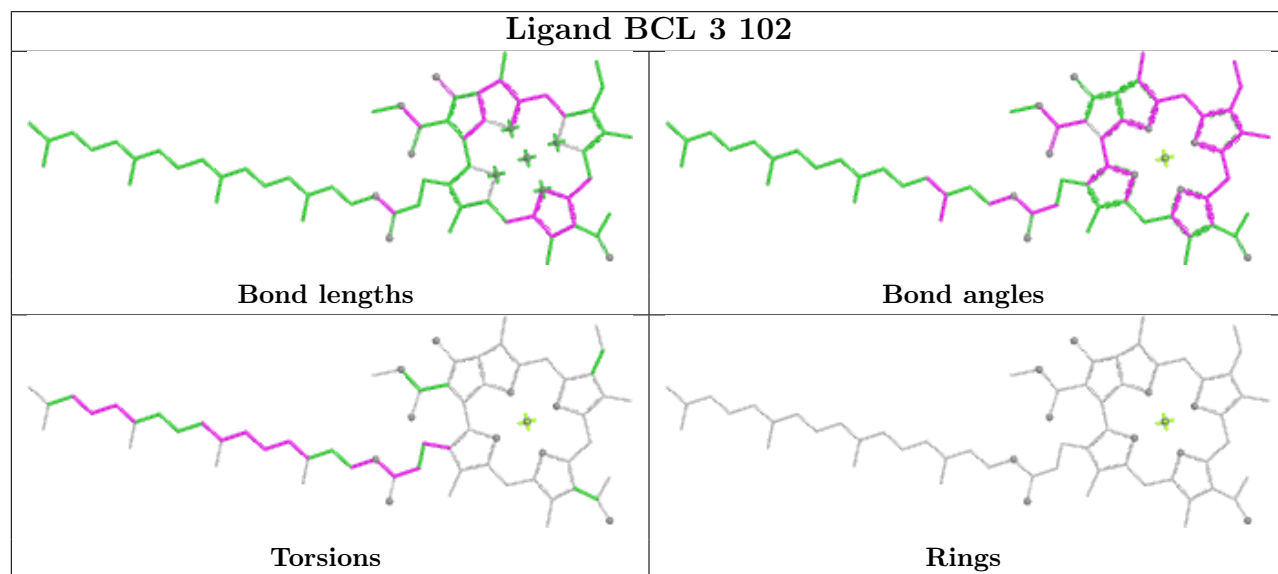
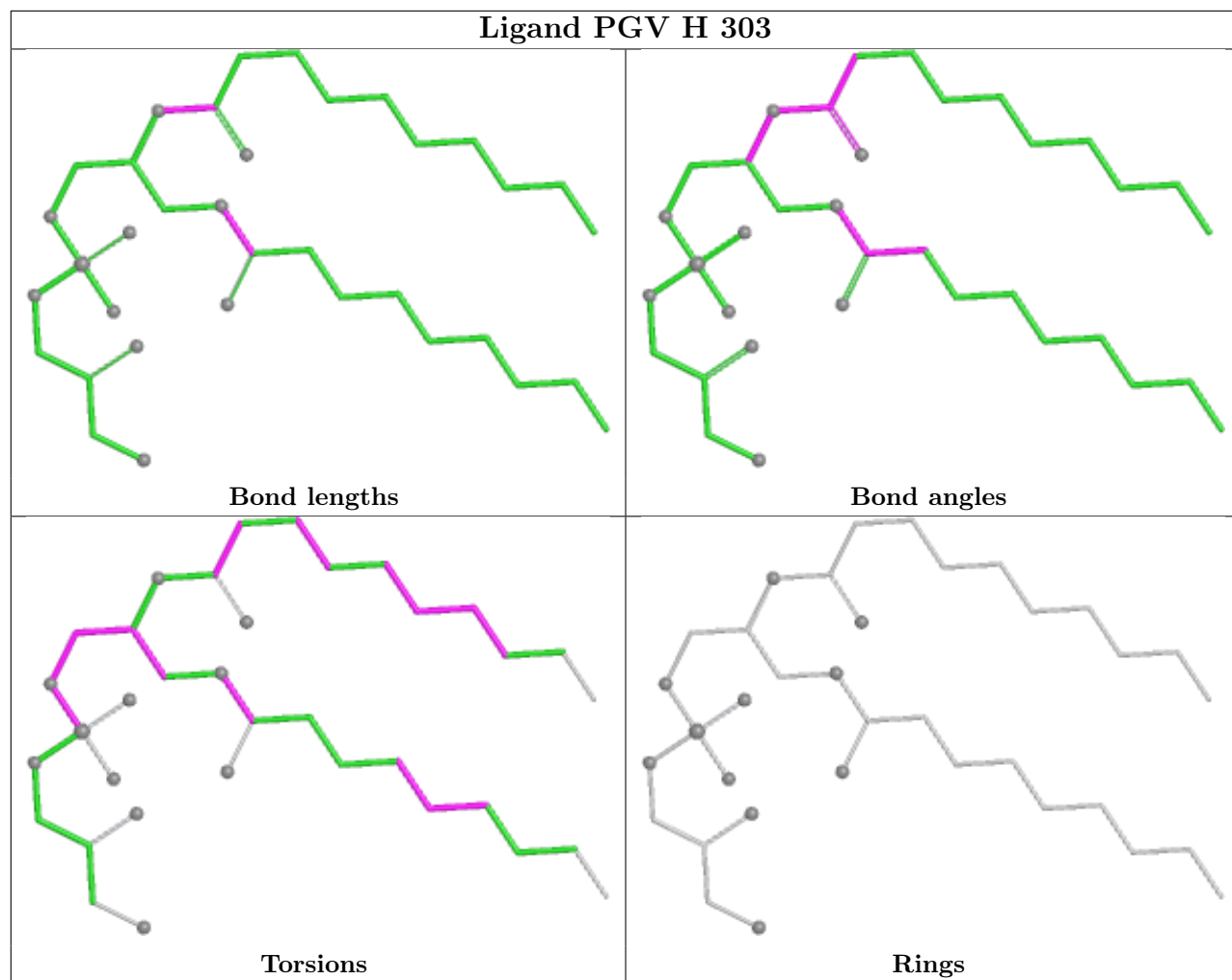
Bond angles

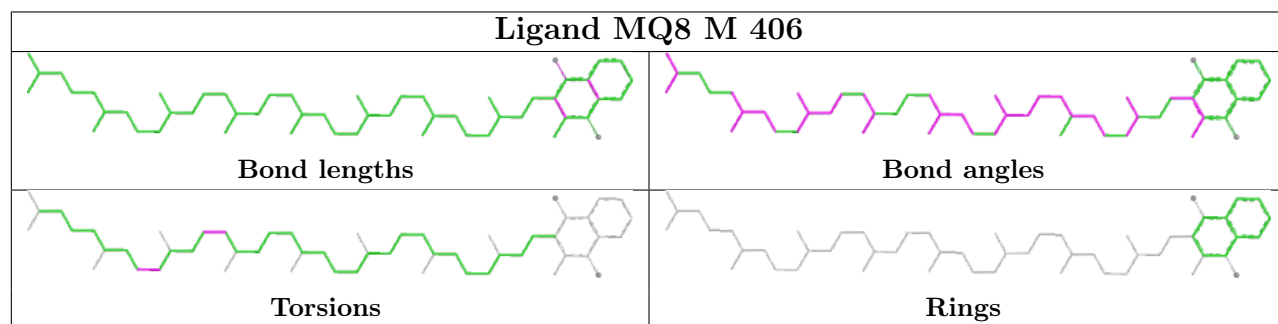
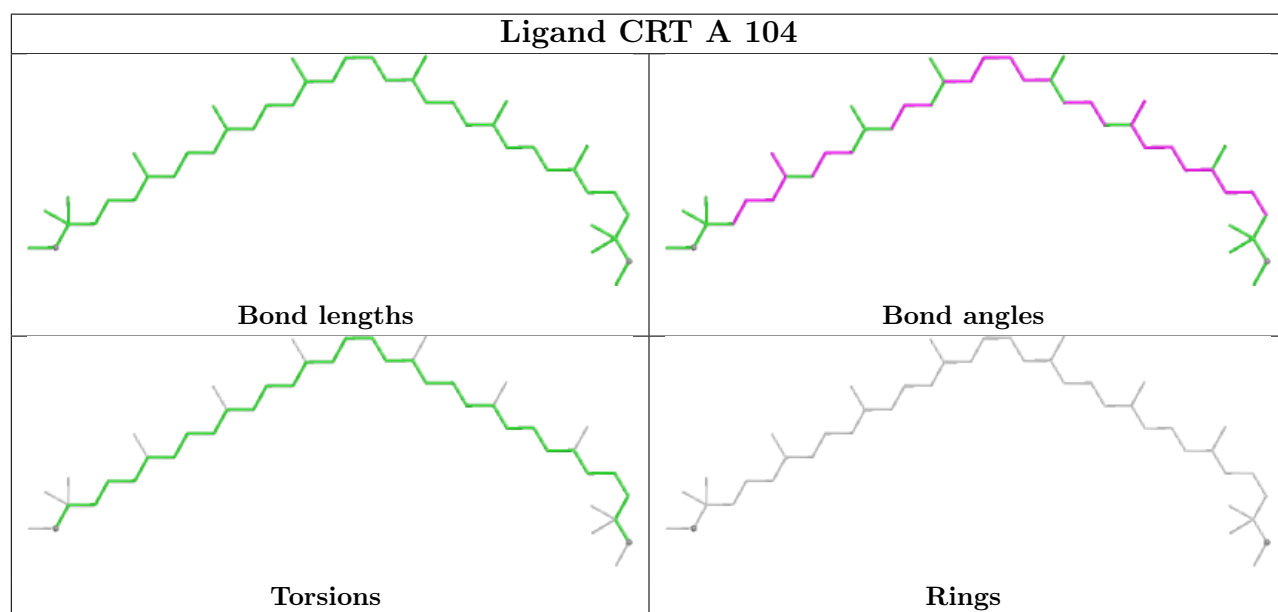
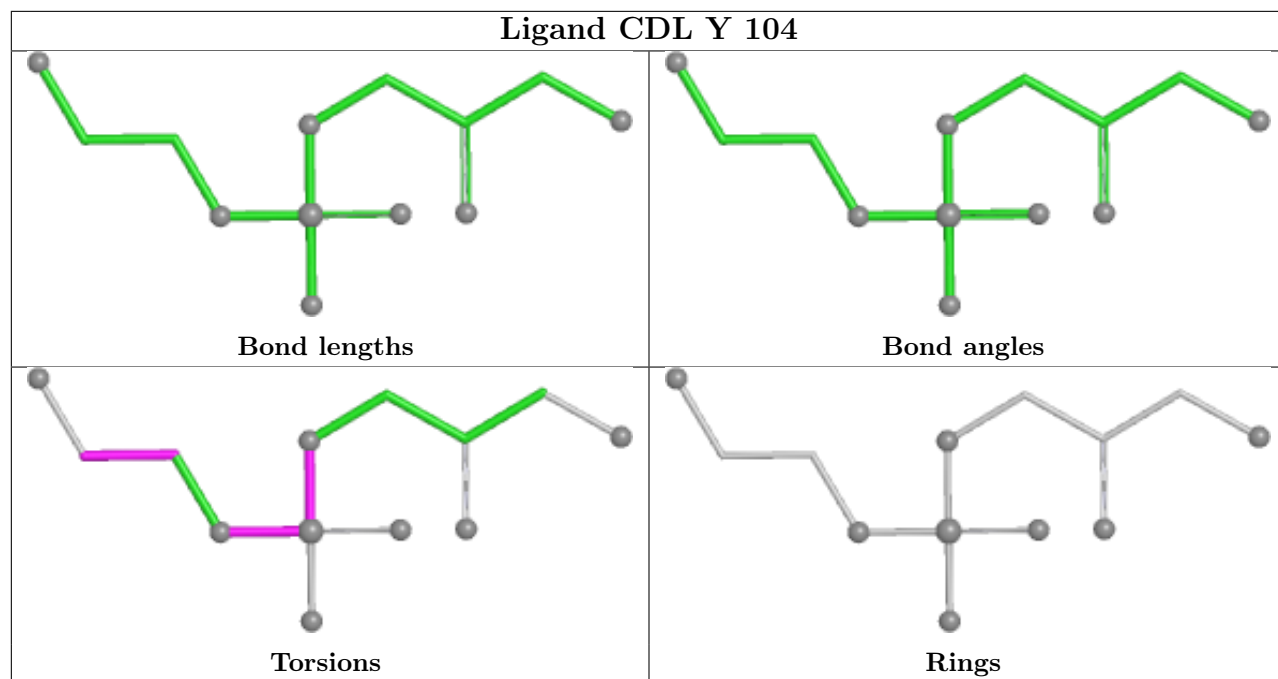


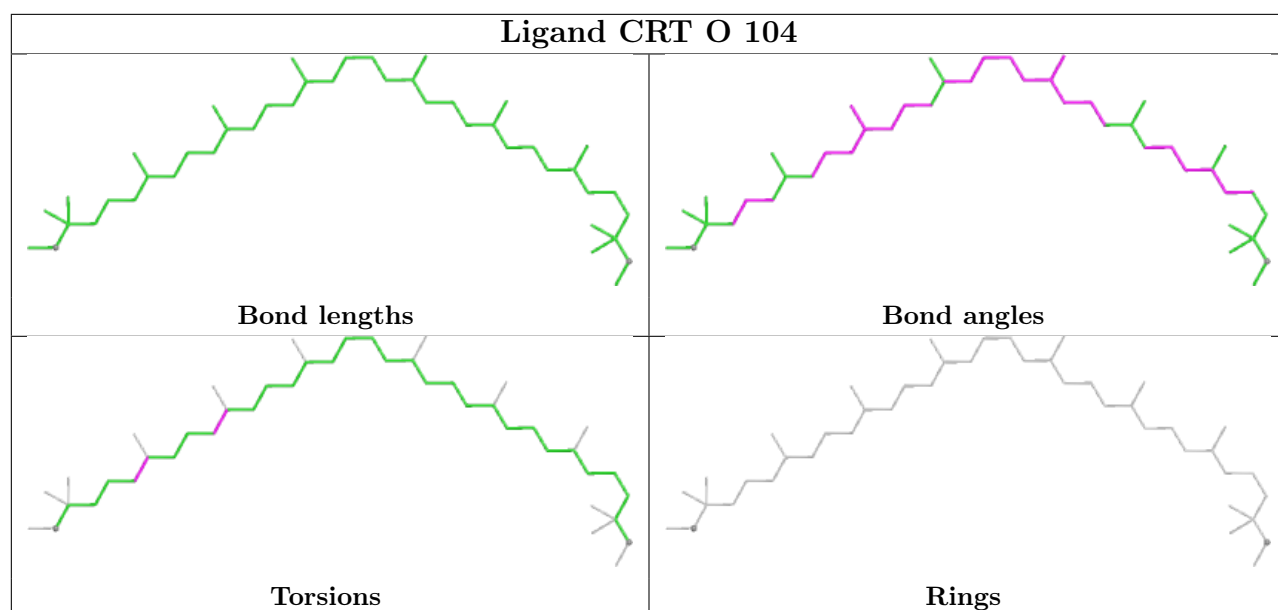
Torsions

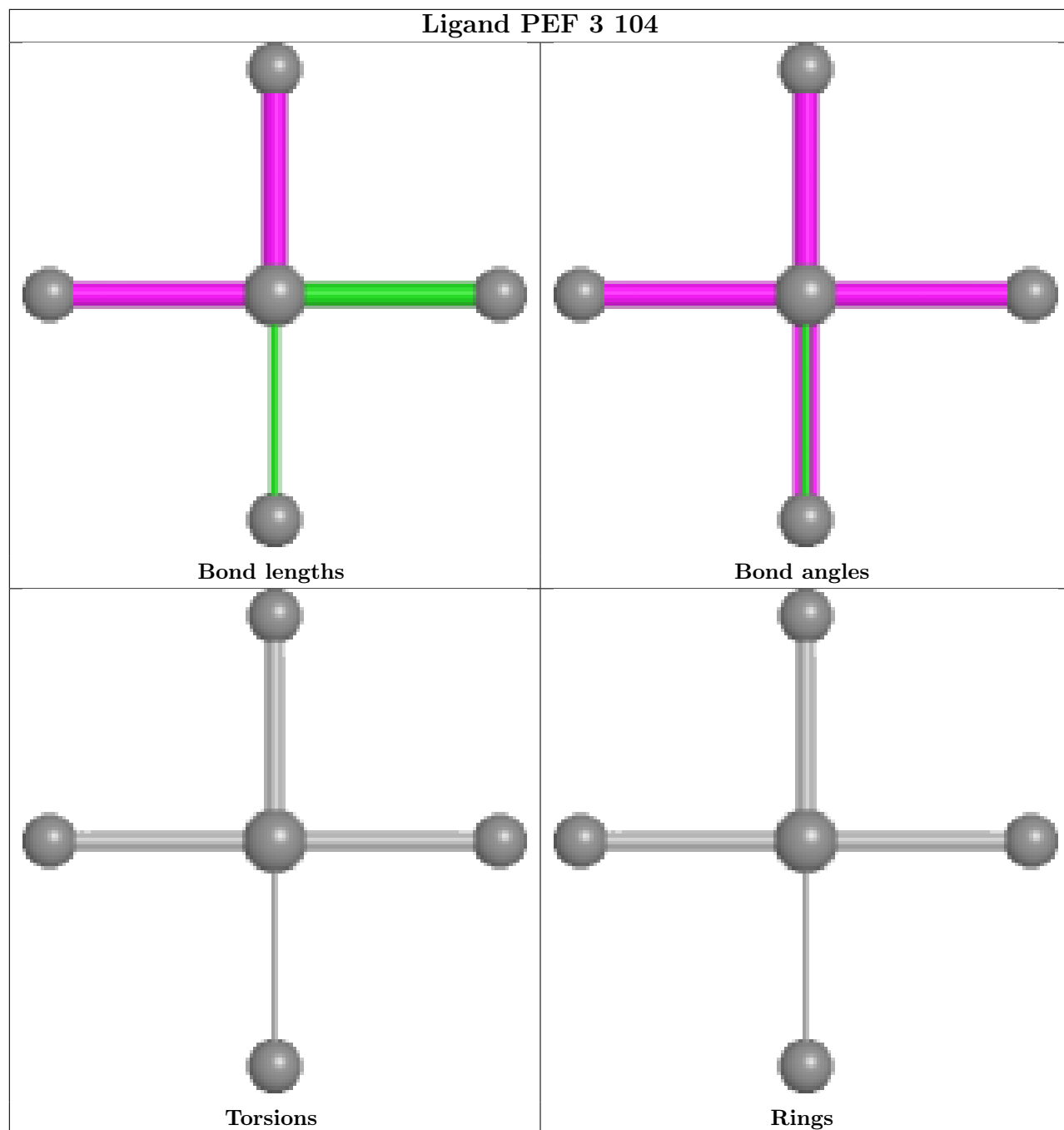


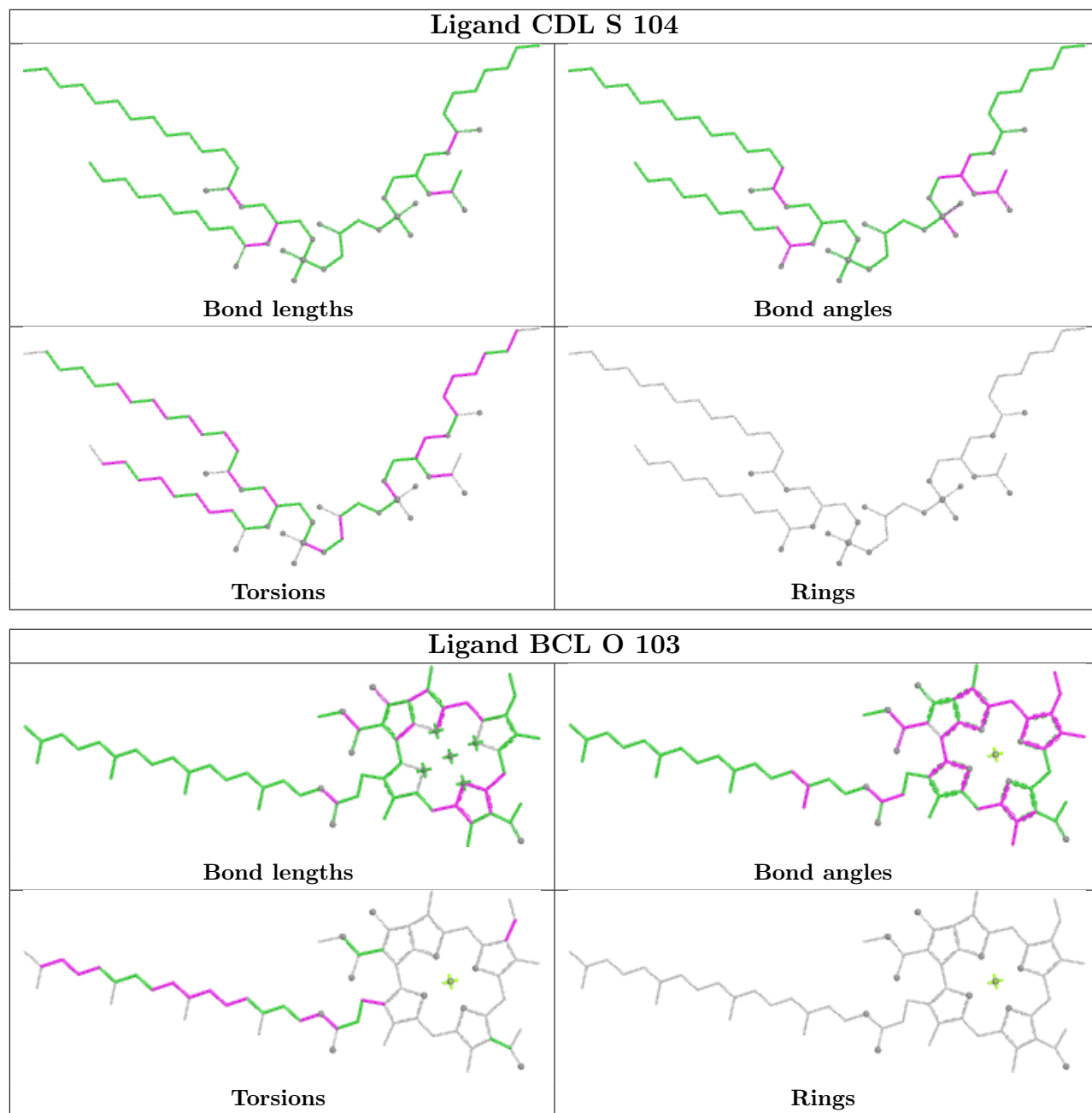
Rings

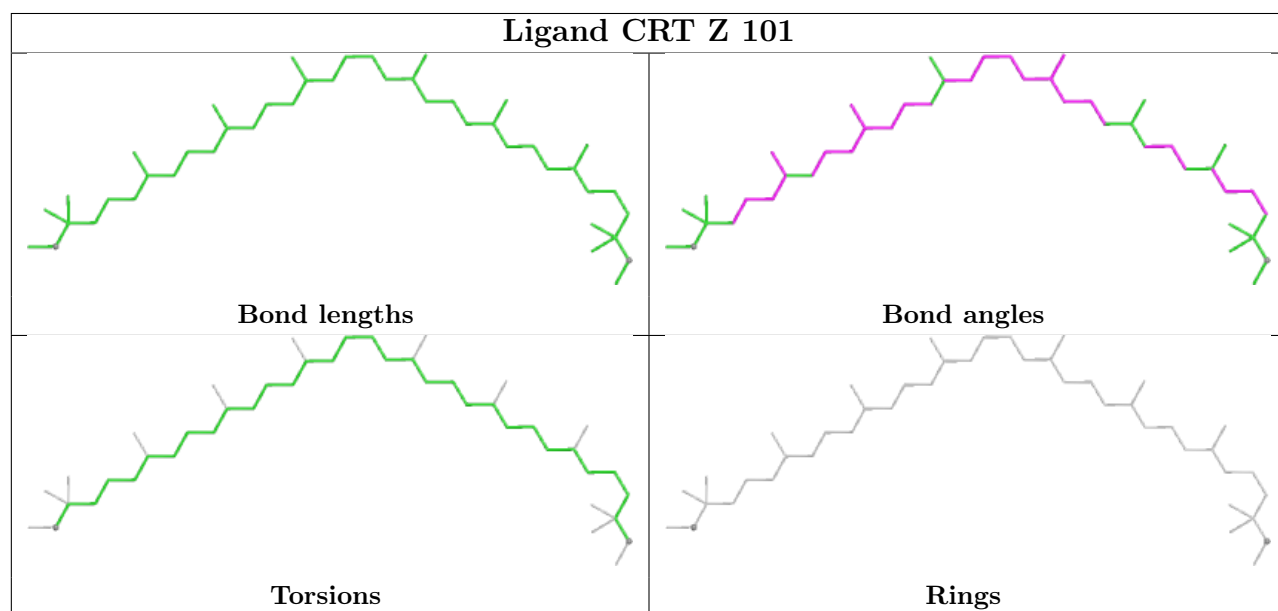
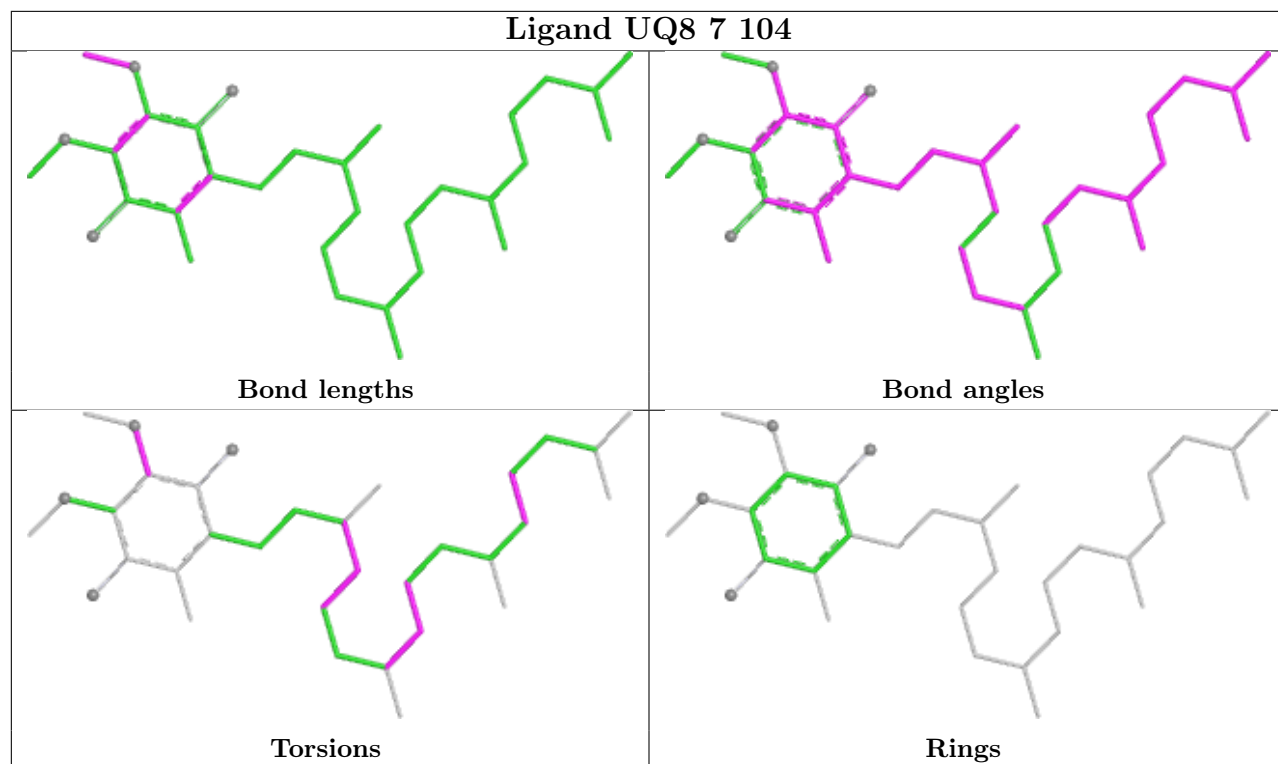


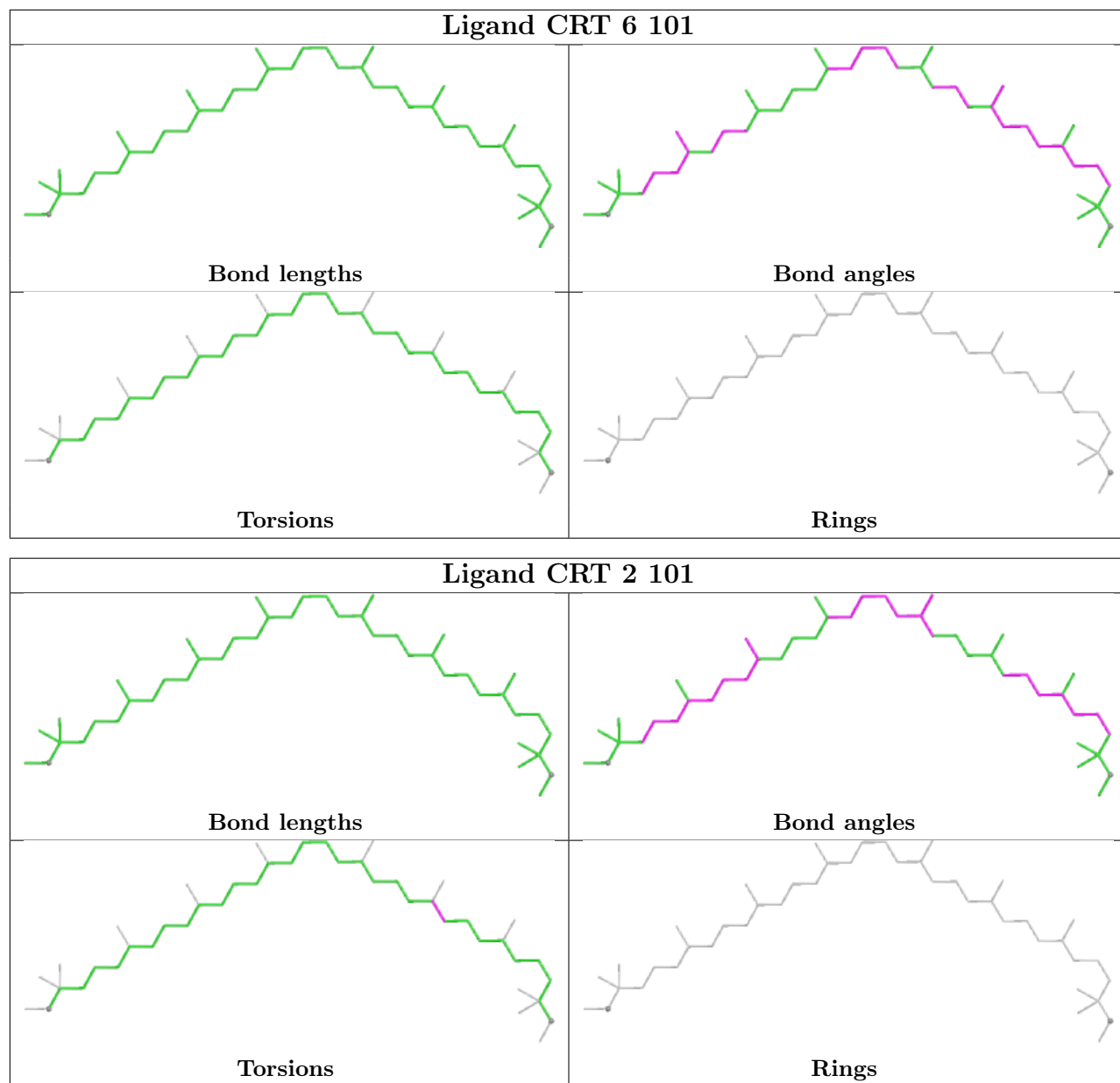


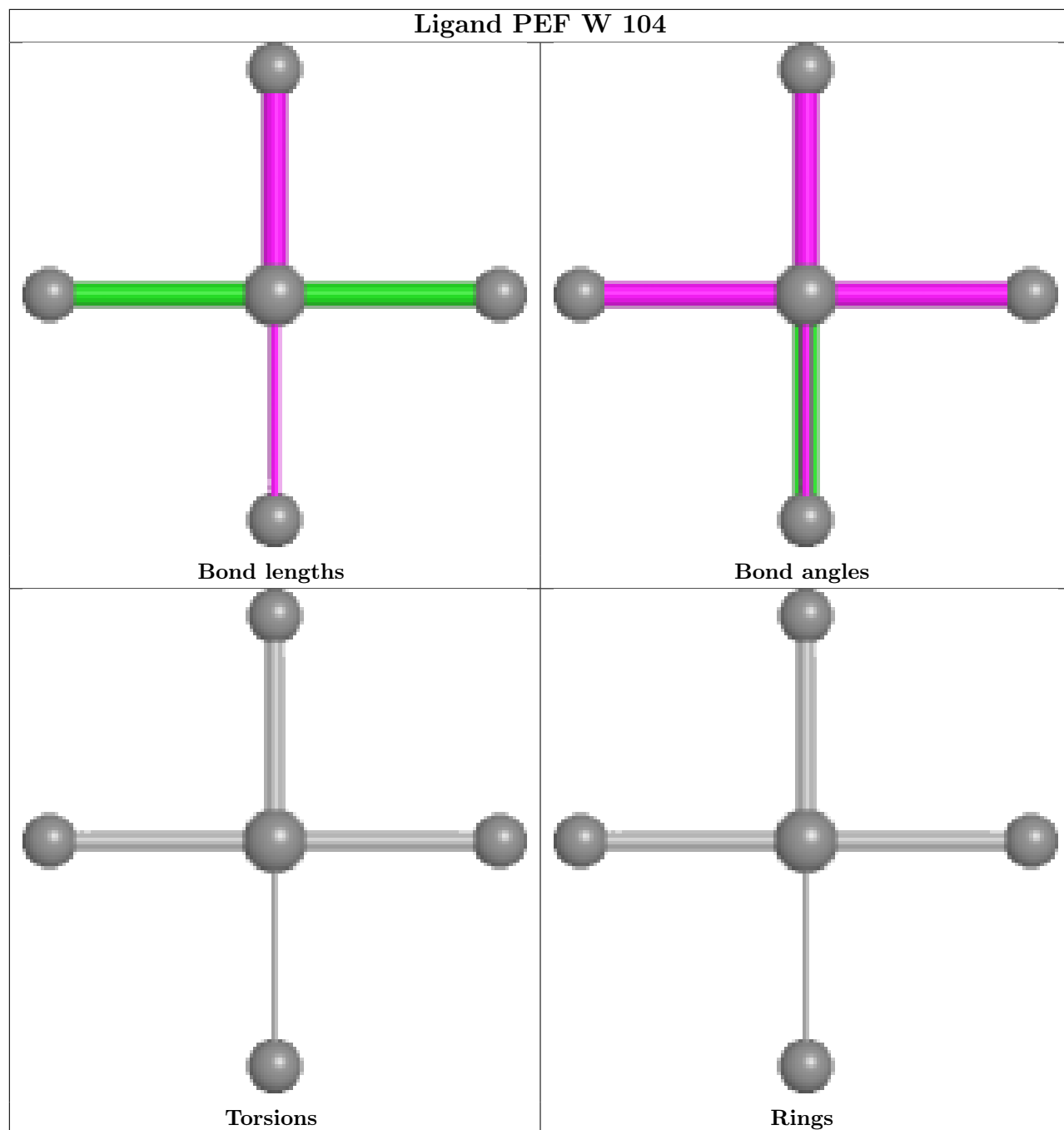


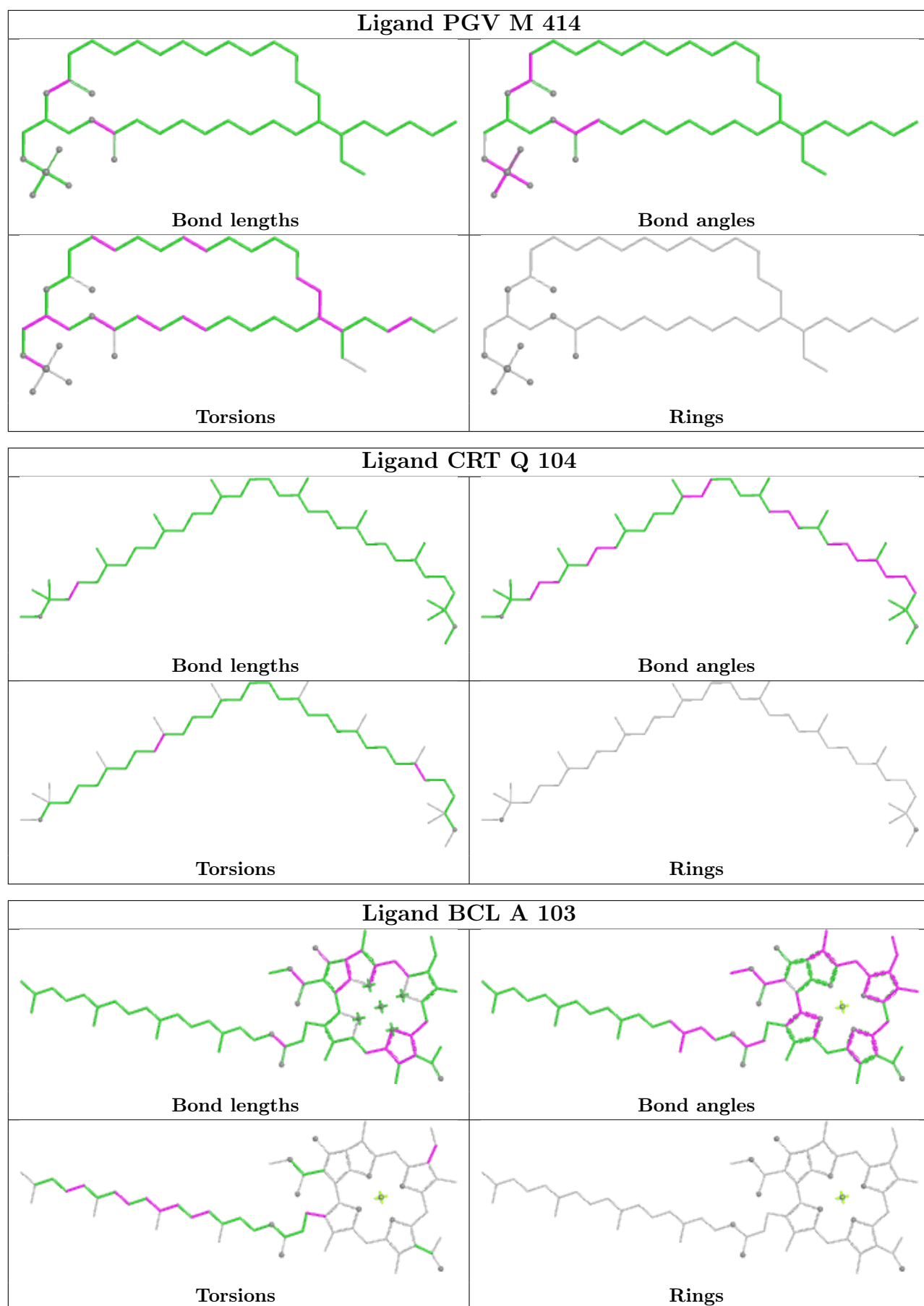


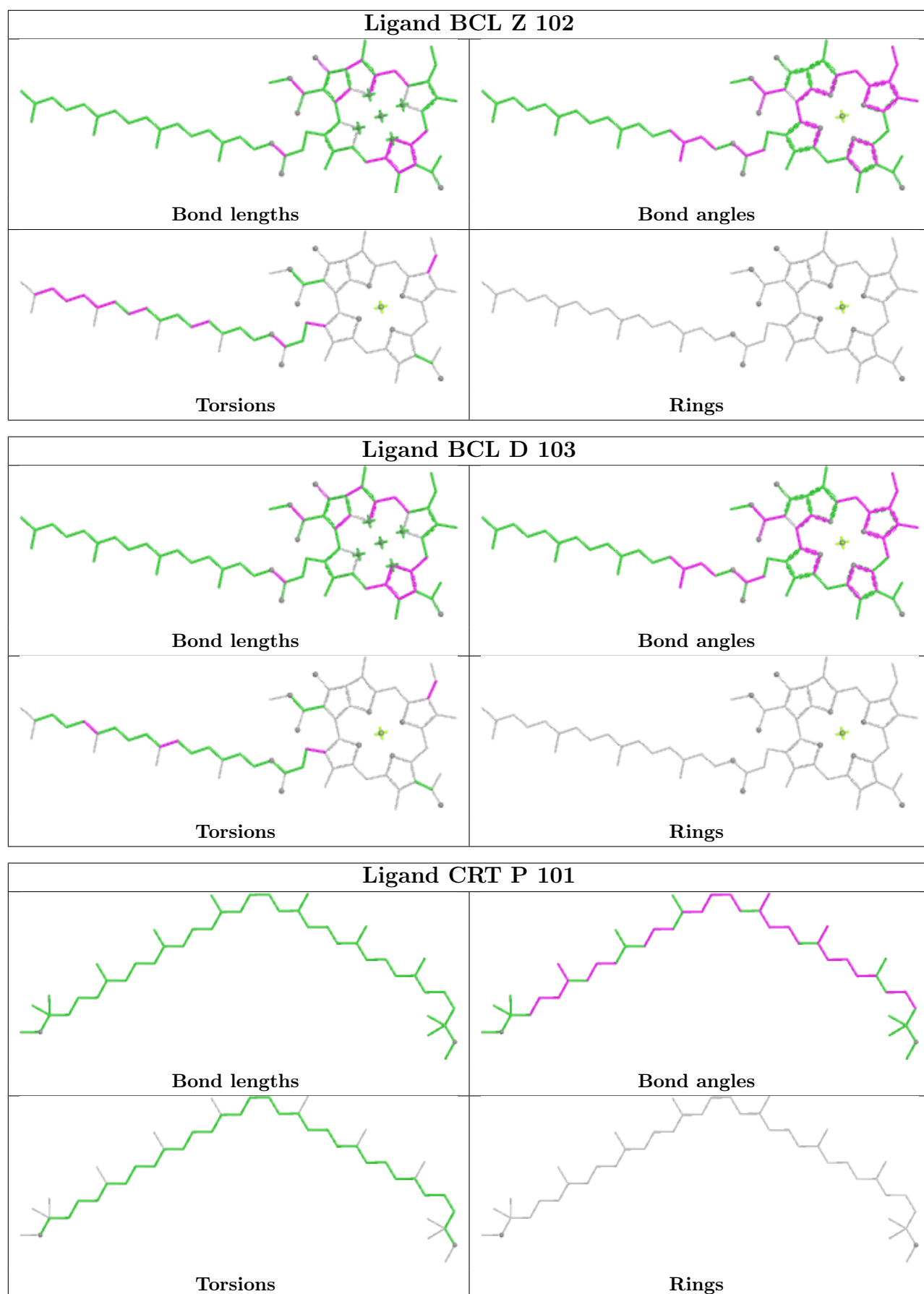


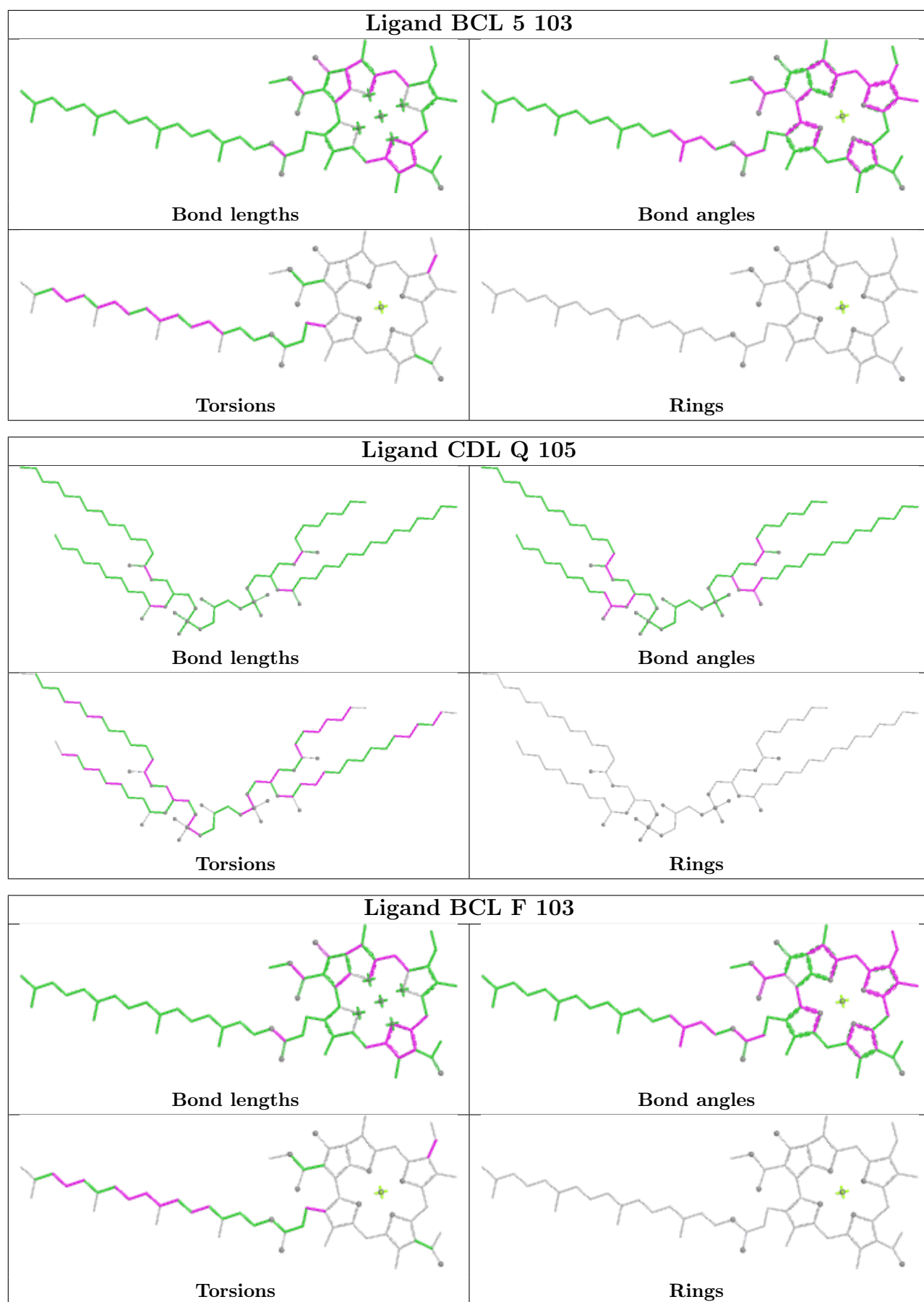




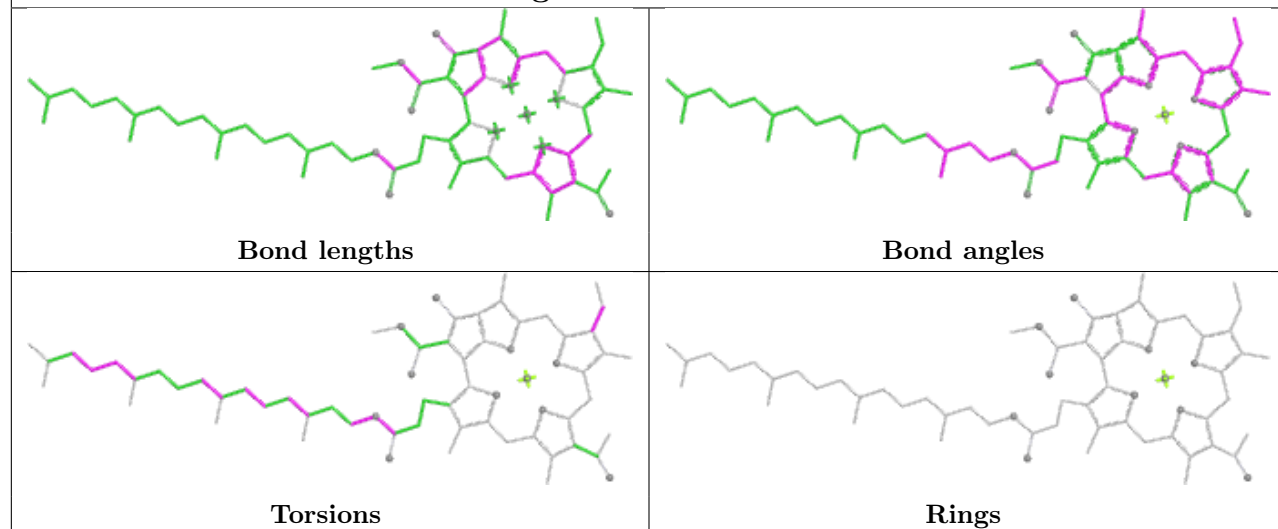




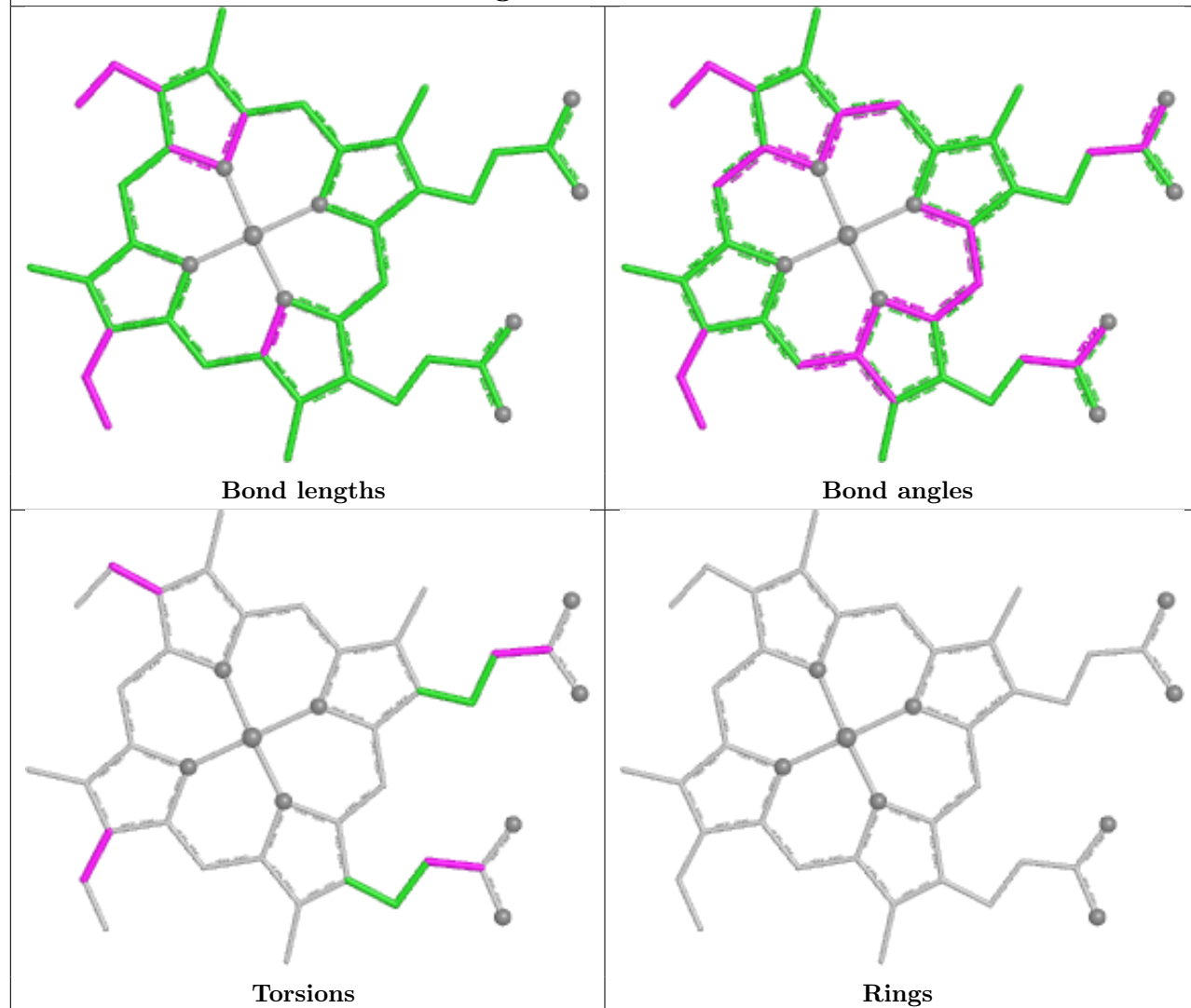


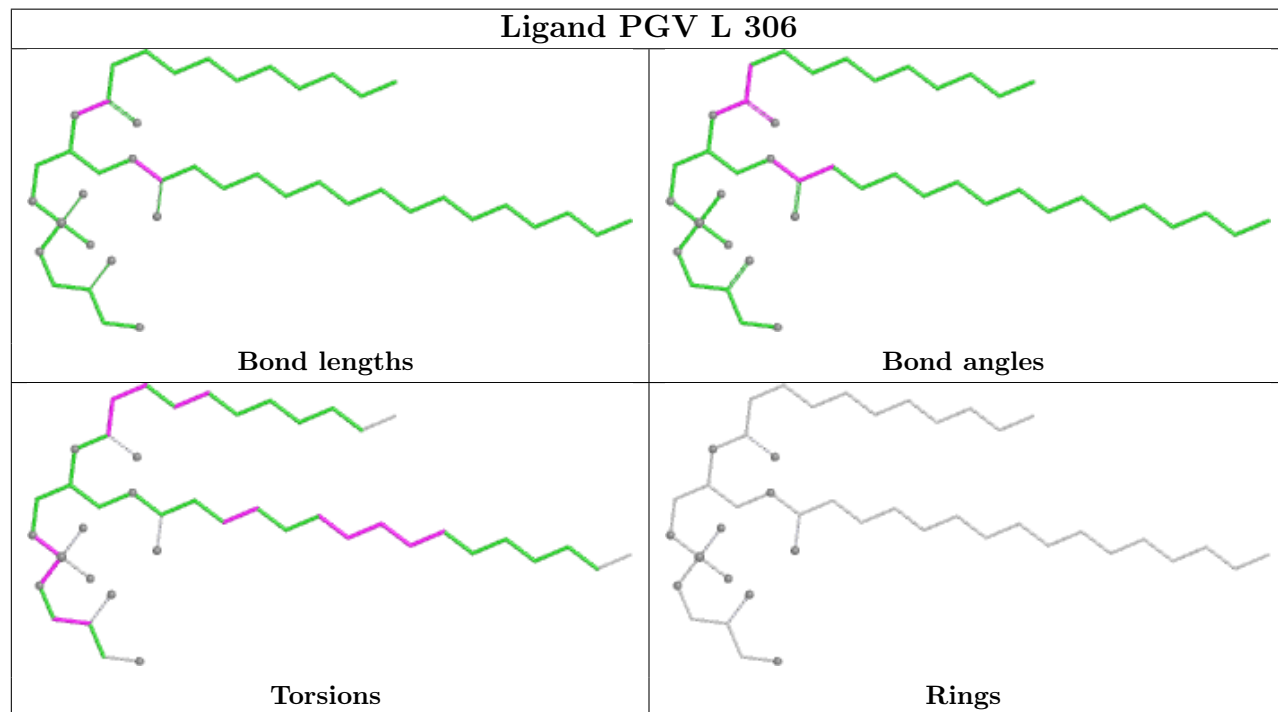
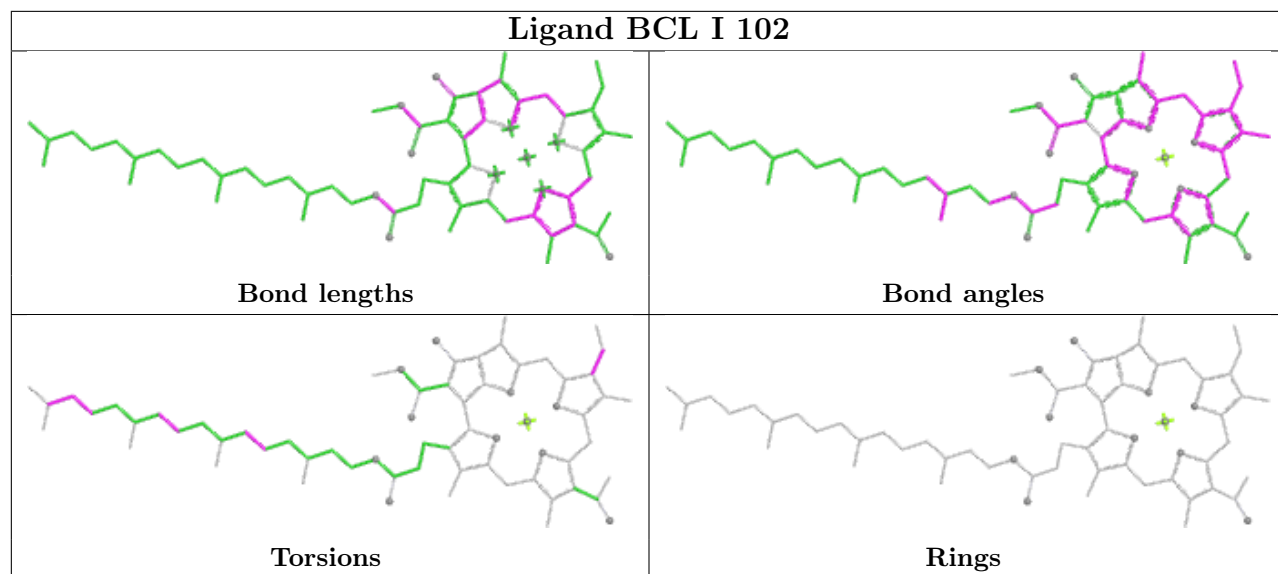


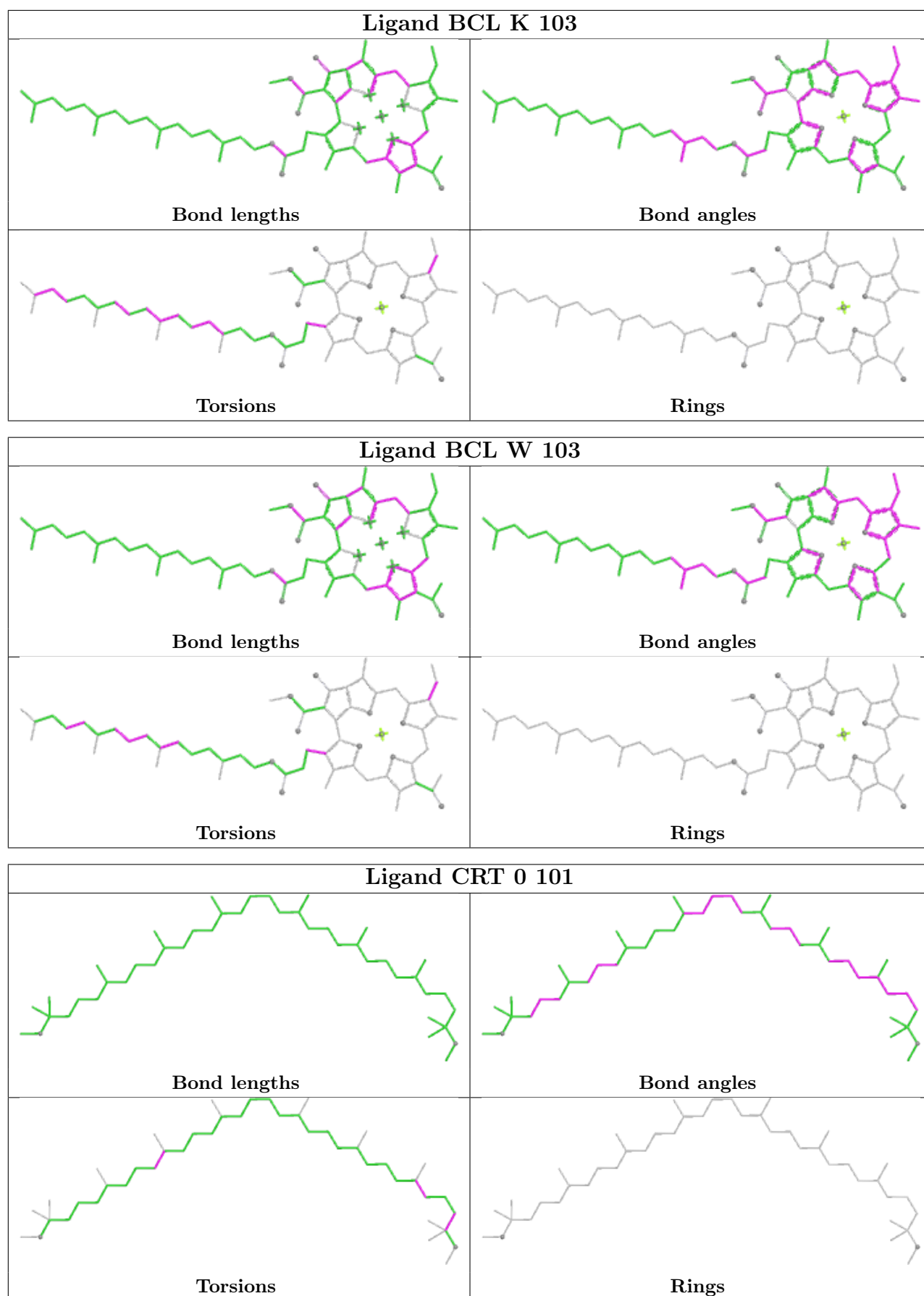
Ligand BCL K 102

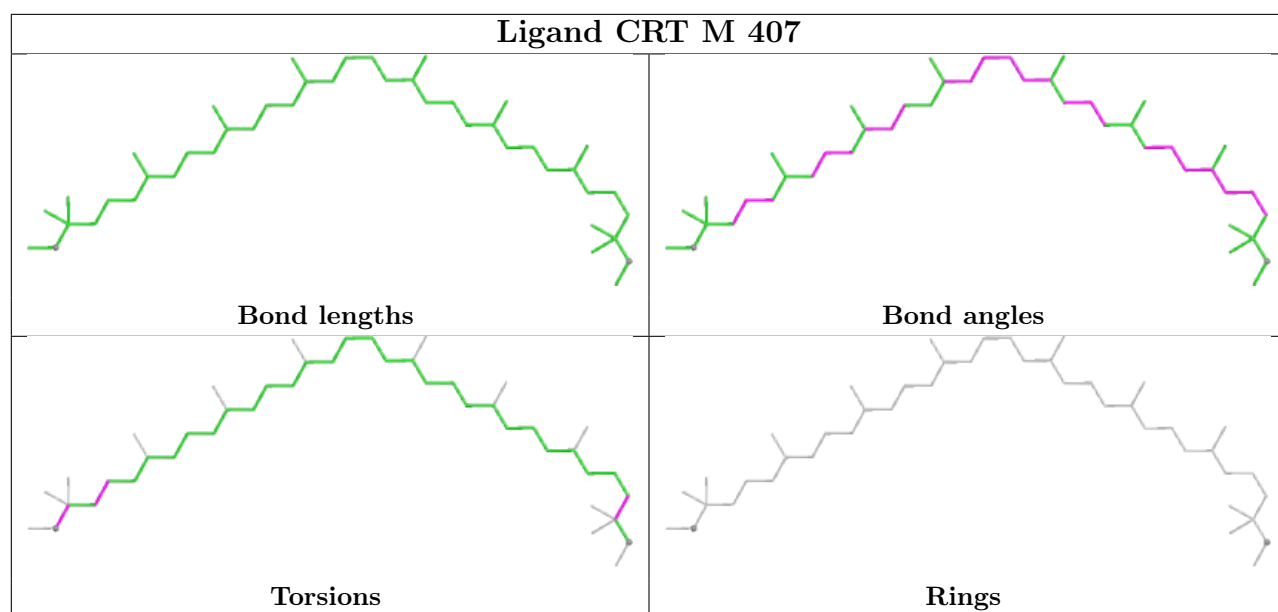


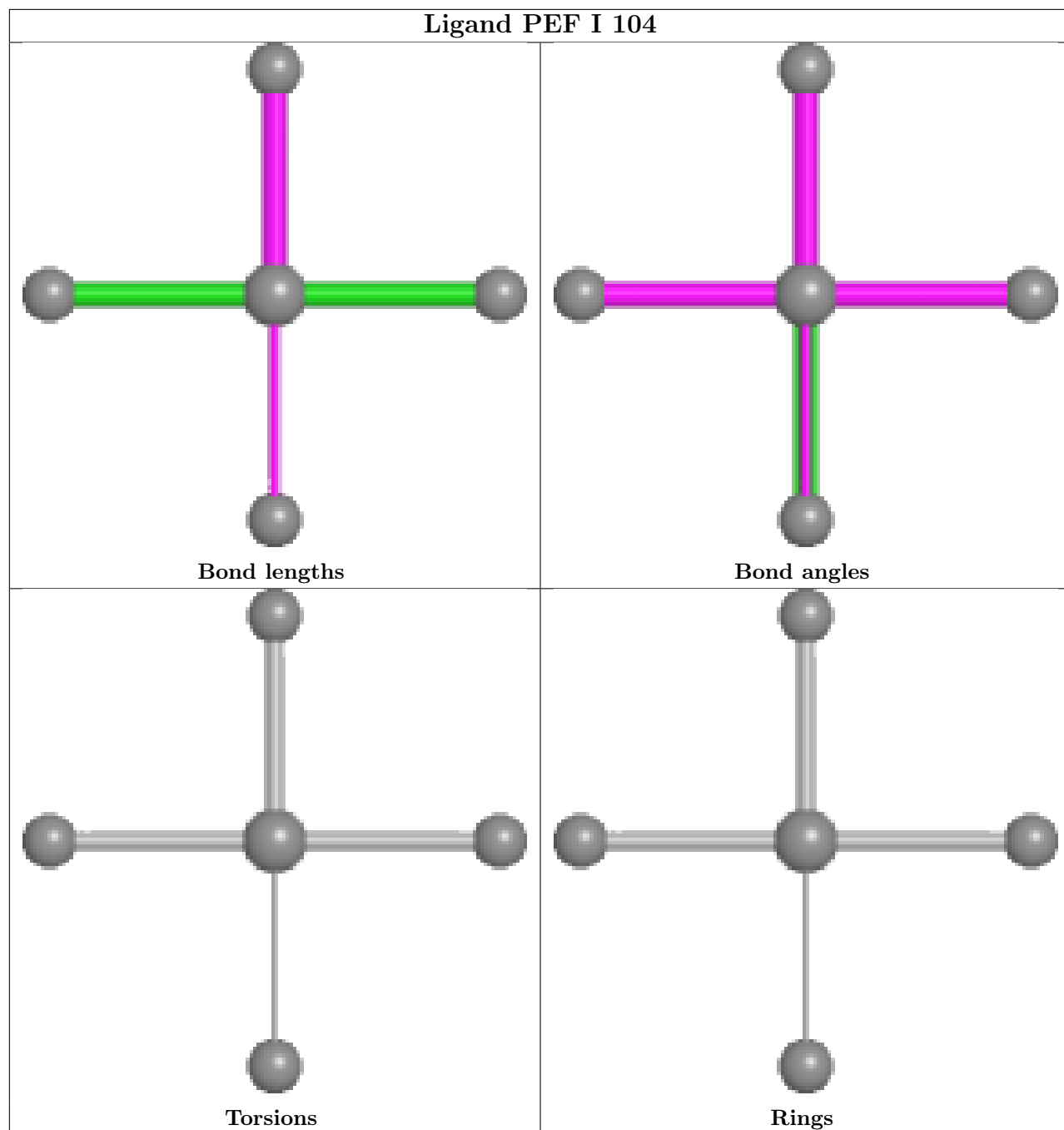
Ligand HEC C 504

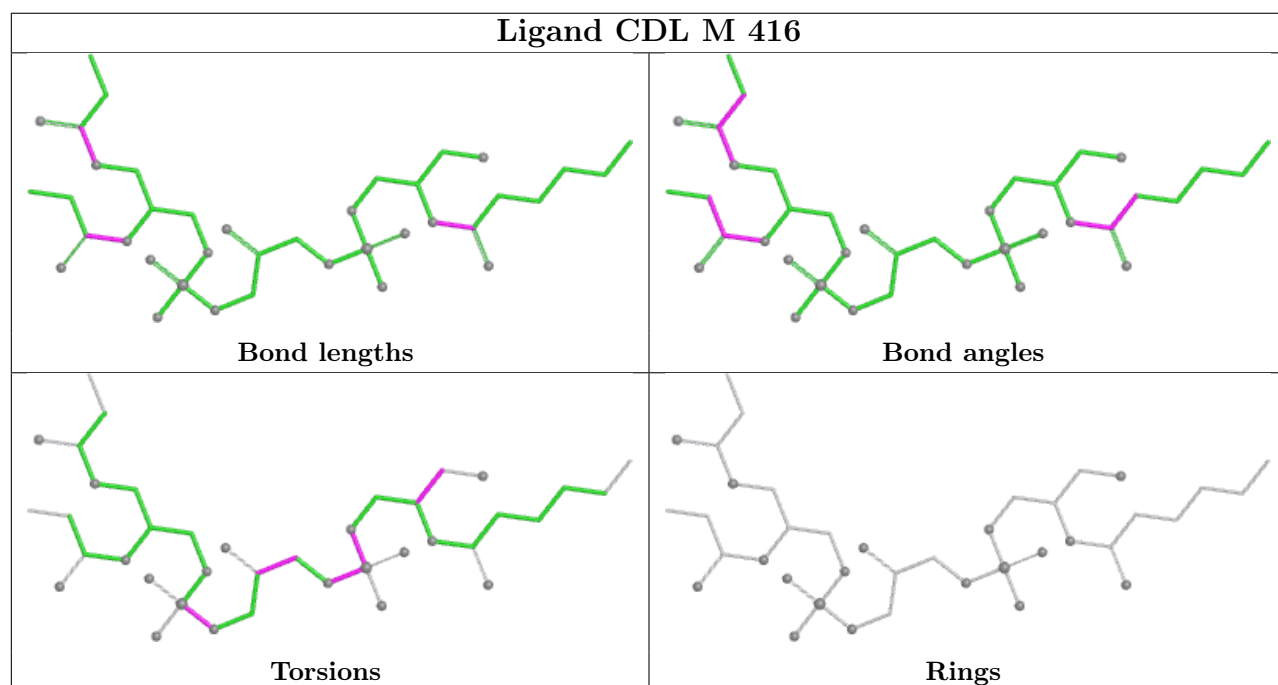
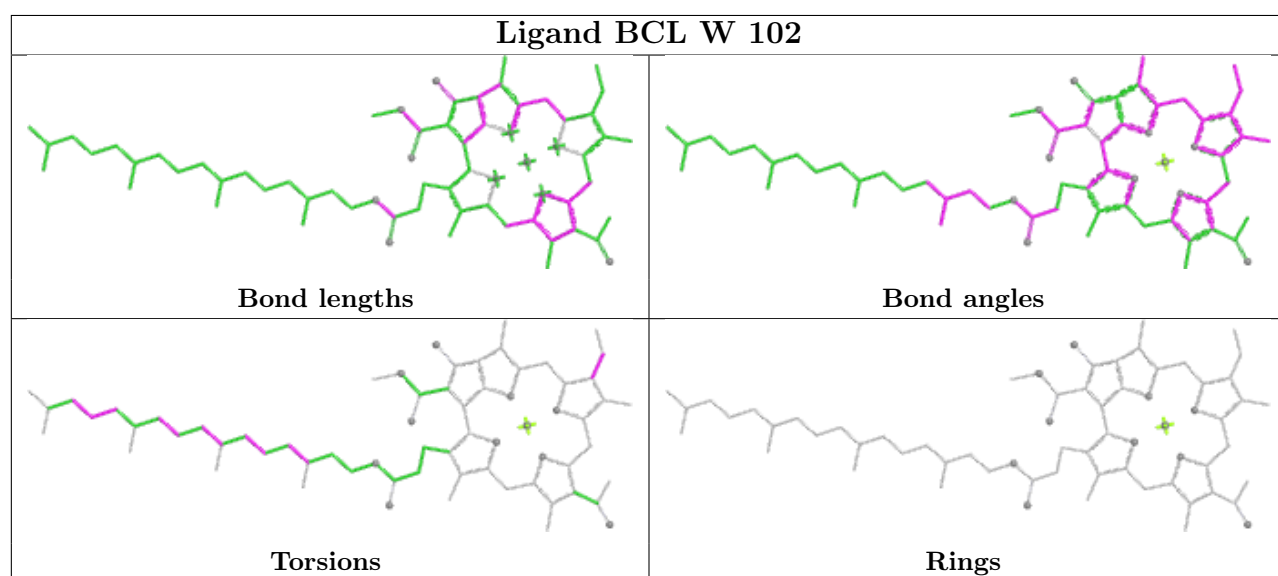
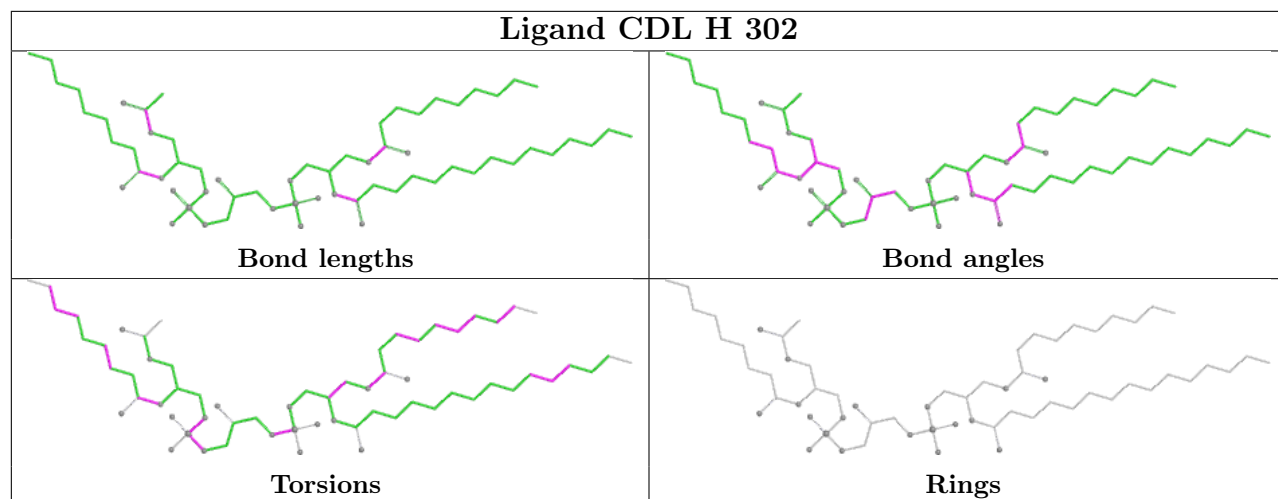


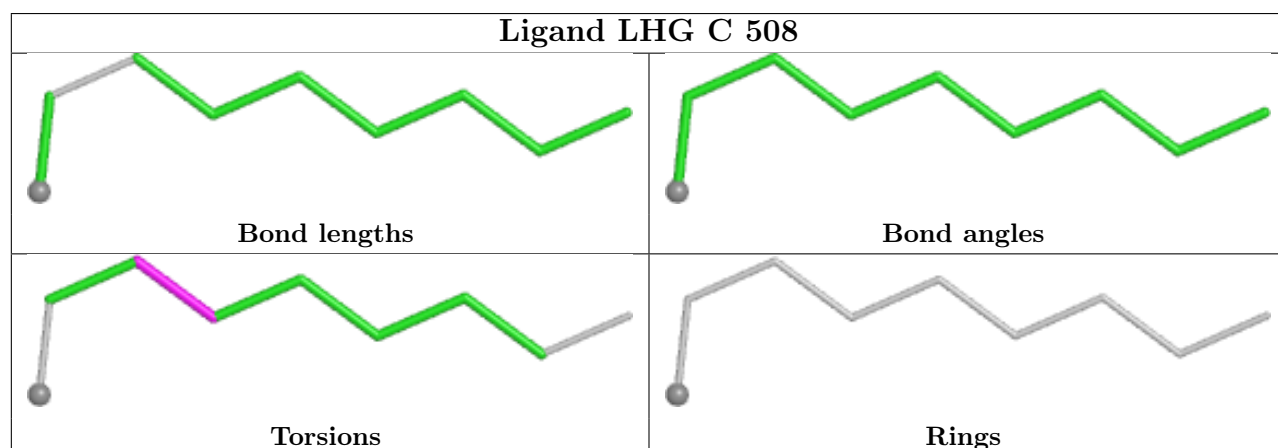
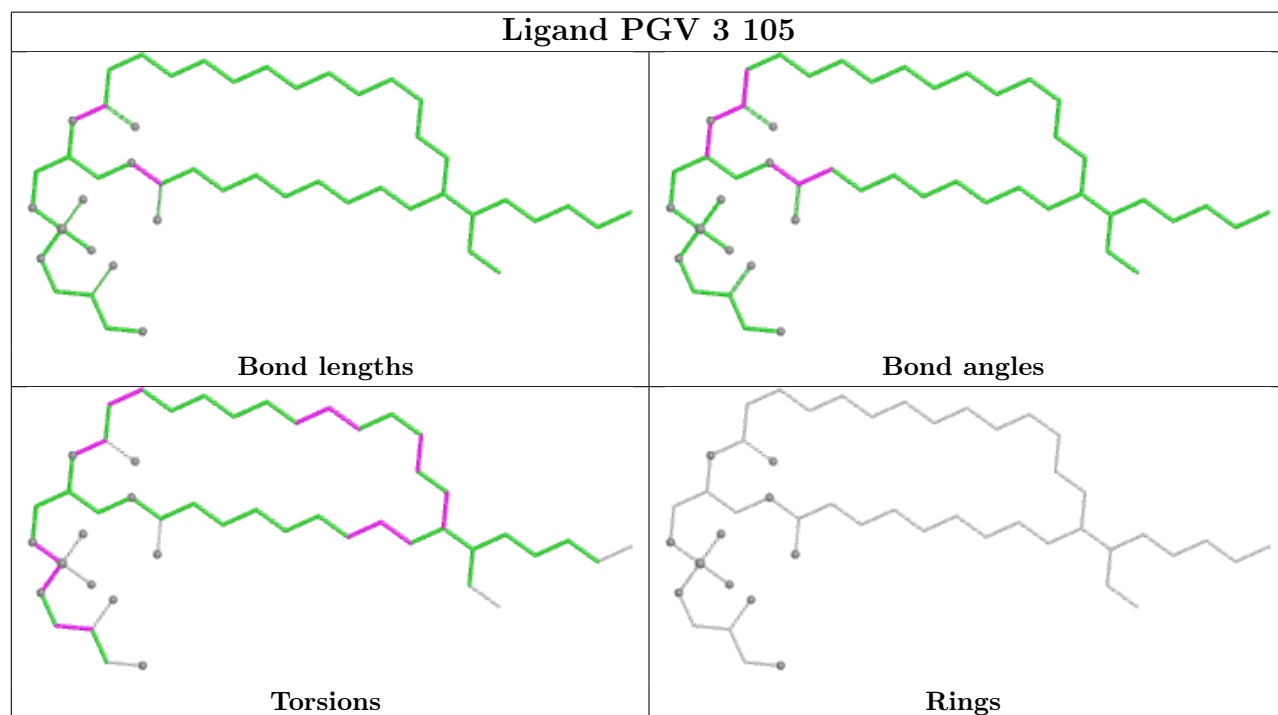
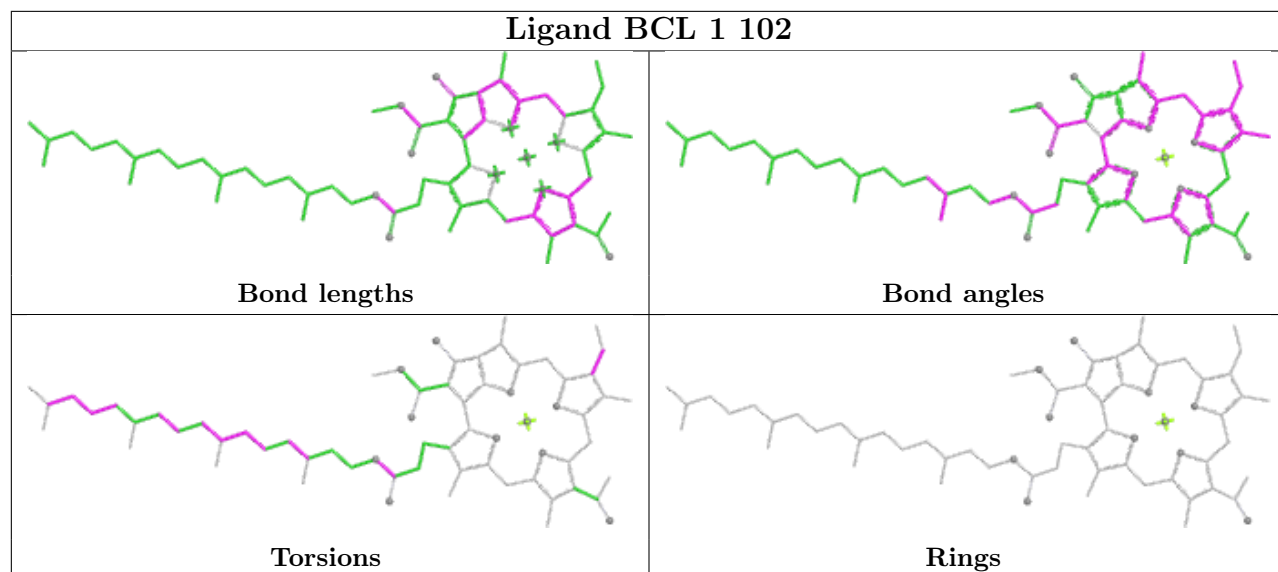


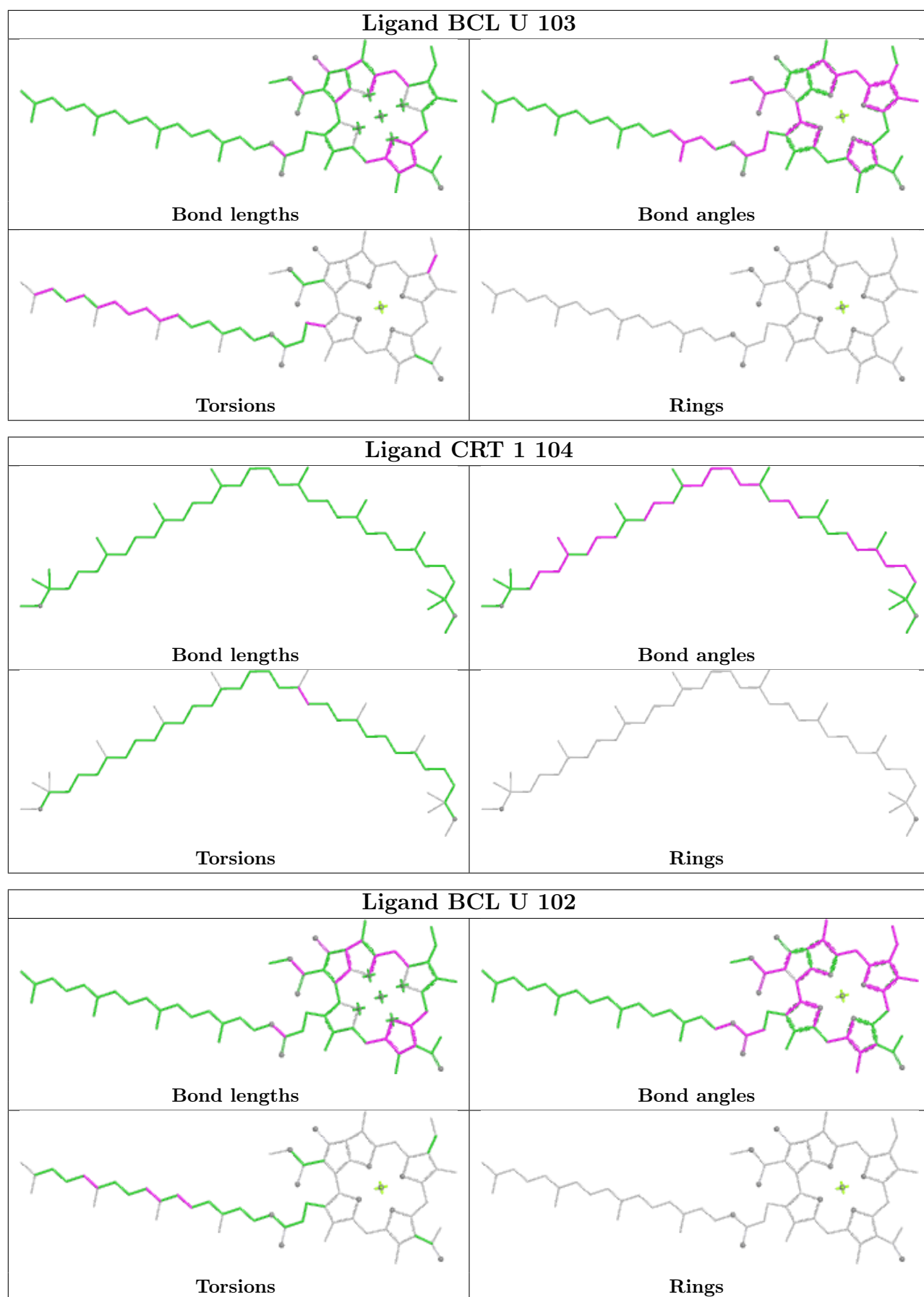


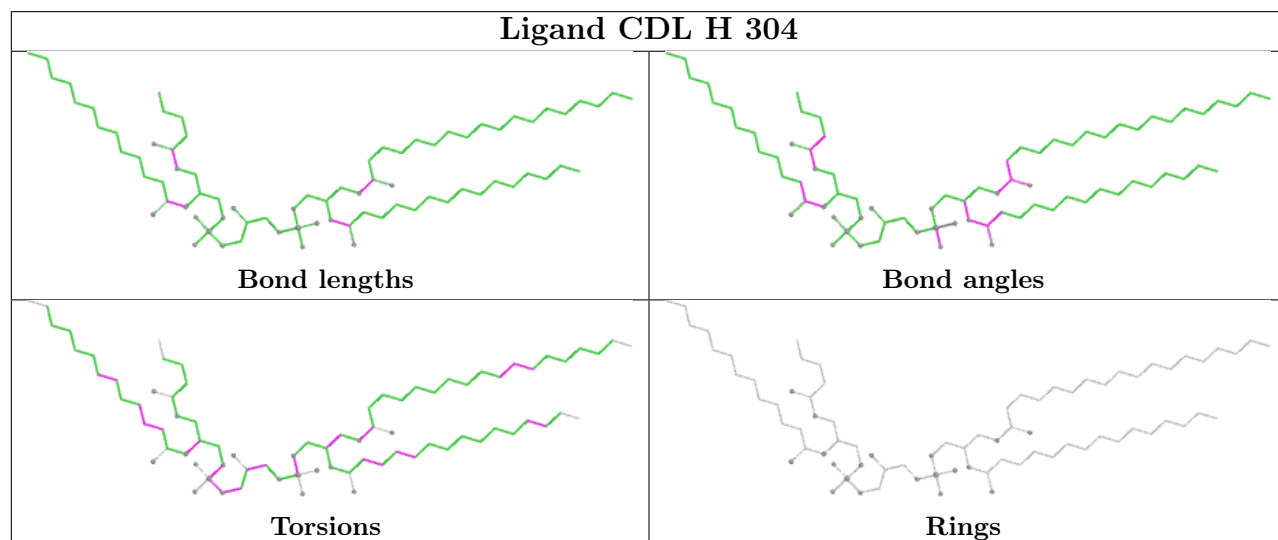
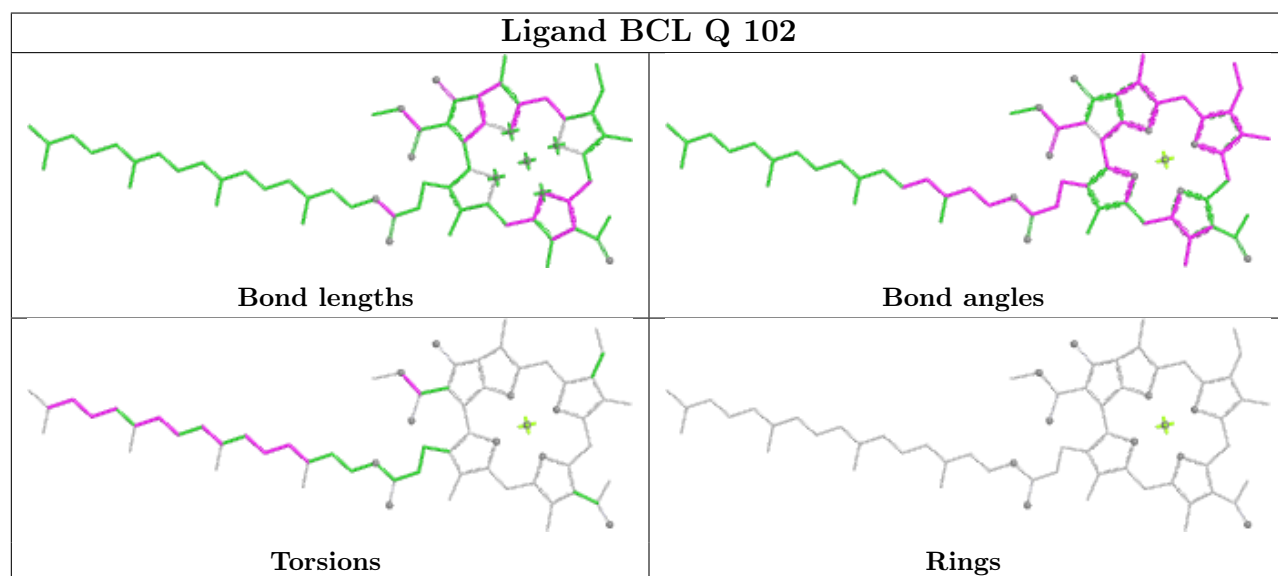
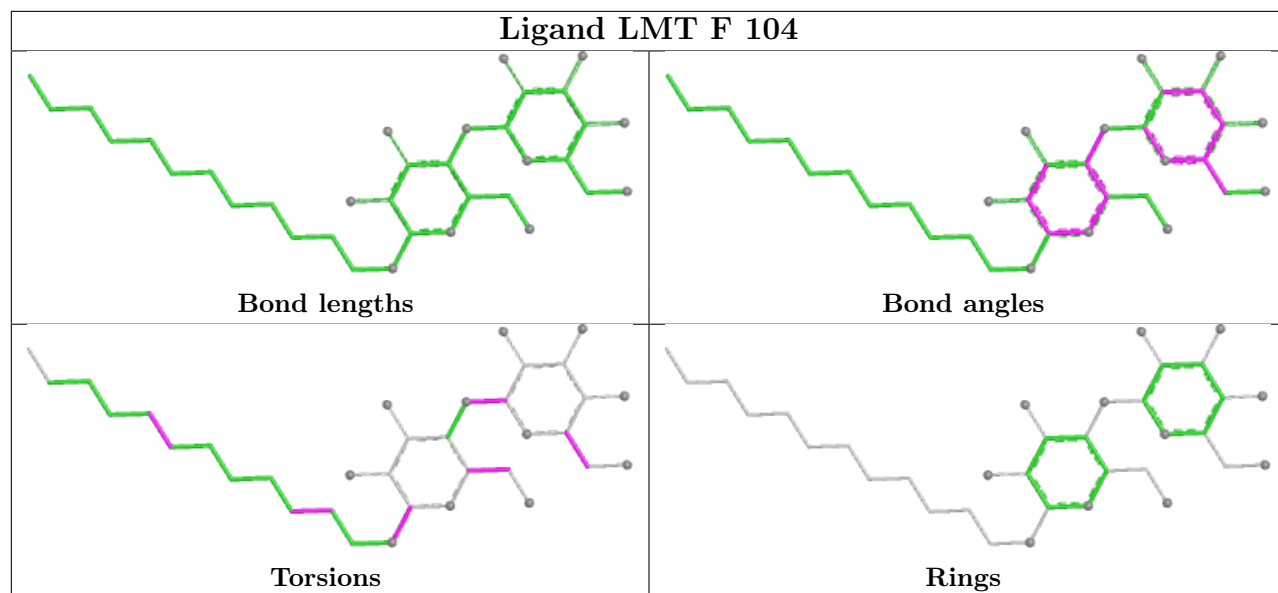


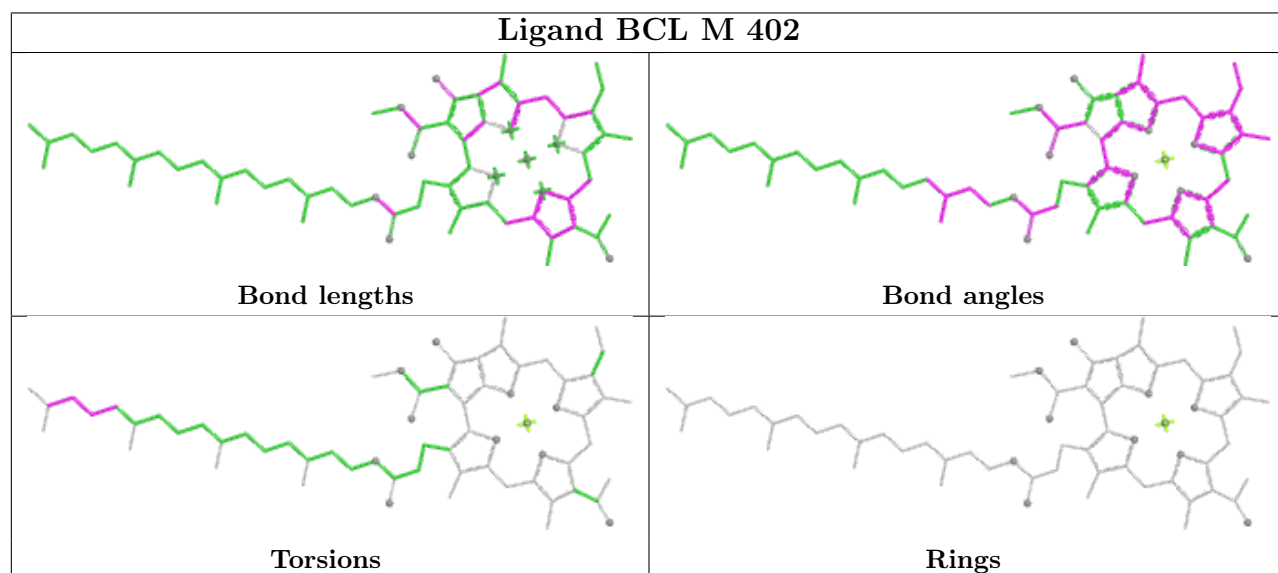
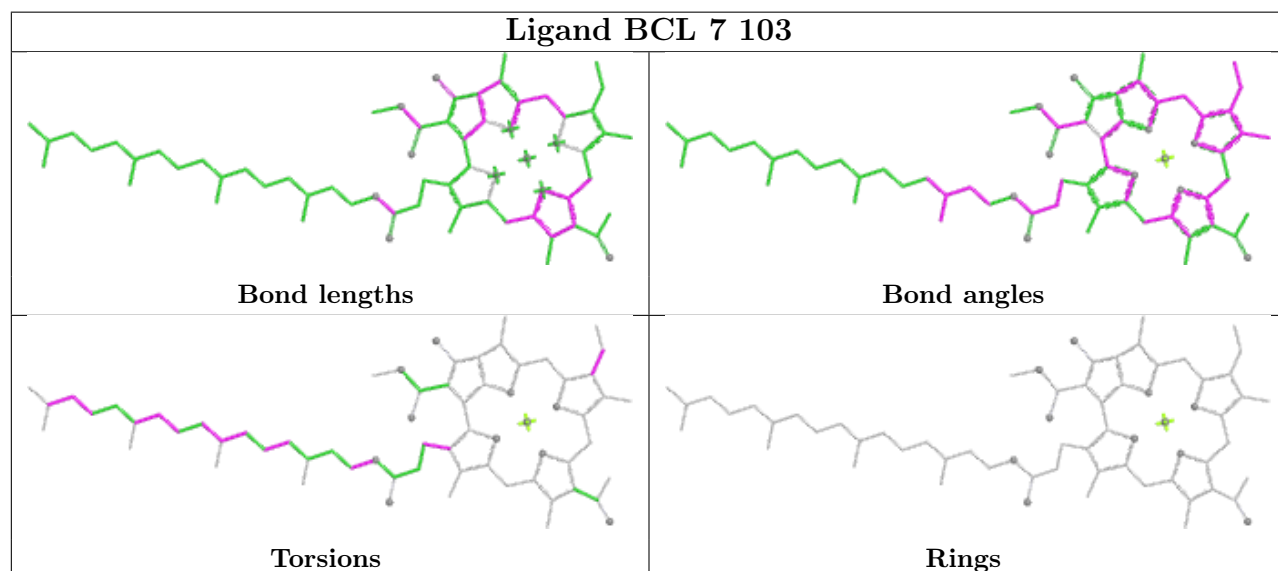
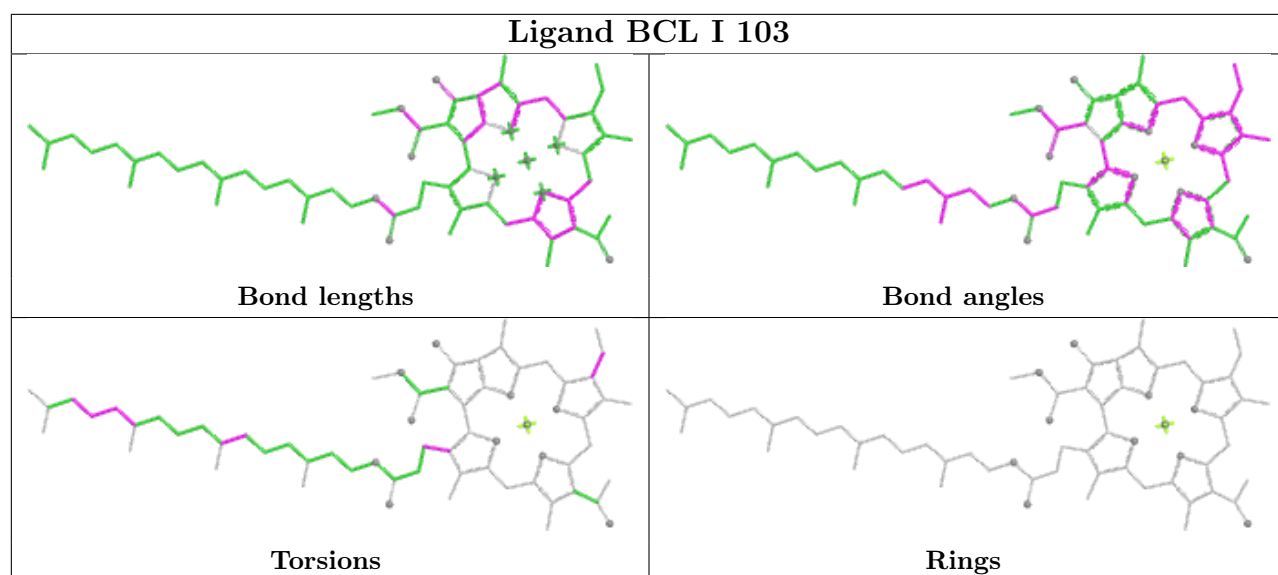


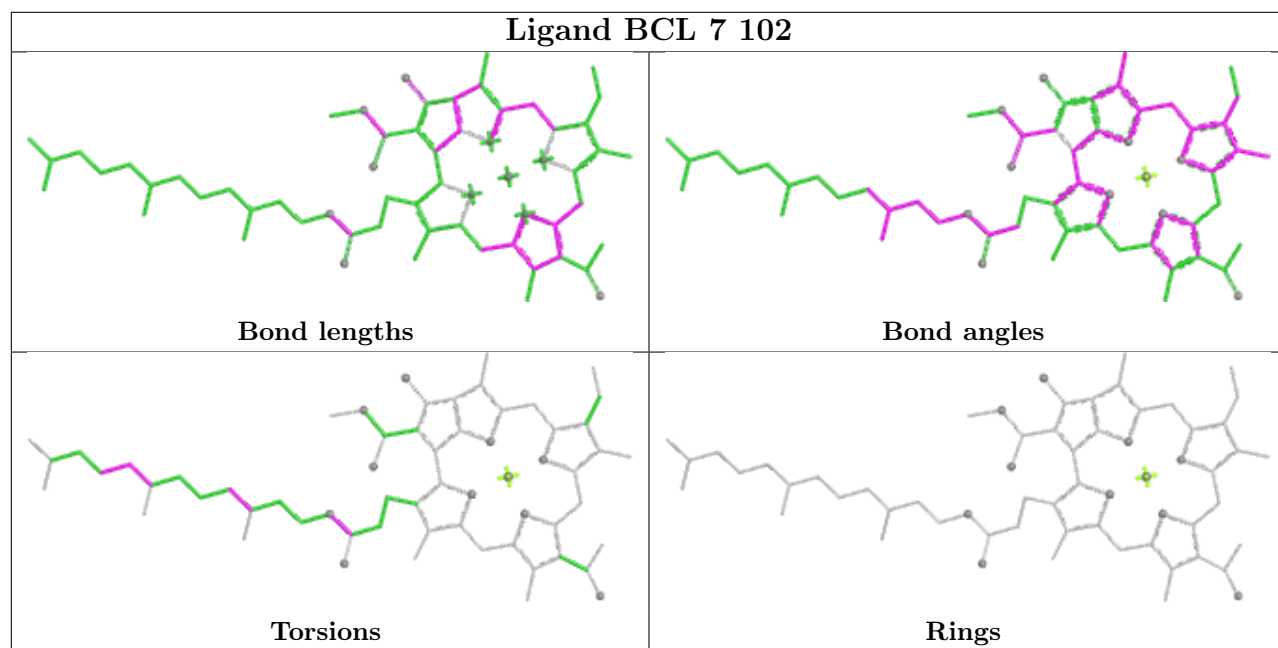
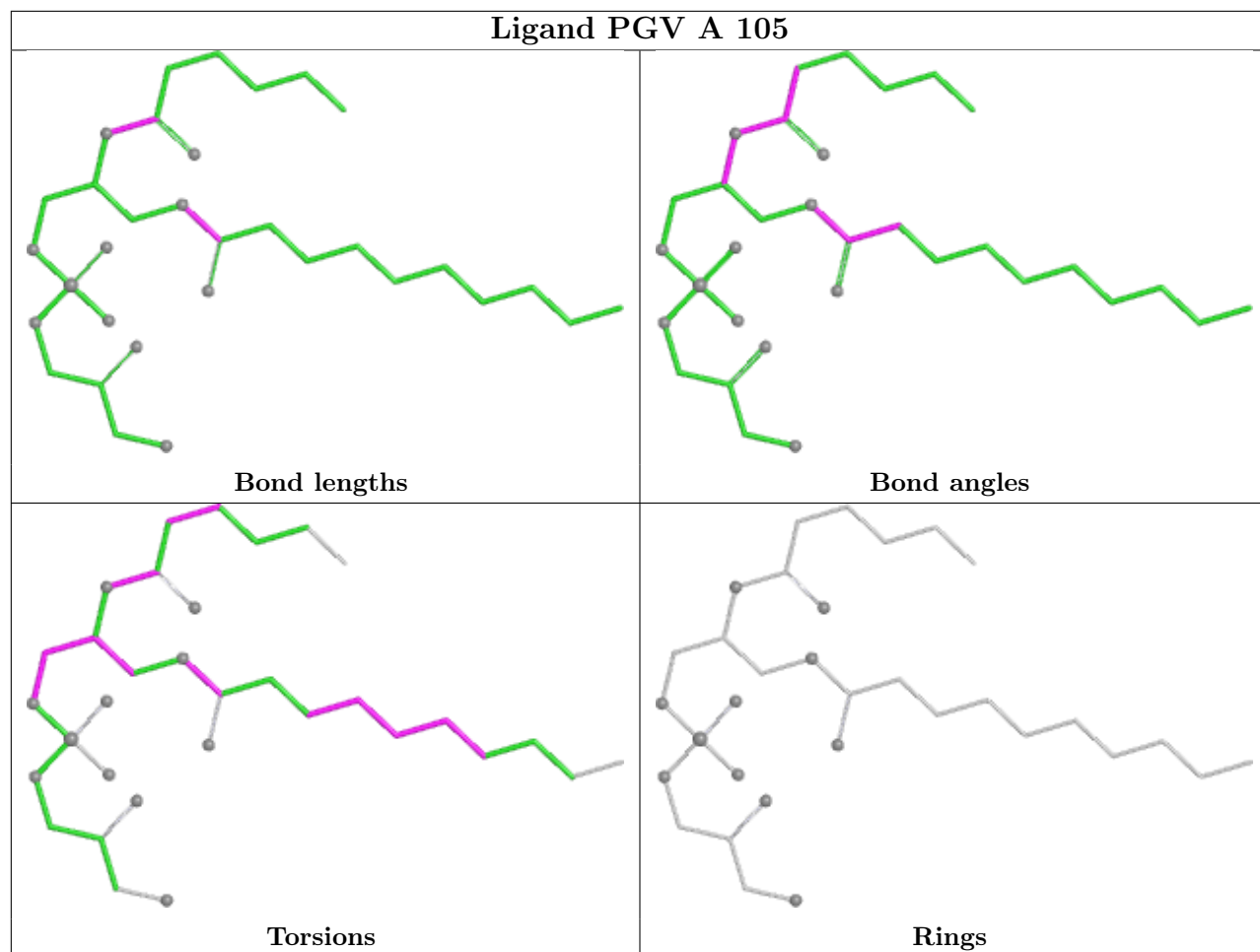


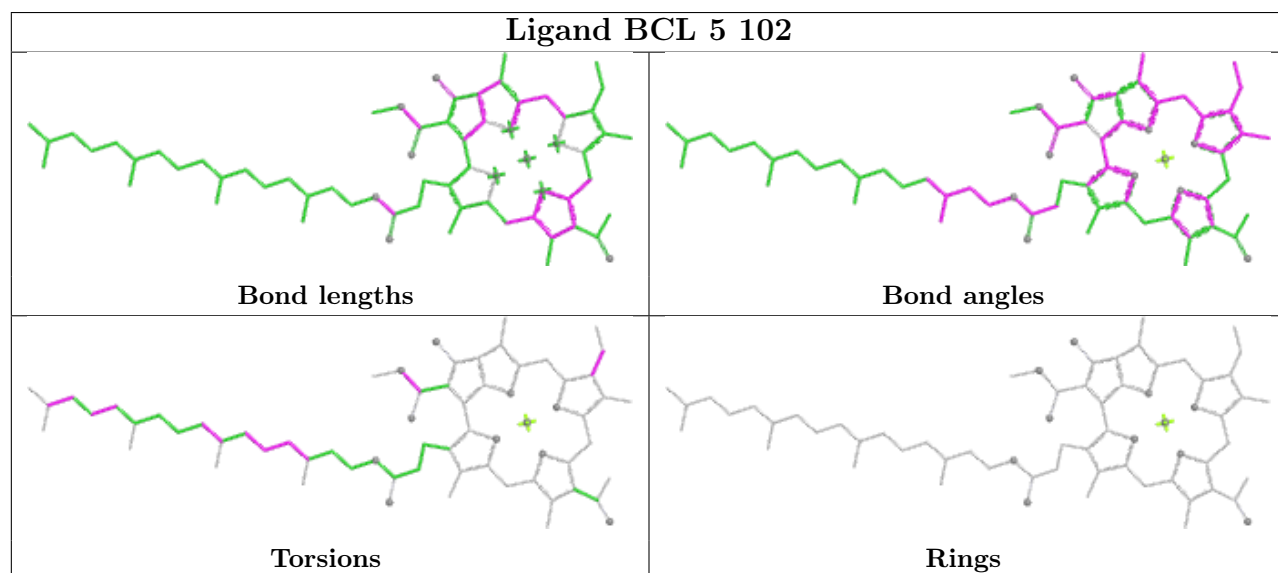
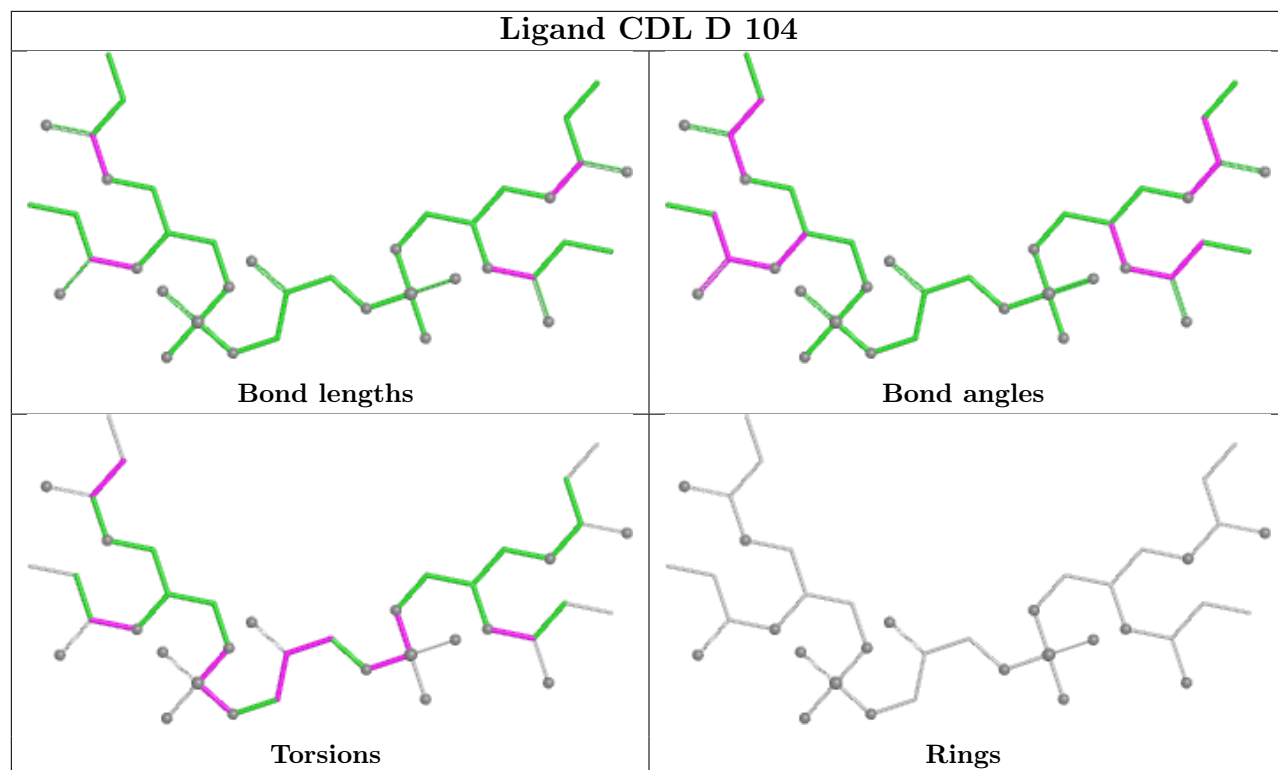


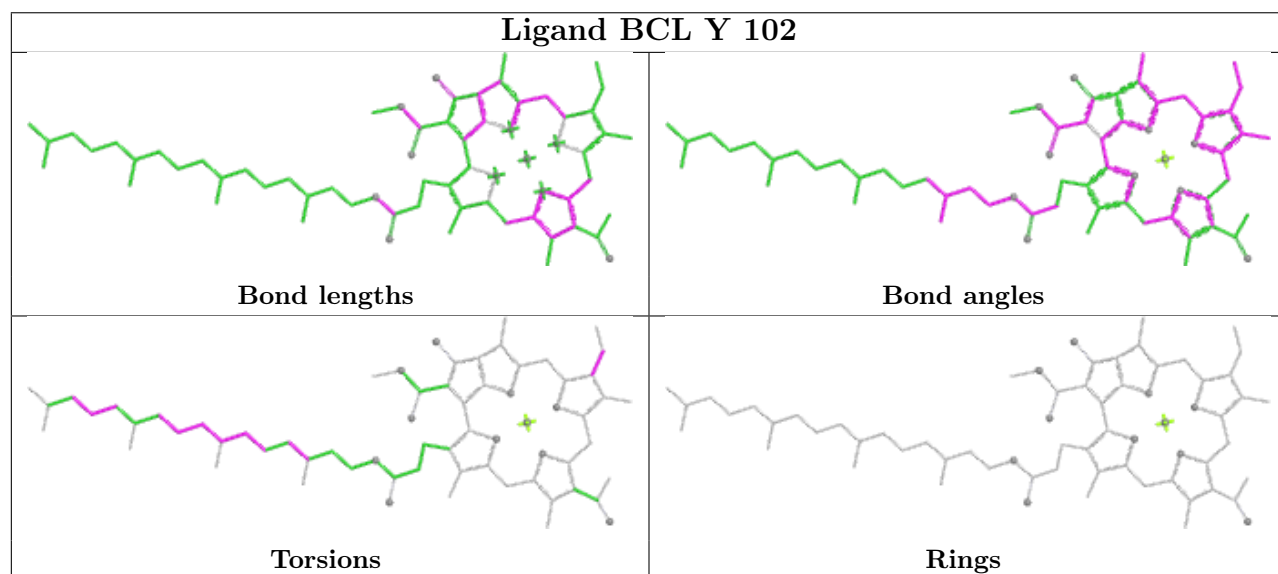
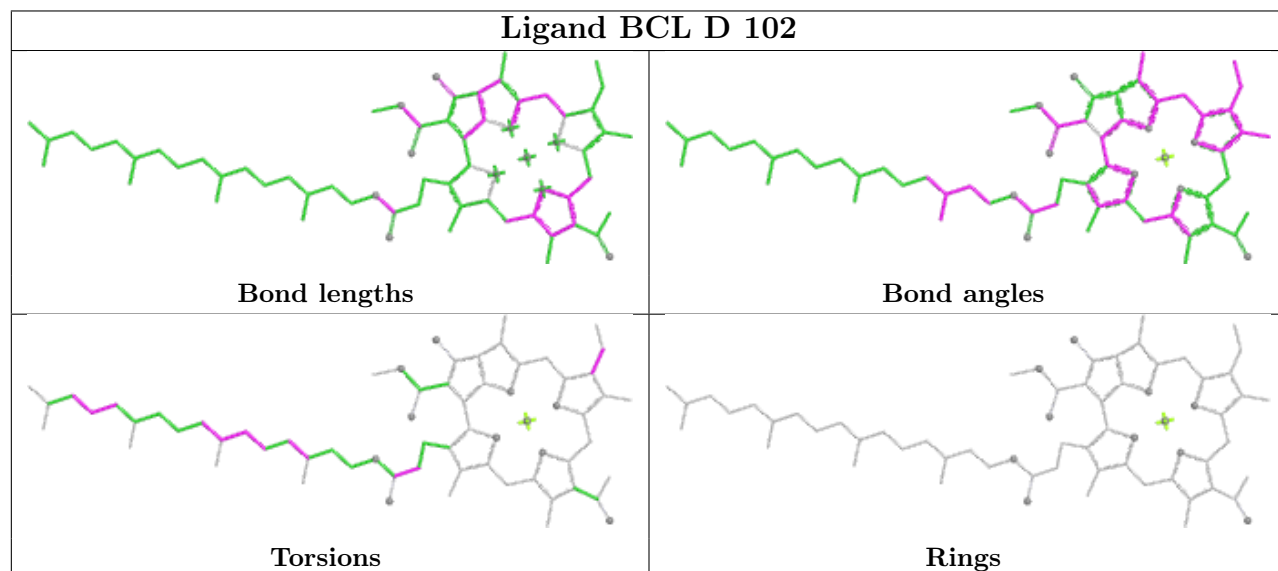
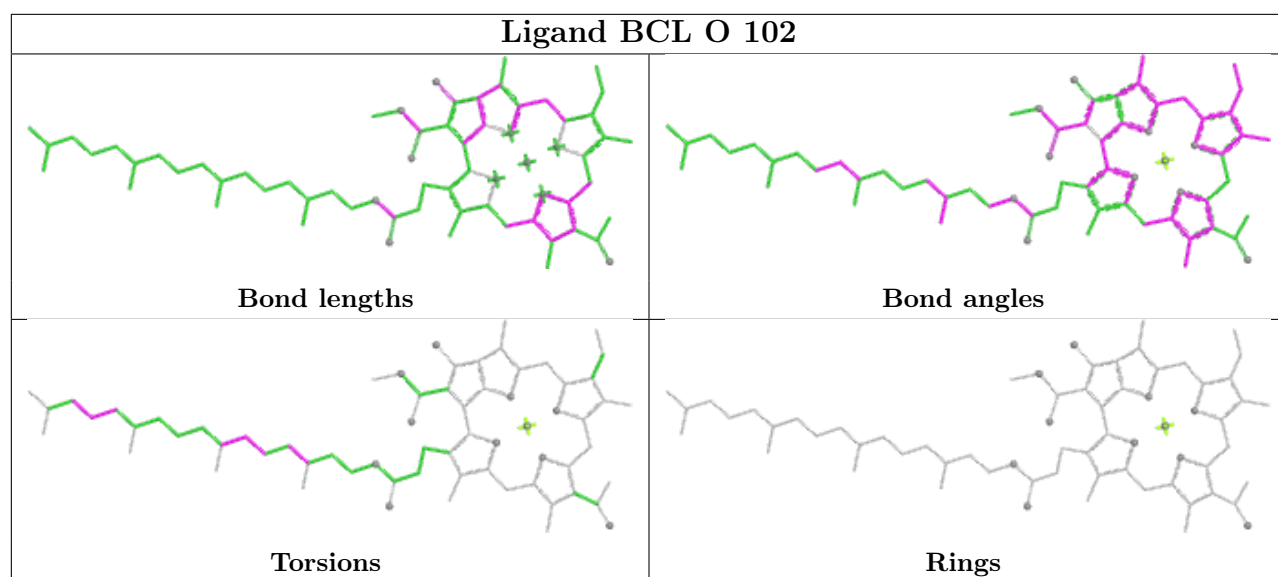


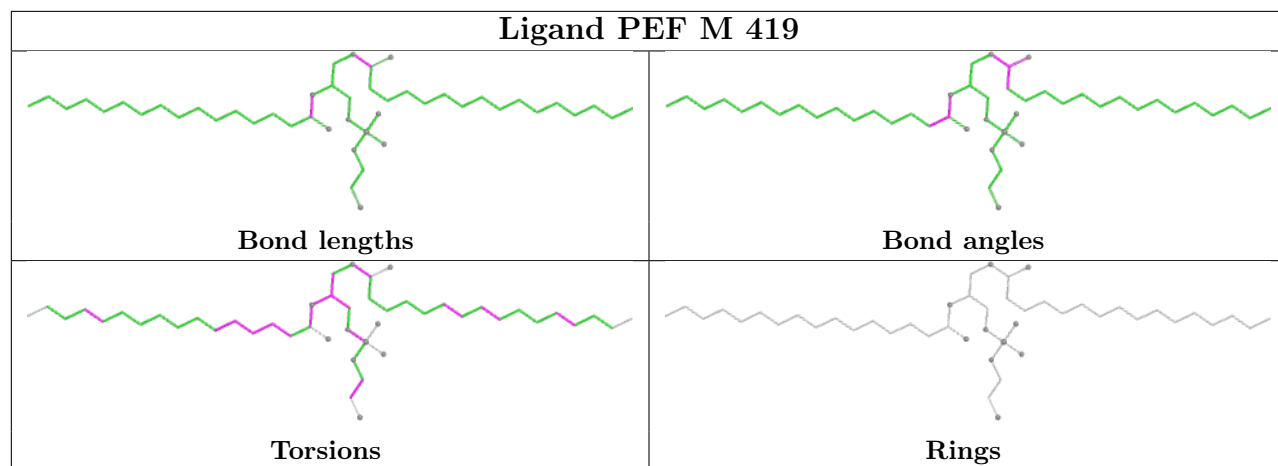


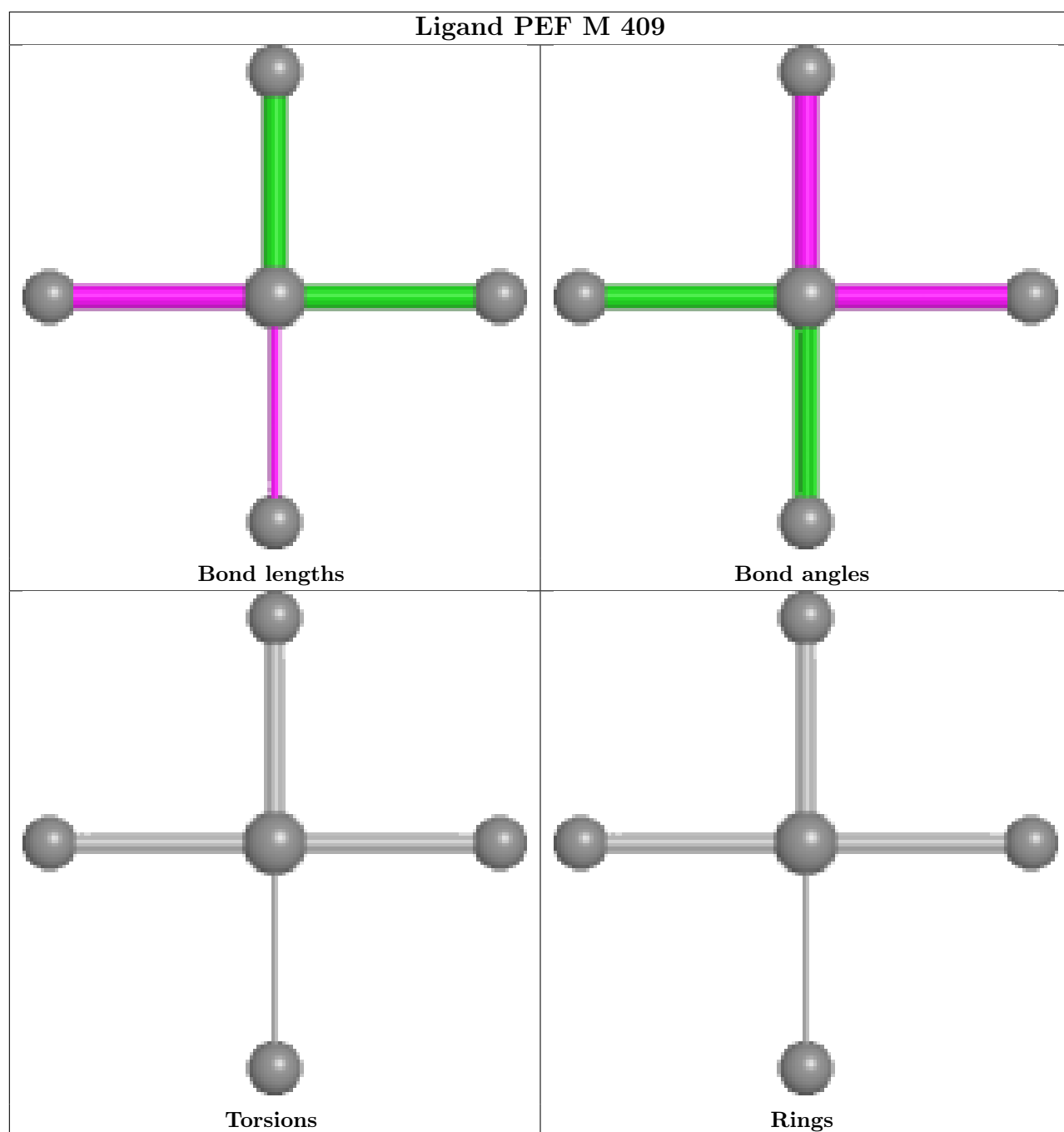


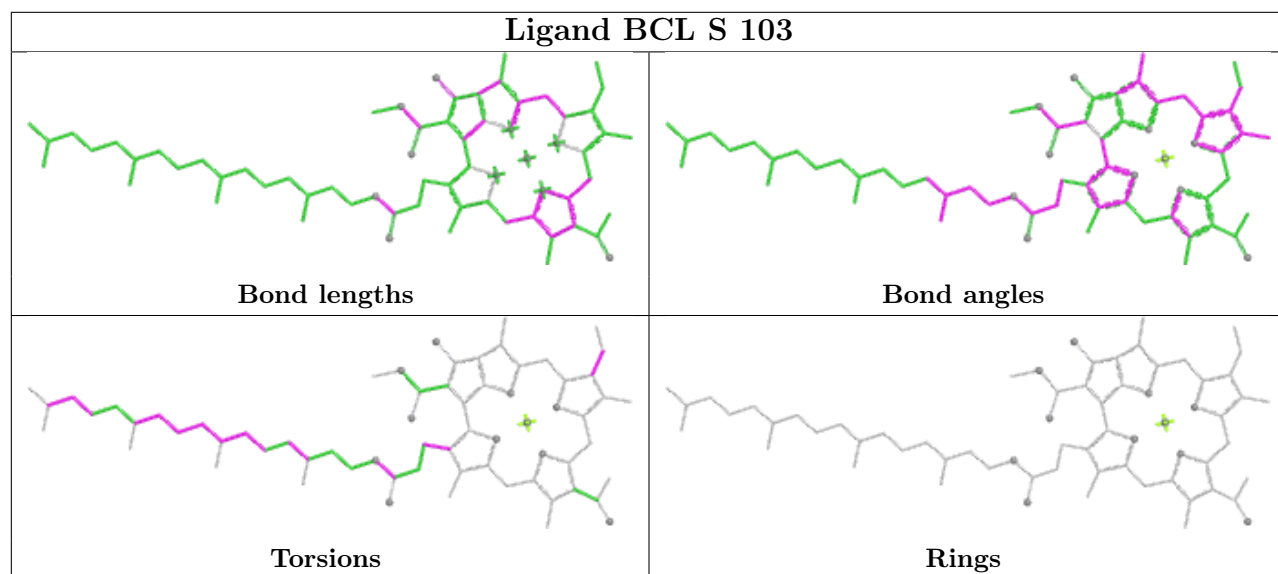
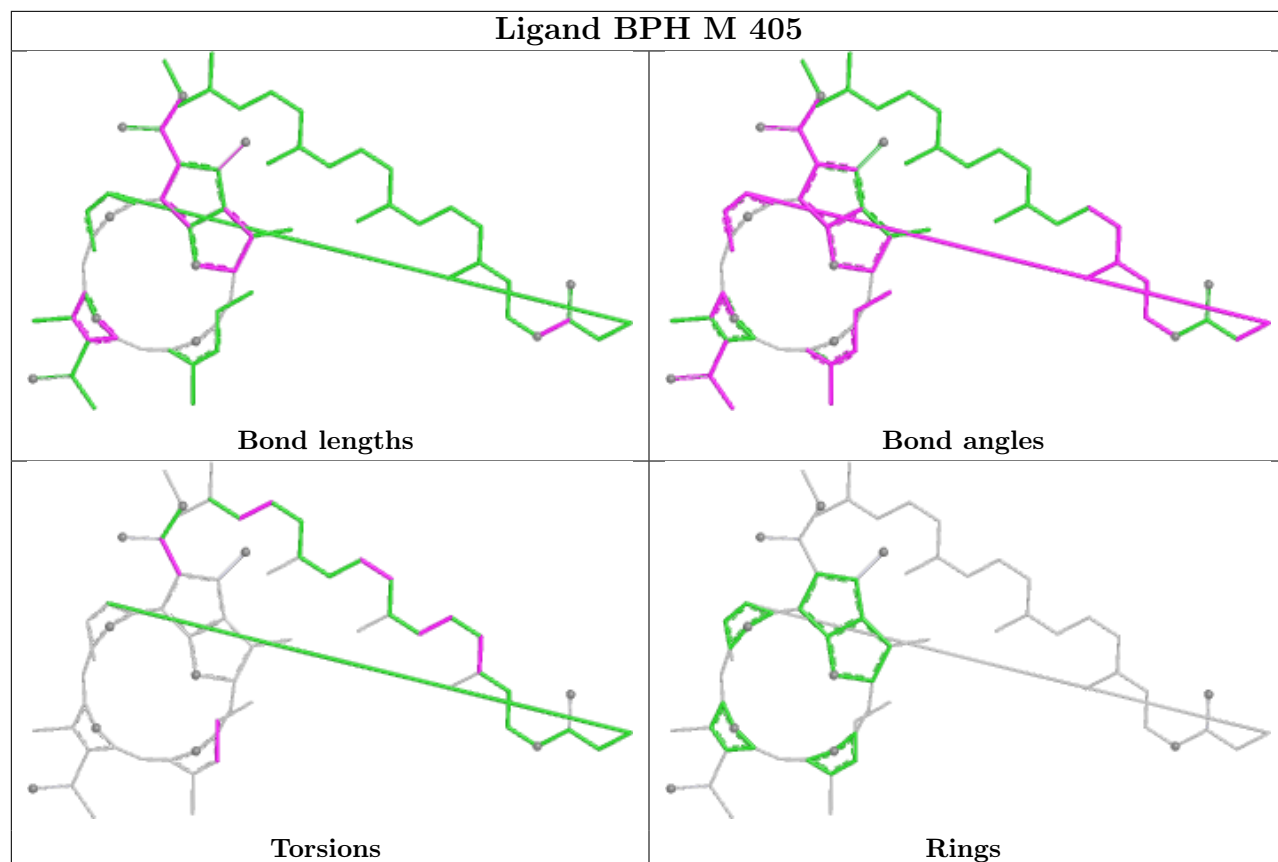


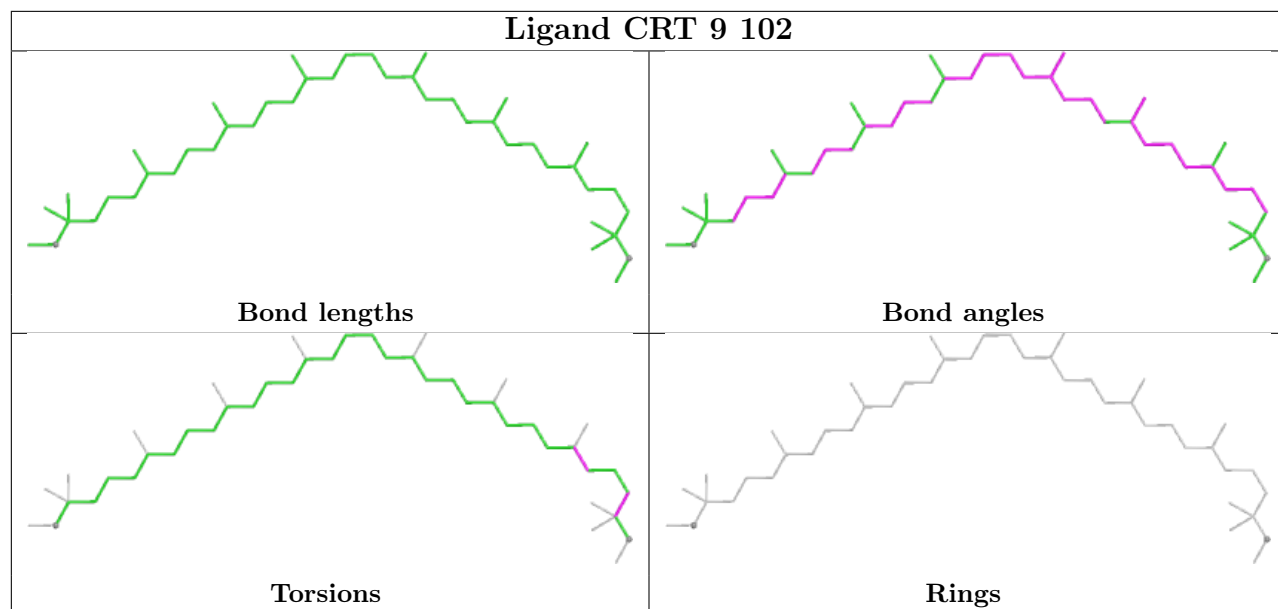


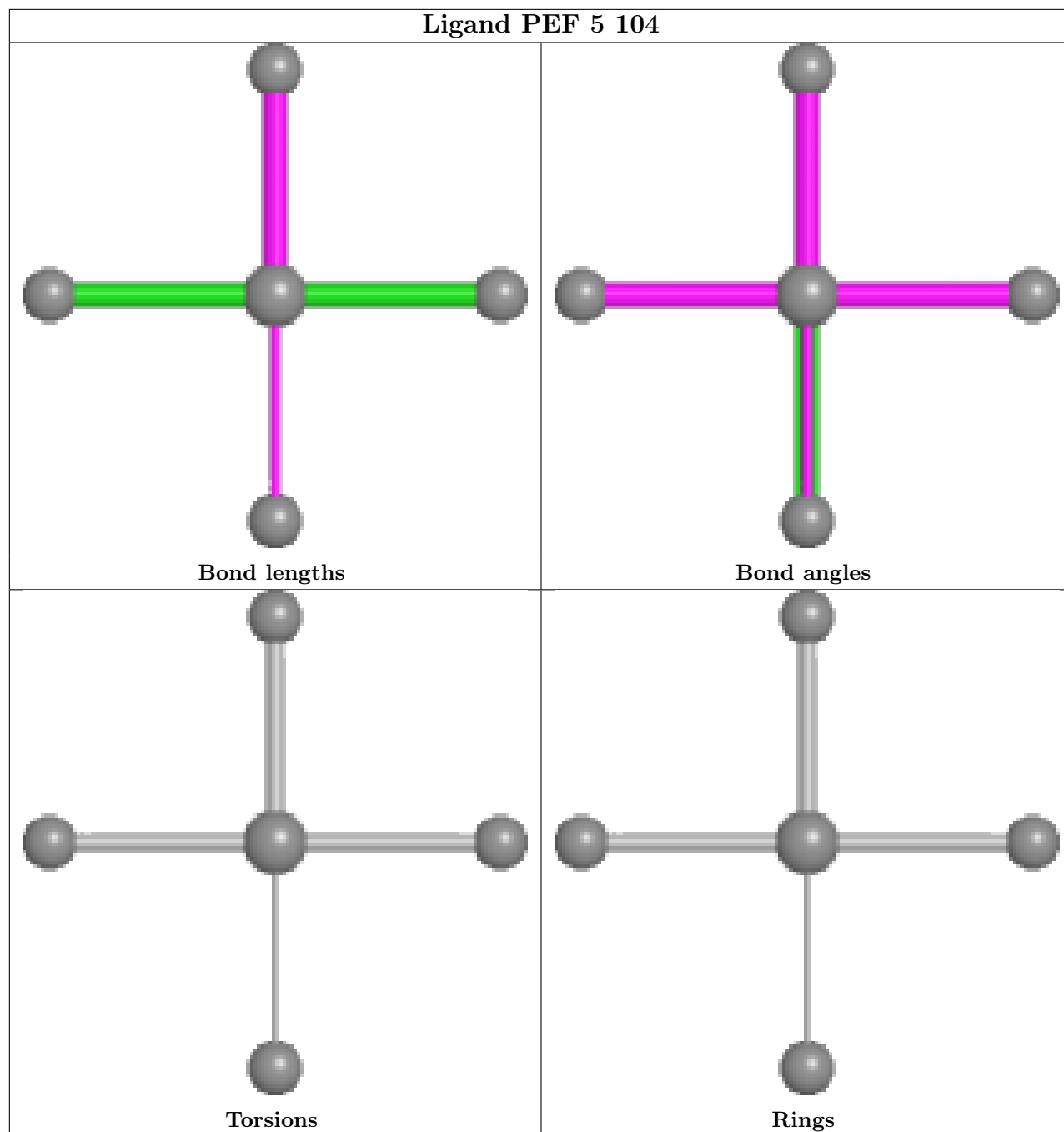


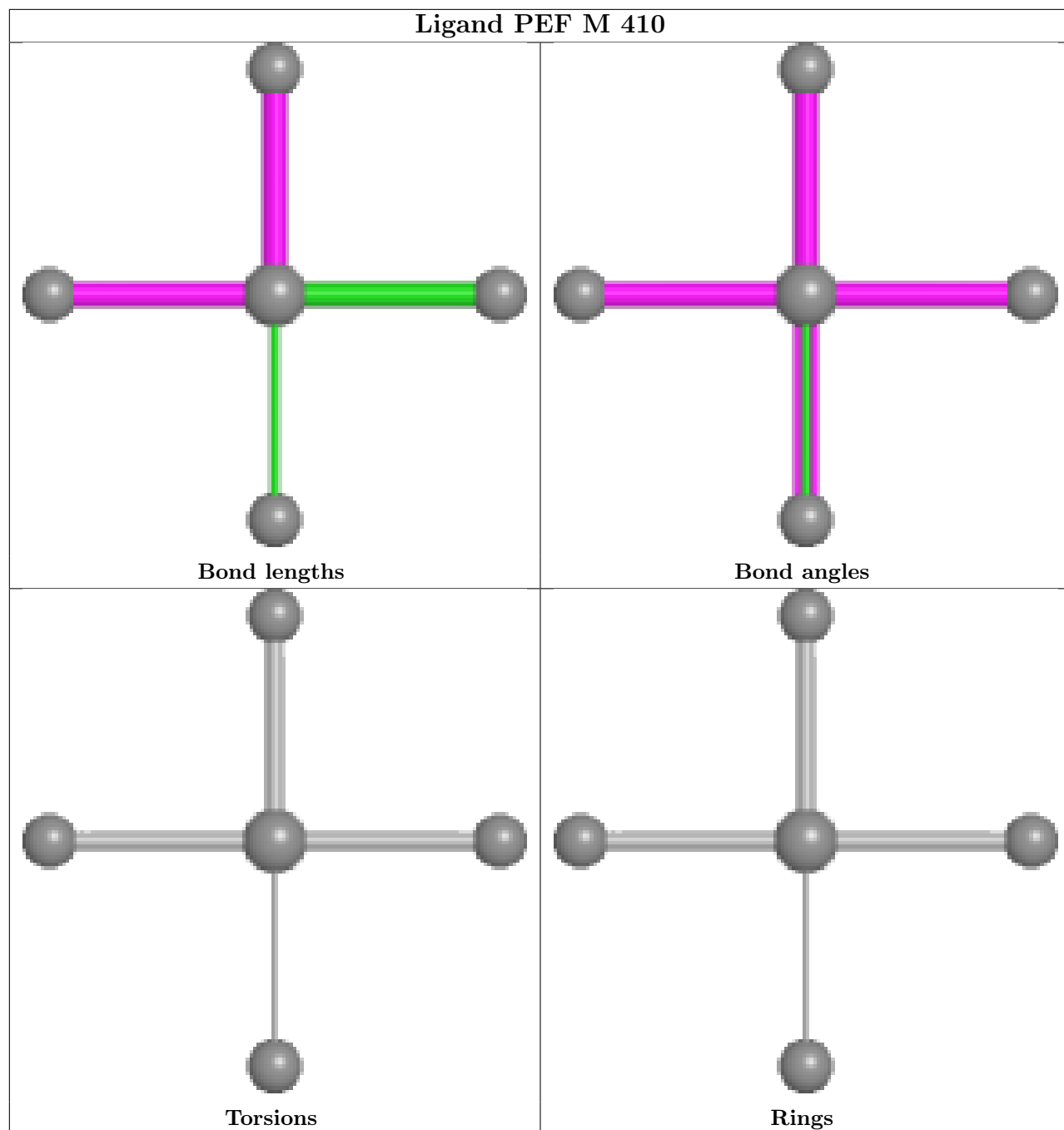


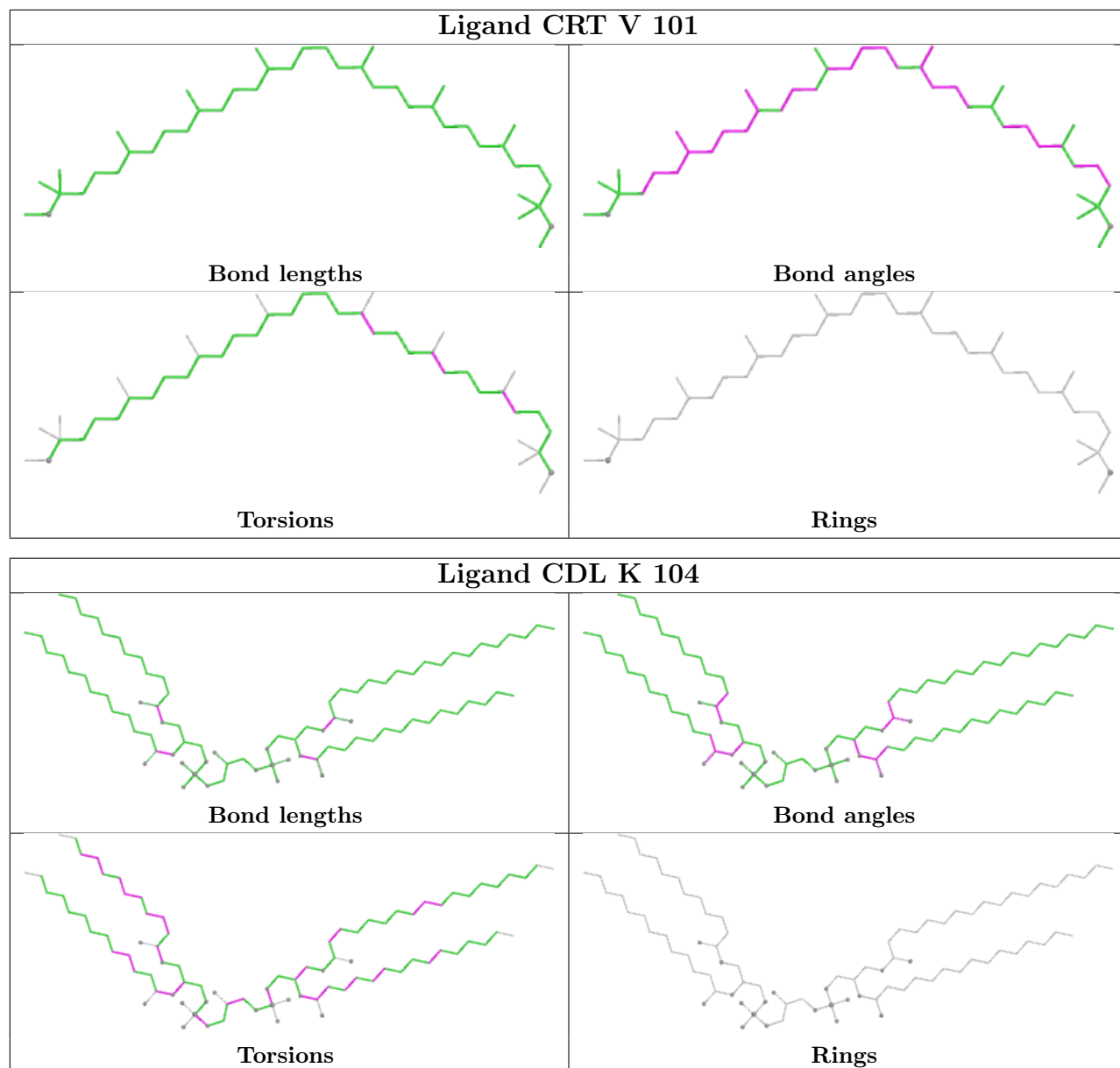


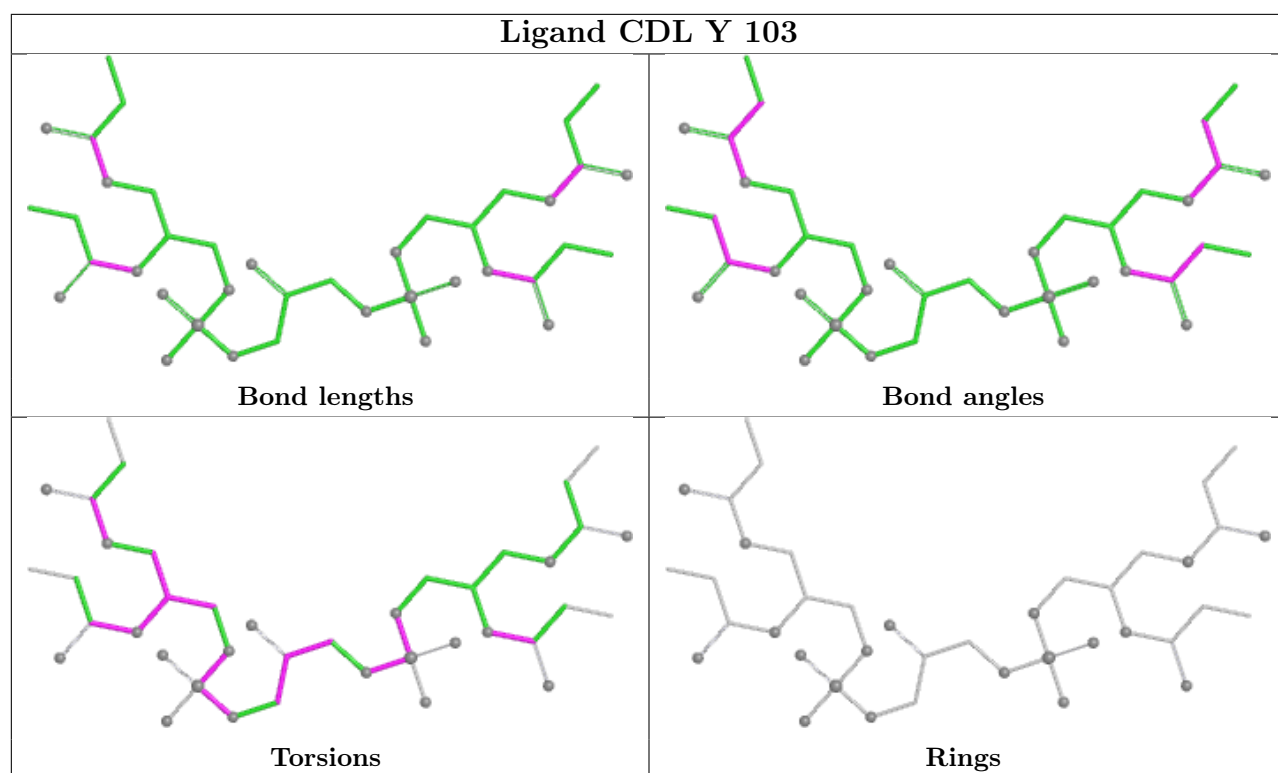


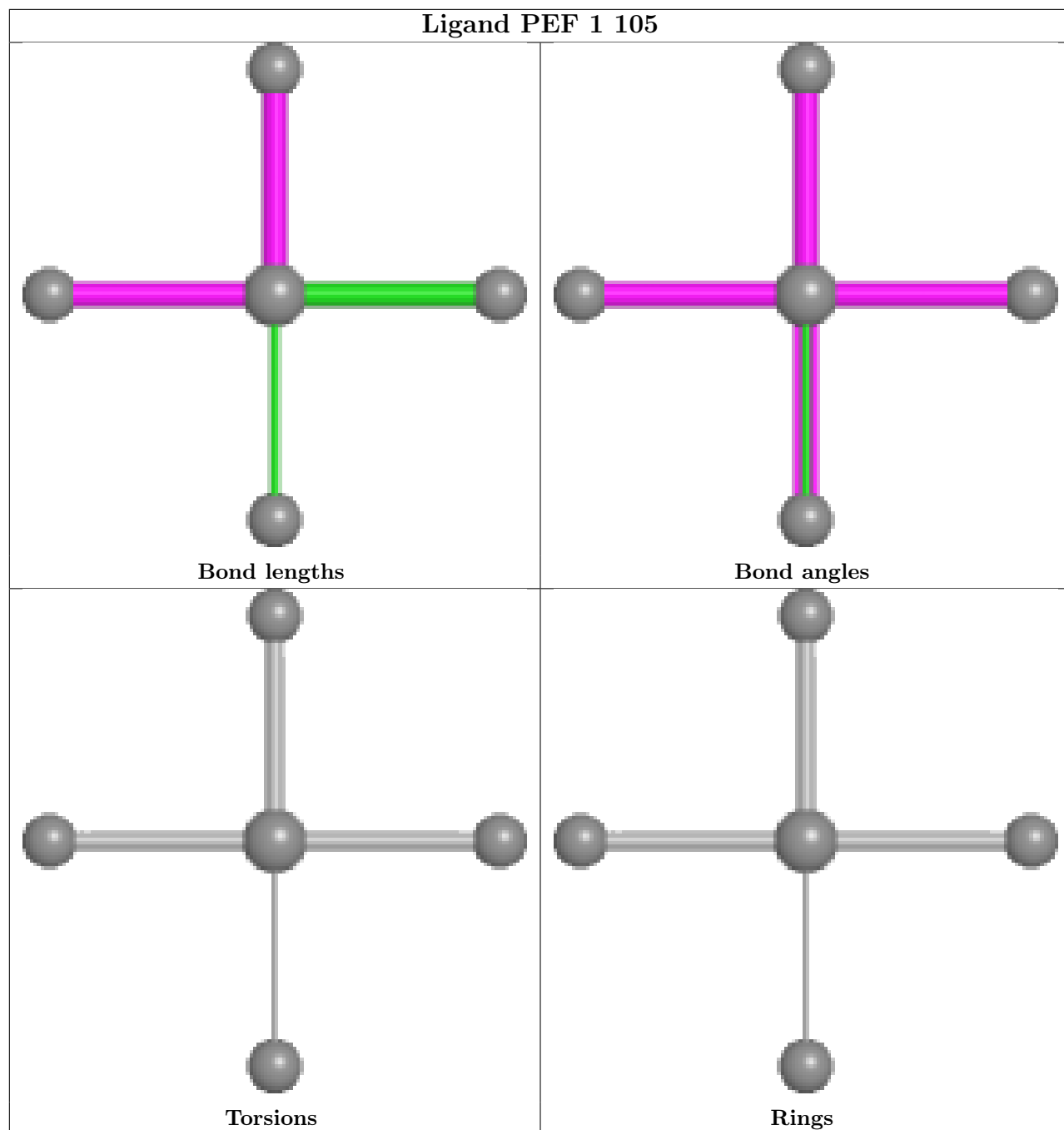


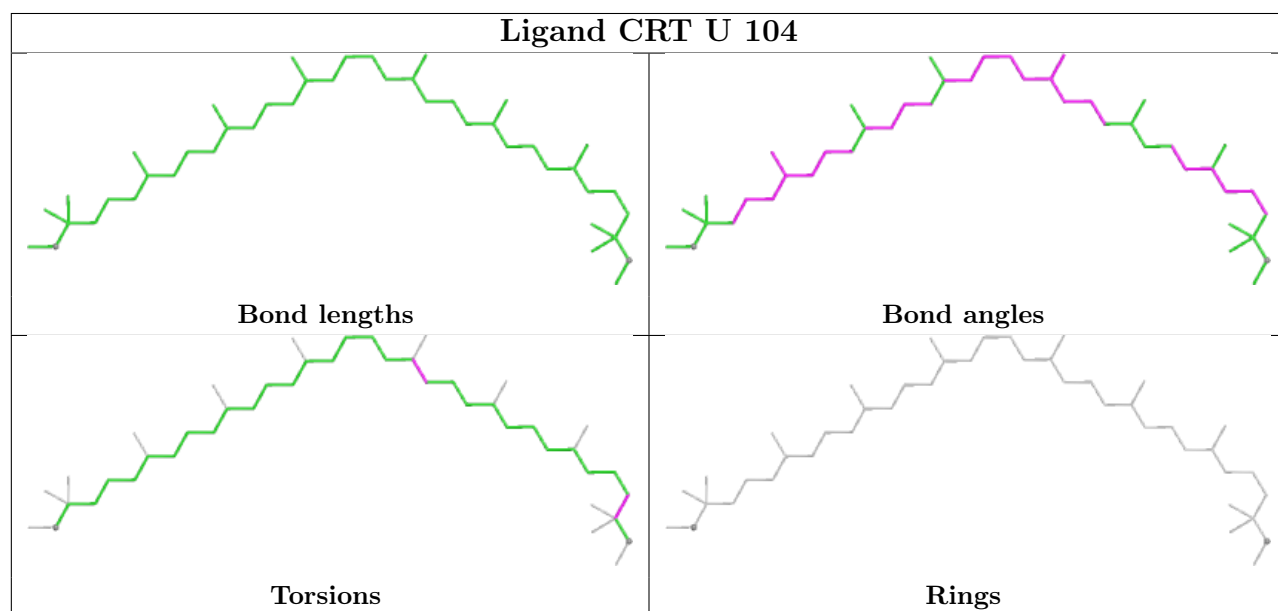
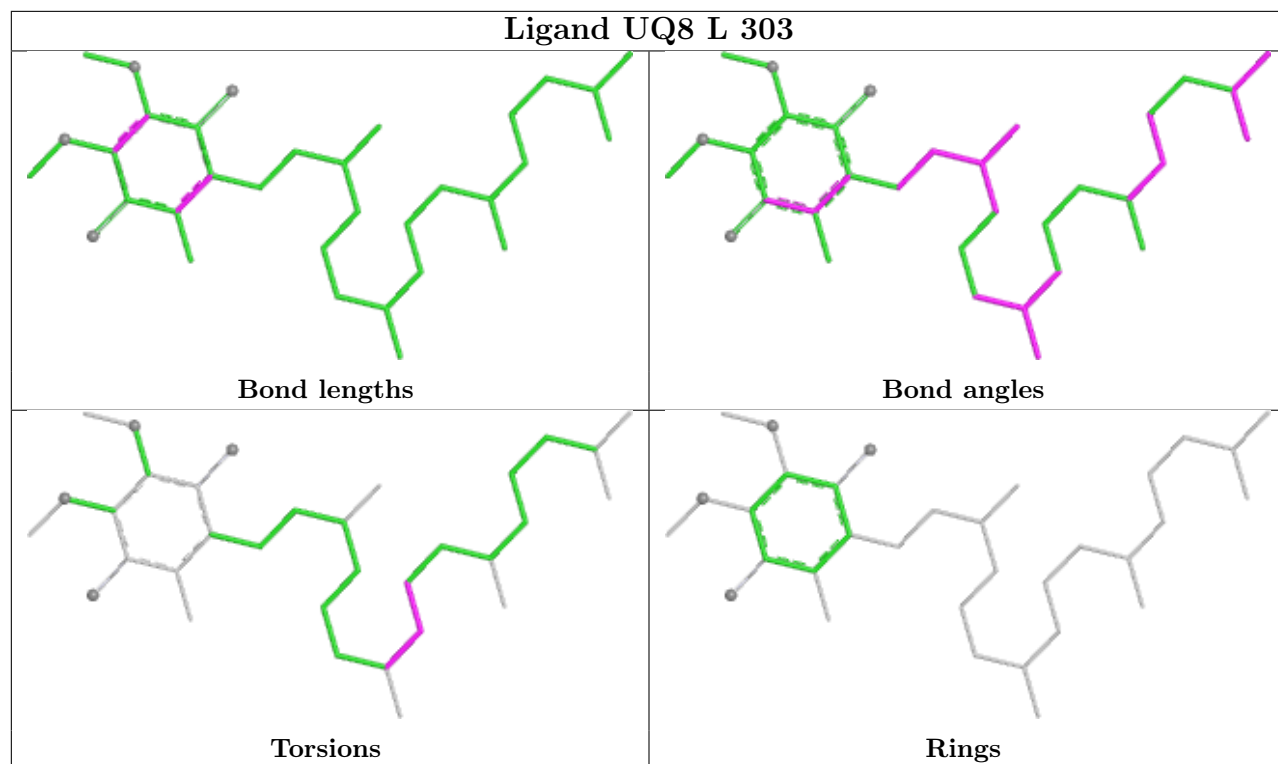




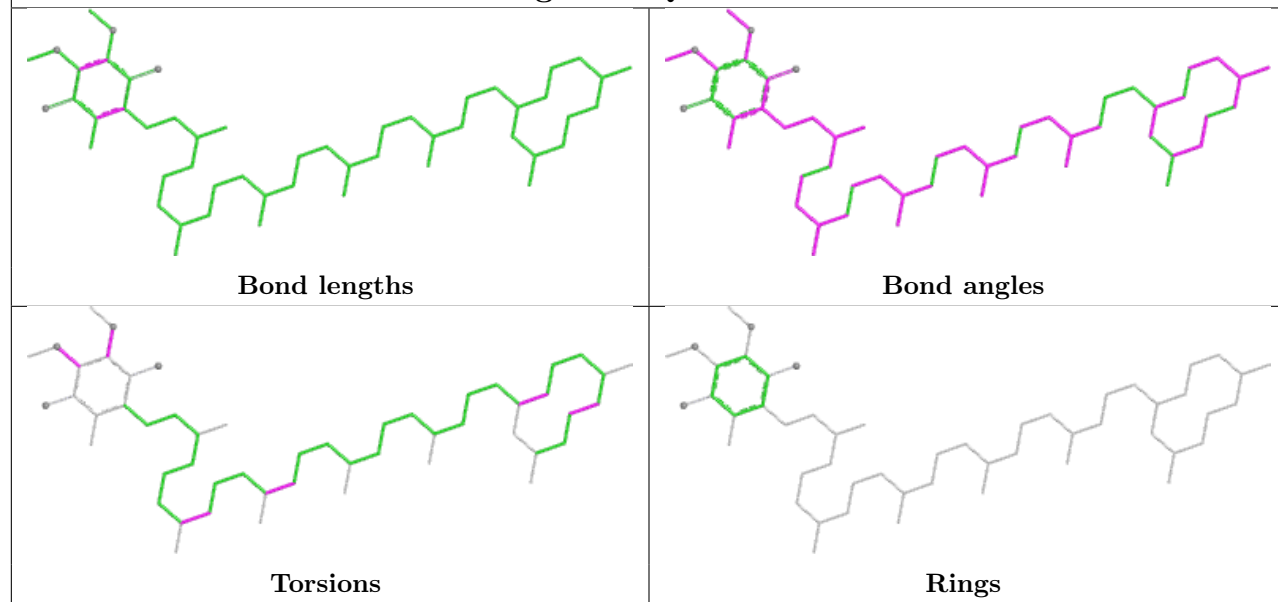




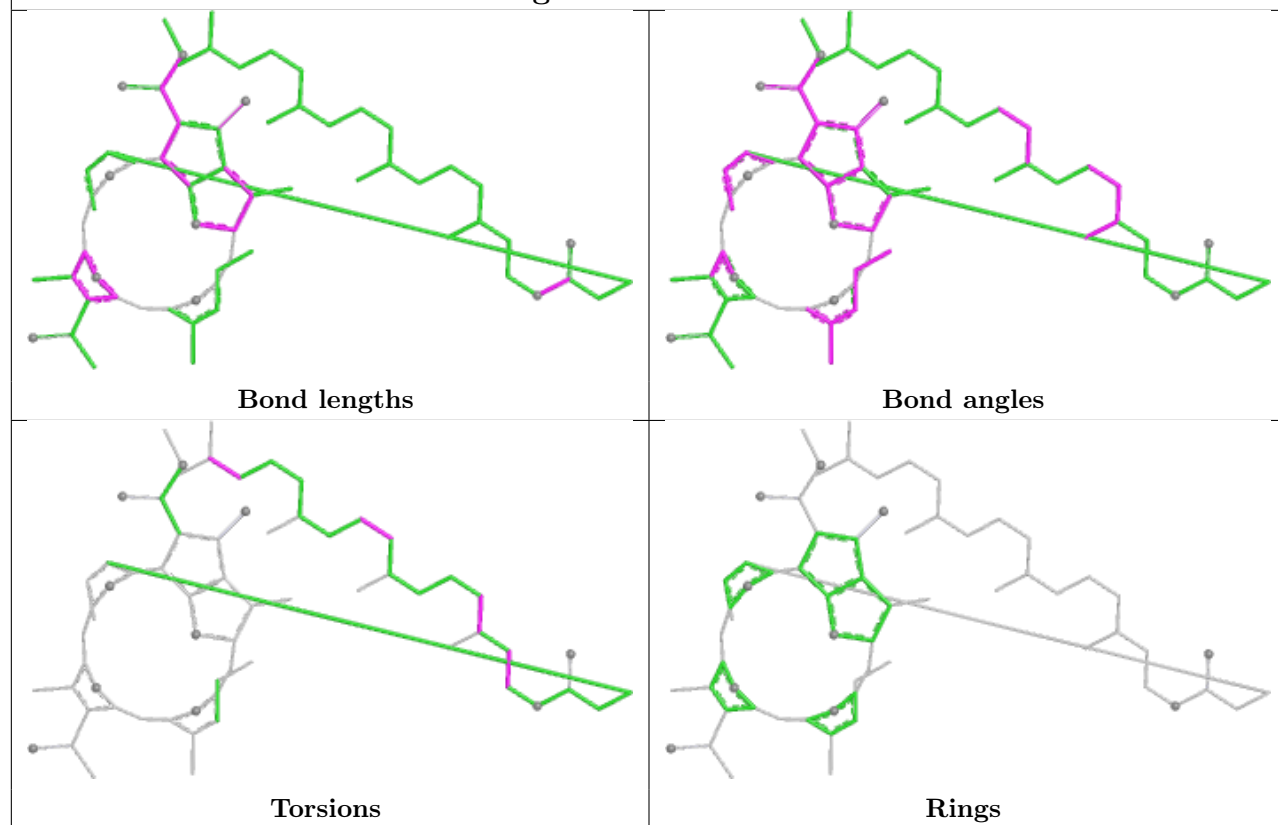


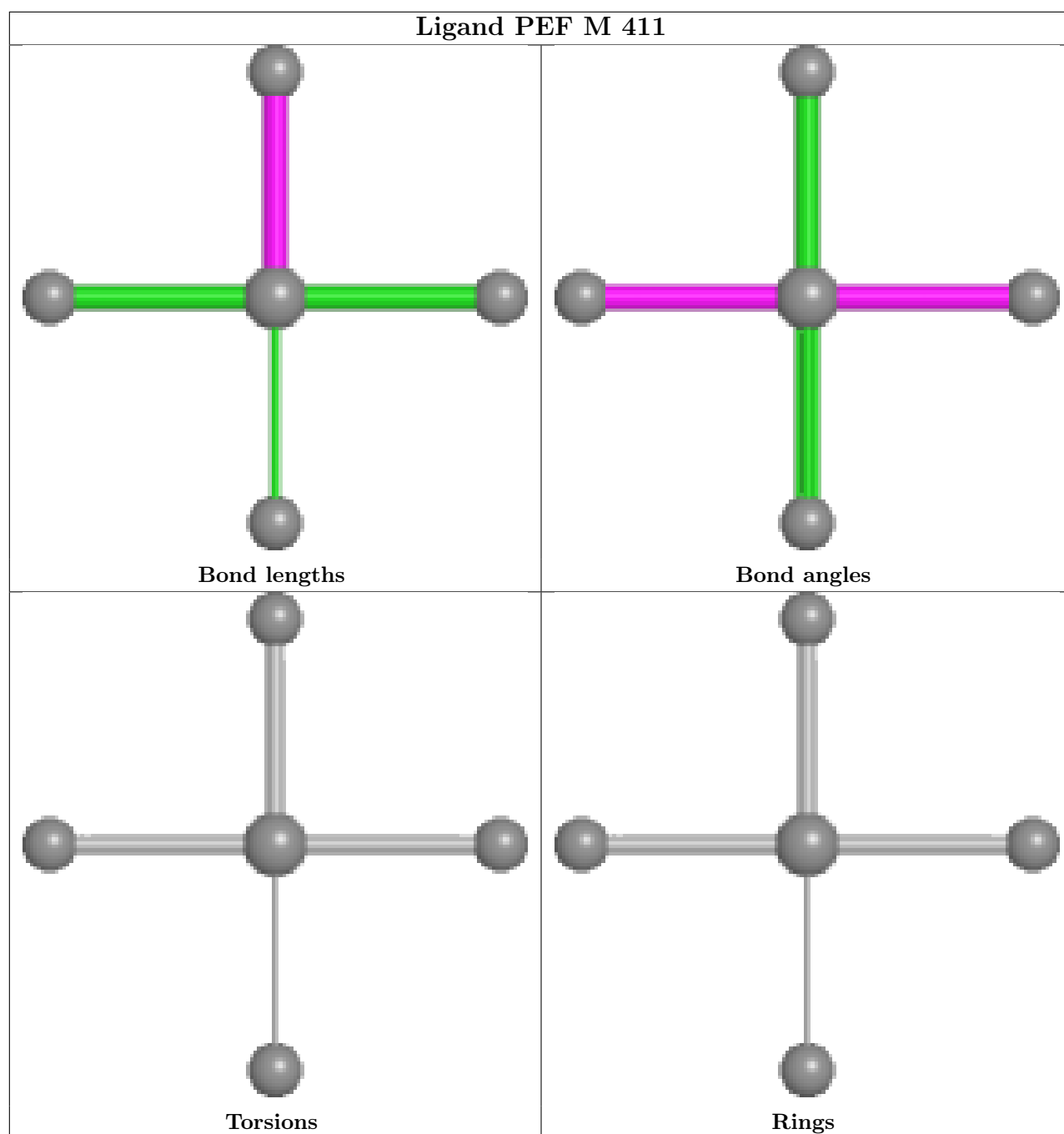


Ligand UQ8 L 308

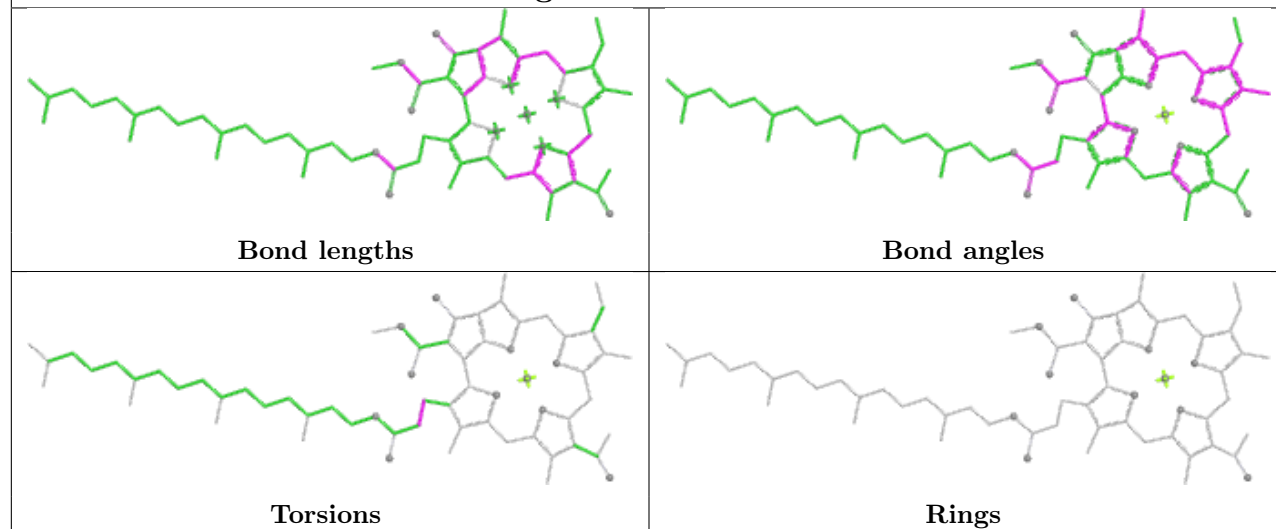


Ligand BPH L 302

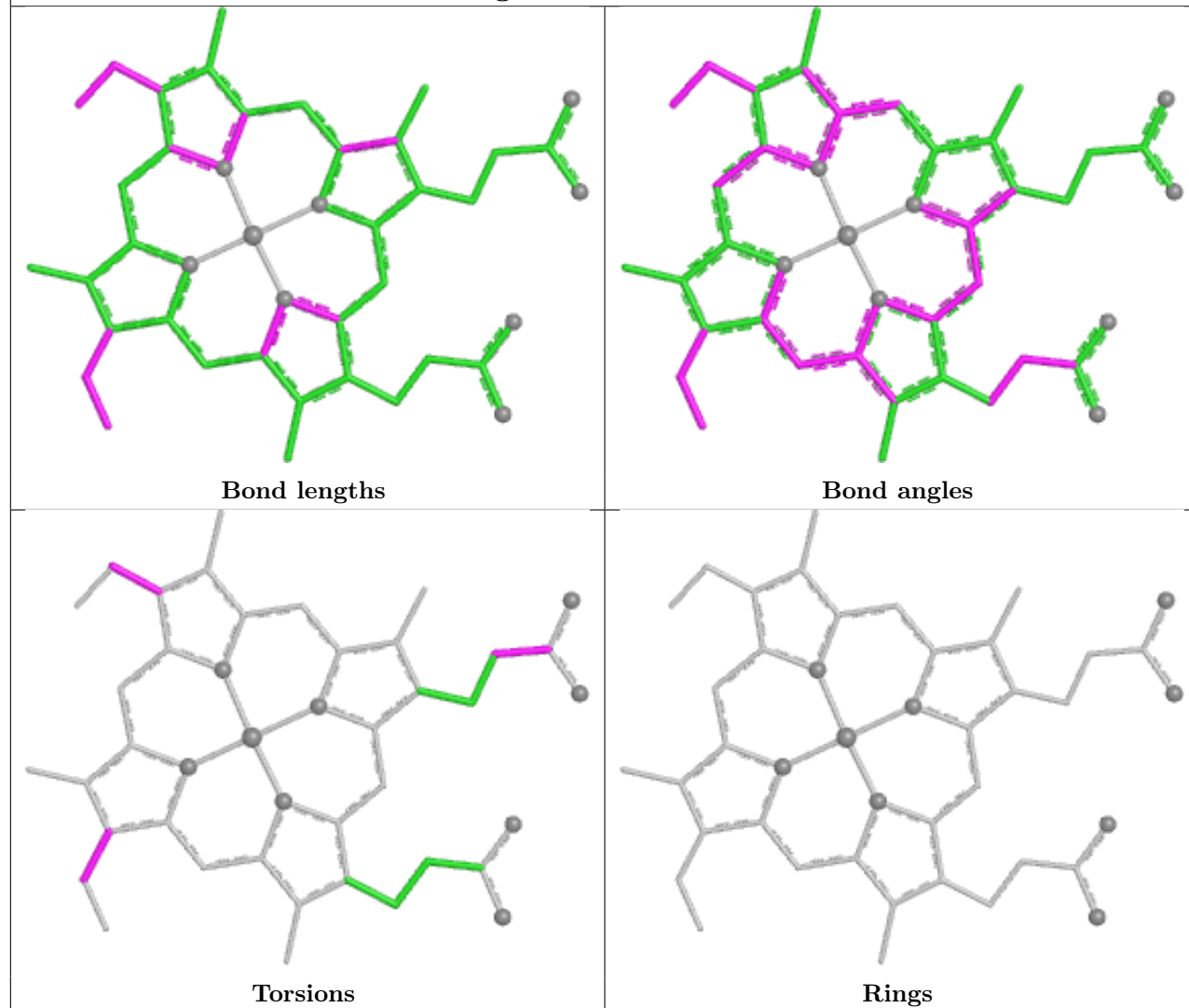




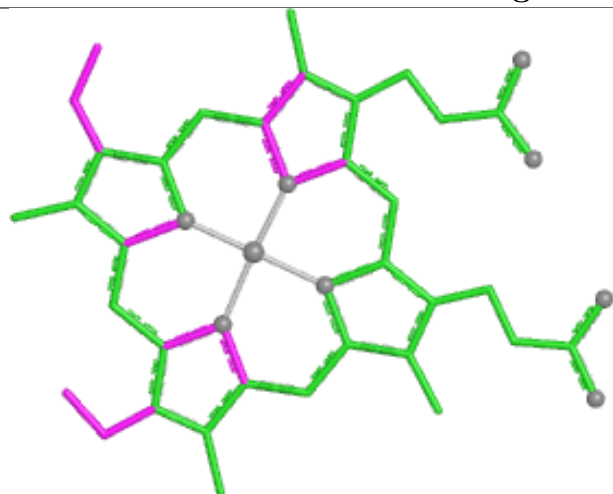
Ligand BCL L 301



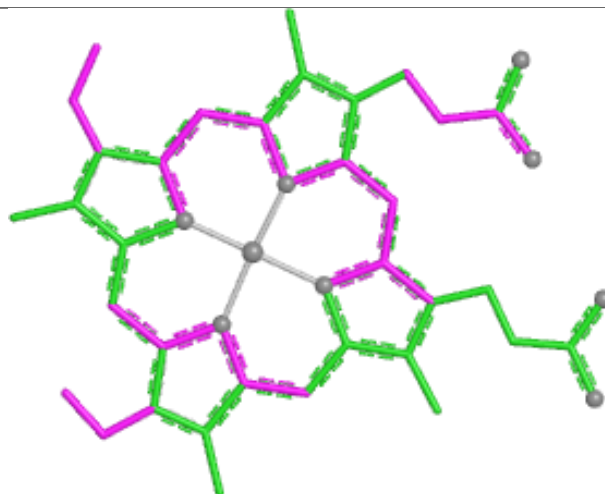
Ligand HEC C 501



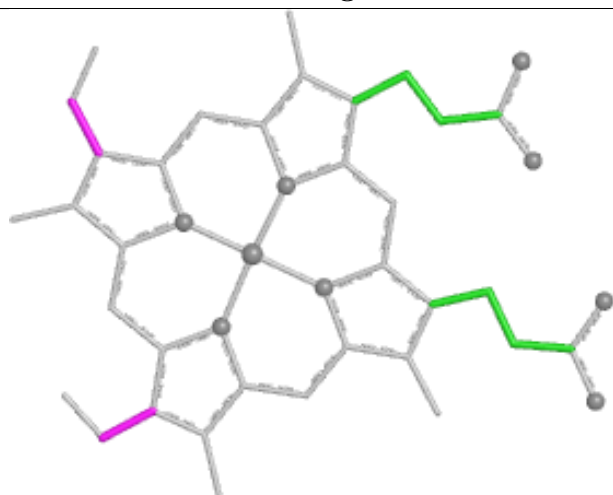
Ligand HEC C 503



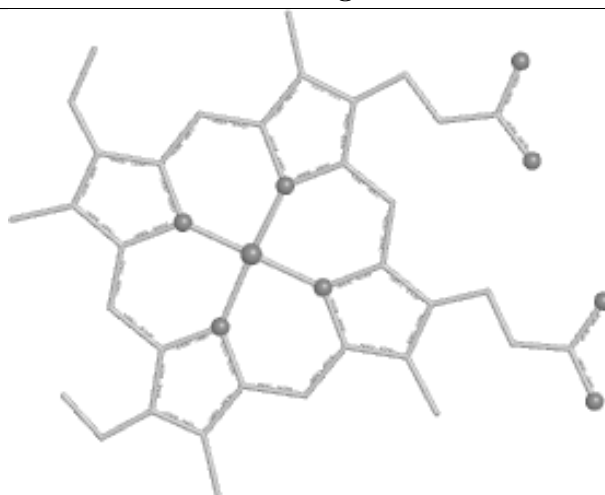
Bond lengths



Bond angles

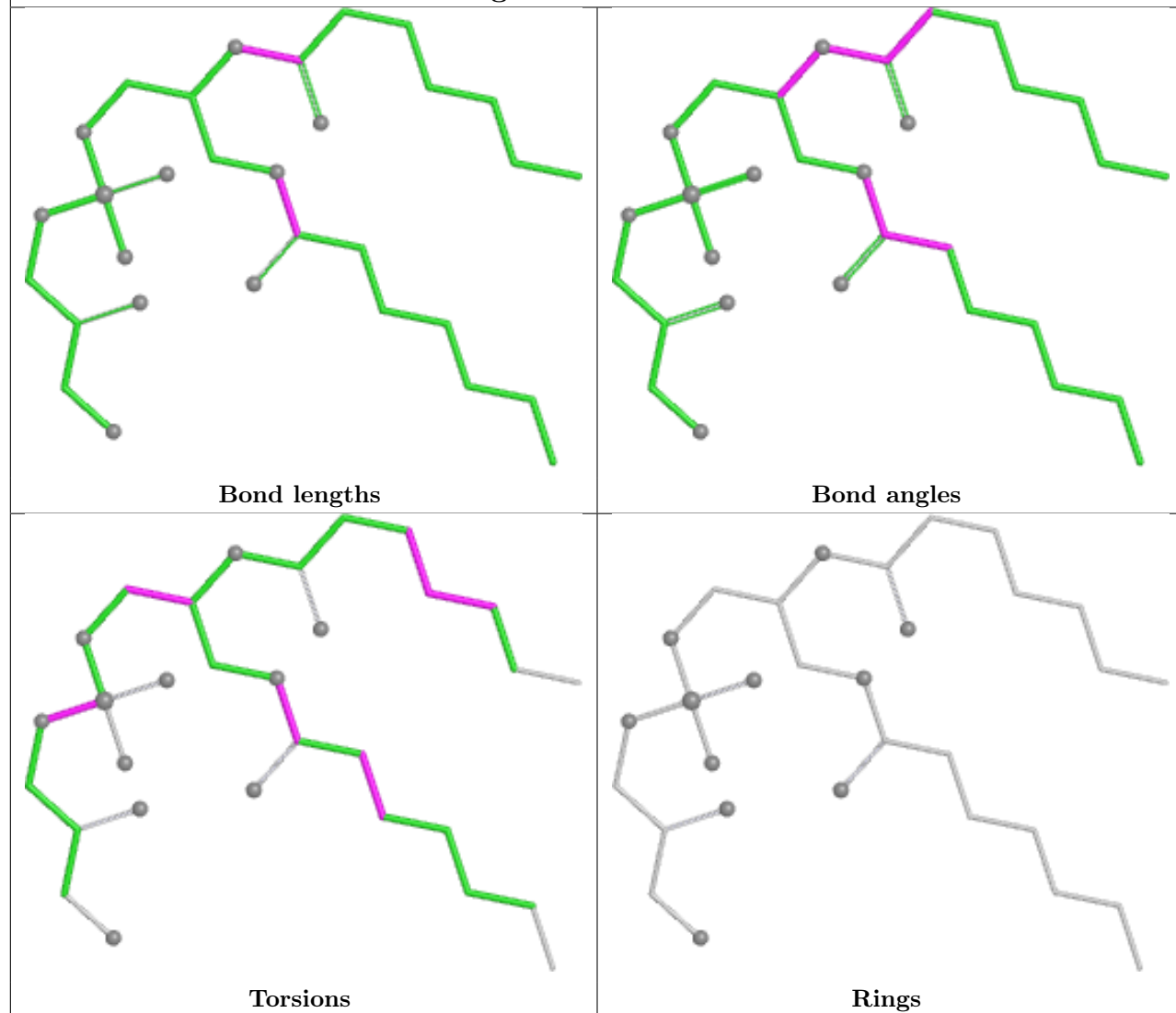


Torsions

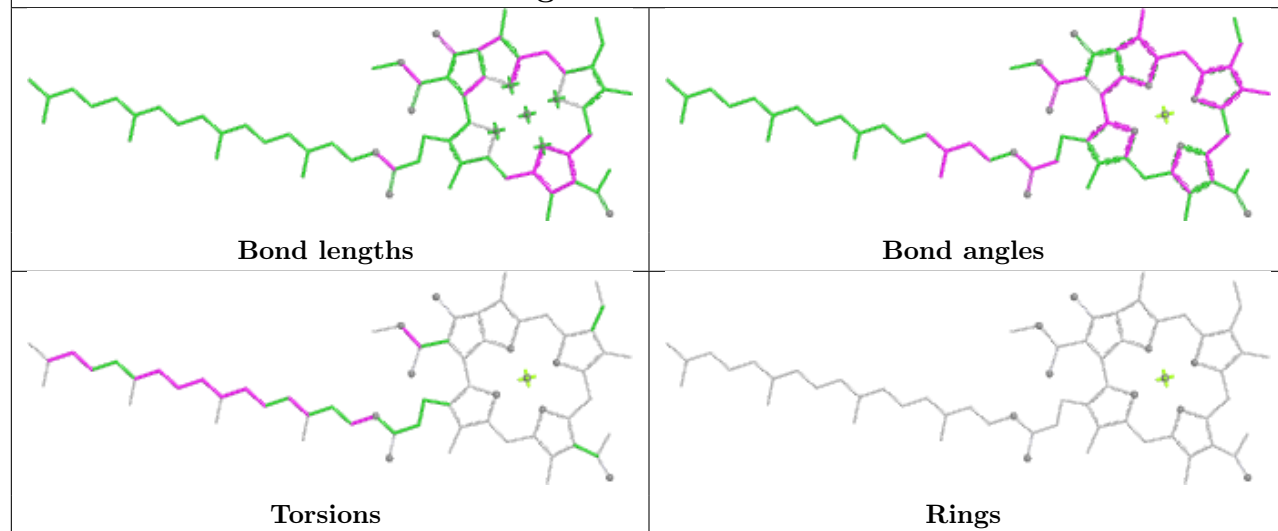


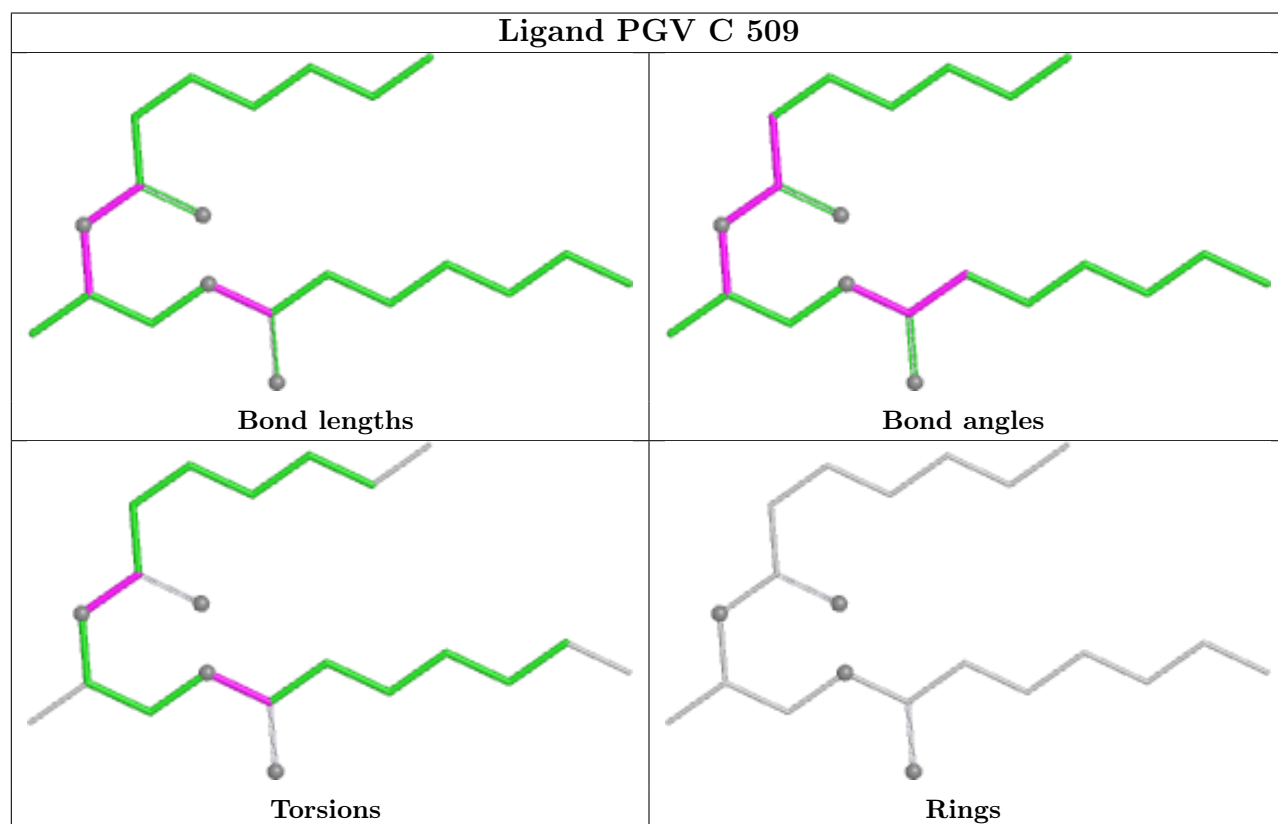
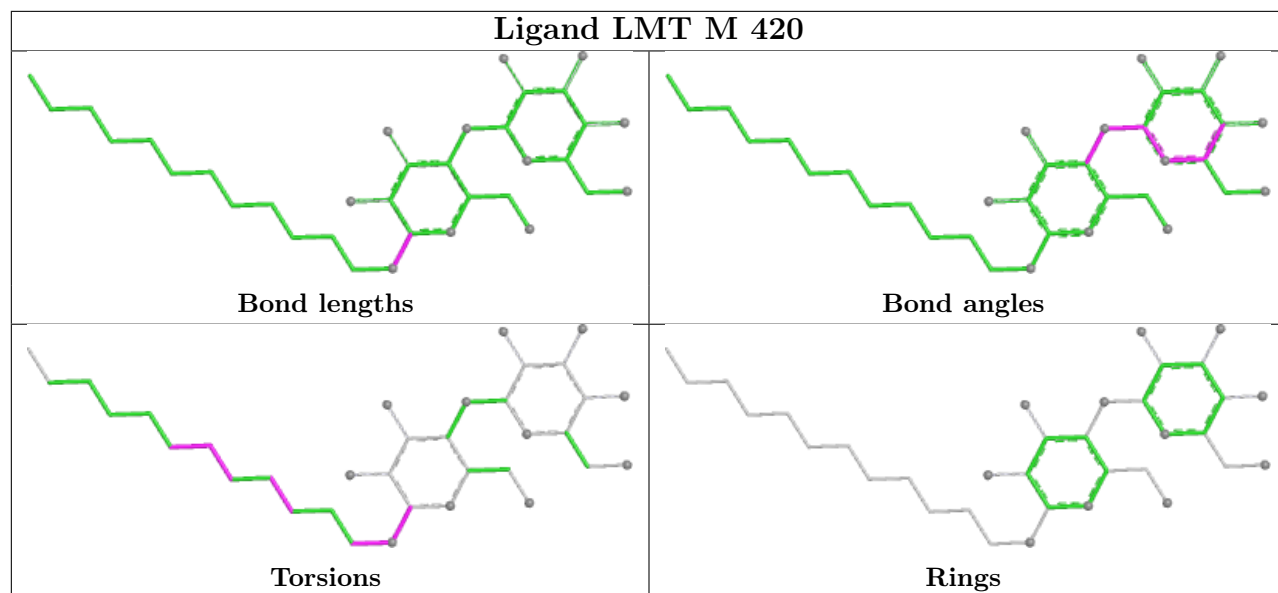
Rings

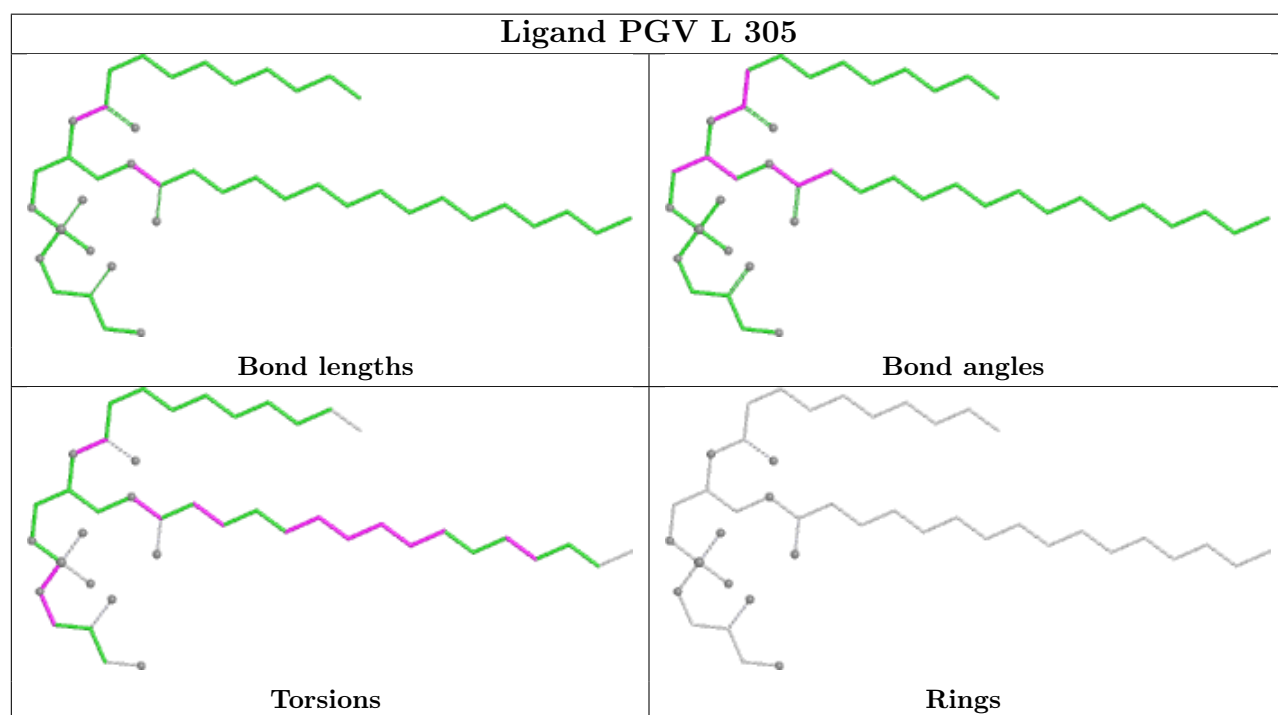
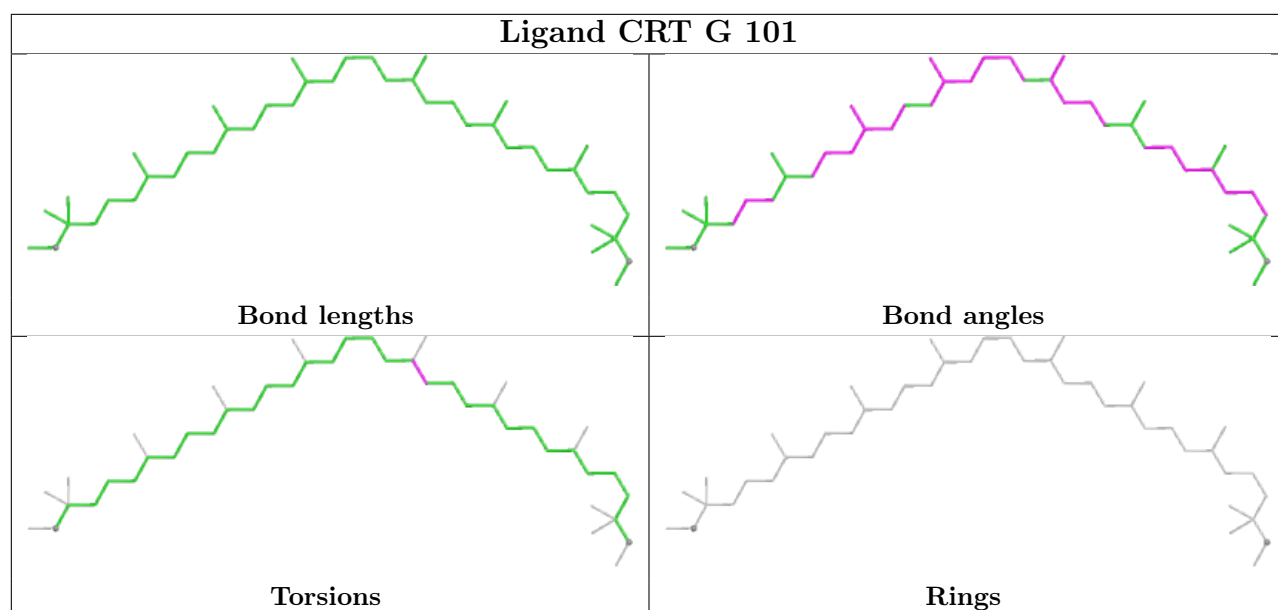
Ligand PGV 1 106

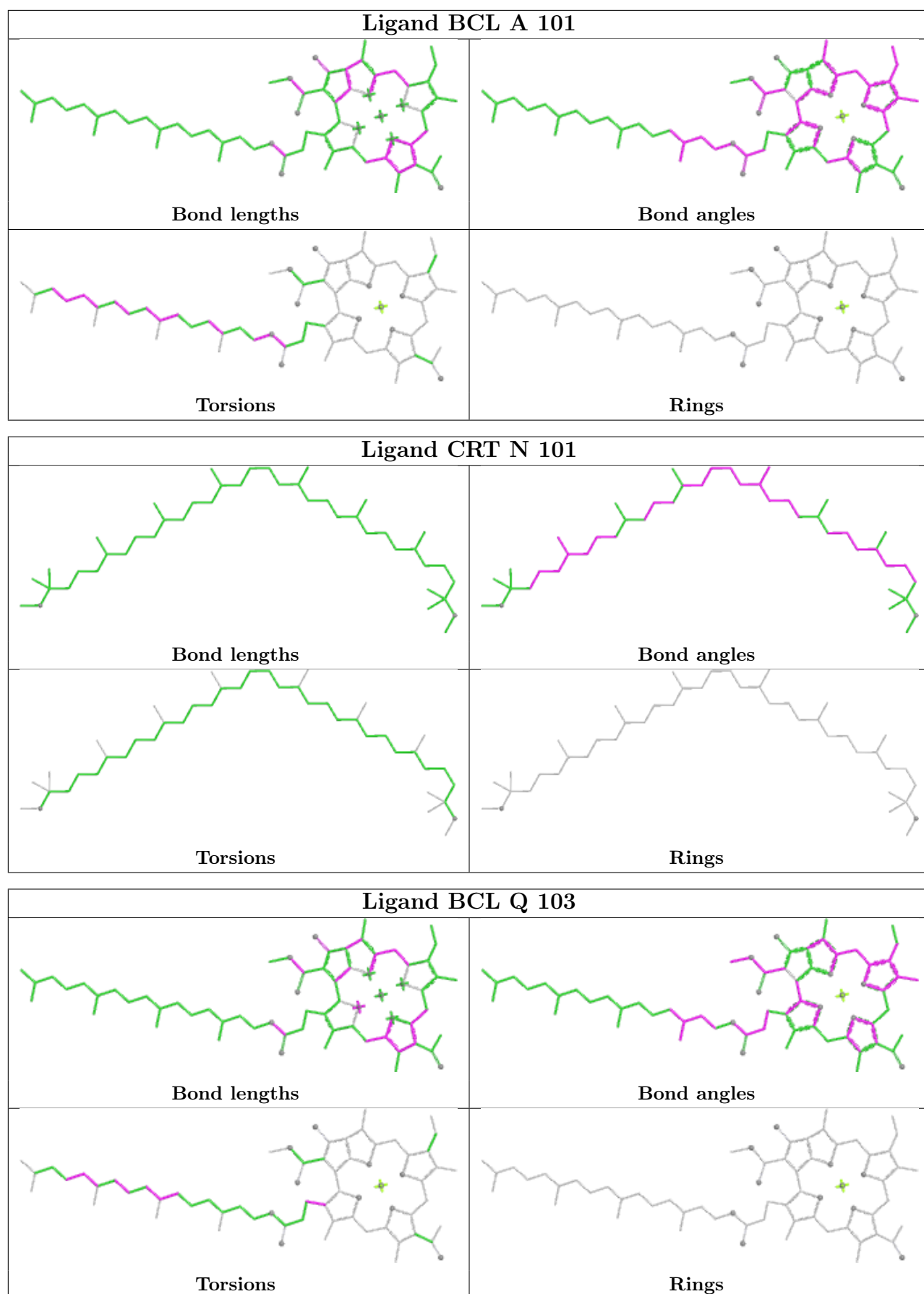


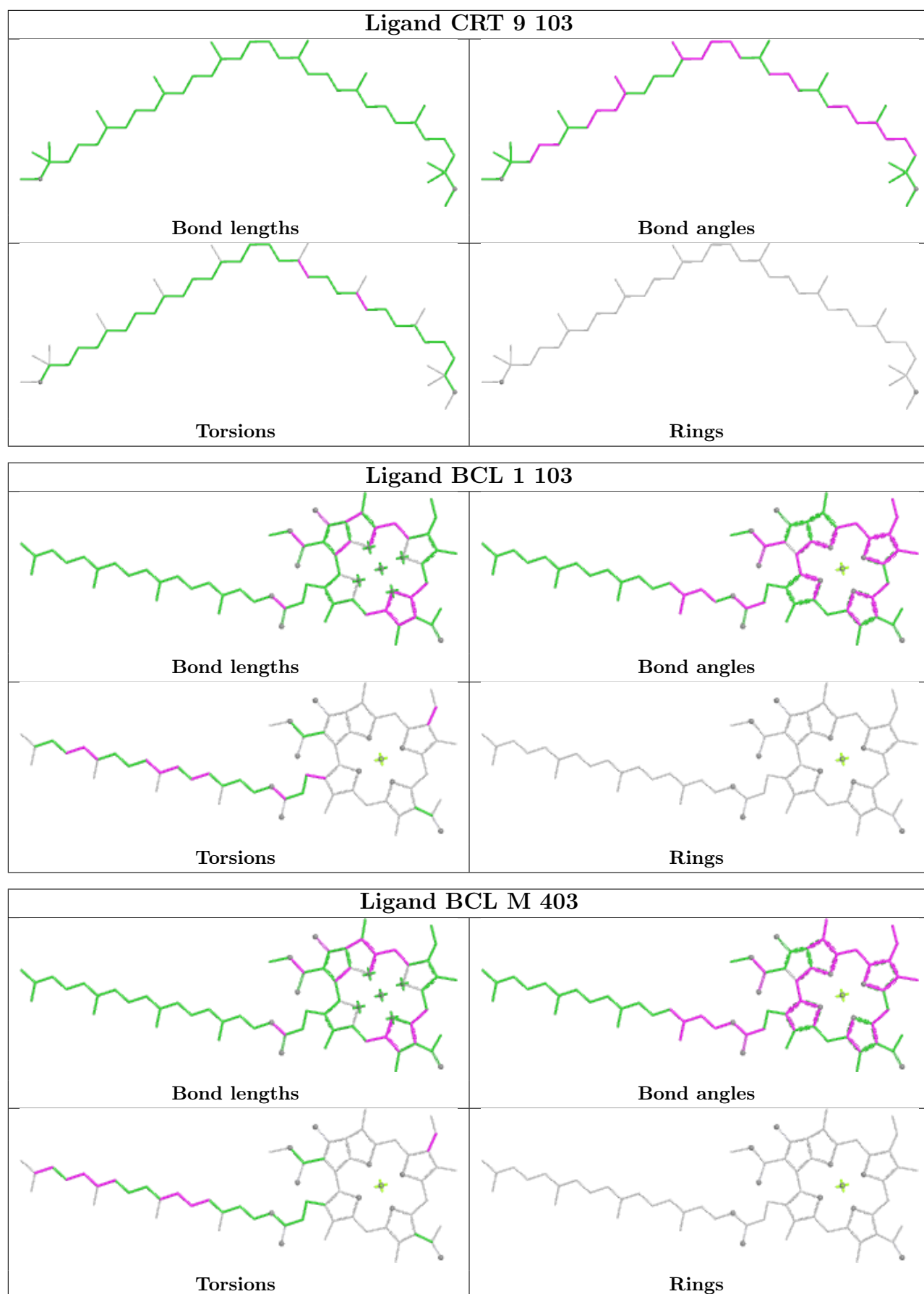
Ligand BCL 9 104











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%)	0.04	1 (0%) 90 91	32, 48, 81, 113	0
2	L	280/281 (99%)	-0.12	2 (0%) 84 86	31, 44, 59, 100	1 (0%)
3	M	318/325 (97%)	-0.10	2 (0%) 85 87	20, 42, 54, 85	2 (0%)
4	H	255/259 (98%)	0.30	4 (1%) 70 74	29, 57, 87, 130	2 (0%)
5	1	56/61 (91%)	0.84	5 (8%) 15 16	58, 75, 118, 138	0
5	3	56/61 (91%)	0.92	6 (10%) 11 11	39, 77, 106, 145	1 (1%)
5	5	54/61 (88%)	0.73	4 (7%) 20 22	54, 70, 95, 114	0
5	7	57/61 (93%)	0.71	3 (5%) 32 34	54, 65, 127, 139	0
5	9	57/61 (93%)	0.68	4 (7%) 22 24	51, 64, 122, 153	0
5	A	54/61 (88%)	0.68	2 (3%) 45 48	55, 67, 98, 117	0
5	D	55/61 (90%)	0.64	3 (5%) 30 32	37, 69, 101, 136	1 (1%)
5	F	55/61 (90%)	0.63	3 (5%) 30 32	40, 70, 126, 136	1 (1%)
5	I	57/61 (93%)	0.72	5 (8%) 15 16	36, 70, 120, 150	1 (1%)
5	K	57/61 (93%)	0.56	3 (5%) 32 34	50, 64, 109, 131	0
5	O	56/61 (91%)	0.36	3 (5%) 31 33	30, 58, 97, 133	1 (1%)
5	Q	57/61 (93%)	0.27	1 (1%) 67 71	36, 49, 87, 143	0
5	S	56/61 (91%)	0.57	5 (8%) 15 16	20, 53, 109, 147	3 (5%)
5	U	58/61 (95%)	0.48	2 (3%) 48 51	43, 56, 117, 144	0
5	W	56/61 (91%)	0.50	1 (1%) 67 71	47, 60, 98, 120	0
5	Y	57/61 (93%)	0.73	6 (10%) 11 12	51, 67, 113, 145	0
6	0	43/47 (91%)	0.59	1 (2%) 61 65	64, 74, 91, 116	0
6	2	41/47 (87%)	0.75	1 (2%) 59 63	68, 84, 105, 109	0
6	4	42/47 (89%)	0.71	1 (2%) 59 63	65, 80, 98, 107	0
6	6	42/47 (89%)	0.81	1 (2%) 59 63	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%)	0.73	2 (4%) 35 37	65, 74, 96, 119	0
6	B	42/47 (89%)	0.63	0 100 100	68, 80, 97, 108	0
6	E	38/47 (80%)	0.45	0 100 100	69, 84, 113, 118	0
6	G	42/47 (89%)	0.53	0 100 100	66, 88, 125, 148	0
6	J	42/47 (89%)	0.74	4 (9%) 14 14	64, 82, 107, 112	0
6	N	42/47 (89%)	0.59	1 (2%) 59 63	57, 75, 95, 102	0
6	P	42/47 (89%)	0.22	1 (2%) 59 63	49, 63, 84, 88	0
6	R	41/47 (87%)	0.38	1 (2%) 59 63	46, 58, 80, 82	0
6	T	43/47 (91%)	0.48	1 (2%) 61 65	49, 61, 82, 97	0
6	V	42/47 (89%)	0.77	3 (7%) 22 23	53, 72, 101, 116	0
6	X	41/47 (87%)	0.53	2 (4%) 35 37	60, 78, 103, 108	0
6	Z	40/47 (85%)	0.48	0 100 100	63, 80, 101, 107	0
All	All	2726/2997 (90%)	0.36	84 (3%) 51 55	20, 60, 101, 153	13 (0%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	9	58	LEU	4.6
5	S	58	LEU	4.3
6	8	9	LEU	4.2
5	1	59	GLY	4.1
6	R	6	LEU	3.9
6	8	6	LEU	3.9
5	A	6	ALA	3.9
5	3	59	GLY	3.9
5	F	59	GLY	3.7
5	3	58	LEU	3.6
5	F	58	LEU	3.6
5	7	14	ILE	3.6
6	V	37	LEU	3.2
5	K	3	THR	3.1
5	I	3	THR	3.0
6	V	35	ALA	3.0
5	3	29	ILE	2.9
2	L	2	ALA	2.9
5	S	4	MET	2.9
5	Y	59	GLY	2.9
6	6	5	SER	2.8

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Mol	Chain	Res	Type	RSRZ
5	O	59	GLY	2.8
5	U	6	ALA	2.8
3	M	319	THR	2.8
5	I	6	ALA	2.7
3	M	236	ASP	2.7
6	X	6	LEU	2.7
6	T	4	LYS	2.7
5	1	57	ALA	2.7
6	V	26	TYR	2.7
1	C	59	VAL	2.7
6	2	6	LEU	2.6
5	K	14	ILE	2.6
5	5	6	ALA	2.6
5	1	58	LEU	2.5
5	Y	14	ILE	2.5
5	3	14	ILE	2.5
5	U	58	LEU	2.5
6	N	6	LEU	2.5
5	9	14	ILE	2.5
6	J	26	TYR	2.5
6	0	6	LEU	2.5
5	1	6	ALA	2.5
5	Y	6	ALA	2.4
5	9	59	GLY	2.4
5	3	55	TYR	2.4
5	Y	17	PRO	2.4
6	J	5	SER	2.4
5	7	58	LEU	2.4
2	L	59	THR	2.4
5	S	3	THR	2.4
5	Y	4	MET	2.4
5	K	8	LEU	2.3
5	5	59	GLY	2.3
4	H	87	VAL	2.3
4	H	259	LEU	2.3
5	W	6	ALA	2.3
5	Y	13	LEU	2.3
5	5	13	LEU	2.3
4	H	166	THR	2.3
6	J	41	LEU	2.3
5	A	58	LEU	2.2
6	J	31	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
6	4	5	SER	2.2
5	F	6	ALA	2.2
5	1	29	ILE	2.2
5	I	4	MET	2.2
5	5	8	LEU	2.2
6	P	37	LEU	2.2
5	D	59	GLY	2.2
5	O	4	MET	2.2
5	7	3	THR	2.2
5	3	4	MET	2.1
5	Q	3	THR	2.1
5	D	58	LEU	2.1
5	O	55	TYR	2.1
5	9	3	THR	2.1
5	S	8	LEU	2.1
4	H	5	ILE	2.0
6	X	33	VAL	2.0
5	D	21	LEU	2.0
5	I	8	LEU	2.0
5	S	19	ARG	2.0
5	I	24	ILE	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
20	PEF	U	106	5/47	0.54	0.09	156,156,159,160	0
20	PEF	M	408	5/47	0.57	0.10	161,162,163,165	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	PEF	5	104	5/47	0.60	0.11	126,127,129,131	0
22	CDL	Y	103	40/100	0.66	0.17	114,129,148,149	0
20	PEF	W	104	5/47	0.71	0.08	146,148,148,149	0
22	CDL	D	104	40/100	0.74	0.19	116,142,163,164	0
22	CDL	S	104	62/100	0.77	0.16	73,116,153,162	0
20	PEF	U	105	5/47	0.77	0.16	113,115,116,118	0
10	SO4	M	413	5/5	0.78	0.12	125,126,126,130	0
15	UQ8	L	309	18/53	0.80	0.24	102,114,125,132	0
21	LDA	M	412	14/16	0.81	0.20	65,82,109,113	0
20	PEF	1	105	5/47	0.81	0.10	119,119,121,121	0
20	PEF	3	104	5/47	0.81	0.10	136,137,138,142	0
10	SO4	C	507	5/5	0.81	0.12	113,114,117,120	0
16	UNL	4	101	12/-	0.82	0.22	72,88,103,105	0
12	PGV	C	509	21/51	0.82	0.22	81,101,108,113	0
16	UNL	J	103	12/-	0.82	0.20	74,79,93,94	0
16	UNL	P	102	12/-	0.82	0.23	67,74,82,82	0
12	PGV	3	105	51/51	0.83	0.20	76,101,155,158	0
20	PEF	M	410	5/47	0.83	0.10	94,98,100,102	0
16	UNL	8	101	12/-	0.83	0.20	64,74,96,96	0
21	LDA	O	105	14/16	0.84	0.23	61,75,110,112	0
16	UNL	T	101	12/-	0.84	0.19	45,68,81,82	0
22	CDL	Q	105	75/100	0.84	0.17	62,97,142,143	0
20	PEF	I	104	5/47	0.84	0.09	99,107,109,112	0
12	PGV	L	306	44/51	0.84	0.17	53,75,98,108	0
21	LDA	V	102	16/16	0.85	0.17	60,77,119,122	0
16	UNL	R	101	12/-	0.85	0.19	57,68,75,77	0
15	UQ8	L	308	53/53	0.85	0.20	60,90,99,104	0
16	UNL	X	101	12/-	0.85	0.20	68,76,82,85	0
15	UQ8	M	418	18/53	0.85	0.17	61,74,96,102	0
9	GOL	C	506	6/6	0.86	0.14	63,68,72,75	0
16	UNL	0	103	12/-	0.86	0.20	77,84,87,87	0
21	LDA	J	102	16/16	0.86	0.17	74,90,112,114	0
22	CDL	Y	104	13/100	0.86	0.14	107,120,124,128	0
23	LMT	M	420	35/35	0.86	0.15	64,99,112,121	0
12	PGV	M	415	37/51	0.87	0.13	60,83,116,121	0
20	PEF	M	409	5/47	0.87	0.10	56,67,83,95	0
12	PGV	1	106	31/51	0.87	0.17	83,102,125,129	0
10	SO4	L	304	5/5	0.87	0.11	136,137,138,138	0
15	UQ8	7	104	33/53	0.87	0.17	60,74,94,100	0
16	UNL	B	101	12/-	0.88	0.16	69,80,88,91	0
12	PGV	M	414	46/51	0.88	0.15	52,74,89,94	0
12	PGV	A	105	33/51	0.88	0.17	60,93,108,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CDL	H	302	64/100	0.88	0.15	75,89,107,113	0
16	UNL	L	307	12/-	0.88	0.21	79,88,96,96	0
23	LMT	F	104	35/35	0.88	0.13	61,78,92,92	0
20	PEF	K	105	27/47	0.89	0.16	63,85,92,97	0
22	CDL	K	104	86/100	0.89	0.15	56,92,114,120	0
16	UNL	E	101	12/-	0.89	0.20	78,93,101,102	0
16	UNL	G	102	12/-	0.89	0.19	77,85,93,93	0
16	UNL	Z	103	12/-	0.90	0.17	68,80,92,95	0
16	UNL	M	417	9/-	0.91	0.15	58,64,73,75	0
16	UNL	2	102	12/-	0.91	0.17	71,80,90,92	0
22	CDL	M	416	39/100	0.91	0.13	46,80,113,119	0
12	PGV	L	305	43/51	0.91	0.14	45,76,104,109	0
9	GOL	H	301	6/6	0.91	0.13	58,78,82,84	0
20	PEF	M	419	47/47	0.91	0.14	58,75,93,97	0
19	CRT	J	101	44/44	0.92	0.14	59,74,97,100	0
19	CRT	1	104	44/44	0.92	0.13	58,78,96,99	0
19	CRT	2	101	44/44	0.92	0.14	67,78,94,99	0
13	BCL	1	103	66/66	0.92	0.13	49,70,97,104	0
16	UNL	6	102	12/-	0.92	0.17	76,81,91,93	0
13	BCL	3	102	66/66	0.92	0.13	61,75,105,110	0
12	PGV	D	105	35/51	0.92	0.12	55,72,100,113	0
22	CDL	H	304	79/100	0.92	0.14	44,73,107,111	0
12	PGV	H	303	36/51	0.93	0.13	47,59,82,89	0
13	BCL	1	102	66/66	0.93	0.12	59,67,107,113	0
19	CRT	9	102	44/44	0.93	0.12	53,68,100,105	0
18	MQ8	M	406	53/53	0.93	0.14	36,53,116,123	0
13	BCL	3	103	66/66	0.93	0.12	53,69,93,96	0
19	CRT	N	101	44/44	0.93	0.12	50,67,86,94	0
13	BCL	5	102	66/66	0.94	0.12	55,69,109,111	0
19	CRT	U	104	44/44	0.94	0.11	48,72,91,96	0
19	CRT	Z	101	44/44	0.94	0.13	58,72,99,100	0
13	BCL	7	102	61/66	0.94	0.11	53,64,96,103	0
13	BCL	7	103	66/66	0.94	0.11	53,63,95,102	0
19	CRT	6	101	44/44	0.94	0.11	48,69,84,87	0
11	LHG	C	508	9/49	0.94	0.12	52,61,67,69	0
19	CRT	M	407	44/44	0.94	0.10	31,39,82,90	0
19	CRT	A	104	44/44	0.94	0.13	62,74,97,101	0
21	LDA	I	105	16/16	0.94	0.14	36,70,75,77	0
19	CRT	G	101	44/44	0.94	0.12	61,80,114,123	0
13	BCL	O	103	66/66	0.94	0.11	41,51,89,96	0
13	BCL	5	103	66/66	0.95	0.10	50,62,90,98	0
13	BCL	K	102	66/66	0.95	0.11	50,63,102,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	BCL	A	101	66/66	0.95	0.10	54,69,113,118	0
13	BCL	9	104	66/66	0.95	0.10	54,63,103,106	0
13	BCL	0	102	66/66	0.95	0.10	54,65,97,108	0
15	UQ8	L	303	33/53	0.95	0.11	36,45,77,85	0
19	CRT	9	103	44/44	0.95	0.11	51,67,94,105	0
19	CRT	0	101	44/44	0.95	0.10	51,68,88,95	0
13	BCL	S	103	66/66	0.95	0.10	40,48,90,96	0
13	BCL	W	102	66/66	0.95	0.12	48,59,114,118	0
13	BCL	W	103	66/66	0.95	0.10	49,60,94,97	0
13	BCL	Y	102	66/66	0.95	0.11	49,60,110,113	0
13	BCL	Z	102	66/66	0.95	0.11	52,64,98,103	0
13	BCL	A	103	66/66	0.95	0.11	58,70,104,109	0
13	BCL	D	102	66/66	0.95	0.11	55,70,117,121	0
13	BCL	F	102	66/66	0.95	0.10	57,69,114,117	0
13	BCL	F	103	66/66	0.95	0.11	55,70,107,113	0
13	BCL	I	102	66/66	0.95	0.10	61,68,100,104	0
13	BCL	D	103	66/66	0.96	0.10	57,69,91,92	0
13	BCL	K	103	66/66	0.96	0.09	47,58,98,102	0
13	BCL	M	403	66/66	0.96	0.09	26,35,84,90	0
19	CRT	O	104	44/44	0.96	0.09	37,51,75,82	0
20	PEF	M	411	5/47	0.96	0.07	40,45,52,54	0
19	CRT	P	101	44/44	0.96	0.09	38,55,77,80	0
19	CRT	Q	104	44/44	0.96	0.09	42,55,73,76	0
13	BCL	Q	102	66/66	0.96	0.10	40,48,94,99	0
19	CRT	V	101	44/44	0.96	0.09	41,62,85,87	0
13	BCL	Q	103	66/66	0.96	0.09	39,47,84,93	0
14	BPH	L	302	65/65	0.96	0.08	29,40,54,59	0
13	BCL	S	102	66/66	0.96	0.09	38,49,96,110	0
13	BCL	I	103	66/66	0.96	0.09	51,65,93,95	0
13	BCL	U	102	66/66	0.96	0.09	42,53,101,104	0
13	BCL	U	103	66/66	0.96	0.10	44,55,92,101	0
13	BCL	M	404	66/66	0.97	0.06	27,34,45,54	0
13	BCL	O	102	66/66	0.97	0.09	44,54,102,112	0
13	BCL	L	301	66/66	0.97	0.07	27,34,43,70	0
14	BPH	M	405	65/65	0.97	0.08	29,38,111,115	0
13	BCL	M	402	66/66	0.98	0.06	30,39,54,62	0
7	HEC	C	502	43/43	0.98	0.06	39,46,52,55	0
7	HEC	C	503	43/43	0.98	0.06	29,35,42,46	0
7	HEC	C	504	43/43	0.98	0.06	34,40,47,54	0
7	HEC	C	501	43/43	0.98	0.07	52,60,67,75	0
8	MG	C	505	1/1	0.99	0.02	36,36,36,36	0
24	CA	A	102	1/1	0.99	0.03	64,64,64,64	0

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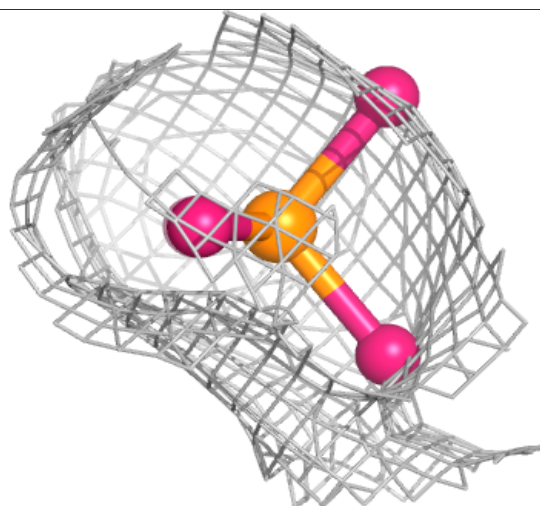
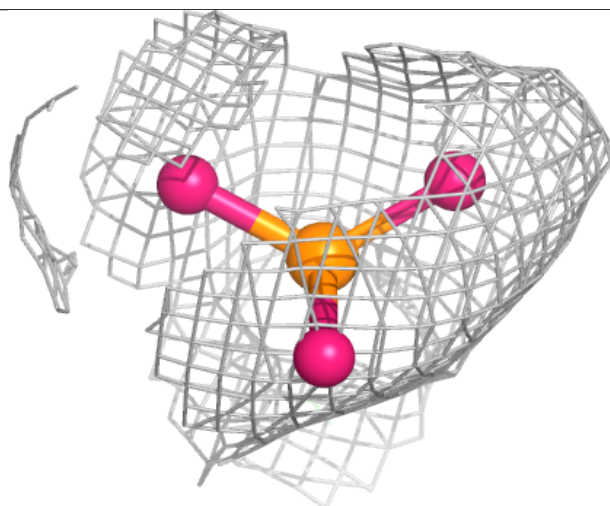
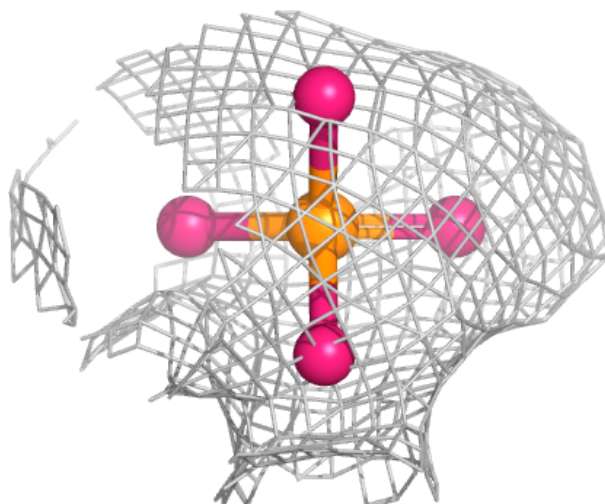
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CA	Y	101	1/1	0.99	0.03	60,60,60,60	0
24	CA	1	101	1/1	0.99	0.03	60,60,60,60	0
24	CA	3	101	1/1	0.99	0.05	68,68,68,68	0
24	CA	5	101	1/1	0.99	0.03	68,68,68,68	0
24	CA	9	101	1/1	0.99	0.03	67,67,67,67	0
24	CA	O	101	1/1	1.00	0.02	56,56,56,56	0
24	CA	Q	101	1/1	1.00	0.02	47,47,47,47	0
24	CA	S	101	1/1	1.00	0.02	44,44,44,44	0
24	CA	U	101	1/1	1.00	0.02	48,48,48,48	0
24	CA	W	101	1/1	1.00	0.02	52,52,52,52	0
17	FE	M	401	1/1	1.00	0.02	39,39,39,39	0
24	CA	D	101	1/1	1.00	0.02	64,64,64,64	0
24	CA	F	101	1/1	1.00	0.02	65,65,65,65	0
24	CA	I	101	1/1	1.00	0.02	64,64,64,64	0
24	CA	7	101	1/1	1.00	0.02	67,67,67,67	0
24	CA	K	101	1/1	1.00	0.02	63,63,63,63	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.

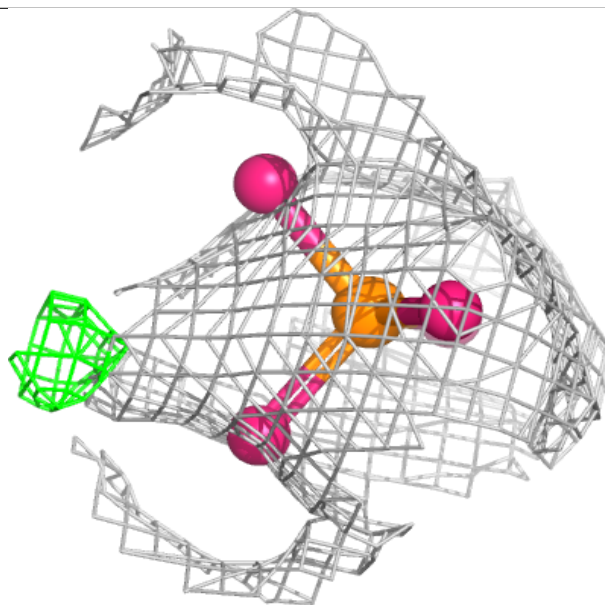
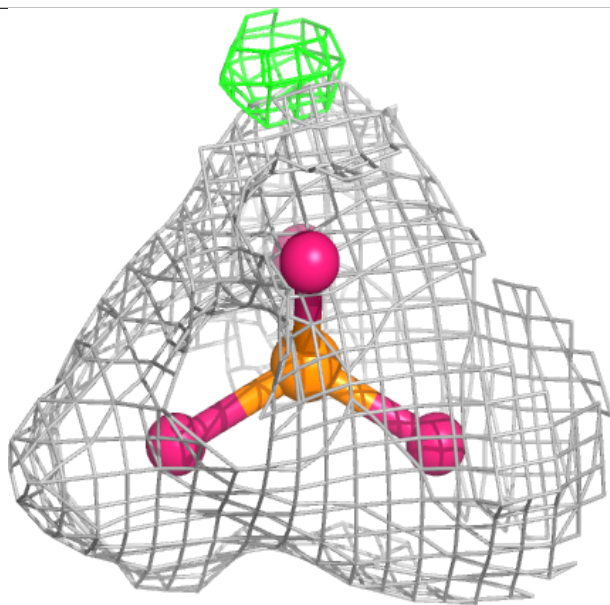
Electron density around PEF U 106:

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



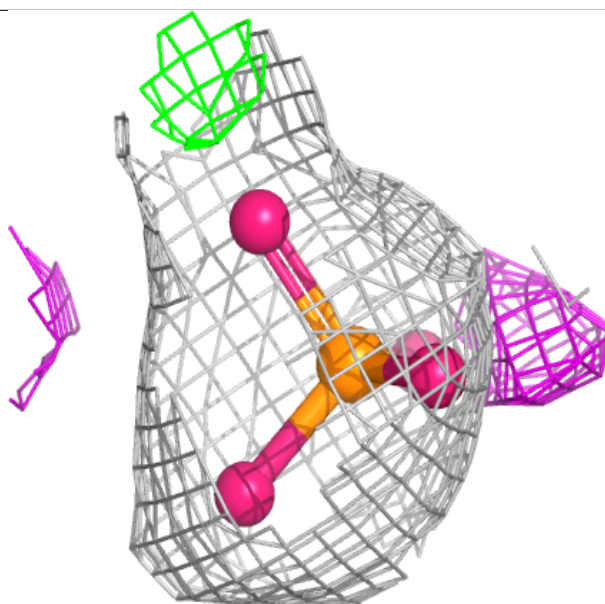
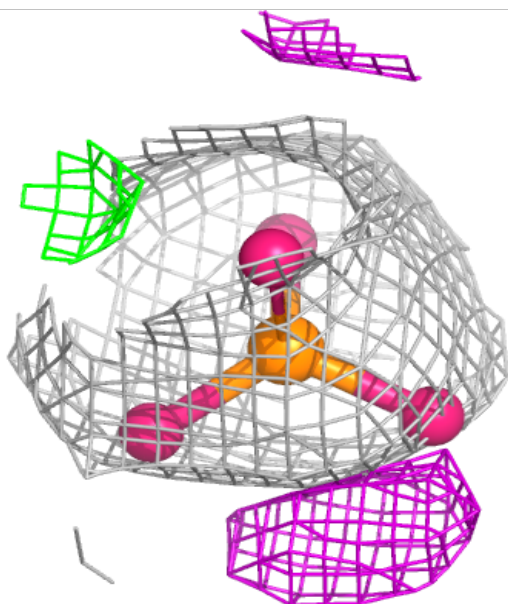
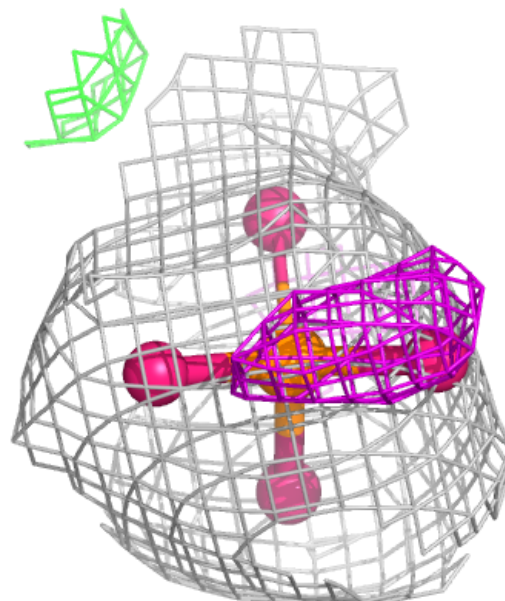
Electron density around PEF M 408:

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



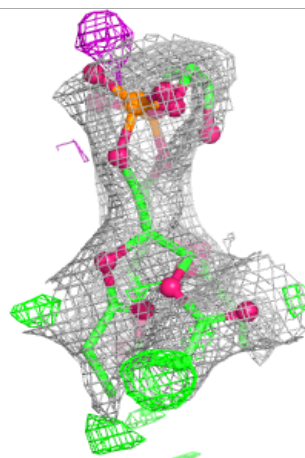
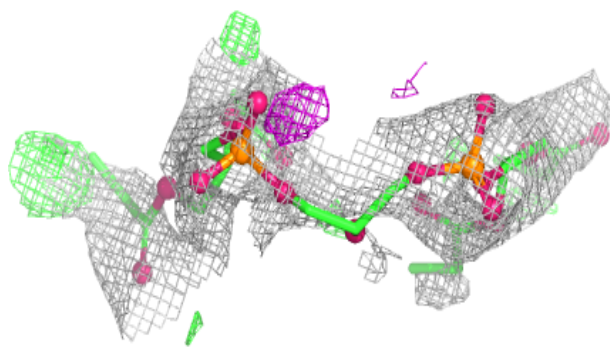
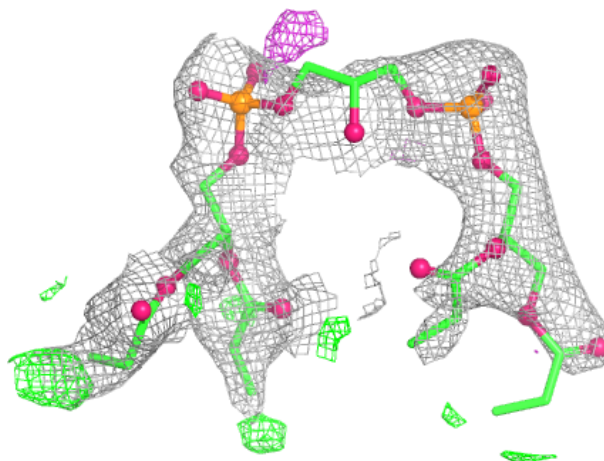
Electron density around PEF 5 104:

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



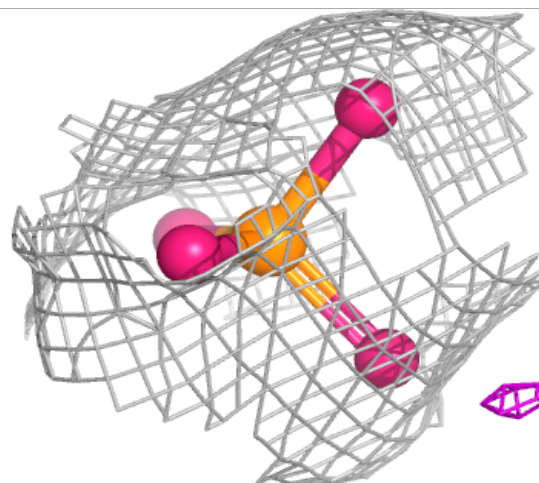
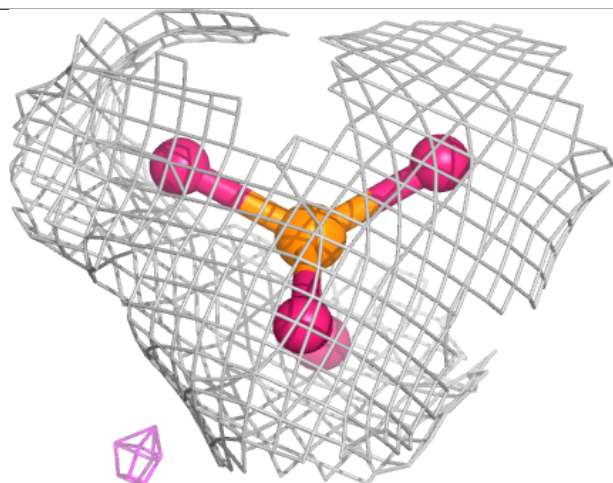
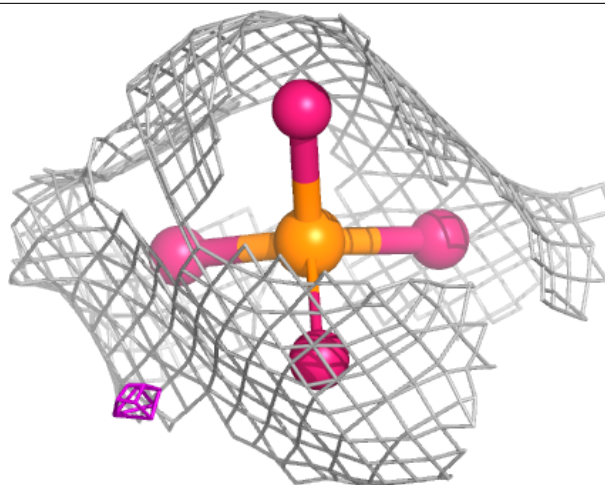
Electron density around CDL Y 103:

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



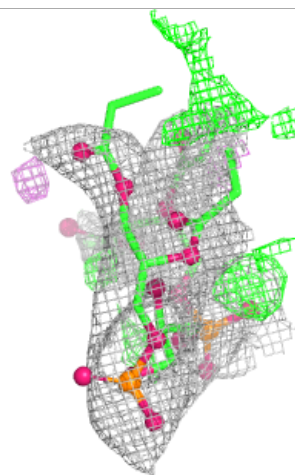
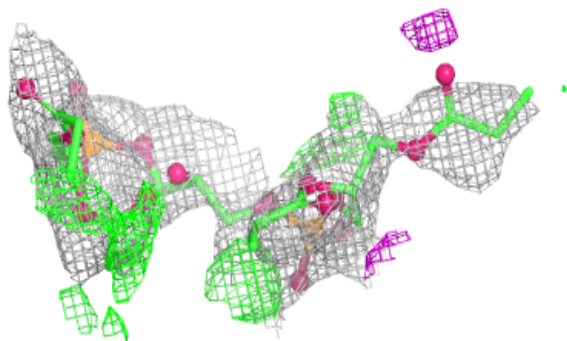
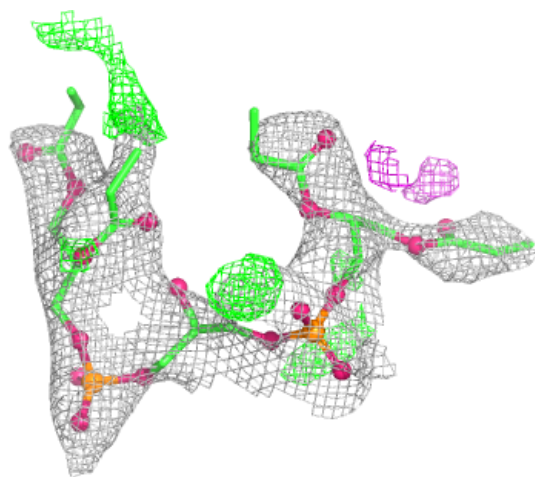
Electron density around PEF W 104:

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



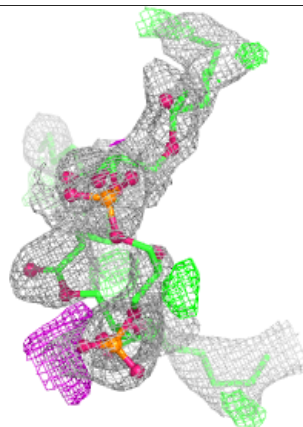
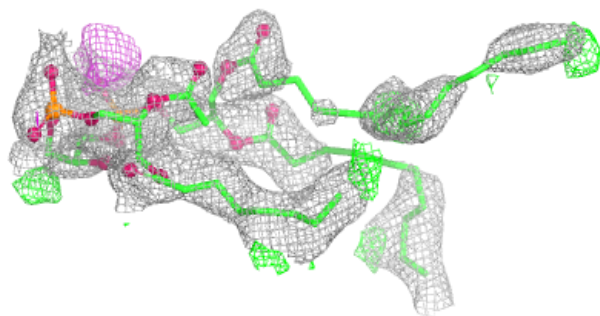
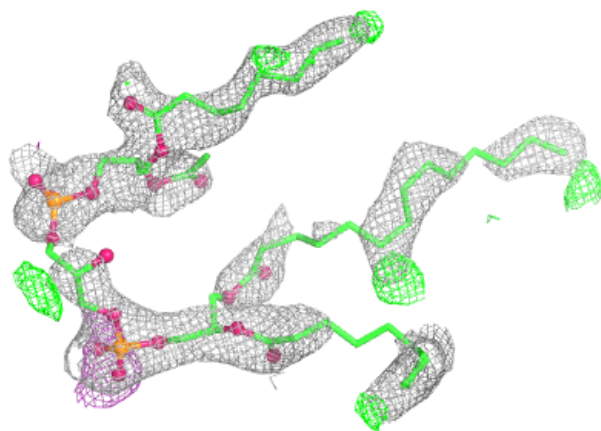
Electron density around CDL D 104:

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



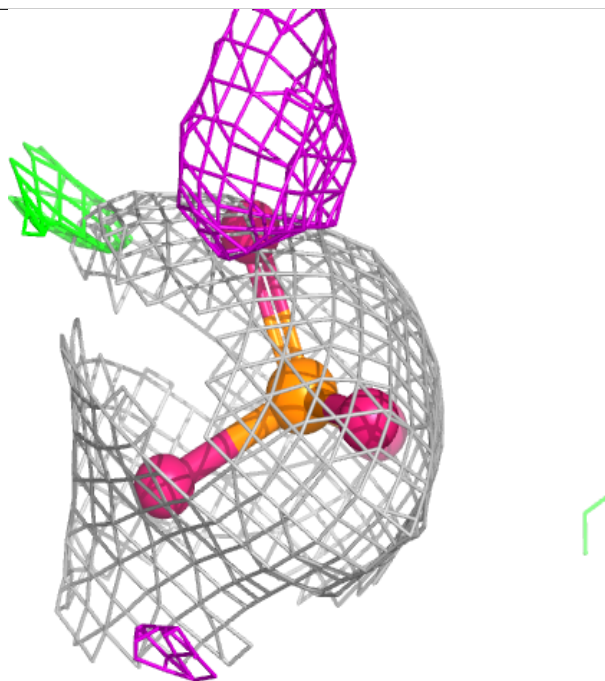
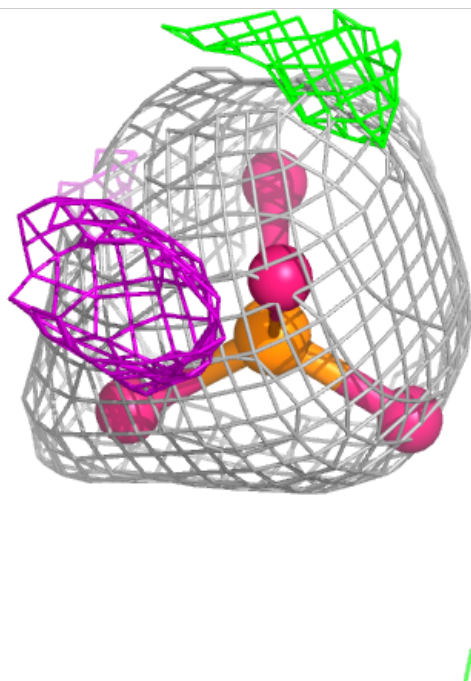
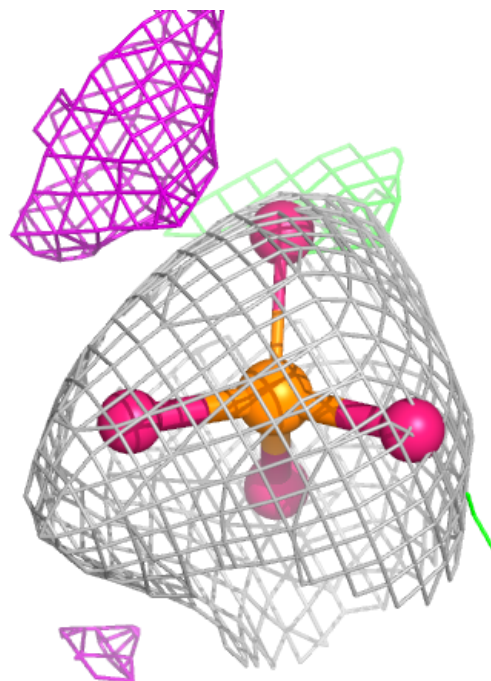
Electron density around CDL S 104:

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



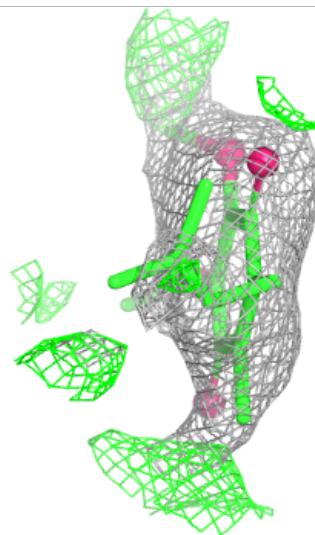
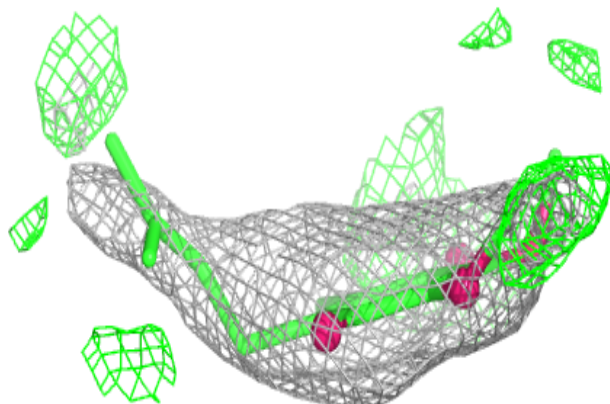
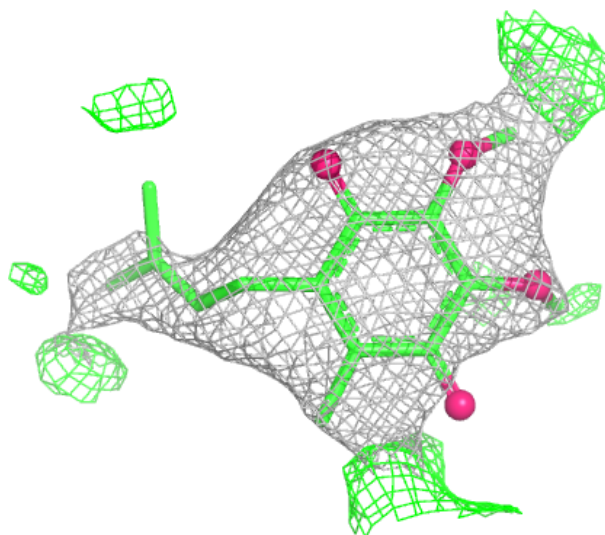
Electron density around PEF U 105:

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



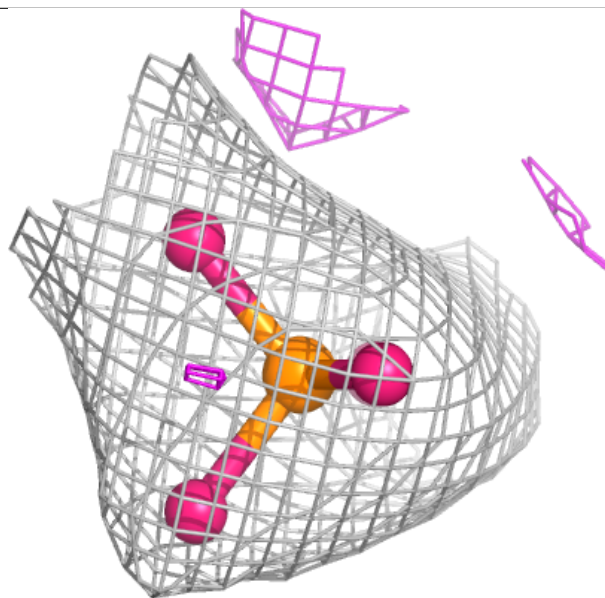
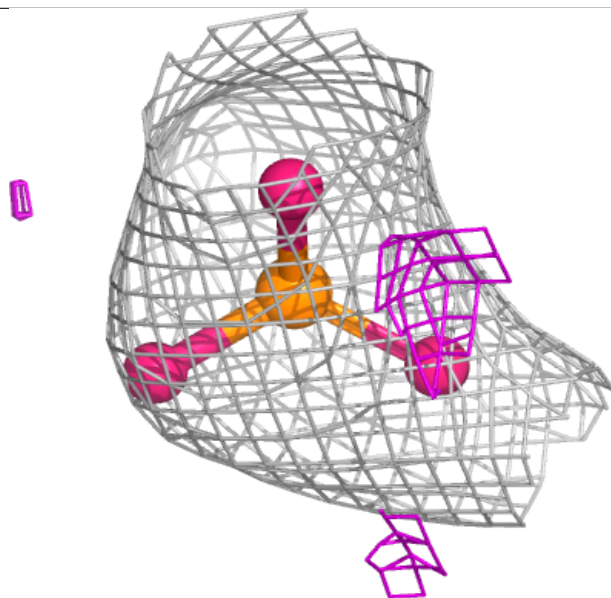
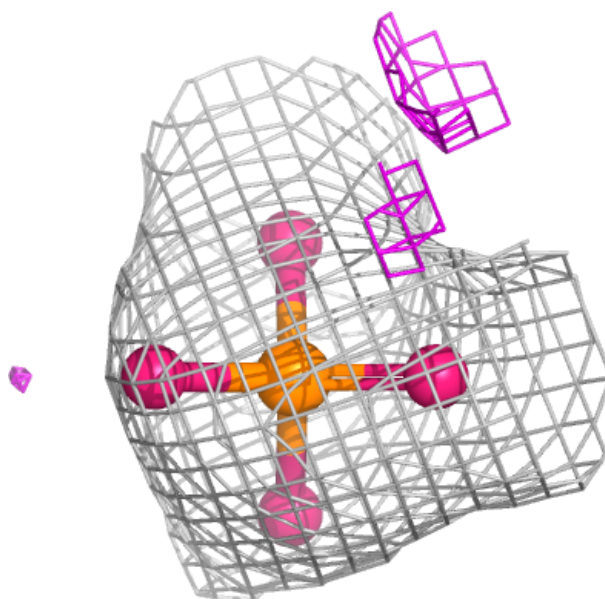
Electron density around UQ8 L 309:

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



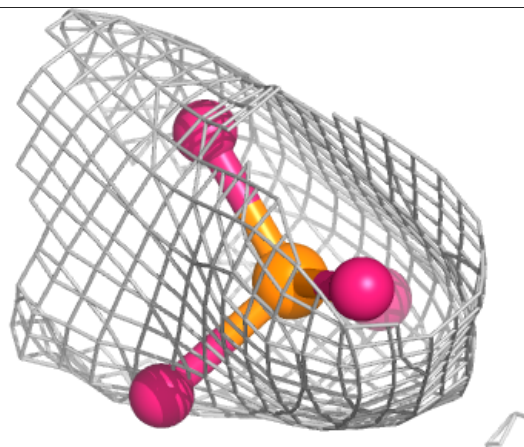
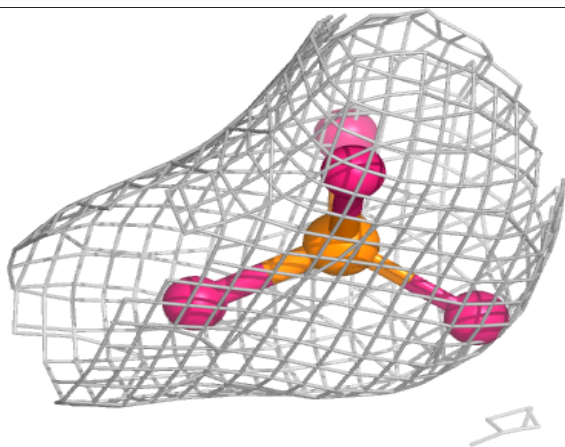
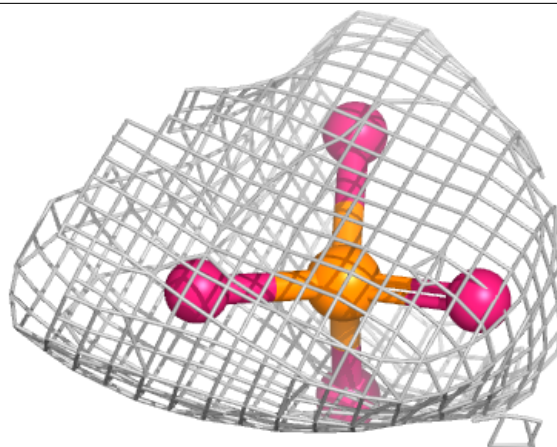
Electron density around PEF 1 105:

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



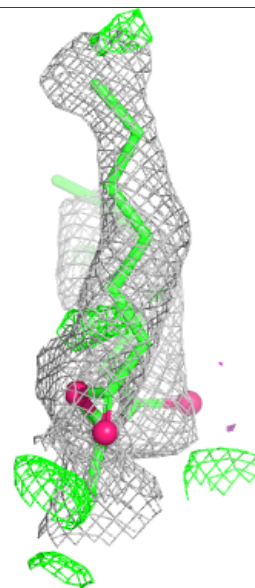
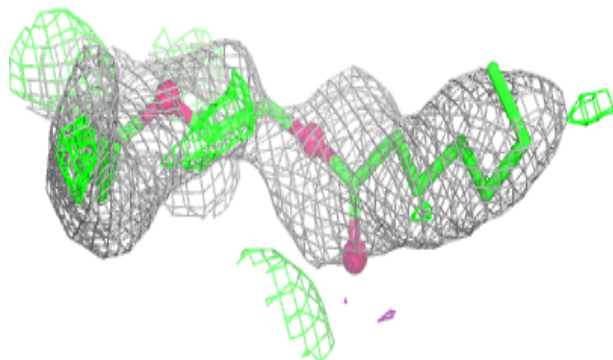
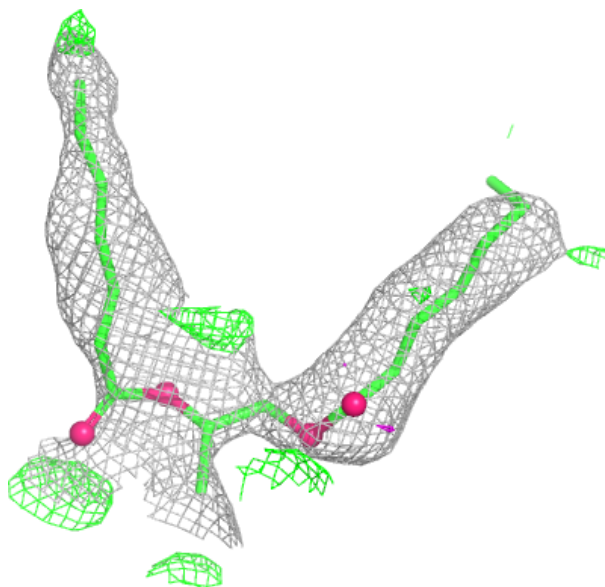
Electron density around PEF 3 104:

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



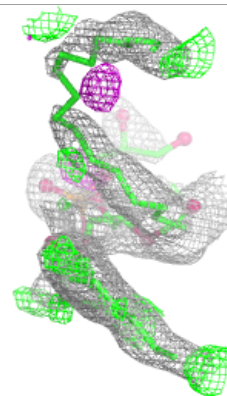
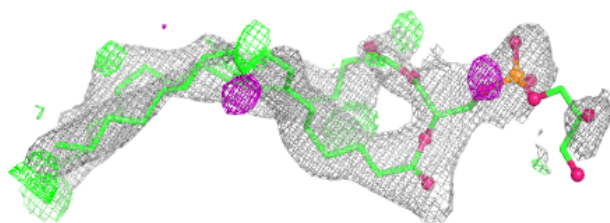
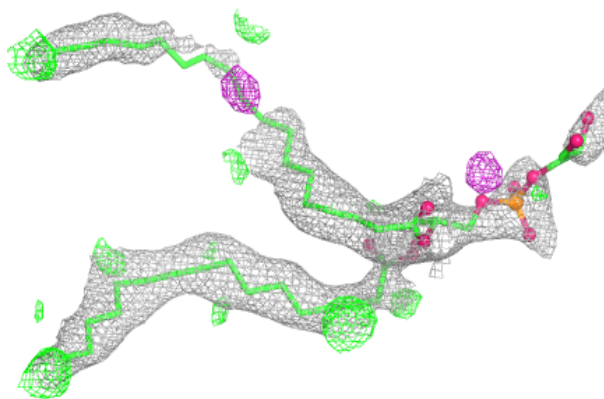
Electron density around PGV C 509:

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



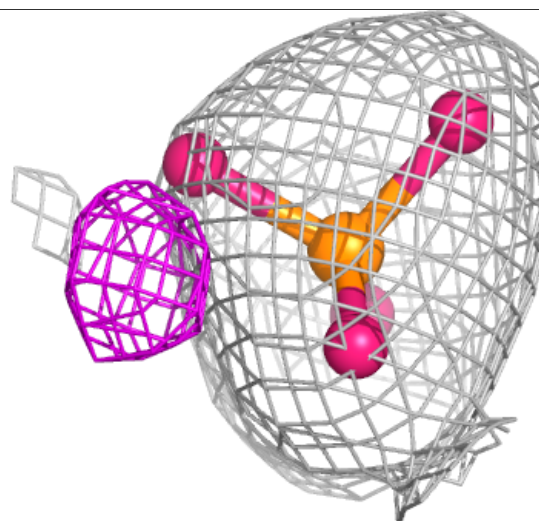
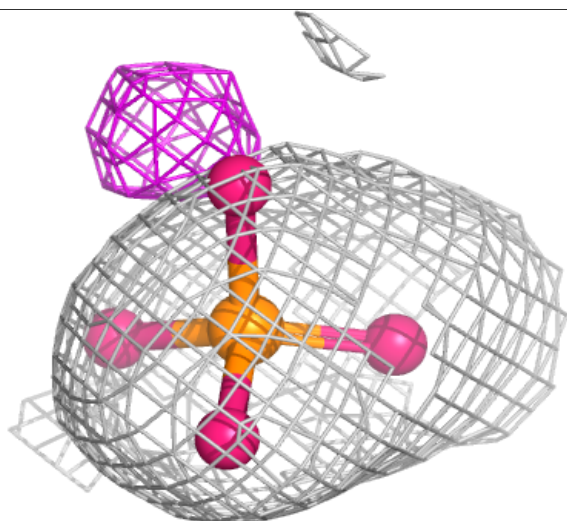
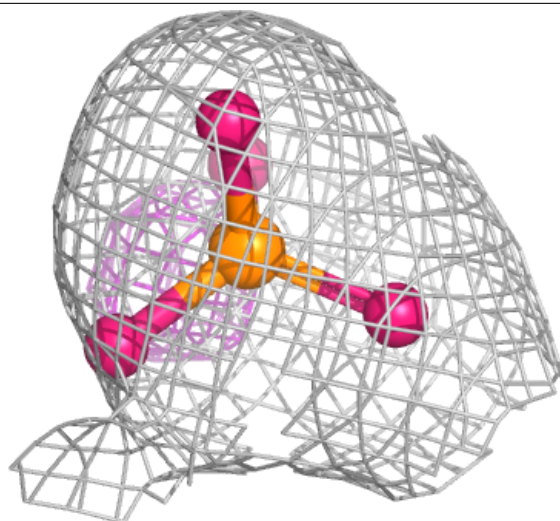
Electron density around PGV 3 105:

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



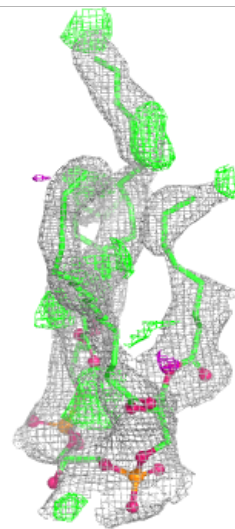
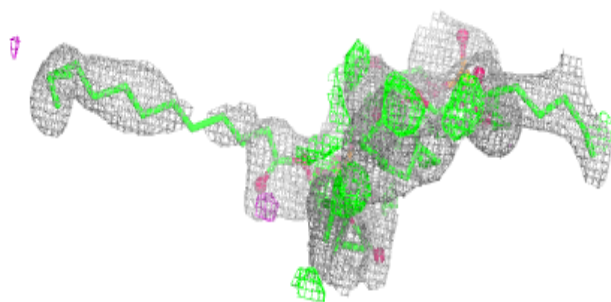
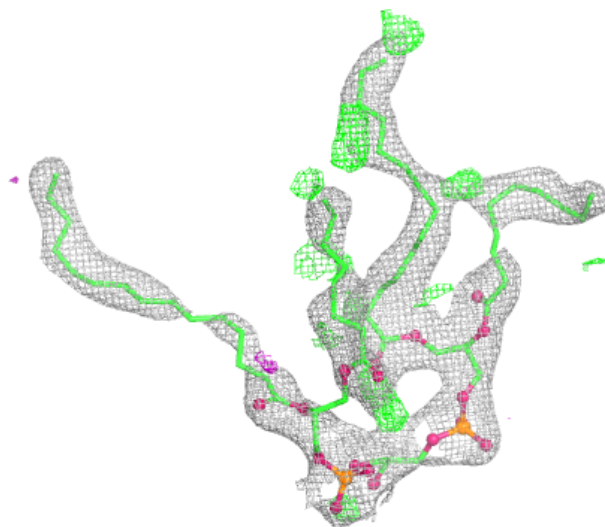
Electron density around PEF M 410:

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



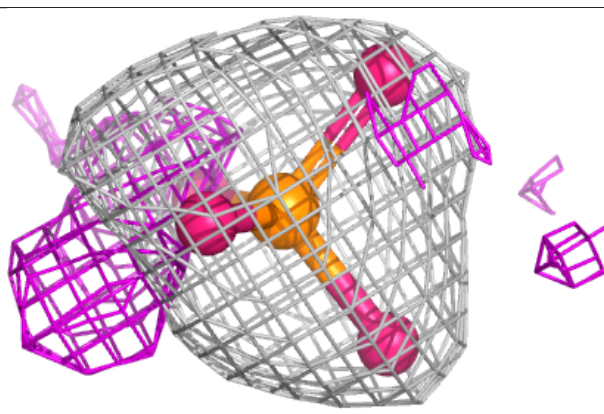
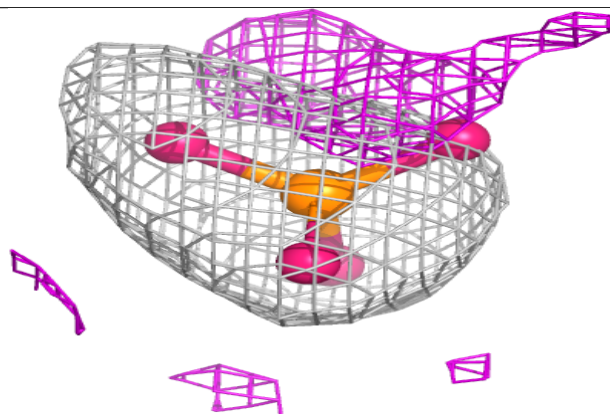
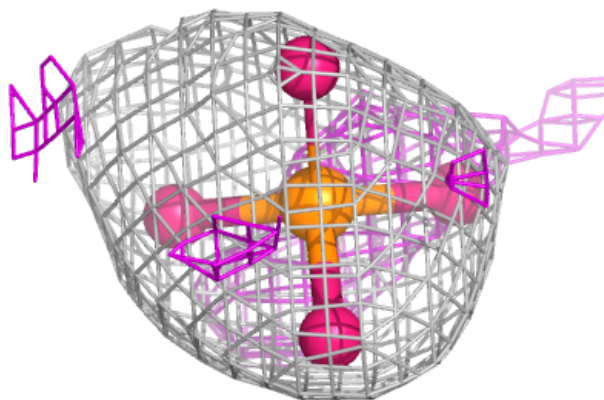
Electron density around CDL Q 105:

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

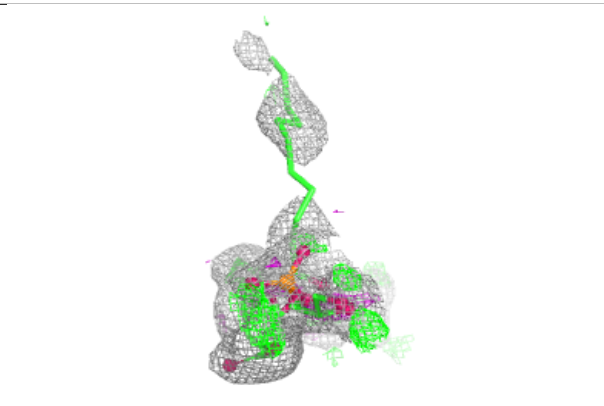
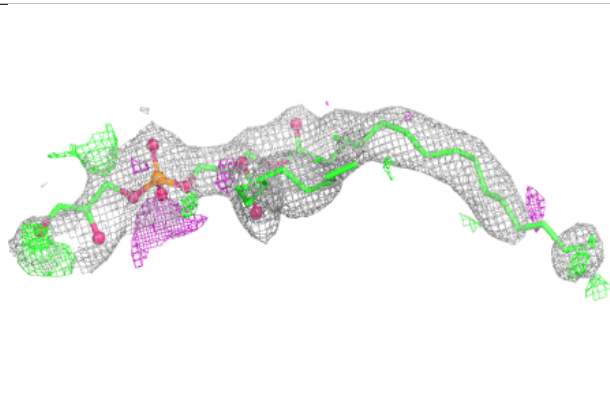
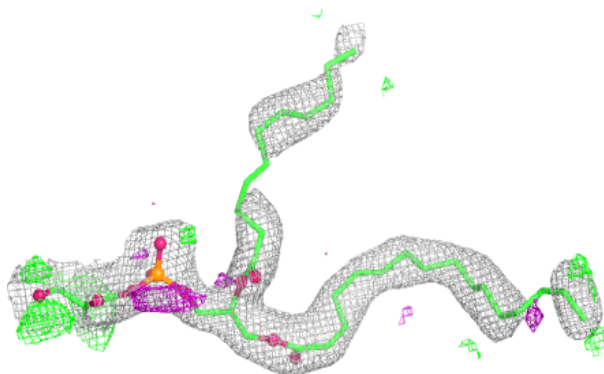


Electron density around PEF I 104:

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

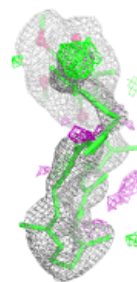
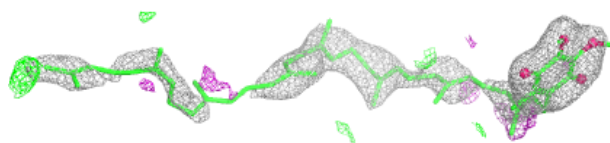
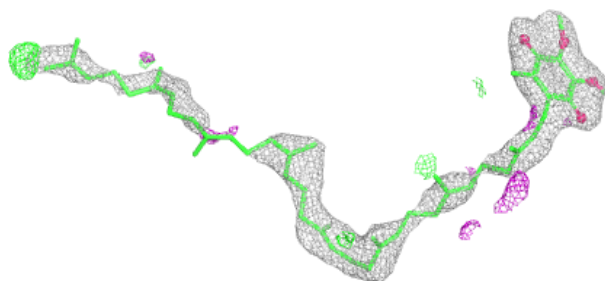
**Electron density around PGV L 306:**

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

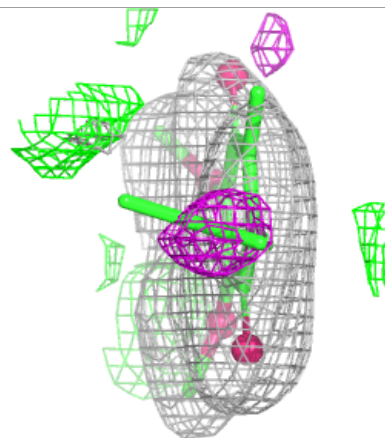
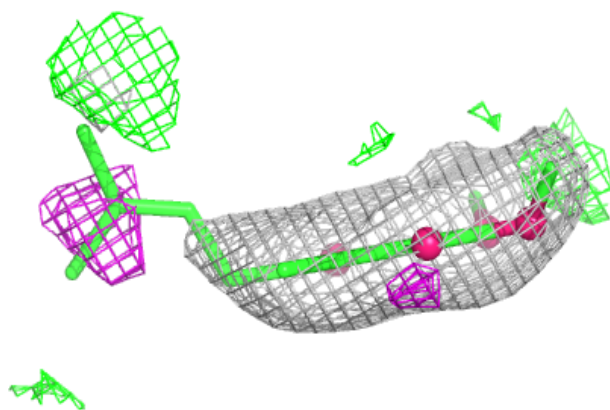
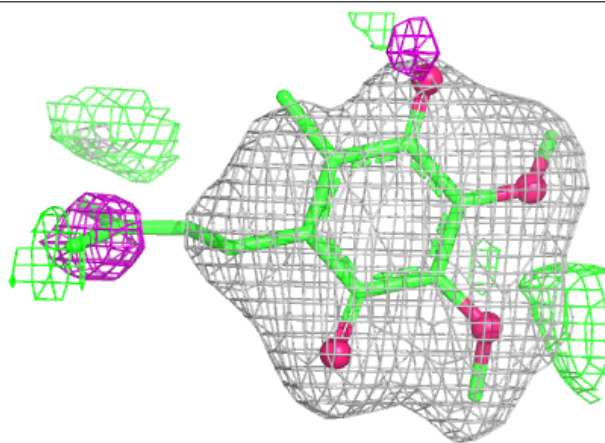


Electron density around UQ8 L 308:

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

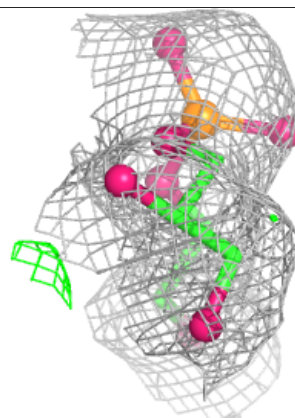
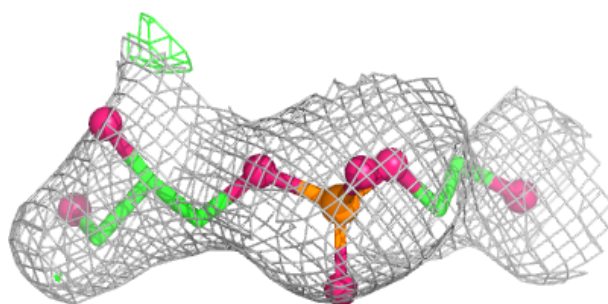
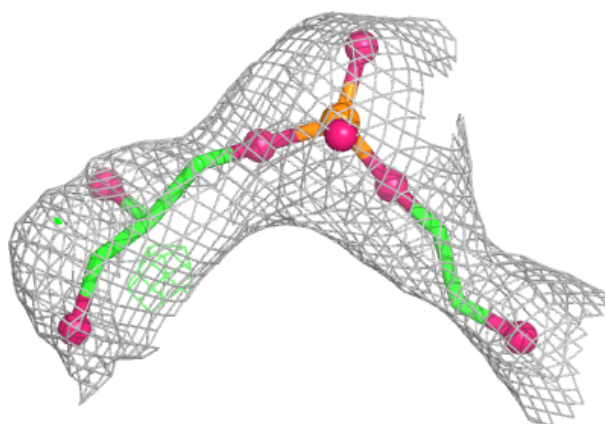
**Electron density around UQ8 M 418:**

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

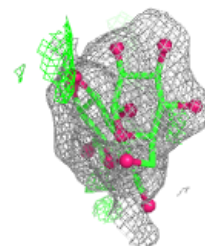
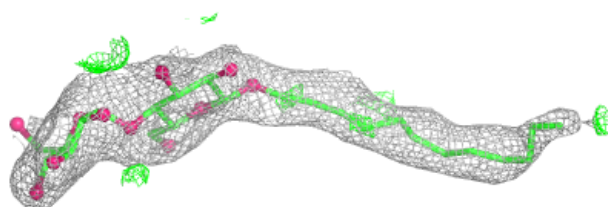
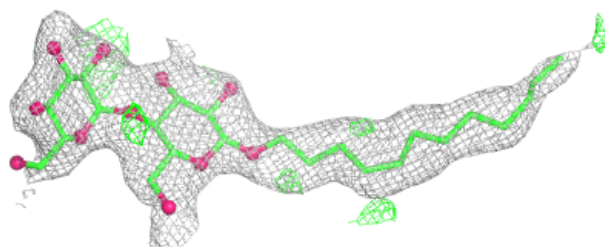


Electron density around CDL Y 104:

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

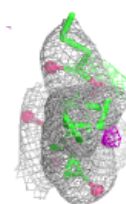
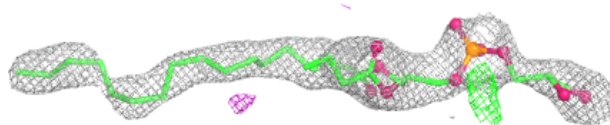
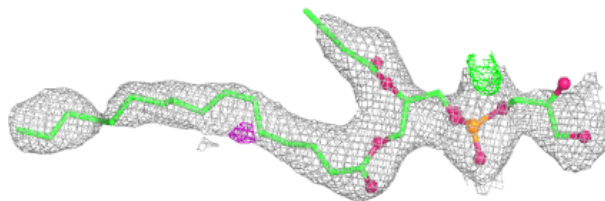
**Electron density around LMT M 420:**

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



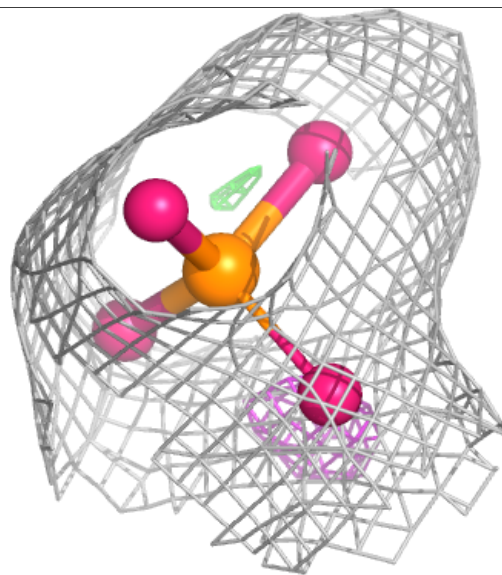
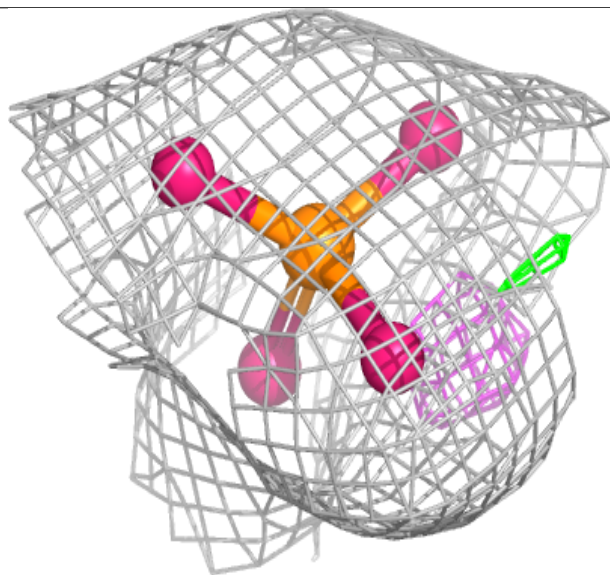
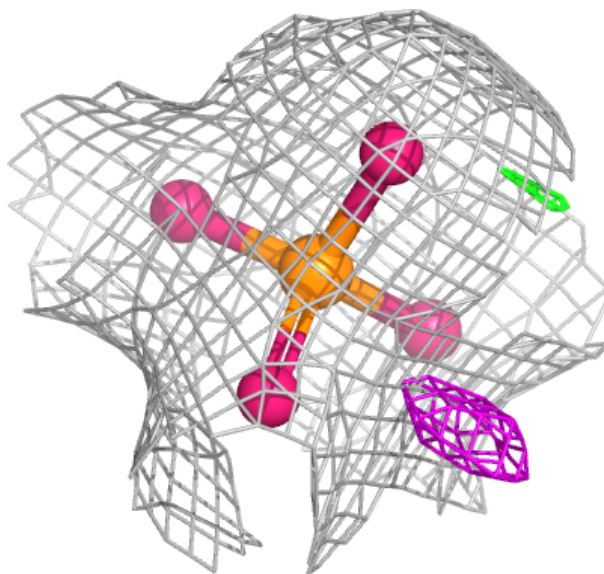
Electron density around PGV M 415:

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



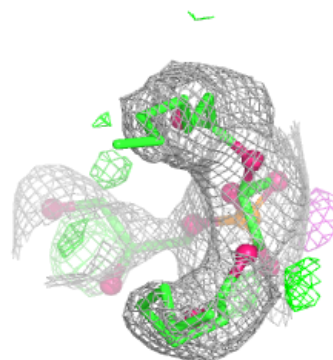
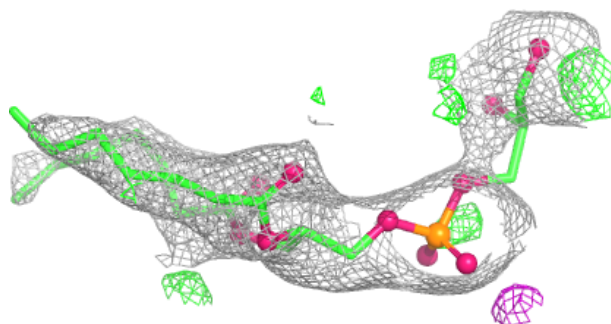
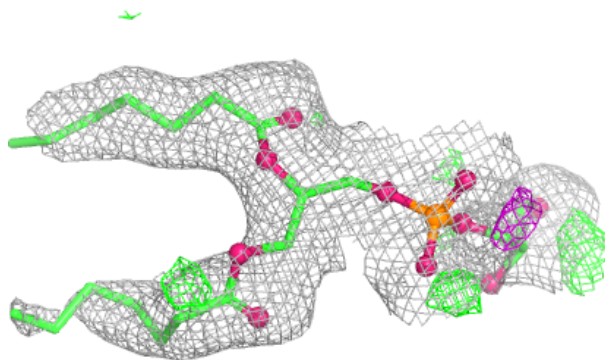
Electron density around PEF M 409:

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

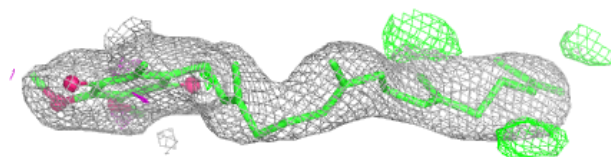
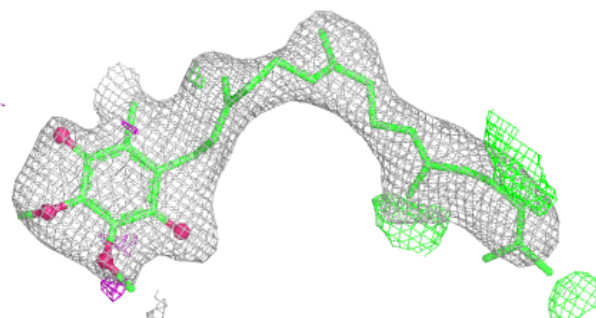


Electron density around PGV 1 106:

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

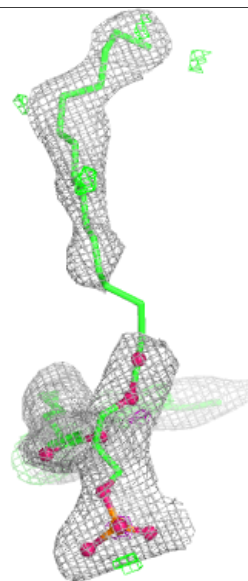
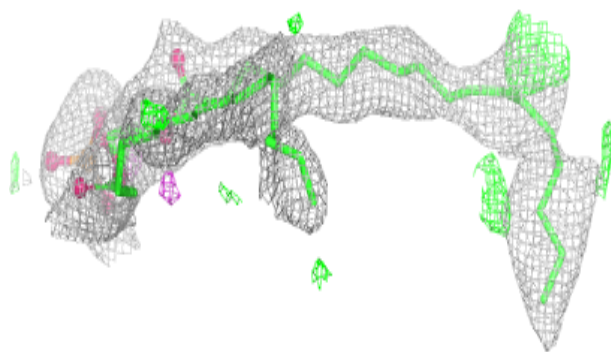
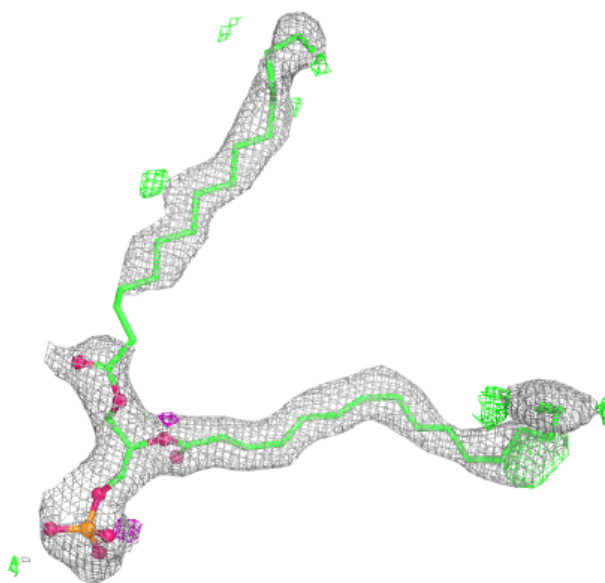
**Electron density around UQ8 7 104:**

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



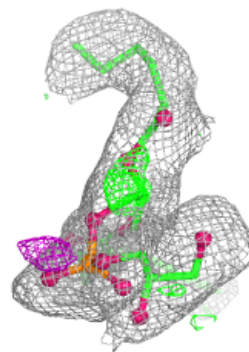
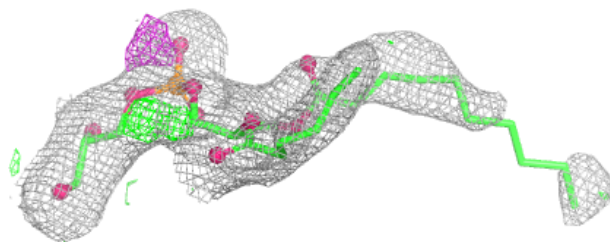
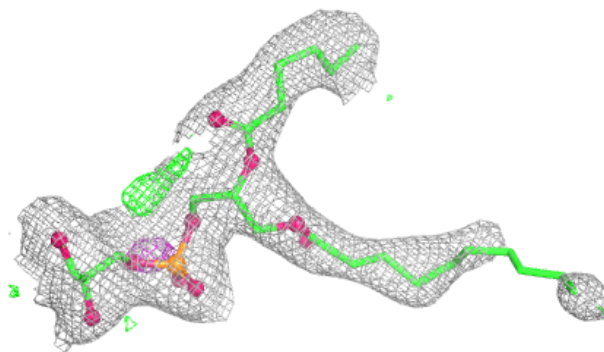
Electron density around PGV M 414:

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



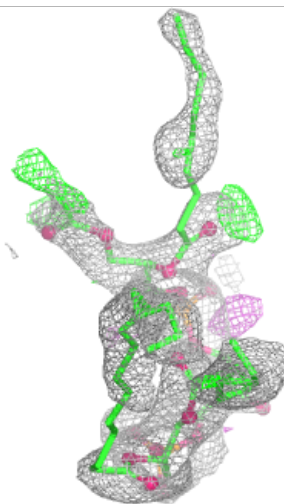
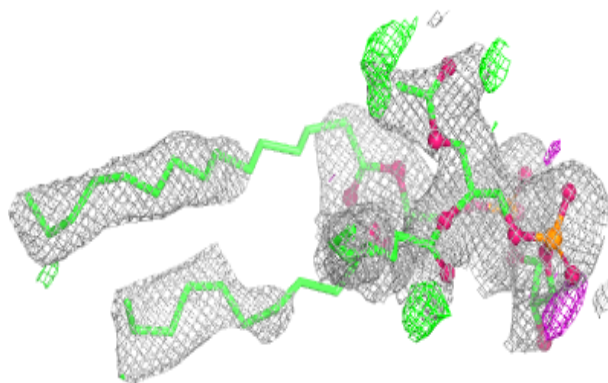
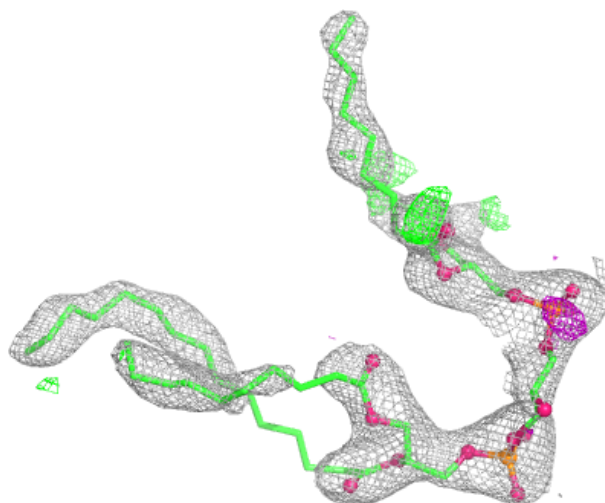
Electron density around PGV A 105:

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



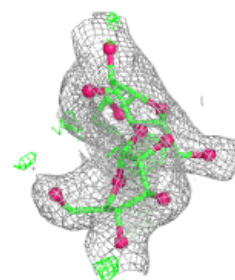
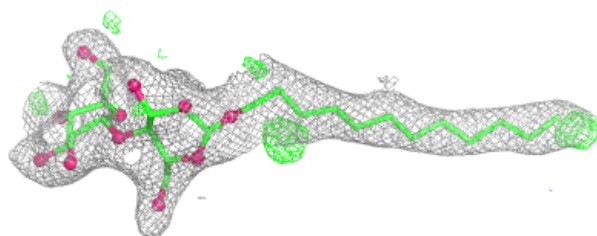
Electron density around CDL H 302:

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

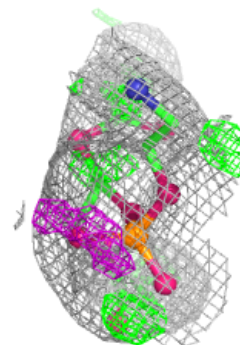
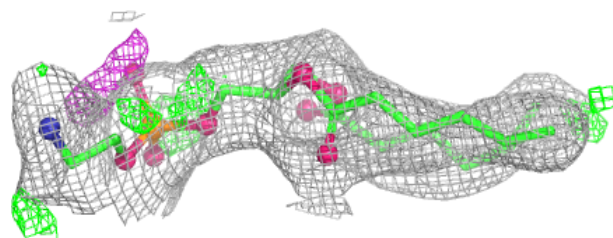
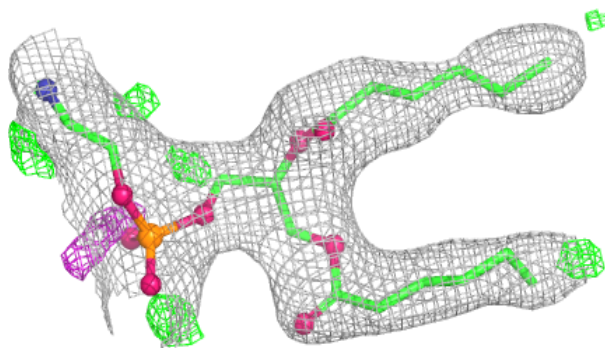


Electron density around LMT F 104:

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

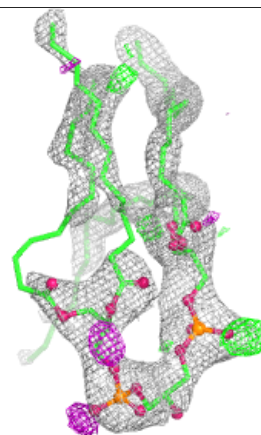
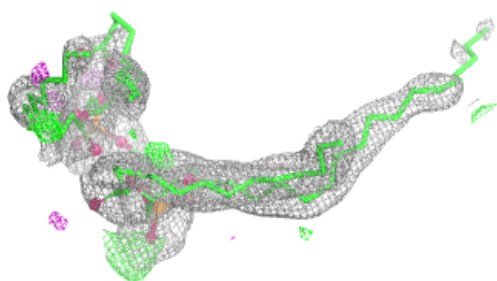
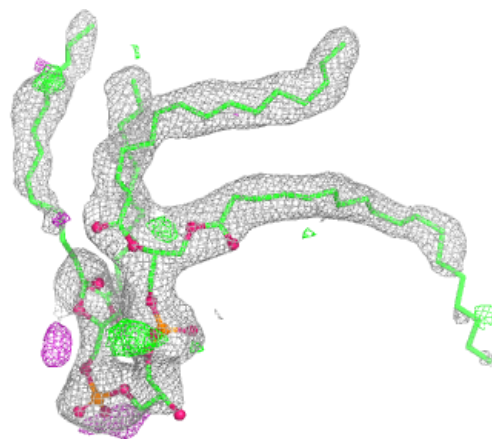
**Electron density around PEF K 105:**

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



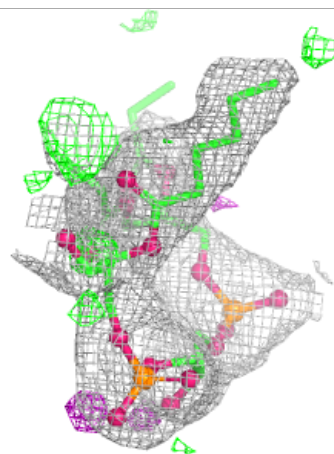
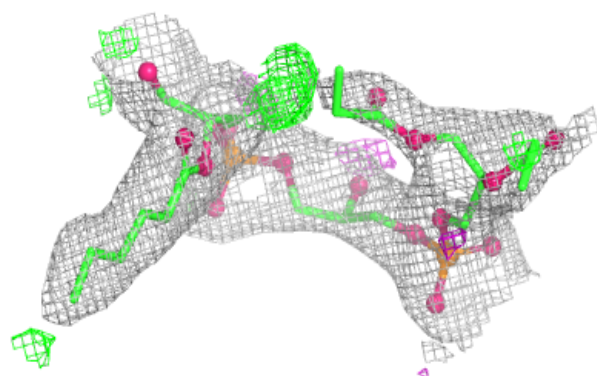
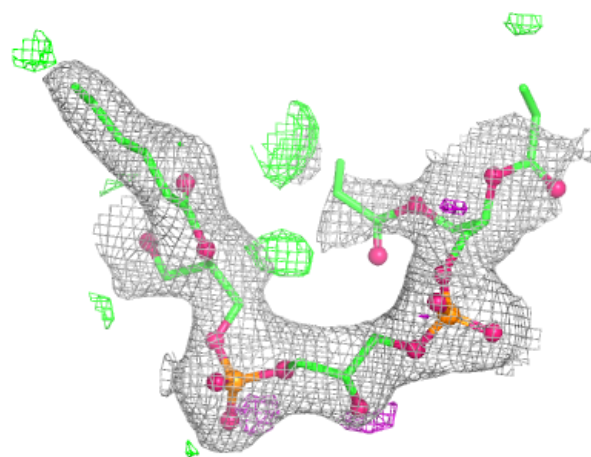
Electron density around CDL K 104:

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



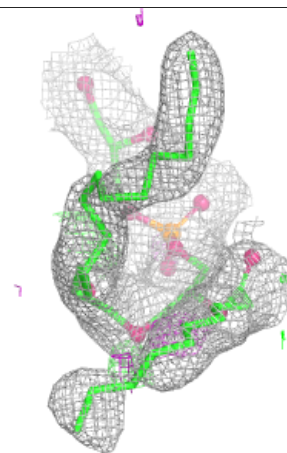
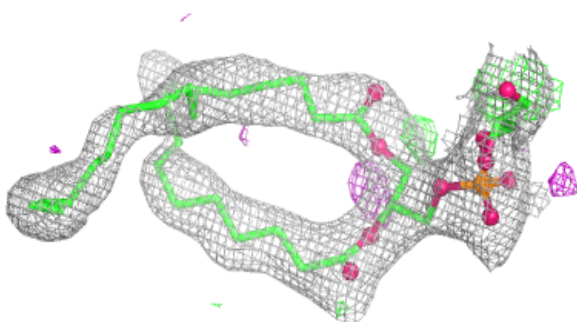
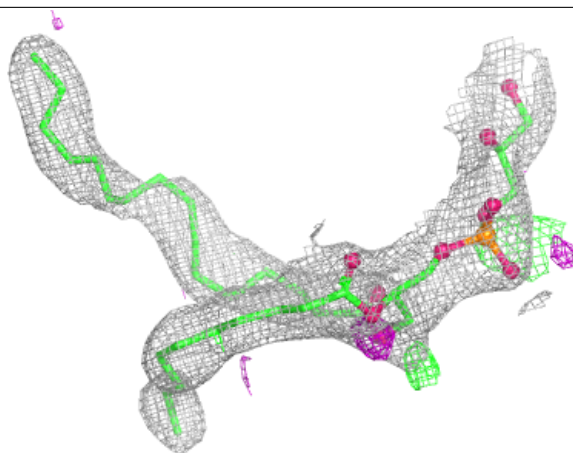
Electron density around CDL M 416:

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

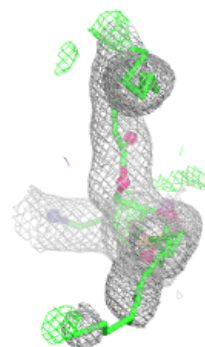
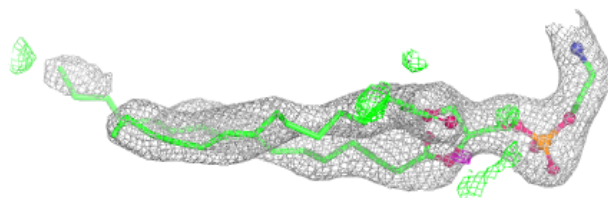
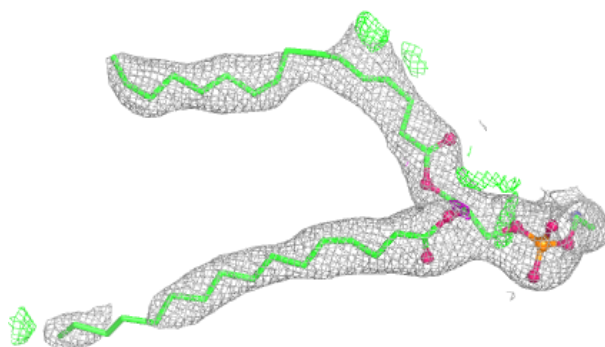


Electron density around PGV L 305:

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

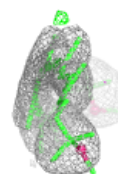
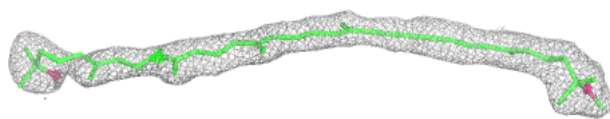
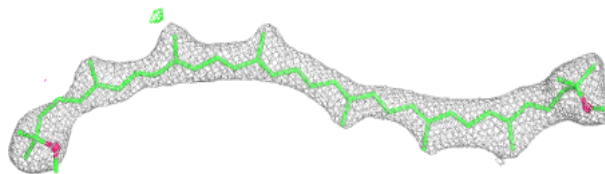
**Electron density around PEF M 419:**

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

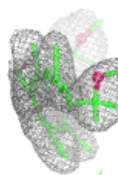
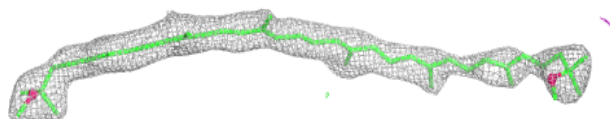
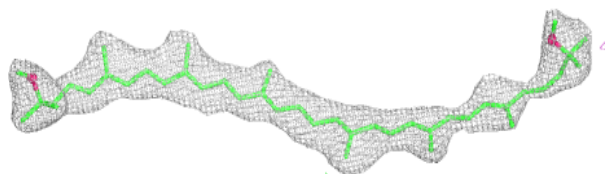


Electron density around CRT J 101:

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

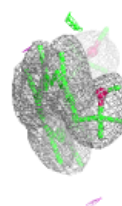
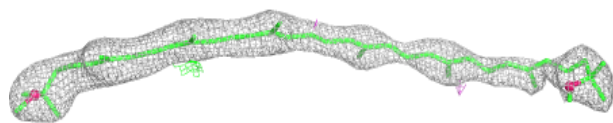
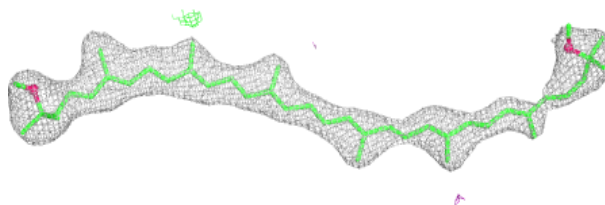
**Electron density around CRT 1 104:**

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



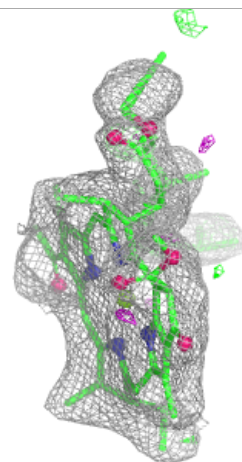
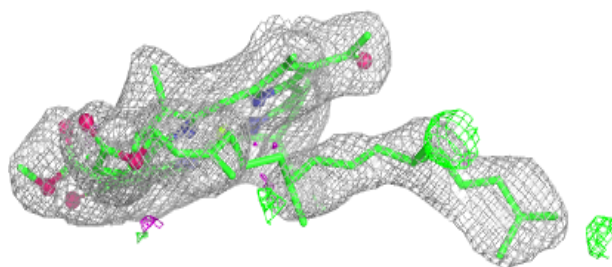
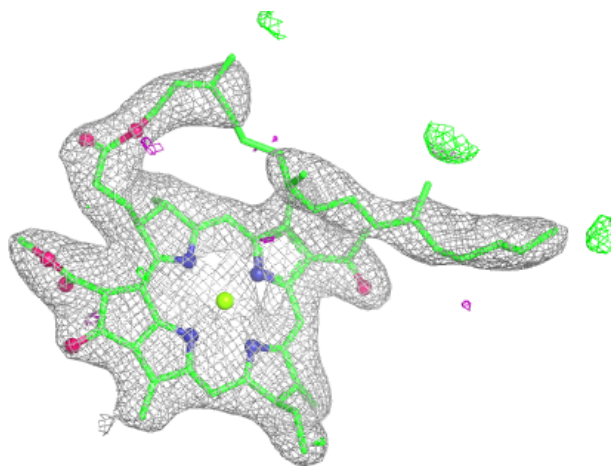
Electron density around CRT 2 101:

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



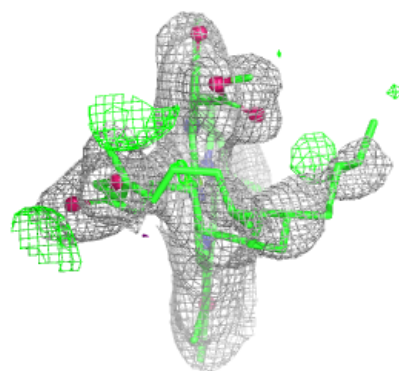
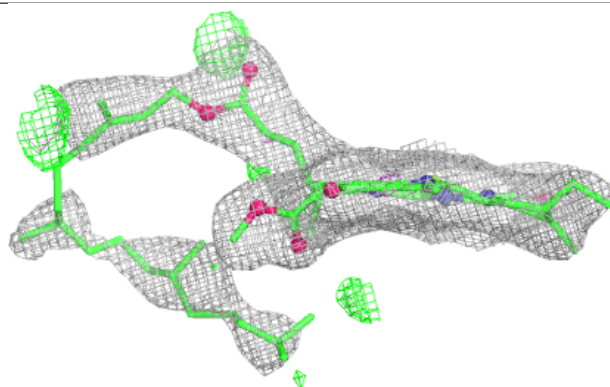
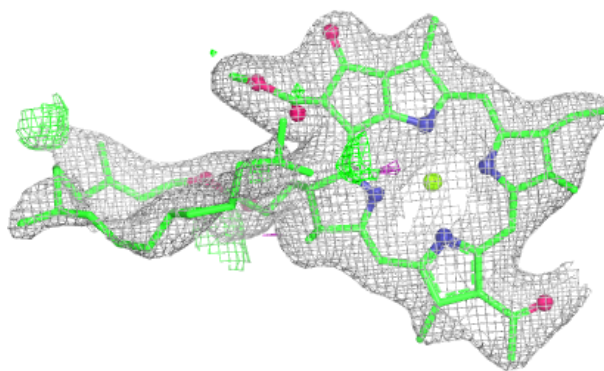
Electron density around BCL 1 103:

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

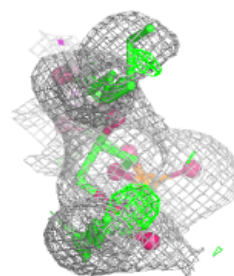
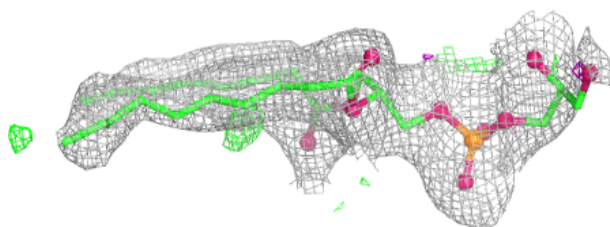
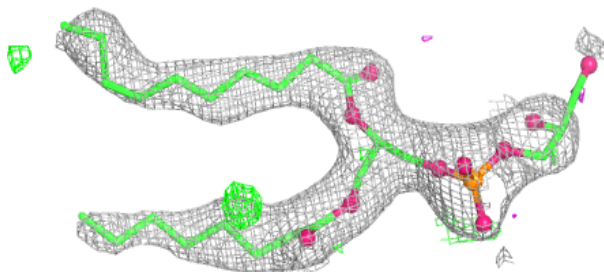


Electron density around BCL 3 102:

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

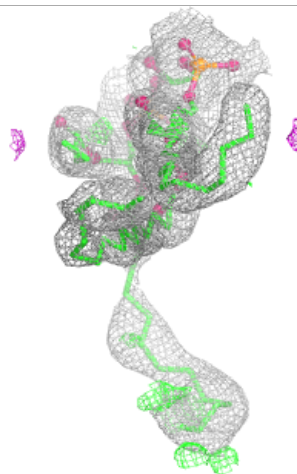
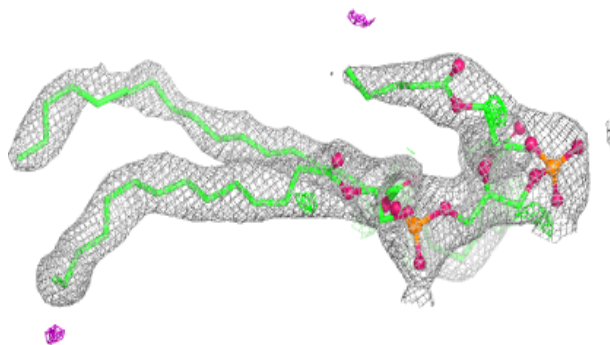
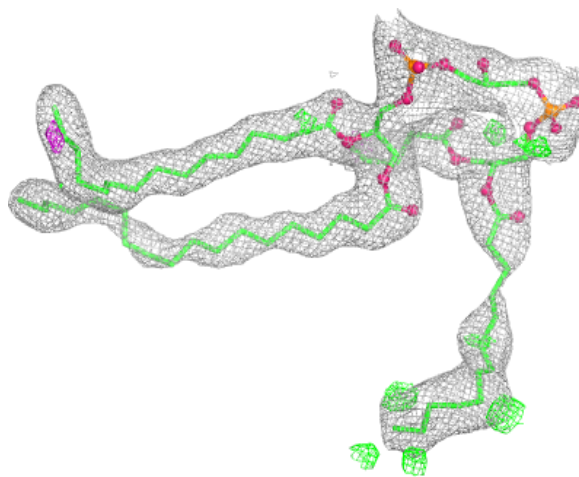
**Electron density around PGV D 105:**

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



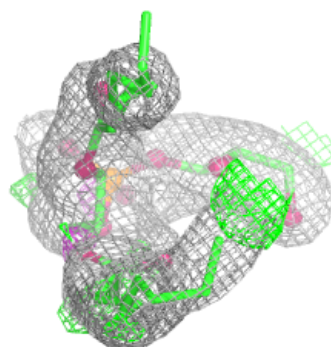
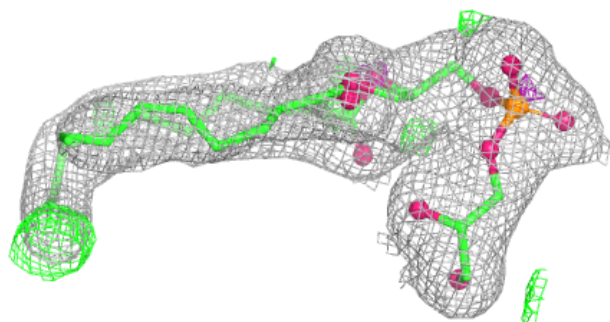
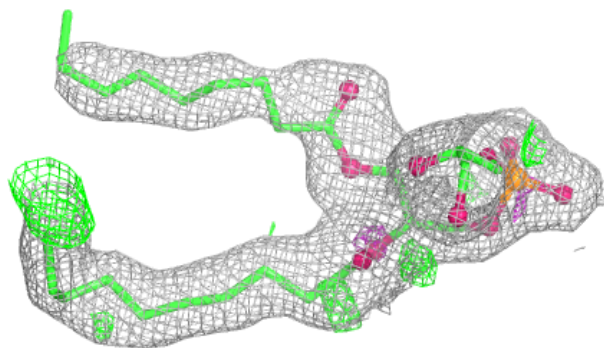
Electron density around CDL H 304:

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

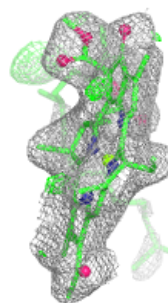
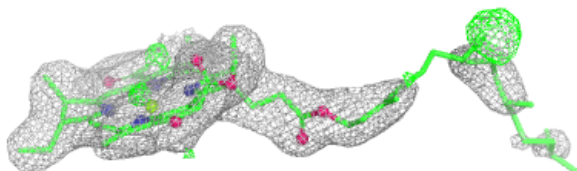


Electron density around PGV H 303:

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

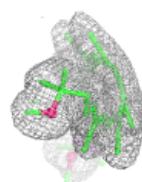
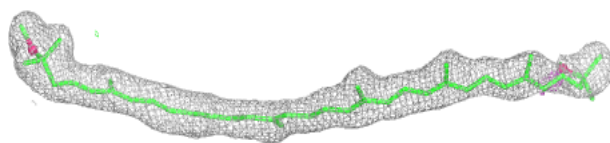
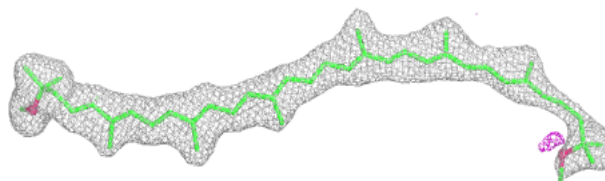
**Electron density around BCL 1 102:**

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

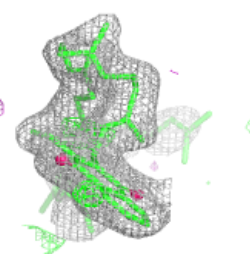
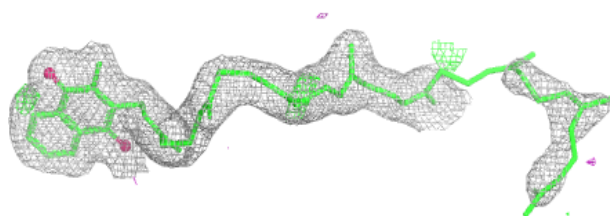
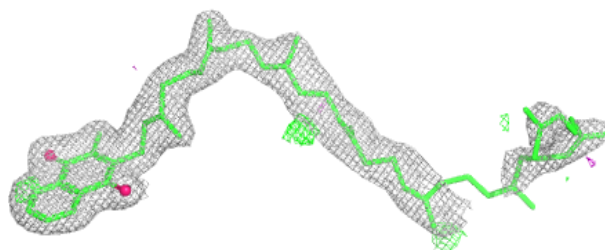


Electron density around CRT 9 102:

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

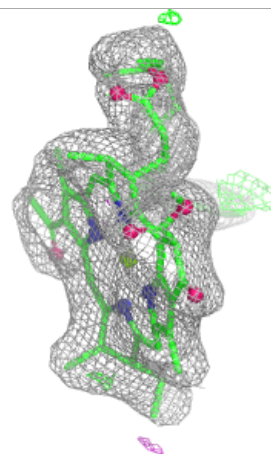
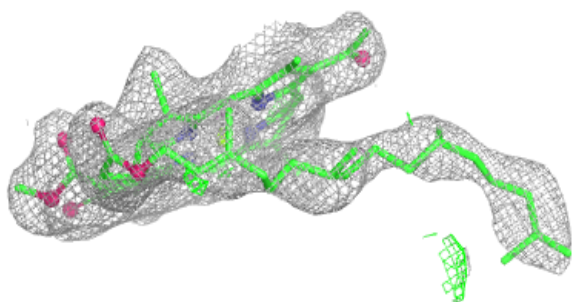
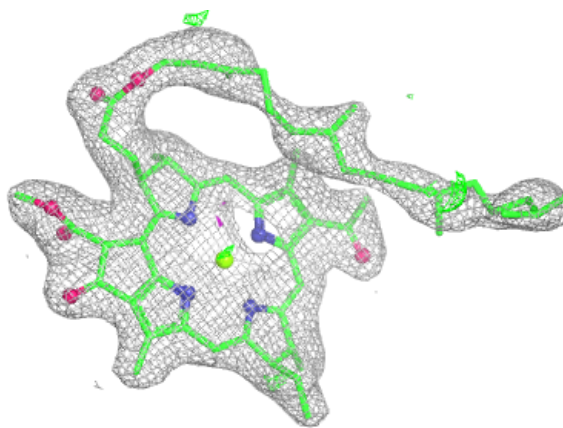
**Electron density around MQ8 M 406:**

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



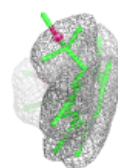
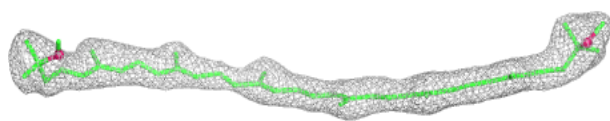
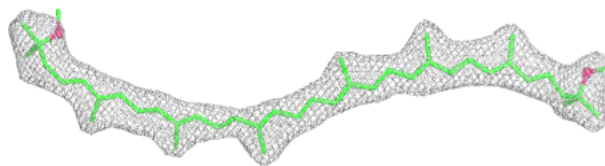
Electron density around BCL 3 103:

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

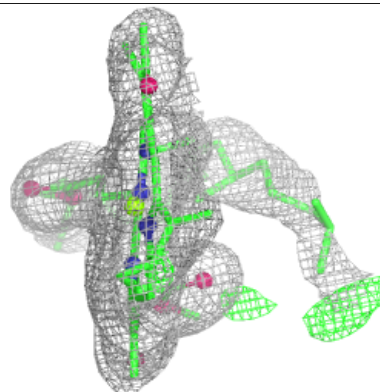
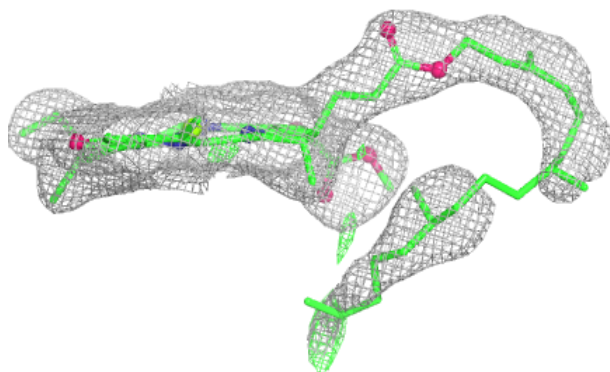
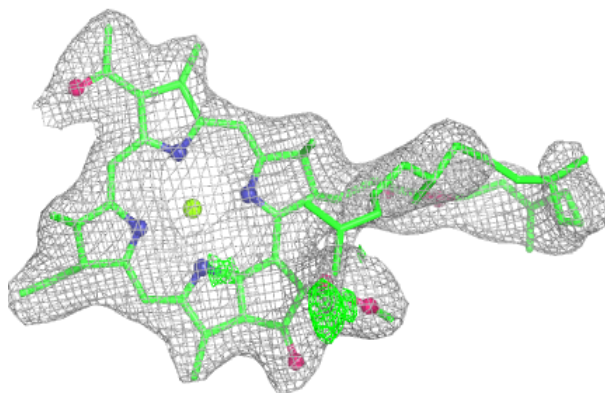


Electron density around CRT N 101:

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

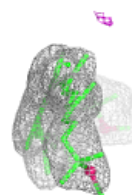
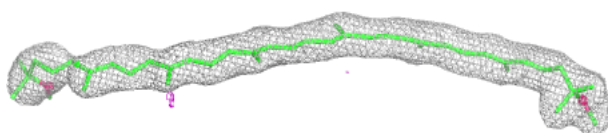
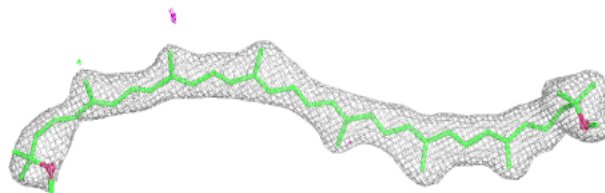
**Electron density around BCL 5 102:**

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

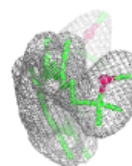
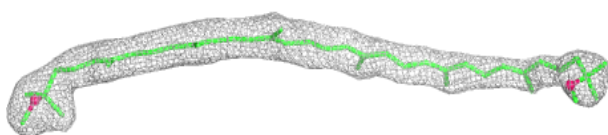
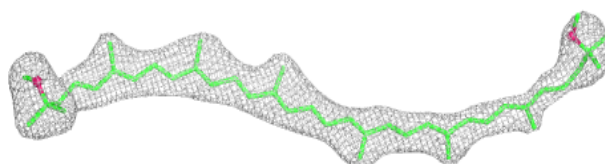


Electron density around CRT U 104:

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

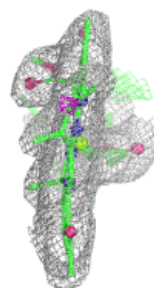
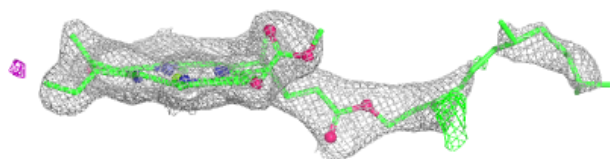
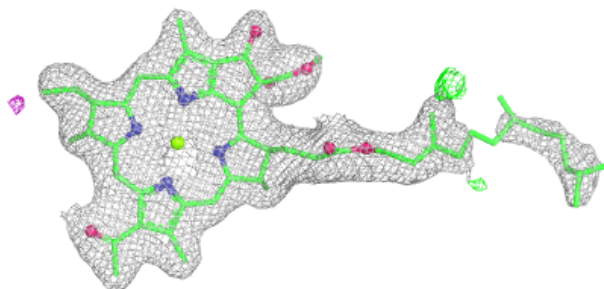
**Electron density around CRT Z 101:**

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



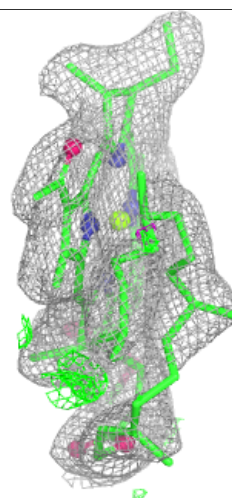
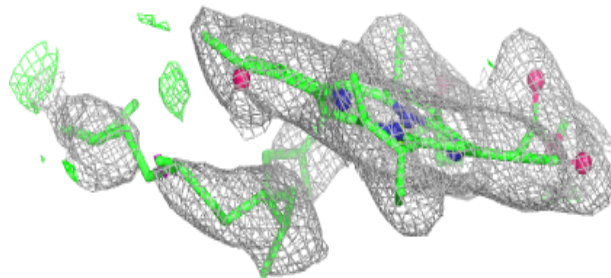
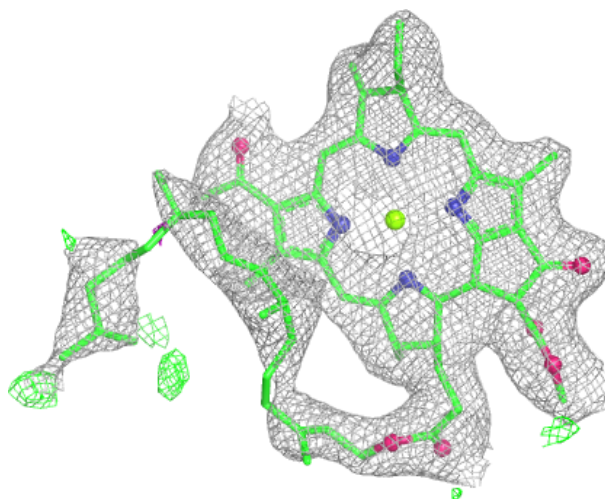
Electron density around BCL 7 102:

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



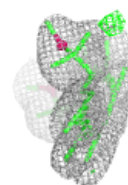
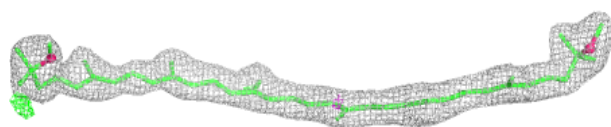
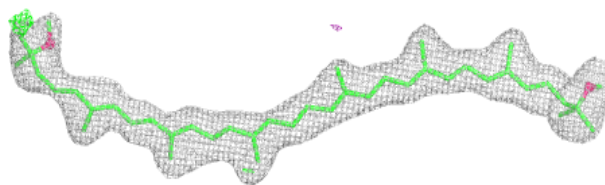
Electron density around BCL 7 103:

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

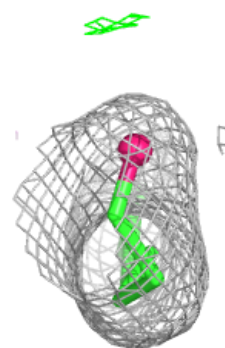
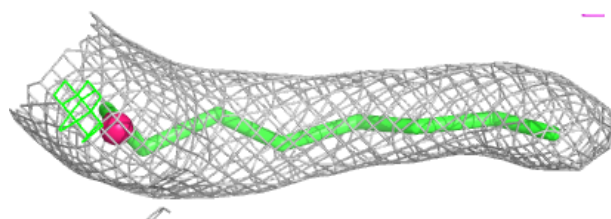
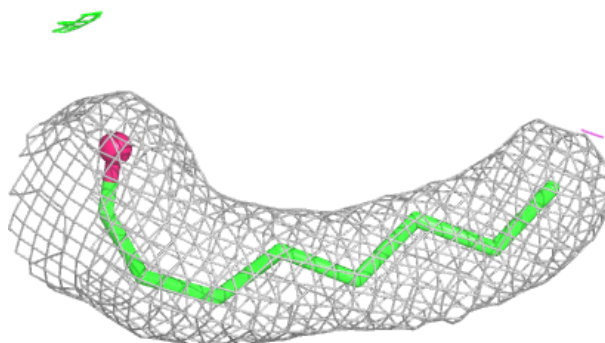


Electron density around CRT 6 101:

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

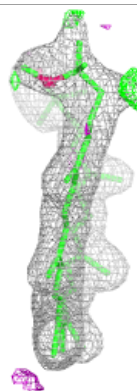
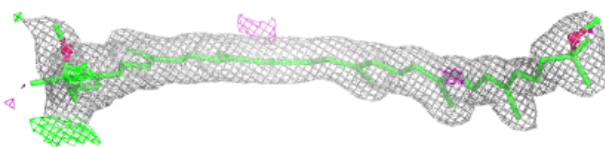
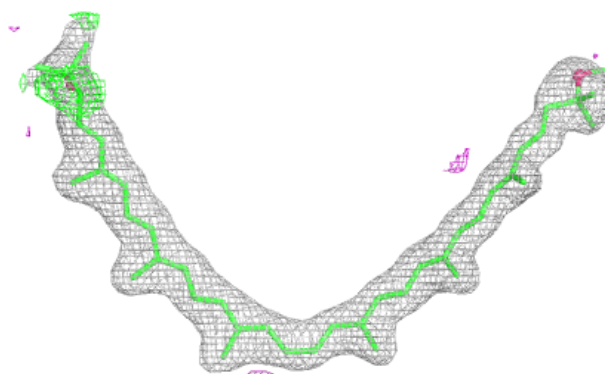
**Electron density around LHG C 508:**

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

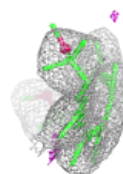
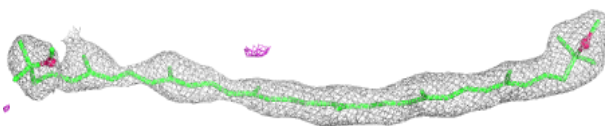
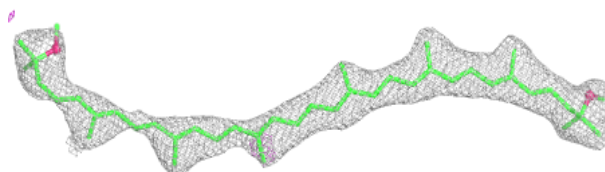


Electron density around CRT M 407:

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

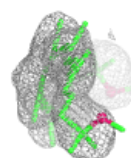
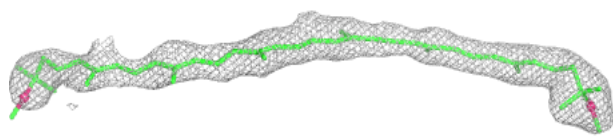
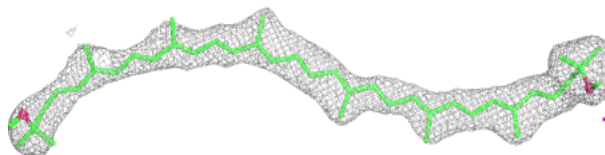
**Electron density around CRT A 104:**

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

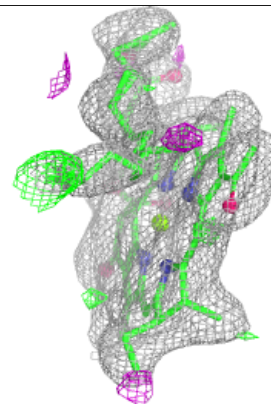
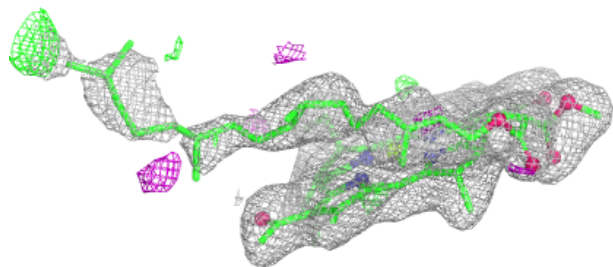
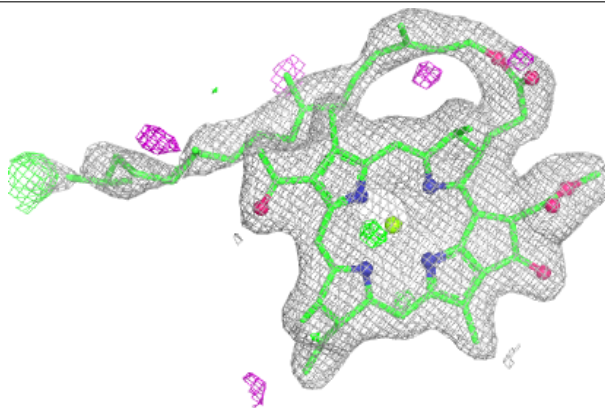


Electron density around CRT G 101:

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

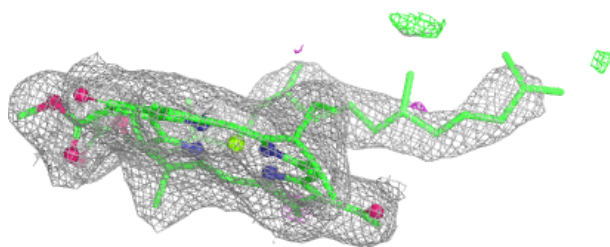
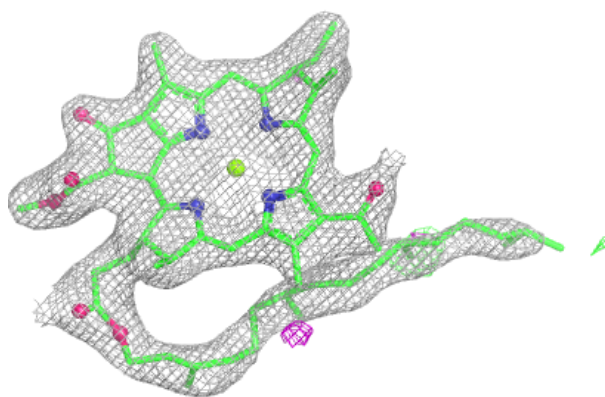
**Electron density around BCL O 103:**

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

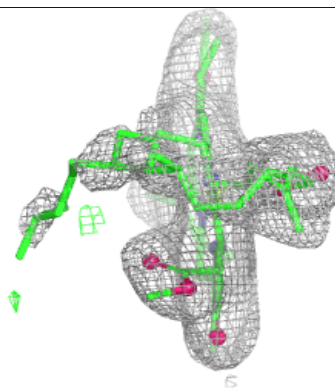
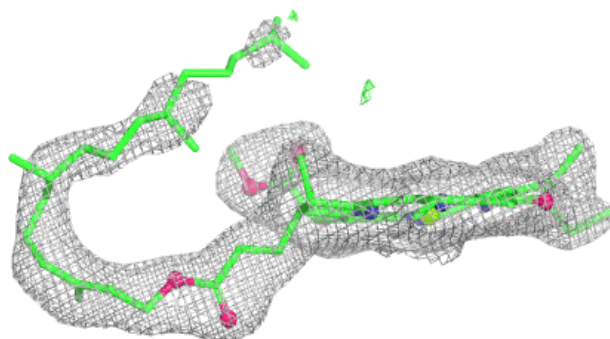
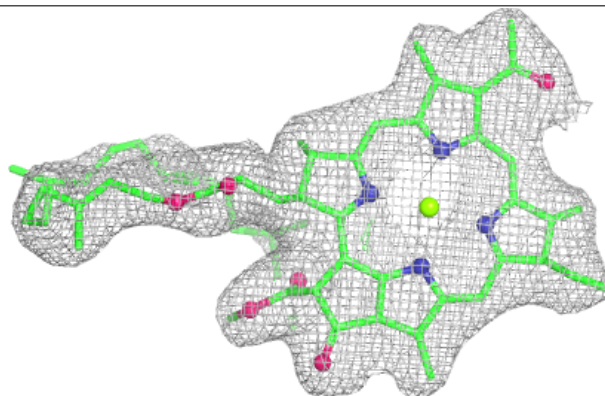


Electron density around BCL 5 103:

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

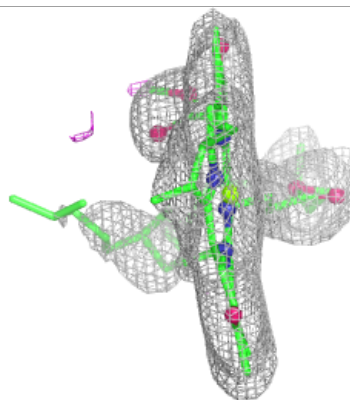
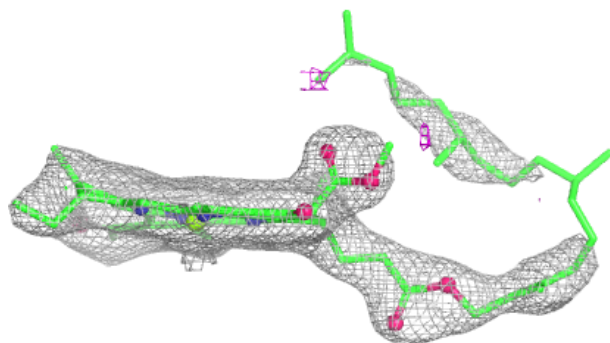
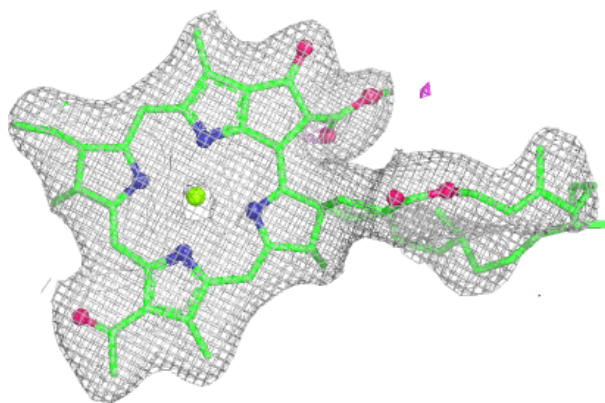
**Electron density around BCL K 102:**

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

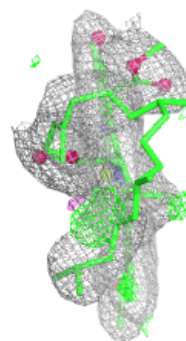
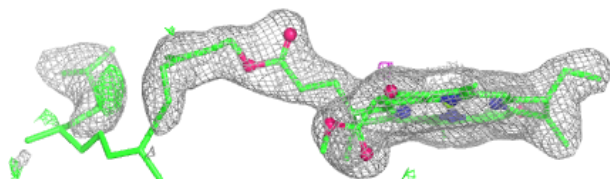
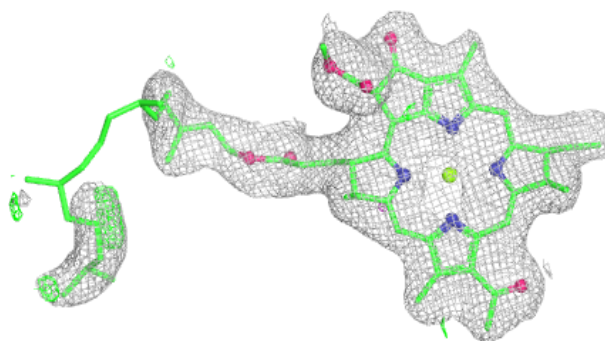


Electron density around BCL A 101:

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

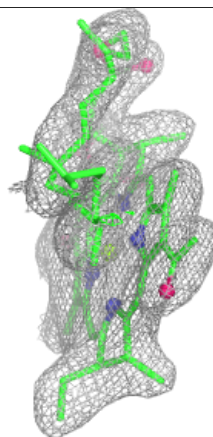
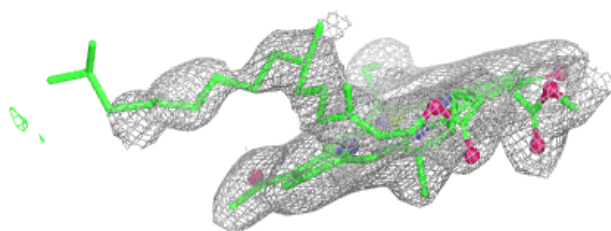
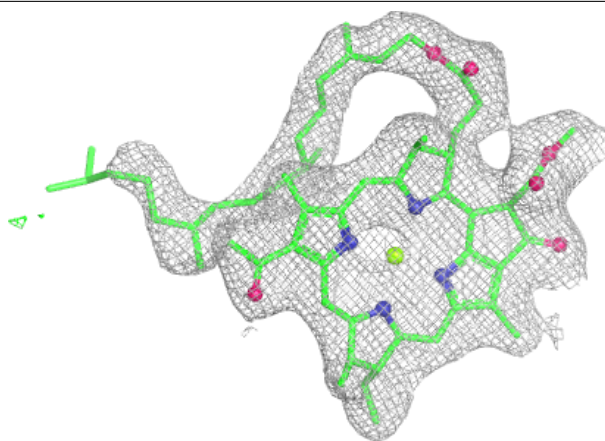
**Electron density around BCL 9 104:**

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

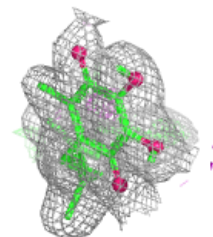
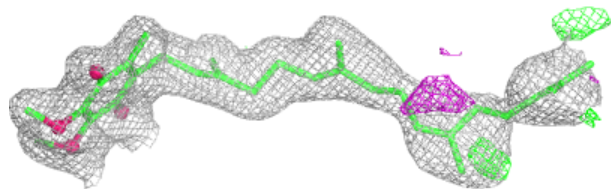
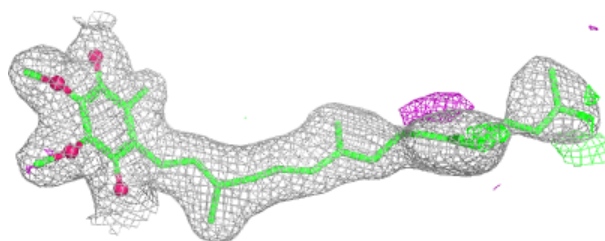


Electron density around BCL 0 102:

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

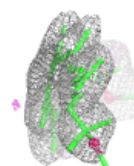
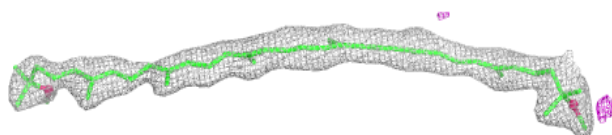
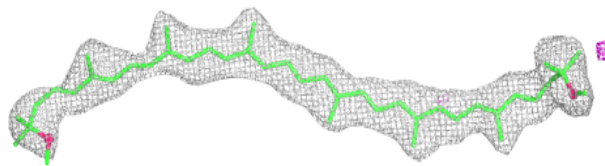
**Electron density around UQ8 L 303:**

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

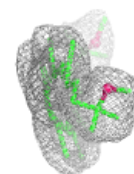
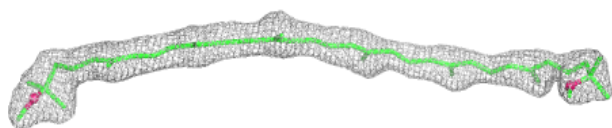
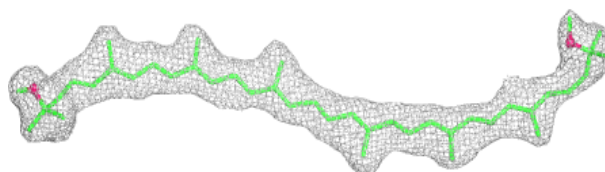


Electron density around CRT 9 103:

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

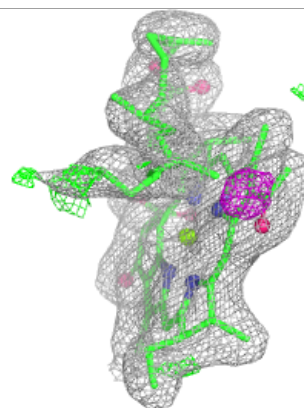
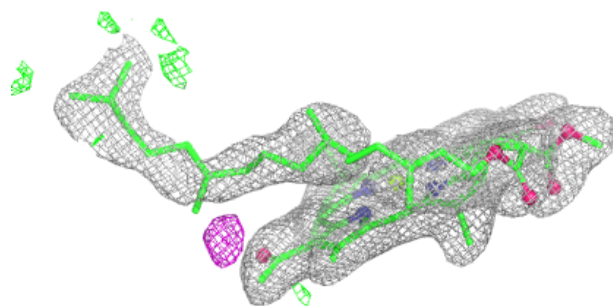
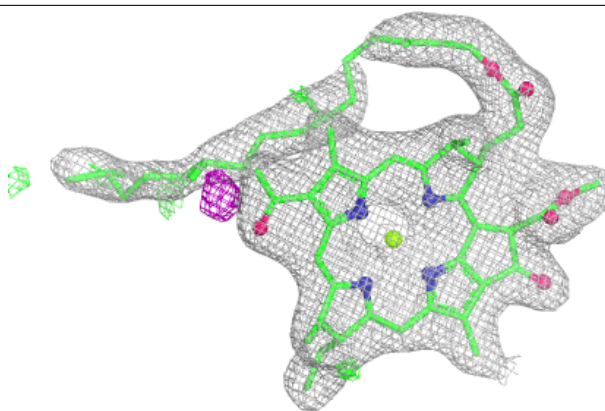
**Electron density around CRT 0 101:**

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

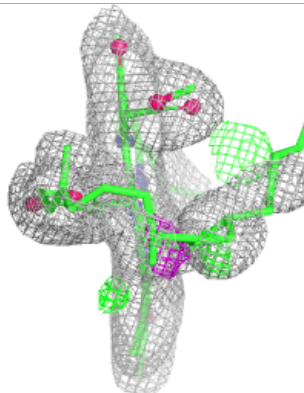
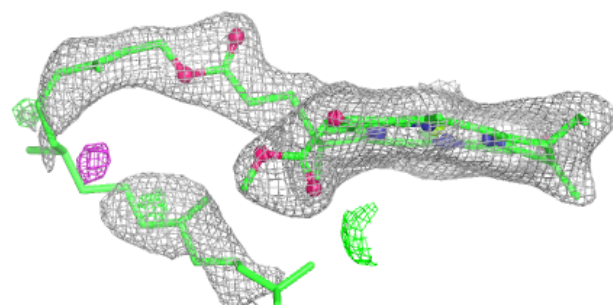
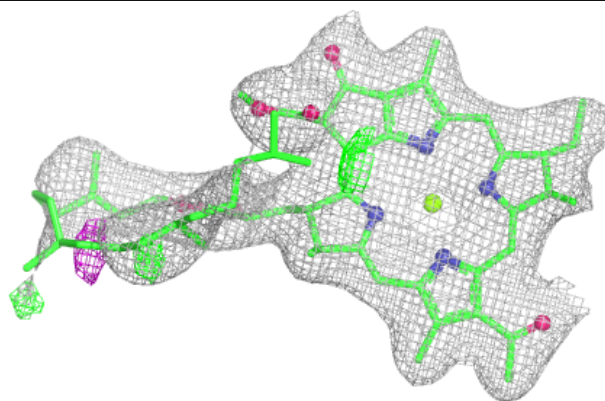


Electron density around BCL S 103:

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

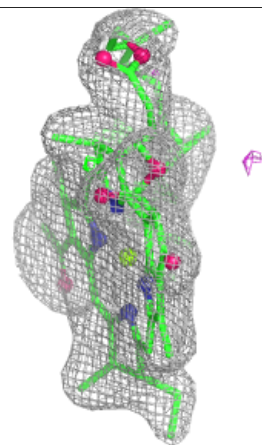
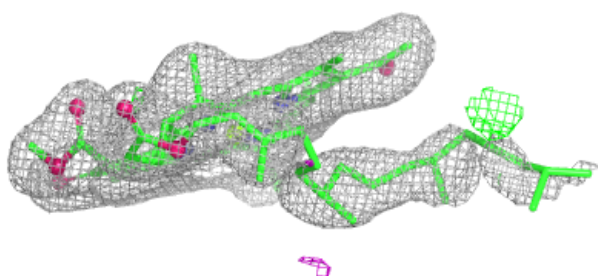
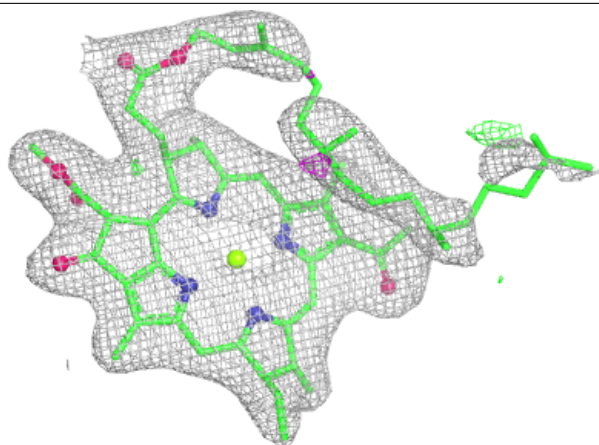
**Electron density around BCL W 102:**

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

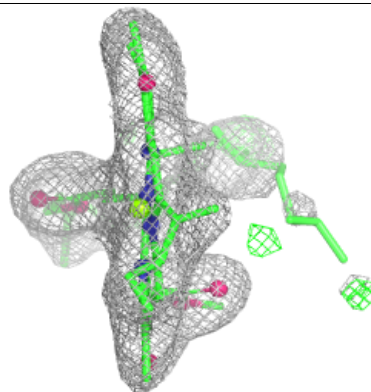
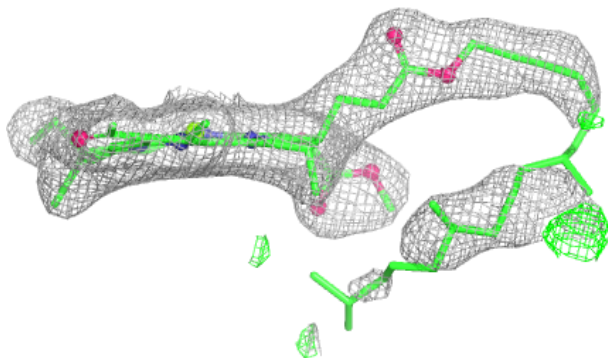
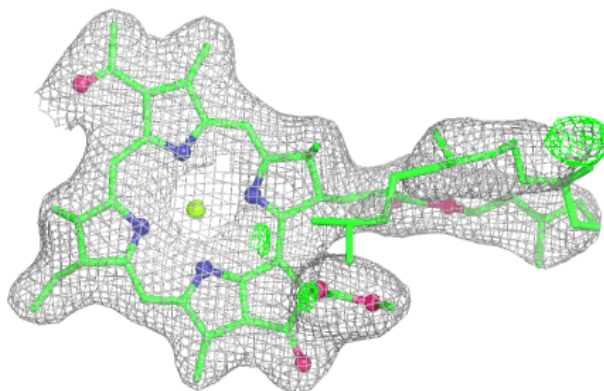


Electron density around BCL W 103:

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

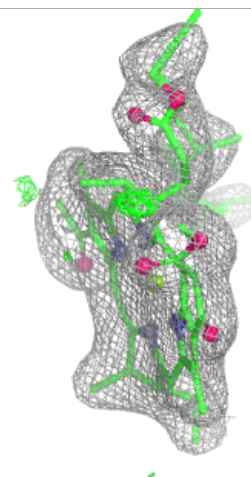
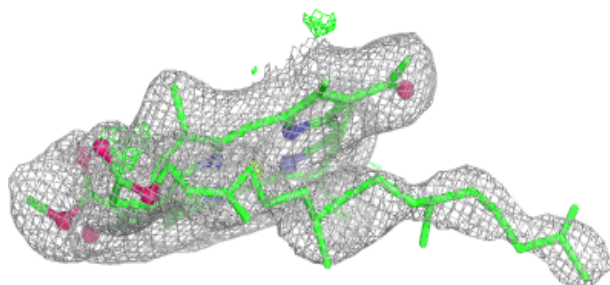
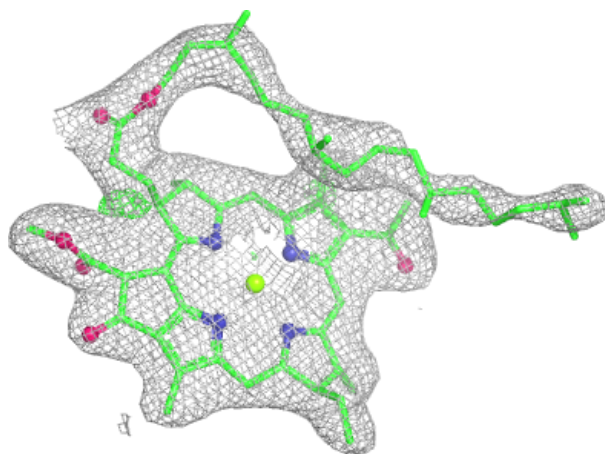
**Electron density around BCL Y 102:**

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



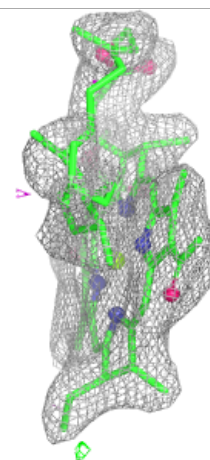
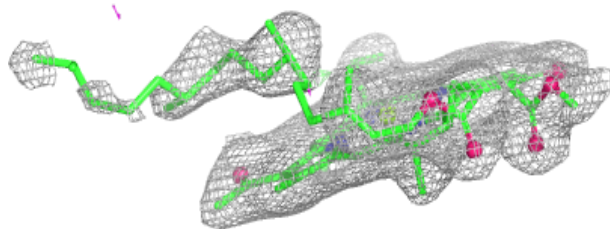
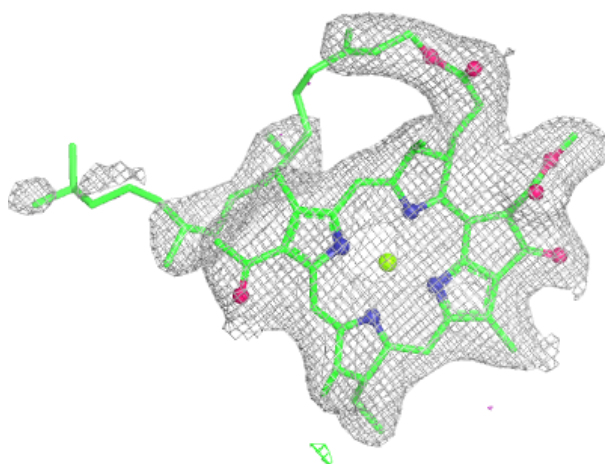
Electron density around BCL Z 102:

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



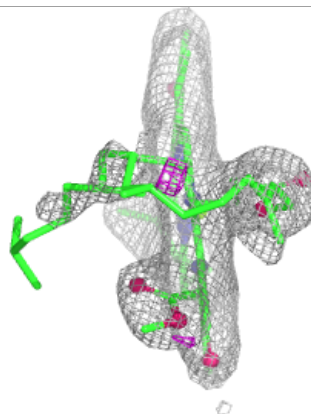
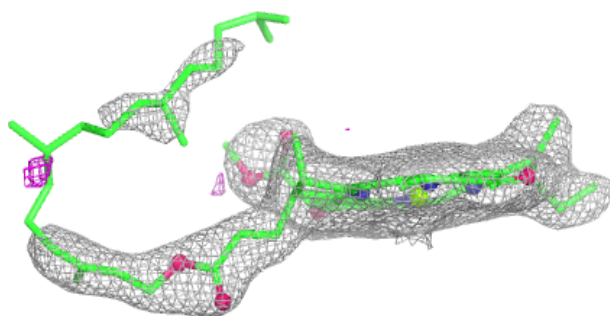
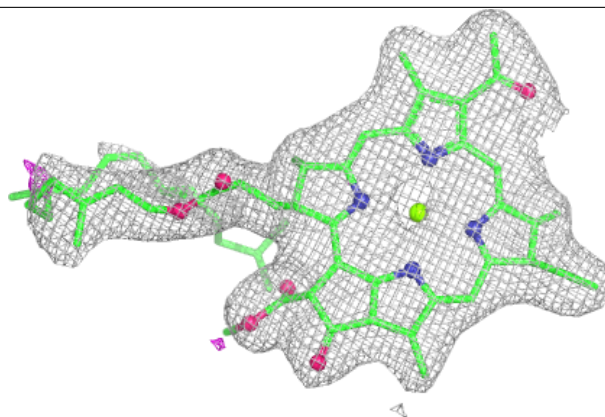
Electron density around BCL A 103:

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

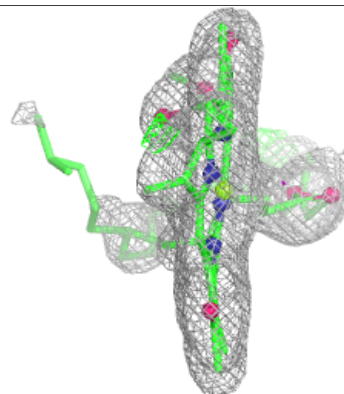
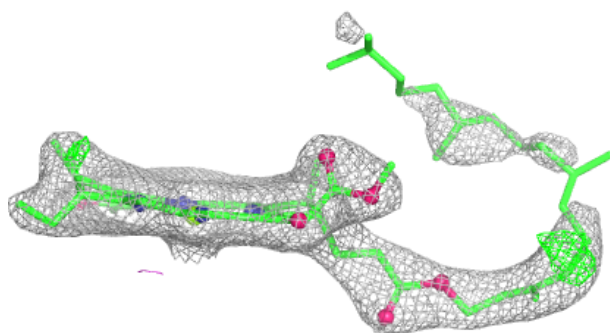
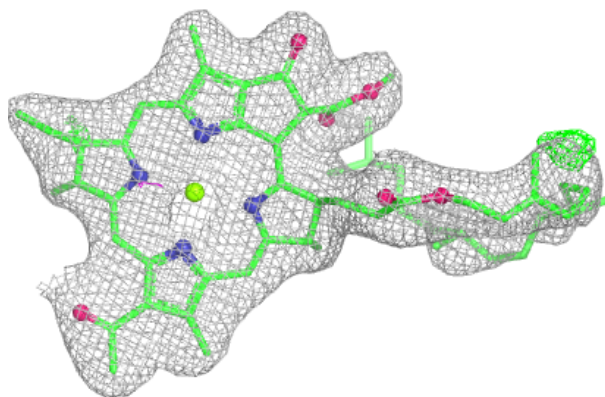


Electron density around BCL D 102:

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

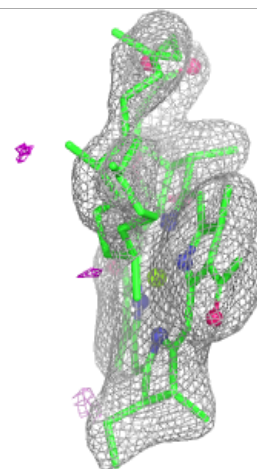
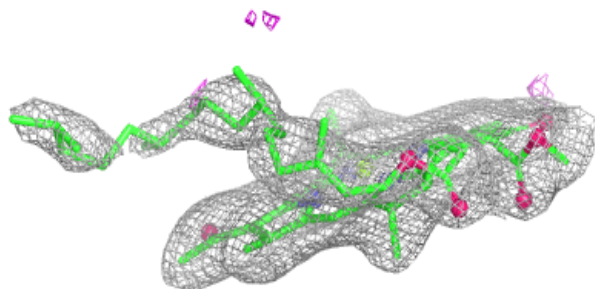
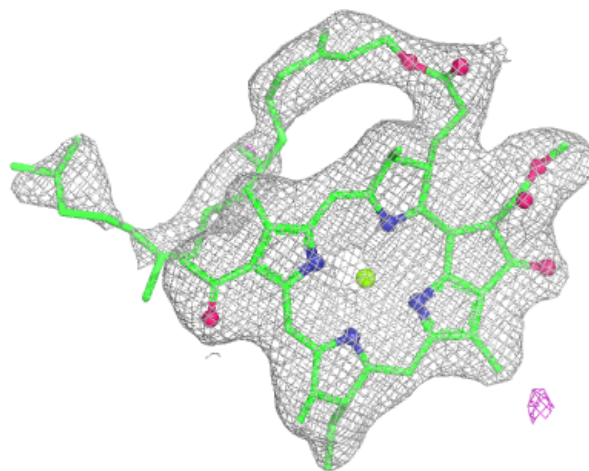
**Electron density around BCL F 102:**

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



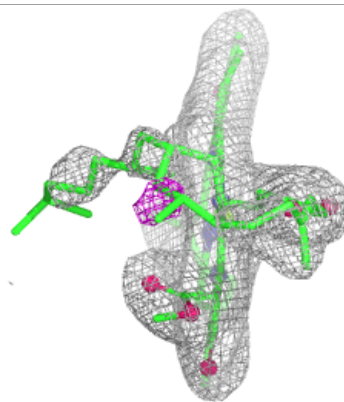
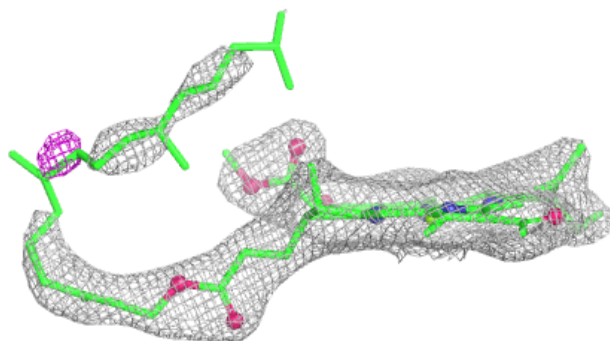
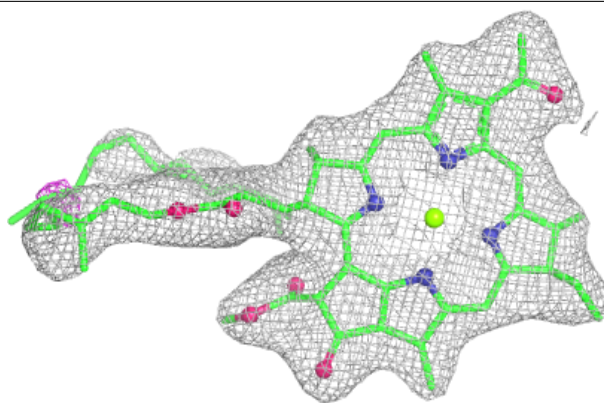
Electron density around BCL F 103:

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



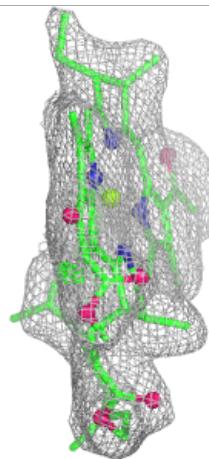
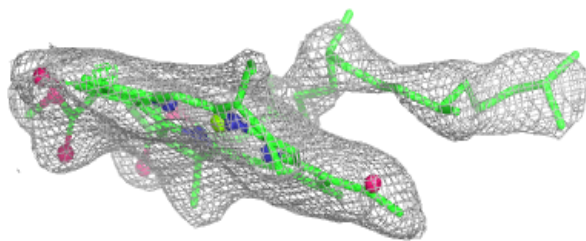
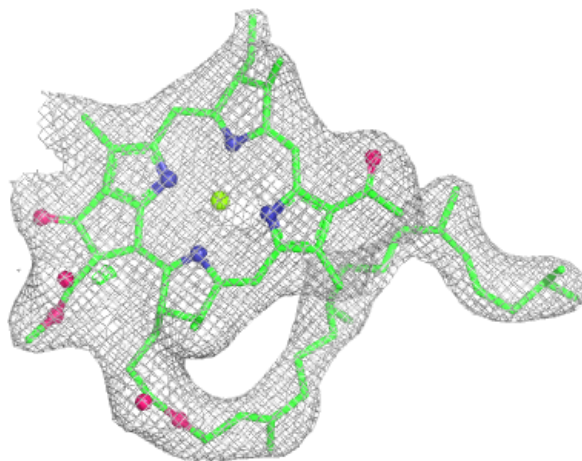
Electron density around BCL I 102:

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



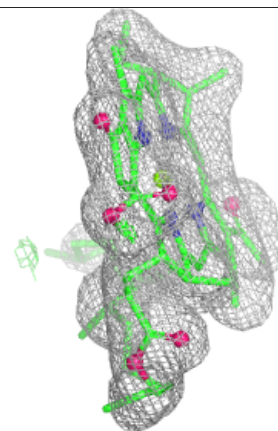
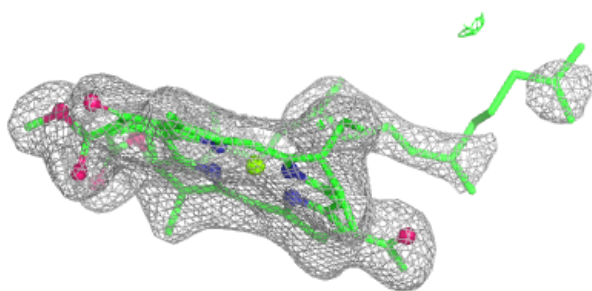
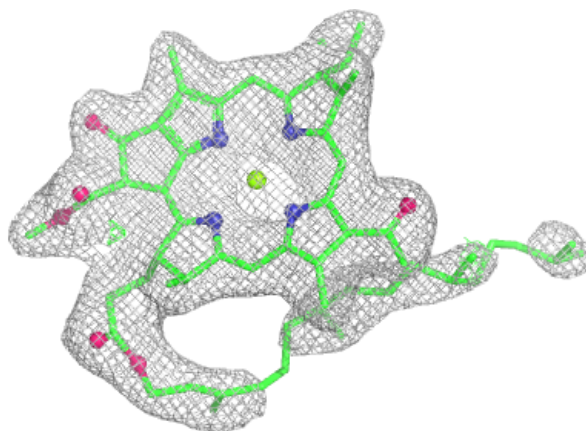
Electron density around BCL D 103:

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



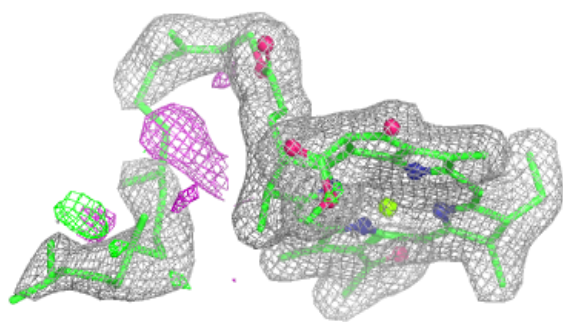
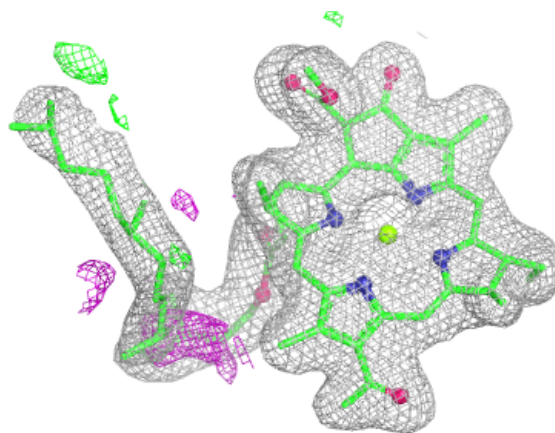
Electron density around BCL K 103:

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

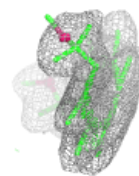
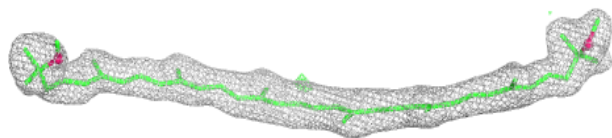
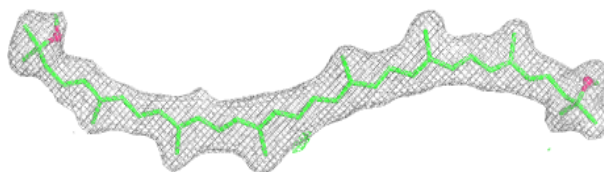


Electron density around BCL M 403:

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

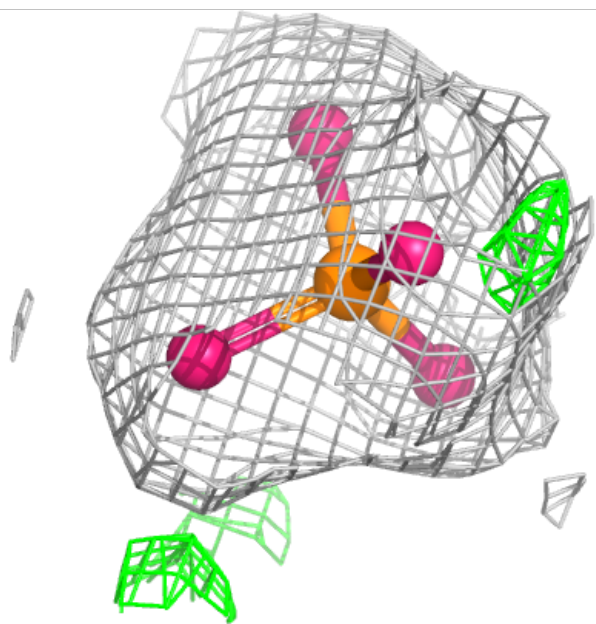
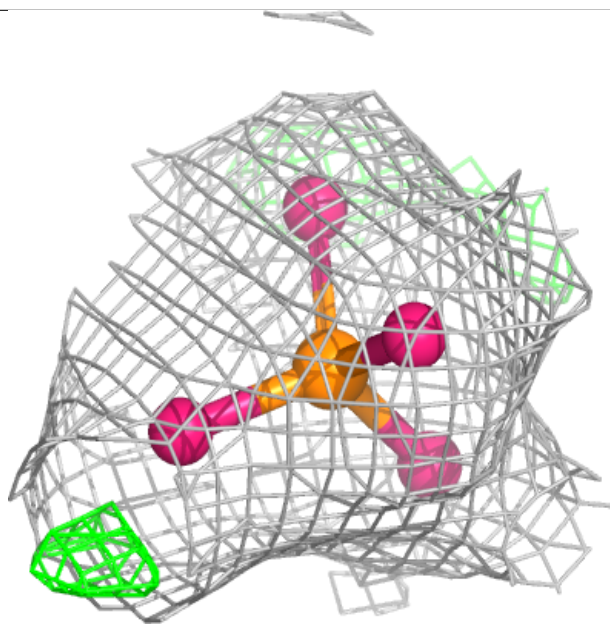
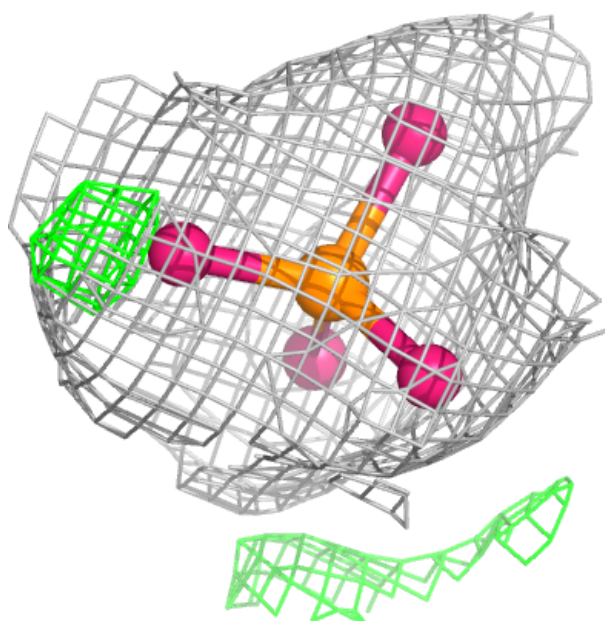
**Electron density around CRT O 104:**

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



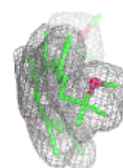
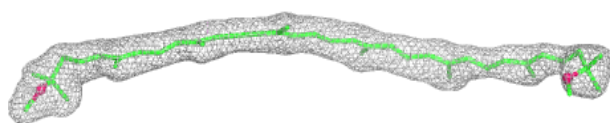
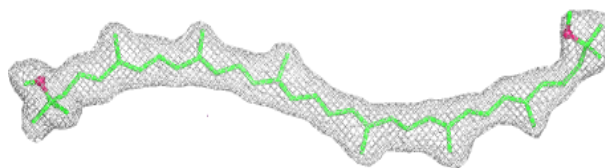
Electron density around PEF M 411:

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

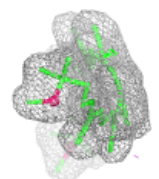
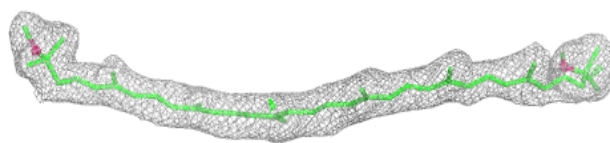
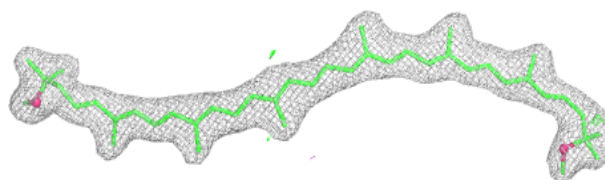


Electron density around CRT P 101:

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

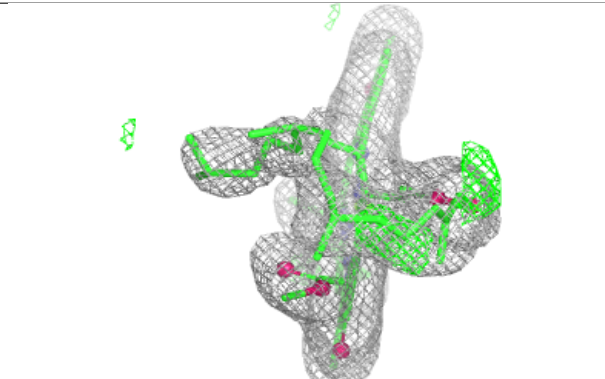
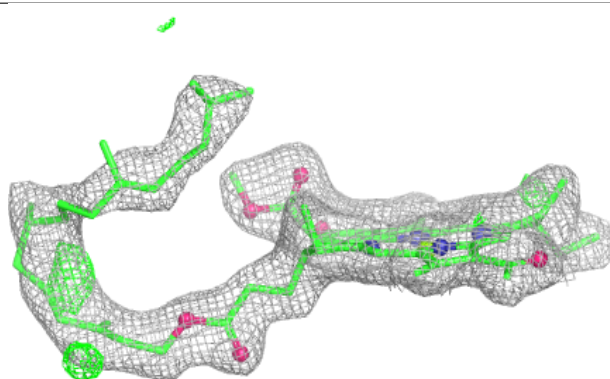
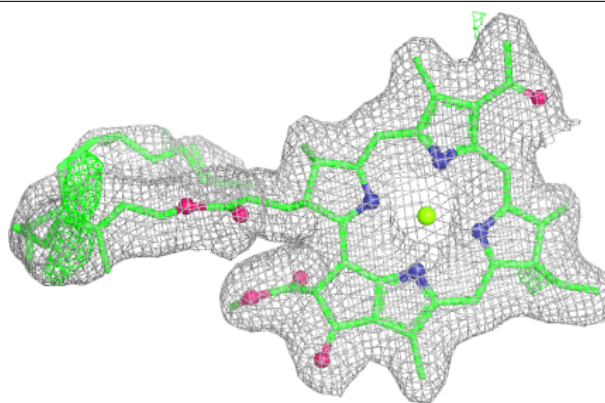
**Electron density around CRT Q 104:**

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

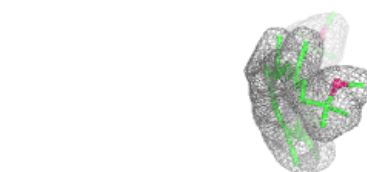
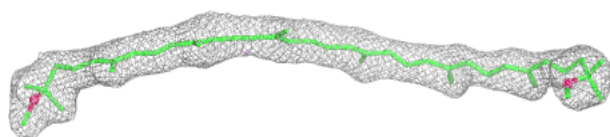
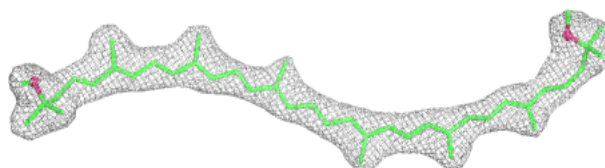


Electron density around BCL Q 102:

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

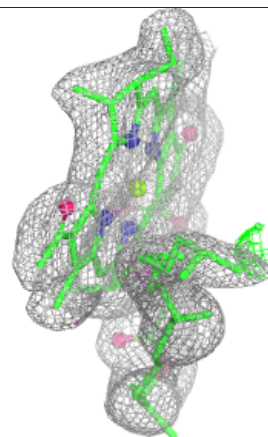
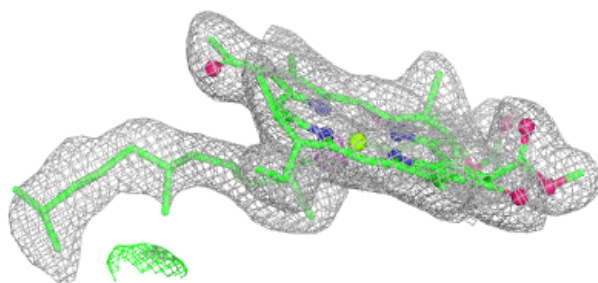
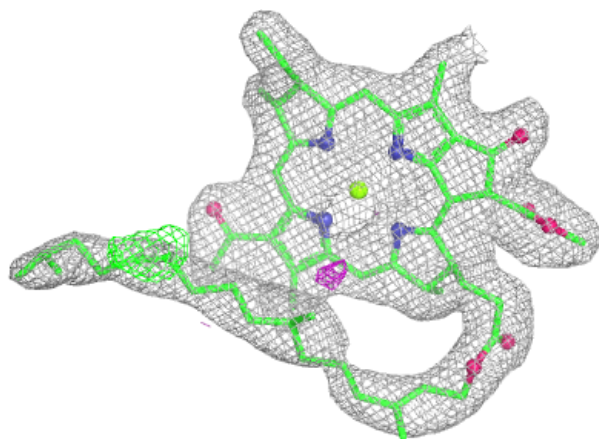
**Electron density around CRT V 101:**

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



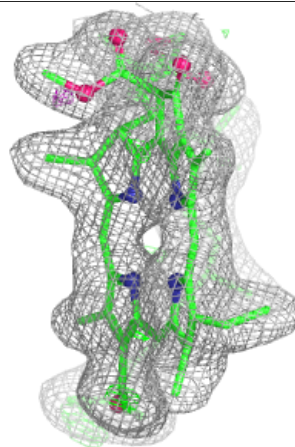
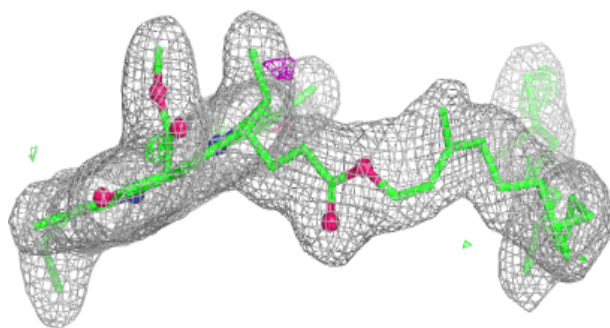
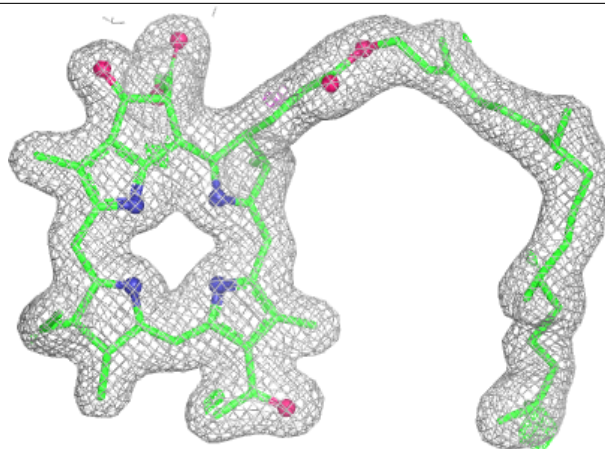
Electron density around BCL Q 103:

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

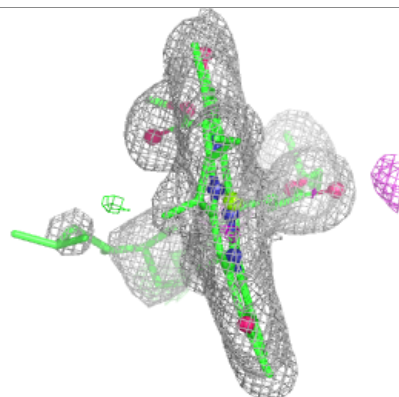
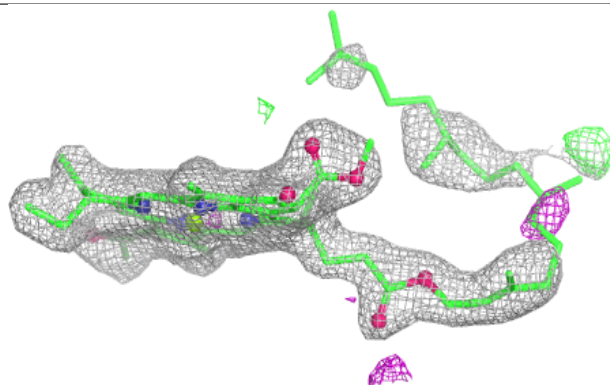
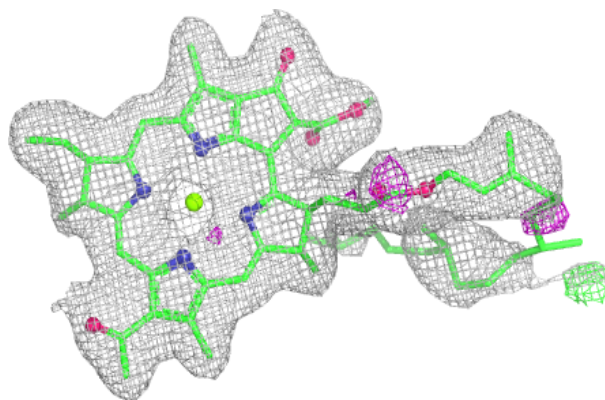


Electron density around BPH L 302:

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

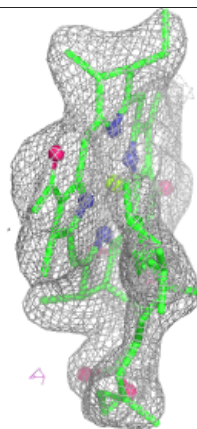
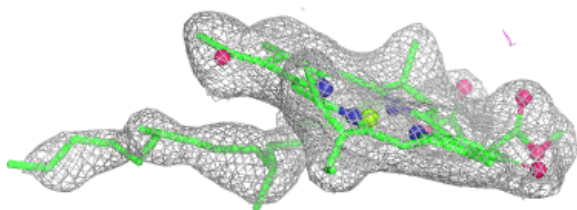
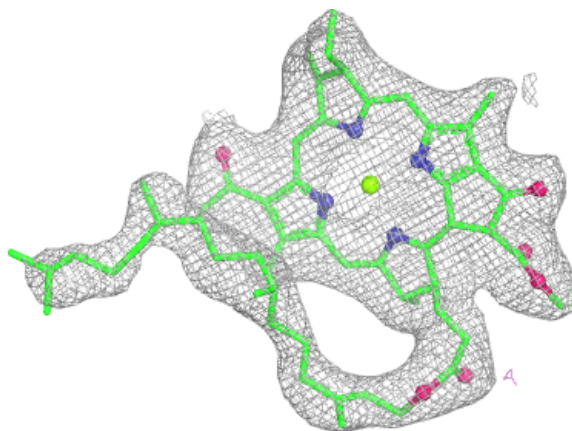
**Electron density around BCL S 102:**

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

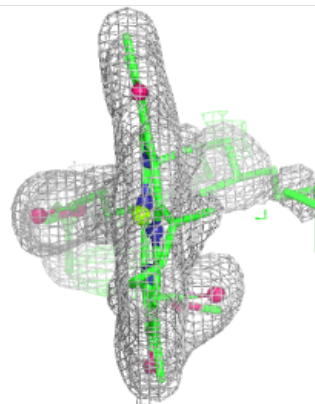
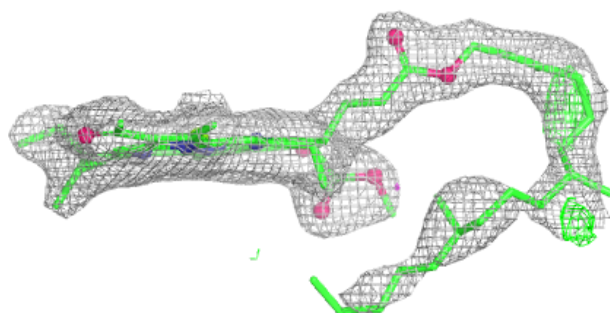
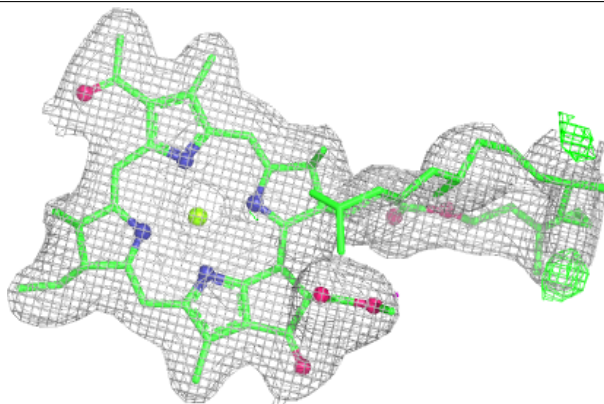


Electron density around BCL I 103:

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

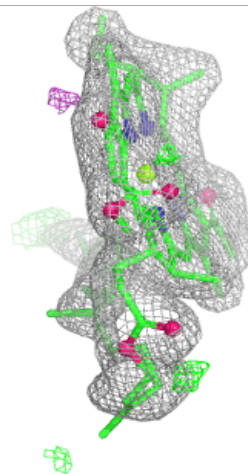
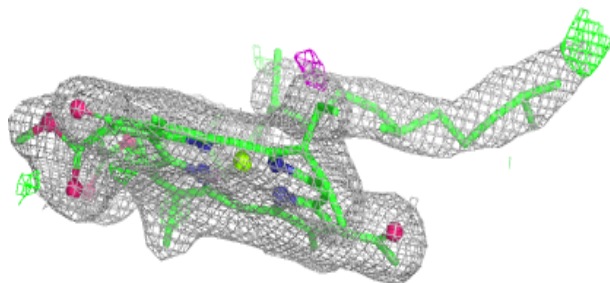
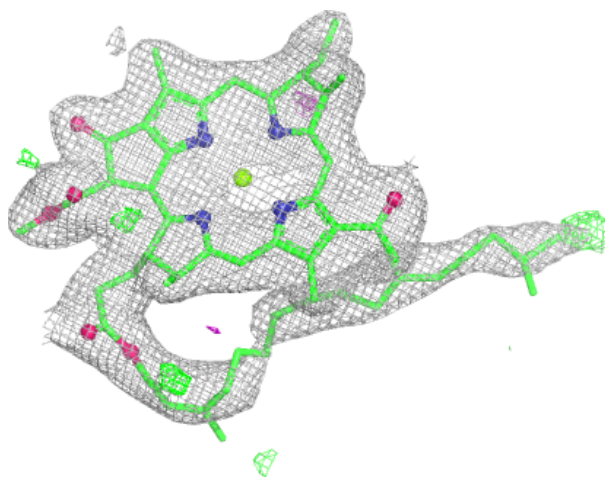
**Electron density around BCL U 102:**

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



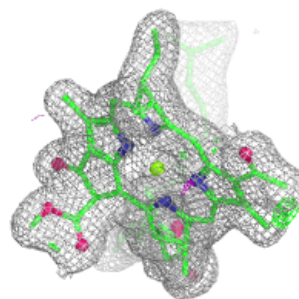
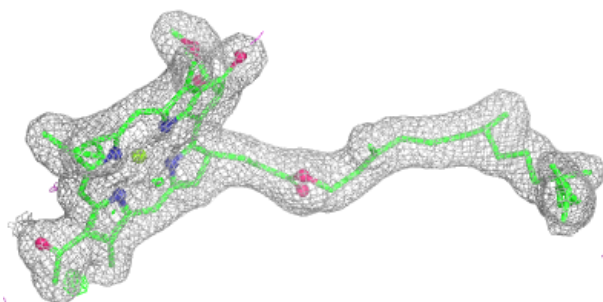
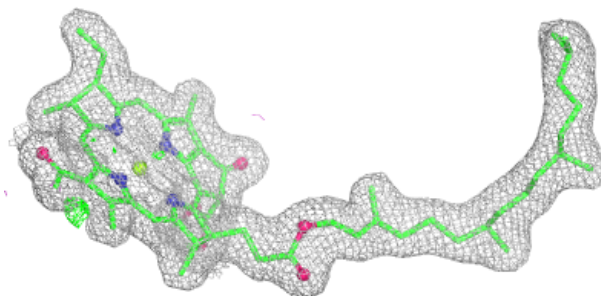
Electron density around BCL U 103:

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

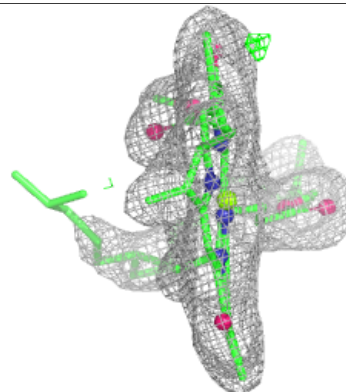
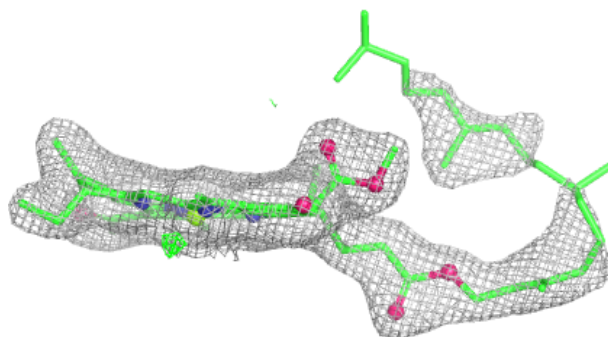
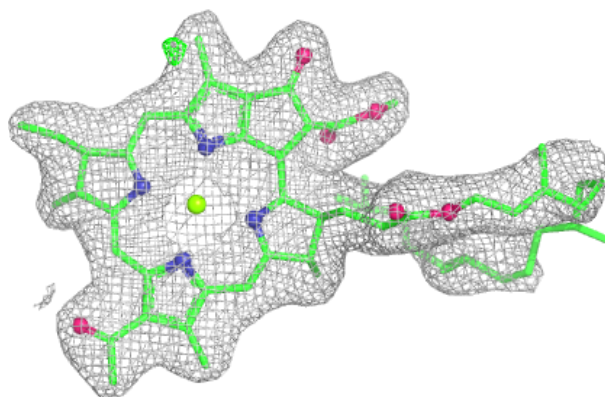


Electron density around BCL M 404:

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

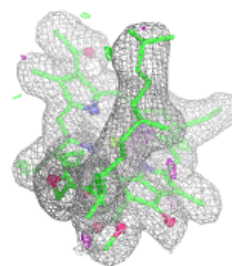
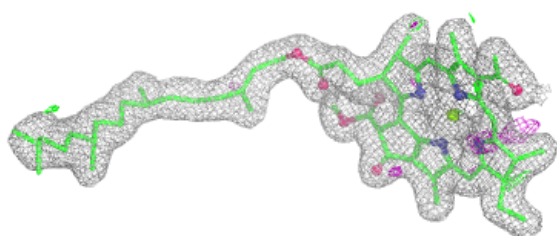
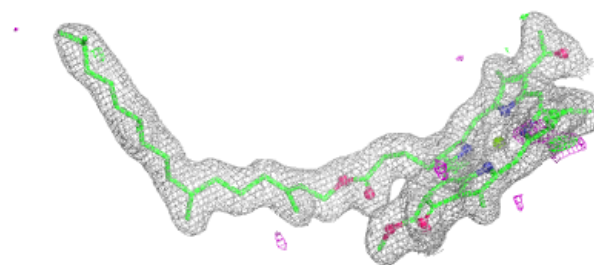
**Electron density around BCL O 102:**

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

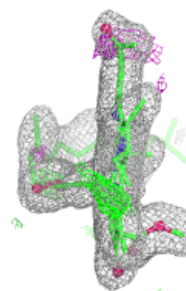
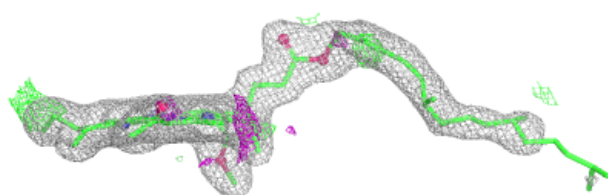
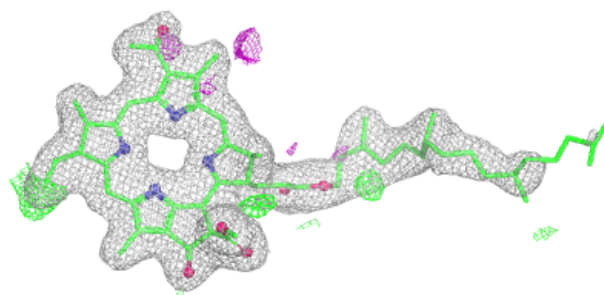


Electron density around BCL L 301:

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

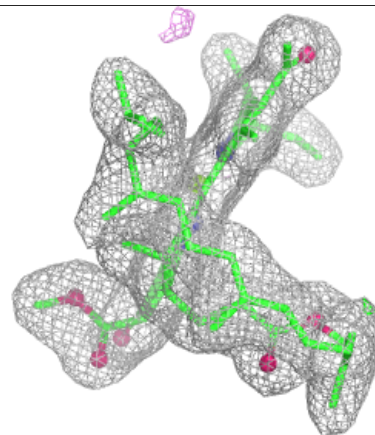
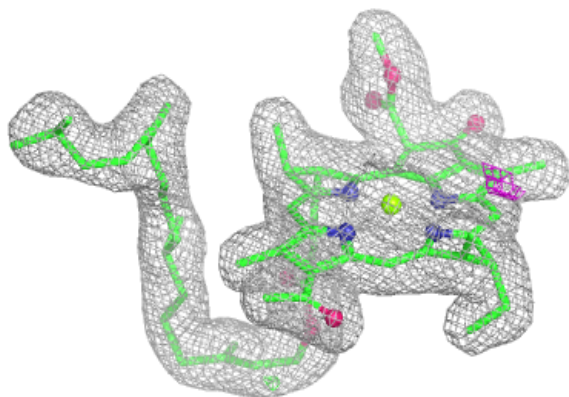
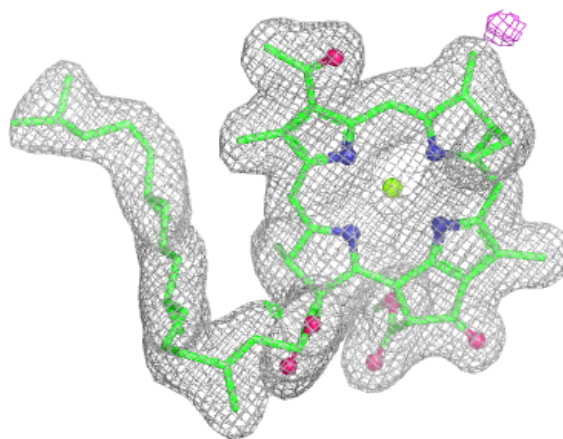
**Electron density around BPH M 405:**

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



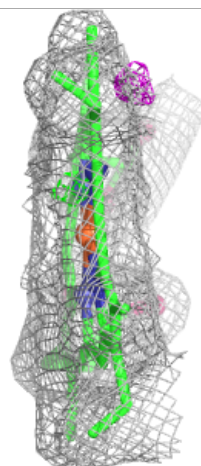
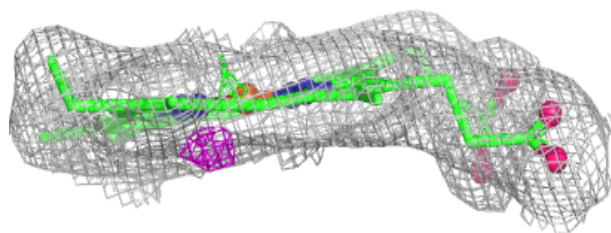
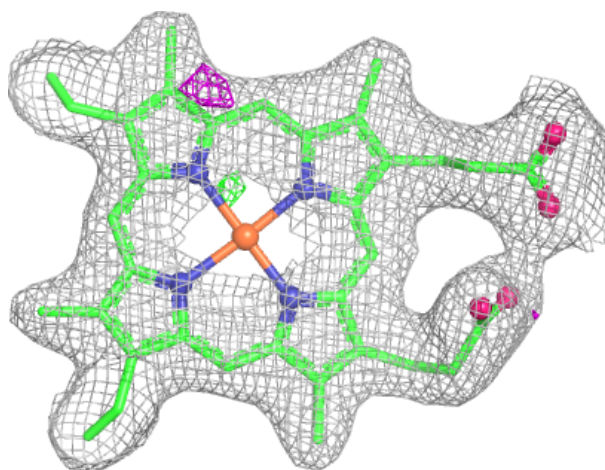
Electron density around BCL M 402:

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



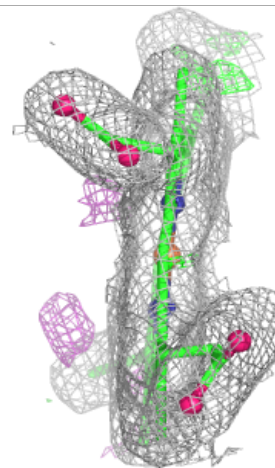
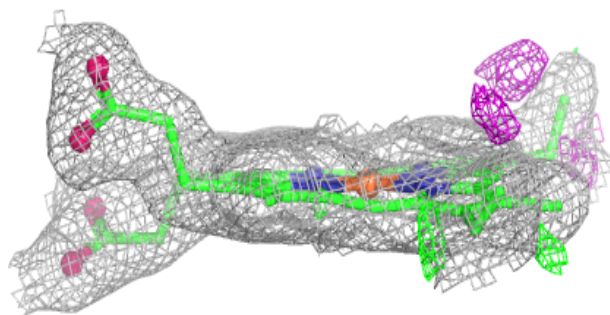
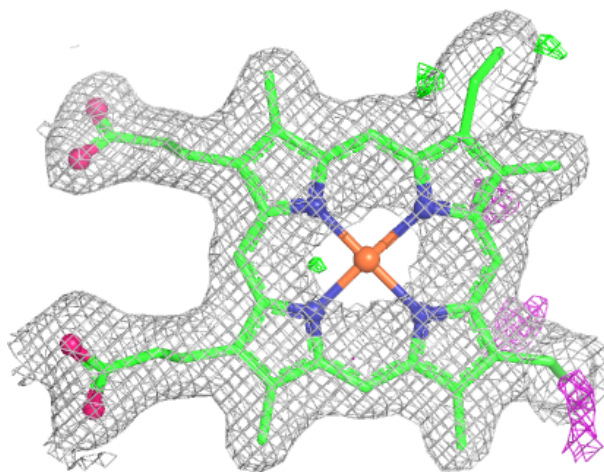
Electron density around HEC C 502:

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



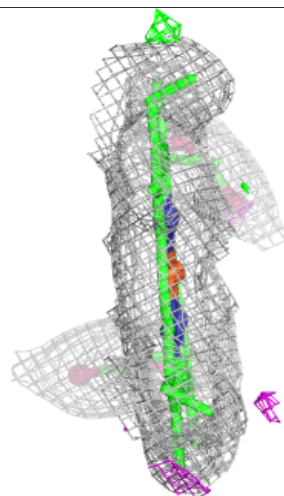
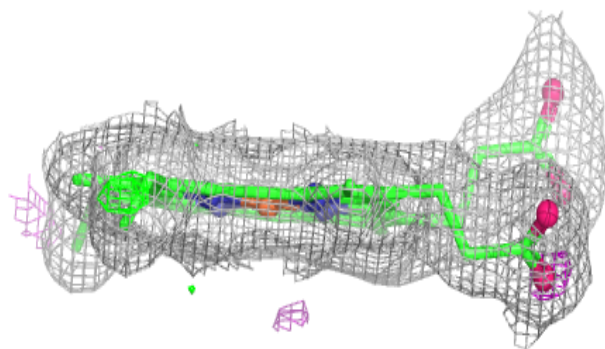
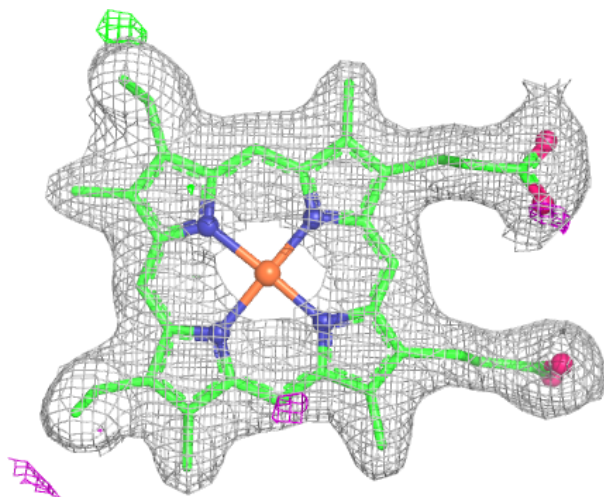
Electron density around HEC C 503:

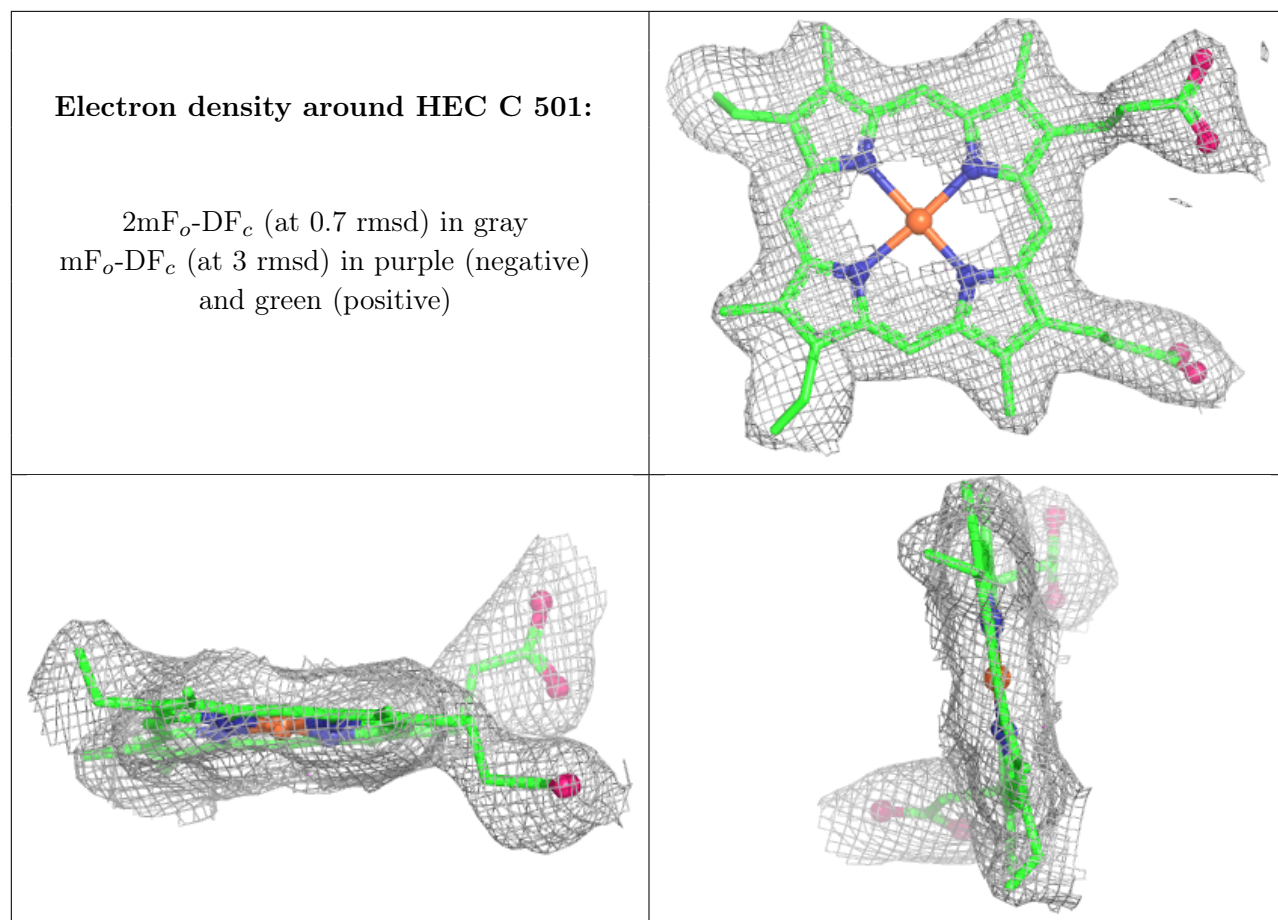
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.