



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 05:55 PM JST

PDB ID : 7C52 / pdb_00007c52
Title : Co-crystal structure of a photosynthetic LH1-RC in complex with electron donor HiPIP
Authors : Yu, L.-J.; Wang-Otomo, Z.-Y.
Deposited on : 2020-05-18
Resolution : 2.89 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:

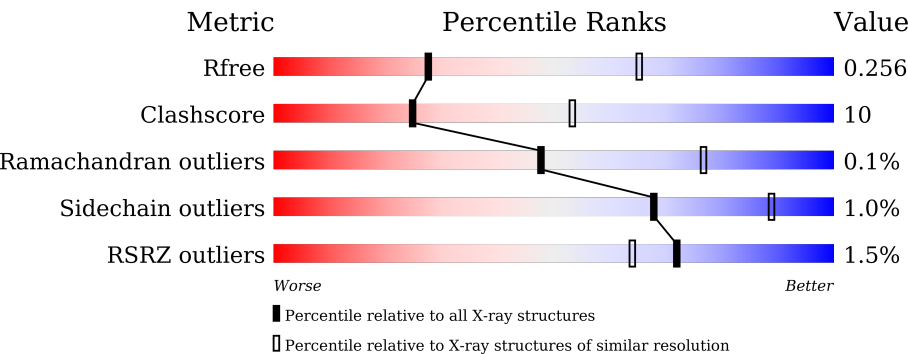
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	311	%92%8%
2	L	281	2%87%12%
3	M	325	%84%14%•
4	H	259	2%87%11%•
5	1	61	3%79%13%8%
5	3	61	84%8%8%

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	R	47	
6	T	47	
6	V	47	
6	X	47	
6	Z	47	
7	b	83	

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
21	PEF	1	103	-	X	-	-
21	PEF	3	104	-	X	-	-
21	PEF	I	103	-	X	-	-
21	PEF	M	407	-	X	-	-
21	PEF	M	409	-	X	-	-
21	PEF	W	105	-	X	-	-
21	PEF	W	106	-	X	-	-
8	HEC	C	501	X	-	-	-
8	HEC	C	502	X	-	-	-
8	HEC	C	503	X	-	-	-
8	HEC	C	504	X	-	-	-

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 27405 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
			1973	1269	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			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	57	Total	C	N	O	S	0	0	0
			454	301	74	78	1			
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
			465	310	74	79	2			
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
			447	297	73	76	1			
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			

Continued on next page...

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

- | Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | b | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 616 | 383 | 110 | 118 | 5 | | | |

- # HEC
-
- Chemical structure diagram of the HEC (Hexaethylcyclen) ligand complexed with an iron(II) ion (Fe). The ligand is a macrocyclic polyamine with six nitrogen atoms (N1-N6) coordinated to the central Fe atom. The ligand is substituted with various side chains: C1C, C1B, C1A, C1D, C2C, C2B, C2A, C2D, C3C, C3B, C3A, C3D, C4C, C4B, C4A, C4D, C5C, C5B, C5A, C5D, C6C, C6B, C6A, C6D. The side chains are labeled with letters A through D, indicating different environments. The structure is shown in a 3D perspective view.

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

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

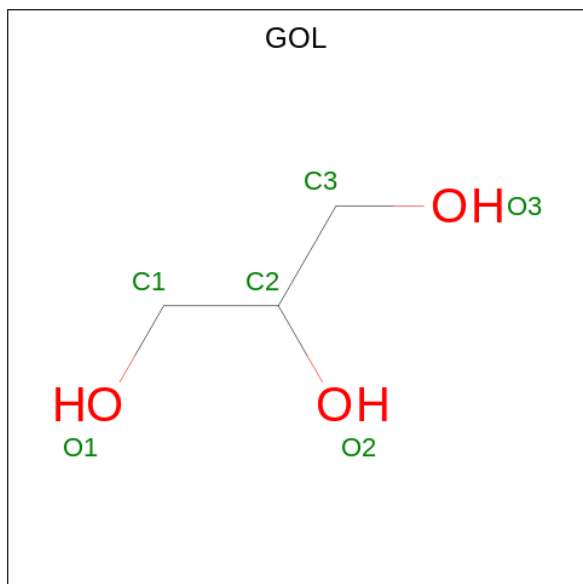
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total 1	Ca 1	0	0
9	A	1	Total 1	Ca 1	0	0
9	D	1	Total 1	Ca 1	0	0
9	F	1	Total 1	Ca 1	0	0
9	I	1	Total 1	Ca 1	0	0
9	K	1	Total 1	Ca 1	0	0
9	O	1	Total 1	Ca 1	0	0
9	Q	1	Total 1	Ca 1	0	0
9	S	1	Total 1	Ca 1	0	0
9	U	1	Total 1	Ca 1	0	0
9	W	1	Total 1	Ca 1	0	0
9	Y	1	Total 1	Ca 1	0	0
9	1	1	Total 1	Ca 1	0	0
9	3	1	Total 1	Ca 1	0	0
9	5	1	Total 1	Ca 1	0	0
9	7	1	Total 1	Ca 1	0	0

Continued on next page...

Continued from previous page...

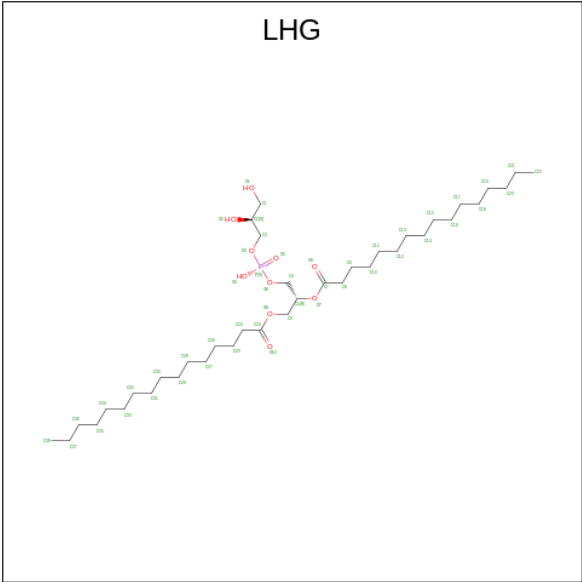
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	9	1	Total	Ca	0	0
			1	1		

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



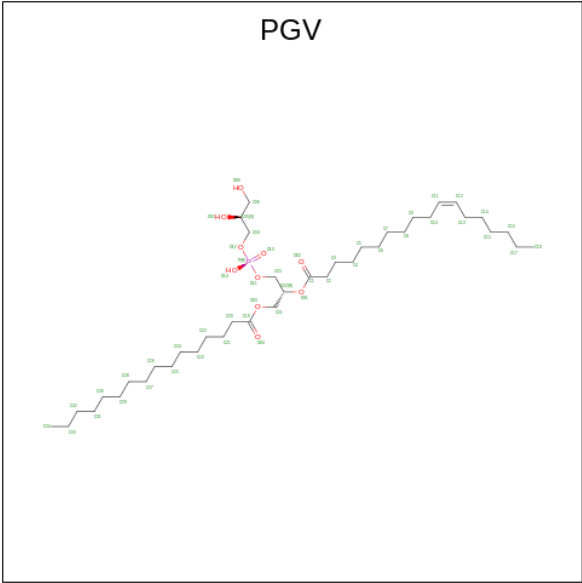
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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).



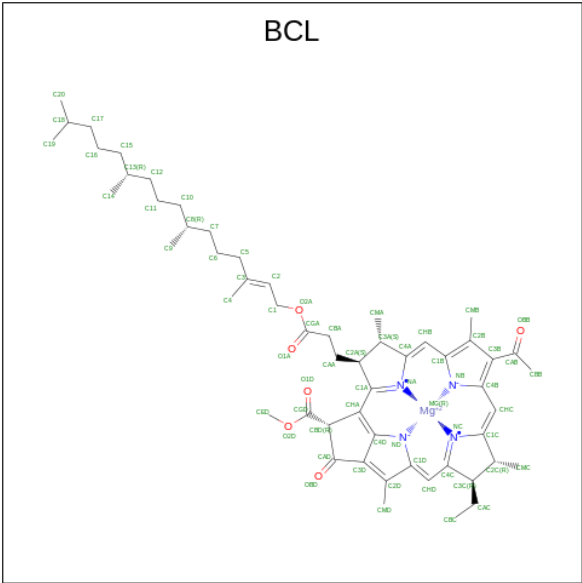
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	O		0	0
			21	17	4			
12	L	1	Total	C	O	P	0	0
			43	32	10	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	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		
12	9	1	Total	C	O	P	0	0
			33	22	10	1		

- Molecule 13 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



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

Continued on next page...

Continued from previous page...

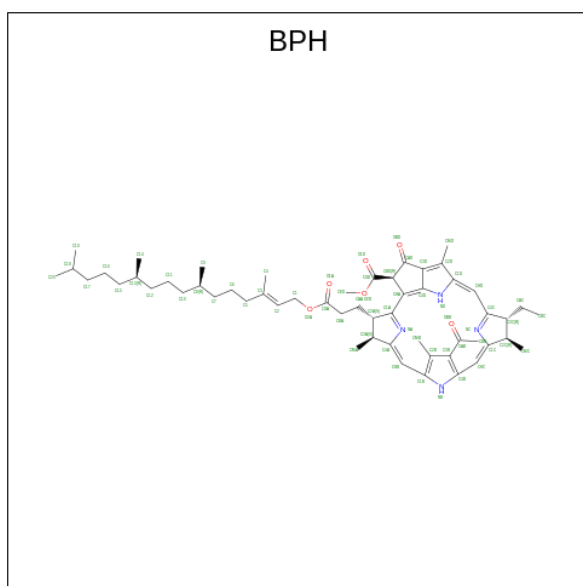
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	D	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	D	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	F	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
13	F	1	Total 66	C 55	Mg 1	N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

Continued on next page...

Continued from previous page...

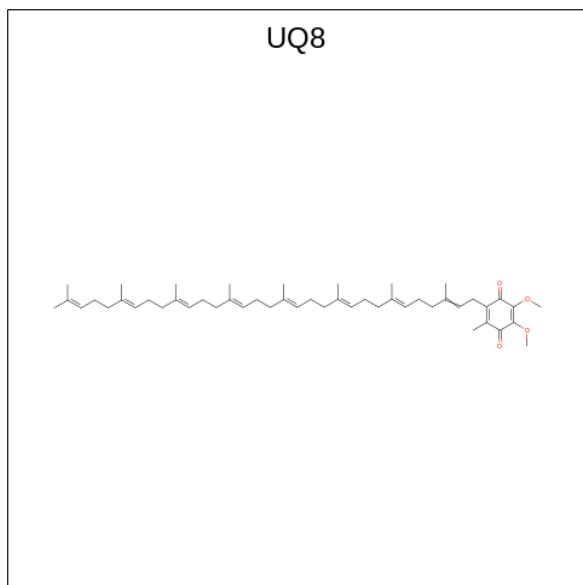
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	Y	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
13	Y	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
13	1	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
13	2	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
13	3	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
13	4	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
13	5	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
13	5	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
13	7	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
13	7	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
13	9	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
13	9	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



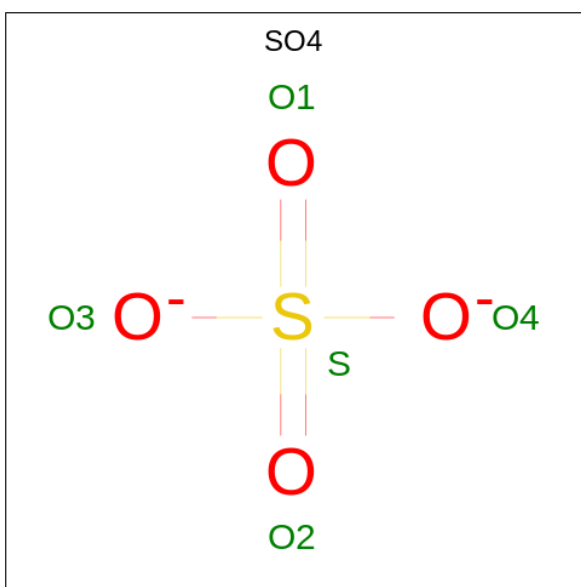
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	L	1	Total	C	N	O	0	0
			65	55	4	6		
14	M	1	Total	C	N	O	0	0
			65	55	4	6		

- 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
			33	29	4		
15	L	1	Total	C	O	0	0
			18	14	4		
15	M	1	Total	C	O	0	0
			18	14	4		

- Molecule 16 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

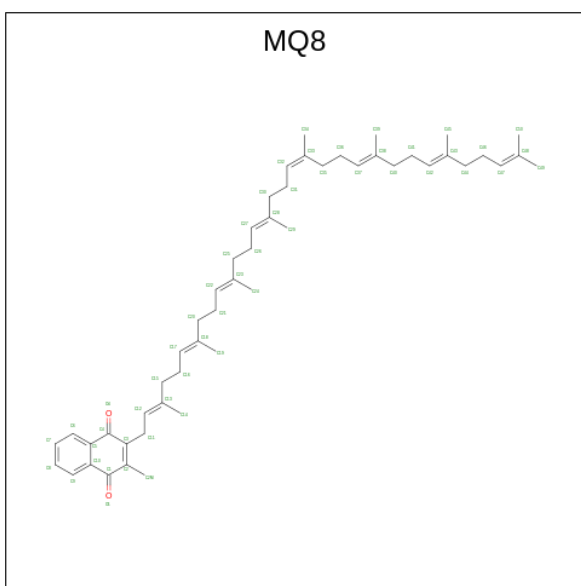


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	L	1	Total	O	S	0	0
			5	4	1		

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

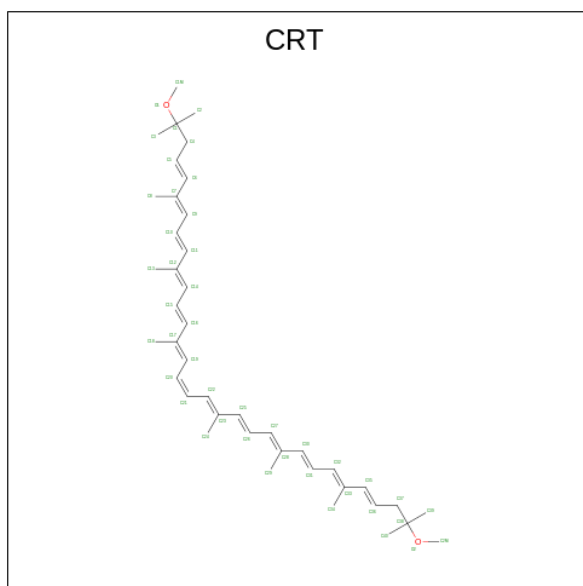
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	M	1	Total	Fe	0	0
			1	1		

- 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: $C_{42}H_{60}O_2$).



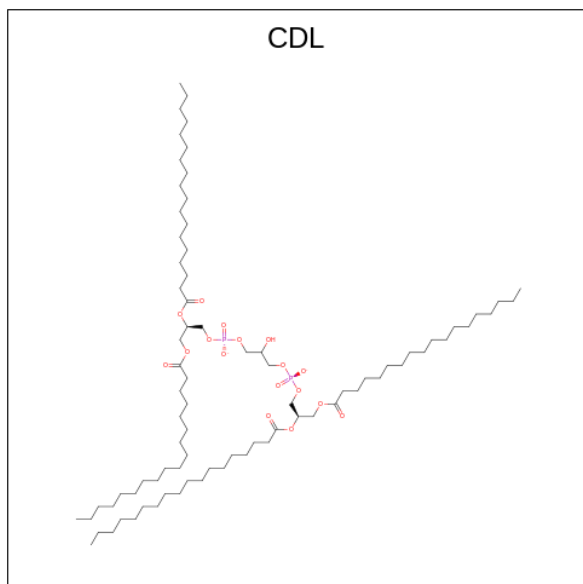
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	M	1	Total	C	O	0	0
			44	42	2		
19	A	1	Total	C	O	0	0
			44	42	2		
19	B	1	Total	C	O	0	0
			44	42	2		
19	G	1	Total	C	O	0	0
			44	42	2		
19	J	1	Total	C	O	0	0
			44	42	2		
19	N	1	Total	C	O	0	0
			44	42	2		
19	O	1	Total	C	O	0	0
			44	42	2		
19	P	1	Total	C	O	0	0
			44	42	2		
19	T	1	Total	C	O	0	0
			44	42	2		
19	V	1	Total	C	O	0	0
			44	42	2		
19	W	1	Total	C	O	0	0
			44	42	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	Z	1	Total	C	O	0	0
			44	42	2		
19	2	1	Total	C	O	0	0
			44	42	2		
19	3	1	Total	C	O	0	0
			44	42	2		
19	4	1	Total	C	O	0	0
			44	42	2		
19	8	1	Total	C	O	0	0
			44	42	2		
19	0	1	Total	C	O	0	0
			44	42	2		

- Molecule 20 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



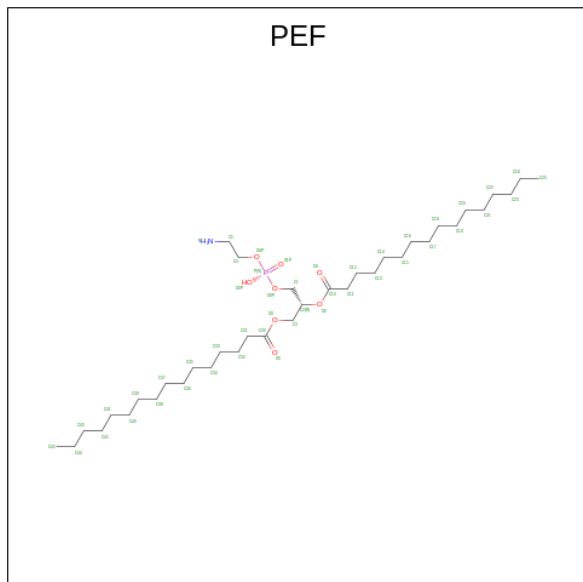
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	M	1	Total	C	O	P	0	0
			100	81	17	2		
20	M	1	Total	C	O	P	0	0
			39	21	16	2		
20	H	1	Total	C	O	P	0	0
			79	60	17	2		
20	D	1	Total	C	O	P	0	0
			40	21	17	2		
20	D	1	Total	C	O	P	0	0
			64	45	17	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	O	1	Total	C	O	P	0	0
			86	67	17	2		
20	S	1	Total	C	O	P	0	0
			75	56	17	2		
20	U	1	Total	C	O	P	0	0
			62	43	17	2		
20	Y	1	Total	C	O	P	0	0
			40	21	17	2		
20	1	1	Total	C	O	P	0	0
			13	5	7	1		

- Molecule 21 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: $C_{37}H_{74}NO_8P$).



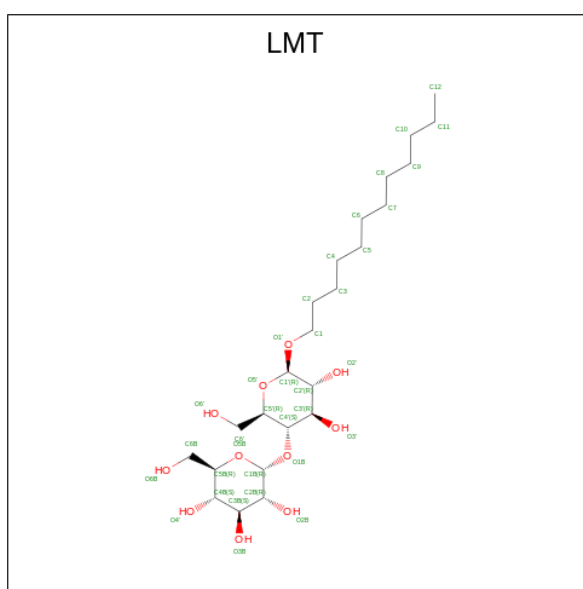
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	M	1	Total	O	P		0	0
			5	4	1			
21	M	1	Total	O	P		0	0
			5	4	1			
21	M	1	Total	O	P		0	0
			5	4	1			
21	H	1	Total	O	P		0	0
			5	4	1			
21	I	1	Total	O	P		0	0
			5	4	1			
21	K	1	Total	C	N	O	P	
			27	17	1	8	1	

Continued on next page...

Continued from previous page...

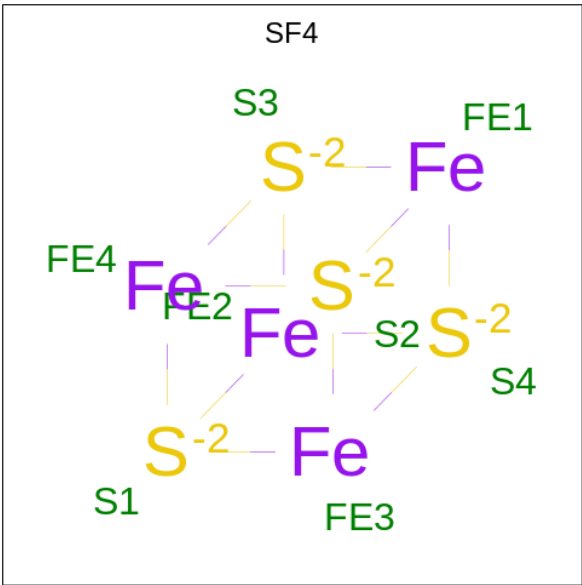
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	W	1	Total	O	P	0	0
			5	4	1		
21	W	1	Total	O	P	0	0
			5	4	1		
21	1	1	Total	O	P	0	0
			5	4	1		
21	3	1	Total	O	P	0	0
			5	4	1		

- Molecule 22 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	M	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		

- Molecule 23 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

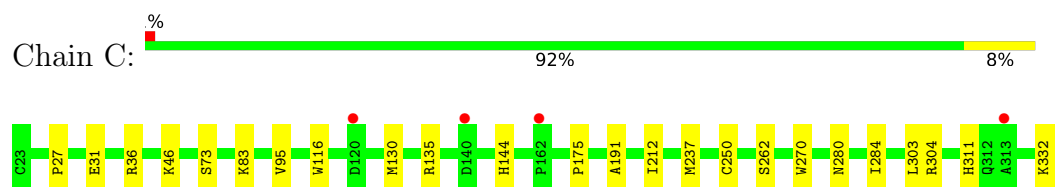


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	b	1	Total	Fe	S	0	0
			8	4	4		

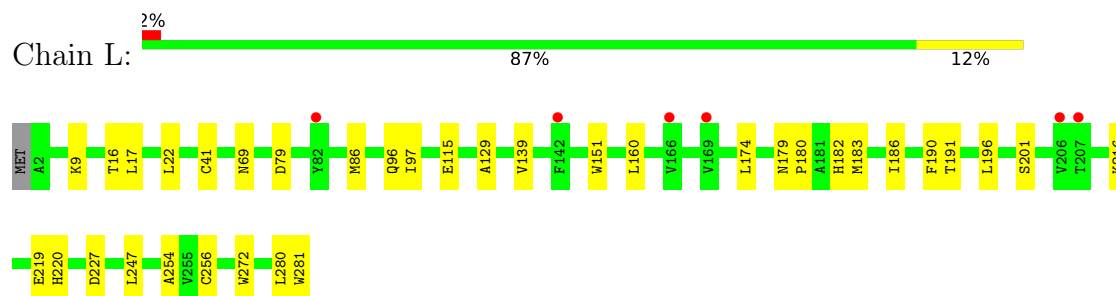
3 Residue-property plots [i](#)

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

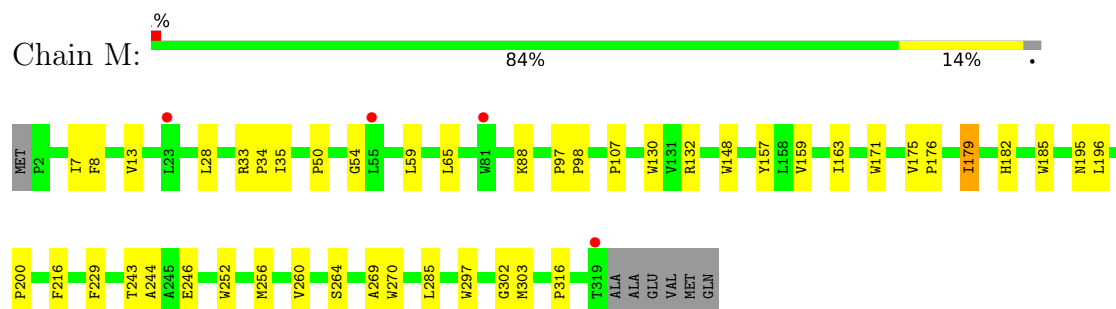
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



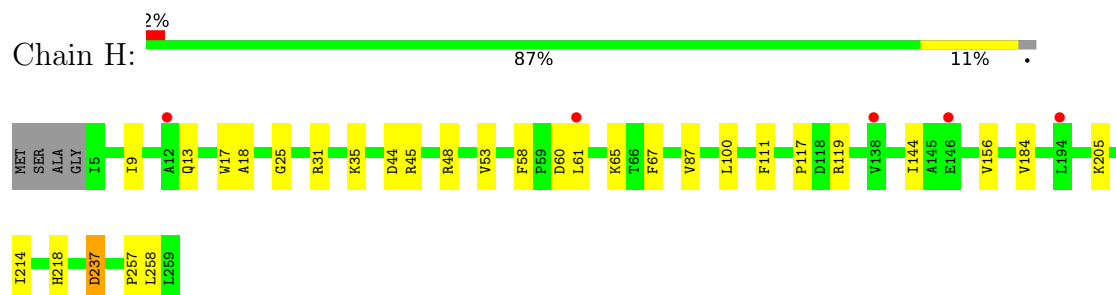
- Molecule 2: Photosynthetic reaction center L subunit



- Molecule 3: Photosynthetic reaction center M subunit



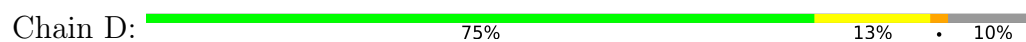
- Molecule 4: Photosynthetic reaction center H subunit



- Molecule 5: LH1 alpha polypeptide



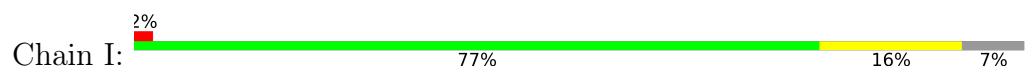
- Molecule 5: LH1 alpha polypeptide



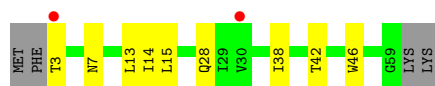
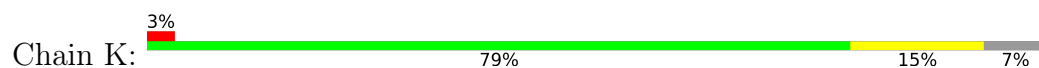
- Molecule 5: LH1 alpha polypeptide



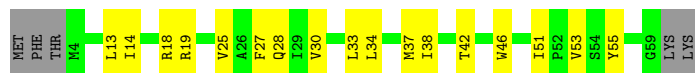
- Molecule 5: LH1 alpha polypeptide



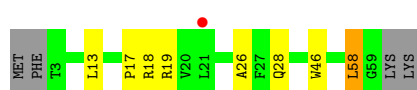
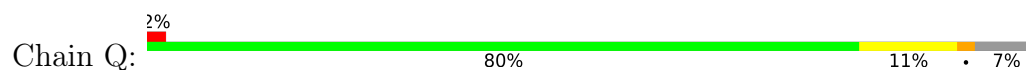
- Molecule 5: LH1 alpha polypeptide



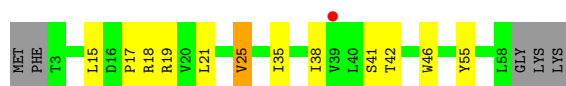
- Molecule 5: LH1 alpha polypeptide



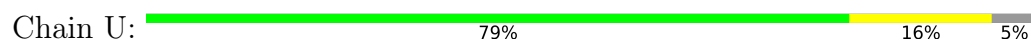
- Molecule 5: LH1 alpha polypeptide



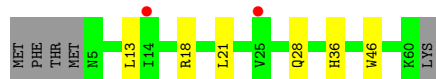
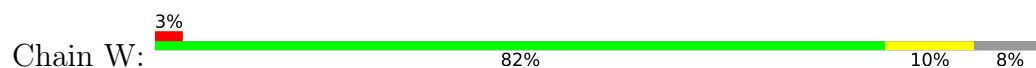
- Molecule 5: LH1 alpha polypeptide



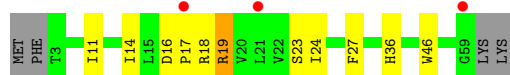
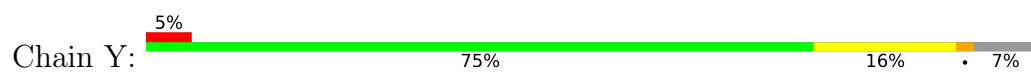
- Molecule 5: LH1 alpha polypeptide



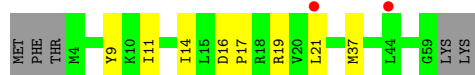
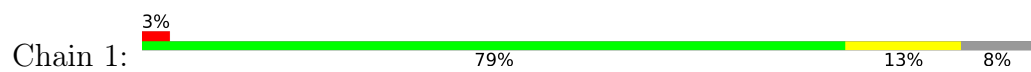
- Molecule 5: LH1 alpha polypeptide



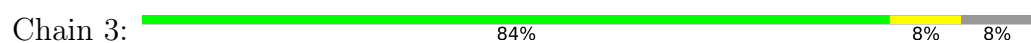
- Molecule 5: LH1 alpha polypeptide



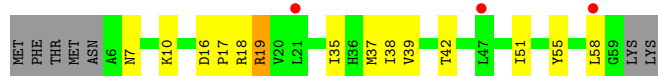
- Molecule 5: LH1 alpha polypeptide



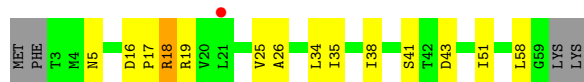
- Molecule 5: LH1 alpha polypeptide



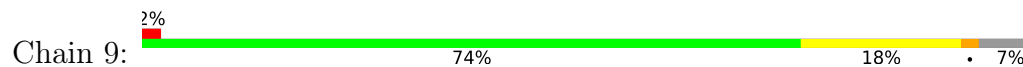
- Molecule 5: LH1 alpha polypeptide



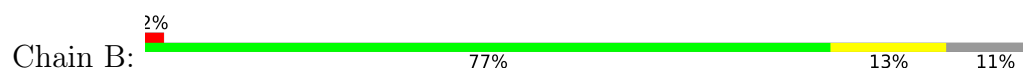
- Molecule 5: LH1 alpha polypeptide



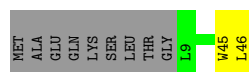
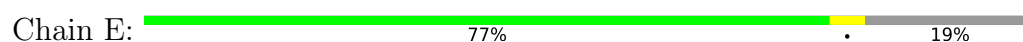
- Molecule 5: LH1 alpha polypeptide



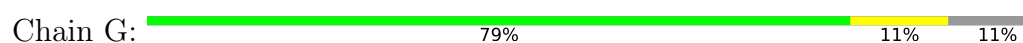
- Molecule 6: LH1 beta polypeptide



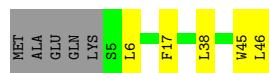
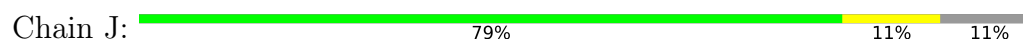
- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide

Chain P:  72% 17% 11%



- Molecule 6: LH1 beta polypeptide

Chain R:  74% 11% 13%



- Molecule 6: LH1 beta polypeptide

Chain T:  2% 81% 11% 9%



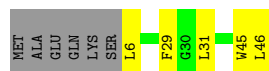
- Molecule 6: LH1 beta polypeptide

Chain V:  81% 9% 11%



- Molecule 6: LH1 beta polypeptide

Chain X:  77% 11% 13%



- Molecule 6: LH1 beta polypeptide

Chain Z:  66% 19% 15%



- Molecule 6: LH1 beta polypeptide

Chain 2:  62% 26% 13%



- Molecule 6: LH1 beta polypeptide

Chain 4:  70% 19% 11%



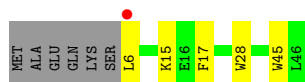
- Molecule 6: LH1 beta polypeptide

Chain 6:  74% 13% 11%



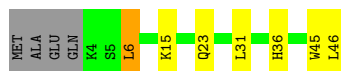
- Molecule 6: LH1 beta polypeptide

Chain 8:  2% 77% 11% 13%



- Molecule 6: LH1 beta polypeptide

Chain 0:  77% 13% 9%



- Molecule 7: High-potential iron-sulfur protein

Chain b:  2% 81% 18%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.44Å 183.34Å 123.86Å 90.00° 112.58° 90.00°	Depositor
Resolution (Å)	29.99 – 2.89 29.99 – 2.89	Depositor EDS
% Data completeness (in resolution range)	97.6 (29.99-2.89) 97.5 (29.99-2.89)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.219 , 0.248 0.226 , 0.256	Depositor DCC
R_{free} test set	4316 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	103.8	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27405	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: GOL, HEC, SF4, PGV, CDL, CRT, BCL, BPH, MQ8, LMT, SO4, UQ8, PEF, LHG, FE, 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	0.17	0/2487	0.50	0/3396
2	L	0.17	0/2326	0.48	0/3177
3	M	0.17	0/2658	0.45	0/3637
4	H	0.21	0/2031	0.53	0/2769
5	1	0.34	0/456	0.59	0/625
5	3	0.19	0/467	0.46	0/638
5	5	0.48	1/443 (0.2%)	0.78	2/607 (0.3%)
5	7	0.52	1/466 (0.2%)	0.67	3/638 (0.5%)
5	9	0.24	0/466	0.58	0/638
5	A	0.16	0/443	0.50	0/607
5	D	0.25	0/457	0.62	2/626 (0.3%)
5	F	0.27	0/457	0.61	0/626
5	I	0.20	0/472	0.53	0/646
5	K	0.14	0/463	0.44	0/635
5	O	0.21	0/467	0.60	0/638
5	Q	0.16	0/466	0.53	1/638 (0.2%)
5	S	0.25	0/480	0.55	0/658
5	U	0.28	0/475	0.62	0/649
5	W	0.23	0/460	0.58	1/629 (0.2%)
5	Y	0.57	2/466 (0.4%)	0.63	2/638 (0.3%)
6	0	0.14	0/373	0.39	0/506
6	2	0.15	0/358	0.39	0/487
6	4	0.14	0/364	0.40	0/495
6	6	0.19	0/364	0.46	0/495
6	8	0.15	0/358	0.44	0/487
6	B	0.12	0/364	0.38	0/495
6	E	0.15	0/339	0.42	0/461
6	G	0.12	0/364	0.39	0/495
6	J	0.16	0/364	0.43	0/495
6	N	0.17	0/364	0.38	0/495
6	P	0.12	0/364	0.33	0/495
6	R	0.13	0/358	0.33	0/487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	T	0.13	0/373	0.42	0/506
6	V	0.19	0/364	0.36	0/495
6	X	0.15	0/358	0.39	0/487
6	Z	0.13	0/350	0.33	0/476
7	b	0.17	0/631	0.48	0/859
All	All	0.22	4/23316 (0.0%)	0.50	11/31831 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	7	18	ARG	CG-CD	-8.82	1.25	1.52
5	Y	19	ARG	CG-CD	-8.09	1.28	1.52
5	5	19	ARG	CZ-NH1	5.88	1.41	1.32
5	Y	19	ARG	CB-CG	-5.44	1.36	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	7	18	ARG	CB-CG-CD	-8.19	92.46	111.30
5	5	19	ARG	CG-CD-NE	-6.69	97.28	112.00
5	Y	19	ARG	CG-CD-NE	-5.99	98.82	112.00
5	7	18	ARG	NE-CZ-NH2	-5.79	113.99	119.20
5	7	18	ARG	CD-NE-CZ	-5.77	116.32	124.40
5	Y	19	ARG	CD-NE-CZ	-5.45	116.78	124.40
5	5	19	ARG	NE-CZ-NH2	-5.37	114.36	119.20
5	D	18	ARG	NE-CZ-NH2	5.23	123.91	119.20
5	Q	18	ARG	CB-CA-C	5.17	119.07	110.90
5	W	18	ARG	NE-CZ-NH1	-5.08	116.42	121.50
5	D	18	ARG	CD-NE-CZ	-5.04	117.34	124.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2417	0	2328	19	0
2	L	2236	0	2201	33	0
3	M	2555	0	2528	39	0
4	H	1973	0	1968	37	0
5	1	447	0	468	18	0
5	3	455	0	484	6	0
5	5	434	0	460	22	0
5	7	457	0	482	22	0
5	9	457	0	482	14	0
5	A	434	0	460	14	0
5	D	445	0	471	12	0
5	F	445	0	471	12	0
5	I	460	0	487	10	0
5	K	454	0	475	8	0
5	O	455	0	484	18	0
5	Q	457	0	482	8	0
5	S	465	0	494	18	0
5	U	466	0	495	18	0
5	W	451	0	479	5	0
5	Y	457	0	482	14	0
6	0	360	0	352	9	0
6	2	345	0	334	15	0
6	4	351	0	339	9	0
6	6	351	0	339	9	0
6	8	345	0	334	5	0
6	B	351	0	339	7	0
6	E	326	0	313	1	0
6	G	351	0	339	6	0
6	J	351	0	339	5	0
6	N	351	0	339	10	0
6	P	351	0	339	8	0
6	R	345	0	334	6	0
6	T	360	0	352	6	0
6	V	351	0	339	6	0
6	X	345	0	334	7	0
6	Z	337	0	323	15	0
7	b	616	0	589	11	0
8	C	172	0	120	5	0
9	1	1	0	0	0	0
9	3	1	0	0	0	0
9	5	1	0	0	0	0
9	7	1	0	0	0	0
9	9	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	F	1	0	0	0	0
9	I	1	0	0	0	0
9	K	1	0	0	0	0
9	O	1	0	0	0	0
9	Q	1	0	0	0	0
9	S	1	0	0	0	0
9	U	1	0	0	0	0
9	W	1	0	0	0	0
9	Y	1	0	0	0	0
10	C	6	0	8	1	0
10	H	6	0	8	0	0
11	C	9	0	12	0	0
12	1	31	0	32	1	0
12	3	51	0	76	6	0
12	9	33	0	36	5	0
12	C	21	0	23	0	0
12	D	35	0	40	2	0
12	H	36	0	42	2	0
12	L	87	0	120	12	0
12	M	83	0	116	8	0
13	1	66	0	74	5	0
13	2	66	0	74	10	0
13	3	66	0	74	3	0
13	4	66	0	74	6	0
13	5	132	0	148	6	0
13	7	127	0	135	10	0
13	9	132	0	148	8	0
13	A	132	0	148	9	0
13	D	132	0	148	4	0
13	F	132	0	148	11	0
13	I	66	0	74	3	0
13	J	66	0	74	3	0
13	K	132	0	148	8	0
13	L	198	0	222	12	0
13	M	66	0	74	0	0
13	O	66	0	74	6	0
13	P	66	0	74	5	0
13	Q	132	0	148	9	0
13	S	132	0	148	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	U	132	0	148	12	0
13	W	132	0	148	11	0
13	Y	132	0	148	16	0
14	L	65	0	74	4	0
14	M	65	0	74	7	0
15	L	137	0	167	19	0
15	M	18	0	15	1	0
16	L	5	0	0	0	0
17	M	1	0	0	0	0
18	M	53	0	72	5	0
19	0	44	0	60	5	0
19	2	44	0	60	6	0
19	3	44	0	60	2	0
19	4	44	0	60	6	0
19	8	44	0	60	5	0
19	A	44	0	60	8	0
19	B	44	0	60	6	0
19	G	44	0	60	5	0
19	J	44	0	60	2	0
19	M	44	0	60	7	0
19	N	44	0	60	4	0
19	O	44	0	60	0	0
19	P	44	0	60	4	0
19	T	44	0	60	3	0
19	V	44	0	60	3	0
19	W	44	0	60	1	0
19	Z	44	0	60	5	0
20	1	13	0	7	0	0
20	D	104	0	96	10	0
20	H	79	0	105	6	0
20	M	139	0	184	7	0
20	O	86	0	119	13	0
20	S	75	0	94	12	0
20	U	62	0	68	9	0
20	Y	40	0	24	3	0
21	1	5	0	0	2	0
21	3	5	0	0	0	0
21	H	5	0	0	0	0
21	I	5	0	0	0	0
21	K	27	0	27	2	0
21	M	15	0	0	0	0
21	W	10	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	H	35	0	46	8	0
22	M	35	0	46	0	0
23	b	8	0	0	0	0
All	All	27405	0	28180	542	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (542) 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)
5:1:16:ASP:HB3	5:1:19:ARG:HE	1.25	1.00
5:U:11:ILE:HD12	5:U:14:ILE:HD11	1.48	0.94
4:H:258:LEU:O	5:5:19:ARG:NH2	2.10	0.85
5:D:18:ARG:NH1	20:D:105:CDL:OB4	2.13	0.82
2:L:96:GLN:HG2	15:L:309:UQ8:H4M	1.63	0.80
5:S:19:ARG:HH11	20:S:104:CDL:PB2	2.05	0.79
5:U:18:ARG:NH1	20:U:104:CDL:O1	2.15	0.78
5:1:11:ILE:HD12	5:1:14:ILE:HD11	1.65	0.78
5:D:18:ARG:NH2	20:D:105:CDL:OA3	2.16	0.78
5:5:16:ASP:HB3	5:5:19:ARG:NH1	2.00	0.76
5:1:19:ARG:NH1	21:1:103:PEF:O2P	2.19	0.76
5:A:19:ARG:NH2	20:D:105:CDL:O1	2.16	0.76
5:1:16:ASP:HB3	5:1:19:ARG:NE	2.02	0.74
6:6:6:LEU:CB	5:7:18:ARG:HH22	1.99	0.74
4:H:44:ASP:H	12:9:104:PGV:H062	1.52	0.74
5:U:18:ARG:HH12	20:U:104:CDL:C1	2.01	0.73
13:P:102:BCL:H42	13:Q:101:BCL:H202	1.70	0.72
2:L:17:LEU:O	4:H:258:LEU:N	2.21	0.72
5:U:18:ARG:NH1	20:U:104:CDL:C1	2.53	0.72
6:6:6:LEU:HB2	5:7:18:ARG:HH22	1.57	0.70
6:4:17:PHE:HA	19:4:101:CRT:H6	1.74	0.68
4:H:258:LEU:O	5:5:19:ARG:CZ	2.41	0.68
4:H:45:ARG:NH1	5:A:14:ILE:O	2.28	0.67
5:D:25:VAL:HG11	20:D:105:CDL:H521	1.75	0.67
5:S:18:ARG:HH22	5:S:19:ARG:HE	1.42	0.67
2:L:86[B]:MET:HG2	5:7:41:SER:HB3	1.77	0.67
5:K:15:LEU:HD23	5:O:18:ARG:HG3	1.77	0.66
6:2:17:PHE:HA	19:2:101:CRT:H6	1.76	0.66
5:5:16:ASP:OD1	5:5:18:ARG:HG2	1.96	0.66
3:M:28:LEU:HD12	3:M:54:GLY:HA2	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:308:PGV:H202	12:M:410:PGV:H222	1.79	0.64
5:D:14:ILE:HD11	19:G:101:CRT:H23	1.77	0.64
6:2:29:PHE:CE1	13:2:102:BCL:H2	2.32	0.64
3:M:130:TRP:HZ3	20:O:104:CDL:H511	1.62	0.64
19:3:103:CRT:H371	13:7:101:BCL:HMB2	1.78	0.64
13:W:104:BCL:H51	13:Y:101:BCL:H162	1.78	0.64
2:L:180:PRO:HA	2:L:183:MET:HE3	1.80	0.64
4:H:45:ARG:HD3	4:H:53:VAL:HG11	1.80	0.63
5:F:10:LYS:NZ	6:G:11:ASP:OD1	2.30	0.63
13:U:103:BCL:H2	6:V:29:PHE:CE1	2.34	0.63
5:1:16:ASP:CB	5:1:19:ARG:HH11	2.13	0.62
13:Y:103:BCL:H2	6:Z:29:PHE:CE1	2.35	0.62
6:4:29:PHE:CE1	13:4:102:BCL:H11	2.35	0.62
14:L:303:BPH:HBB3	14:L:303:BPH:HHC	1.82	0.61
12:L:307:PGV:H62	12:D:106:PGV:H62	1.82	0.61
12:3:105:PGV:H251	5:5:37:MET:HG3	1.83	0.61
5:Y:18:ARG:HH12	20:Y:104:CDL:CB2	2.14	0.60
2:L:17:LEU:HD22	4:H:258:LEU:HD11	1.84	0.60
12:L:308:PGV:H62	4:H:258:LEU:HD12	1.83	0.60
13:4:102:BCL:H42	13:5:101:BCL:H162	1.83	0.60
5:O:25:VAL:HG11	20:O:104:CDL:H331	1.82	0.60
1:C:116:TRP:NE1	7:b:79:THR:OG1	2.32	0.60
3:M:200:PRO:HB3	12:H:303:PGV:H22	1.84	0.59
5:Q:28:GLN:HB3	13:Q:101:BCL:H42	1.83	0.59
13:S:101:BCL:HMA3	13:S:101:BCL:H203	1.85	0.59
2:L:16:THR:OG1	4:H:257:PRO:HB3	2.03	0.59
5:S:18:ARG:HH22	5:S:19:ARG:NE	2.00	0.59
6:2:29:PHE:CD1	13:2:102:BCL:H2	2.37	0.59
5:Y:36:HIS:CE1	13:Y:103:BCL:HMD3	2.38	0.58
6:Z:17:PHE:HA	19:Z:101:CRT:H6	1.85	0.58
4:H:45:ARG:NH2	6:B:6:LEU:O	2.33	0.58
19:B:101:CRT:H1M1	5:9:14:ILE:HD11	1.85	0.58
6:6:6:LEU:HD22	5:7:18:ARG:HH12	1.68	0.58
18:M:404:MQ8:H241	20:H:305:CDL:H772	1.85	0.58
20:O:104:CDL:H531	20:O:104:CDL:H371	1.85	0.58
20:H:305:CDL:OA3	5:A:19:ARG:NH2	2.36	0.58
6:P:17:PHE:HA	19:P:101:CRT:H6	1.86	0.57
19:2:101:CRT:H342	13:3:101:BCL:HBA2	1.85	0.57
3:M:157:TYR:CZ	19:M:405:CRT:H293	2.39	0.57
6:B:45:TRP:CD1	6:B:46:LEU:HG	2.40	0.57
19:B:101:CRT:H372	5:D:36:HIS:CG	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:45:ARG:NH2	4:H:53:VAL:HG21	2.20	0.57
5:1:16:ASP:HB2	5:1:19:ARG:HH11	1.69	0.57
5:Y:11:ILE:HD12	5:Y:14:ILE:HD11	1.85	0.57
5:U:18:ARG:NH1	20:U:104:CDL:H1	2.19	0.57
19:A:104:CRT:H27	13:D:103:BCL:O1A	2.05	0.56
5:1:16:ASP:CB	5:1:19:ARG:HE	2.11	0.56
13:S:103:BCL:H42	13:U:101:BCL:H151	1.87	0.56
5:Y:19:ARG:NH2	20:Y:104:CDL:O1	2.38	0.56
13:L:305:BCL:H161	15:L:311:UQ8:H3M	1.86	0.56
6:B:21:PHE:HA	19:B:101:CRT:H14	1.87	0.56
5:D:18:ARG:NH1	20:D:105:CDL:HB21	2.21	0.56
5:F:16:ASP:HB3	5:F:19:ARG:HE	1.71	0.56
5:7:35:ILE:HG12	19:8:101:CRT:H403	1.88	0.56
7:b:33:ARG:NH1	7:b:78:TRP:O	2.38	0.56
5:7:5:ASN:ND2	6:0:23:GLN:OE1	2.38	0.55
20:H:305:CDL:H862	20:H:305:CDL:H592	1.87	0.55
13:F:103:BCL:O1A	19:G:101:CRT:H27	2.07	0.55
5:W:46:TRP:CE2	13:W:101:BCL:H2C	2.41	0.55
5:9:53:VAL:CG2	5:9:58:LEU:HD11	2.36	0.55
3:M:65:LEU:HD21	14:M:402:BPH:H112	1.89	0.55
3:M:171:TRP:HZ2	19:M:405:CRT:H402	1.72	0.55
19:A:104:CRT:H27	13:D:103:BCL:H12	1.88	0.55
5:D:38:ILE:O	5:D:42:THR:HG23	2.07	0.55
5:7:16:ASP:OD1	5:7:18:ARG:HG2	2.07	0.55
2:L:151:TRP:HE1	15:L:309:UQ8:H3MA	1.71	0.55
14:M:402:BPH:HBC3	14:M:402:BPH:HHD	1.88	0.55
5:I:21:LEU:HD21	19:J:101:CRT:C14	2.37	0.55
2:L:190:PHE:HB3	14:M:402:BPH:CBB	2.37	0.54
5:7:43:ASP:HB2	5:9:48:ASP:OD1	2.07	0.54
5:W:36:HIS:CE1	13:W:104:BCL:HMD3	2.42	0.54
5:5:7:ASN:HB3	5:5:10:LYS:HD2	1.88	0.54
1:C:27:PRO:HG3	12:3:105:PGV:H32	1.90	0.54
4:H:258:LEU:HA	5:5:19:ARG:NH2	2.23	0.54
19:2:101:CRT:H27	13:2:102:BCL:O1A	2.07	0.54
2:L:201:SER:HG	3:M:270:TRP:CD1	2.25	0.54
13:W:104:BCL:H2C	6:X:45:TRP:CE2	2.43	0.54
19:Z:101:CRT:H292	13:1:101:BCL:H51	1.90	0.54
4:H:58:PHE:HB3	20:D:105:CDL:H122	1.88	0.53
19:A:104:CRT:H371	13:F:101:BCL:HMB2	1.90	0.53
5:1:16:ASP:HB2	5:1:19:ARG:NH1	2.22	0.53
5:D:43:ASP:N	5:F:48:ASP:OD1	2.37	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:44:PRO:O	5:S:55:TYR:OH	2.26	0.53
5:U:25:VAL:HG11	20:U:104:CDL:H122	1.91	0.53
13:Q:101:BCL:H141	13:Q:101:BCL:H203	1.89	0.53
3:M:59:LEU:HD13	5:Q:26:ALA:HA	1.90	0.53
5:S:19:ARG:NH1	20:S:104:CDL:OB5	2.42	0.53
13:U:103:BCL:H92	6:V:32:VAL:HG12	1.91	0.53
19:V:101:CRT:H371	13:W:101:BCL:HMB2	1.90	0.53
13:Y:103:BCL:H2	6:Z:29:PHE:CD1	2.44	0.53
6:N:43:ARG:HG3	5:O:55:TYR:CZ	2.44	0.53
5:W:13:LEU:O	6:X:6:LEU:HB3	2.09	0.52
6:4:40:TRP:CE2	13:4:102:BCL:H18	2.44	0.52
2:L:182:HIS:CE1	2:L:186:ILE:HD11	2.44	0.52
20:D:104:CDL:OB4	5:F:19:ARG:HG2	2.09	0.52
13:A:103:BCL:H2C	6:B:45:TRP:CE2	2.45	0.52
19:4:101:CRT:H27	13:4:102:BCL:O1A	2.10	0.52
5:7:51:ILE:HD11	5:9:58:LEU:O	2.10	0.52
13:K:103:BCL:H202	6:N:40:TRP:CE2	2.45	0.52
5:F:36:HIS:CE1	13:F:103:BCL:HMD3	2.44	0.52
5:U:23:SER:OG	20:U:104:CDL:H712	2.10	0.52
5:O:19:ARG:NH1	20:O:104:CDL:PB2	2.83	0.52
5:S:19:ARG:NH2	20:S:104:CDL:OB9	2.43	0.52
6:2:43:ARG:HG3	5:3:55:TYR:CZ	2.44	0.52
1:C:175:PRO:HB2	5:S:41[B]:SER:O	2.10	0.51
5:Y:23:SER:HB3	13:1:101:BCL:H172	1.91	0.51
3:M:34:PRO:HG3	3:M:50:PRO:HD3	1.92	0.51
1:C:284:ILE:HG21	1:C:304:ARG:HB3	1.93	0.51
12:L:307:PGV:H82	5:D:37:MET:HE1	1.92	0.51
15:L:309:UQ8:H28	5:7:26:ALA:HB1	1.93	0.51
4:H:35:LYS:HB3	4:H:61:LEU:HD22	1.91	0.51
1:C:135:ARG:HB3	1:C:332:LYS:HG3	1.91	0.51
1:C:175:PRO:HB2	5:S:41[A]:SER:O	2.10	0.51
13:5:101:BCL:H43	6:6:28:TRP:CZ2	2.46	0.51
5:D:23:SER:OG	20:D:105:CDL:OA9	2.25	0.51
13:L:302:BCL:H152	14:L:303:BPH:H3A	1.92	0.51
3:M:8:PHE:CD1	20:M:412:CDL:H512	2.45	0.51
3:M:256:MET:CE	18:M:404:MQ8:H142	2.41	0.51
19:B:101:CRT:C1M	5:9:14:ILE:HD11	2.41	0.51
1:C:280:ASN:OD1	1:C:304:ARG:HB2	2.11	0.51
13:F:103:BCL:H13	13:F:103:BCL:HBB2	1.93	0.51
1:C:191:ALA:HB3	1:C:237:MET:HE3	1.93	0.50
13:A:103:BCL:H12	19:B:101:CRT:H27	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:48:ARG:HE	6:0:6:LEU:HD12	1.77	0.50
13:9:103:BCL:O1A	19:0:101:CRT:H27	2.11	0.50
5:3:51:ILE:HD13	5:5:58:LEU:HD23	1.92	0.50
5:K:28:GLN:HB3	13:K:101:BCL:H12	1.93	0.50
5:S:21:LEU:O	5:S:25:VAL:HG13	2.12	0.50
6:2:21:PHE:CD2	19:2:101:CRT:H14	2.47	0.50
4:H:17:TRP:CD1	22:H:304:LMT:H61	2.47	0.50
2:L:9:LYS:HA	4:H:87:VAL:HG13	1.93	0.50
5:U:11:ILE:CD1	5:U:14:ILE:HD11	2.32	0.50
6:2:40:TRP:CE2	13:2:102:BCL:H18	2.47	0.50
13:2:102:BCL:HED3	13:2:102:BCL:HBA2	1.93	0.50
2:L:17:LEU:N	2:L:115:GLU:OE1	2.38	0.49
6:G:17:PHE:HB2	19:G:101:CRT:H21A	1.94	0.49
13:9:103:BCL:H2C	6:0:45:TRP:CE2	2.47	0.49
2:L:196:LEU:HD11	3:M:269:ALA:HB1	1.94	0.49
15:L:309:UQ8:H46A	6:6:21:PHE:HE1	1.76	0.49
4:H:258:LEU:C	5:5:19:ARG:NH2	2.70	0.49
13:7:103:BCL:H2C	6:8:45:TRP:CD2	2.47	0.49
20:M:406:CDL:H571	20:M:406:CDL:H342	1.94	0.49
5:Y:17:PRO:HB3	6:Z:17:PHE:CE2	2.48	0.49
4:H:156:VAL:HG21	4:H:184:VAL:HG22	1.95	0.49
13:7:103:BCL:H2C	6:8:45:TRP:CE2	2.47	0.49
13:L:305:BCL:H203	15:L:311:UQ8:H3MA	1.94	0.49
3:M:35:ILE:HD11	12:M:411:PGV:H21	1.94	0.49
13:W:104:BCL:H11	6:X:29:PHE:CE1	2.48	0.49
5:1:17:PRO:HG2	6:2:9:LEU:HD21	1.95	0.49
5:I:36:HIS:CE1	13:J:102:BCL:HMD3	2.48	0.49
13:K:103:BCL:O1A	19:N:101:CRT:H27	2.13	0.49
6:Z:21:PHE:CD2	19:Z:101:CRT:H14	2.48	0.49
6:2:45:TRP:CD1	6:2:46:LEU:HG	2.48	0.48
5:I:38:ILE:HG12	21:K:104:PEF:H312	1.95	0.48
5:A:28:GLN:HB3	13:A:101:BCL:H12	1.95	0.48
13:W:101:BCL:H171	6:X:31:LEU:HD21	1.96	0.48
13:Y:103:BCL:O1A	19:Z:101:CRT:H27	2.13	0.48
5:5:51:ILE:HD13	5:7:58:LEU:HD23	1.95	0.48
5:5:51:ILE:CD1	5:7:58:LEU:HD23	2.44	0.48
4:H:18:ALA:HB2	22:H:304:LMT:H121	1.94	0.48
19:P:101:CRT:H27	13:P:102:BCL:O1A	2.13	0.48
5:U:19:ARG:HD2	20:U:104:CDL:HB61	1.95	0.48
13:5:103:BCL:H162	13:5:103:BCL:H141	1.62	0.48
5:7:17:PRO:HB3	6:8:17:PHE:CE2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:309:UQ8:H26	5:7:26:ALA:HB1	1.96	0.48
6:J:17:PHE:HA	19:J:101:CRT:H6	1.95	0.48
13:Q:101:BCL:H43	6:R:28:TRP:CZ2	2.47	0.48
5:Y:24:ILE:HG12	13:1:101:BCL:H112	1.96	0.48
13:5:103:BCL:H11	6:6:29:PHE:CE1	2.49	0.48
7:b:43:CYS:HB2	7:b:71:VAL:HA	1.96	0.48
2:L:129:ALA:HB1	2:L:247:LEU:HD21	1.95	0.48
22:H:304:LMT:H6D	5:F:41[A]:SER:HA	1.95	0.48
13:I:101:BCL:HMA3	13:I:101:BCL:H203	1.95	0.48
6:P:21:PHE:CD1	19:P:101:CRT:H14	2.49	0.48
5:1:19:ARG:NH2	21:1:103:PEF:O1P	2.46	0.48
20:M:406:CDL:H351	20:M:406:CDL:H621	1.94	0.47
5:I:5:ASN:OD1	5:I:7:ASN:N	2.40	0.47
20:O:104:CDL:H401	20:O:104:CDL:H551	1.96	0.47
5:1:17:PRO:HG2	6:2:9:LEU:CD2	2.44	0.47
5:1:37:MET:SD	12:1:105:PGV:H232	2.55	0.47
3:M:256:MET:HE3	18:M:404:MQ8:H142	1.96	0.47
19:M:405:CRT:H21A	15:M:413:UQ8:H1MA	1.96	0.47
5:I:13:LEU:O	6:J:6:LEU:HB3	2.13	0.47
13:K:101:BCL:H43	6:N:28:TRP:CZ2	2.49	0.47
13:S:101:BCL:H13	13:S:101:BCL:H102	1.60	0.47
5:I:5:ASN:ND2	6:N:23:GLN:OE1	2.44	0.47
5:Q:13:LEU:O	6:R:6:LEU:HA	2.15	0.47
6:Z:46:LEU:HB3	6:2:42:TYR:CE1	2.49	0.47
3:M:130:TRP:CZ3	20:O:104:CDL:H511	2.46	0.47
5:K:13:LEU:HB3	6:N:5:SER:HB2	1.96	0.47
20:S:104:CDL:H121	20:S:104:CDL:H341	1.97	0.47
5:1:17:PRO:HB3	6:2:17:PHE:CZ	2.50	0.47
7:b:48:PHE:HD1	7:b:62:GLN:HE21	1.61	0.47
1:C:144:HIS:HE1	8:C:504:HEC:NC	2.09	0.47
6:6:9:LEU:HD22	6:6:13:GLU:HB3	1.95	0.47
7:b:48:PHE:O	7:b:62:GLN:HG3	2.15	0.47
12:L:307:PGV:H202	5:D:37:MET:HE2	1.95	0.47
3:M:260:VAL:HB	3:M:264:SER:OG	2.15	0.47
4:H:60:ASP:OD1	4:H:61:LEU:N	2.40	0.47
5:O:19:ARG:NH1	20:O:104:CDL:OB3	2.43	0.47
2:L:96:GLN:CG	15:L:309:UQ8:H4M	2.39	0.47
13:L:305:BCL:H72	14:M:402:BPH:HMB2	1.96	0.47
5:Q:19:ARG:HG2	20:S:104:CDL:HA4	1.97	0.47
5:S:17:PRO:HB3	6:T:17:PHE:CE2	2.50	0.47
5:A:18:ARG:NH1	12:9:104:PGV:H012	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:104:CRT:H372	5:F:36:HIS:CD2	2.50	0.46
3:M:252:TRP:CE3	3:M:256:MET:HE2	2.51	0.46
13:F:103:BCL:H51	13:I:101:BCL:H171	1.96	0.46
6:N:21:PHE:CD2	19:N:101:CRT:H14	2.50	0.46
5:O:13:LEU:HB3	6:P:5:SER:HB2	1.97	0.46
5:U:11:ILE:HD12	5:U:14:ILE:CD1	2.33	0.46
2:L:191:THR:OG1	13:L:305:BCL:H12	2.16	0.46
13:L:301:BCL:H13	13:L:301:BCL:H172	1.71	0.46
14:L:303:BPH:HH C	14:L:303:BPH:CBB	2.45	0.46
22:H:304:LMT:H6D	5:F:41[B]:SER:HA	1.96	0.46
20:O:104:CDL:H522	20:O:104:CDL:H131	1.97	0.46
2:L:179:ASN:HB3	2:L:182:HIS:HB3	1.97	0.46
5:S:38:ILE:O	5:S:42:THR:HG23	2.16	0.46
13:U:103:BCL:HBA2	13:U:103:BCL:HED3	1.96	0.46
5:D:18:ARG:HH22	20:D:105:CDL:PA1	2.39	0.46
12:9:104:PGV:H041	12:9:104:PGV:H032	1.98	0.46
2:L:160:LEU:HD12	3:M:303:MET:O	2.16	0.46
5:S:18:ARG:HH12	5:S:19:ARG:CZ	2.29	0.46
13:9:103:BCL:H2C	6:0:45:TRP:CD2	2.51	0.46
3:M:179:ILE:O	3:M:182:HIS:ND1	2.39	0.46
13:A:101:BCL:H203	13:A:101:BCL:HMA3	1.97	0.46
6:T:45:TRP:CD1	6:T:46:LEU:HG	2.51	0.46
13:W:104:BCL:H121	13:W:104:BCL:H161	1.74	0.46
13:Y:103:BCL:H142	13:Y:103:BCL:H102	1.98	0.46
5:3:37[B]:MET:SD	12:3:105:PGV:H12	2.56	0.46
5:7:25:VAL:HG21	13:7:101:BCL:H13	1.97	0.46
2:L:97:ILE:HG21	5:9:37:MET:HE1	1.96	0.45
2:L:151:TRP:HB3	15:L:309:UQ8:H4MB	1.98	0.45
5:Q:28:GLN:CB	13:Q:101:BCL:H42	2.44	0.45
2:L:41:CYS:SG	15:L:310:UQ8:H1MB	2.57	0.45
13:S:101:BCL:H43	6:T:28:TRP:CE2	2.51	0.45
13:S:103:BCL:H2C	6:T:45:TRP:CD2	2.51	0.45
5:3:51:ILE:HD11	5:5:58:LEU:HB3	1.99	0.45
5:9:53:VAL:HG21	5:9:58:LEU:HD11	1.98	0.45
5:O:19:ARG:NH1	20:O:104:CDL:OB4	2.49	0.45
19:T:101:CRT:H243	20:U:104:CDL:H172	1.99	0.45
5:5:19:ARG:HE	5:5:19:ARG:HB2	0.99	0.45
2:L:281:TRP:CG	3:M:88:LYS:HB2	2.51	0.45
13:L:301:BCL:H161	13:L:301:BCL:H192	1.67	0.45
5:A:36:HIS:CG	19:0:101:CRT:H372	2.52	0.45
6:P:29:PHE:CE1	13:P:102:BCL:H11	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:18:ARG:NH2	5:Y:19:ARG:NH1	2.64	0.45
13:Y:101:BCL:OBB	13:Y:101:BCL:HHC	2.17	0.45
12:3:105:PGV:H212	12:3:105:PGV:H241	1.62	0.45
20:S:104:CDL:H131	20:S:104:CDL:H171	1.98	0.45
12:M:411:PGV:H261	12:M:411:PGV:H232	1.85	0.45
6:V:17:PHE:HA	19:V:101:CRT:H6	1.98	0.45
5:1:16:ASP:CB	5:1:19:ARG:NH1	2.78	0.45
6:6:6:LEU:HB3	5:7:18:ARG:HH22	1.80	0.45
2:L:69:ASN:ND2	3:M:302:GLY:O	2.48	0.45
15:L:310:UQ8:H15	15:L:310:UQ8:H12	1.68	0.45
3:M:285:LEU:HD21	21:K:104:PEF:H141	1.99	0.45
6:2:29:PHE:O	6:2:33:VAL:HG23	2.16	0.45
3:M:13:VAL:HG12	4:H:144:ILE:HD13	1.99	0.45
5:A:58:LEU:HA	5:A:58:LEU:HD13	1.65	0.45
5:1:16:ASP:CB	5:1:19:ARG:NE	2.77	0.45
5:7:19:ARG:HA	5:7:19:ARG:HD3	1.71	0.45
1:C:311:HIS:CE1	8:C:504:HEC:NA	2.84	0.45
5:I:21:LEU:O	5:I:25:VAL:HG23	2.17	0.45
6:P:40:TRP:CE2	13:P:102:BCL:H18	2.51	0.45
3:M:7:ILE:HD12	12:M:410:PGV:H92	1.98	0.45
13:D:103:BCL:HHC	13:D:103:BCL:OBB	2.17	0.45
13:D:103:BCL:H202	6:G:38:LEU:HD13	1.98	0.45
5:U:28:GLN:CB	13:U:101:BCL:H42	2.47	0.45
13:W:104:BCL:H2C	6:X:45:TRP:CD2	2.52	0.45
13:Y:101:BCL:H43	6:Z:28:TRP:CE2	2.52	0.45
5:K:38:ILE:O	5:K:42:THR:HG23	2.16	0.44
5:1:9:TYR:CE1	6:2:15:LYS:HG3	2.52	0.44
13:5:103:BCL:H162	13:5:103:BCL:H192	1.85	0.44
5:7:38:ILE:O	5:7:41:SER:OG	2.34	0.44
13:7:103:BCL:H112	13:7:103:BCL:H152	1.45	0.44
7:b:33:ARG:HA	7:b:34:PRO:HD3	1.88	0.44
15:L:309:UQ8:H27	15:L:309:UQ8:H30	1.80	0.44
15:L:310:UQ8:H25	15:L:310:UQ8:H22	1.68	0.44
6:J:46:LEU:HB3	6:N:42:TYR:CE1	2.51	0.44
13:K:103:BCL:H11	6:N:29:PHE:CE1	2.51	0.44
13:2:102:BCL:HHC	13:2:102:BCL:OBB	2.17	0.44
14:L:303:BPH:H172	12:L:307:PGV:H342	1.99	0.44
13:5:101:BCL:H142	13:5:101:BCL:H111	1.86	0.44
13:A:101:BCL:H62	13:A:101:BCL:H41	1.81	0.44
13:O:101:BCL:H62	13:O:101:BCL:H41	1.78	0.44
5:1:16:ASP:H	5:1:19:ARG:HH11	1.65	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:17:TRP:CG	22:H:304:LMT:H61	2.52	0.44
22:H:304:LMT:H71	5:F:38:ILE:HG12	1.99	0.44
5:K:46:TRP:CE2	13:K:101:BCL:H2C	2.52	0.44
3:M:175:VAL:HG22	3:M:185:TRP:CE2	2.52	0.44
4:H:205:LYS:HA	4:H:205:LYS:HD2	1.88	0.44
5:O:34:LEU:HA	5:O:37[A]:MET:HE2	2.00	0.44
13:2:102:BCL:H52	13:2:102:BCL:H12	1.76	0.44
13:O:101:BCL:H43	6:P:28:TRP:CZ2	2.52	0.44
13:3:101:BCL:H41	13:3:101:BCL:H62	1.76	0.44
6:4:6:LEU:HD23	5:5:18:ARG:HH21	1.82	0.44
5:9:46:TRP:CE2	13:9:101:BCL:H2C	2.53	0.44
13:A:101:BCL:HMB1	19:0:101:CRT:H371	2.00	0.44
5:O:27:PHE:HB2	20:O:104:CDL:H762	2.00	0.44
6:Z:45:TRP:CD1	6:Z:46:LEU:HG	2.53	0.44
12:L:308:PGV:C11	15:L:309:UQ8:H26A	2.48	0.44
15:L:310:UQ8:H10	15:L:310:UQ8:H7A	1.55	0.44
5:5:16:ASP:HB3	5:5:19:ARG:CZ	2.47	0.44
5:5:17:PRO:HB3	6:6:17:PHE:CZ	2.53	0.44
13:L:305:BCL:H161	13:L:305:BCL:H141	1.49	0.43
18:M:404:MQ8:H412	18:M:404:MQ8:H441	1.77	0.43
19:M:405:CRT:H20	19:M:405:CRT:H181	1.84	0.43
5:S:19:ARG:NH2	20:S:104:CDL:CB7	2.81	0.43
13:S:101:BCL:H43	6:T:28:TRP:CZ2	2.53	0.43
13:W:101:BCL:H62	13:W:101:BCL:H41	1.73	0.43
13:Y:103:BCL:OB	13:Y:103:BCL:HH	2.18	0.43
6:Z:46:LEU:HB3	6:2:42:TYR:CZ	2.53	0.43
6:4:21:PHE:HA	19:4:101:CRT:H14	1.99	0.43
1:C:31:GLU:OE2	10:C:506:GOL:H2	2.18	0.43
12:M:411:PGV:P	20:S:104:CDL:HB31	2.58	0.43
5:K:14:ILE:HG22	5:O:18:ARG:HB2	2.00	0.43
5:O:38:ILE:O	5:O:42:THR:HG23	2.18	0.43
5:O:46:TRP:CE2	13:O:101:BCL:H2C	2.54	0.43
13:O:101:BCL:O1D	13:O:101:BCL:H202	2.18	0.43
5:W:21:LEU:HD23	5:W:21:LEU:HA	1.90	0.43
1:C:130:MET:HB3	8:C:502:HEC:C4B	2.47	0.43
18:M:404:MQ8:H312	18:M:404:MQ8:H351	1.78	0.43
4:H:9:ILE:HA	4:H:13:GLN:OE1	2.18	0.43
5:A:46:TRP:HA	6:B:43:ARG:HH12	1.82	0.43
13:J:102:BCL:H111	13:J:102:BCL:H152	1.67	0.43
19:T:101:CRT:H372	5:U:36:HIS:CD2	2.54	0.43
1:C:46:LYS:HD3	12:3:105:PGV:H062	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:309:UQ8:H32	15:L:309:UQ8:H35	1.78	0.43
20:M:406:CDL:H202	4:H:25:GLY:HA3	2.00	0.43
5:O:51:ILE:HD11	5:Q:58:LEU:HB2	2.01	0.43
13:2:102:BCL:H192	13:2:102:BCL:H162	1.74	0.43
6:O:45:TRP:CD1	6:O:46:LEU:HG	2.53	0.43
1:C:303:LEU:HB2	8:C:502:HEC:HBD1	2.01	0.43
20:H:305:CDL:H172	20:H:305:CDL:H202	1.86	0.43
19:A:104:CRT:H372	5:F:36:HIS:CG	2.54	0.43
19:N:101:CRT:H10	19:N:101:CRT:H81	1.85	0.43
6:8:15:LYS:HA	6:8:15:LYS:HD2	1.80	0.43
2:L:219:GLU:OE1	2:L:219:GLU:N	2.45	0.43
20:H:305:CDL:H862	20:H:305:CDL:H831	1.81	0.43
13:F:103:BCL:H193	6:J:38:LEU:HD13	2.01	0.43
5:U:23:SER:HA	20:U:104:CDL:H731	2.00	0.43
5:Y:19:ARG:NH2	20:Y:104:CDL:OA2	2.49	0.43
5:1:21:LEU:HD23	5:1:21:LEU:HA	1.78	0.43
13:7:101:BCL:H61	13:7:101:BCL:H41	1.96	0.43
2:L:190:PHE:CD2	14:M:402:BPH:HBB1	2.54	0.43
5:O:28:GLN:CB	13:O:101:BCL:H42	2.49	0.43
6:Z:31:LEU:HD23	6:Z:31:LEU:HA	1.68	0.43
19:Z:101:CRT:H10	19:Z:101:CRT:H81	1.84	0.43
5:9:49:ASP:O	5:9:51:ILE:HG13	2.18	0.43
7:b:57:ASP:O	7:b:70:ASN:HA	2.19	0.43
13:L:305:BCL:OBB	19:M:405:CRT:H243	2.19	0.43
3:M:98:PRO:CG	3:M:107:PRO:HG3	2.48	0.43
4:H:258:LEU:HA	5:5:19:ARG:HH21	1.83	0.43
20:O:104:CDL:H342	20:O:104:CDL:H311	1.80	0.43
13:4:102:BCL:HHC	13:4:102:BCL:OBB	2.18	0.43
15:L:304:UQ8:H7	15:L:304:UQ8:H10	1.75	0.43
19:M:405:CRT:H2M3	5:O:38:ILE:HA	2.00	0.43
4:H:48:ARG:NE	6:O:6:LEU:HD12	2.33	0.43
13:U:101:BCL:HED1	6:V:28:TRP:CZ3	2.54	0.43
6:X:46:LEU:HB3	6:Z:42:TYR:CE1	2.53	0.43
19:O:101:CRT:H10	19:O:101:CRT:H81	1.90	0.43
7:b:49:MET:HE2	7:b:49:MET:HB3	1.92	0.43
4:H:100:LEU:HB2	4:H:111:PHE:CZ	2.53	0.42
5:U:46:TRP:CE2	13:U:101:BCL:H2C	2.54	0.42
6:X:31:LEU:HD12	6:X:31:LEU:HA	1.91	0.42
5:5:51:ILE:HD11	5:7:58:LEU:HB3	2.01	0.42
15:L:310:UQ8:H16A	5:7:34:LEU:HD13	2.00	0.42
6:J:45:TRP:CD2	13:J:102:BCL:H2C	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:17:PRO:HB3	6:R:17:PHE:CZ	2.54	0.42
13:Q:103:BCL:H2C	6:R:45:TRP:CD2	2.55	0.42
6:4:44:PRO:O	5:5:55:TYR:OH	2.33	0.42
19:8:101:CRT:H36	19:8:101:CRT:H341	1.91	0.42
7:b:53:VAL:HB	7:b:60:GLY:HA3	2.00	0.42
2:L:139:VAL:HG21	2:L:254:ALA:HB1	2.02	0.42
19:4:101:CRT:H10	19:4:101:CRT:H81	1.84	0.42
7:b:58:TRP:HA	7:b:69:ILE:O	2.19	0.42
3:M:243:THR:HB	4:H:117:PRO:HD2	2.02	0.42
14:M:402:BPH:H161	20:S:104:CDL:H752	2.00	0.42
13:A:103:BCL:H161	13:A:103:BCL:H192	1.66	0.42
19:B:101:CRT:H10	19:B:101:CRT:H81	1.84	0.42
5:Y:27:PHE:HB2	13:1:101:BCL:H152	2.00	0.42
13:1:101:BCL:HHC	13:1:101:BCL:OBB	2.20	0.42
5:9:35:ILE:O	5:9:39:VAL:HG23	2.19	0.42
5:9:46:TRP:CD2	13:9:101:BCL:H2C	2.55	0.42
4:H:214:ILE:HB	4:H:218:HIS:HB2	2.01	0.42
5:A:18:ARG:HD3	6:0:6:LEU:HD22	2.01	0.42
19:W:102:CRT:H10	19:W:102:CRT:H81	1.91	0.42
5:5:35:ILE:O	5:5:39:VAL:HG23	2.19	0.42
5:S:46:TRP:CD2	13:S:101:BCL:H2C	2.55	0.42
20:S:104:CDL:H362	20:S:104:CDL:C14	2.50	0.42
5:W:28:GLN:HB3	13:W:101:BCL:H12	2.02	0.42
3:M:196:LEU:HD12	3:M:196:LEU:HA	1.82	0.42
3:M:200:PRO:HG3	3:M:297:TRP:CH2	2.54	0.42
4:H:17:TRP:NE1	22:H:304:LMT:H41	2.35	0.42
12:L:307:PGV:H222	12:L:307:PGV:H251	1.82	0.42
12:M:410:PGV:H312	12:M:410:PGV:H281	1.88	0.42
5:A:17:PRO:HB3	6:B:17:PHE:CZ	2.54	0.42
5:Q:46:TRP:CE2	13:Q:101:BCL:H2C	2.55	0.42
6:4:32:VAL:HG12	13:4:102:BCL:H61	2.01	0.42
13:7:101:BCL:H43	6:8:28:TRP:CH2	2.55	0.42
5:I:38:ILE:O	5:I:42:THR:HG23	2.19	0.42
13:P:102:BCL:H192	13:P:102:BCL:H152	2.01	0.42
8:C:503:HEC:HBB1	2:L:174:LEU:HD22	2.02	0.41
5:K:46:TRP:CD2	13:K:101:BCL:H2C	2.55	0.41
13:K:101:BCL:HMD3	6:N:36:HIS:CE1	2.55	0.41
6:P:37:LEU:HD23	6:P:37:LEU:HA	1.87	0.41
13:Y:103:BCL:H193	6:Z:40:TRP:CH2	2.55	0.41
6:4:45:TRP:CD1	6:4:46:LEU:HG	2.54	0.41
1:C:73:SER:HB2	1:C:83:LYS:HB3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:308:PGV:H52	12:L:308:PGV:H81	1.73	0.41
4:H:119:ARG:HD2	4:H:237:ASP:CG	2.45	0.41
13:I:101:BCL:HHC	13:I:101:BCL:OBB	2.20	0.41
5:O:18:ARG:HD2	20:O:104:CDL:HA21	2.02	0.41
13:7:103:BCL:HBA2	13:7:103:BCL:HED3	2.02	0.41
2:L:179:ASN:HB3	2:L:182:HIS:CB	2.49	0.41
12:L:307:PGV:H42	12:D:106:PGV:H51	2.01	0.41
3:M:33:ARG:HD3	12:M:411:PGV:H062	2.01	0.41
4:H:17:TRP:CE2	22:H:304:LMT:H41	2.54	0.41
12:H:303:PGV:H262	20:H:305:CDL:H841	2.01	0.41
13:O:101:BCL:HHC	13:O:101:BCL:OBB	2.21	0.41
5:S:46:TRP:CE2	13:S:101:BCL:H2C	2.55	0.41
13:U:101:BCL:HHC	13:U:101:BCL:OBB	2.19	0.41
5:Y:36:HIS:NE2	13:Y:103:BCL:HMD3	2.35	0.41
13:Y:103:BCL:HED1	6:Z:28:TRP:HZ2	1.86	0.41
2:L:216:LYS:HD2	2:L:220:HIS:CD2	2.56	0.41
13:L:305:BCL:OBB	13:L:305:BCL:HHC	2.21	0.41
5:A:38:ILE:O	5:A:42:THR:HG23	2.20	0.41
19:N:101:CRT:H241	19:N:101:CRT:H26	1.85	0.41
13:Q:101:BCL:H141	13:Q:101:BCL:H162	1.72	0.41
13:Y:103:BCL:H52	13:Y:103:BCL:H12	1.81	0.41
6:2:21:PHE:HA	19:2:101:CRT:H11	2.03	0.41
19:3:103:CRT:H10	19:3:103:CRT:H81	1.79	0.41
5:5:10:LYS:HB2	19:8:101:CRT:H5	2.02	0.41
5:9:15:LEU:HD13	12:9:104:PGV:H261	2.01	0.41
13:A:101:BCL:HHB	19:0:101:CRT:H35	2.02	0.41
19:A:104:CRT:H36	19:A:104:CRT:H341	1.88	0.41
6:E:45:TRP:CD1	6:E:46:LEU:HG	2.56	0.41
5:F:17:PRO:HB3	6:G:17:PHE:CZ	2.56	0.41
6:N:45:TRP:CD1	6:N:46:LEU:HG	2.55	0.41
13:S:103:BCL:H93	13:S:103:BCL:H61	1.61	0.41
13:U:103:BCL:O1A	19:V:101:CRT:H27	2.20	0.41
19:4:101:CRT:H26	19:4:101:CRT:H241	1.91	0.41
6:0:15:LYS:HD2	6:0:15:LYS:HA	1.88	0.41
13:L:301:BCL:H151	12:L:307:PGV:H321	2.02	0.41
19:M:405:CRT:H10	19:M:405:CRT:H81	1.87	0.41
5:O:30:VAL:HG11	20:O:104:CDL:H601	2.02	0.41
19:T:101:CRT:C31	13:U:101:BCL:HBA2	2.50	0.41
13:Y:103:BCL:H141	6:Z:45:TRP:CZ2	2.55	0.41
5:7:35:ILE:HD12	13:7:103:BCL:O1D	2.21	0.41
13:9:103:BCL:H101	6:0:36:HIS:CD2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:ARG:HB3	2:L:79:ASP:OD1	2.21	0.41
1:C:250:CYS:O	1:C:262:SER:HB3	2.21	0.41
1:C:270:TRP:CG	3:M:316:PRO:HG2	2.55	0.41
19:2:101:CRT:H35	13:3:101:BCL:HMB1	2.02	0.41
13:7:101:BCL:OBB	13:7:101:BCL:HHC	2.21	0.41
12:L:308:PGV:C20	12:M:410:PGV:H222	2.49	0.41
15:L:310:UQ8:H12	15:L:310:UQ8:H10A	1.84	0.41
20:S:104:CDL:H362	20:S:104:CDL:H142	2.03	0.41
6:4:21:PHE:CD2	19:4:101:CRT:H14	2.55	0.41
19:8:101:CRT:H20	19:8:101:CRT:H181	1.94	0.41
3:M:130:TRP:CH2	20:M:406:CDL:H781	2.56	0.41
3:M:229:PHE:HB2	3:M:244:ALA:HB2	2.02	0.41
5:A:56:GLN:HE22	5:9:49:ASP:HB3	1.85	0.41
19:A:104:CRT:H10	19:A:104:CRT:H81	1.80	0.41
20:D:105:CDL:H741	12:9:104:PGV:H42	2.02	0.41
5:F:13:LEU:O	6:G:6:LEU:HB3	2.21	0.41
19:G:101:CRT:H20	19:G:101:CRT:H181	1.90	0.41
5:O:33:LEU:O	5:O:37[A]:MET:HG3	2.20	0.41
5:S:15:LEU:HD23	5:U:18:ARG:HG3	2.03	0.41
5:U:17:PRO:HB3	6:V:17:PHE:CE2	2.56	0.41
5:Y:16:ASP:OD2	5:Y:19:ARG:HG2	2.20	0.41
13:2:102:BCL:H62	13:2:102:BCL:H41	1.92	0.41
5:3:19:ARG:HD3	5:3:19:ARG:HA	1.95	0.41
1:C:95:VAL:HG21	7:b:63:LEU:O	2.21	0.41
2:L:227:ASP:O	3:M:132:ARG:NH2	2.54	0.41
19:A:104:CRT:H35	13:F:101:BCL:HBB	2.02	0.41
5:U:17:PRO:HB3	6:V:17:PHE:CZ	2.55	0.41
5:Y:19:ARG:HA	5:Y:19:ARG:HD3	1.75	0.41
5:5:38:ILE:O	5:5:42:THR:HG23	2.21	0.41
3:M:97:PRO:HD3	3:M:176:PRO:HB3	2.02	0.40
3:M:159:VAL:HA	3:M:163:ILE:HB	2.03	0.40
13:F:101:BCL:H43	6:G:28:TRP:CZ2	2.56	0.40
5:S:17:PRO:HB3	6:T:17:PHE:CZ	2.56	0.40
13:U:103:BCL:H161	13:U:103:BCL:H192	1.79	0.40
5:Y:46:TRP:CE3	13:Y:101:BCL:HAC2	2.56	0.40
13:2:102:BCL:HBB2	13:2:102:BCL:H121	2.03	0.40
3:M:246:GLU:OE2	4:H:117:PRO:HD3	2.21	0.40
13:F:101:BCL:H141	13:F:101:BCL:H161	1.88	0.40
5:U:36:HIS:CG	13:U:103:BCL:HMD1	2.56	0.40
19:8:101:CRT:H371	13:9:101:BCL:HMB1	2.02	0.40
4:H:65:LYS:HE2	4:H:67:PHE:CZ	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:32:GLY:HA2	13:A:103:BCL:O1D	2.21	0.40
13:F:103:BCL:H152	13:F:103:BCL:H112	1.80	0.40
19:P:101:CRT:H20	19:P:101:CRT:H181	1.96	0.40
13:Y:101:BCL:H171	6:Z:31:LEU:HD13	2.04	0.40
5:3:41:SER:O	12:3:105:PGV:H011	2.21	0.40
5:9:46:TRP:NE1	13:9:101:BCL:HHC	2.37	0.40
2:L:22:LEU:HB2	5:7:19:ARG:HB2	2.04	0.40
14:M:402:BPH:H141	20:S:104:CDL:H751	2.03	0.40
5:I:37:MET:HE2	5:I:37:MET:HA	2.04	0.40
2:L:183:MET:HE1	2:L:272:TRP:CZ2	2.57	0.40
13:L:302:BCL:HHC	13:L:302:BCL:OBB	2.21	0.40
3:M:8:PHE:HB2	20:M:412:CDL:HB22	2.02	0.40
3:M:148:TRP:HE1	20:M:406:CDL:H711	1.86	0.40
4:H:31:ARG:HA	4:H:31:ARG:HD2	1.86	0.40
5:A:17:PRO:HB3	6:B:17:PHE:CE1	2.56	0.40
13:F:103:BCL:H161	13:F:103:BCL:H192	1.83	0.40
19:G:101:CRT:H2M3	5:I:37:MET:HE3	2.04	0.40
5:K:7:ASN:HB2	6:P:20:ILE:HD11	2.03	0.40
13:Q:103:BCL:HAA1	6:R:32:VAL:HG11	2.02	0.40
5:S:35:ILE:HD12	13:S:103:BCL:O1D	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	309/311 (99%)	296 (96%)	13 (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	51
4	H	255/259 (98%)	254 (100%)	1 (0%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	55 (100%)	0	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%)	1 (2%)	1 (2%)	6	23
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%)	55 (98%)	1 (2%)	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
6	X	39/47 (83%)	39 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Z	38/47 (81%)	38 (100%)	0	0	100	100
7	b	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
All	All	2748/2987 (92%)	2707 (98%)	38 (1%)	3 (0%)	48	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	58	LEU
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	260/260 (100%)	258 (99%)	2 (1%)	73	90
2	L	229/229 (100%)	227 (99%)	2 (1%)	70	90
3	M	258/261 (99%)	257 (100%)	1 (0%)	84	94
4	H	210/211 (100%)	209 (100%)	1 (0%)	81	93
5	1	50/56 (89%)	50 (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%)	50 (96%)	2 (4%)	29	64
5	A	49/56 (88%)	48 (98%)	1 (2%)	48	78
5	D	51/56 (91%)	51 (100%)	0	100	100
5	F	51/56 (91%)	50 (98%)	1 (2%)	48	78
5	I	53/56 (95%)	52 (98%)	1 (2%)	50	79
5	K	51/56 (91%)	50 (98%)	1 (2%)	48	78
5	O	52/56 (93%)	50 (96%)	2 (4%)	29	64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Q	52/56 (93%)	51 (98%)	1 (2%)	50	79
5	S	54/56 (96%)	53 (98%)	1 (2%)	50	79
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%)	52 (100%)	0	100	100
6	0	36/39 (92%)	34 (94%)	2 (6%)	19	50
6	2	34/39 (87%)	33 (97%)	1 (3%)	37	71
6	4	35/39 (90%)	35 (100%)	0	100	100
6	6	35/39 (90%)	34 (97%)	1 (3%)	37	71
6	8	34/39 (87%)	33 (97%)	1 (3%)	37	71
6	B	35/39 (90%)	35 (100%)	0	100	100
6	E	32/39 (82%)	32 (100%)	0	100	100
6	G	35/39 (90%)	35 (100%)	0	100	100
6	J	35/39 (90%)	35 (100%)	0	100	100
6	N	35/39 (90%)	35 (100%)	0	100	100
6	P	35/39 (90%)	35 (100%)	0	100	100
6	R	34/39 (87%)	33 (97%)	1 (3%)	37	71
6	T	36/39 (92%)	35 (97%)	1 (3%)	38	72
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
7	b	61/61 (100%)	60 (98%)	1 (2%)	55	83
All	All	2395/2542 (94%)	2371 (99%)	24 (1%)	68	89

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	212	ILE
1	C	333	THR
2	L	256	CYS
2	L	280	LEU
3	M	216	PHE
4	H	237	ASP
5	A	58	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	F	14	ILE
5	I	4	MET
5	K	3	THR
5	O	14	ILE
5	O	53	VAL
5	Q	58	LEU
6	R	6	LEU
5	S	25	VAL
6	T	31	LEU
6	2	6	LEU
6	6	6	LEU
6	8	6	LEU
5	9	3	THR
5	9	53	VAL
6	0	6	LEU
6	0	31	LEU
7	b	33	ARG

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

Mol	Chain	Res	Type
1	C	42	ASN
2	L	172	GLN
2	L	175	HIS
2	L	210	GLN
2	L	222	ASN
3	M	80	HIS
4	H	7	HIS
5	D	7	ASN
5	I	7	ASN
5	Q	7	ASN
5	5	7	ASN
5	7	7	ASN

5.3.3 RNA ⓘ

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 120 ligands modelled in this entry, 18 are monoatomic - leaving 102 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$
19	CRT	0	101	-	41,43,43	0.75	0	50,54,54	1.49	9 (18%)
20	CDL	U	104	-	61,61,99	1.17	4 (6%)	67,73,111	1.62	14 (20%)
12	PGV	3	105	-	50,50,50	0.94	2 (4%)	53,56,56	0.97	2 (3%)
13	BCL	D	103	6	69,74,74	1.16	4 (5%)	83,115,115	1.50	15 (18%)
19	CRT	N	101	-	41,43,43	0.75	0	50,54,54	1.83	14 (28%)
20	CDL	H	305	-	78,78,99	1.05	4 (5%)	84,90,111	1.05	5 (5%)
21	PEF	W	106	-	4,4,46	2.63	2 (50%)	6,6,51	1.83	2 (33%)
8	HEC	C	501	1	50,50,50	1.86	9 (18%)	68,82,82	2.28	25 (36%)
13	BCL	Q	103	6	69,74,74	1.19	4 (5%)	83,115,115	1.59	15 (18%)
20	CDL	O	104	-	85,85,99	1.00	4 (4%)	91,97,111	1.26	11 (12%)
22	LMT	H	304	-	36,36,36	0.52	0	47,47,47	1.31	8 (17%)
19	CRT	G	101	-	41,43,43	0.71	0	50,54,54	1.56	11 (22%)
12	PGV	D	106	-	34,34,50	1.12	2 (5%)	37,40,56	1.05	3 (8%)
20	CDL	D	105	-	63,63,99	1.08	4 (6%)	69,75,111	1.27	6 (8%)
20	CDL	M	412	3	38,38,99	1.31	3 (7%)	43,49,111	1.34	5 (11%)
20	CDL	1	104	-	12,12,99	0.44	0	13,15,111	0.58	0
18	MQ8	M	404	-	54,54,54	1.36	2 (3%)	66,69,69	1.50	14 (21%)
13	BCL	U	101	5	69,74,74	1.18	3 (4%)	83,115,115	1.60	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BCL	1	101	5	69,74,74	1.16	5 (7%)	83,115,115	1.61	12 (14%)
13	BCL	P	102	6	69,74,74	1.23	3 (4%)	83,115,115	1.72	16 (19%)
21	PEF	K	104	-	26,26,46	1.31	2 (7%)	29,31,51	1.27	2 (6%)
21	PEF	H	302	-	4,4,46	2.48	1 (25%)	6,6,51	2.44	2 (33%)
19	CRT	O	103	-	41,43,43	0.71	0	50,54,54	1.52	9 (18%)
20	CDL	M	406	-	99,99,99	0.93	4 (4%)	105,111,111	1.14	7 (6%)
13	BCL	4	102	6	69,74,74	1.15	5 (7%)	83,115,115	1.58	13 (15%)
13	BCL	L	301	2	69,74,74	1.13	4 (5%)	83,115,115	1.55	13 (15%)
13	BCL	5	103	6	69,74,74	1.17	5 (7%)	83,115,115	1.61	15 (18%)
21	PEF	M	407	-	4,4,46	2.63	2 (50%)	6,6,51	1.84	2 (33%)
13	BCL	Y	101	5	69,74,74	1.14	5 (7%)	83,115,115	1.54	11 (13%)
19	CRT	W	102	-	41,43,43	0.74	0	50,54,54	1.59	13 (26%)
12	PGV	L	307	-	42,42,50	0.99	2 (4%)	45,48,56	1.22	4 (8%)
14	BPH	M	402	-	59,70,70	2.46	14 (23%)	61,101,101	2.25	20 (32%)
19	CRT	V	101	-	41,43,43	0.70	0	50,54,54	1.62	12 (24%)
8	HEC	C	504	1	50,50,50	1.71	8 (16%)	68,82,82	1.93	18 (26%)
13	BCL	A	103	6	69,74,74	1.14	5 (7%)	83,115,115	1.47	12 (14%)
23	SF4	b	101	7	0,12,12	-	-	-	-	-
12	PGV	C	508	1	20,20,50	1.45	3 (15%)	22,22,56	1.56	3 (13%)
13	BCL	K	101	5	69,74,74	1.18	5 (7%)	83,115,115	1.65	16 (19%)
8	HEC	C	502	1	50,50,50	1.81	10 (20%)	68,82,82	2.06	20 (29%)
13	BCL	3	101	5	69,74,74	1.22	3 (4%)	83,115,115	1.95	19 (22%)
13	BCL	2	102	6	69,74,74	1.27	6 (8%)	83,115,115	1.73	13 (15%)
20	CDL	Y	104	-	39,39,99	1.48	5 (12%)	45,51,111	2.01	14 (31%)
15	UQ8	L	309	-	53,53,53	1.18	2 (3%)	64,67,67	1.77	18 (28%)
12	PGV	9	104	-	32,32,50	1.16	2 (6%)	35,38,56	1.31	6 (17%)
21	PEF	W	105	-	4,4,46	2.68	2 (50%)	6,6,51	1.65	2 (33%)
13	BCL	9	103	6	69,74,74	1.20	3 (4%)	83,115,115	1.58	14 (16%)
19	CRT	Z	101	-	41,43,43	0.72	0	50,54,54	1.74	14 (28%)
12	PGV	H	303	-	35,35,50	1.10	2 (5%)	38,41,56	1.19	4 (10%)
21	PEF	M	408	-	4,4,46	1.71	2 (50%)	6,6,51	1.28	1 (16%)
13	BCL	S	101	5	69,74,74	1.20	4 (5%)	83,115,115	1.52	14 (16%)
13	BCL	W	101	5	69,74,74	1.16	5 (7%)	83,115,115	1.57	14 (16%)
8	HEC	C	503	1	50,50,50	1.69	10 (20%)	68,82,82	1.90	17 (25%)
20	CDL	S	104	-	74,74,99	1.18	4 (5%)	80,86,111	1.34	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	UQ8	L	311	-	18,18,53	2.10	2 (11%)	22,25,67	1.05	1 (4%)
13	BCL	I	101	5	69,74,74	1.19	7 (10%)	83,115,115	1.59	14 (16%)
13	BCL	K	103	6	69,74,74	1.16	4 (5%)	83,115,115	1.60	15 (18%)
19	CRT	T	101	-	41,43,43	0.76	0	50,54,54	1.66	13 (26%)
19	CRT	4	101	-	41,43,43	0.70	0	50,54,54	1.64	13 (26%)
13	BCL	F	101	5	69,74,74	1.14	4 (5%)	83,115,115	1.75	18 (21%)
13	BCL	Y	103	6	69,74,74	1.18	5 (7%)	83,115,115	1.61	18 (21%)
13	BCL	J	102	6	69,74,74	1.13	5 (7%)	83,115,115	1.56	16 (19%)
13	BCL	L	302	2	69,74,74	1.14	5 (7%)	83,115,115	1.43	10 (12%)
13	BCL	M	401	3	69,74,74	1.19	5 (7%)	83,115,115	1.53	13 (15%)
15	UQ8	M	413	-	18,18,53	2.13	2 (11%)	22,25,67	1.27	2 (9%)
10	GOL	C	506	-	5,5,5	0.90	0	5,5,5	1.00	0
22	LMT	M	414	-	36,36,36	0.42	0	47,47,47	0.77	0
19	CRT	M	405	-	41,43,43	0.74	0	50,54,54	1.57	10 (20%)
19	CRT	2	101	-	41,43,43	0.70	0	50,54,54	1.62	11 (22%)
21	PEF	1	103	-	4,4,46	2.61	2 (50%)	6,6,51	2.77	3 (50%)
16	SO4	L	306	-	4,4,4	0.14	0	6,6,6	0.05	0
19	CRT	A	104	-	41,43,43	0.71	0	50,54,54	1.67	13 (26%)
15	UQ8	L	304	-	33,33,53	1.48	2 (6%)	40,43,67	1.86	12 (30%)
21	PEF	I	103	-	4,4,46	2.63	2 (50%)	6,6,51	1.83	2 (33%)
13	BCL	7	101	5	64,69,74	1.21	4 (6%)	77,109,115	1.74	14 (18%)
13	BCL	D	101	5	69,74,74	1.16	3 (4%)	83,115,115	1.69	18 (21%)
19	CRT	J	101	-	41,43,43	0.80	0	50,54,54	1.50	10 (20%)
13	BCL	Q	101	5	69,74,74	1.17	3 (4%)	83,115,115	1.75	17 (20%)
21	PEF	3	104	-	4,4,46	2.63	2 (50%)	6,6,51	1.84	2 (33%)
13	BCL	O	101	5	69,74,74	1.13	4 (5%)	83,115,115	1.63	14 (16%)
12	PGV	1	105	-	30,30,50	1.22	2 (6%)	33,36,56	1.17	2 (6%)
12	PGV	M	411	-	36,36,50	1.06	2 (5%)	39,42,56	1.24	4 (10%)
19	CRT	3	103	-	41,43,43	0.71	0	50,54,54	1.69	14 (28%)
19	CRT	P	101	-	41,43,43	0.74	0	50,54,54	1.59	7 (14%)
13	BCL	S	103	6	69,74,74	1.26	4 (5%)	83,115,115	1.75	15 (18%)
21	PEF	M	409	-	4,4,46	2.64	2 (50%)	6,6,51	1.85	2 (33%)
13	BCL	A	101	5	69,74,74	1.16	5 (7%)	83,115,115	1.63	15 (18%)
19	CRT	8	101	-	41,43,43	0.73	0	50,54,54	1.57	13 (26%)
13	BCL	9	101	5	69,74,74	1.15	5 (7%)	83,115,115	1.49	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	PGV	L	308	-	43,43,50	0.98	2 (4%)	46,49,56	1.13	3 (6%)
13	BCL	L	305	3	69,74,74	1.13	4 (5%)	83,115,115	1.70	17 (20%)
10	GOL	H	301	-	5,5,5	0.93	0	5,5,5	0.94	0
13	BCL	7	103	6	69,74,74	1.21	4 (5%)	83,115,115	1.43	12 (14%)
15	UQ8	L	310	-	33,33,53	1.47	2 (6%)	40,43,67	1.82	13 (32%)
13	BCL	W	104	6	69,74,74	1.16	4 (5%)	83,115,115	1.50	13 (15%)
13	BCL	5	101	5	69,74,74	1.19	6 (8%)	83,115,115	1.72	17 (20%)
13	BCL	U	103	6	69,74,74	1.24	5 (7%)	83,115,115	1.62	17 (20%)
19	CRT	B	101	-	41,43,43	0.73	0	50,54,54	1.62	12 (24%)
12	PGV	M	410	-	45,45,50	1.05	2 (4%)	49,50,56	0.95	3 (6%)
13	BCL	F	103	6	69,74,74	1.16	4 (5%)	83,115,115	1.46	12 (14%)
14	BPH	L	303	-	59,70,70	2.57	15 (25%)	61,101,101	2.04	14 (22%)
20	CDL	D	104	-	39,39,99	1.45	4 (10%)	45,51,111	1.40	7 (15%)
11	LHG	C	507	1	8,8,48	0.29	0	7,7,54	1.04	1 (14%)

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
19	CRT	0	101	-	-	4/51/51/51	-
20	CDL	U	104	-	-	33/71/71/110	-
12	PGV	3	105	-	-	17/55/55/55	-
13	BCL	D	103	6	-	7/41/137/137	-
19	CRT	N	101	-	-	0/51/51/51	-
20	CDL	H	305	-	-	29/89/89/110	-
8	HEC	C	501	1	1/1/3/7	6/14/54/54	-
13	BCL	Q	103	6	-	8/41/137/137	-
20	CDL	O	104	-	-	35/96/96/110	-
22	LMT	H	304	-	-	9/21/61/61	0/2/2/2
19	CRT	G	101	-	-	2/51/51/51	-
12	PGV	D	106	-	-	16/39/39/55	-
20	CDL	D	105	-	-	26/73/73/110	-
20	CDL	M	412	3	-	7/48/48/110	-
20	CDL	1	104	-	-	8/13/13/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	MQ8	M	404	-	-	2/47/67/67	0/2/2/2
13	BCL	U	101	5	-	4/41/137/137	-
13	BCL	1	101	5	-	14/41/137/137	-
13	BCL	P	102	6	-	13/41/137/137	-
21	PEF	K	104	-	-	6/30/30/50	-
19	CRT	O	103	-	-	1/51/51/51	-
20	CDL	M	406	-	-	47/110/110/110	-
13	BCL	4	102	6	-	14/41/137/137	-
13	BCL	L	301	2	-	3/41/137/137	-
13	BCL	5	103	6	-	14/41/137/137	-
13	BCL	Y	101	5	-	8/41/137/137	-
19	CRT	W	102	-	-	3/51/51/51	-
12	PGV	L	307	-	-	22/47/47/55	-
14	BPH	M	402	-	-	8/37/105/105	0/5/6/6
19	CRT	V	101	-	-	5/51/51/51	-
8	HEC	C	504	1	1/1/3/7	6/14/54/54	-
13	BCL	A	103	6	-	11/41/137/137	-
23	SF4	b	101	7	-	-	0/6/5/5
12	PGV	C	508	1	-	6/21/21/55	-
13	BCL	K	101	5	-	10/41/137/137	-
8	HEC	C	502	1	1/1/3/7	7/14/54/54	-
13	BCL	3	101	5	-	19/41/137/137	-
13	BCL	2	102	6	-	14/41/137/137	-
20	CDL	Y	104	-	-	20/50/50/110	-
15	UQ8	L	309	-	-	16/51/75/75	0/1/1/1
12	PGV	9	104	-	-	14/37/37/55	-
13	BCL	9	103	6	-	11/41/137/137	-
19	CRT	Z	101	-	-	0/51/51/51	-
12	PGV	H	303	-	-	11/40/40/55	-
13	BCL	S	101	5	-	10/41/137/137	-
13	BCL	W	101	5	-	10/41/137/137	-
8	HEC	C	503	1	1/1/3/7	2/14/54/54	-
20	CDL	S	104	-	-	40/85/85/110	-
15	UQ8	L	311	-	-	2/9/33/75	0/1/1/1
13	BCL	I	101	5	-	8/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCL	K	103	6	-	13/41/137/137	-
19	CRT	T	101	-	-	3/51/51/51	-
19	CRT	4	101	-	-	1/51/51/51	-
13	BCL	F	101	5	-	12/41/137/137	-
13	BCL	Y	103	6	-	14/41/137/137	-
13	BCL	J	102	6	-	10/41/137/137	-
13	BCL	L	302	2	-	1/41/137/137	-
13	BCL	M	401	3	-	6/41/137/137	-
15	UQ8	M	413	-	-	0/9/33/75	0/1/1/1
10	GOL	C	506	-	-	2/4/4/4	-
22	LMT	M	414	-	-	6/21/61/61	0/2/2/2
19	CRT	M	405	-	-	5/51/51/51	-
19	CRT	2	101	-	-	1/51/51/51	-
19	CRT	A	104	-	-	0/51/51/51	-
15	UQ8	L	304	-	-	3/27/51/75	0/1/1/1
13	BCL	7	101	5	-	6/35/131/137	-
13	BCL	D	101	5	-	8/41/137/137	-
19	CRT	J	101	-	-	2/51/51/51	-
13	BCL	Q	101	5	-	15/41/137/137	-
13	BCL	O	101	5	-	6/41/137/137	-
12	PGV	1	105	-	-	11/35/35/55	-
12	PGV	M	411	-	-	15/41/41/55	-
19	CRT	3	103	-	-	0/51/51/51	-
19	CRT	P	101	-	-	1/51/51/51	-
13	BCL	S	103	6	-	18/41/137/137	-
13	BCL	A	101	5	-	11/41/137/137	-
19	CRT	8	101	-	-	4/51/51/51	-
13	BCL	9	101	5	-	16/41/137/137	-
12	PGV	L	308	-	-	25/48/48/55	-
13	BCL	L	305	3	-	15/41/137/137	-
10	GOL	H	301	-	-	2/4/4/4	-
13	BCL	7	103	6	-	12/41/137/137	-
15	UQ8	L	310	-	-	9/27/51/75	0/1/1/1
13	BCL	W	104	6	-	7/41/137/137	-
13	BCL	5	101	5	-	9/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCL	U	103	6	-	13/41/137/137	-
19	CRT	B	101	-	-	5/51/51/51	-
12	PGV	M	410	-	-	15/47/47/55	-
13	BCL	F	103	6	-	10/41/137/137	-
14	BPH	L	303	-	-	6/37/105/105	0/5/6/6
20	CDL	D	104	-	-	23/50/50/110	-
11	LHG	C	507	1	-	3/5/6/53	-

All (313) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	L	303	BPH	C1B-C2B	9.20	1.49	1.39
14	L	303	BPH	C1D-C2D	8.35	1.48	1.39
14	M	402	BPH	C1B-C2B	8.27	1.48	1.39
14	M	402	BPH	C1D-C2D	8.05	1.48	1.39
15	M	413	UQ8	C6-C1	8.02	1.49	1.35
15	L	311	UQ8	C6-C1	7.96	1.49	1.35
18	M	404	MQ8	C3-C2	7.92	1.49	1.35
15	L	304	UQ8	C6-C1	7.53	1.49	1.35
15	L	310	UQ8	C6-C1	7.31	1.48	1.35
15	L	309	UQ8	C6-C1	7.27	1.48	1.35
14	L	303	BPH	C3B-C2B	5.73	1.49	1.39
8	C	501	HEC	FE-NB	5.27	2.11	1.94
13	S	103	BCL	MG-NA	5.21	2.18	2.06
14	L	303	BPH	O2D-CGD	5.20	1.45	1.33
13	2	102	BCL	MG-NA	5.19	2.18	2.06
14	M	402	BPH	C4D-CHA	5.19	1.47	1.39
8	C	503	HEC	FE-NB	5.19	2.10	1.94
20	S	104	CDL	OB8-CB7	5.19	1.48	1.33
14	M	402	BPH	C3D-C2D	5.17	1.48	1.39
8	C	504	HEC	FE-NB	5.17	2.10	1.94
14	M	402	BPH	O2D-CGD	5.16	1.45	1.33
14	L	303	BPH	C3B-C4B	5.15	1.50	1.41
14	L	303	BPH	C4D-CHA	5.15	1.47	1.39
14	L	303	BPH	C3D-C2D	5.13	1.48	1.39
13	Y	103	BCL	MG-NA	5.13	2.18	2.06
13	U	103	BCL	MG-NA	5.13	2.18	2.06
13	3	101	BCL	MG-NA	5.09	2.18	2.06
13	Q	103	BCL	MG-NA	5.08	2.18	2.06
13	5	103	BCL	MG-NA	5.08	2.18	2.06
13	Y	101	BCL	MG-NA	5.03	2.18	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	7	103	BCL	MG-NA	5.02	2.18	2.06
13	A	103	BCL	MG-NA	5.01	2.18	2.06
18	M	404	MQ8	C10-C5	5.00	1.49	1.40
13	M	401	BCL	MG-NA	5.00	2.18	2.06
13	W	104	BCL	MG-NA	4.98	2.18	2.06
13	S	101	BCL	MG-NA	4.95	2.18	2.06
14	M	402	BPH	C3B-C2B	4.94	1.48	1.39
8	C	502	HEC	FE-NB	4.94	2.10	1.94
13	P	102	BCL	MG-NA	4.93	2.18	2.06
13	F	103	BCL	MG-NA	4.90	2.17	2.06
13	4	102	BCL	MG-NA	4.90	2.17	2.06
13	K	103	BCL	MG-NA	4.89	2.17	2.06
13	L	301	BCL	MG-NA	4.88	2.17	2.06
13	J	102	BCL	MG-NA	4.87	2.17	2.06
13	W	101	BCL	MG-NA	4.85	2.17	2.06
13	1	101	BCL	MG-NA	4.82	2.17	2.06
13	9	103	BCL	MG-NA	4.82	2.17	2.06
13	U	101	BCL	MG-NA	4.80	2.17	2.06
13	A	101	BCL	MG-NA	4.78	2.17	2.06
13	D	101	BCL	MG-NA	4.76	2.17	2.06
13	5	101	BCL	MG-NA	4.76	2.17	2.06
13	I	101	BCL	MG-NA	4.76	2.17	2.06
13	D	103	BCL	MG-NA	4.75	2.17	2.06
14	M	402	BPH	C3B-C4B	4.70	1.49	1.41
13	O	101	BCL	MG-NA	4.70	2.17	2.06
13	9	101	BCL	MG-NA	4.70	2.17	2.06
14	M	402	BPH	OBD-CAD	4.67	1.28	1.22
13	7	101	BCL	MG-NA	4.67	2.17	2.06
13	K	101	BCL	MG-NA	4.67	2.17	2.06
14	L	303	BPH	OBD-CAD	4.66	1.28	1.22
21	1	103	PEF	P-O1P	4.65	1.61	1.50
13	F	101	BCL	MG-NA	4.64	2.17	2.06
13	L	302	BCL	MG-NA	4.59	2.17	2.06
13	L	305	BCL	MG-NA	4.58	2.17	2.06
13	Q	101	BCL	MG-NA	4.56	2.17	2.06
21	W	105	PEF	P-O1P	4.55	1.61	1.50
21	M	409	PEF	P-O1P	4.54	1.61	1.50
21	W	106	PEF	P-O1P	4.51	1.61	1.50
21	I	103	PEF	P-O1P	4.51	1.61	1.50
21	M	407	PEF	P-O1P	4.50	1.61	1.50
21	3	104	PEF	P-O1P	4.50	1.61	1.50
12	M	410	PGV	O03-C19	4.49	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	M	412	CDL	OA8-CA7	4.48	1.46	1.33
21	K	104	PEF	O2-C10	4.46	1.46	1.34
20	H	305	CDL	OA6-CA5	4.45	1.46	1.34
12	1	105	PGV	O03-C19	4.40	1.46	1.33
20	M	406	CDL	OB8-CB7	4.40	1.46	1.33
20	S	104	CDL	OA8-CA7	4.39	1.46	1.33
20	U	104	CDL	OB8-CB7	4.37	1.46	1.33
12	M	410	PGV	O01-C1	4.37	1.46	1.34
20	D	105	CDL	OA6-CA5	4.36	1.46	1.34
20	H	305	CDL	OA8-CA7	4.35	1.46	1.33
21	H	302	PEF	P-O1P	4.34	1.61	1.50
12	9	104	PGV	O03-C19	4.32	1.46	1.33
20	M	406	CDL	OB6-CB5	4.31	1.46	1.34
12	1	105	PGV	O01-C1	4.31	1.46	1.34
20	O	104	CDL	OA6-CA5	4.30	1.46	1.34
20	D	105	CDL	OB8-CB7	4.30	1.45	1.33
12	D	106	PGV	O03-C19	4.29	1.45	1.33
20	D	104	CDL	OA8-CA7	4.29	1.45	1.33
8	C	502	HEC	C1A-C2A	-4.29	1.37	1.45
20	O	104	CDL	OA8-CA7	4.28	1.45	1.33
14	M	402	BPH	O2A-CGA	4.27	1.45	1.33
20	D	104	CDL	OB8-CB7	4.27	1.45	1.33
12	3	105	PGV	O03-C19	4.26	1.45	1.33
8	C	502	HEC	CBC-CAC	-4.26	1.32	1.51
20	Y	104	CDL	OB8-CB7	4.25	1.45	1.33
20	H	305	CDL	OB8-CB7	4.25	1.45	1.33
12	3	105	PGV	O01-C1	4.25	1.46	1.34
12	H	303	PGV	O01-C1	4.24	1.46	1.34
20	U	104	CDL	OB6-CB5	4.24	1.44	1.35
21	K	104	PEF	O3-C30	4.21	1.45	1.33
20	Y	104	CDL	OB6-CB5	4.20	1.46	1.34
20	U	104	CDL	OA8-CA7	4.20	1.45	1.33
12	L	308	PGV	O03-C19	4.18	1.45	1.33
12	H	303	PGV	O03-C19	4.18	1.45	1.33
12	C	508	PGV	O03-C19	4.16	1.45	1.33
20	O	104	CDL	OB8-CB7	4.16	1.45	1.33
12	9	104	PGV	O01-C1	4.15	1.46	1.34
12	L	307	PGV	O01-C1	4.15	1.46	1.34
20	D	104	CDL	OA6-CA5	4.15	1.46	1.34
12	M	411	PGV	O03-C19	4.15	1.45	1.33
20	M	412	CDL	OA6-CA5	4.14	1.46	1.34
20	M	406	CDL	OA8-CA7	4.14	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	M	412	CDL	OB6-CB5	4.14	1.46	1.34
20	Y	104	CDL	OA6-CA5	4.13	1.45	1.34
20	S	104	CDL	OB6-CB5	4.12	1.45	1.34
20	S	104	CDL	OA6-CA5	4.11	1.45	1.34
12	C	508	PGV	O01-C1	4.11	1.45	1.34
8	C	504	HEC	CBB-CAB	-4.11	1.33	1.51
8	C	501	HEC	C4A-C3A	-4.09	1.37	1.45
12	D	106	PGV	O01-C1	4.08	1.45	1.34
8	C	501	HEC	CBC-CAC	-4.08	1.33	1.51
12	L	307	PGV	O03-C19	4.08	1.45	1.33
12	L	308	PGV	O01-C1	4.06	1.45	1.34
12	M	411	PGV	O01-C1	4.06	1.45	1.34
8	C	501	HEC	CBB-CAB	-4.05	1.33	1.51
20	D	104	CDL	OB6-CB5	4.05	1.45	1.34
8	C	503	HEC	CBC-CAC	-4.04	1.33	1.51
20	H	305	CDL	OB6-CB5	4.03	1.45	1.34
8	C	503	HEC	FE-NC	4.03	2.08	1.95
14	L	303	BPH	O2A-CGA	4.02	1.45	1.33
8	C	503	HEC	CBB-CAB	-4.01	1.33	1.51
8	C	504	HEC	FE-NC	3.97	2.08	1.95
20	M	406	CDL	OA6-CA5	3.92	1.45	1.34
8	C	504	HEC	CBC-CAC	-3.92	1.34	1.51
20	O	104	CDL	OB6-CB5	3.89	1.45	1.34
8	C	502	HEC	C4A-C3A	-3.89	1.37	1.45
13	U	103	BCL	MG-NC	3.87	2.15	2.06
8	C	502	HEC	CBB-CAB	-3.84	1.34	1.51
20	Y	104	CDL	OA8-CA7	3.84	1.44	1.33
13	3	101	BCL	MG-NC	3.84	2.15	2.06
20	D	105	CDL	OB6-CB5	3.81	1.45	1.34
13	2	102	BCL	MG-NC	3.80	2.15	2.06
20	U	104	CDL	OA6-CA5	3.72	1.44	1.34
13	5	101	BCL	MG-NC	3.67	2.15	2.06
8	C	501	HEC	C1A-C2A	-3.66	1.38	1.45
13	1	101	BCL	MG-NC	3.64	2.14	2.06
13	S	103	BCL	MG-NC	3.63	2.14	2.06
13	Q	101	BCL	MG-NC	3.60	2.14	2.06
13	W	104	BCL	MG-NC	3.59	2.14	2.06
13	5	103	BCL	MG-NC	3.59	2.14	2.06
13	O	101	BCL	MG-NC	3.59	2.14	2.06
13	Y	101	BCL	MG-NC	3.57	2.14	2.06
13	L	302	BCL	MG-NC	3.56	2.14	2.06
13	7	101	BCL	MG-NC	3.55	2.14	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Q	103	BCL	MG-NC	3.54	2.14	2.06
13	9	101	BCL	MG-NC	3.54	2.14	2.06
8	C	502	HEC	FE-NC	3.53	2.07	1.95
13	W	101	BCL	MG-NC	3.53	2.14	2.06
13	Y	103	BCL	MG-NC	3.51	2.14	2.06
13	I	101	BCL	MG-NC	3.50	2.14	2.06
13	M	401	BCL	C3B-C4B	3.50	1.47	1.41
13	S	101	BCL	MG-NC	3.49	2.14	2.06
13	L	305	BCL	MG-NC	3.48	2.14	2.06
13	U	101	BCL	MG-NC	3.48	2.14	2.06
8	C	501	HEC	C4D-ND	-3.48	1.31	1.38
13	9	103	BCL	C3B-C4B	3.46	1.47	1.41
14	M	402	BPH	CHA-CBD	-3.43	1.47	1.51
13	K	103	BCL	MG-NC	3.43	2.14	2.06
13	S	103	BCL	C3B-C4B	3.41	1.47	1.41
13	P	102	BCL	C3B-C4B	3.41	1.47	1.41
13	P	102	BCL	MG-NC	3.41	2.14	2.06
13	A	101	BCL	MG-NC	3.40	2.14	2.06
8	C	502	HEC	C1D-ND	-3.39	1.34	1.40
14	L	303	BPH	CHA-CBD	-3.38	1.47	1.51
13	D	103	BCL	MG-NC	3.37	2.14	2.06
13	F	101	BCL	MG-NC	3.37	2.14	2.06
8	C	503	HEC	C1D-ND	-3.36	1.34	1.40
13	K	101	BCL	MG-NC	3.35	2.14	2.06
13	F	103	BCL	MG-NC	3.35	2.14	2.06
13	3	101	BCL	C3B-C4B	3.35	1.47	1.41
8	C	504	HEC	C1D-ND	-3.33	1.34	1.40
15	L	309	UQ8	C4-C3	3.33	1.49	1.36
13	A	103	BCL	MG-NC	3.32	2.14	2.06
13	4	102	BCL	MG-NC	3.32	2.14	2.06
8	C	501	HEC	C1B-NB	-3.32	1.32	1.38
13	Q	103	BCL	C3B-C4B	3.30	1.47	1.41
13	K	103	BCL	C3B-C4B	3.28	1.47	1.41
13	9	103	BCL	MG-NC	3.27	2.14	2.06
13	7	103	BCL	C3B-C4B	3.26	1.47	1.41
13	D	101	BCL	MG-NC	3.24	2.14	2.06
13	7	103	BCL	MG-NC	3.23	2.13	2.06
13	S	101	BCL	C3B-C4B	3.22	1.47	1.41
13	Q	101	BCL	C3B-C4B	3.21	1.47	1.41
15	M	413	UQ8	C4-C3	3.20	1.49	1.36
13	F	101	BCL	C3B-C4B	3.20	1.47	1.41
13	A	103	BCL	C3B-C4B	3.18	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	501	HEC	FE-NC	3.18	2.05	1.95
13	J	102	BCL	MG-NC	3.18	2.13	2.06
13	U	103	BCL	C3B-C4B	3.17	1.47	1.41
15	L	310	UQ8	C4-C3	3.17	1.49	1.36
13	A	101	BCL	C3B-C4B	3.14	1.46	1.41
15	L	304	UQ8	C4-C3	3.13	1.49	1.36
13	L	301	BCL	MG-NC	3.12	2.13	2.06
13	5	101	BCL	C3B-C4B	3.12	1.46	1.41
13	K	101	BCL	C3B-C4B	3.11	1.46	1.41
13	W	101	BCL	C3B-C4B	3.11	1.46	1.41
13	7	101	BCL	C3B-C4B	3.09	1.46	1.41
13	L	302	BCL	C3B-C4B	3.09	1.46	1.41
13	F	103	BCL	C3B-C4B	3.08	1.46	1.41
13	5	103	BCL	C3B-C4B	3.07	1.46	1.41
15	L	311	UQ8	C4-C3	3.07	1.48	1.36
13	D	101	BCL	C3B-C4B	3.06	1.46	1.41
13	9	101	BCL	C3B-C4B	3.05	1.46	1.41
13	4	102	BCL	C3B-C4B	3.04	1.46	1.41
8	C	503	HEC	C4B-NB	-3.02	1.35	1.40
13	J	102	BCL	C3B-C4B	3.01	1.46	1.41
13	D	103	BCL	C3B-C4B	3.01	1.46	1.41
13	W	104	BCL	C3B-C4B	3.01	1.46	1.41
13	O	101	BCL	C3B-C4B	2.96	1.46	1.41
13	U	101	BCL	C3B-C4B	2.95	1.46	1.41
13	Y	103	BCL	C3B-C4B	2.92	1.46	1.41
13	M	401	BCL	MG-NC	2.92	2.13	2.06
13	2	102	BCL	C3B-C4B	2.90	1.46	1.41
8	C	504	HEC	C4B-NB	-2.88	1.35	1.40
13	1	101	BCL	C3B-C4B	2.87	1.46	1.41
13	I	101	BCL	C3B-C4B	2.85	1.46	1.41
13	L	301	BCL	C3B-C4B	2.84	1.46	1.41
13	2	102	BCL	O2A-CGA	-2.80	1.25	1.33
13	Y	101	BCL	C3B-C4B	2.73	1.46	1.41
14	L	303	BPH	C1D-ND	-2.73	1.33	1.38
14	M	402	BPH	C1D-ND	-2.67	1.33	1.38
13	L	305	BCL	CHD-C1D	2.63	1.43	1.38
14	L	303	BPH	C2C-C3C	-2.54	1.52	1.54
8	C	502	HEC	C4B-NB	-2.52	1.36	1.40
13	A	101	BCL	CHD-C1D	2.51	1.43	1.38
13	M	401	BCL	CHD-C1D	2.50	1.43	1.38
13	2	102	BCL	O1A-CGA	-2.49	1.15	1.22
8	C	502	HEC	C4D-ND	-2.49	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	D	105	CDL	OA8-CA7	2.48	1.45	1.33
14	M	402	BPH	C2C-C3C	-2.46	1.52	1.54
13	W	101	BCL	CHD-C1D	2.45	1.43	1.38
8	C	504	HEC	C4B-C3B	2.44	1.49	1.45
13	L	301	BCL	CHD-C1D	2.41	1.43	1.38
13	Y	103	BCL	C1D-C2D	-2.39	1.40	1.45
8	C	504	HEC	C4D-ND	-2.39	1.33	1.38
14	L	303	BPH	C4B-NB	-2.38	1.34	1.38
13	U	103	BCL	C1D-C2D	-2.37	1.40	1.45
13	Q	103	BCL	C1D-C2D	-2.36	1.40	1.45
13	L	305	BCL	C3B-C4B	2.36	1.45	1.41
13	L	302	BCL	CHD-C1D	2.35	1.43	1.38
13	Y	101	BCL	CHD-C1D	2.33	1.42	1.38
21	W	105	PEF	P-O4P	2.31	1.61	1.54
8	C	503	HEC	C1A-C2A	-2.29	1.41	1.45
21	M	408	PEF	P-O4P	2.29	1.61	1.54
21	I	103	PEF	P-O4P	2.29	1.61	1.54
21	M	408	PEF	P-O3P	2.28	1.61	1.54
21	W	106	PEF	P-O3P	2.28	1.61	1.54
21	M	409	PEF	P-O4P	2.28	1.61	1.54
13	D	103	BCL	C1D-C2D	-2.28	1.40	1.45
13	I	101	BCL	C1-C2	2.28	1.55	1.49
8	C	501	HEC	FE-NA	2.27	2.02	1.95
21	M	407	PEF	P-O3P	2.27	1.61	1.54
21	3	104	PEF	P-O3P	2.27	1.61	1.54
13	Y	101	BCL	C1D-ND	2.26	1.40	1.37
13	7	103	BCL	C1D-C2D	-2.26	1.40	1.45
13	5	101	BCL	C5-C3	2.26	1.56	1.51
12	C	508	PGV	O01-C02	-2.26	1.43	1.47
13	9	101	BCL	CHD-C1D	2.24	1.42	1.38
13	1	101	BCL	CHD-C1D	2.24	1.42	1.38
13	I	101	BCL	CHD-C1D	2.24	1.42	1.38
13	K	101	BCL	CHD-C1D	2.22	1.42	1.38
14	L	303	BPH	C1B-NB	-2.22	1.34	1.38
13	A	103	BCL	CHD-C1D	2.21	1.42	1.38
13	W	104	BCL	C1D-C2D	-2.19	1.41	1.45
13	O	101	BCL	CHD-C1D	2.18	1.42	1.38
14	L	303	BPH	CBD-CGD	-2.17	1.49	1.52
13	1	101	BCL	C1D-ND	2.16	1.40	1.37
13	U	103	BCL	C16-C15	2.16	1.61	1.52
8	C	503	HEC	C4A-C3A	-2.16	1.41	1.45
13	Y	103	BCL	CHD-C1D	2.15	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	W	101	BCL	C1D-ND	2.15	1.40	1.37
13	9	101	BCL	C1D-ND	2.15	1.40	1.37
13	4	102	BCL	C1D-C2D	-2.14	1.41	1.45
14	M	402	BPH	C4B-NB	-2.14	1.34	1.38
13	5	101	BCL	C1-C2	2.14	1.55	1.49
8	C	503	HEC	C4D-ND	-2.14	1.34	1.38
14	M	402	BPH	CBD-CGD	-2.13	1.49	1.52
21	1	103	PEF	P-O4P	2.12	1.61	1.54
13	2	102	BCL	CHD-C1D	2.12	1.42	1.38
13	J	102	BCL	C1D-C2D	-2.11	1.41	1.45
13	4	102	BCL	CHD-C1D	2.11	1.42	1.38
13	F	103	BCL	C1D-C2D	-2.11	1.41	1.45
13	7	101	BCL	CHD-C1D	2.10	1.42	1.38
13	A	101	BCL	C1D-ND	2.10	1.40	1.37
13	K	101	BCL	C1-C2	2.08	1.55	1.49
13	5	101	BCL	C1D-ND	2.08	1.40	1.37
13	S	103	BCL	CHD-C1D	2.08	1.42	1.38
13	I	101	BCL	C5-C3	2.07	1.55	1.51
13	K	103	BCL	C1D-C2D	-2.07	1.41	1.45
13	F	101	BCL	CHD-C1D	2.07	1.42	1.38
20	Y	104	CDL	PA1-OA5	2.06	1.67	1.59
13	J	102	BCL	CHD-C1D	2.06	1.42	1.38
13	5	103	BCL	C1D-C2D	-2.06	1.41	1.45
13	M	401	BCL	C3D-C4D	-2.05	1.39	1.44
13	L	302	BCL	C1D-ND	2.05	1.40	1.37
13	S	101	BCL	C1D-ND	2.03	1.40	1.37
13	5	103	BCL	CHD-C1D	2.02	1.42	1.38
8	C	503	HEC	C4B-C3B	2.01	1.48	1.45
13	A	103	BCL	C1D-ND	2.01	1.40	1.37
13	I	101	BCL	C1D-ND	2.01	1.40	1.37
8	C	502	HEC	C1B-NB	-2.00	1.34	1.38

All (1037) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	3	101	BCL	C1-O2A-CGA	7.91	137.19	116.44
13	S	103	BCL	C1-O2A-CGA	6.62	133.82	116.44
14	M	402	BPH	O2D-CGD-CBD	6.38	119.07	111.00
13	L	305	BCL	C1-C2-C3	-6.15	115.40	126.04
14	M	402	BPH	C2B-C1B-NB	6.15	113.77	109.53
19	N	101	CRT	C21-C22-C23	-6.08	118.63	127.31
13	Q	101	BCL	C1-C2-C3	-6.01	115.65	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L	303	BPH	CMC-C2C-C1C	5.91	127.32	114.38
14	M	402	BPH	CMC-C2C-C1C	5.83	127.14	114.38
13	3	101	BCL	CHD-C1D-ND	-5.80	119.12	124.45
13	Q	101	BCL	CHD-C1D-ND	-5.76	119.16	124.45
14	M	402	BPH	C4A-C3A-C2A	-5.67	97.44	102.84
13	O	101	BCL	CHD-C1D-ND	-5.66	119.25	124.45
13	F	101	BCL	CHD-C1D-ND	-5.64	119.27	124.45
13	1	101	BCL	C1-O2A-CGA	5.56	131.03	116.44
13	L	305	BCL	CHD-C1D-ND	-5.53	119.37	124.45
13	U	101	BCL	CHD-C1D-ND	-5.53	119.37	124.45
13	D	101	BCL	CHD-C1D-ND	-5.52	119.38	124.45
13	2	102	BCL	C1-O2A-CGA	5.51	130.89	116.44
13	A	101	BCL	CHD-C1D-ND	-5.49	119.41	124.45
13	7	101	BCL	C1-C2-C3	-5.49	116.55	126.04
13	5	101	BCL	CHD-C1D-ND	-5.48	119.41	124.45
13	I	101	BCL	CHD-C1D-ND	-5.47	119.43	124.45
20	U	104	CDL	CB4-OB6-CB5	-5.42	107.79	117.90
13	A	101	BCL	C4D-CHA-C1A	5.41	127.84	121.25
13	7	101	BCL	CHD-C1D-ND	-5.41	119.48	124.45
14	M	402	BPH	CAC-C3C-C4C	5.41	125.83	113.73
13	W	101	BCL	CHD-C1D-ND	-5.38	119.51	124.45
13	5	101	BCL	C11-C10-C8	-5.38	98.53	115.92
19	P	101	CRT	C21-C22-C23	-5.38	119.64	127.31
13	1	101	BCL	CHD-C1D-ND	-5.37	119.52	124.45
13	5	103	BCL	C1-C2-C3	-5.36	116.78	126.04
13	F	101	BCL	C4D-CHA-C1A	5.34	127.75	121.25
13	S	101	BCL	C4D-CHA-C1A	5.33	127.74	121.25
13	L	302	BCL	CHD-C1D-ND	-5.33	119.56	124.45
13	L	301	BCL	CHD-C1D-ND	-5.32	119.56	124.45
13	I	101	BCL	C4D-CHA-C1A	5.32	127.72	121.25
13	U	101	BCL	C4D-CHA-C1A	5.31	127.71	121.25
13	M	401	BCL	CHD-C1D-ND	-5.28	119.61	124.45
13	M	401	BCL	C4D-CHA-C1A	5.24	127.62	121.25
13	K	101	BCL	CHD-C1D-ND	-5.24	119.64	124.45
13	3	101	BCL	O2A-CGA-O1A	-5.24	110.38	123.59
21	H	302	PEF	O3P-P-O2P	5.23	124.75	107.97
13	D	101	BCL	C4D-CHA-C1A	5.22	127.60	121.25
15	L	304	UQ8	C15-C14-C16	5.18	123.99	115.27
13	Y	101	BCL	CHD-C1D-ND	-5.17	119.71	124.45
13	L	301	BCL	C4D-CHA-C1A	5.11	127.47	121.25
13	S	101	BCL	CHD-C1D-ND	-5.11	119.76	124.45
13	K	101	BCL	C4D-CHA-C1A	5.10	127.46	121.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	P	102	BCL	C1-C2-C3	5.10	134.86	126.04
13	F	101	BCL	C1-O2A-CGA	5.09	129.80	116.44
13	2	102	BCL	C16-C15-C13	-5.07	99.53	115.92
13	9	103	BCL	C4D-CHA-C1A	5.07	127.42	121.25
13	W	101	BCL	C4D-CHA-C1A	5.06	127.40	121.25
13	W	104	BCL	C4D-CHA-C1A	5.06	127.40	121.25
19	Z	101	CRT	C21-C22-C23	-5.05	120.11	127.31
13	Q	101	BCL	C4D-CHA-C1A	5.05	127.39	121.25
15	L	310	UQ8	C7-C8-C9	-5.04	118.39	126.79
13	U	103	BCL	CHD-C1D-ND	-5.04	119.82	124.45
14	L	303	BPH	C2B-C1B-NB	5.02	112.99	109.53
13	9	101	BCL	CHD-C1D-ND	-5.02	119.84	124.45
13	F	103	BCL	C4D-CHA-C1A	5.01	127.35	121.25
8	C	501	HEC	CAB-C3B-C4B	-5.01	118.31	124.81
13	4	102	BCL	C4D-CHA-C1A	5.01	127.35	121.25
13	9	103	BCL	CHD-C1D-ND	-5.01	119.85	124.45
13	Y	103	BCL	C4D-CHA-C1A	5.00	127.33	121.25
13	O	101	BCL	C4D-CHA-C1A	5.00	127.33	121.25
20	Y	104	CDL	CA4-OA6-CA5	-4.99	105.49	117.79
14	L	303	BPH	CAC-C3C-C4C	4.99	124.90	113.73
13	W	104	BCL	CHD-C1D-ND	-4.99	119.87	124.45
13	2	102	BCL	CHD-C1D-ND	-4.98	119.88	124.45
13	Y	101	BCL	C4D-CHA-C1A	4.97	127.30	121.25
19	W	102	CRT	C21-C22-C23	-4.95	120.24	127.31
13	K	103	BCL	CHD-C1D-ND	-4.94	119.92	124.45
13	2	102	BCL	C4D-CHA-C1A	4.92	127.23	121.25
13	5	103	BCL	CHD-C1D-ND	-4.91	119.94	124.45
8	C	501	HEC	CHC-C4B-NB	4.91	130.42	124.37
20	S	104	CDL	OB6-CB5-C51	4.90	122.07	111.50
13	D	103	BCL	C4D-CHA-C1A	4.90	127.22	121.25
13	9	101	BCL	C4D-CHA-C1A	4.90	127.21	121.25
13	7	101	BCL	C4D-CHA-C1A	4.90	127.21	121.25
13	Q	103	BCL	CHD-C1D-ND	-4.88	119.97	124.45
20	D	105	CDL	OA6-CA5-C11	4.86	121.98	111.50
13	Q	103	BCL	C4D-CHA-C1A	4.85	127.15	121.25
13	3	101	BCL	C4D-CHA-C1A	4.85	127.15	121.25
19	V	101	CRT	C21-C22-C23	-4.84	120.40	127.31
13	9	103	BCL	C1-O2A-CGA	4.82	129.09	116.44
20	U	104	CDL	OB6-CB5-C51	4.80	119.92	111.09
19	B	101	CRT	C21-C22-C23	-4.80	120.46	127.31
13	P	102	BCL	CHD-C1D-ND	-4.80	120.05	124.45
13	F	103	BCL	CHD-C1D-ND	-4.78	120.06	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	S	103	BCL	CHD-C1D-ND	-4.77	120.07	124.45
8	C	502	HEC	CHA-C4D-ND	4.76	129.59	124.42
19	M	405	CRT	C21-C22-C23	-4.75	120.53	127.31
13	S	103	BCL	C4D-CHA-C1A	4.73	127.00	121.25
13	3	101	BCL	O2A-CGA-CBA	4.72	126.72	111.91
13	1	101	BCL	C4D-CHA-C1A	4.69	126.95	121.25
8	C	501	HEC	C2A-C1A-NA	-4.68	105.77	110.32
8	C	502	HEC	CAB-C3B-C4B	-4.67	118.75	124.81
13	A	103	BCL	CHD-C1D-ND	-4.67	120.16	124.45
13	J	102	BCL	C4D-CHA-C1A	4.65	126.90	121.25
20	Y	104	CDL	OA6-CA5-C11	4.64	123.73	110.80
13	7	103	BCL	C4D-CHA-C1A	4.62	126.87	121.25
19	3	103	CRT	C21-C22-C23	-4.61	120.72	127.31
13	L	302	BCL	C4D-CHA-C1A	4.60	126.85	121.25
21	1	103	PEF	O4P-P-O1P	-4.57	94.18	110.89
13	L	305	BCL	C4D-CHA-C1A	4.57	126.81	121.25
13	D	103	BCL	CHD-C1D-ND	-4.56	120.26	124.45
13	4	102	BCL	CHD-C1D-ND	-4.56	120.26	124.45
12	L	307	PGV	O01-C1-C2	4.54	121.28	111.50
8	C	504	HEC	CHC-C4B-NB	4.53	129.96	124.37
13	D	101	BCL	C17-C16-C15	4.53	134.03	113.24
13	5	101	BCL	C4D-CHA-C1A	4.52	126.75	121.25
13	U	103	BCL	C4D-CHA-C1A	4.51	126.73	121.25
14	L	303	BPH	O2D-CGD-CBD	4.46	116.64	111.00
19	8	101	CRT	C21-C22-C23	-4.45	120.96	127.31
8	C	503	HEC	C4B-NB-C1B	4.44	109.66	105.07
8	C	503	HEC	CHC-C4B-NB	4.44	129.85	124.37
8	C	501	HEC	C3B-C4B-NB	-4.44	105.23	110.17
13	J	102	BCL	CHD-C1D-ND	-4.44	120.38	124.45
19	2	101	CRT	C21-C22-C23	-4.42	121.00	127.31
20	O	104	CDL	OA6-CA5-C11	4.42	121.03	111.50
20	M	406	CDL	OB6-CB5-C51	4.42	121.02	111.50
19	0	101	CRT	C21-C22-C23	-4.41	121.02	127.31
21	K	104	PEF	O2-C10-C11	4.41	121.00	111.50
12	H	303	PGV	O01-C1-C2	4.40	120.98	111.50
19	O	103	CRT	C21-C22-C23	-4.38	121.05	127.31
13	P	102	BCL	C4A-NA-C1A	4.37	108.67	106.71
13	K	101	BCL	C11-C10-C8	-4.37	101.79	115.92
13	5	103	BCL	C4D-CHA-C1A	4.36	126.56	121.25
8	C	504	HEC	C4B-NB-C1B	4.35	109.57	105.07
13	7	103	BCL	CHD-C1D-ND	-4.35	120.46	124.45
8	C	502	HEC	C4B-NB-C1B	4.33	109.55	105.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	103	BCL	C4D-CHA-C1A	4.33	126.52	121.25
13	Y	103	BCL	CHD-C1D-ND	-4.31	120.49	124.45
8	C	502	HEC	CHA-C1A-NA	4.31	129.10	124.44
20	M	406	CDL	OA6-CA5-C11	4.29	120.74	111.50
12	L	308	PGV	O01-C1-C2	4.27	120.70	111.50
12	1	105	PGV	O01-C1-C2	4.25	120.65	111.50
13	P	102	BCL	C4D-CHA-C1A	4.23	126.39	121.25
13	A	101	BCL	C1-O2A-CGA	4.22	127.52	116.44
12	M	411	PGV	O01-C1-C2	4.22	120.59	111.50
8	C	502	HEC	CHB-C1B-NB	4.20	128.98	124.42
14	L	303	BPH	C4D-CHA-CBD	-4.18	106.63	108.52
8	C	501	HEC	C4B-NB-C1B	4.13	109.34	105.07
8	C	502	HEC	CHC-C4B-NB	4.12	129.46	124.37
13	K	103	BCL	C1-C2-C3	-4.12	118.92	126.04
13	Y	101	BCL	C4A-NA-C1A	4.11	108.55	106.71
13	S	103	BCL	C1-C2-C3	-4.11	118.94	126.04
13	J	102	BCL	C4A-NA-C1A	4.10	108.55	106.71
12	3	105	PGV	O01-C1-C2	4.10	120.34	111.50
19	3	103	CRT	C10-C9-C7	-4.10	121.47	127.31
12	9	104	PGV	O01-C1-C2	4.09	120.32	111.50
13	7	101	BCL	C4A-NA-C1A	4.06	108.53	106.71
13	L	305	BCL	C1D-ND-C4D	-4.05	103.46	106.33
20	D	105	CDL	OB6-CB5-C51	4.04	120.21	111.50
8	C	504	HEC	C4C-NC-C1C	4.04	109.31	105.35
19	T	101	CRT	C21-C22-C23	-4.04	121.55	127.31
19	A	104	CRT	C21-C22-C23	-4.04	121.55	127.31
8	C	501	HEC	C4A-NA-C1A	4.02	109.28	105.35
20	U	104	CDL	CA6-CA4-CA3	-4.02	102.28	111.79
12	C	508	PGV	O01-C1-C2	4.02	120.16	111.50
8	C	501	HEC	CHB-C1B-NB	4.01	128.78	124.42
13	2	102	BCL	C4A-NA-C1A	4.01	108.51	106.71
20	O	104	CDL	CB4-OB6-CB5	-4.00	107.95	117.79
20	S	104	CDL	CB4-OB6-CB5	-3.97	108.03	117.79
8	C	502	HEC	C3B-C4B-NB	-3.95	105.77	110.17
13	4	102	BCL	C4A-NA-C1A	3.94	108.48	106.71
13	K	103	BCL	C4A-NA-C1A	3.94	108.48	106.71
8	C	503	HEC	C4C-NC-C1C	3.93	109.19	105.35
13	L	301	BCL	C1D-ND-C4D	-3.93	103.55	106.33
20	H	305	CDL	OB6-CB5-C51	3.92	119.95	111.50
13	O	101	BCL	C11-C10-C8	-3.92	103.26	115.92
13	S	103	BCL	C4A-NA-C1A	3.91	108.47	106.71
13	Y	103	BCL	C4A-NA-C1A	3.91	108.47	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	104	CRT	C10-C9-C7	-3.91	121.73	127.31
15	L	304	UQ8	C7-C8-C9	-3.91	120.29	126.79
13	O	101	BCL	C4A-NA-C1A	3.89	108.45	106.71
8	C	504	HEC	C3B-C4B-NB	-3.88	105.84	110.17
13	Q	101	BCL	C16-C15-C13	-3.88	103.37	115.92
18	M	404	MQ8	C16-C17-C18	-3.88	118.32	127.66
13	W	104	BCL	C4A-NA-C1A	3.87	108.44	106.71
13	P	102	BCL	C6-C5-C3	3.86	123.58	113.45
13	K	103	BCL	C4D-CHA-C1A	3.86	125.95	121.25
20	S	104	CDL	OA6-CA5-C11	3.86	119.81	111.50
12	C	508	PGV	C02-O01-C1	-3.85	112.93	117.88
13	A	103	BCL	C4A-NA-C1A	3.85	108.44	106.71
20	U	104	CDL	OA6-CA5-C11	3.84	119.78	111.50
13	Q	103	BCL	C1D-ND-C4D	-3.84	103.61	106.33
8	C	503	HEC	CHA-C1A-NA	3.84	128.60	124.44
13	Q	103	BCL	C4A-NA-C1A	3.84	108.43	106.71
19	4	101	CRT	C21-C22-C23	-3.84	121.83	127.31
15	L	304	UQ8	C16-C14-C13	-3.83	113.37	121.12
13	U	101	BCL	C1-C2-C3	-3.82	119.44	126.04
13	1	101	BCL	C1-C2-C3	3.82	132.64	126.04
13	U	103	BCL	C1D-ND-C4D	-3.81	103.62	106.33
8	C	504	HEC	CHB-C1B-NB	3.81	128.56	124.42
13	9	101	BCL	C4A-NA-C1A	3.80	108.42	106.71
19	G	101	CRT	C21-C22-C23	-3.80	121.89	127.31
13	U	103	BCL	C20-C18-C19	-3.80	92.99	110.51
13	5	101	BCL	C4A-NA-C1A	3.79	108.41	106.71
13	D	101	BCL	C1D-ND-C4D	-3.79	103.65	106.33
8	C	501	HEC	CHD-C1D-ND	3.78	129.04	124.37
21	M	409	PEF	O3P-P-O2P	3.77	120.07	107.97
21	3	104	PEF	O4P-P-O2P	3.77	120.07	107.97
13	U	101	BCL	C4A-NA-C1A	3.76	108.40	106.71
21	M	407	PEF	O4P-P-O2P	3.76	120.03	107.97
13	F	103	BCL	C4A-NA-C1A	3.75	108.39	106.71
21	I	103	PEF	O3P-P-O2P	3.75	120.00	107.97
13	U	101	BCL	C1D-ND-C4D	-3.74	103.67	106.33
21	W	106	PEF	O4P-P-O2P	3.72	119.91	107.97
13	D	101	BCL	C4A-NA-C1A	3.71	108.38	106.71
8	C	503	HEC	C3B-C4B-NB	-3.71	106.04	110.17
13	L	305	BCL	CAB-C3B-C2B	3.71	133.89	128.34
20	O	104	CDL	OB6-CB5-C51	3.68	119.44	111.50
20	D	105	CDL	CB4-OB6-CB5	-3.68	108.73	117.79
19	Z	101	CRT	C20-C19-C17	-3.68	122.06	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	K	103	BCL	C1D-ND-C4D	-3.66	103.73	106.33
13	Y	101	BCL	C1D-ND-C4D	-3.66	103.73	106.33
14	M	402	BPH	C3D-C4D-ND	3.66	112.71	107.72
13	K	101	BCL	C1D-ND-C4D	-3.65	103.74	106.33
8	C	504	HEC	CHA-C4D-ND	3.65	128.38	124.42
14	L	303	BPH	C1A-C2A-C3A	-3.65	99.37	102.84
19	T	101	CRT	C10-C9-C7	-3.64	122.11	127.31
13	5	103	BCL	C4A-NA-C1A	3.64	108.34	106.71
13	P	102	BCL	C1D-ND-C4D	-3.64	103.75	106.33
13	K	101	BCL	C4A-NA-C1A	3.63	108.34	106.71
13	7	103	BCL	C4A-NA-C1A	3.62	108.33	106.71
13	5	103	BCL	C1D-ND-C4D	-3.62	103.76	106.33
22	H	304	LMT	C3'-C4'-C5'	-3.61	102.64	110.93
20	D	104	CDL	OA6-CA5-C11	3.61	120.88	110.80
13	M	401	BCL	C4A-NA-C1A	3.61	108.33	106.71
14	L	303	BPH	CBC-CAC-C3C	-3.58	106.55	113.77
13	7	101	BCL	C1D-ND-C4D	-3.58	103.79	106.33
20	Y	104	CDL	OB8-CB7-C71	3.58	120.77	111.38
20	M	412	CDL	OA8-CA7-C31	3.57	120.74	111.38
19	N	101	CRT	C10-C9-C7	-3.57	122.22	127.31
8	C	502	HEC	C1D-ND-C4D	3.56	108.75	105.07
8	C	503	HEC	CHB-C1B-NB	3.56	128.28	124.42
13	K	101	BCL	C1-O2A-CGA	3.56	125.77	116.44
14	L	303	BPH	C3D-C4D-ND	3.56	112.57	107.72
20	M	406	CDL	CA4-OA6-CA5	-3.54	109.08	117.79
8	C	503	HEC	CHA-C4D-ND	3.54	128.26	124.42
15	L	309	UQ8	C7-C8-C9	-3.53	120.92	126.79
15	L	309	UQ8	O5-C5-C6	-3.53	115.37	121.55
8	C	501	HEC	CHB-C1B-C2B	-3.52	119.49	124.98
13	F	101	BCL	C4A-NA-C1A	3.51	108.28	106.71
13	A	101	BCL	C4A-NA-C1A	3.51	108.28	106.71
20	H	305	CDL	OA6-CA5-C11	3.50	119.04	111.50
13	I	101	BCL	C1D-ND-C4D	-3.50	103.85	106.33
13	2	102	BCL	C1D-ND-C4D	-3.49	103.85	106.33
13	Q	101	BCL	C1D-ND-C4D	-3.49	103.86	106.33
13	5	101	BCL	C1D-ND-C4D	-3.49	103.86	106.33
8	C	501	HEC	C1D-ND-C4D	3.49	108.67	105.07
21	1	103	PEF	O3P-P-O2P	3.48	119.14	107.97
13	F	103	BCL	C1D-ND-C4D	-3.48	103.87	106.33
13	S	103	BCL	C1D-ND-C4D	-3.47	103.87	106.33
19	2	101	CRT	C10-C9-C7	-3.47	122.36	127.31
13	3	101	BCL	C1D-ND-C4D	-3.47	103.87	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S	104	CDL	OB8-CB7-C71	3.46	122.76	111.91
19	4	101	CRT	C10-C9-C7	-3.46	122.37	127.31
13	Y	103	BCL	C1-O2A-CGA	3.44	125.48	116.44
8	C	504	HEC	CHD-C1D-ND	3.44	128.62	124.37
20	M	412	CDL	OB6-CB5-C51	3.43	118.90	111.50
13	4	102	BCL	C1-C2-C3	3.43	131.97	126.04
13	S	101	BCL	C1D-ND-C4D	-3.43	103.90	106.33
13	W	104	BCL	C1D-ND-C4D	-3.42	103.90	106.33
13	J	102	BCL	C1-C2-C3	-3.41	120.14	126.04
8	C	503	HEC	CHD-C1D-ND	3.41	128.58	124.37
19	N	101	CRT	C21-C20-C19	-3.41	116.50	123.47
20	Y	104	CDL	OB6-CB5-C51	3.40	120.29	110.80
13	M	401	BCL	C1D-ND-C4D	-3.40	103.92	106.33
12	M	410	PGV	O01-C1-C2	3.40	118.83	111.50
22	H	304	LMT	C1B-O5B-C5B	3.40	120.36	113.69
13	O	101	BCL	C1D-ND-C4D	-3.39	103.92	106.33
13	F	101	BCL	C1D-ND-C4D	-3.39	103.93	106.33
13	W	101	BCL	C1D-ND-C4D	-3.38	103.93	106.33
19	Z	101	CRT	C10-C9-C7	-3.38	122.49	127.31
13	D	103	BCL	C4A-NA-C1A	3.38	108.22	106.71
12	D	106	PGV	O01-C1-C2	3.38	118.78	111.50
13	9	103	BCL	C1D-ND-C4D	-3.38	103.94	106.33
13	1	101	BCL	C1D-ND-C4D	-3.37	103.94	106.33
20	D	104	CDL	OA8-CA7-C31	3.36	120.19	111.38
13	M	401	BCL	CHA-C1A-NA	-3.36	118.71	126.40
13	7	103	BCL	C1D-ND-C4D	-3.36	103.95	106.33
13	U	103	BCL	C4A-NA-C1A	3.35	108.21	106.71
13	D	103	BCL	C1D-ND-C4D	-3.35	103.95	106.33
19	M	405	CRT	C20-C19-C17	-3.35	122.53	127.31
13	9	103	BCL	C4A-NA-C1A	3.34	108.21	106.71
8	C	501	HEC	CAB-C3B-C2B	3.34	133.24	127.53
13	A	101	BCL	C1D-ND-C4D	-3.34	103.97	106.33
13	Q	101	BCL	C4A-NA-C1A	3.33	108.20	106.71
20	M	412	CDL	OA6-CA5-C11	3.33	120.08	110.80
19	O	103	CRT	C21-C20-C19	-3.32	116.67	123.47
21	W	105	PEF	O3P-P-O2P	3.31	118.61	107.97
13	9	101	BCL	C1D-ND-C4D	-3.30	103.99	106.33
13	1	101	BCL	C4A-NA-C1A	3.30	108.19	106.71
8	C	503	HEC	C1D-ND-C4D	3.28	108.46	105.07
13	Y	101	BCL	CAB-C3B-C2B	3.28	133.25	128.34
20	D	104	CDL	OB8-CB7-C71	3.28	119.98	111.38
13	W	101	BCL	C4A-NA-C1A	3.28	108.18	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	V	101	CRT	C20-C19-C17	-3.28	122.63	127.31
13	4	102	BCL	C1D-ND-C4D	-3.28	104.01	106.33
8	C	501	HEC	CHD-C4C-NC	3.28	129.88	123.85
8	C	503	HEC	CAB-C3B-C4B	-3.28	120.56	124.81
13	J	102	BCL	CHA-C1A-NA	-3.27	118.91	126.40
13	I	101	BCL	C4A-NA-C1A	3.27	108.17	106.71
14	L	303	BPH	C4A-C3A-C2A	-3.26	99.74	102.84
15	L	309	UQ8	C35-C34-C36	3.26	120.75	115.27
13	L	301	BCL	CAB-C3B-C2B	3.25	133.20	128.34
19	4	101	CRT	C20-C19-C17	-3.24	122.68	127.31
20	O	104	CDL	OB8-CB7-C71	3.24	122.07	111.91
20	Y	104	CDL	OA2-PA1-OA3	-3.23	96.45	109.07
20	M	406	CDL	OA8-CA7-C31	3.23	122.03	111.91
19	T	101	CRT	C5-C6-C7	-3.23	121.02	125.89
13	Y	103	BCL	C1D-ND-C4D	-3.22	104.05	106.33
13	D	101	BCL	C1-O2A-CGA	3.21	124.88	116.44
13	A	103	BCL	C1D-ND-C4D	-3.21	104.05	106.33
13	7	103	BCL	CHA-C1A-NA	-3.21	119.04	126.40
13	L	302	BCL	C1D-ND-C4D	-3.20	104.06	106.33
8	C	502	HEC	C4C-NC-C1C	3.20	108.48	105.35
13	5	101	BCL	C1-C2-C3	-3.20	120.52	126.04
13	K	103	BCL	CHA-C1A-NA	-3.19	119.08	126.40
12	9	104	PGV	O03-C19-C20	3.19	121.92	111.91
13	U	103	BCL	CHA-C1A-NA	-3.19	119.09	126.40
13	4	102	BCL	CHA-C1A-NA	-3.19	119.09	126.40
19	J	101	CRT	C10-C9-C7	-3.19	122.76	127.31
13	3	101	BCL	CHA-C1A-NA	-3.19	119.10	126.40
14	M	402	BPH	CMC-C2C-C3C	3.18	126.79	113.99
13	5	103	BCL	CHA-C1A-NA	-3.18	119.12	126.40
13	P	102	BCL	C1-O2A-CGA	3.18	124.78	116.44
8	C	501	HEC	C1C-CHC-C4B	-3.17	118.82	126.34
14	M	402	BPH	CBA-CAA-C2A	-3.17	104.55	113.81
13	Y	103	BCL	CHA-C1A-NA	-3.17	119.15	126.40
13	F	103	BCL	CHA-C1A-NA	-3.15	119.17	126.40
12	M	411	PGV	C02-O01-C1	-3.15	110.05	117.79
20	D	104	CDL	OB6-CB5-C51	3.14	119.57	110.80
13	J	102	BCL	C2A-C1A-CHA	3.14	129.35	123.86
13	D	101	BCL	CHA-C1A-NA	-3.14	119.20	126.40
8	C	502	HEC	CHB-C1B-C2B	-3.14	120.07	124.98
20	O	104	CDL	OA8-CA7-C31	3.14	121.76	111.91
19	P	101	CRT	C32-C31-C30	-3.13	113.46	123.22
20	Y	104	CDL	OA8-CA7-C31	3.13	119.58	111.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	504	HEC	C1D-ND-C4D	3.12	108.30	105.07
8	C	504	HEC	CAB-C3B-C4B	-3.12	120.76	124.81
13	J	102	BCL	C1D-ND-C4D	-3.12	104.12	106.33
15	L	309	UQ8	C12-C13-C14	-3.11	120.17	127.66
13	2	102	BCL	CAB-C3B-C2B	3.11	132.99	128.34
19	N	101	CRT	C32-C31-C30	-3.11	113.52	123.22
14	L	303	BPH	CMC-C2C-C3C	3.10	126.49	113.99
13	Y	103	BCL	O2A-CGA-O1A	-3.09	115.79	123.59
18	M	404	MQ8	C29-C28-C30	3.09	120.47	115.27
13	A	103	BCL	CHA-C1A-NA	-3.09	119.33	126.40
13	S	103	BCL	CHA-C1A-NA	-3.08	119.35	126.40
13	Q	103	BCL	CHA-C1A-NA	-3.08	119.36	126.40
13	W	101	BCL	C17-C16-C15	3.07	127.36	113.24
8	C	501	HEC	CHA-C4D-ND	3.07	127.76	124.42
19	A	104	CRT	C36-C35-C33	-3.06	121.26	125.89
15	L	309	UQ8	C15-C14-C16	3.06	120.42	115.27
13	P	102	BCL	CHA-C1A-NA	-3.06	119.40	126.40
19	G	101	CRT	C26-C27-C28	-3.05	122.95	127.31
15	L	310	UQ8	C12-C13-C14	-3.05	120.31	127.66
13	D	103	BCL	CHA-C1A-NA	-3.05	119.42	126.40
13	D	103	BCL	CAB-C3B-C2B	3.04	132.89	128.34
19	B	101	CRT	C10-C9-C7	-3.03	122.99	127.31
13	U	103	BCL	C2A-C1A-CHA	3.03	129.15	123.86
19	J	101	CRT	C5-C6-C7	-3.03	121.32	125.89
19	4	101	CRT	C26-C27-C28	-3.02	122.99	127.31
13	I	101	BCL	CAB-C3B-C2B	3.02	132.87	128.34
13	7	103	BCL	C2A-C1A-CHA	3.02	129.13	123.86
15	L	304	UQ8	C10-C9-C11	3.02	120.34	115.27
18	M	404	MQ8	C45-C43-C44	3.01	120.33	115.27
13	9	103	BCL	CHA-C1A-NA	-3.01	119.51	126.40
13	U	101	BCL	CAB-C3B-C2B	3.00	132.84	128.34
8	C	504	HEC	CBC-CAC-C3C	3.00	120.70	112.43
20	S	104	CDL	CB6-CB4-CB3	3.00	118.87	111.79
19	M	405	CRT	C10-C9-C7	-2.99	123.04	127.31
13	W	104	BCL	CHA-C1A-NA	-2.99	119.55	126.40
8	C	502	HEC	CBB-CAB-C3B	2.99	120.67	112.43
8	C	502	HEC	CAB-C3B-C2B	2.99	132.64	127.53
19	4	101	CRT	C5-C6-C7	-2.99	121.38	125.89
13	2	102	BCL	CHA-C1A-NA	-2.99	119.56	126.40
14	M	402	BPH	CBC-CAC-C3C	-2.99	107.75	113.77
13	L	301	BCL	C4A-NA-C1A	2.99	108.05	106.71
13	4	102	BCL	C2A-C1A-CHA	2.98	129.07	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Y	103	BCL	CAB-C3B-C2B	2.98	132.81	128.34
13	S	101	BCL	C1-C2-C3	-2.97	120.90	126.04
13	F	101	BCL	O2A-CGA-O1A	-2.97	116.09	123.59
13	5	103	BCL	C17-C16-C15	2.96	126.83	113.24
13	S	101	BCL	CHA-C1A-NA	-2.96	119.62	126.40
20	Y	104	CDL	OA6-CA4-CA3	2.96	119.11	108.40
20	S	104	CDL	OA8-CA7-C31	2.95	121.17	111.91
19	4	101	CRT	C32-C31-C30	-2.95	114.02	123.22
19	N	101	CRT	C29-C28-C30	2.95	122.72	118.08
13	4	102	BCL	CAB-C3B-C2B	2.94	132.75	128.34
13	9	101	BCL	CHC-C4B-NB	-2.93	121.15	124.26
19	8	101	CRT	C21-C20-C19	-2.93	117.47	123.47
19	3	103	CRT	C21-C20-C19	-2.93	117.48	123.47
15	L	310	UQ8	O5-C5-C6	-2.93	116.42	121.55
20	Y	104	CDL	PA1-OA2-CA2	2.92	138.82	121.68
13	Q	103	BCL	C16-C15-C13	2.92	125.37	115.92
8	C	501	HEC	CAD-CBD-CGD	2.92	119.89	113.60
13	L	301	BCL	CHA-C1A-NA	-2.92	119.71	126.40
15	L	309	UQ8	C1M-C1-C6	-2.92	119.64	124.40
13	W	101	BCL	CAB-C3B-C2B	2.92	132.71	128.34
13	Y	103	BCL	C2A-C1A-CHA	2.91	128.95	123.86
8	C	503	HEC	CBC-CAC-C3C	2.91	120.45	112.43
13	Q	101	BCL	C17-C16-C15	-2.91	99.88	113.24
21	1	103	PEF	O4P-P-O3P	2.91	117.30	107.97
19	P	101	CRT	C21-C20-C19	-2.90	117.54	123.47
8	C	501	HEC	CBC-CAC-C3C	2.89	120.41	112.43
13	Q	103	BCL	O2A-C1-C2	-2.89	101.03	108.64
19	Z	101	CRT	C32-C31-C30	-2.89	114.20	123.22
13	D	101	BCL	CAB-C3B-C2B	2.89	132.67	128.34
13	9	101	BCL	CAB-C3B-C2B	2.88	132.66	128.34
19	8	101	CRT	C10-C9-C7	-2.88	123.20	127.31
13	Q	101	BCL	CHC-C4B-NB	-2.88	121.21	124.26
20	Y	104	CDL	O1-C1-CA2	2.88	119.64	109.56
15	L	310	UQ8	C1M-C1-C6	-2.87	119.71	124.40
13	O	101	BCL	CAB-C3B-C2B	2.87	132.64	128.34
13	5	101	BCL	CHC-C4B-NB	-2.87	121.22	124.26
20	D	105	CDL	OB8-CB7-C71	2.87	120.91	111.91
13	A	101	BCL	CHA-C1A-NA	-2.87	119.83	126.40
13	K	103	BCL	C2A-C1A-CHA	2.87	128.87	123.86
13	I	101	BCL	CHA-C1A-NA	-2.86	119.84	126.40
8	C	502	HEC	CHA-C4D-C3D	-2.86	120.63	124.84
13	1	101	BCL	CAB-C3B-C2B	2.86	132.62	128.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	504	HEC	CHB-C1B-C2B	-2.86	120.52	124.98
13	S	101	BCL	C4A-NA-C1A	2.85	107.99	106.71
13	7	101	BCL	CHC-C4B-NB	-2.85	121.24	124.26
19	B	101	CRT	C32-C31-C30	-2.85	114.33	123.22
13	K	101	BCL	CAB-C3B-C2B	2.85	132.60	128.34
15	L	309	UQ8	C37-C38-C39	-2.84	120.81	127.66
19	W	102	CRT	C21-C20-C19	-2.84	117.65	123.47
13	P	102	BCL	C2A-C1A-CHA	2.84	128.83	123.86
8	C	501	HEC	C4C-CHD-C1D	-2.84	119.60	126.34
13	O	101	BCL	C1-C2-C3	-2.84	121.13	126.04
13	K	103	BCL	CHC-C4B-NB	-2.84	121.25	124.26
13	F	101	BCL	O2A-CGA-CBA	2.84	120.81	111.91
13	Q	103	BCL	C2A-C1A-CHA	2.83	128.81	123.86
8	C	504	HEC	CHA-C1A-NA	2.83	127.50	124.44
20	Y	104	CDL	OA6-CA5-OA7	-2.83	116.87	123.70
8	C	501	HEC	CHA-C1A-C2A	2.82	129.51	124.94
13	W	101	BCL	C1-C2-C3	-2.82	121.17	126.04
13	Y	101	BCL	CHA-C1A-NA	-2.82	119.94	126.40
13	W	104	BCL	CAB-C3B-C2B	2.82	132.56	128.34
19	J	101	CRT	C21-C22-C23	-2.81	123.30	127.31
12	L	307	PGV	C02-O01-C1	-2.81	110.87	117.79
19	T	101	CRT	C8-C7-C9	-2.81	118.99	122.92
13	9	103	BCL	C1-C2-C3	-2.80	121.19	126.04
20	U	104	CDL	OB8-CB7-C71	2.80	120.70	111.91
13	Q	101	BCL	CHA-C1A-NA	-2.80	119.98	126.40
13	A	103	BCL	C2A-C1A-CHA	2.80	128.76	123.86
13	3	101	BCL	C4A-NA-C1A	2.80	107.96	106.71
19	M	405	CRT	C31-C32-C33	-2.80	123.32	127.31
13	1	101	BCL	CHA-C1A-NA	-2.79	120.01	126.40
20	M	412	CDL	CA4-OA6-CA5	-2.79	110.92	117.79
13	L	302	BCL	CHA-C1A-NA	-2.79	120.02	126.40
18	M	404	MQ8	C24-C23-C25	2.78	119.95	115.27
13	7	101	BCL	CAB-C3B-C2B	2.78	132.51	128.34
20	Y	104	CDL	OA5-PA1-OA3	2.78	119.92	109.07
13	L	302	BCL	CAB-C3B-C2B	2.78	132.50	128.34
13	9	101	BCL	CHA-C1A-NA	-2.78	120.04	126.40
13	5	101	BCL	C4-C3-C5	-2.77	110.61	115.27
13	S	103	BCL	C2A-C1A-CHA	2.77	128.71	123.86
13	3	101	BCL	CHC-C4B-NB	-2.77	121.32	124.26
19	M	405	CRT	C14-C15-C16	-2.77	114.57	123.22
13	F	101	BCL	CHC-C4B-NB	-2.77	121.33	124.26
15	L	310	UQ8	C15-C14-C16	2.77	119.93	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	U	101	BCL	CHA-C1A-NA	-2.77	120.06	126.40
12	L	308	PGV	O03-C19-C20	2.77	120.59	111.91
20	M	412	CDL	CB3-CB4-CB6	-2.77	105.33	111.80
13	F	101	BCL	C11-C10-C8	-2.76	106.98	115.92
15	L	310	UQ8	C10-C9-C11	2.76	119.92	115.27
13	F	103	BCL	C2A-C1A-CHA	2.76	128.68	123.86
13	F	103	BCL	CAB-C3B-C2B	2.75	132.46	128.34
13	W	101	BCL	CHC-C4B-NB	-2.75	121.34	124.26
18	M	404	MQ8	C41-C42-C43	-2.75	121.04	127.66
13	7	101	BCL	CHA-C1A-NA	-2.74	120.11	126.40
13	O	101	BCL	C1-O2A-CGA	2.74	123.64	116.44
8	C	504	HEC	CHD-C4C-NC	2.74	128.88	123.85
13	W	104	BCL	C2A-C1A-CHA	2.74	128.64	123.86
15	L	310	UQ8	C20-C19-C21	2.73	119.87	115.27
20	H	305	CDL	OA8-CA7-C31	2.73	120.48	111.91
22	H	304	LMT	C1'-C2'-C3'	2.73	115.68	110.00
13	F	101	BCL	CHA-C1A-NA	-2.73	120.14	126.40
15	L	309	UQ8	C30-C29-C31	2.73	119.86	115.27
13	L	305	BCL	CHA-C1A-NA	-2.73	120.15	126.40
12	L	307	PGV	O03-C19-C20	2.73	120.47	111.91
13	Y	103	BCL	O2A-CGA-CBA	2.73	120.47	111.91
19	G	101	CRT	C20-C19-C17	-2.72	123.42	127.31
12	H	303	PGV	C02-O01-C1	-2.72	111.08	117.79
20	U	104	CDL	OA8-CA7-C31	2.72	120.44	111.91
19	3	103	CRT	C14-C15-C16	-2.71	114.75	123.22
19	2	101	CRT	C5-C6-C7	-2.71	121.80	125.89
19	Z	101	CRT	C21-C20-C19	-2.71	117.92	123.47
13	D	103	BCL	C1-O2A-CGA	2.71	123.56	116.44
13	J	102	BCL	CAB-C3B-C2B	2.71	132.40	128.34
15	L	309	UQ8	C10-C9-C11	2.71	119.83	115.27
19	Z	101	CRT	C14-C15-C16	-2.71	114.77	123.22
13	L	305	BCL	C11-C12-C13	-2.71	107.17	115.92
19	B	101	CRT	C21-C20-C19	-2.70	117.93	123.47
13	I	101	BCL	CHC-C4B-NB	-2.70	121.40	124.26
13	I	101	BCL	C11-C10-C8	-2.70	107.19	115.92
8	C	504	HEC	CAA-CBA-CGA	-2.70	107.80	113.60
13	K	101	BCL	CHA-C1A-NA	-2.70	120.22	126.40
8	C	504	HEC	CBB-CAB-C3B	2.70	119.86	112.43
19	T	101	CRT	C14-C15-C16	-2.70	114.81	123.22
15	L	304	UQ8	C1M-C1-C6	-2.70	120.00	124.40
13	L	301	BCL	C2A-C1A-CHA	2.69	128.57	123.86
13	D	101	BCL	CHC-C4B-NB	-2.69	121.41	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	W	101	BCL	CHA-C1A-NA	-2.69	120.23	126.40
13	S	103	BCL	C6-C5-C3	2.69	120.50	113.45
13	U	103	BCL	C16-C15-C13	-2.68	107.25	115.92
13	A	101	BCL	CHC-C4B-NB	-2.68	121.42	124.26
19	A	104	CRT	C21-C20-C19	-2.68	117.98	123.47
13	1	101	BCL	CHC-C4B-NB	-2.68	121.42	124.26
13	M	401	BCL	CHC-C4B-NB	-2.67	121.43	124.26
13	A	103	BCL	CAB-C3B-C2B	2.67	132.34	128.34
13	O	101	BCL	CHA-C1A-NA	-2.67	120.28	126.40
15	L	309	UQ8	C22-C23-C24	-2.67	121.23	127.66
13	5	101	BCL	CHA-C1A-NA	-2.67	120.28	126.40
12	L	308	PGV	C02-O01-C1	-2.67	111.22	117.79
13	J	102	BCL	CHC-C4B-NB	-2.67	121.43	124.26
19	A	104	CRT	C14-C15-C16	-2.67	114.90	123.22
8	C	502	HEC	C2A-C1A-NA	-2.66	107.73	110.32
15	L	309	UQ8	C20-C19-C21	2.66	119.74	115.27
13	P	102	BCL	CAA-CBA-CGA	-2.66	105.49	113.25
8	C	502	HEC	CHD-C1D-ND	2.65	127.65	124.37
19	W	102	CRT	C10-C9-C7	-2.65	123.52	127.31
20	U	104	CDL	CB2-C1-CA2	2.65	120.59	112.79
13	A	101	BCL	CAB-C3B-C2B	2.65	132.31	128.34
19	J	101	CRT	C8-C7-C9	-2.65	119.22	122.92
19	P	101	CRT	C29-C28-C30	2.65	122.25	118.08
19	3	103	CRT	C5-C6-C7	-2.65	121.89	125.89
19	V	101	CRT	C14-C15-C16	-2.64	114.96	123.22
13	U	103	BCL	C17-C16-C15	-2.64	101.11	113.24
13	P	102	BCL	CHC-C4B-NB	-2.64	121.47	124.26
13	K	101	BCL	CHC-C4B-NB	-2.64	121.47	124.26
19	0	101	CRT	C10-C9-C7	-2.64	123.55	127.31
13	F	101	BCL	CAB-C3B-C2B	2.63	132.28	128.34
19	2	101	CRT	C21-C20-C19	-2.63	118.09	123.47
13	O	101	BCL	CHC-C4B-NB	-2.63	121.48	124.26
8	C	501	HEC	CHC-C1C-C2C	-2.62	119.82	127.24
12	D	106	PGV	O03-C19-C20	2.62	120.13	111.91
13	L	302	BCL	C2A-C1A-CHA	2.62	128.44	123.86
13	5	101	BCL	CAB-C3B-C2B	2.61	132.25	128.34
13	K	103	BCL	C1-O2A-CGA	2.61	123.29	116.44
20	U	104	CDL	CA4-OA6-CA5	-2.61	111.37	117.79
13	5	103	BCL	C2A-C1A-CHA	2.61	128.42	123.86
20	O	104	CDL	CA4-OA6-CA5	-2.60	111.38	117.79
19	P	101	CRT	C10-C9-C7	-2.60	123.59	127.31
13	9	103	BCL	CHC-C4B-NB	-2.60	121.50	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	103	BCL	CHC-C4B-NB	-2.60	121.51	124.26
13	P	102	BCL	CAB-C3B-C2B	2.60	132.23	128.34
20	S	104	CDL	CB6-OB8-CB7	2.59	126.73	117.12
8	C	502	HEC	C1A-CHA-C4D	-2.59	120.47	126.06
15	L	309	UQ8	C17-C18-C19	-2.59	121.42	127.66
20	M	406	CDL	OB8-CB7-C71	2.59	120.03	111.91
19	3	103	CRT	C18-C17-C16	2.59	122.16	118.08
13	Q	101	BCL	CAB-C3B-C2B	2.58	132.21	128.34
15	L	311	UQ8	C10-C9-C11	2.58	120.31	114.60
14	M	402	BPH	C4-C3-C2	-2.58	117.05	123.68
15	L	304	UQ8	C16-C17-C18	-2.58	103.40	111.88
13	I	101	BCL	C4-C3-C5	-2.58	110.93	115.27
13	D	103	BCL	C1-C2-C3	-2.58	121.58	126.04
13	K	103	BCL	CAB-C3B-C2B	2.58	132.20	128.34
13	U	101	BCL	C4-C3-C5	-2.58	110.94	115.27
13	U	101	BCL	C16-C15-C13	2.57	124.24	115.92
19	2	101	CRT	C32-C31-C30	-2.57	115.19	123.22
19	N	101	CRT	C2-C1-C4	-2.57	106.91	110.86
20	M	406	CDL	OA8-CA7-OA9	-2.56	117.12	123.59
13	5	103	BCL	CAB-C3B-C2B	2.56	132.17	128.34
15	L	309	UQ8	C40-C39-C41	2.56	119.57	115.27
13	S	101	BCL	C4-C3-C5	-2.56	110.97	115.27
22	H	304	LMT	C4B-C3B-C2B	-2.56	106.36	110.82
18	M	404	MQ8	C34-C33-C35	2.55	119.56	115.27
13	7	103	BCL	CHC-C4B-NB	-2.54	121.56	124.26
19	V	101	CRT	C32-C31-C30	-2.54	115.28	123.22
13	9	103	BCL	C16-C15-C13	2.54	124.14	115.92
13	I	101	BCL	C1-C2-C3	-2.54	121.65	126.04
12	1	105	PGV	O03-C19-C20	2.54	119.87	111.91
12	H	303	PGV	O03-C19-C20	2.53	119.86	111.91
8	C	501	HEC	CAD-C3D-C4D	2.53	129.08	124.66
13	L	305	BCL	C2A-C1A-CHA	2.53	128.29	123.86
13	U	103	BCL	CAB-C3B-C2B	2.53	132.13	128.34
8	C	504	HEC	C3C-C4C-NC	-2.53	107.32	110.15
15	M	413	UQ8	C4M-O4-C4	2.53	125.42	116.47
13	L	305	BCL	C6-C7-C8	2.53	124.08	115.92
19	2	101	CRT	C35-C33-C32	-2.52	115.07	118.94
19	M	405	CRT	C5-C6-C7	-2.52	122.08	125.89
19	4	101	CRT	C34-C33-C35	2.52	122.04	118.08
13	4	102	BCL	CHC-C4B-NB	-2.52	121.59	124.26
13	S	101	BCL	CHC-C4B-NB	-2.52	121.59	124.26
13	D	103	BCL	C2A-C1A-CHA	2.51	128.26	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	502	HEC	CBC-CAC-C3C	2.51	119.36	112.43
13	S	103	BCL	CHC-C4B-NB	-2.51	121.60	124.26
19	B	101	CRT	C26-C27-C28	-2.51	123.73	127.31
20	Y	104	CDL	CA6-CA4-CA3	-2.51	105.86	111.79
19	G	101	CRT	C14-C15-C16	-2.51	115.40	123.22
13	U	101	BCL	CHC-C4B-NB	-2.50	121.61	124.26
20	U	104	CDL	PA1-OA5-CA3	-2.50	107.01	121.68
13	S	103	BCL	CMB-C2B-C1B	-2.50	121.56	125.37
15	L	304	UQ8	C21-C22-C23	-2.50	103.67	111.88
19	M	405	CRT	C24-C23-C22	-2.50	119.42	122.92
13	U	103	BCL	CHC-C4B-NB	-2.50	121.61	124.26
13	W	101	BCL	C1C-NC-C4C	2.50	107.83	106.71
13	Y	101	BCL	CHC-C4B-NB	-2.50	121.61	124.26
8	C	501	HEC	CHD-C4C-C3C	-2.50	119.91	125.36
13	9	103	BCL	C2A-C1A-CHA	2.50	128.22	123.86
13	F	103	BCL	CHC-C4B-NB	-2.49	121.62	124.26
19	B	101	CRT	C29-C28-C30	2.49	122.00	118.08
19	2	101	CRT	C34-C33-C35	2.49	122.00	118.08
19	T	101	CRT	C29-C28-C30	2.49	121.99	118.08
8	C	504	HEC	CHA-C4D-C3D	-2.48	121.19	124.84
13	S	101	BCL	CMB-C2B-C1B	-2.48	121.59	125.37
13	9	103	BCL	CAB-C3B-C2B	2.48	132.06	128.34
21	H	302	PEF	O4P-P-O1P	-2.48	101.81	110.89
19	T	101	CRT	C21-C20-C19	-2.48	118.39	123.47
13	9	103	BCL	CMB-C2B-C1B	-2.47	121.60	125.37
8	C	502	HEC	CHB-C4A-NA	2.47	127.11	124.44
13	L	302	BCL	CHC-C4B-NB	-2.47	121.64	124.26
19	G	101	CRT	C32-C31-C30	-2.47	115.51	123.22
19	B	101	CRT	C5-C6-C7	-2.47	122.16	125.89
13	M	401	BCL	CMB-C2B-C1B	-2.47	121.61	125.37
8	C	501	HEC	CHC-C1C-NC	2.47	128.39	123.85
19	W	102	CRT	C20-C19-C17	-2.47	123.79	127.31
13	K	103	BCL	CMB-C2B-C1B	-2.46	121.62	125.37
13	S	103	BCL	CAB-C3B-C2B	2.46	132.03	128.34
13	5	101	BCL	C5-C3-C2	2.46	126.10	121.12
19	N	101	CRT	C8-C7-C9	-2.46	119.48	122.92
14	L	303	BPH	CED-O2D-CGD	2.46	121.49	115.94
21	M	408	PEF	O2P-P-O1P	2.45	119.88	110.89
8	C	503	HEC	C3C-C4C-NC	-2.45	107.40	110.15
19	O	103	CRT	C32-C31-C30	-2.45	115.58	123.22
13	2	102	BCL	CHC-C4B-NB	-2.45	121.67	124.26
8	C	502	HEC	C4A-NA-C1A	2.44	107.74	105.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	0	101	CRT	C36-C35-C33	-2.44	122.20	125.89
13	D	103	BCL	CHC-C4B-NB	-2.44	121.67	124.26
19	A	104	CRT	C32-C31-C30	-2.44	115.59	123.22
13	K	101	BCL	C11-C12-C13	-2.44	108.02	115.92
14	L	303	BPH	CBA-CAA-C2A	-2.44	106.67	113.81
19	A	104	CRT	C20-C19-C17	-2.44	123.82	127.31
22	H	304	LMT	O1B-C4'-C3'	2.44	113.78	107.28
19	3	103	CRT	C20-C19-C17	-2.44	123.83	127.31
20	H	305	CDL	CB4-OB6-CB5	-2.44	111.79	117.79
8	C	501	HEC	CAC-C3C-C4C	2.44	128.30	124.92
13	3	101	BCL	CAB-C3B-C2B	2.43	131.98	128.34
13	5	103	BCL	CHC-C4B-NB	-2.43	121.68	124.26
22	H	304	LMT	O5'-C1'-C2'	2.43	115.49	110.35
15	L	309	UQ8	C25-C24-C26	2.43	119.36	115.27
15	L	310	UQ8	O4-C4-C5	2.43	124.77	116.56
13	9	101	BCL	C2A-C1A-CHA	2.42	128.10	123.86
13	M	401	BCL	C4B-C3B-C2B	-2.42	104.46	108.36
22	H	304	LMT	O5B-C5B-C4B	2.42	114.09	109.69
19	4	101	CRT	C14-C15-C16	-2.42	115.67	123.22
19	N	101	CRT	C34-C33-C35	2.42	121.88	118.08
13	W	101	BCL	C4B-C3B-C2B	-2.41	104.48	108.36
19	Z	101	CRT	C26-C27-C28	-2.41	123.87	127.31
15	L	309	UQ8	C3M-O3-C3	2.41	125.01	116.47
19	V	101	CRT	C26-C27-C28	-2.41	123.87	127.31
13	J	102	BCL	O2A-CGA-O1A	-2.41	117.52	123.59
13	Q	101	BCL	CBA-CAA-C2A	-2.41	106.76	113.86
13	U	103	BCL	CMB-C2B-C1B	-2.41	121.70	125.37
13	D	101	BCL	C4B-C3B-C2B	-2.41	104.49	108.36
13	7	103	BCL	CAB-C3B-C2B	2.40	131.94	128.34
13	S	103	BCL	C4B-C3B-C2B	-2.40	104.49	108.36
13	Q	101	BCL	C4-C3-C5	-2.40	111.24	115.27
13	9	103	BCL	C4B-C3B-C2B	-2.40	104.50	108.36
13	A	101	BCL	C2A-C1A-CHA	2.40	128.05	123.86
15	M	413	UQ8	C10-C9-C11	2.40	119.90	114.60
13	5	101	BCL	C4B-C3B-C2B	-2.39	104.51	108.36
19	W	102	CRT	C32-C31-C30	-2.39	115.75	123.22
13	U	103	BCL	C2D-C1D-ND	2.39	111.87	110.10
13	Q	101	BCL	C4B-C3B-C2B	-2.39	104.51	108.36
13	A	103	BCL	C4B-C3B-C2B	-2.39	104.51	108.36
19	Z	101	CRT	C18-C17-C16	2.39	121.85	118.08
13	D	101	BCL	C2A-C1A-CHA	2.39	128.04	123.86
13	W	104	BCL	CHC-C4B-NB	-2.39	121.73	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	7	101	BCL	CBA-CAA-C2A	-2.39	106.81	113.86
13	K	103	BCL	C4B-C3B-C2B	-2.39	104.52	108.36
13	5	101	BCL	CMB-C2B-C1B	-2.39	121.73	125.37
15	L	310	UQ8	C22-C23-C24	-2.39	119.59	127.75
18	M	404	MQ8	C50-C48-C49	2.39	119.87	114.60
19	T	101	CRT	C32-C31-C30	-2.39	115.77	123.22
19	8	101	CRT	C32-C31-C30	-2.39	115.77	123.22
13	3	101	BCL	C4B-C3B-C2B	-2.38	104.52	108.36
20	D	104	CDL	CA4-OA6-CA5	-2.38	111.93	117.79
19	V	101	CRT	C9-C10-C11	-2.38	115.79	123.22
19	T	101	CRT	C1-C4-C5	2.38	119.36	113.06
13	W	101	BCL	OBb-CAB-CBB	-2.38	114.46	119.73
13	P	102	BCL	C4B-C3B-C2B	-2.38	104.53	108.36
14	M	402	BPH	C4D-CHA-CBD	-2.38	107.44	108.52
15	L	309	UQ8	C46-C44-C45	2.38	119.85	114.60
13	K	101	BCL	C4B-C3B-C2B	-2.38	104.54	108.36
19	T	101	CRT	C13-C12-C11	2.38	121.82	118.08
19	N	101	CRT	C30-C28-C27	-2.38	115.30	118.94
13	5	101	BCL	C11-C12-C13	-2.38	108.24	115.92
19	2	101	CRT	C20-C19-C17	-2.38	123.92	127.31
13	M	401	BCL	CAB-C3B-C2B	2.37	131.89	128.34
15	L	304	UQ8	C25-C24-C26	2.37	119.84	114.60
13	D	101	BCL	C11-C10-C8	-2.37	108.25	115.92
13	9	101	BCL	C4B-C3B-C2B	-2.37	104.55	108.36
18	M	404	MQ8	C26-C27-C28	-2.37	121.95	127.66
12	M	410	PGV	O14-P-O13	2.37	119.96	110.68
8	C	503	HEC	CHB-C1B-C2B	-2.37	121.28	124.98
13	Y	101	BCL	C4B-C3B-C2B	-2.37	104.55	108.36
19	W	102	CRT	C9-C10-C11	-2.37	115.83	123.22
19	V	101	CRT	C21-C20-C19	-2.37	118.63	123.47
19	O	103	CRT	C34-C33-C35	2.36	121.80	118.08
19	N	101	CRT	C20-C19-C17	-2.36	123.94	127.31
13	D	101	BCL	CMB-C2B-C1B	-2.36	121.77	125.37
19	3	103	CRT	C32-C31-C30	-2.36	115.85	123.22
12	M	410	PGV	O03-C19-C20	2.36	119.31	111.91
20	S	104	CDL	OB6-CB5-OB7	-2.36	118.00	123.70
13	S	101	BCL	C4B-C3B-C2B	-2.36	104.57	108.36
13	A	101	BCL	C4B-C3B-C2B	-2.35	104.57	108.36
13	Q	101	BCL	C2A-C1A-CHA	2.35	127.97	123.86
8	C	501	HEC	CBB-CAB-C3B	2.35	118.92	112.43
13	Y	103	BCL	CHC-C4B-NB	-2.35	121.77	124.26
13	7	103	BCL	C4B-C3B-C2B	-2.35	104.58	108.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	J	101	CRT	C18-C17-C16	2.35	121.78	118.08
13	Q	103	BCL	CHC-C4B-NB	-2.35	121.77	124.26
13	2	102	BCL	C2A-C1A-CHA	2.35	127.97	123.86
13	2	102	BCL	C4B-C3B-C2B	-2.35	104.58	108.36
13	A	101	BCL	C1C-NC-C4C	2.35	107.76	106.71
13	Q	101	BCL	CMB-C2B-C1B	-2.35	121.80	125.37
13	U	103	BCL	C4B-C3B-C2B	-2.35	104.59	108.36
15	L	310	UQ8	C4M-O4-C4	2.34	124.78	116.47
13	4	102	BCL	C4B-C3B-C2B	-2.34	104.59	108.36
13	U	101	BCL	OBB-CAB-CBB	-2.34	114.54	119.73
13	7	101	BCL	C4B-C3B-C2B	-2.34	104.59	108.36
13	3	101	BCL	C11-C10-C8	-2.34	108.35	115.92
19	4	101	CRT	C21-C20-C19	-2.34	118.67	123.47
19	3	103	CRT	C27-C26-C25	-2.34	115.91	123.22
19	N	101	CRT	C27-C26-C25	-2.34	115.92	123.22
13	4	102	BCL	CMB-C2B-C1B	-2.34	121.81	125.37
13	Y	103	BCL	CMB-C2B-C1B	-2.34	121.81	125.37
13	J	102	BCL	C4B-C3B-C2B	-2.34	104.60	108.36
19	8	101	CRT	C29-C28-C30	2.34	121.76	118.08
19	M	405	CRT	C13-C12-C11	2.33	121.75	118.08
13	I	101	BCL	C4B-C3B-C2B	-2.33	104.61	108.36
13	L	301	BCL	CHC-C4B-NB	-2.33	121.79	124.26
13	O	101	BCL	C4B-C3B-C2B	-2.33	104.61	108.36
13	F	101	BCL	C4B-C3B-C2B	-2.33	104.61	108.36
21	M	409	PEF	O4P-P-O1P	-2.33	102.38	110.89
14	M	402	BPH	C4-C3-C5	2.32	119.18	115.27
13	Q	103	BCL	C1-C2-C3	-2.32	122.03	126.04
13	P	102	BCL	CMB-C2B-C1B	-2.32	121.83	125.37
13	3	101	BCL	CMB-C2B-C1B	-2.32	121.83	125.37
19	Z	101	CRT	C29-C28-C30	2.32	121.73	118.08
13	M	401	BCL	OBB-CAB-CBB	-2.32	114.59	119.73
19	N	101	CRT	C18-C17-C16	2.32	121.73	118.08
13	Y	103	BCL	C4B-C3B-C2B	-2.32	104.63	108.36
19	J	101	CRT	C13-C12-C11	2.32	121.73	118.08
13	L	301	BCL	OBB-CAB-CBB	-2.32	114.60	119.73
19	8	101	CRT	C18-C17-C16	2.32	121.73	118.08
13	U	103	BCL	C19-C18-C17	-2.32	97.23	111.54
19	W	102	CRT	C14-C15-C16	-2.31	116.00	123.22
13	Y	101	BCL	OBB-CAB-CBB	-2.31	114.60	119.73
13	D	103	BCL	C4B-C3B-C2B	-2.31	104.64	108.36
19	G	101	CRT	C9-C10-C11	-2.31	116.00	123.22
13	A	103	BCL	CMB-C2B-C1B	-2.31	121.85	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	5	103	BCL	CMB-C2B-C1B	-2.31	121.85	125.37
13	M	401	BCL	C4D-C3D-CAD	-2.31	105.37	108.10
13	L	305	BCL	C4A-NA-C1A	2.31	107.75	106.71
13	Q	103	BCL	C2D-C1D-ND	2.31	111.81	110.10
13	9	101	BCL	OBB-CAB-CBB	-2.31	114.61	119.73
13	U	101	BCL	C4B-C3B-C2B	-2.31	104.64	108.36
13	J	102	BCL	CMB-C2B-C1B	-2.31	121.85	125.37
19	J	101	CRT	C14-C15-C16	-2.31	116.01	123.22
13	7	103	BCL	CMB-C2B-C1B	-2.31	121.85	125.37
13	Q	103	BCL	CMB-C2B-C1B	-2.31	121.86	125.37
19	M	405	CRT	C18-C17-C16	2.31	121.71	118.08
13	1	101	BCL	C4B-C3B-C2B	-2.31	104.65	108.36
19	G	101	CRT	C29-C28-C30	2.30	121.71	118.08
15	L	309	UQ8	C8-C7-C6	-2.30	105.84	112.05
13	K	101	BCL	C4-C3-C5	-2.30	111.40	115.27
13	K	101	BCL	OBB-CAB-CBB	-2.30	114.63	119.73
18	M	404	MQ8	C39-C38-C40	2.30	119.14	115.27
19	A	104	CRT	C8-C7-C9	-2.30	119.70	122.92
13	L	302	BCL	C4B-C3B-C2B	-2.30	104.66	108.36
8	C	504	HEC	CAB-C3B-C2B	2.30	131.46	127.53
13	A	101	BCL	C6-C5-C3	2.30	119.48	113.45
13	W	104	BCL	C4B-C3B-C2B	-2.30	104.67	108.36
13	S	101	BCL	CAB-C3B-C2B	2.29	131.78	128.34
13	2	102	BCL	OBB-CAB-CBB	-2.29	114.66	119.73
19	3	103	CRT	C31-C32-C33	-2.29	124.04	127.31
19	J	101	CRT	C32-C31-C30	-2.29	116.08	123.22
13	4	102	BCL	OBB-CAB-CBB	-2.29	114.66	119.73
19	0	101	CRT	C21-C20-C19	-2.29	118.79	123.47
13	F	103	BCL	C4B-C3B-C2B	-2.28	104.68	108.36
13	S	103	BCL	OBB-CAB-CBB	-2.28	114.67	119.73
13	A	101	BCL	OBB-CAB-CBB	-2.28	114.67	119.73
14	M	402	BPH	O2D-CGD-O1D	-2.28	119.38	123.84
13	Q	103	BCL	C4B-C3B-C2B	-2.28	104.69	108.36
13	3	101	BCL	OBB-CAB-CBB	-2.28	114.68	119.73
13	9	103	BCL	OBB-CAB-CBB	-2.28	114.69	119.73
20	H	305	CDL	OB8-CB7-C71	2.28	119.05	111.91
13	L	301	BCL	C4B-C3B-C2B	-2.28	104.70	108.36
19	W	102	CRT	C13-C12-C11	2.27	121.66	118.08
13	3	101	BCL	C16-C15-C13	2.27	123.27	115.92
13	A	101	BCL	CMB-C2B-C1B	-2.27	121.91	125.37
13	D	103	BCL	OBB-CAB-CBB	-2.27	114.69	119.73
13	D	101	BCL	OBB-CAB-CBB	-2.27	114.69	119.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	103	CRT	C8-C7-C9	-2.27	119.74	122.92
13	I	101	BCL	C2A-C1A-CHA	2.27	127.83	123.86
8	C	503	HEC	CAB-C3B-C2B	2.27	131.41	127.53
13	K	101	BCL	CMB-C2B-C1B	-2.27	121.92	125.37
15	L	310	UQ8	C25-C24-C26	2.27	119.61	114.60
19	8	101	CRT	C20-C19-C17	-2.26	124.08	127.31
13	5	103	BCL	C4B-C3B-C2B	-2.26	104.72	108.36
21	W	106	PEF	O3P-P-O1P	-2.26	102.62	110.89
13	F	101	BCL	OBB-CAB-CBB	-2.26	114.72	119.73
13	Y	103	BCL	OBB-CAB-CBB	-2.26	114.72	119.73
19	A	104	CRT	C29-C28-C30	2.26	121.64	118.08
12	C	508	PGV	O03-C19-C20	2.26	119.00	111.91
13	L	302	BCL	OBB-CAB-CBB	-2.26	114.73	119.73
22	H	304	LMT	O5'-C5'-C6'	2.25	112.04	106.44
13	L	302	BCL	CMB-C2B-C1B	-2.25	121.94	125.37
13	O	101	BCL	CMB-C2B-C1B	-2.25	121.94	125.37
13	Q	101	BCL	OBB-CAB-CBB	-2.25	114.74	119.73
19	V	101	CRT	C34-C33-C35	2.25	121.63	118.08
13	D	103	BCL	CMB-C2B-C1B	-2.25	121.94	125.37
21	M	407	PEF	O3P-P-O1P	-2.25	102.66	110.89
19	3	103	CRT	C13-C12-C11	2.25	121.62	118.08
13	Y	103	BCL	C16-C15-C13	2.25	123.18	115.92
13	I	101	BCL	OBB-CAB-CBB	-2.25	114.75	119.73
13	W	101	BCL	C11-C10-C8	-2.24	108.66	115.92
13	F	101	BCL	C1C-NC-C4C	2.24	107.71	106.71
13	A	103	BCL	C11-C12-C13	-2.24	108.67	115.92
13	D	101	BCL	C16-C15-C13	2.24	123.16	115.92
19	0	101	CRT	C32-C31-C30	-2.24	116.22	123.22
20	U	104	CDL	OB6-CB5-OB7	-2.24	118.52	122.96
13	5	101	BCL	OBB-CAB-CBB	-2.24	114.77	119.73
21	I	103	PEF	O4P-P-O1P	-2.24	102.71	110.89
13	F	101	BCL	CMB-C2B-C1B	-2.24	121.96	125.37
21	3	104	PEF	O3P-P-O1P	-2.24	102.71	110.89
13	5	101	BCL	C2A-C1A-CHA	2.23	127.77	123.86
19	B	101	CRT	C34-C33-C35	2.23	121.60	118.08
19	4	101	CRT	C13-C12-C11	2.23	121.60	118.08
14	M	402	BPH	C2D-C1D-ND	2.23	111.07	109.53
19	O	103	CRT	C27-C26-C25	-2.23	116.25	123.22
12	M	411	PGV	O03-C19-C20	2.23	118.91	111.91
13	F	101	BCL	C1-C2-C3	-2.23	122.19	126.04
19	Z	101	CRT	C27-C26-C25	-2.23	116.26	123.22
13	F	103	BCL	CMB-C2B-C1B	-2.23	121.98	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	P	102	BCL	OBB-CAB-CBB	-2.23	114.79	119.73
13	7	101	BCL	OBB-CAB-CBB	-2.23	114.79	119.73
13	W	104	BCL	OBB-CAB-CBB	-2.22	114.80	119.73
13	9	101	BCL	CMB-C2B-C1B	-2.22	121.99	125.37
14	M	402	BPH	CMB-C2B-C3B	2.22	128.83	124.68
19	O	103	CRT	C18-C17-C16	2.22	121.57	118.08
12	9	104	PGV	O03-C19-O04	-2.22	117.99	123.59
13	U	103	BCL	OBB-CAB-CBB	-2.22	114.81	119.73
13	Y	103	BCL	C6-C7-C8	-2.22	108.75	115.92
21	K	104	PEF	O3-C30-C31	2.22	118.86	111.91
8	C	502	HEC	C4A-CHB-C1B	-2.22	121.28	126.06
20	O	104	CDL	O1-C1-CA2	-2.21	101.79	109.56
13	M	401	BCL	C16-C15-C13	-2.21	108.77	115.92
13	J	102	BCL	OBB-CAB-CBB	-2.21	114.83	119.73
19	A	104	CRT	C18-C17-C16	2.21	121.56	118.08
19	T	101	CRT	C6-C7-C9	2.21	122.33	118.94
13	A	103	BCL	OBB-CAB-CBB	-2.21	114.84	119.73
13	1	101	BCL	OBB-CAB-CBB	-2.21	114.84	119.73
19	8	101	CRT	C9-C10-C11	-2.21	116.33	123.22
19	W	102	CRT	C27-C26-C25	-2.21	116.33	123.22
13	2	102	BCL	CMB-C2B-C1B	-2.21	122.01	125.37
19	3	103	CRT	C29-C28-C30	2.21	121.55	118.08
13	K	101	BCL	C1C-NC-C4C	2.20	107.70	106.71
19	P	101	CRT	C18-C17-C16	2.20	121.55	118.08
13	K	103	BCL	OBB-CAB-CBB	-2.20	114.85	119.73
19	A	104	CRT	C27-C26-C25	-2.20	116.34	123.22
12	9	104	PGV	C03-C02-C01	-2.20	106.58	111.79
19	V	101	CRT	C13-C12-C11	2.20	121.54	118.08
13	Q	103	BCL	CAB-C3B-C2B	2.20	131.63	128.34
13	F	103	BCL	OBB-CAB-CBB	-2.20	114.86	119.73
20	O	104	CDL	OB8-CB7-OB9	-2.20	118.05	123.59
8	C	503	HEC	CBB-CAB-C3B	2.20	118.48	112.43
13	5	101	BCL	C16-C15-C13	2.20	123.02	115.92
19	G	101	CRT	C13-C12-C11	2.19	121.53	118.08
19	V	101	CRT	C10-C9-C7	-2.19	124.18	127.31
19	G	101	CRT	C21-C20-C19	-2.19	118.98	123.47
13	P	102	BCL	C17-C16-C15	-2.19	103.16	113.24
13	5	103	BCL	C16-C15-C13	-2.19	108.83	115.92
13	W	101	BCL	CMB-C2B-C1B	-2.19	122.03	125.37
19	B	101	CRT	C18-C17-C16	2.19	121.53	118.08
19	Z	101	CRT	C34-C33-C35	2.19	121.53	118.08
13	7	103	BCL	OBB-CAB-CBB	-2.19	114.88	119.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	8	101	CRT	C8-C7-C6	2.19	121.52	118.08
13	F	101	BCL	C2A-C1A-CHA	2.19	127.68	123.86
19	W	102	CRT	C5-C6-C7	-2.19	122.59	125.89
13	O	101	BCL	OBB-CAB-CBB	-2.18	114.89	119.73
13	S	101	BCL	C2A-C1A-CHA	2.18	127.67	123.86
19	G	101	CRT	C18-C17-C16	2.18	121.51	118.08
13	L	301	BCL	O2A-C1-C2	-2.17	102.93	108.64
19	B	101	CRT	C8-C7-C9	-2.17	119.89	122.92
13	K	101	BCL	C2A-C1A-CHA	2.17	127.65	123.86
13	W	104	BCL	O2A-CGA-O1A	-2.17	118.12	123.59
19	V	101	CRT	C29-C28-C30	2.17	121.49	118.08
19	V	101	CRT	C18-C17-C16	2.16	121.49	118.08
11	C	507	LHG	C27-C26-C25	-2.16	103.44	114.42
13	D	101	BCL	C2D-C1D-ND	2.16	111.70	110.10
13	L	305	BCL	C2D-C1D-ND	2.16	111.70	110.10
13	W	104	BCL	CMB-C2B-C1B	-2.16	122.08	125.37
13	7	101	BCL	CMB-C2B-C1B	-2.16	122.08	125.37
13	S	101	BCL	OBB-CAB-CBB	-2.16	114.94	119.73
13	M	401	BCL	C2A-C1A-CHA	2.15	127.63	123.86
19	T	101	CRT	C18-C17-C16	2.15	121.47	118.08
19	Z	101	CRT	C8-C7-C6	2.15	121.47	118.08
13	1	101	BCL	CMB-C2B-C1B	-2.15	122.10	125.37
18	M	404	MQ8	C2M-C2-C3	-2.15	120.90	124.40
18	M	404	MQ8	C21-C22-C23	-2.15	122.49	127.66
19	B	101	CRT	C20-C19-C17	-2.15	124.25	127.31
19	W	102	CRT	C29-C28-C30	2.14	121.45	118.08
13	S	101	BCL	C1-O2A-CGA	2.14	122.07	116.44
19	8	101	CRT	C27-C26-C25	-2.14	116.53	123.22
12	L	307	PGV	O01-C1-O02	-2.14	118.53	123.70
19	8	101	CRT	C14-C15-C16	-2.14	116.54	123.22
20	D	105	CDL	OA6-CA5-OA7	-2.14	118.53	123.70
19	N	101	CRT	C14-C15-C16	-2.14	116.55	123.22
14	L	303	BPH	C3B-C4B-NB	2.14	111.23	108.04
13	L	305	BCL	C16-C15-C13	-2.13	109.02	115.92
19	0	101	CRT	C31-C32-C33	-2.13	124.26	127.31
19	J	101	CRT	C29-C28-C30	2.13	121.43	118.08
13	4	102	BCL	C16-C15-C13	-2.13	109.04	115.92
13	7	101	BCL	C4-C3-C5	-2.13	111.69	115.27
20	U	104	CDL	OB8-CB6-CB4	2.13	114.62	108.43
19	A	104	CRT	C5-C6-C7	-2.13	122.68	125.89
19	0	101	CRT	C27-C26-C25	-2.12	116.59	123.22
14	M	402	BPH	C1-O2A-CGA	2.12	122.02	116.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	J	102	BCL	C17-C16-C15	-2.12	103.48	113.24
13	A	101	BCL	O2A-CGA-O1A	-2.12	118.23	123.59
19	G	101	CRT	C8-C7-C6	2.12	121.42	118.08
13	W	104	BCL	C2D-C1D-ND	2.12	111.67	110.10
19	O	103	CRT	C9-C10-C11	-2.12	116.60	123.22
20	O	104	CDL	CB2-C1-CA2	-2.12	106.55	112.79
13	I	101	BCL	CMB-C2B-C1B	-2.12	122.14	125.37
19	8	101	CRT	C15-C14-C12	-2.12	124.29	127.31
15	L	310	UQ8	O4-C4-C3	-2.12	115.66	123.64
19	4	101	CRT	C29-C28-C30	2.12	121.41	118.08
13	Y	101	BCL	CMB-C2B-C1B	-2.11	122.15	125.37
13	S	103	BCL	C9-C8-C10	-2.11	103.64	111.29
8	C	503	HEC	C1A-CHA-C4D	-2.11	121.50	126.06
12	9	104	PGV	O03-C01-C02	2.11	114.58	108.43
19	3	103	CRT	C34-C33-C35	2.11	121.40	118.08
21	W	105	PEF	O4P-P-O1P	-2.11	103.18	110.89
13	F	101	BCL	C6-C5-C3	2.11	118.98	113.45
13	D	103	BCL	C2D-C1D-ND	2.11	111.66	110.10
13	K	103	BCL	C2D-C1D-ND	2.11	111.66	110.10
19	2	101	CRT	C8-C7-C9	-2.10	119.97	122.92
13	U	101	BCL	CMB-C2B-C1B	-2.10	122.17	125.37
15	L	304	UQ8	C7-C6-C5	2.10	121.00	118.48
20	D	105	CDL	CA4-OA6-CA5	-2.10	112.62	117.79
13	L	301	BCL	CMB-C2B-C1B	-2.10	122.17	125.37
19	2	101	CRT	C14-C15-C16	-2.10	116.67	123.22
13	3	101	BCL	C2A-C1A-CHA	2.10	127.52	123.86
15	L	304	UQ8	C11-C12-C13	-2.09	105.00	111.88
13	L	301	BCL	C17-C16-C15	-2.09	103.62	113.24
15	L	304	UQ8	C20-C19-C21	2.09	118.79	115.27
13	Q	103	BCL	OBB-CAB-CBB	-2.09	115.09	119.73
19	T	101	CRT	C34-C33-C35	2.09	121.37	118.08
12	3	105	PGV	O03-C19-C20	2.09	118.47	111.91
13	L	305	BCL	CAC-C3C-C4C	2.09	117.22	112.58
13	D	101	BCL	C1C-NC-C4C	2.09	107.65	106.71
13	K	103	BCL	C11-C12-C13	-2.09	109.16	115.92
13	L	305	BCL	C1C-NC-C4C	2.08	107.64	106.71
13	5	103	BCL	OBB-CAB-CBB	-2.08	115.11	119.73
13	L	305	BCL	C4B-C3B-C2B	-2.08	105.01	108.36
18	M	404	MQ8	C14-C13-C15	2.08	118.77	115.27
8	C	503	HEC	O2D-CGD-CBD	2.08	120.71	114.03
13	D	103	BCL	C17-C16-C15	-2.08	103.69	113.24
19	0	101	CRT	C8-C7-C9	-2.08	120.01	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	402	BPH	C3B-C4B-NB	2.08	111.15	108.04
13	Y	101	BCL	C2A-C1A-CHA	2.08	127.49	123.86
19	4	101	CRT	C26-C25-C23	-2.08	120.58	126.42
13	5	103	BCL	C2D-C1D-ND	2.07	111.63	110.10
19	N	101	CRT	C13-C12-C11	2.07	121.35	118.08
20	U	104	CDL	O1-C1-CB2	-2.07	102.29	109.56
13	Y	103	BCL	C11-C12-C13	-2.07	109.22	115.92
19	M	405	CRT	C9-C10-C11	-2.07	116.75	123.22
19	8	101	CRT	C36-C35-C33	-2.07	122.76	125.89
14	M	402	BPH	CMA-C3A-C4A	-2.07	109.85	114.38
13	J	102	BCL	O2A-C1-C2	-2.07	103.20	108.64
20	U	104	CDL	OB4-PB2-OB3	2.06	122.43	112.24
19	2	101	CRT	C18-C17-C16	2.06	121.32	118.08
13	U	101	BCL	C2A-C1A-CHA	2.06	127.46	123.86
20	U	104	CDL	OA6-CA5-OA7	-2.06	118.73	123.70
13	U	101	BCL	C2D-C1D-ND	2.06	111.62	110.10
20	O	104	CDL	OA6-CA5-OA7	-2.05	118.74	123.70
13	L	305	BCL	CHC-C4B-NB	-2.05	122.08	124.26
19	W	102	CRT	C8-C7-C9	-2.05	120.05	122.92
19	0	101	CRT	C13-C12-C11	2.05	121.31	118.08
19	O	103	CRT	C10-C9-C7	-2.05	124.38	127.31
13	J	102	BCL	O2A-CGA-CBA	2.05	118.34	111.91
14	M	402	BPH	CGD-CBD-CAD	-2.05	104.09	110.73
12	M	411	PGV	O14-P-O13	2.05	122.38	112.24
20	D	104	CDL	CB4-OB6-CB5	-2.05	112.74	117.79
12	H	303	PGV	O01-C1-O02	-2.05	118.75	123.70
15	L	304	UQ8	C12-C11-C9	-2.05	106.25	112.98
20	D	104	CDL	OA6-CA5-OA7	-2.04	118.77	123.70
13	L	305	BCL	OB6-CAB-CBB	-2.04	115.20	119.73
20	O	104	CDL	OA8-CA7-OA9	-2.04	118.44	123.59
13	Q	101	BCL	C2D-C1D-ND	2.04	111.61	110.10
13	F	103	BCL	C2D-C1D-ND	2.04	111.61	110.10
18	M	404	MQ8	C46-C47-C48	-2.04	120.78	127.75
12	D	106	PGV	C02-O01-C1	-2.04	112.77	117.79
13	3	101	BCL	C1-C2-C3	-2.04	122.52	126.04
19	A	104	CRT	C9-C10-C11	-2.04	116.86	123.22
20	Y	104	CDL	CB4-OB6-CB5	-2.04	112.78	117.79
13	3	101	BCL	CBA-CAA-C2A	2.03	119.87	113.86
14	M	402	BPH	C4C-C3C-C2C	-2.03	100.91	102.84
15	L	310	UQ8	C17-C18-C19	-2.03	122.77	127.66
13	7	103	BCL	C2D-C1D-ND	2.03	111.60	110.10
19	J	101	CRT	C21-C20-C19	-2.03	119.32	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Y	103	BCL	C2D-C1D-ND	2.02	111.60	110.10
8	C	501	HEC	O2A-CGA-CBA	2.02	120.53	114.03
20	M	406	CDL	C12-C11-CA5	-2.02	106.27	113.62
19	W	102	CRT	C18-C17-C16	2.02	121.26	118.08
13	7	101	BCL	C11-C10-C8	-2.02	109.39	115.92
15	L	309	UQ8	C42-C43-C44	-2.02	120.85	127.75
20	Y	104	CDL	OA4-PA1-OA3	2.02	122.21	112.24
19	O	103	CRT	C29-C28-C30	2.02	121.25	118.08
12	9	104	PGV	C02-O01-C1	-2.01	112.83	117.79
19	Z	101	CRT	C13-C12-C11	2.01	121.25	118.08
13	U	103	BCL	O2A-CGA-O1A	-2.01	118.52	123.59
19	Z	101	CRT	C31-C32-C33	-2.01	124.44	127.31
13	D	101	BCL	C6-C5-C3	2.01	118.72	113.45
13	U	101	BCL	C11-C12-C13	-2.01	109.43	115.92
18	M	404	MQ8	C31-C32-C33	-2.01	122.82	127.66
20	S	104	CDL	PB2-OB5-CB3	2.01	133.45	121.68
19	P	101	CRT	C24-C23-C22	-2.01	120.11	122.92
19	B	101	CRT	C14-C15-C16	-2.01	116.96	123.22
19	4	101	CRT	C8-C7-C9	-2.01	120.11	122.92
13	3	101	BCL	CHC-C1C-NC	-2.00	121.74	124.51
13	O	101	BCL	C2A-C1A-CHA	2.00	127.36	123.86
14	L	303	BPH	C11-C10-C8	-2.00	109.45	115.92

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	C	501	HEC	NA
8	C	502	HEC	NA
8	C	503	HEC	NA
8	C	504	HEC	NA

All (932) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	H	301	GOL	C1-C2-C3-O3
11	C	507	LHG	C23-C24-C25-C26
12	C	508	PGV	O02-C1-O01-C02
12	L	308	PGV	C03-O11-P-O14
12	L	308	PGV	O12-C04-C05-O05
12	M	410	PGV	C03-O11-P-O12
12	M	411	PGV	C04-C05-C06-O06
12	H	303	PGV	C04-O12-P-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	D	106	PGV	O12-C04-C05-O05
12	1	105	PGV	C03-O11-P-O12
12	1	105	PGV	C03-O11-P-O13
12	1	105	PGV	C04-O12-P-O13
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	O12-C04-C05-C06
13	L	305	BCL	C4C-C3C-CAC-CBC
13	M	401	BCL	CHA-CBD-CGD-O1D
13	M	401	BCL	CHA-CBD-CGD-O2D
13	M	401	BCL	CAD-CBD-CGD-O1D
13	M	401	BCL	CAD-CBD-CGD-O2D
13	A	101	BCL	C14-C13-C15-C16
13	A	103	BCL	C4C-C3C-CAC-CBC
13	F	101	BCL	C4C-C3C-CAC-CBC
13	F	103	BCL	C1A-C2A-CAA-CBA
13	I	101	BCL	C4C-C3C-CAC-CBC
13	J	102	BCL	C1A-C2A-CAA-CBA
13	J	102	BCL	C2C-C3C-CAC-CBC
13	J	102	BCL	C4C-C3C-CAC-CBC
13	K	103	BCL	C4C-C3C-CAC-CBC
13	Q	101	BCL	C2-C3-C5-C6
13	Q	101	BCL	C4-C3-C5-C6
13	Q	103	BCL	C1A-C2A-CAA-CBA
13	S	103	BCL	C6-C7-C8-C9
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	101	BCL	C2C-C3C-CAC-CBC
13	W	101	BCL	C4C-C3C-CAC-CBC
13	W	101	BCL	C4-C3-C5-C6
13	W	104	BCL	C1A-C2A-CAA-CBA
13	Y	101	BCL	C2C-C3C-CAC-CBC
13	Y	101	BCL	C4C-C3C-CAC-CBC
13	Y	103	BCL	C2C-C3C-CAC-CBC
13	Y	103	BCL	C4C-C3C-CAC-CBC
13	1	101	BCL	C2C-C3C-CAC-CBC
13	1	101	BCL	C4C-C3C-CAC-CBC
13	2	102	BCL	C2C-C3C-CAC-CBC
13	2	102	BCL	C4C-C3C-CAC-CBC
13	2	102	BCL	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	3	101	BCL	C2-C3-C5-C6
13	3	101	BCL	C4-C3-C5-C6
13	4	102	BCL	C11-C10-C8-C9
13	5	103	BCL	C1A-C2A-CAA-CBA
13	7	101	BCL	C2-C3-C5-C6
13	7	101	BCL	C4-C3-C5-C6
13	7	103	BCL	C11-C10-C8-C9
13	9	103	BCL	C1A-C2A-CAA-CBA
13	9	103	BCL	C2C-C3C-CAC-CBC
13	9	103	BCL	C4C-C3C-CAC-CBC
14	M	402	BPH	C2C-C3C-CAC-CBC
15	L	304	UQ8	C15-C14-C16-C17
15	L	304	UQ8	C13-C14-C16-C17
15	L	309	UQ8	C35-C34-C36-C37
15	L	309	UQ8	C33-C34-C36-C37
15	L	310	UQ8	C12-C11-C9-C10
15	L	310	UQ8	C12-C11-C9-C8
18	M	404	MQ8	C33-C35-C36-C37
18	M	404	MQ8	C38-C40-C41-C42
19	M	405	CRT	O1-C1-C4-C5
19	M	405	CRT	C2-C1-C4-C5
19	M	405	CRT	C3-C1-C4-C5
19	M	405	CRT	C39-C38-O2-C2M
19	B	101	CRT	C5-C6-C7-C8
19	8	101	CRT	C10-C11-C12-C13
20	M	406	CDL	CB2-OB2-PB2-OB3
20	M	406	CDL	CB2-OB2-PB2-OB4
20	M	406	CDL	CB2-OB2-PB2-OB5
20	M	406	CDL	OB7-CB5-OB6-CB4
20	M	406	CDL	C51-CB5-OB6-CB4
20	M	412	CDL	CB3-OB5-PB2-OB2
20	M	412	CDL	CB3-OB5-PB2-OB4
20	H	305	CDL	O1-C1-CB2-OB2
20	H	305	CDL	CA2-C1-CB2-OB2
20	H	305	CDL	CA2-OA2-PA1-OA4
20	H	305	CDL	CA3-OA5-PA1-OA2
20	H	305	CDL	CA3-OA5-PA1-OA3
20	H	305	CDL	CA3-OA5-PA1-OA4
20	H	305	CDL	CB3-OB5-PB2-OB4
20	D	104	CDL	O1-C1-CA2-OA2
20	D	104	CDL	O1-C1-CB2-OB2
20	D	104	CDL	CA2-OA2-PA1-OA3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	D	104	CDL	CA3-OA5-PA1-OA4
20	D	104	CDL	CB2-OB2-PB2-OB3
20	D	104	CDL	CB2-OB2-PB2-OB4
20	D	104	CDL	CB2-OB2-PB2-OB5
20	D	104	CDL	CB3-OB5-PB2-OB4
20	D	104	CDL	C71-CB7-OB8-CB6
20	D	105	CDL	CB2-C1-CA2-OA2
20	D	105	CDL	O1-C1-CB2-OB2
20	D	105	CDL	CA2-OA2-PA1-OA3
20	D	105	CDL	CA2-OA2-PA1-OA4
20	D	105	CDL	OA7-CA5-OA6-CA4
20	D	105	CDL	C11-CA5-OA6-CA4
20	O	104	CDL	CA2-OA2-PA1-OA3
20	O	104	CDL	OB7-CB5-OB6-CB4
20	S	104	CDL	CA2-OA2-PA1-OA3
20	S	104	CDL	CB2-OB2-PB2-OB3
20	S	104	CDL	OB5-CB3-CB4-OB6
20	S	104	CDL	OB6-CB4-CB6-OB8
20	U	104	CDL	CA2-OA2-PA1-OA3
20	U	104	CDL	CA2-OA2-PA1-OA4
20	U	104	CDL	CB3-OB5-PB2-OB3
20	U	104	CDL	OB5-CB3-CB4-OB6
20	Y	104	CDL	O1-C1-CB2-OB2
20	Y	104	CDL	CA2-OA2-PA1-OA3
20	Y	104	CDL	CA2-OA2-PA1-OA4
20	Y	104	CDL	CA3-OA5-PA1-OA3
20	Y	104	CDL	CB2-OB2-PB2-OB3
20	Y	104	CDL	CB2-OB2-PB2-OB4
20	Y	104	CDL	CB3-OB5-PB2-OB3
20	1	104	CDL	CB3-OB5-PB2-OB2
20	1	104	CDL	CB3-OB5-PB2-OB3
20	1	104	CDL	CB3-OB5-PB2-OB4
20	1	104	CDL	CB3-CB4-CB6-OB8
22	M	414	LMT	C2'-C1'-O1'-C1
22	M	414	LMT	O5'-C1'-O1'-C1
22	H	304	LMT	C2'-C1'-O1'-C1
20	U	104	CDL	C51-CB5-OB6-CB4
20	D	104	CDL	OB9-CB7-OB8-CB6
12	C	508	PGV	O04-C19-O03-C01
12	D	106	PGV	O04-C19-O03-C01
13	9	103	BCL	C3-C5-C6-C7
12	C	508	PGV	C20-C19-O03-C01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	D	106	PGV	C20-C19-O03-C01
12	C	508	PGV	C2-C1-O01-C02
20	O	104	CDL	C51-CB5-OB6-CB4
13	A	101	BCL	C4-C3-C5-C6
14	M	402	BPH	C4-C3-C5-C6
13	A	101	BCL	C2-C3-C5-C6
13	W	101	BCL	C2-C3-C5-C6
13	3	101	BCL	C3-C5-C6-C7
20	U	104	CDL	OA9-CA7-OA8-CA6
12	9	104	PGV	O12-C04-C05-O05
20	M	406	CDL	O1-C1-CA2-OA2
20	S	104	CDL	O1-C1-CB2-OB2
20	O	104	CDL	C31-CA7-OA8-CA6
12	3	105	PGV	C2-C1-O01-C02
12	9	104	PGV	C2-C1-O01-C02
12	L	308	PGV	C19-C20-C21-C22
20	U	104	CDL	C31-CA7-OA8-CA6
22	H	304	LMT	O5'-C5'-C6'-O6'
20	O	104	CDL	OA9-CA7-OA8-CA6
13	1	101	BCL	C4-C3-C5-C6
13	1	101	BCL	C2-C3-C5-C6
14	M	402	BPH	C2-C3-C5-C6
22	H	304	LMT	O5'-C1'-O1'-C1
12	L	308	PGV	O12-C04-C05-C06
12	D	106	PGV	O12-C04-C05-C06
20	M	406	CDL	CB2-C1-CA2-OA2
20	D	104	CDL	CB2-C1-CA2-OA2
20	S	104	CDL	CA2-C1-CB2-OB2
12	9	104	PGV	O02-C1-O01-C02
13	P	102	BCL	C3-C5-C6-C7
13	4	102	BCL	C8-C10-C11-C12
13	S	101	BCL	CBD-CGD-O2D-CED
13	9	101	BCL	CBD-CGD-O2D-CED
20	U	104	CDL	OB7-CB5-OB6-CB4
13	3	101	BCL	C5-C6-C7-C8
8	C	502	HEC	C2B-C3B-CAB-CBB
13	P	102	BCL	C8-C10-C11-C12
13	Q	101	BCL	C5-C6-C7-C8
13	5	101	BCL	C5-C6-C7-C8
20	H	305	CDL	OB6-CB4-CB6-OB8
13	L	305	BCL	C6-C7-C8-C9
13	L	305	BCL	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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	101	BCL	C14-C13-C15-C16
13	K	103	BCL	C6-C7-C8-C9
13	K	103	BCL	C11-C10-C8-C9
13	P	102	BCL	C6-C7-C8-C9
13	P	102	BCL	C11-C10-C8-C9
13	Q	101	BCL	C11-C12-C13-C14
13	Q	103	BCL	C14-C13-C15-C16
13	S	101	BCL	C14-C13-C15-C16
13	U	103	BCL	C11-C12-C13-C14
13	W	104	BCL	C6-C7-C8-C9
13	Y	103	BCL	C14-C13-C15-C16
13	2	102	BCL	C6-C7-C8-C9
13	3	101	BCL	C14-C13-C15-C16
13	5	103	BCL	C11-C12-C13-C14
13	7	103	BCL	C6-C7-C8-C9
13	9	103	BCL	C6-C7-C8-C9
19	W	102	CRT	C15-C16-C17-C18
19	8	101	CRT	C15-C16-C17-C18
19	0	101	CRT	C5-C6-C7-C8
12	3	105	PGV	O02-C1-O01-C02
20	O	104	CDL	C31-C32-C33-C34
13	W	104	BCL	C8-C10-C11-C12
13	O	101	BCL	C13-C15-C16-C17
13	P	102	BCL	C5-C6-C7-C8
20	H	305	CDL	CB5-C51-C52-C53
13	1	101	BCL	C5-C6-C7-C8
10	C	506	GOL	O1-C1-C2-O2
12	9	104	PGV	C1-C2-C3-C4
13	F	101	BCL	C15-C16-C17-C18
13	1	101	BCL	C13-C15-C16-C17
13	I	101	BCL	C5-C6-C7-C8
13	7	101	BCL	C8-C10-C11-C12
13	A	101	BCL	C13-C15-C16-C17
13	Q	101	BCL	C11-C12-C13-C15
13	W	104	BCL	C6-C7-C8-C10
13	9	101	BCL	C11-C10-C8-C7
15	L	309	UQ8	C3-C4-O4-C4M
15	L	310	UQ8	C3-C4-O4-C4M
13	S	101	BCL	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	S	103	BCL	C5-C6-C7-C8
14	M	402	BPH	C5-C6-C7-C8
13	Y	103	BCL	C8-C10-C11-C12
15	L	304	UQ8	C14-C16-C17-C18
15	L	310	UQ8	C9-C11-C12-C13
12	M	411	PGV	O12-C04-C05-O05
12	3	105	PGV	O12-C04-C05-O05
20	D	105	CDL	O1-C1-CA2-OA2
20	O	104	CDL	O1-C1-CB2-OB2
20	S	104	CDL	O1-C1-CA2-OA2
13	Y	101	BCL	C13-C15-C16-C17
13	5	101	BCL	C13-C15-C16-C17
13	W	104	BCL	C13-C15-C16-C17
13	Y	103	BCL	C13-C15-C16-C17
13	Y	103	BCL	C15-C16-C17-C18
13	1	101	BCL	C15-C16-C17-C18
20	M	406	CDL	C71-C72-C73-C74
20	Y	104	CDL	C11-CA5-OA6-CA4
13	A	103	BCL	C13-C15-C16-C17
13	Q	103	BCL	C13-C15-C16-C17
13	W	101	BCL	C13-C15-C16-C17
12	L	308	PGV	C03-O11-P-O12
12	L	308	PGV	C04-O12-P-O11
12	D	106	PGV	C03-O11-P-O12
12	3	105	PGV	C03-O11-P-O12
20	M	406	CDL	CB3-OB5-PB2-OB2
20	M	412	CDL	CB2-OB2-PB2-OB5
20	H	305	CDL	CB3-OB5-PB2-OB2
20	D	104	CDL	CB3-OB5-PB2-OB2
20	D	105	CDL	CA2-OA2-PA1-OA5
20	D	105	CDL	CB2-OB2-PB2-OB5
20	D	105	CDL	CB3-OB5-PB2-OB2
20	S	104	CDL	CB2-OB2-PB2-OB5
20	S	104	CDL	CB3-OB5-PB2-OB2
20	U	104	CDL	CA2-OA2-PA1-OA5
20	Y	104	CDL	CA2-OA2-PA1-OA5
20	Y	104	CDL	CA3-OA5-PA1-OA2
20	Y	104	CDL	CB2-OB2-PB2-OB5
13	J	102	BCL	C15-C16-C17-C18
13	U	101	BCL	C5-C6-C7-C8
22	H	304	LMT	C4'-C5'-C6'-O6'
12	M	411	PGV	O12-C04-C05-C06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	D	104	CDL	CA2-C1-CB2-OB2
20	D	105	CDL	CA2-C1-CB2-OB2
20	O	104	CDL	CA2-C1-CB2-OB2
20	S	104	CDL	CB2-C1-CA2-OA2
13	Q	101	BCL	C15-C16-C17-C18
13	Q	103	BCL	C10-C11-C12-C13
12	M	410	PGV	C20-C19-O03-C01
20	M	406	CDL	C31-CA7-OA8-CA6
12	L	307	PGV	C2-C1-O01-C02
20	O	104	CDL	C11-CA5-OA6-CA4
20	S	104	CDL	C37-C38-C39-C40
13	9	101	BCL	C16-C17-C18-C19
12	L	308	PGV	C7-C8-C9-C10
20	M	406	CDL	C40-C41-C42-C43
20	M	406	CDL	C51-C52-C53-C54
12	L	307	PGV	O02-C1-O01-C02
13	Q	101	BCL	C10-C11-C12-C13
20	O	104	CDL	CA7-C31-C32-C33
20	M	406	CDL	C14-C15-C16-C17
20	M	406	CDL	C34-C35-C36-C37
20	U	104	CDL	C14-C15-C16-C17
20	U	104	CDL	C33-C34-C35-C36
20	D	105	CDL	C59-C60-C61-C62
12	9	104	PGV	C19-C20-C21-C22
20	H	305	CDL	C11-C12-C13-C14
13	F	101	BCL	C13-C15-C16-C17
13	P	102	BCL	C16-C17-C18-C20
13	Q	101	BCL	C16-C17-C18-C19
13	5	101	BCL	C16-C17-C18-C19
14	L	303	BPH	C4-C3-C5-C6
12	M	410	PGV	C30-C31-C32-C33
20	M	406	CDL	C12-C13-C14-C15
13	A	103	BCL	C11-C10-C8-C9
13	S	103	BCL	C11-C10-C8-C9
13	S	103	BCL	C11-C12-C13-C14
13	U	103	BCL	C6-C7-C8-C9
13	7	101	BCL	C11-C10-C8-C9
13	9	103	BCL	C11-C12-C13-C14
12	1	105	PGV	C19-C20-C21-C22
12	1	105	PGV	C3-C4-C5-C6
13	U	103	BCL	C8-C10-C11-C12
13	2	102	BCL	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	3	101	BCL	O1A-CGA-O2A-C1
20	M	406	CDL	C61-C62-C63-C64
20	S	104	CDL	C35-C36-C37-C38
22	M	414	LMT	C5-C6-C7-C8
10	C	506	GOL	O1-C1-C2-C3
19	8	101	CRT	C10-C11-C12-C14
20	O	104	CDL	OA7-CA5-OA6-CA4
20	Y	104	CDL	OA7-CA5-OA6-CA4
12	L	307	PGV	C23-C24-C25-C26
12	L	307	PGV	C24-C25-C26-C27
13	I	101	BCL	C16-C17-C18-C19
13	9	101	BCL	C16-C17-C18-C20
14	L	303	BPH	C16-C17-C18-C19
13	7	103	BCL	C10-C11-C12-C13
20	H	305	CDL	C78-C79-C80-C81
20	O	104	CDL	C33-C34-C35-C36
20	S	104	CDL	CB5-C51-C52-C53
13	F	103	BCL	C10-C11-C12-C13
12	M	410	PGV	O04-C19-O03-C01
12	L	307	PGV	C29-C30-C31-C32
20	S	104	CDL	C73-C74-C75-C76
12	L	307	PGV	C26-C27-C28-C29
13	F	103	BCL	C3A-C2A-CAA-CBA
13	S	103	BCL	C3A-C2A-CAA-CBA
13	U	103	BCL	C3A-C2A-CAA-CBA
13	W	104	BCL	C3A-C2A-CAA-CBA
13	5	103	BCL	C3A-C2A-CAA-CBA
13	9	103	BCL	C3A-C2A-CAA-CBA
13	1	101	BCL	C10-C11-C12-C13
20	M	406	CDL	C42-C43-C44-C45
20	D	105	CDL	C71-C72-C73-C74
13	K	103	BCL	C3-C5-C6-C7
12	L	307	PGV	C19-C20-C21-C22
20	O	104	CDL	CB7-C71-C72-C73
20	S	104	CDL	CA5-C11-C12-C13
20	M	406	CDL	C11-CA5-OA6-CA4
12	L	308	PGV	C23-C24-C25-C26
20	1	104	CDL	OB6-CB4-CB6-OB8
12	D	106	PGV	C4-C5-C6-C7
13	U	103	BCL	C10-C11-C12-C13
20	M	406	CDL	C17-C18-C19-C20
20	M	406	CDL	OA9-CA7-OA8-CA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	4	102	BCL	C5-C6-C7-C8
8	C	502	HEC	C4B-C3B-CAB-CBB
12	9	104	PGV	C22-C23-C24-C25
20	M	406	CDL	C20-C21-C22-C23
13	3	101	BCL	C13-C15-C16-C17
20	S	104	CDL	C14-C15-C16-C17
12	M	410	PGV	C2-C3-C4-C5
21	K	104	PEF	C30-C31-C32-C33
12	M	411	PGV	C29-C30-C31-C32
13	F	101	BCL	C5-C6-C7-C8
13	9	101	BCL	C5-C6-C7-C8
13	D	101	BCL	C4-C3-C5-C6
13	A	101	BCL	C11-C10-C8-C7
13	Q	101	BCL	C11-C10-C8-C7
13	Q	103	BCL	C12-C13-C15-C16
13	S	101	BCL	C12-C13-C15-C16
13	S	103	BCL	C11-C12-C13-C15
13	U	103	BCL	C6-C7-C8-C10
13	W	101	BCL	C11-C10-C8-C7
13	9	103	BCL	C11-C12-C13-C15
13	Y	103	BCL	C3-C5-C6-C7
11	C	507	LHG	C25-C26-C27-C28
13	S	103	BCL	C16-C17-C18-C20
12	3	105	PGV	C11-C10-C9-C8
20	U	104	CDL	OA7-CA5-OA6-CA4
20	O	104	CDL	C60-C61-C62-C63
20	M	406	CDL	CB5-C51-C52-C53
13	K	101	BCL	C13-C15-C16-C17
12	3	105	PGV	C7-C8-C9-C10
12	3	105	PGV	C13-C14-C15-C16
20	H	305	CDL	C59-C60-C61-C62
20	S	104	CDL	C72-C73-C74-C75
12	M	410	PGV	C21-C22-C23-C24
20	H	305	CDL	C71-CB7-OB8-CB6
13	S	103	BCL	C16-C17-C18-C19
13	W	101	BCL	C5-C6-C7-C8
20	U	104	CDL	C71-C72-C73-C74
12	3	105	PGV	C19-C20-C21-C22
12	D	106	PGV	C2-C1-O01-C02
20	U	104	CDL	C11-CA5-OA6-CA4
20	U	104	CDL	OA5-CA3-CA4-OA6
12	M	411	PGV	C27-C28-C29-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	M	414	LMT	C4-C5-C6-C7
20	M	406	CDL	OA7-CA5-OA6-CA4
13	4	102	BCL	C3-C5-C6-C7
13	P	102	BCL	C16-C17-C18-C19
13	Q	101	BCL	C16-C17-C18-C20
20	D	105	CDL	C75-C76-C77-C78
13	K	101	BCL	C4-C3-C5-C6
20	U	104	CDL	CA5-C11-C12-C13
14	L	303	BPH	C2-C3-C5-C6
12	M	410	PGV	C6-C7-C8-C9
13	A	101	BCL	C11-C10-C8-C9
13	F	101	BCL	C11-C10-C8-C9
13	Q	101	BCL	C11-C10-C8-C9
13	W	101	BCL	C11-C10-C8-C9
13	A	103	BCL	C3-C5-C6-C7
19	G	101	CRT	C15-C16-C17-C18
19	V	101	CRT	C5-C6-C7-C8
13	D	103	BCL	C1A-C2A-CAA-CBA
13	K	103	BCL	C1A-C2A-CAA-CBA
13	P	102	BCL	C1A-C2A-CAA-CBA
13	S	103	BCL	C1A-C2A-CAA-CBA
12	1	105	PGV	C2-C1-O01-C02
20	D	104	CDL	C11-CA5-OA6-CA4
13	S	101	BCL	C15-C16-C17-C18
20	D	104	CDL	CA3-OA5-PA1-OA2
20	Y	104	CDL	CB3-OB5-PB2-OB2
20	U	104	CDL	C15-C16-C17-C18
12	M	410	PGV	C19-C20-C21-C22
13	Q	101	BCL	CBD-CGD-O2D-CED
13	9	101	BCL	O1D-CGD-O2D-CED
13	P	102	BCL	C13-C15-C16-C17
12	M	410	PGV	C01-C02-C03-O11
20	S	104	CDL	OA5-CA3-CA4-CA6
20	O	104	CDL	C17-C18-C19-C20
12	M	410	PGV	C13-C14-C15-C16
20	S	104	CDL	C52-C53-C54-C55
20	S	104	CDL	C51-C52-C53-C54
13	S	101	BCL	O1D-CGD-O2D-CED
13	W	104	BCL	C10-C11-C12-C13
13	A	103	BCL	C2C-C3C-CAC-CBC
13	I	101	BCL	C2C-C3C-CAC-CBC
20	M	406	CDL	CA3-CA4-CA6-OA8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	M	406	CDL	CB3-CB4-CB6-OB8
20	S	104	CDL	CA3-CA4-CA6-OA8
20	S	104	CDL	CB3-CB4-CB6-OB8
22	M	414	LMT	O5'-C5'-C6'-O6'
13	Y	101	BCL	C15-C16-C17-C18
20	S	104	CDL	C74-C75-C76-C77
20	M	406	CDL	C52-C53-C54-C55
10	H	301	GOL	O2-C2-C3-O3
12	M	411	PGV	O05-C05-C06-O06
20	M	406	CDL	C53-C54-C55-C56
13	L	305	BCL	C13-C15-C16-C17
20	U	104	CDL	CB7-C71-C72-C73
21	K	104	PEF	C31-C30-O3-C3
20	M	406	CDL	C31-C32-C33-C34
20	S	104	CDL	C59-C60-C61-C62
22	H	304	LMT	O1'-C1-C2-C3
12	D	106	PGV	O02-C1-O01-C02
12	M	410	PGV	C03-O11-P-O13
20	M	406	CDL	OB5-CB3-CB4-OB6
22	H	304	LMT	C11-C10-C9-C8
19	M	405	CRT	C40-C38-O2-C2M
14	L	303	BPH	C8-C10-C11-C12
20	H	305	CDL	OB9-CB7-OB8-CB6
8	C	501	HEC	C2C-C3C-CAC-CBC
19	B	101	CRT	C2-C1-C4-C5
19	B	101	CRT	C3-C1-C4-C5
19	J	101	CRT	C2-C1-C4-C5
19	W	102	CRT	C2-C1-C4-C5
19	0	101	CRT	C2-C1-C4-C5
13	A	103	BCL	C6-C7-C8-C10
13	D	101	BCL	C11-C10-C8-C7
13	D	103	BCL	C12-C13-C15-C16
13	F	101	BCL	C11-C10-C8-C7
13	F	103	BCL	C6-C7-C8-C10
13	J	102	BCL	C12-C13-C15-C16
13	K	103	BCL	C6-C7-C8-C10
13	P	102	BCL	C6-C7-C8-C10
13	U	101	BCL	C11-C10-C8-C7
13	2	102	BCL	C12-C13-C15-C16
13	7	103	BCL	C6-C7-C8-C10
13	D	101	BCL	C11-C10-C8-C9
13	D	103	BCL	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	J	102	BCL	C6-C7-C8-C9
13	Q	103	BCL	C11-C10-C8-C9
13	3	101	BCL	C11-C10-C8-C9
13	5	101	BCL	C11-C10-C8-C9
13	9	101	BCL	C11-C10-C8-C9
13	9	101	BCL	C11-C12-C13-C14
15	L	309	UQ8	C4-C3-O3-C3M
13	Q	101	BCL	C13-C15-C16-C17
13	S	101	BCL	C10-C11-C12-C13
8	C	501	HEC	C2B-C3B-CAB-CBB
8	C	504	HEC	C2B-C3B-CAB-CBB
12	9	104	PGV	O12-C04-C05-C06
12	1	105	PGV	O02-C1-O01-C02
13	S	101	BCL	C13-C15-C16-C17
12	L	308	PGV	C4-C5-C6-C7
12	9	104	PGV	C20-C19-O03-C01
12	H	303	PGV	C01-C02-C03-O11
12	D	106	PGV	C01-C02-C03-O11
20	O	104	CDL	OA5-CA3-CA4-CA6
20	S	104	CDL	OB5-CB3-CB4-CB6
20	U	104	CDL	OA5-CA3-CA4-CA6
20	U	104	CDL	OB5-CB3-CB4-CB6
12	M	411	PGV	C21-C22-C23-C24
20	M	406	CDL	C80-C81-C82-C83
13	A	103	BCL	C10-C11-C12-C13
13	7	103	BCL	C15-C16-C17-C18
13	3	101	BCL	CBA-CGA-O2A-C1
20	H	305	CDL	CA5-C11-C12-C13
13	D	103	BCL	C3A-C2A-CAA-CBA
13	J	102	BCL	C3A-C2A-CAA-CBA
13	3	101	BCL	C3A-C2A-CAA-CBA
13	9	101	BCL	C15-C16-C17-C18
12	9	104	PGV	C23-C24-C25-C26
20	O	104	CDL	C77-C78-C79-C80
20	O	104	CDL	C76-C77-C78-C79
13	A	101	BCL	C15-C16-C17-C18
13	5	103	BCL	C10-C11-C12-C13
13	L	305	BCL	C16-C17-C18-C20
13	I	101	BCL	C16-C17-C18-C20
20	M	406	CDL	C38-C39-C40-C41
12	M	411	PGV	O03-C01-C02-C03
20	H	305	CDL	CB3-CB4-CB6-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	D	104	CDL	CB3-CB4-CB6-OB8
20	O	104	CDL	CB3-CB4-CB6-OB8
22	M	414	LMT	C2-C3-C4-C5
15	L	309	UQ8	C40-C39-C41-C42
12	L	308	PGV	C26-C27-C28-C29
20	H	305	CDL	CA2-OA2-PA1-OA5
20	O	104	CDL	CA2-OA2-PA1-OA5
13	S	103	BCL	O1A-CGA-O2A-C1
21	K	104	PEF	O5-C30-O3-C3
13	J	102	BCL	C13-C15-C16-C17
12	D	106	PGV	O01-C02-C03-O11
20	M	406	CDL	OA5-CA3-CA4-OA6
20	D	105	CDL	OB5-CB3-CB4-OB6
20	Y	104	CDL	OB5-CB3-CB4-OB6
22	H	304	LMT	C6-C7-C8-C9
15	L	310	UQ8	C5-C4-O4-C4M
12	H	303	PGV	O03-C01-C02-O01
20	M	406	CDL	OA6-CA4-CA6-OA8
20	D	104	CDL	OB6-CB4-CB6-OB8
20	O	104	CDL	OB6-CB4-CB6-OB8
14	L	303	BPH	C16-C17-C18-C20
13	D	101	BCL	C15-C16-C17-C18
15	L	310	UQ8	C14-C16-C17-C18
20	D	104	CDL	OA7-CA5-OA6-CA4
13	7	103	BCL	C2-C1-O2A-CGA
13	9	101	BCL	C2-C1-O2A-CGA
13	K	101	BCL	C11-C10-C8-C9
13	U	101	BCL	C11-C10-C8-C9
13	U	101	BCL	C14-C13-C15-C16
13	3	101	BCL	C6-C7-C8-C9
13	5	103	BCL	C11-C10-C8-C9
20	O	104	CDL	C1-CB2-OB2-PB2
20	D	105	CDL	C15-C16-C17-C18
13	F	103	BCL	C3-C5-C6-C7
13	D	103	BCL	C4C-C3C-CAC-CBC
13	S	103	BCL	C4C-C3C-CAC-CBC
13	4	102	BCL	C4C-C3C-CAC-CBC
13	5	103	BCL	C4C-C3C-CAC-CBC
13	7	101	BCL	C4C-C3C-CAC-CBC
19	B	101	CRT	C5-C6-C7-C9
19	0	101	CRT	C5-C6-C7-C9
13	S	103	BCL	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	D	105	CDL	C72-C73-C74-C75
20	O	104	CDL	C11-C12-C13-C14
13	5	101	BCL	C16-C17-C18-C20
13	W	101	BCL	C10-C11-C12-C13
13	5	103	BCL	C13-C15-C16-C17
13	A	101	BCL	C12-C13-C15-C16
13	D	103	BCL	C6-C7-C8-C10
13	K	101	BCL	C11-C10-C8-C7
13	Q	103	BCL	C11-C10-C8-C7
13	U	103	BCL	C11-C10-C8-C7
13	Y	103	BCL	C11-C12-C13-C15
13	2	102	BCL	C11-C10-C8-C7
13	3	101	BCL	C11-C10-C8-C7
13	3	101	BCL	C12-C13-C15-C16
13	4	102	BCL	C6-C7-C8-C10
13	4	102	BCL	C11-C10-C8-C7
13	5	101	BCL	C11-C10-C8-C7
13	7	101	BCL	C11-C10-C8-C7
13	7	103	BCL	C11-C10-C8-C7
13	9	101	BCL	C6-C7-C8-C10
13	9	101	BCL	C11-C12-C13-C15
20	M	406	CDL	C35-C36-C37-C38
12	L	308	PGV	C2-C3-C4-C5
13	S	103	BCL	C15-C16-C17-C18
13	4	102	BCL	C15-C16-C17-C18
13	1	101	BCL	C16-C17-C18-C20
13	L	305	BCL	C5-C6-C7-C8
12	3	105	PGV	C20-C19-O03-C01
13	L	305	BCL	CAD-CBD-CGD-O2D
13	A	101	BCL	CAD-CBD-CGD-O2D
13	D	101	BCL	C5-C6-C7-C8
13	U	103	BCL	C13-C15-C16-C17
12	H	303	PGV	C5-C6-C7-C8
13	5	101	BCL	C4-C3-C5-C6
21	K	104	PEF	C32-C33-C34-C35
12	L	308	PGV	C31-C32-C33-C34
12	H	303	PGV	O01-C02-C03-O11
20	O	104	CDL	OA5-CA3-CA4-OA6
20	S	104	CDL	OA5-CA3-CA4-OA6
13	F	103	BCL	C13-C15-C16-C17
20	M	406	CDL	C44-C45-C46-C47
13	7	103	BCL	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	Y	101	BCL	C5-C6-C7-C8
12	D	106	PGV	O03-C01-C02-O01
20	M	406	CDL	OB6-CB4-CB6-OB8
20	S	104	CDL	OA6-CA4-CA6-OA8
13	S	103	BCL	CBA-CGA-O2A-C1
12	L	307	PGV	C25-C26-C27-C28
12	9	104	PGV	O04-C19-O03-C01
13	Q	101	BCL	O1D-CGD-O2D-CED
12	M	410	PGV	C14-C15-C16-C17
13	D	101	BCL	C2-C3-C5-C6
13	S	101	BCL	C11-C10-C8-C9
13	Y	103	BCL	C11-C12-C13-C14
13	1	101	BCL	C6-C7-C8-C9
13	F	101	BCL	CBD-CGD-O2D-CED
14	M	402	BPH	C8-C10-C11-C12
19	G	101	CRT	C15-C16-C17-C19
19	W	102	CRT	C15-C16-C17-C19
19	8	101	CRT	C15-C16-C17-C19
13	A	103	BCL	C1A-C2A-CAA-CBA
13	Y	103	BCL	C1A-C2A-CAA-CBA
13	2	102	BCL	C1A-C2A-CAA-CBA
13	4	102	BCL	C1A-C2A-CAA-CBA
13	7	103	BCL	C1A-C2A-CAA-CBA
12	D	106	PGV	C04-O12-P-O11
12	1	105	PGV	C04-O12-P-O11
20	D	104	CDL	CA2-OA2-PA1-OA5
20	O	104	CDL	CB2-OB2-PB2-OB5
20	U	104	CDL	C34-C35-C36-C37
8	C	501	HEC	C4B-C3B-CAB-CBB
13	F	101	BCL	C4-C3-C5-C6
12	M	411	PGV	C02-C03-O11-P
13	K	101	BCL	C2-C3-C5-C6
12	L	308	PGV	C03-O11-P-O13
12	L	308	PGV	C04-O12-P-O13
12	H	303	PGV	C03-O11-P-O13
12	D	106	PGV	C03-O11-P-O13
12	3	105	PGV	C04-O12-P-O14
20	M	406	CDL	CB3-OB5-PB2-OB3
20	M	412	CDL	CB2-OB2-PB2-OB3
20	M	412	CDL	CB3-OB5-PB2-OB3
20	H	305	CDL	CA2-OA2-PA1-OA3
20	D	104	CDL	CA3-OA5-PA1-OA3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	D	105	CDL	CB2-OB2-PB2-OB3
20	D	105	CDL	CB3-OB5-PB2-OB4
20	S	104	CDL	CB3-OB5-PB2-OB3
20	Y	104	CDL	CA3-OA5-PA1-OA4
20	Y	104	CDL	CB3-OB5-PB2-OB4
13	L	305	BCL	C16-C17-C18-C19
13	1	101	BCL	C16-C17-C18-C19
13	L	301	BCL	C15-C16-C17-C18
13	K	103	BCL	C10-C11-C12-C13
12	L	307	PGV	C20-C19-O03-C01
13	2	102	BCL	CBA-CGA-O2A-C1
12	L	308	PGV	C01-C02-C03-O11
20	M	406	CDL	OA5-CA3-CA4-CA6
20	M	406	CDL	OB5-CB3-CB4-CB6
20	D	105	CDL	OB5-CB3-CB4-CB6
8	C	501	HEC	C4C-C3C-CAC-CBC
15	L	309	UQ8	C5-C4-O4-C4M
15	L	311	UQ8	C5-C4-O4-C4M
12	L	307	PGV	C5-C6-C7-C8
13	S	103	BCL	C10-C11-C12-C13
13	9	101	BCL	C8-C10-C11-C12
12	H	303	PGV	C20-C21-C22-C23
12	L	308	PGV	C1-C2-C3-C4
12	D	106	PGV	C1-C2-C3-C4
20	S	104	CDL	OB9-CB7-OB8-CB6
20	Y	104	CDL	CA2-C1-CB2-OB2
12	L	308	PGV	O02-C1-O01-C02
12	M	410	PGV	O01-C02-C03-O11
13	L	305	BCL	C2C-C3C-CAC-CBC
13	L	305	BCL	C6-C7-C8-C10
13	L	305	BCL	C11-C12-C13-C15
13	F	101	BCL	C2C-C3C-CAC-CBC
13	J	102	BCL	C6-C7-C8-C10
13	K	101	BCL	C12-C13-C15-C16
13	K	103	BCL	C3A-C2A-CAA-CBA
13	K	103	BCL	C2C-C3C-CAC-CBC
13	Q	103	BCL	C3A-C2A-CAA-CBA
13	U	103	BCL	C2C-C3C-CAC-CBC
13	U	103	BCL	C11-C12-C13-C15
13	1	101	BCL	C6-C7-C8-C10
13	3	101	BCL	C6-C7-C8-C10
20	Y	104	CDL	OA5-CA3-CA4-OA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	C	504	HEC	C4B-C3B-CAB-CBB
14	M	402	BPH	C15-C16-C17-C18
12	L	308	PGV	C2-C1-O01-C02
12	3	105	PGV	O04-C19-O03-C01
12	D	106	PGV	C19-C20-C21-C22
12	D	106	PGV	O03-C01-C02-C03
20	M	406	CDL	C13-C14-C15-C16
12	L	308	PGV	C21-C22-C23-C24
20	O	104	CDL	C36-C37-C38-C39
12	3	105	PGV	C21-C22-C23-C24
12	H	303	PGV	C02-C03-O11-P
12	L	307	PGV	C7-C8-C9-C10
12	L	308	PGV	C3-C4-C5-C6
13	L	305	BCL	C11-C12-C13-C14
13	D	103	BCL	C6-C7-C8-C9
13	J	102	BCL	C14-C13-C15-C16
13	4	102	BCL	C6-C7-C8-C9
13	5	103	BCL	C6-C7-C8-C9
13	9	101	BCL	C6-C7-C8-C9
20	O	104	CDL	C57-C58-C59-C60
12	H	303	PGV	C3-C4-C5-C6
13	W	101	BCL	C15-C16-C17-C18
8	C	503	HEC	C2C-C3C-CAC-CBC
13	M	401	BCL	C13-C15-C16-C17
11	C	507	LHG	C26-C27-C28-C29
20	O	104	CDL	C18-C19-C20-C21
13	K	101	BCL	C5-C6-C7-C8
20	U	104	CDL	CA6-CA4-OA6-CA5
20	Y	104	CDL	OA5-CA3-CA4-CA6
21	K	104	PEF	O4-C10-O2-C2
13	F	101	BCL	CBA-CGA-O2A-C1
13	A	101	BCL	C2-C1-O2A-CGA
22	H	304	LMT	C1-C2-C3-C4
20	M	406	CDL	C73-C74-C75-C76
12	L	307	PGV	C05-C04-O12-P
13	M	401	BCL	CAA-CBA-CGA-O2A
13	5	103	BCL	C15-C16-C17-C18
13	O	101	BCL	C4-C3-C5-C6
13	2	102	BCL	C4-C3-C5-C6
20	S	104	CDL	C16-C17-C18-C19
20	S	104	CDL	C58-C59-C60-C61
13	F	101	BCL	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	1	105	PGV	O03-C01-C02-O01
12	L	307	PGV	C03-O11-P-O12
12	L	307	PGV	C04-O12-P-O11
20	M	406	CDL	CA2-OA2-PA1-OA5
20	M	412	CDL	CA3-OA5-PA1-OA2
20	O	104	CDL	CB3-OB5-PB2-OB2
20	S	104	CDL	CA2-OA2-PA1-OA5
20	S	104	CDL	CA3-OA5-PA1-OA2
20	U	104	CDL	CB2-OB2-PB2-OB5
20	U	104	CDL	CB3-OB5-PB2-OB2
20	1	104	CDL	CB2-OB2-PB2-OB5
19	J	101	CRT	C3-C1-C4-C5
19	0	101	CRT	C3-C1-C4-C5
12	C	508	PGV	C3-C4-C5-C6
13	I	101	BCL	C11-C10-C8-C7
13	S	101	BCL	C11-C10-C8-C7
13	I	101	BCL	C11-C10-C8-C9
13	2	102	BCL	C14-C13-C15-C16
20	S	104	CDL	C71-CB7-OB8-CB6
12	L	307	PGV	C27-C28-C29-C30
19	B	101	CRT	O1-C1-C4-C5
12	M	411	PGV	C28-C29-C30-C31
19	V	101	CRT	C10-C11-C12-C13
20	D	105	CDL	C73-C74-C75-C76
13	Y	103	BCL	CBA-CGA-O2A-C1
12	M	411	PGV	C20-C21-C22-C23
20	D	105	CDL	C71-CB7-OB8-CB6
12	L	307	PGV	O04-C19-O03-C01
20	H	305	CDL	C79-C80-C81-C82
13	2	102	BCL	O1A-CGA-O2A-C1
8	C	504	HEC	CAD-CBD-CGD-O1D
20	Y	104	CDL	OB5-CB3-CB4-CB6
20	O	104	CDL	C37-C38-C39-C40
20	M	406	CDL	C77-C78-C79-C80
13	Y	101	BCL	C4-C3-C5-C6
13	K	101	BCL	C2-C1-O2A-CGA
8	C	501	HEC	CAA-CBA-CGA-O2A
8	C	502	HEC	CAA-CBA-CGA-O1A
8	C	502	HEC	CAD-CBD-CGD-O1D
8	C	503	HEC	C4C-C3C-CAC-CBC
13	L	302	BCL	C2A-CAA-CBA-CGA
13	P	102	BCL	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	L	307	PGV	C28-C29-C30-C31
13	1	101	BCL	C11-C10-C8-C9
13	4	102	BCL	C14-C13-C15-C16
8	C	501	HEC	CAA-CBA-CGA-O1A
14	L	303	BPH	O2A-C1-C2-C3
19	T	101	CRT	C5-C6-C7-C8
13	L	305	BCL	C3-C5-C6-C7
13	O	101	BCL	C15-C16-C17-C18
8	C	502	HEC	CAA-CBA-CGA-O2A
13	K	103	BCL	C4-C3-C5-C6
13	3	101	BCL	C1A-C2A-CAA-CBA
12	H	303	PGV	C2-C3-C4-C5
13	L	305	BCL	C12-C13-C15-C16
13	A	101	BCL	C6-C7-C8-C10
13	K	103	BCL	C11-C10-C8-C7
13	S	103	BCL	C6-C7-C8-C10
13	4	102	BCL	C11-C12-C13-C15
13	7	103	BCL	C11-C12-C13-C15
20	S	104	CDL	C40-C41-C42-C43
8	C	504	HEC	CAD-CBD-CGD-O2D
20	D	104	CDL	C32-C31-CA7-OA8
12	M	410	PGV	C31-C32-C33-C34
12	9	104	PGV	C02-C03-O11-P
13	K	101	BCL	C15-C16-C17-C18
21	K	104	PEF	C11-C10-O2-C2
13	5	103	BCL	C4-C3-C5-C6
20	H	305	CDL	OA7-CA5-OA6-CA4
12	C	508	PGV	O03-C01-C02-O01
8	C	502	HEC	CAD-CBD-CGD-O2D
12	L	307	PGV	C30-C31-C32-C33
15	L	309	UQ8	C34-C36-C37-C38
13	5	103	BCL	C3-C5-C6-C7
13	S	103	BCL	C4-C3-C5-C6
15	L	309	UQ8	C30-C29-C31-C32
15	L	309	UQ8	C20-C19-C21-C22
13	F	103	BCL	C2-C1-O2A-CGA
13	P	102	BCL	C2-C1-O2A-CGA
13	3	101	BCL	C2-C1-O2A-CGA
20	D	105	CDL	OB9-CB7-OB8-CB6
20	D	105	CDL	C61-C62-C63-C64
13	5	101	BCL	C3-C5-C6-C7
20	D	104	CDL	C1-CA2-OA2-PA1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	9	104	PGV	C20-C21-C22-C23
13	K	103	BCL	C15-C16-C17-C18
20	U	104	CDL	CB3-CB4-CB6-OB8
19	V	101	CRT	C5-C6-C7-C9
20	U	104	CDL	C36-C37-C38-C39
13	1	101	BCL	O1A-CGA-O2A-C1
20	S	104	CDL	C32-C31-CA7-OA8
12	M	411	PGV	C22-C23-C24-C25
13	P	102	BCL	C15-C16-C17-C18
20	H	305	CDL	OB5-CB3-CB4-CB6
13	9	103	BCL	C11-C10-C8-C7
13	L	301	BCL	C13-C15-C16-C17
20	U	104	CDL	C72-C71-CB7-OB8
20	O	104	CDL	OA6-CA4-CA6-OA8
13	Q	101	BCL	C3-C5-C6-C7
20	S	104	CDL	C72-C71-CB7-OB8
13	3	101	BCL	CAA-CBA-CGA-O2A
12	L	308	PGV	C22-C23-C24-C25
15	L	309	UQ8	C25-C24-C26-C27
15	L	309	UQ8	C15-C14-C16-C17
15	L	310	UQ8	C15-C14-C16-C17
13	F	101	BCL	C2-C3-C5-C6
13	5	101	BCL	C2-C3-C5-C6
15	L	309	UQ8	C38-C39-C41-C42
15	L	309	UQ8	C28-C29-C31-C32
15	L	309	UQ8	C18-C19-C21-C22
13	4	102	BCL	C11-C12-C13-C14
13	A	103	BCL	C3A-C2A-CAA-CBA
13	Y	103	BCL	C3A-C2A-CAA-CBA
13	2	102	BCL	C3A-C2A-CAA-CBA
13	7	103	BCL	C3A-C2A-CAA-CBA
12	L	307	PGV	O01-C1-C2-C3
14	M	402	BPH	CAD-CBD-CGD-O2D
20	H	305	CDL	CA6-CA4-OA6-CA5
20	O	104	CDL	CA6-CA4-OA6-CA5
22	H	304	LMT	O5B-C1B-O1B-C4'
12	L	308	PGV	O03-C19-C20-C21
15	L	309	UQ8	C29-C31-C32-C33
12	M	411	PGV	C05-C04-O12-P
20	H	305	CDL	OB5-CB3-CB4-OB6
20	O	104	CDL	OB5-CB3-CB4-OB6
12	9	104	PGV	O03-C19-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	7	103	BCL	O2A-C1-C2-C3
12	M	411	PGV	C20-C19-O03-C01
20	D	105	CDL	C76-C77-C78-C79
13	L	305	BCL	CHA-CBD-CGD-O2D
20	M	406	CDL	C74-C75-C76-C77
12	M	410	PGV	O03-C01-C02-O01
20	S	104	CDL	C13-C14-C15-C16
20	U	104	CDL	C40-C41-C42-C43
8	C	504	HEC	CAA-CBA-CGA-O2A
12	3	105	PGV	C9-C10-C11-C12
20	H	305	CDL	C81-C82-C83-C84
14	M	402	BPH	CHA-CBD-CGD-O1D
19	T	101	CRT	C2-C1-C4-C5
20	1	104	CDL	O1-C1-CB2-OB2
20	H	305	CDL	C11-CA5-OA6-CA4
13	D	101	BCL	C6-C7-C8-C10
13	Y	103	BCL	C12-C13-C15-C16
15	L	310	UQ8	C13-C14-C16-C17
20	H	305	CDL	C1-CA2-OA2-PA1
15	L	311	UQ8	C3-C4-O4-C4M
12	L	307	PGV	C22-C23-C24-C25
20	M	406	CDL	C39-C40-C41-C42
8	C	502	HEC	C3D-CAD-CBD-CGD
13	9	103	BCL	C4-C3-C5-C6
12	L	308	PGV	O01-C1-C2-C3
19	T	101	CRT	C27-C28-C30-C31
19	V	101	CRT	C10-C11-C12-C14
19	V	101	CRT	C15-C16-C17-C19
19	4	101	CRT	C15-C16-C17-C19
20	U	104	CDL	CA3-CA4-CA6-OA8
12	L	307	PGV	C03-O11-P-O13
12	H	303	PGV	C04-O12-P-O13
20	M	406	CDL	CA2-OA2-PA1-OA3
20	M	412	CDL	CA3-OA5-PA1-OA3
20	D	104	CDL	CA2-OA2-PA1-OA4
20	U	104	CDL	CA3-OA5-PA1-OA3
20	U	104	CDL	CA3-OA5-PA1-OA4
20	U	104	CDL	CB2-OB2-PB2-OB3
20	1	104	CDL	CB2-OB2-PB2-OB3
20	S	104	CDL	C72-C71-CB7-OB9
20	D	105	CDL	OA5-CA3-CA4-CA6
20	M	406	CDL	C72-C73-C74-C75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	9	101	BCL	C10-C11-C12-C13
12	L	307	PGV	O02-C1-C2-C3
13	L	301	BCL	C16-C17-C18-C19
12	L	308	PGV	O04-C19-C20-C21
12	9	104	PGV	O04-C19-C20-C21
15	L	309	UQ8	C23-C24-C26-C27
13	D	101	BCL	C16-C17-C18-C20
13	Y	103	BCL	C16-C17-C18-C19
8	C	504	HEC	CAA-CBA-CGA-O1A
20	O	104	CDL	CA3-CA4-OA6-CA5
12	1	105	PGV	O01-C1-C2-C3
13	3	101	BCL	C15-C16-C17-C18
13	O	101	BCL	C6-C7-C8-C9
13	9	103	BCL	C11-C10-C8-C9
20	H	305	CDL	C31-C32-C33-C34
20	U	104	CDL	C32-C31-CA7-OA8
12	M	411	PGV	O04-C19-O03-C01
20	O	104	CDL	CA4-CA3-OA5-PA1
13	A	103	BCL	C4-C3-C5-C6
13	9	101	BCL	C4-C3-C5-C6
13	K	103	BCL	C2-C3-C5-C6
13	O	101	BCL	C2-C3-C5-C6
13	O	101	BCL	C6-C7-C8-C10
13	S	103	BCL	C2-C3-C5-C6
13	Y	101	BCL	C2-C3-C5-C6
13	2	102	BCL	C2-C3-C5-C6
13	4	102	BCL	C12-C13-C15-C16
13	5	103	BCL	C2-C3-C5-C6
13	5	103	BCL	C6-C7-C8-C10
13	5	103	BCL	C11-C12-C13-C15
20	H	305	CDL	C71-C72-C73-C74
20	S	104	CDL	CB7-C71-C72-C73
19	O	103	CRT	C27-C28-C30-C31
19	P	101	CRT	C15-C16-C17-C19
19	2	101	CRT	C10-C11-C12-C14
12	L	308	PGV	O02-C1-C2-C3
12	1	105	PGV	O02-C1-C2-C3
13	3	101	BCL	CAA-CBA-CGA-O1A
13	I	101	BCL	C15-C16-C17-C18
13	F	103	BCL	C15-C16-C17-C18
15	L	310	UQ8	C16-C17-C18-C19
13	Y	101	BCL	C10-C11-C12-C13

There are no ring outliers.

83 monomers are involved in 342 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	0	101	CRT	5	0
20	U	104	CDL	9	0
12	3	105	PGV	6	0
13	D	103	BCL	4	0
19	N	101	CRT	4	0
20	H	305	CDL	6	0
13	Q	103	BCL	2	0
20	O	104	CDL	13	0
22	H	304	LMT	8	0
19	G	101	CRT	5	0
12	D	106	PGV	2	0
20	D	105	CDL	9	0
20	M	412	CDL	2	0
18	M	404	MQ8	5	0
13	U	101	BCL	6	0
13	1	101	BCL	5	0
13	P	102	BCL	5	0
21	K	104	PEF	2	0
20	M	406	CDL	5	0
13	4	102	BCL	6	0
13	L	301	BCL	3	0
13	5	103	BCL	3	0
13	Y	101	BCL	5	0
19	W	102	CRT	1	0
12	L	307	PGV	7	0
14	M	402	BPH	7	0
19	V	101	CRT	3	0
8	C	504	HEC	2	0
13	A	103	BCL	4	0
13	K	101	BCL	5	0
8	C	502	HEC	2	0
13	3	101	BCL	3	0
13	2	102	BCL	10	0
20	Y	104	CDL	3	0
15	L	309	UQ8	10	0
12	9	104	PGV	5	0
13	9	103	BCL	4	0
19	Z	101	CRT	5	0
12	H	303	PGV	2	0
13	S	101	BCL	6	0

Continued on next page...

Continued from previous page...

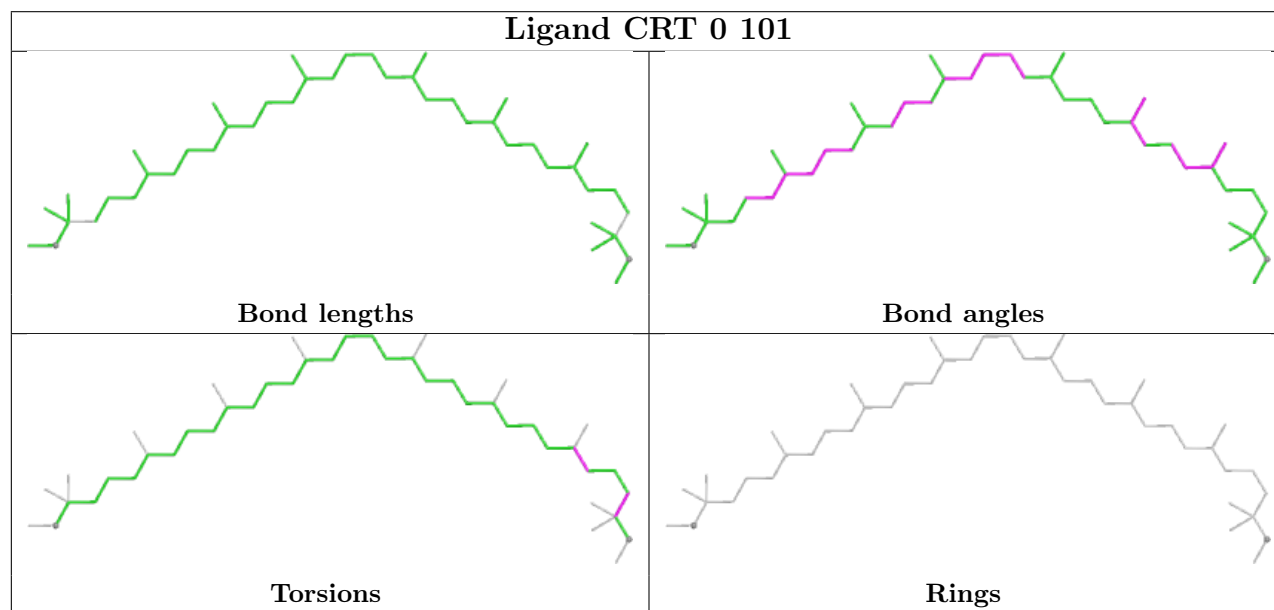
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	W	101	BCL	5	0
8	C	503	HEC	1	0
20	S	104	CDL	12	0
15	L	311	UQ8	2	0
13	I	101	BCL	3	0
13	K	103	BCL	3	0
19	T	101	CRT	3	0
19	4	101	CRT	6	0
13	F	101	BCL	4	0
13	Y	103	BCL	11	0
13	J	102	BCL	3	0
13	L	302	BCL	2	0
15	M	413	UQ8	1	0
10	C	506	GOL	1	0
19	M	405	CRT	7	0
19	2	101	CRT	6	0
21	1	103	PEF	2	0
19	A	104	CRT	8	0
15	L	304	UQ8	1	0
13	7	101	BCL	5	0
19	J	101	CRT	2	0
13	Q	101	BCL	7	0
13	O	101	BCL	6	0
12	1	105	PGV	1	0
12	M	411	PGV	4	0
19	3	103	CRT	2	0
19	P	101	CRT	4	0
13	S	103	BCL	4	0
13	A	101	BCL	5	0
19	8	101	CRT	5	0
13	9	101	BCL	4	0
12	L	308	PGV	5	0
13	L	305	BCL	7	0
13	7	103	BCL	5	0
15	L	310	UQ8	6	0
13	W	104	BCL	6	0
13	5	101	BCL	3	0
13	U	103	BCL	6	0
19	B	101	CRT	6	0
12	M	410	PGV	4	0
13	F	103	BCL	7	0
14	L	303	BPH	4	0

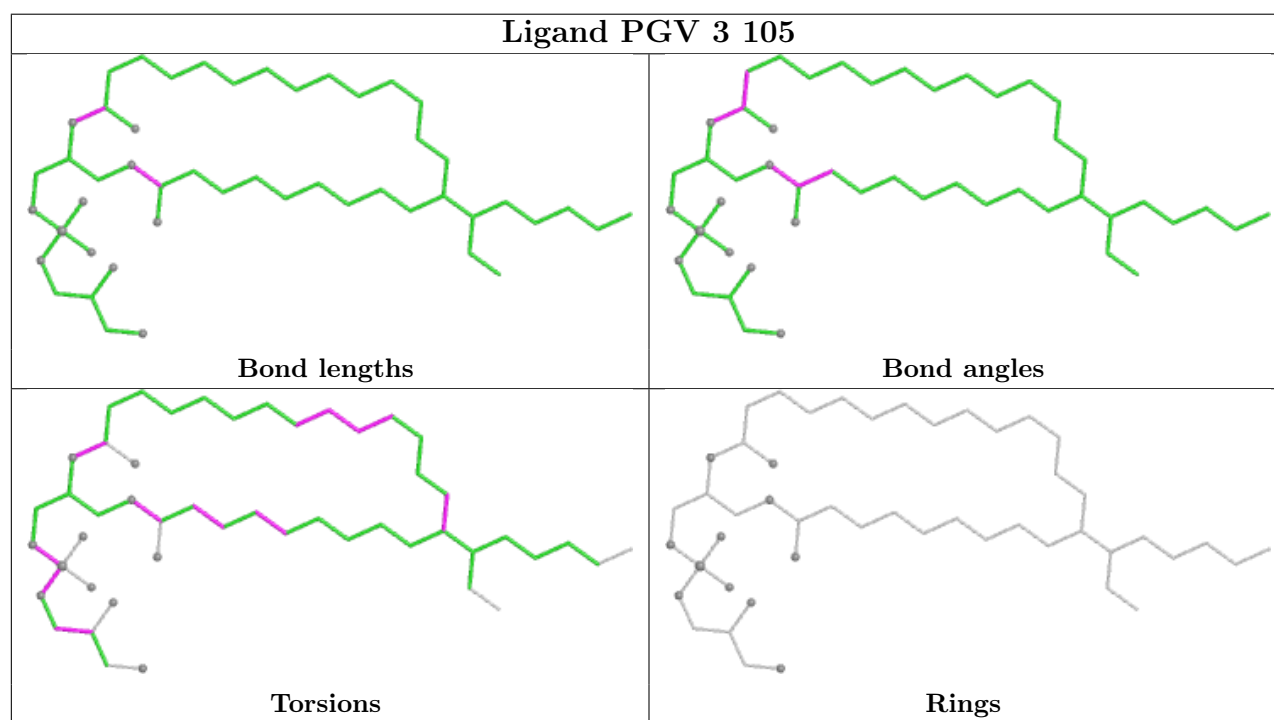
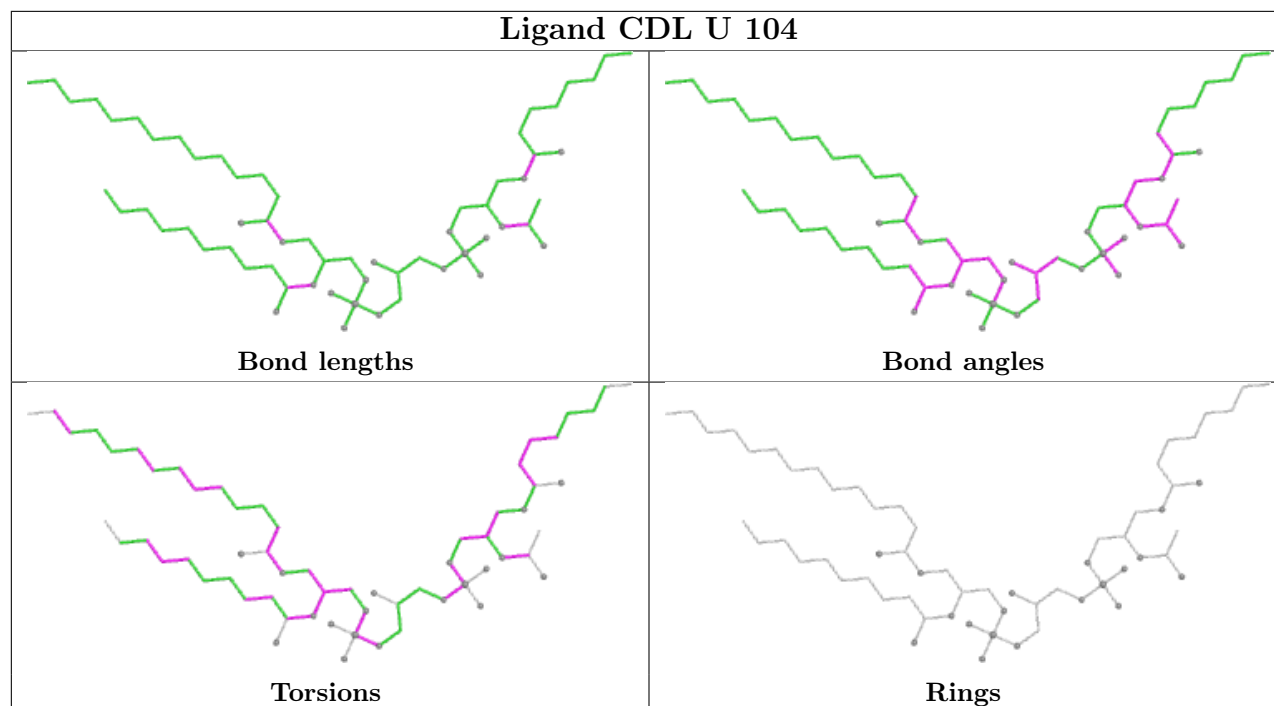
Continued on next page...

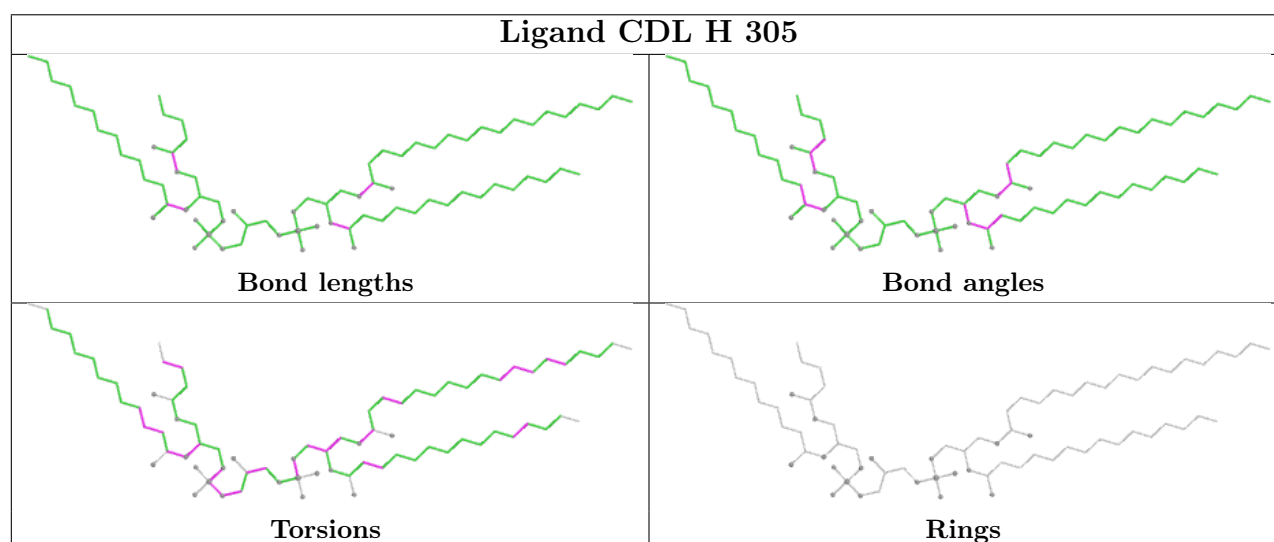
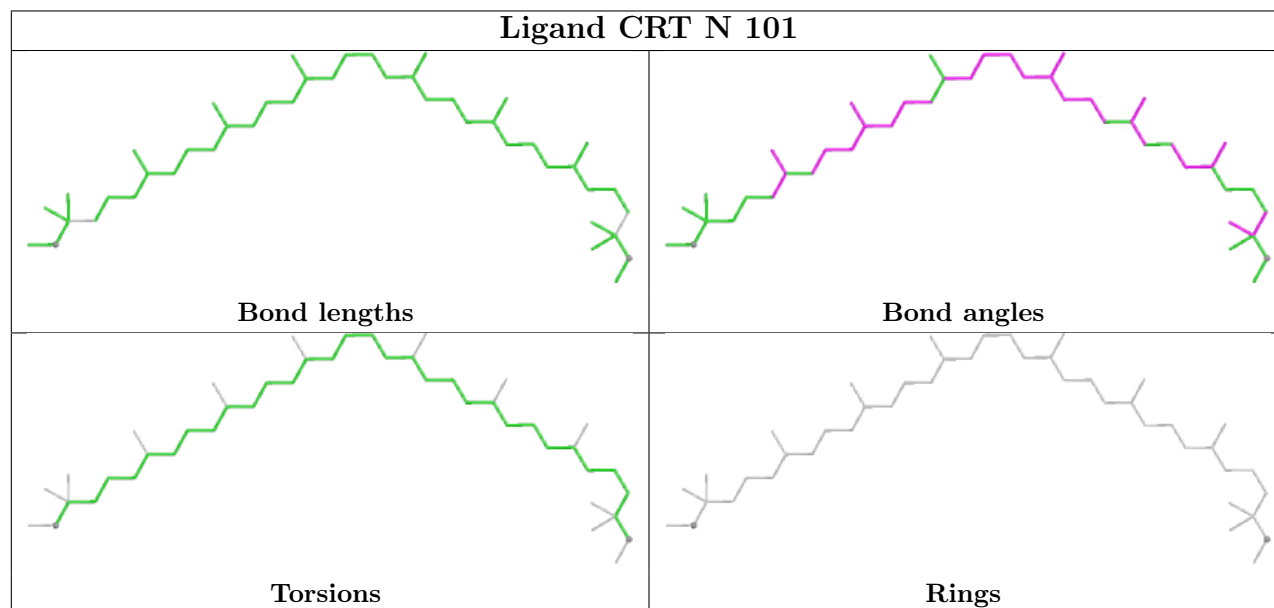
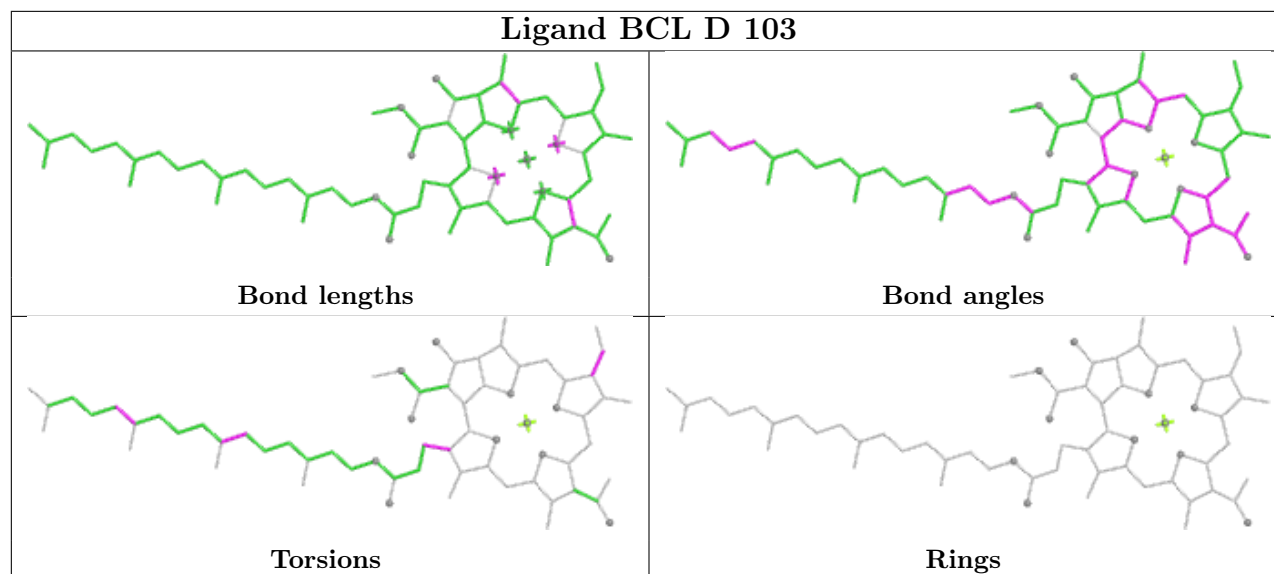
Continued from previous page...

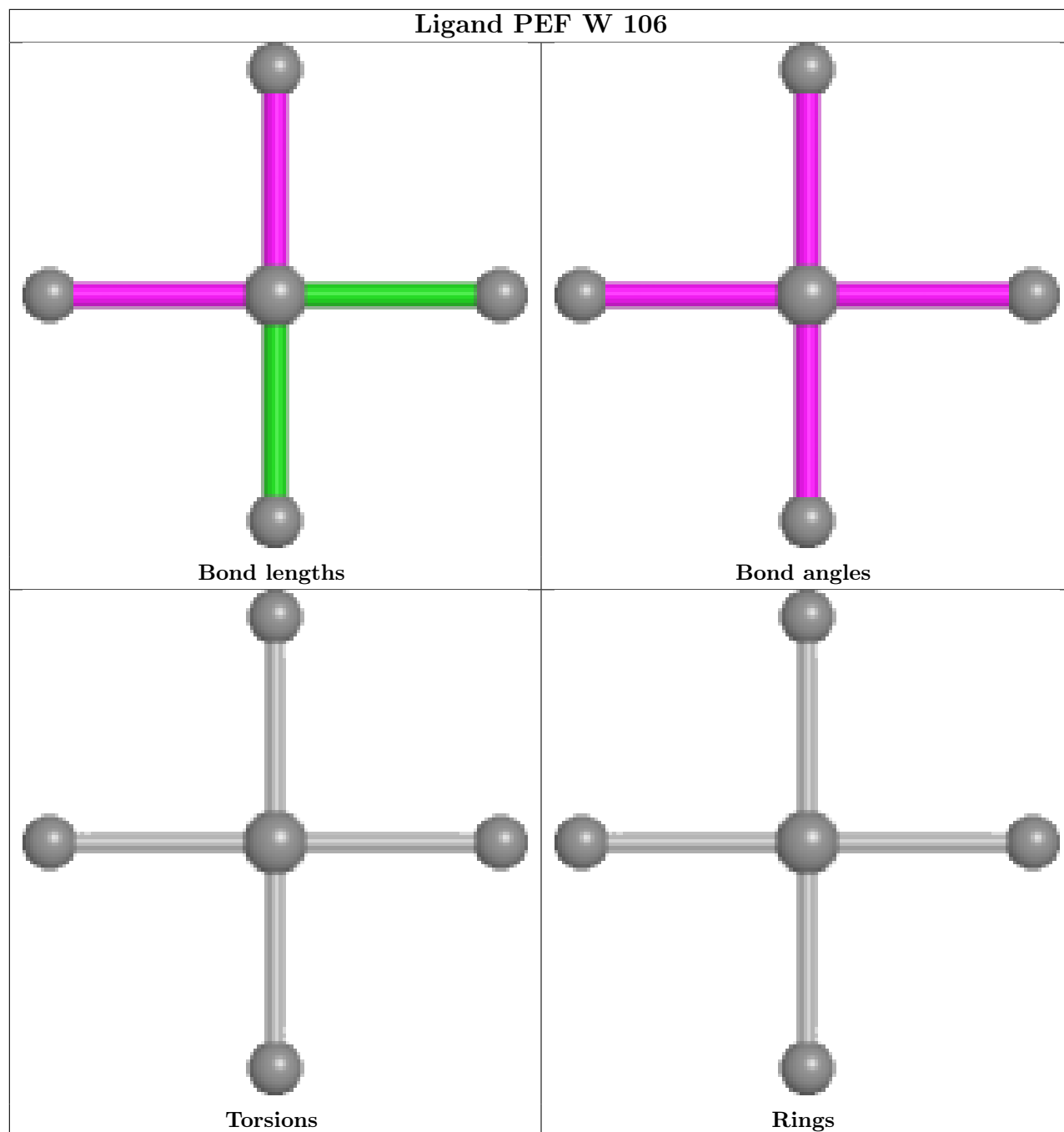
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	D	104	CDL	1	0

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

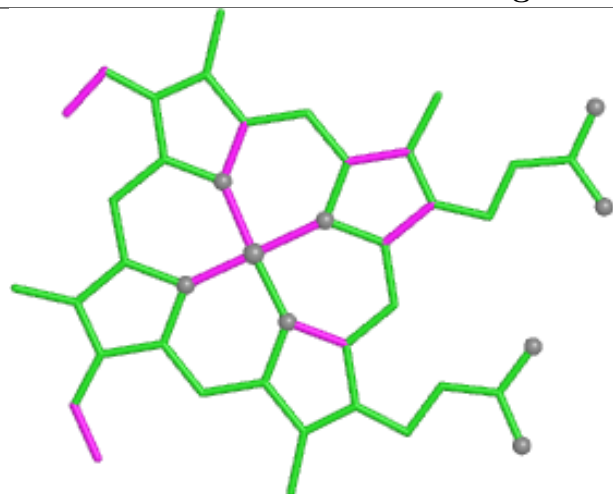




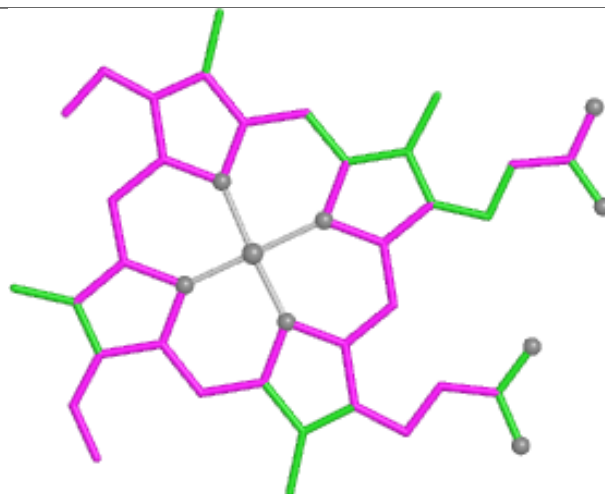




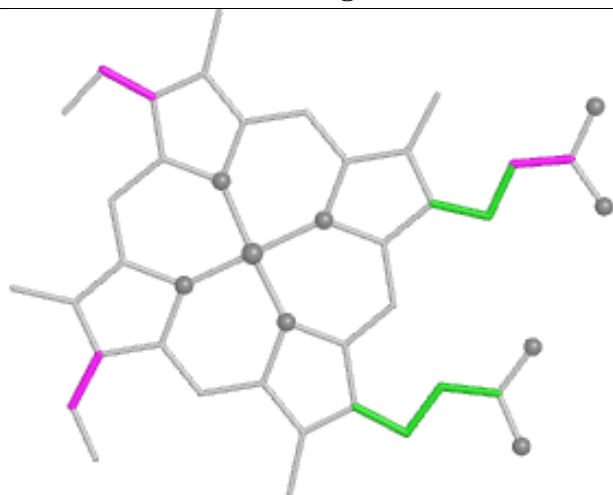
Ligand HEC C 501



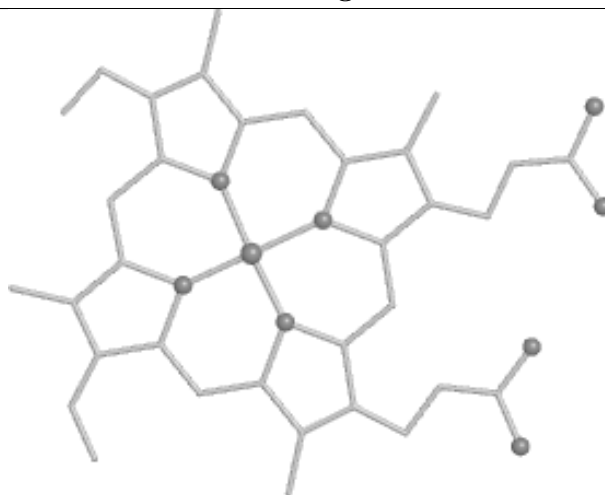
Bond lengths



Bond angles

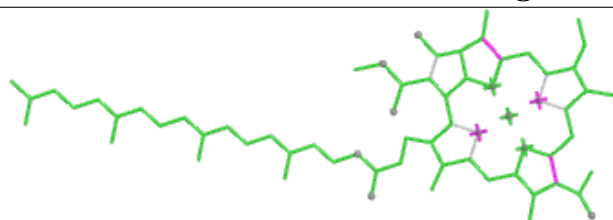


Torsions

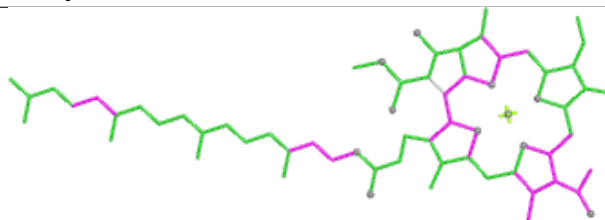


Rings

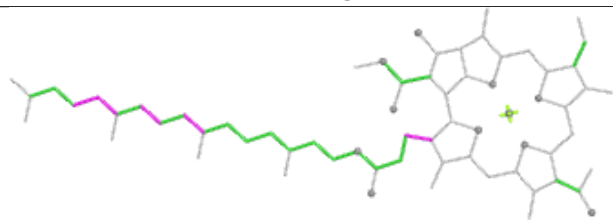
Ligand BCL Q 103



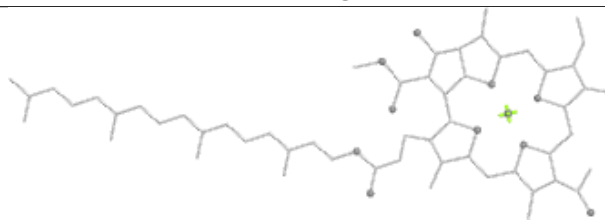
Bond lengths



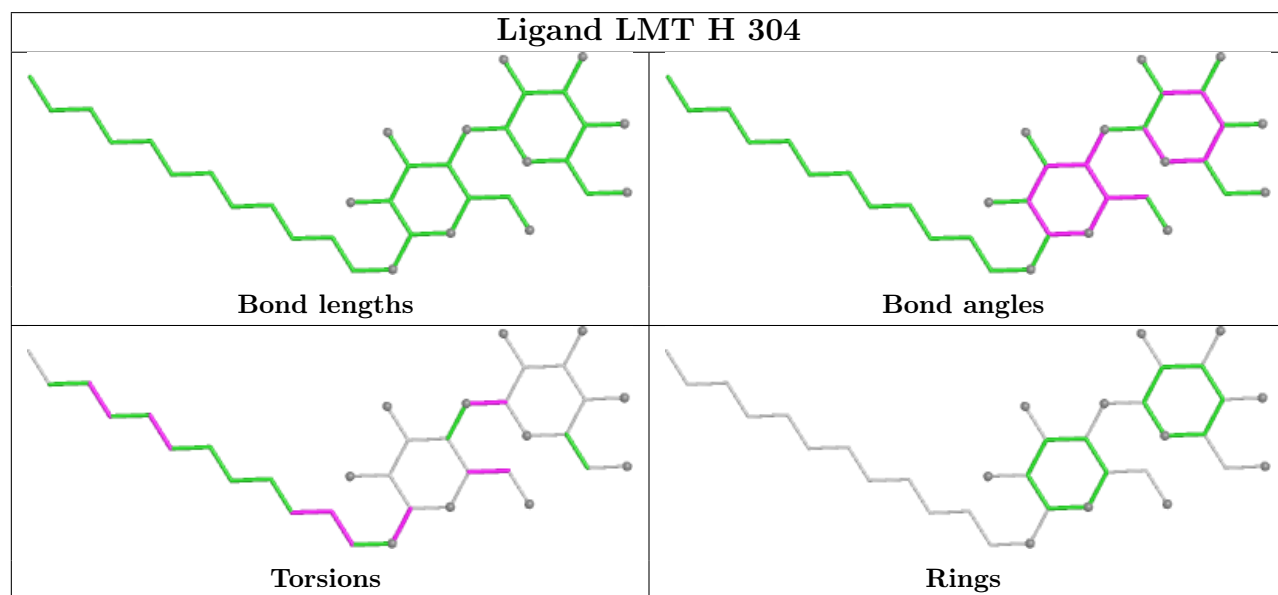
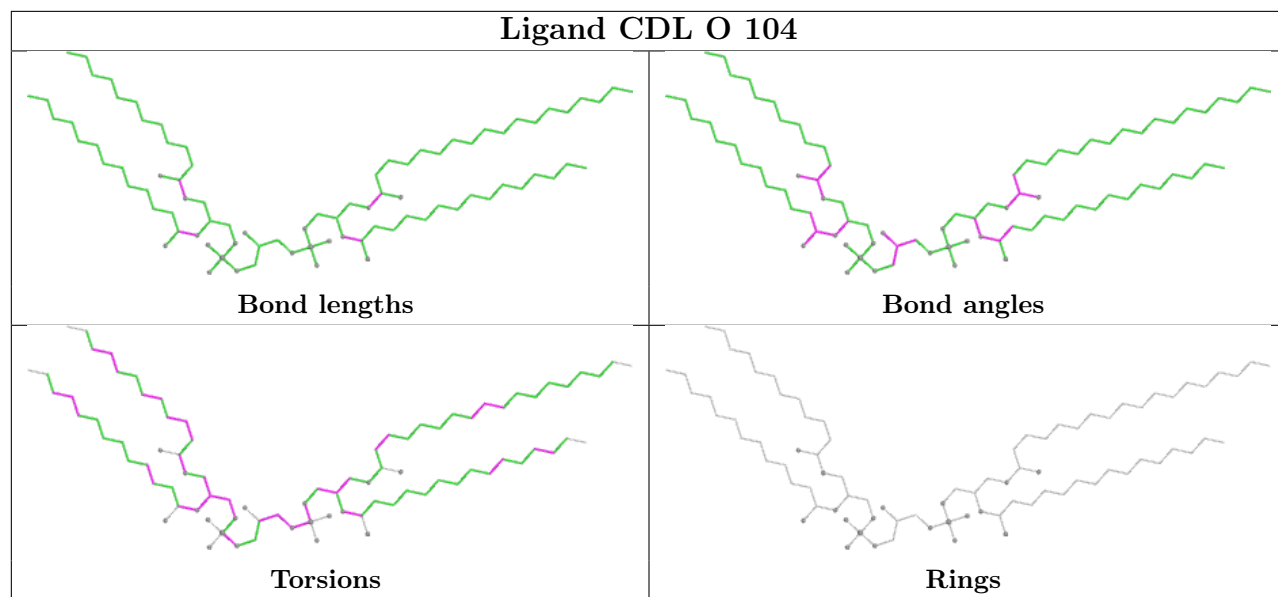
Bond angles

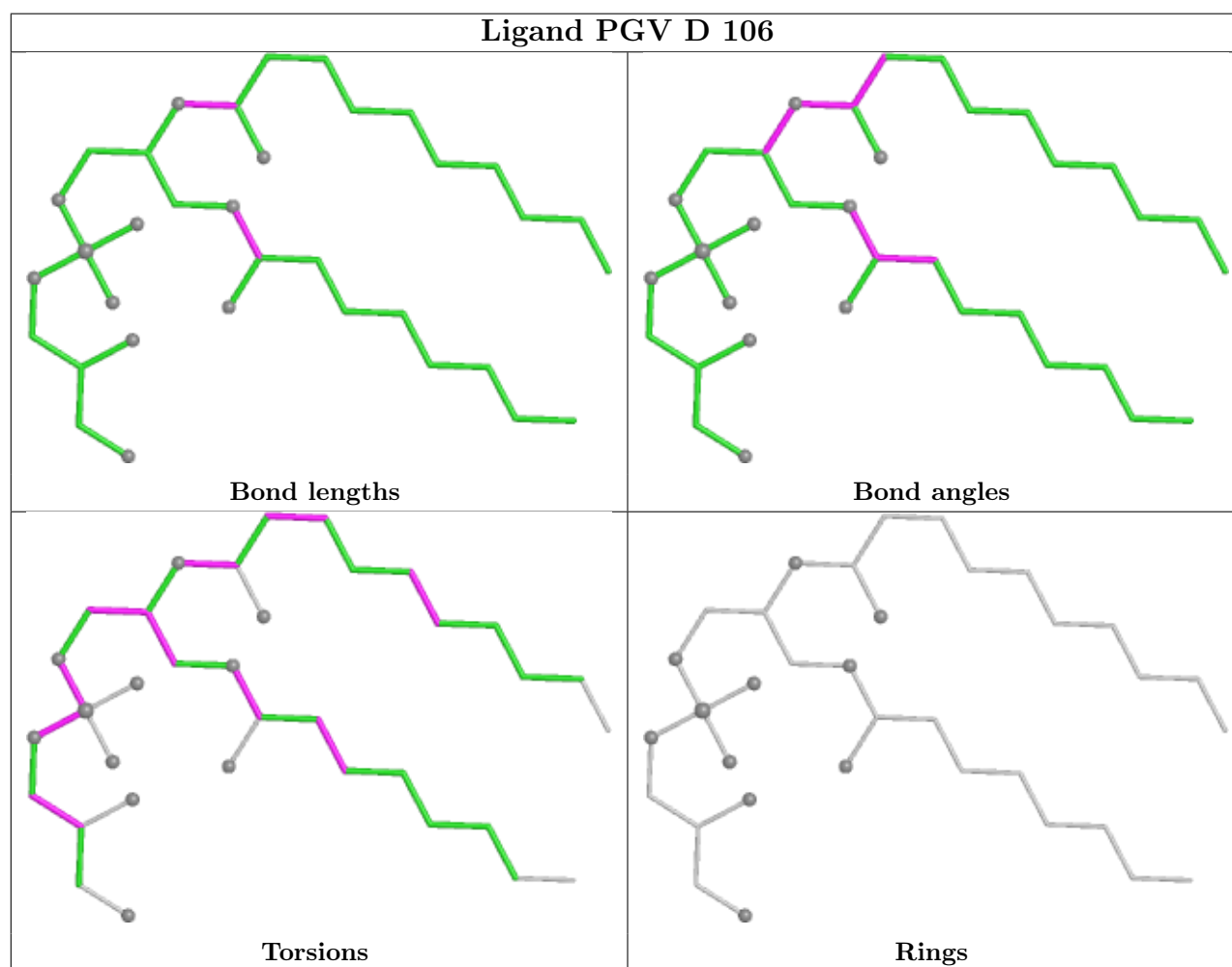
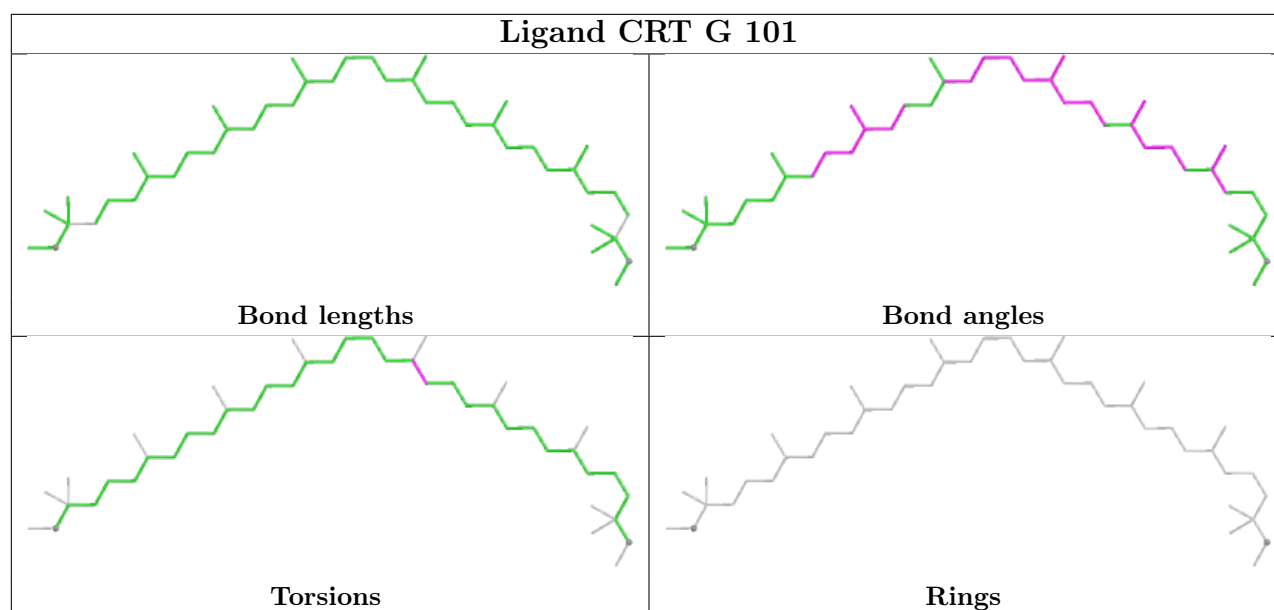


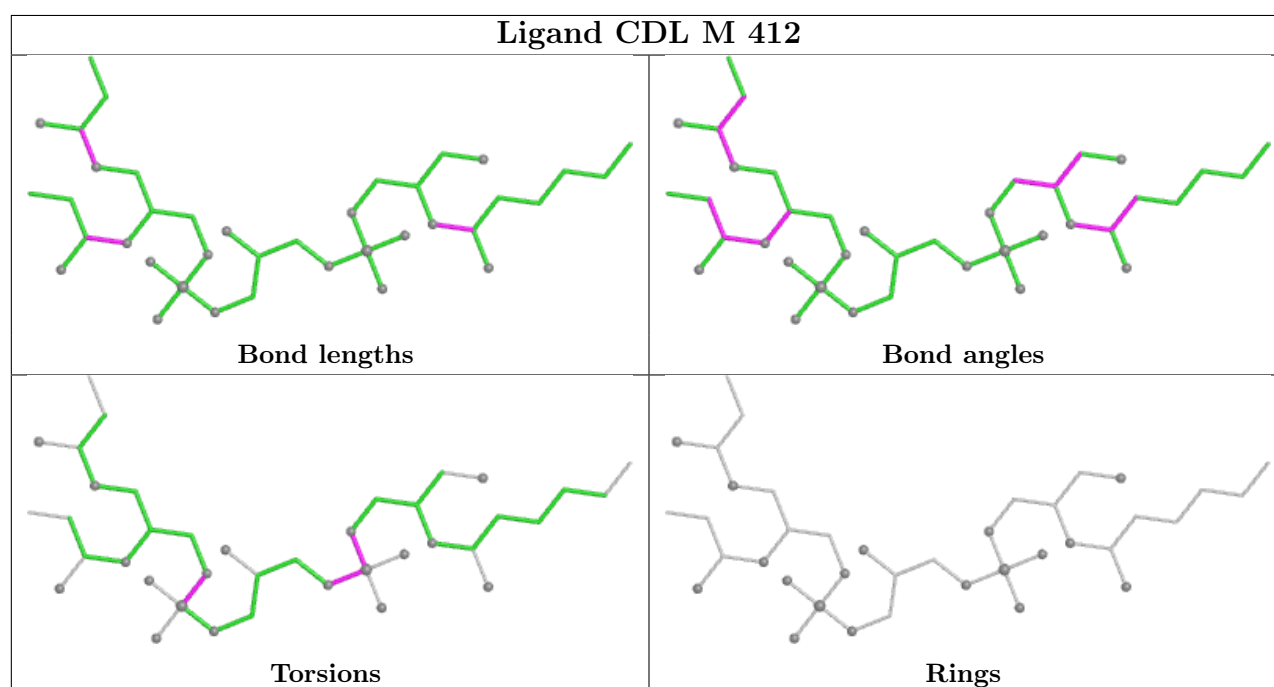
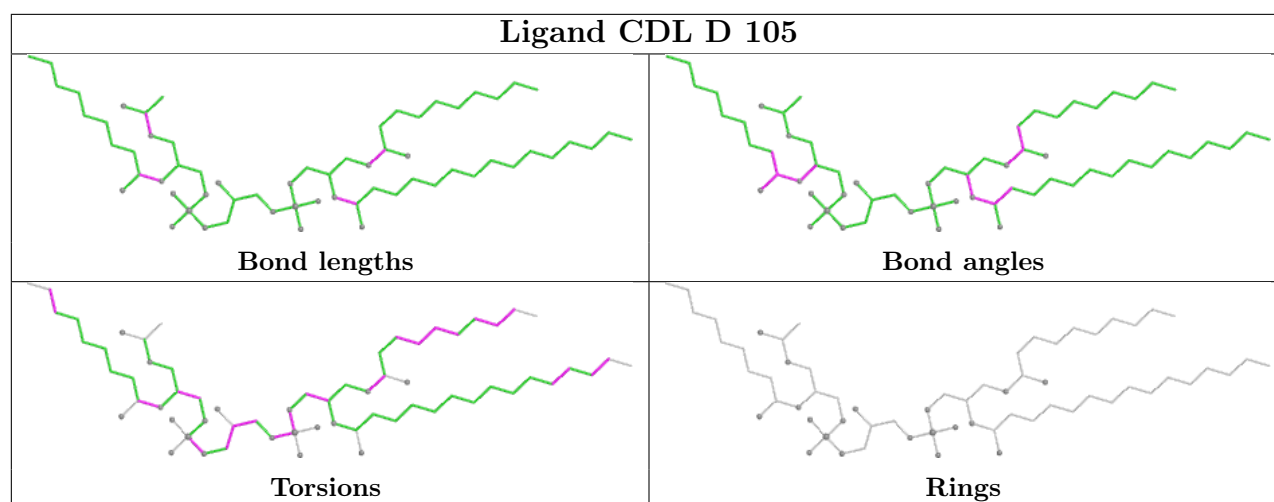
Torsions

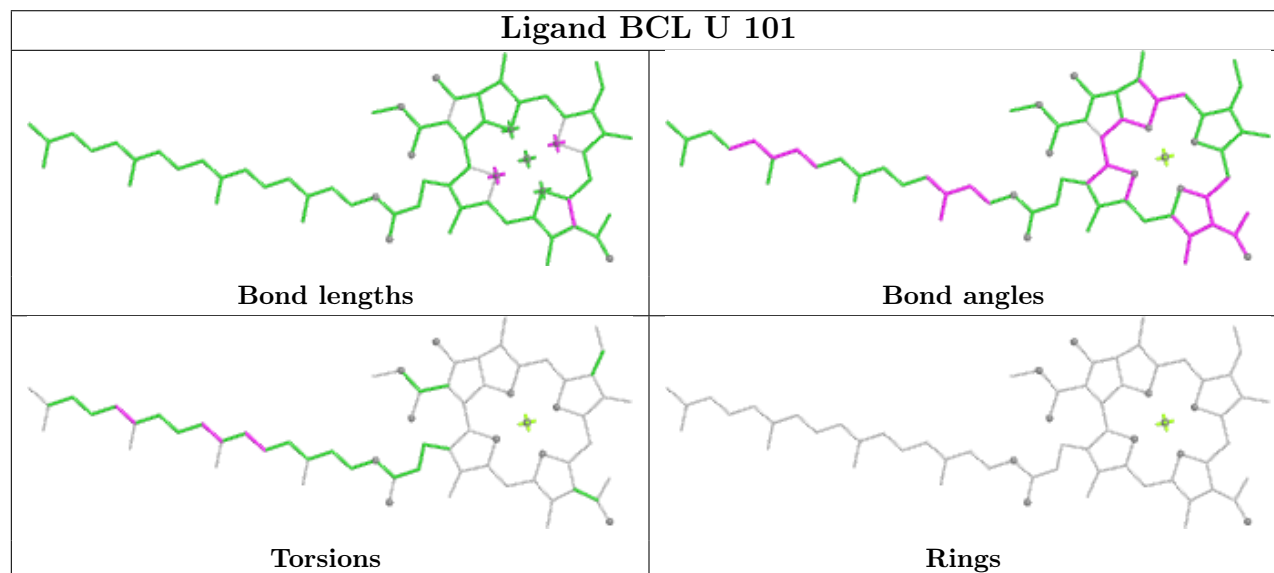
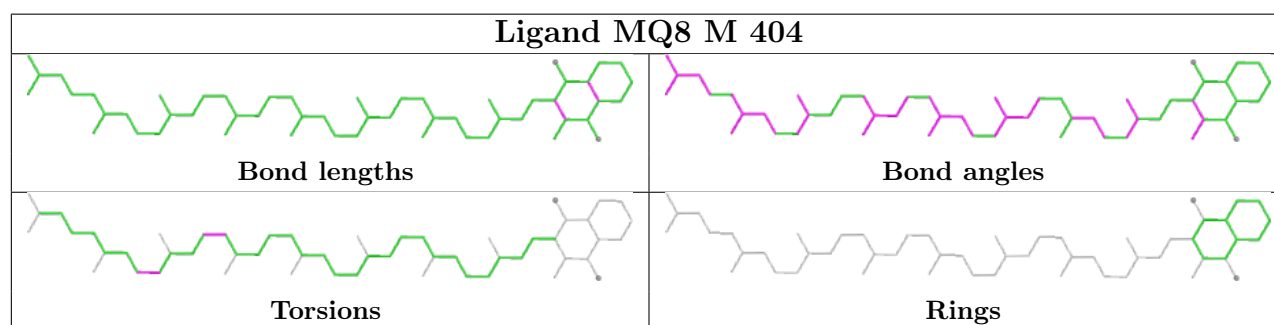
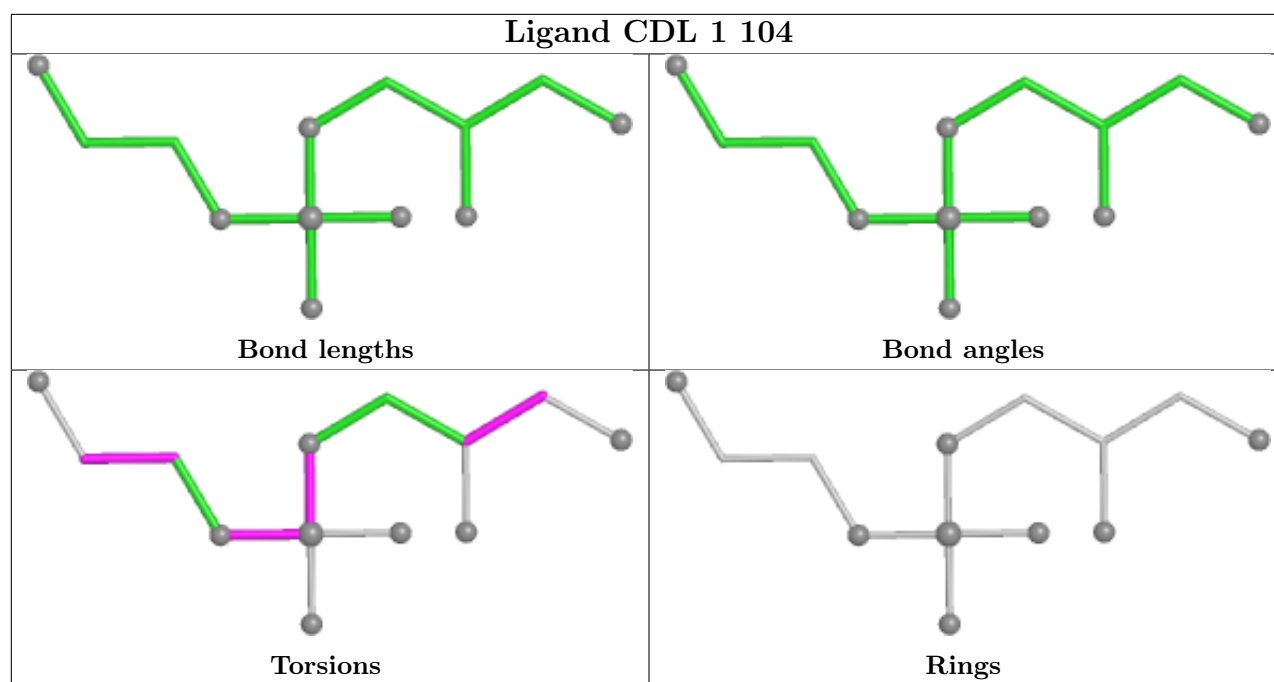


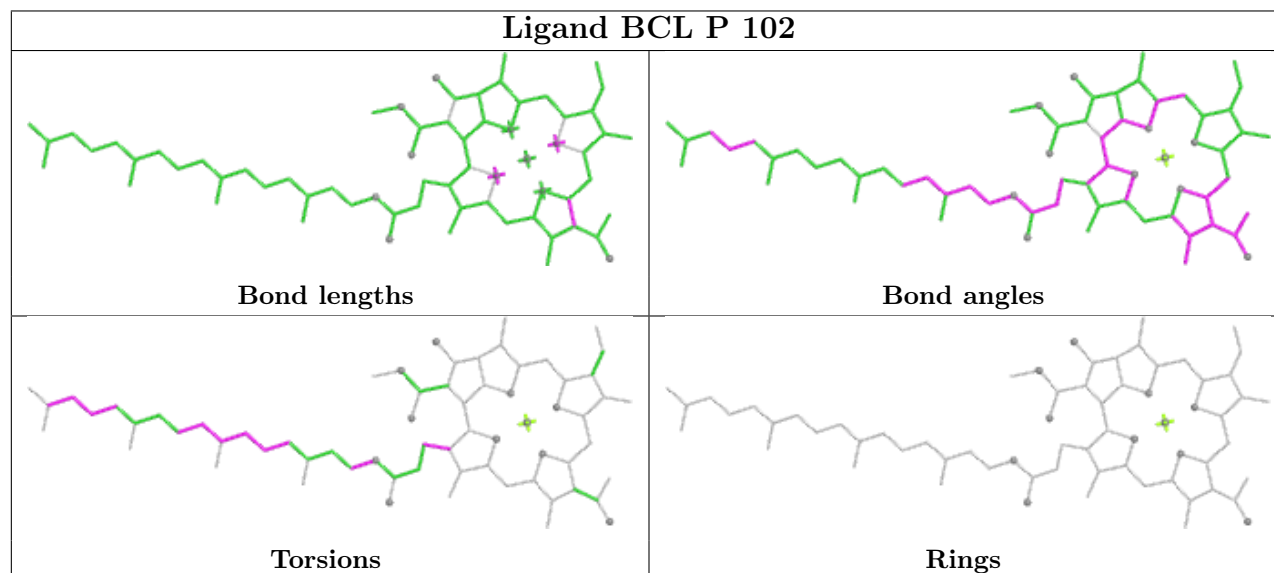
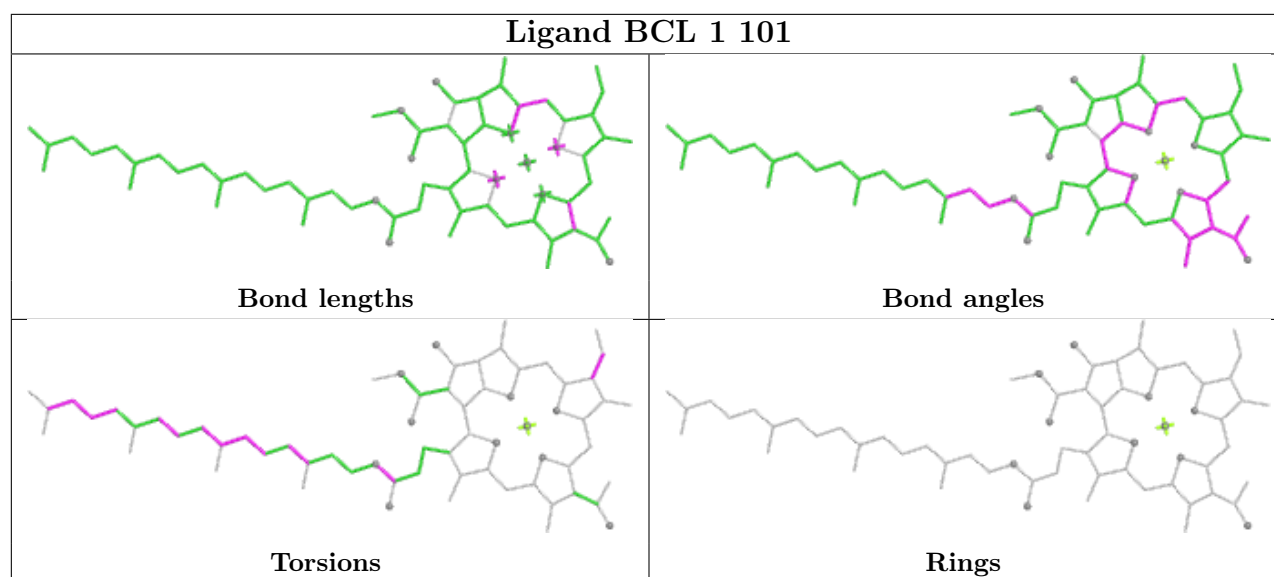
Rings

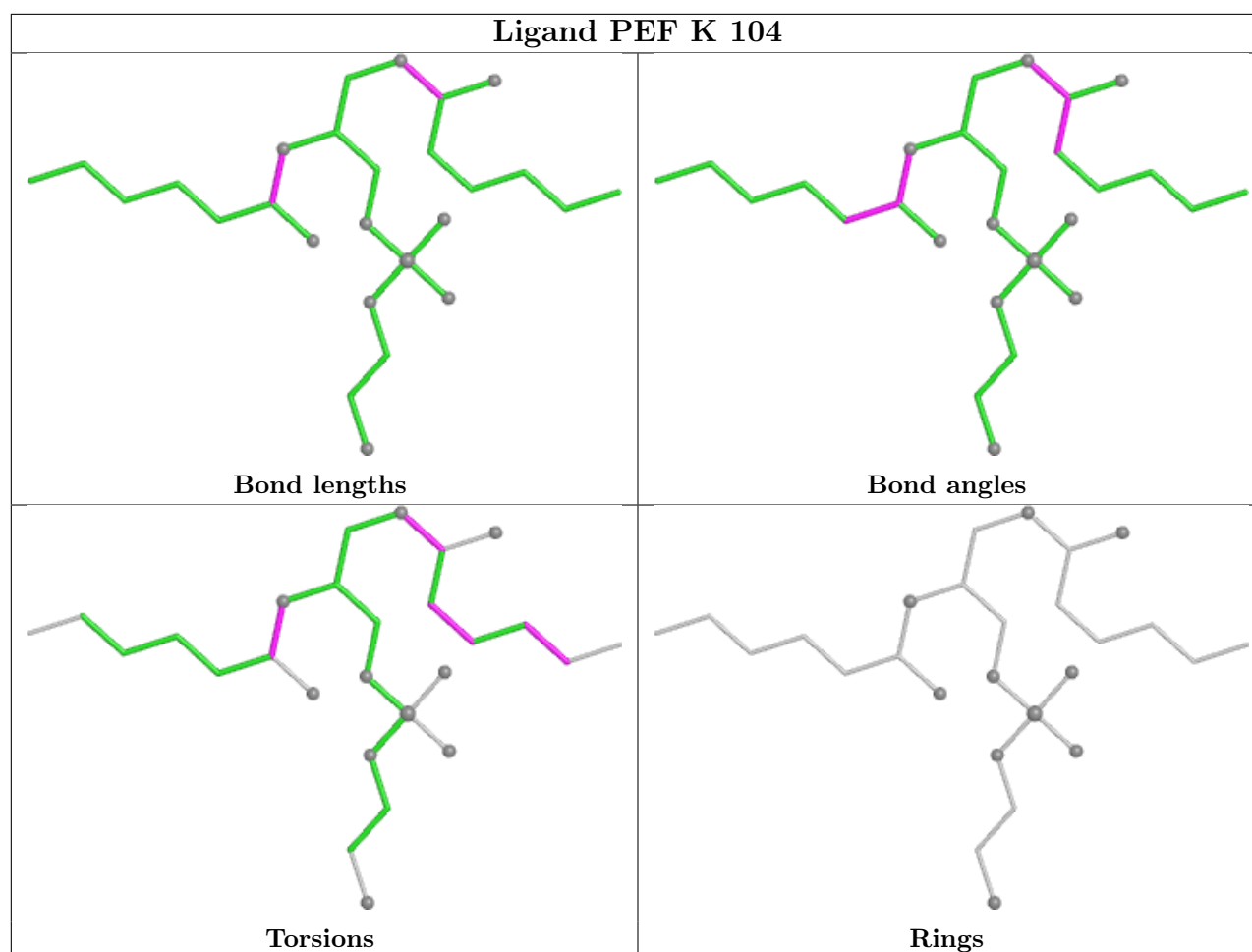


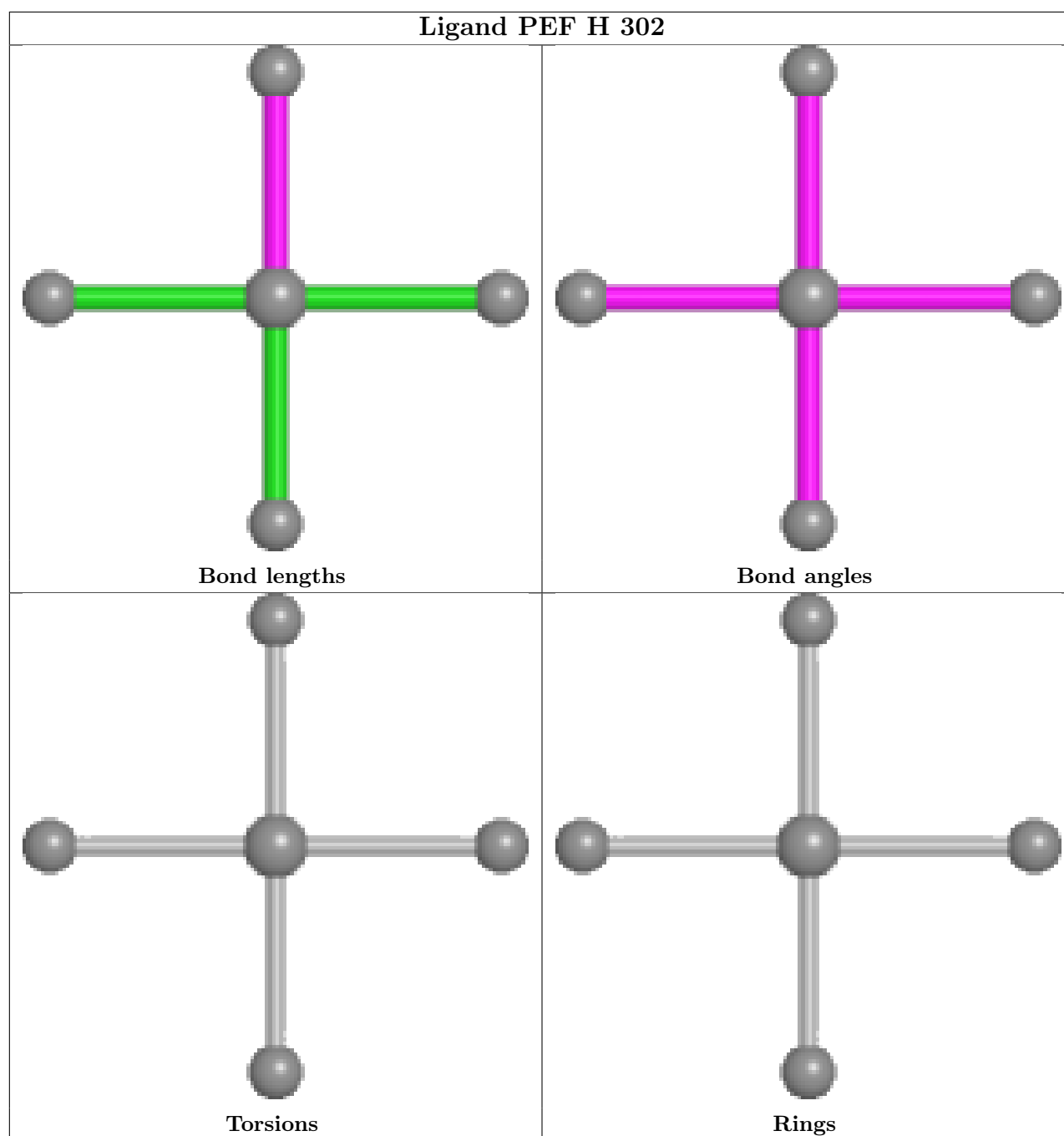


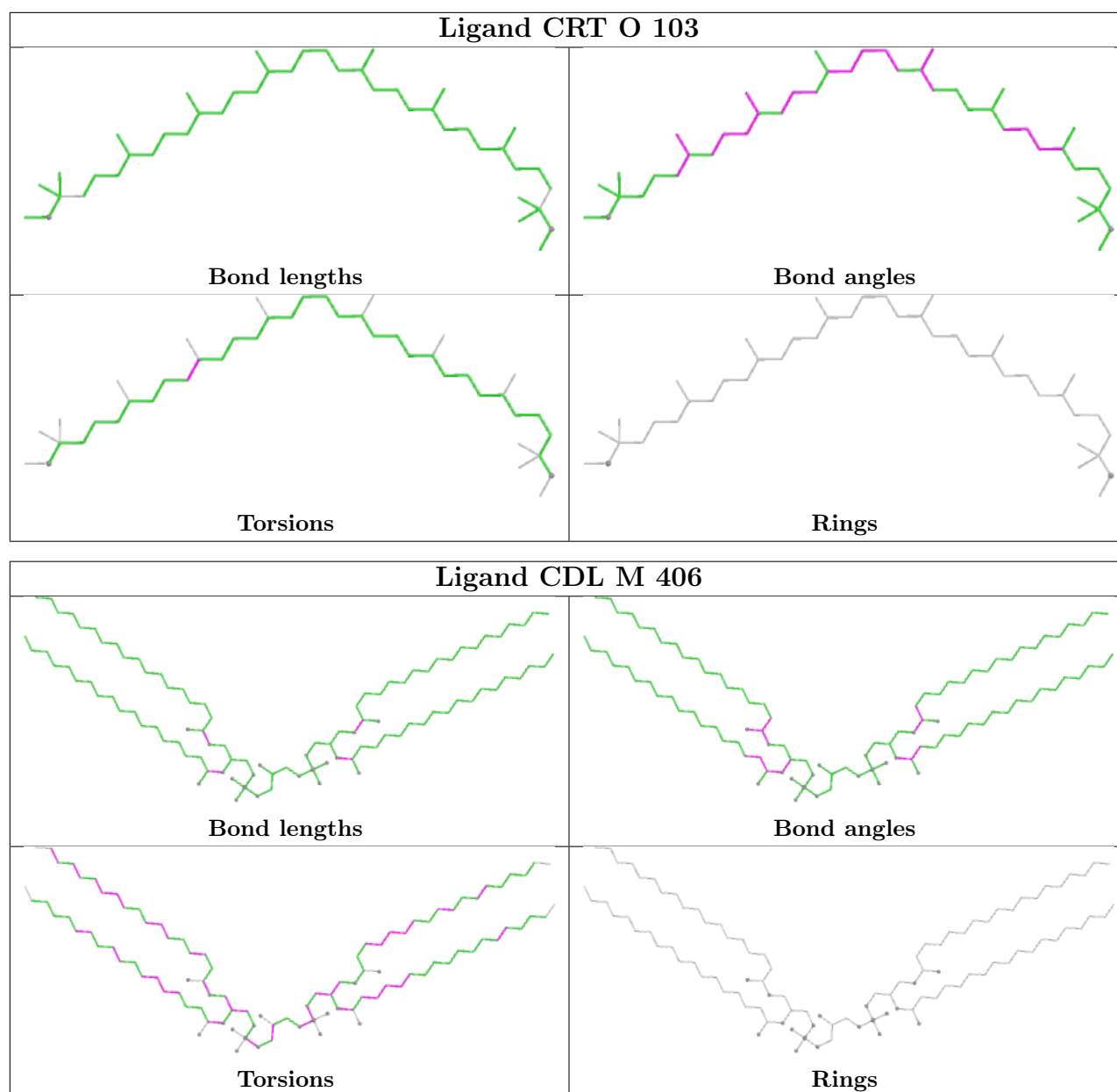


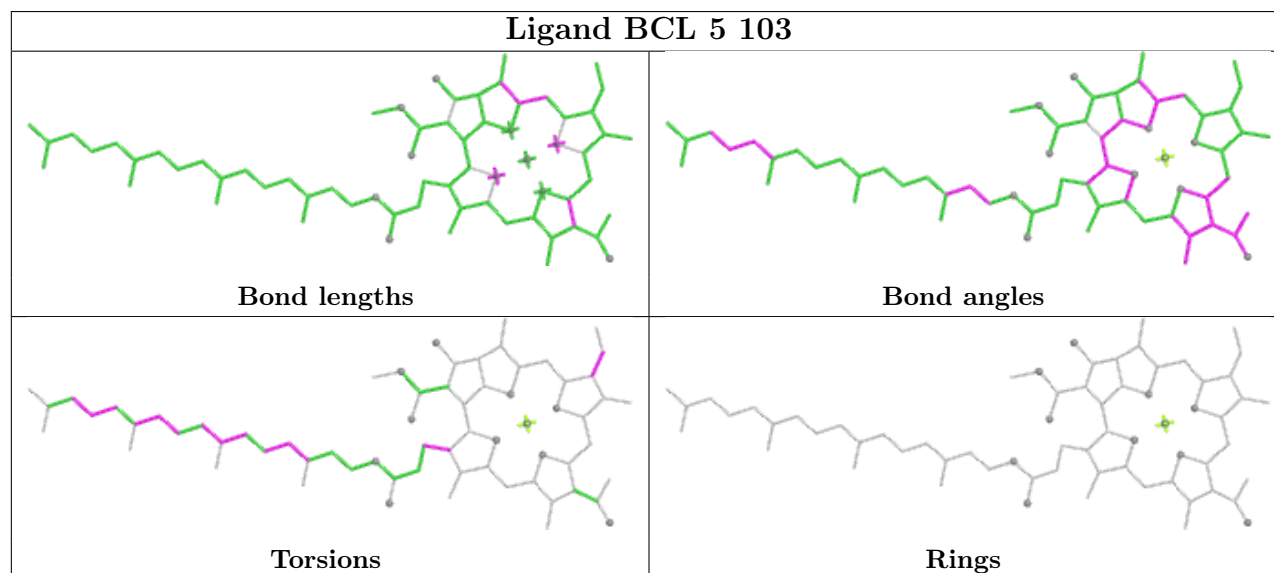
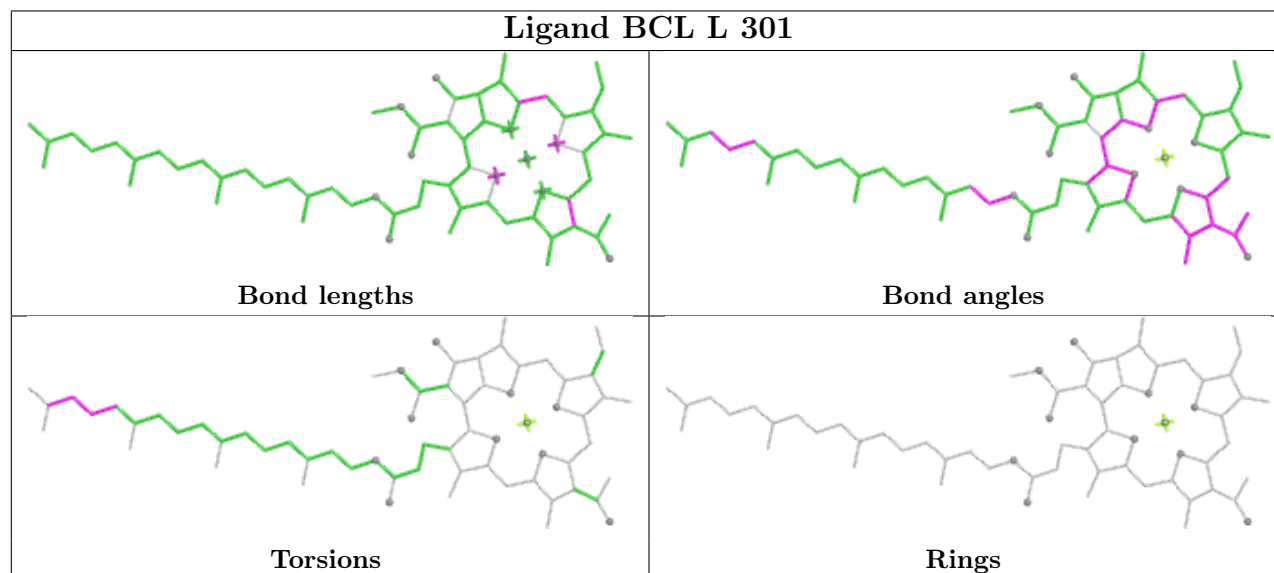
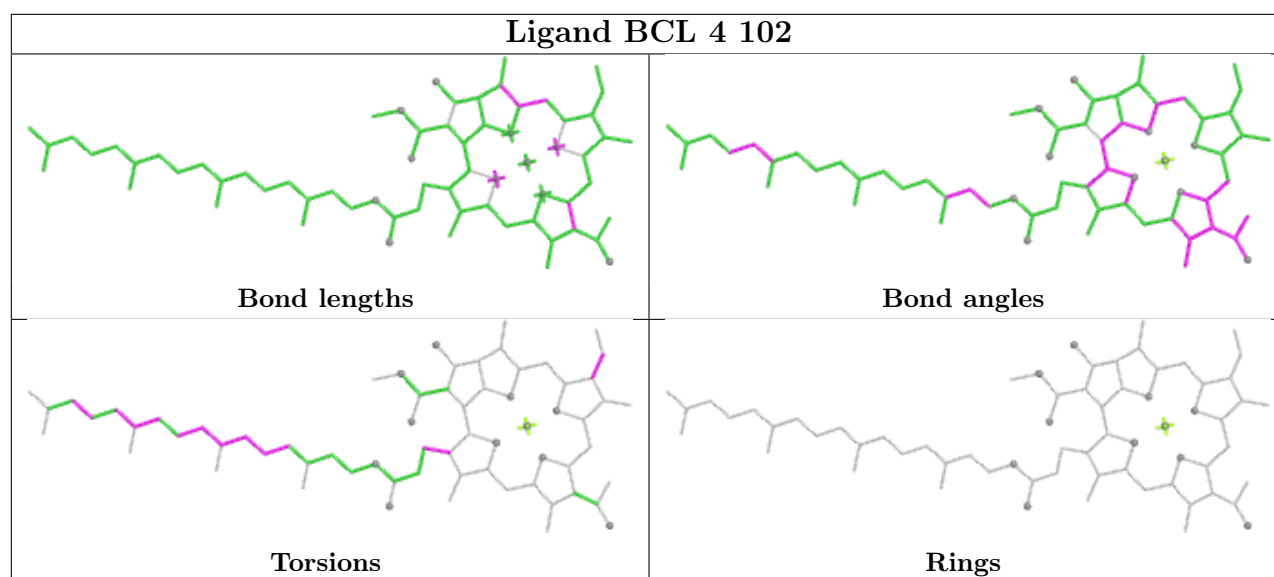


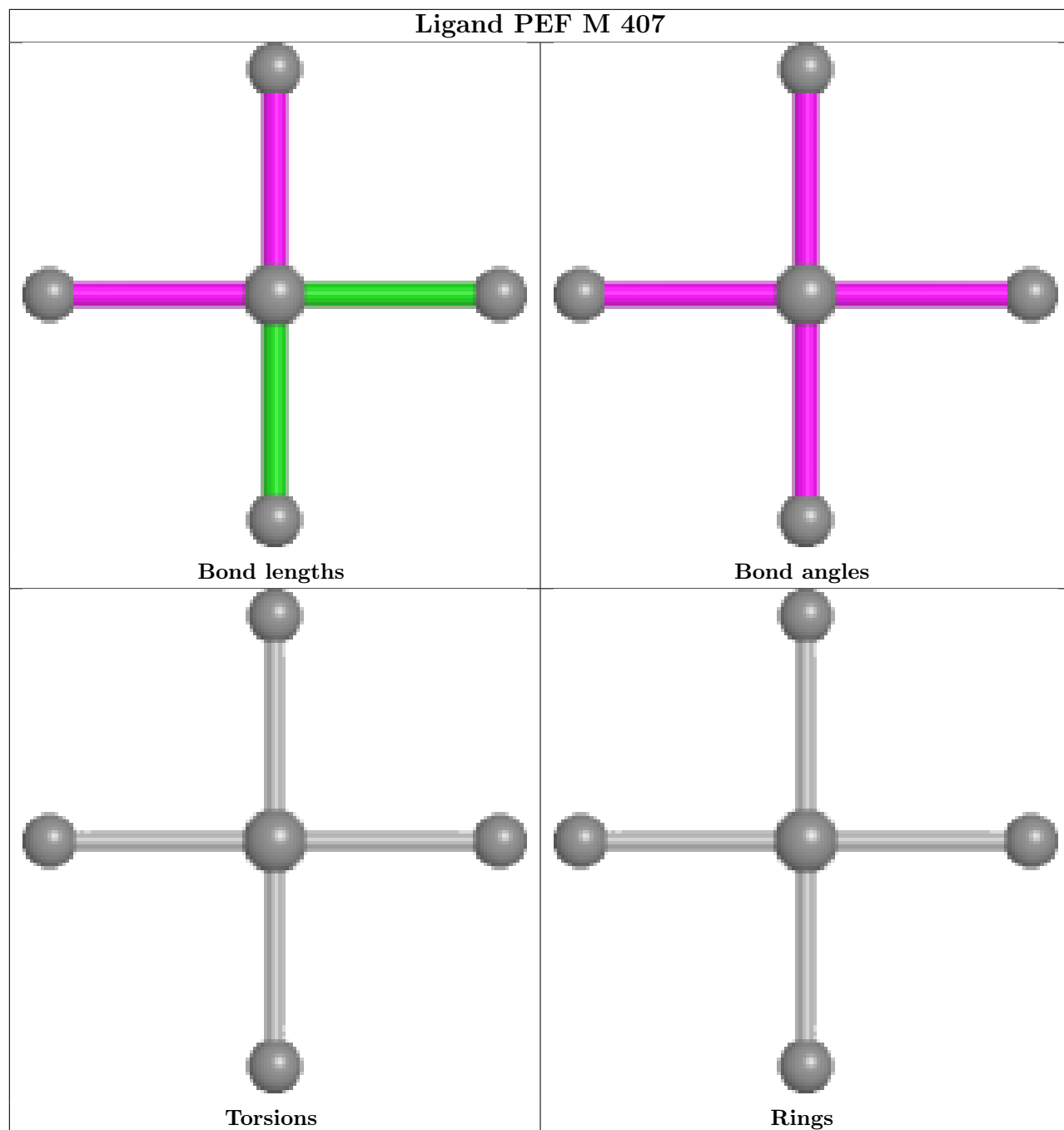


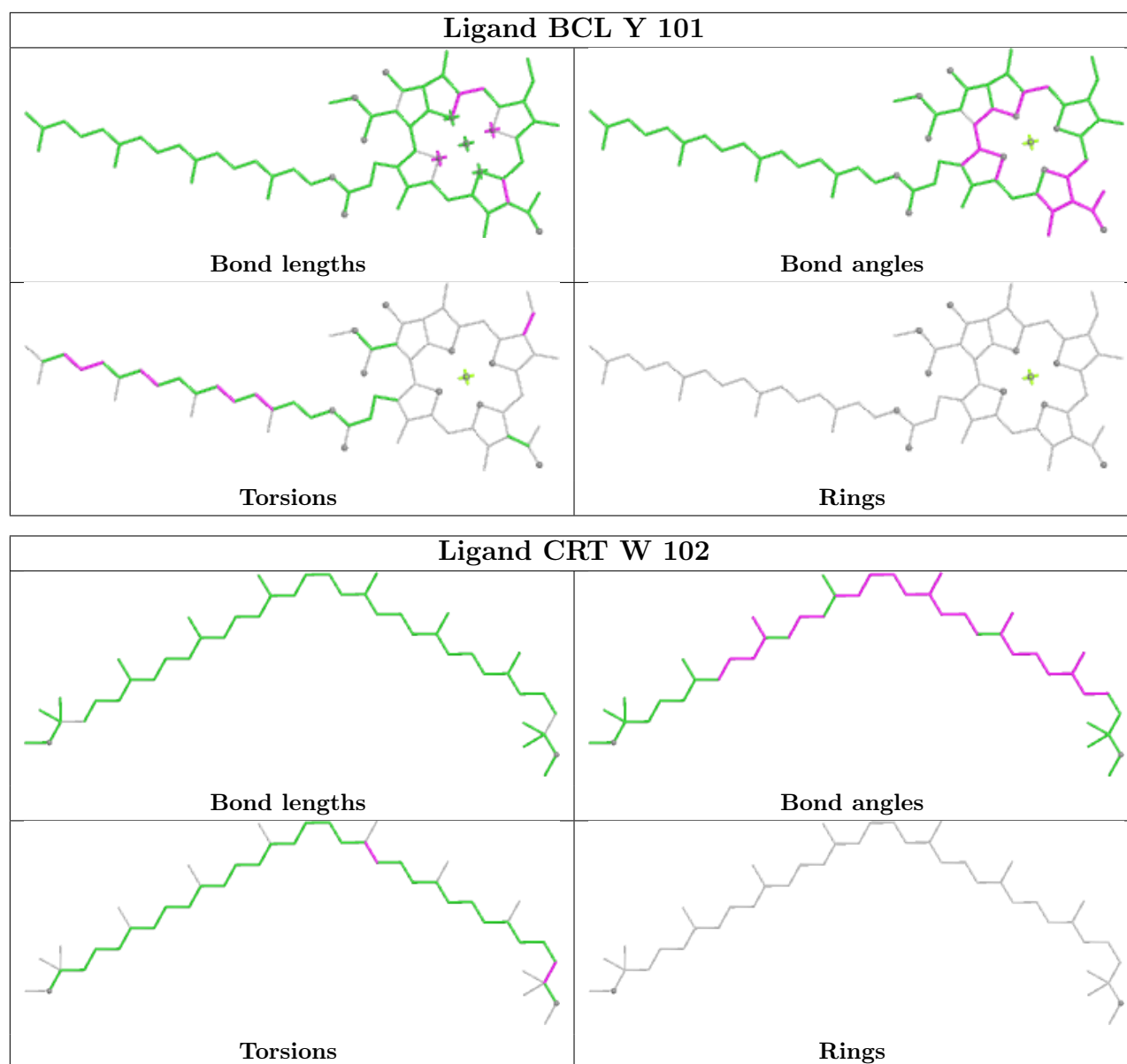


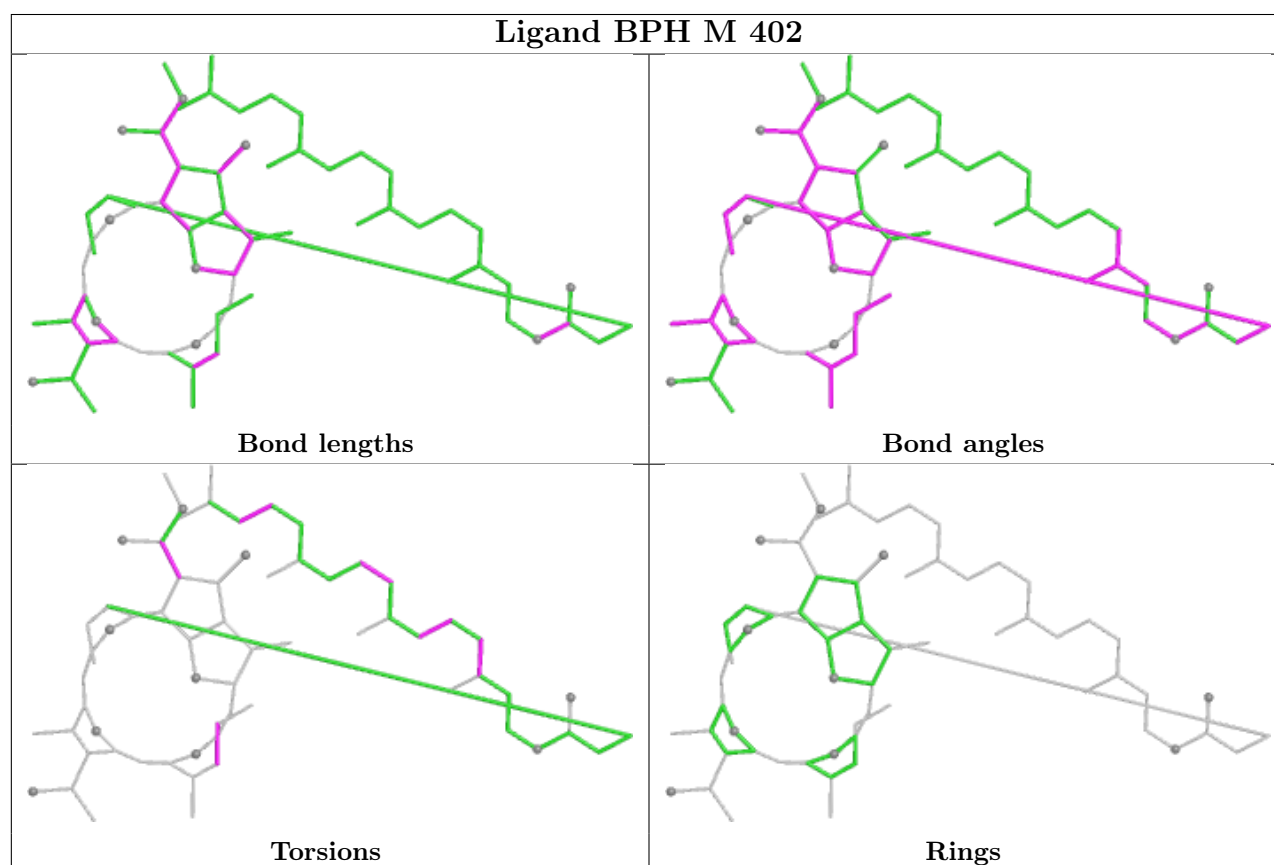
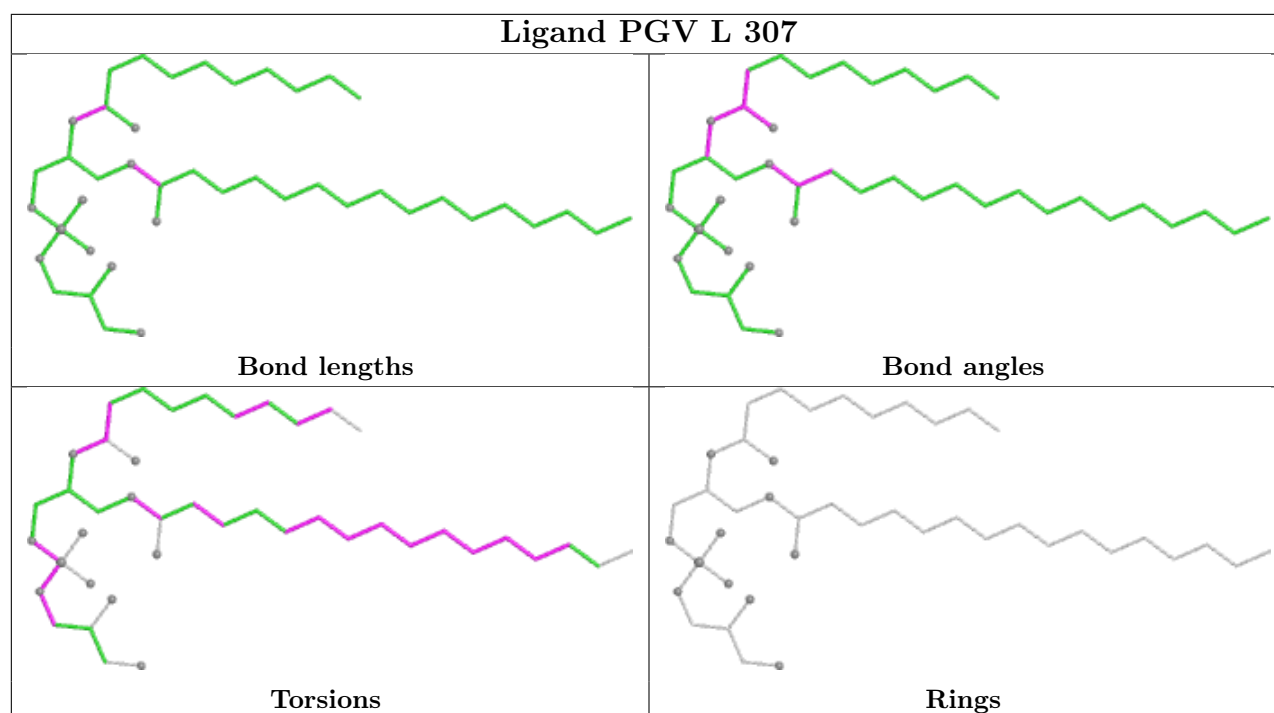


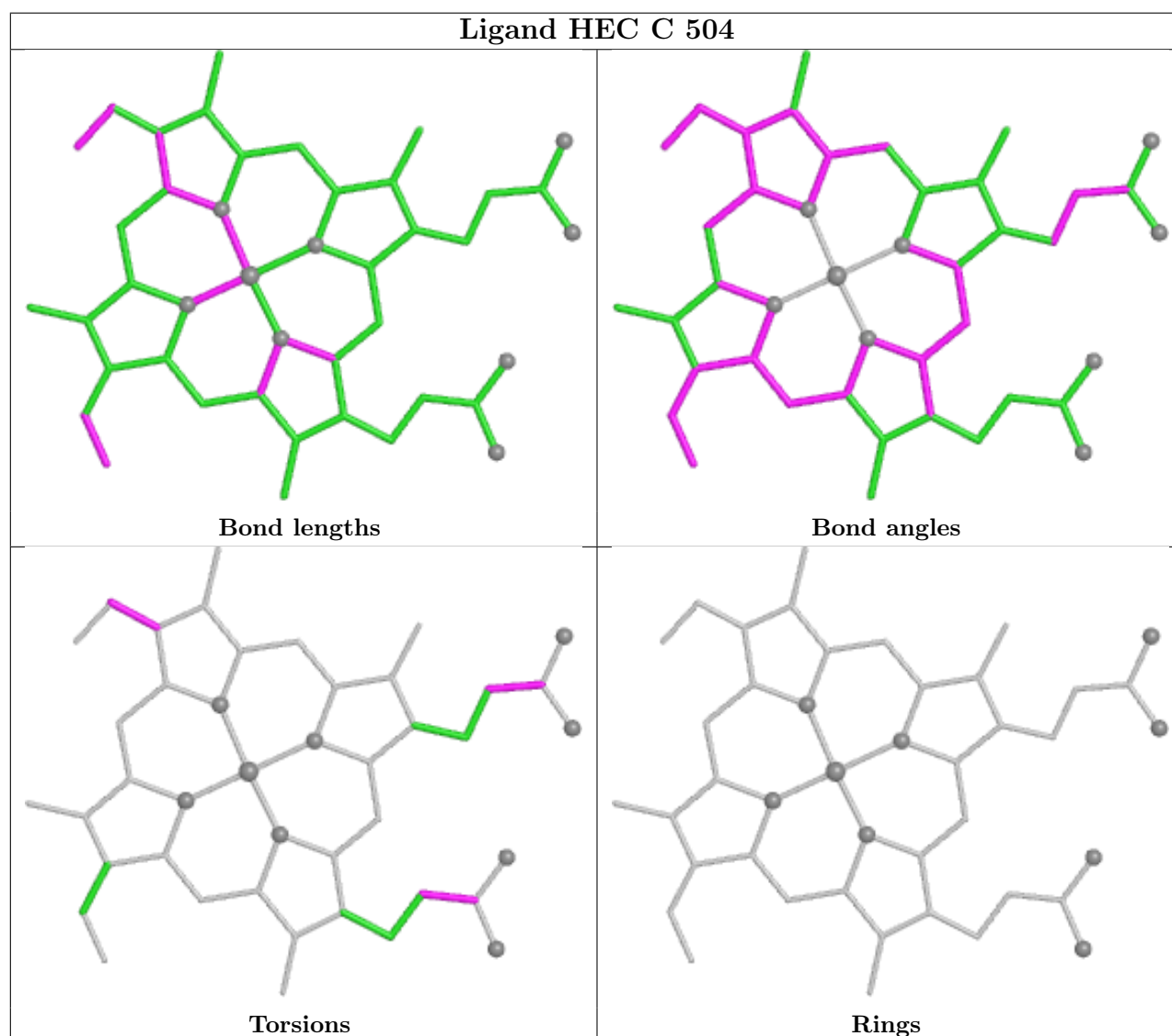
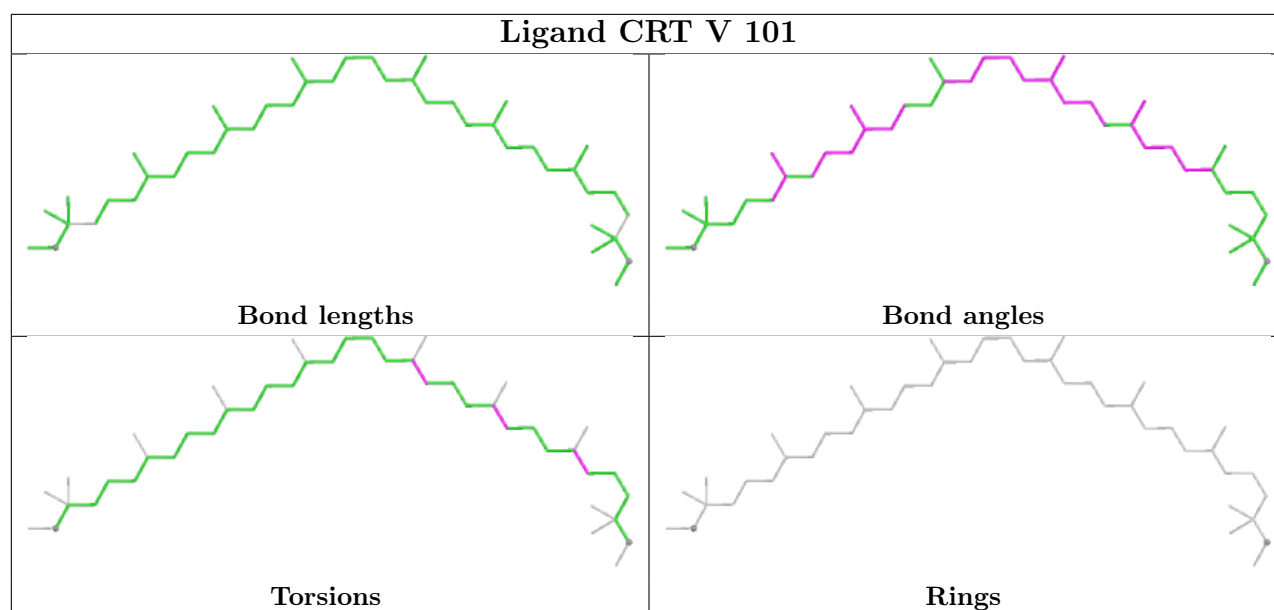


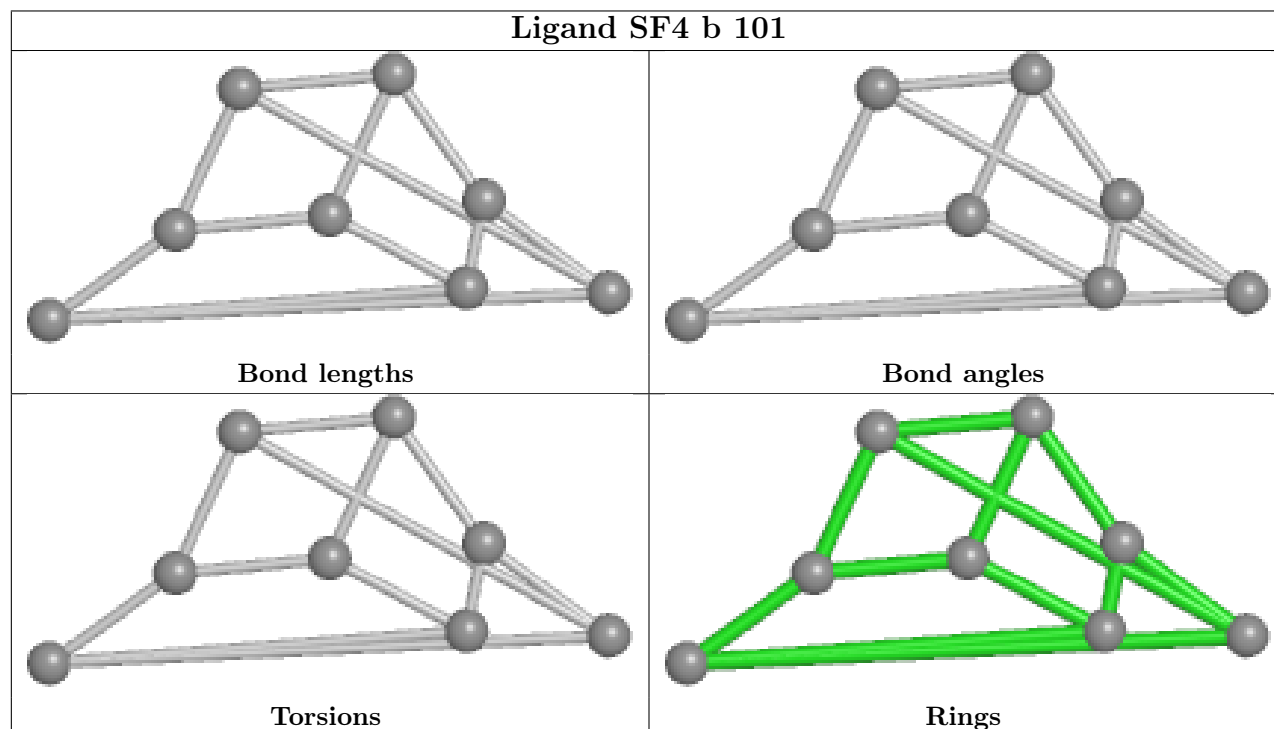
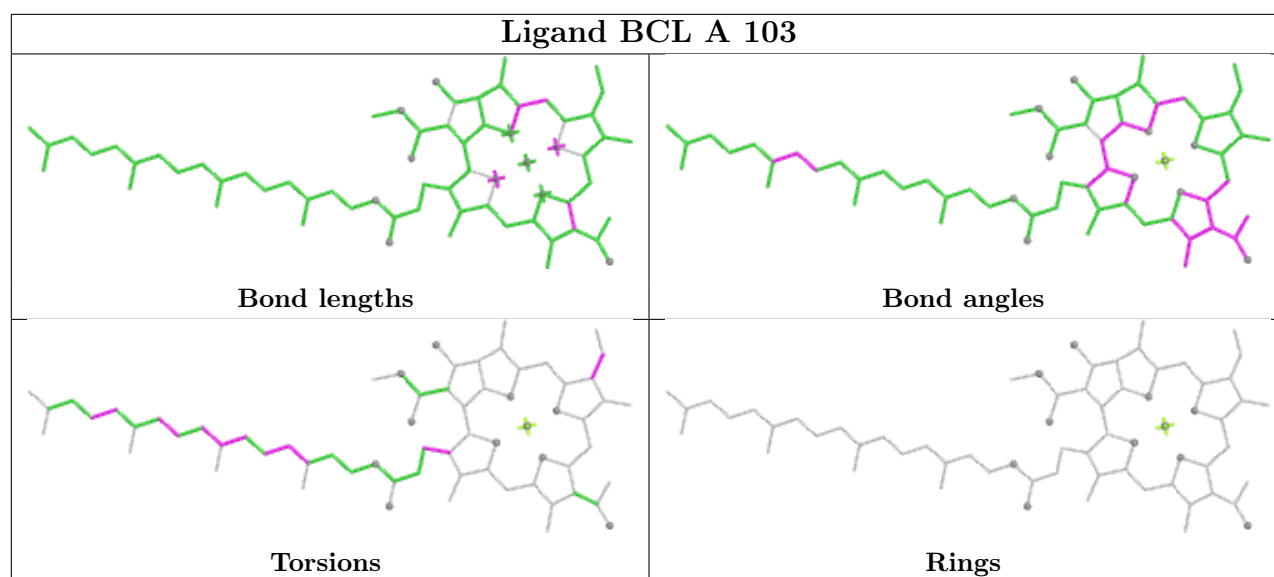


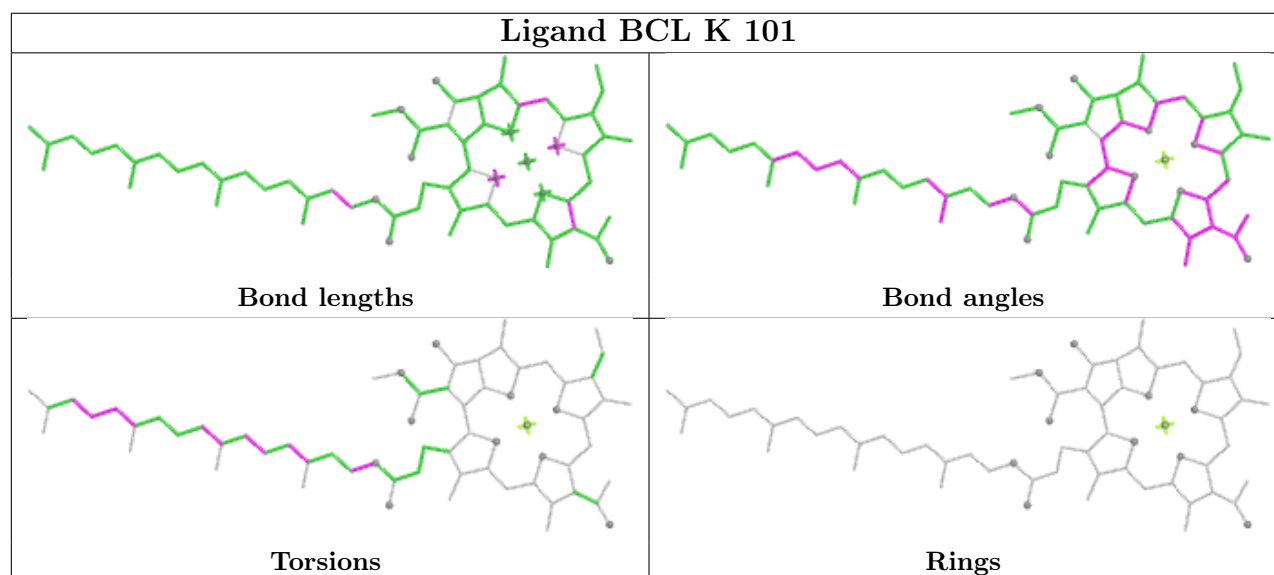
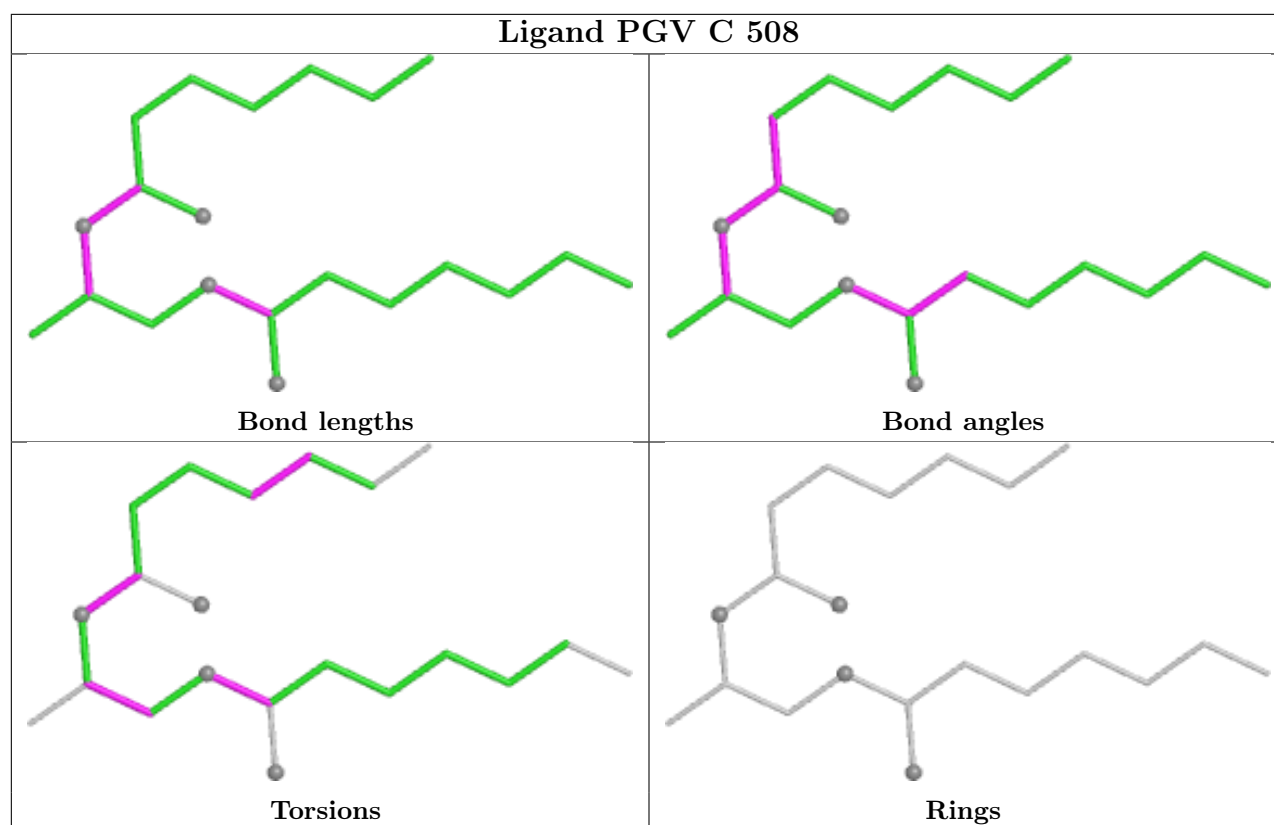




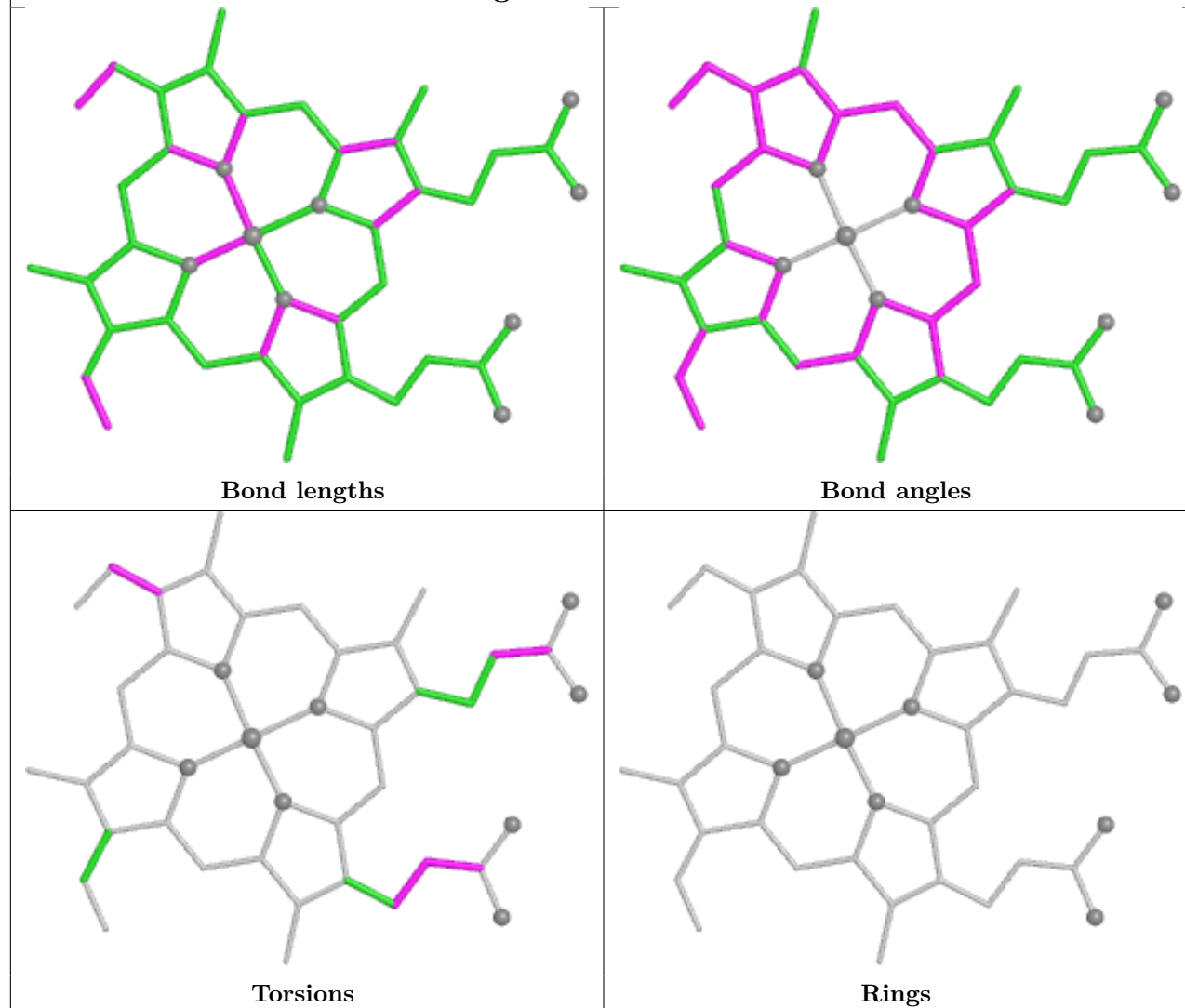




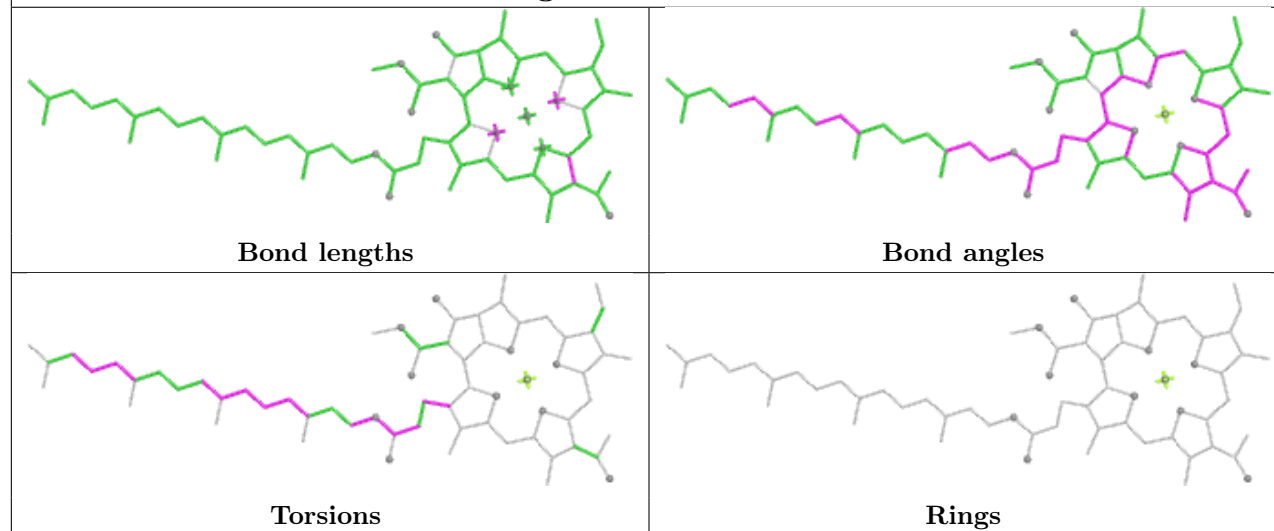


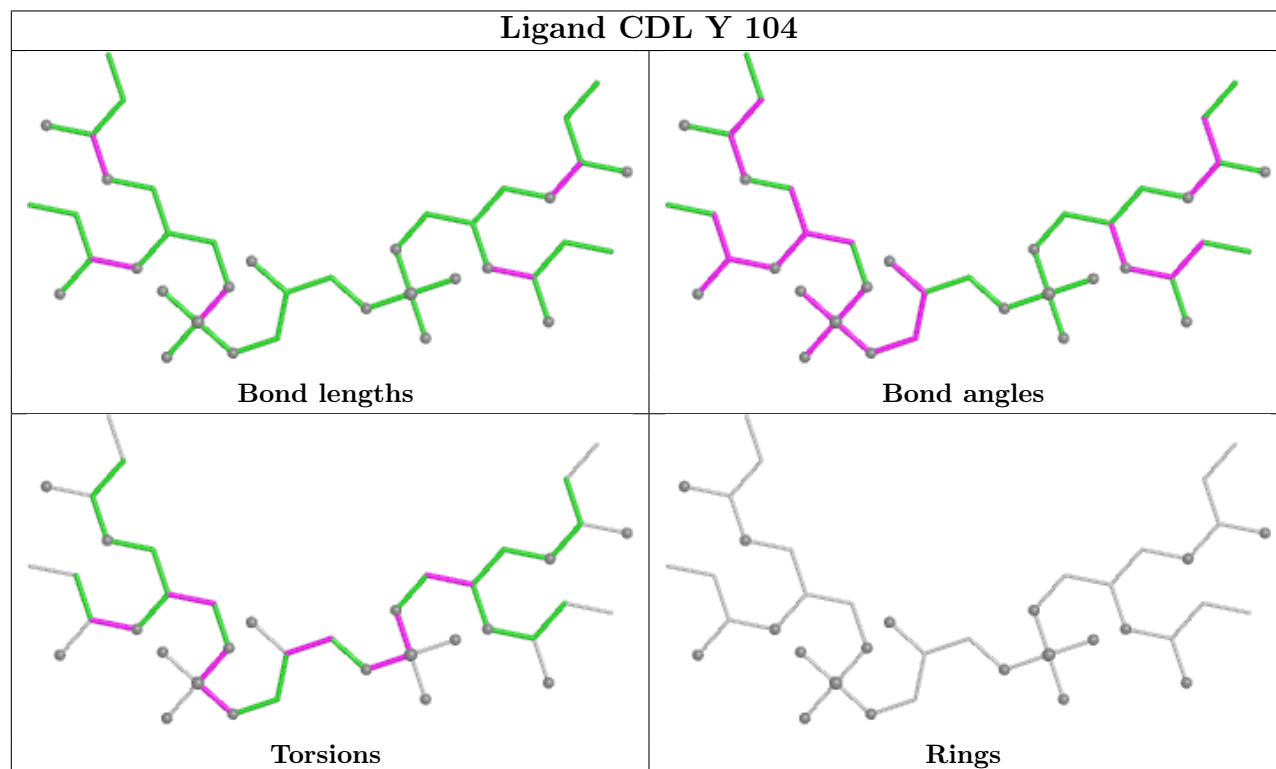
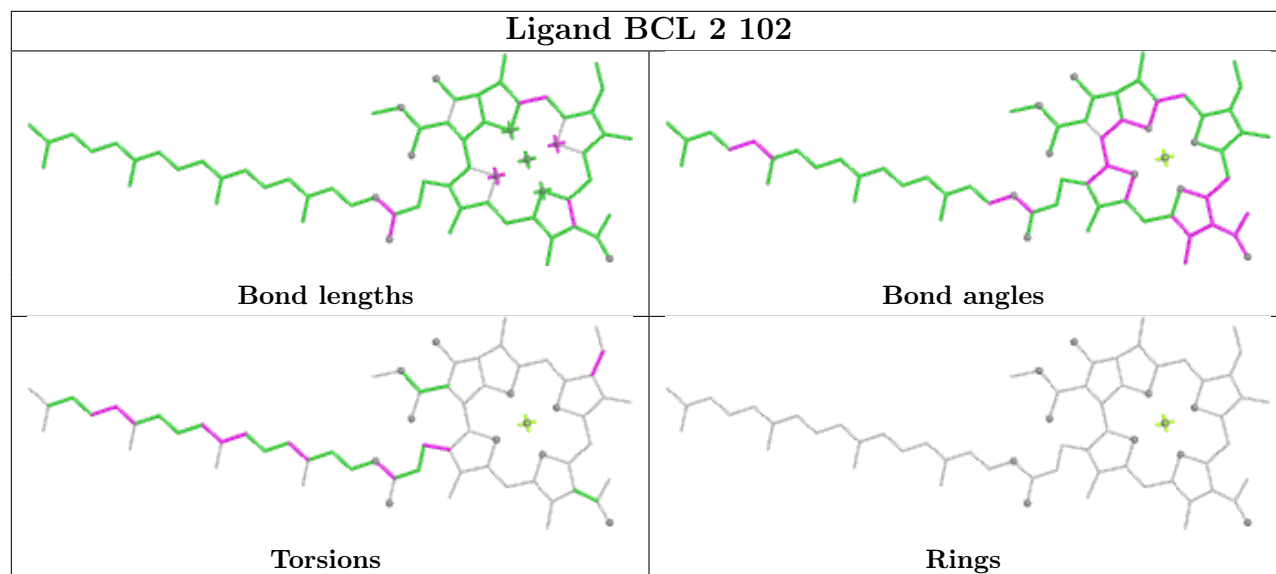


Ligand HEC C 502

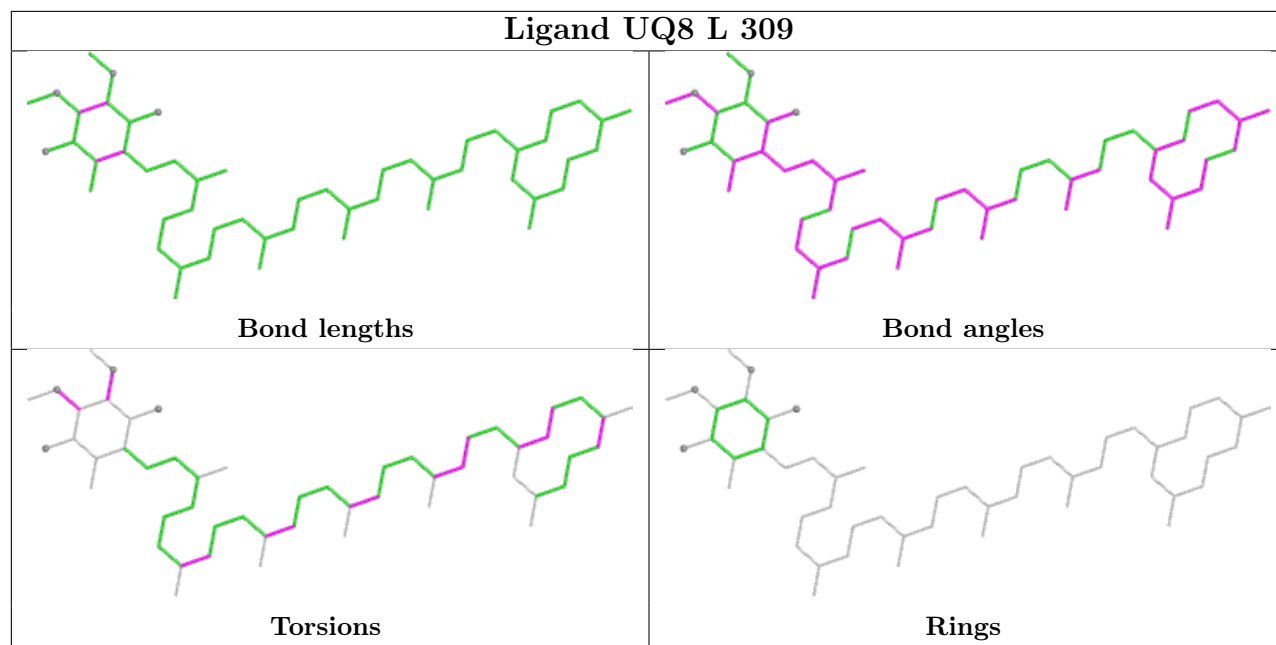


Ligand BCL 3 101

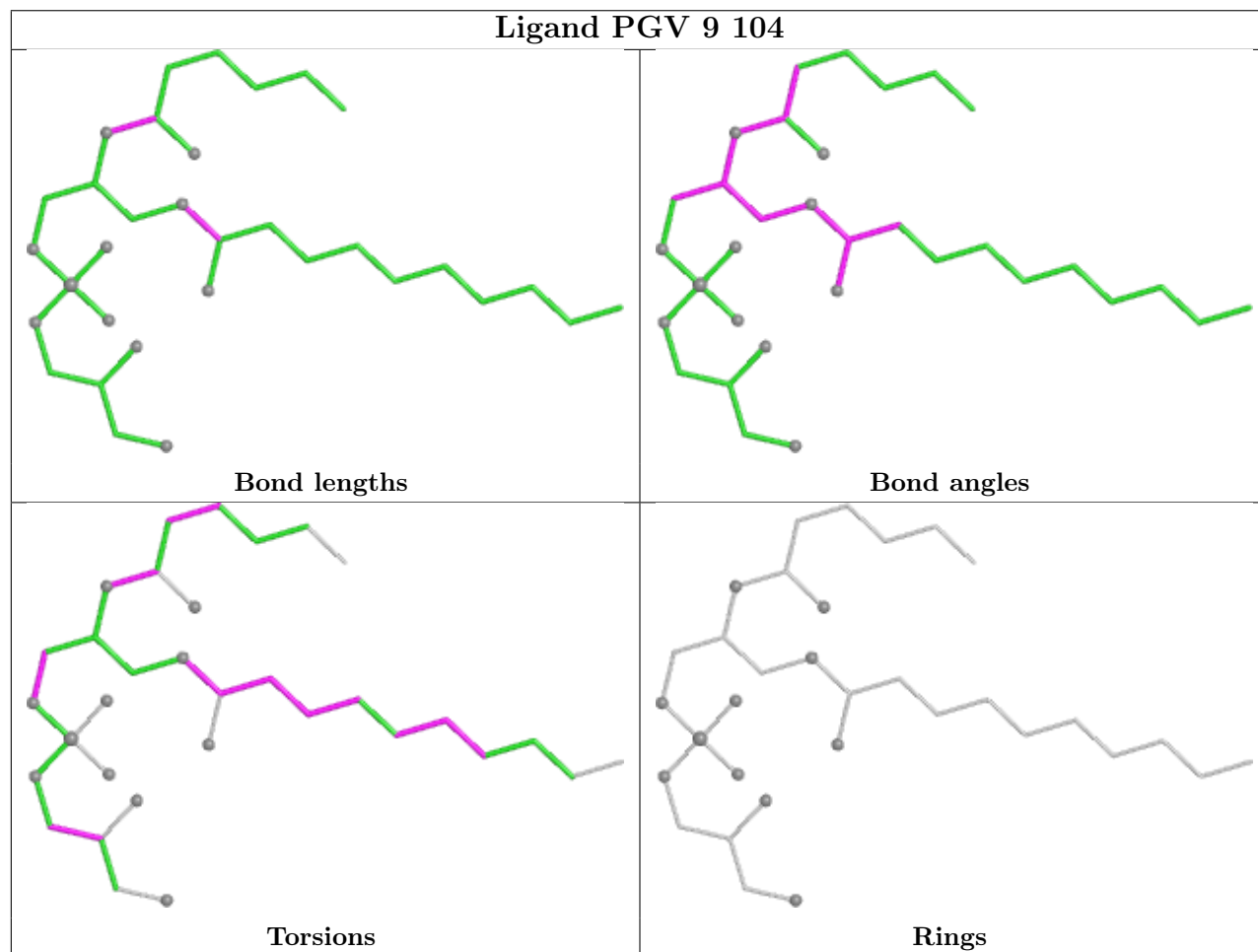


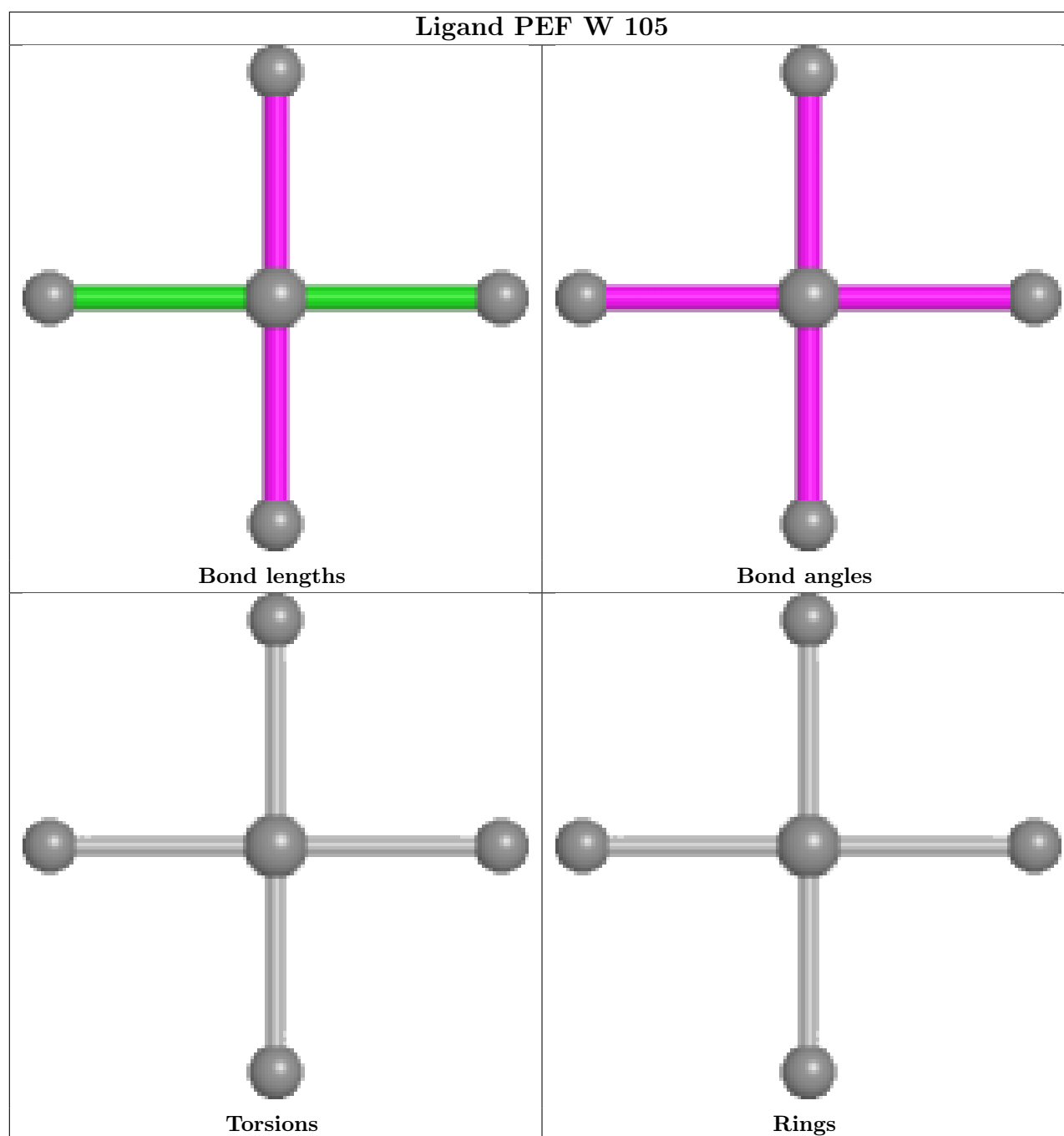


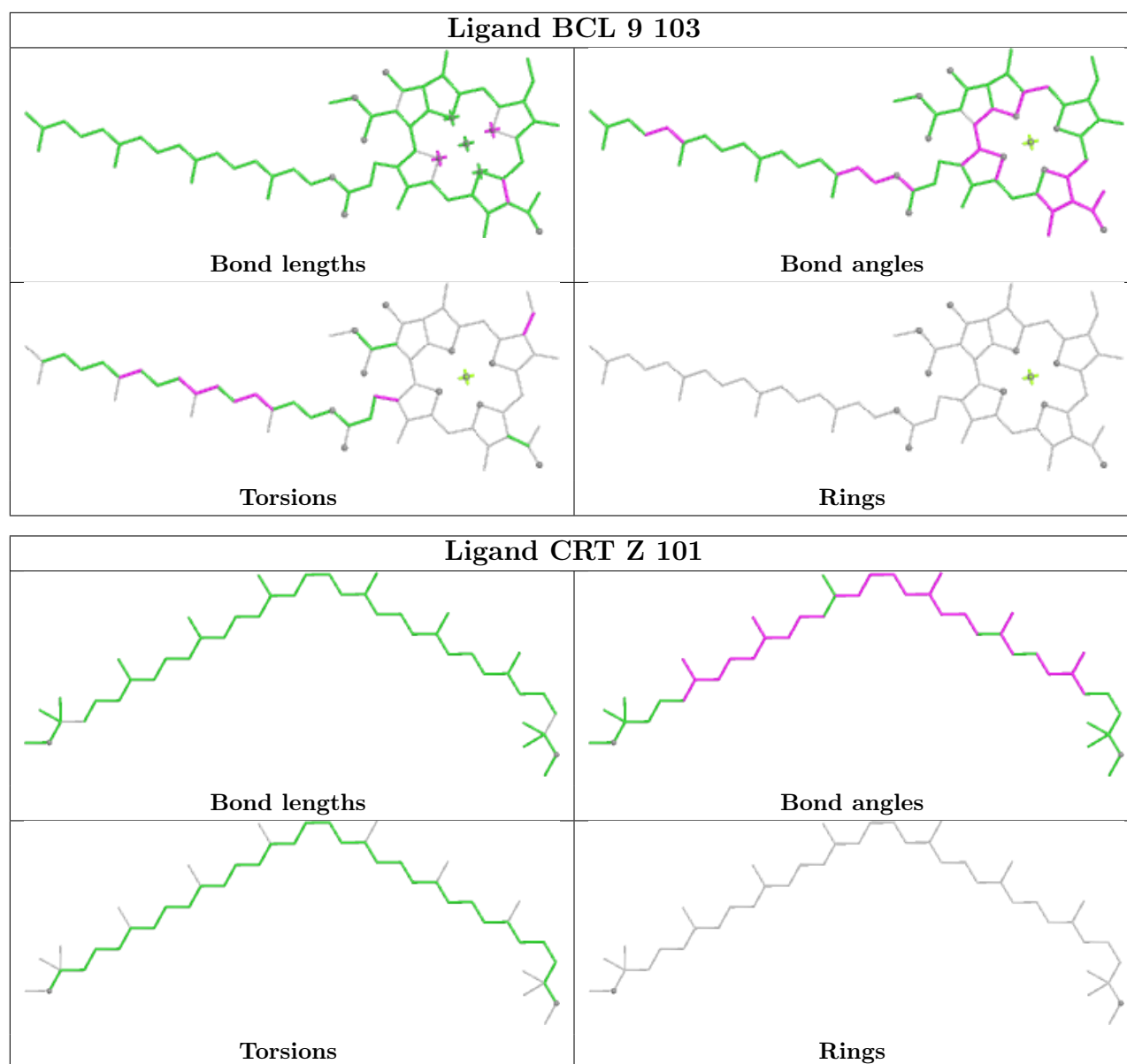
Ligand UQ8 L 309

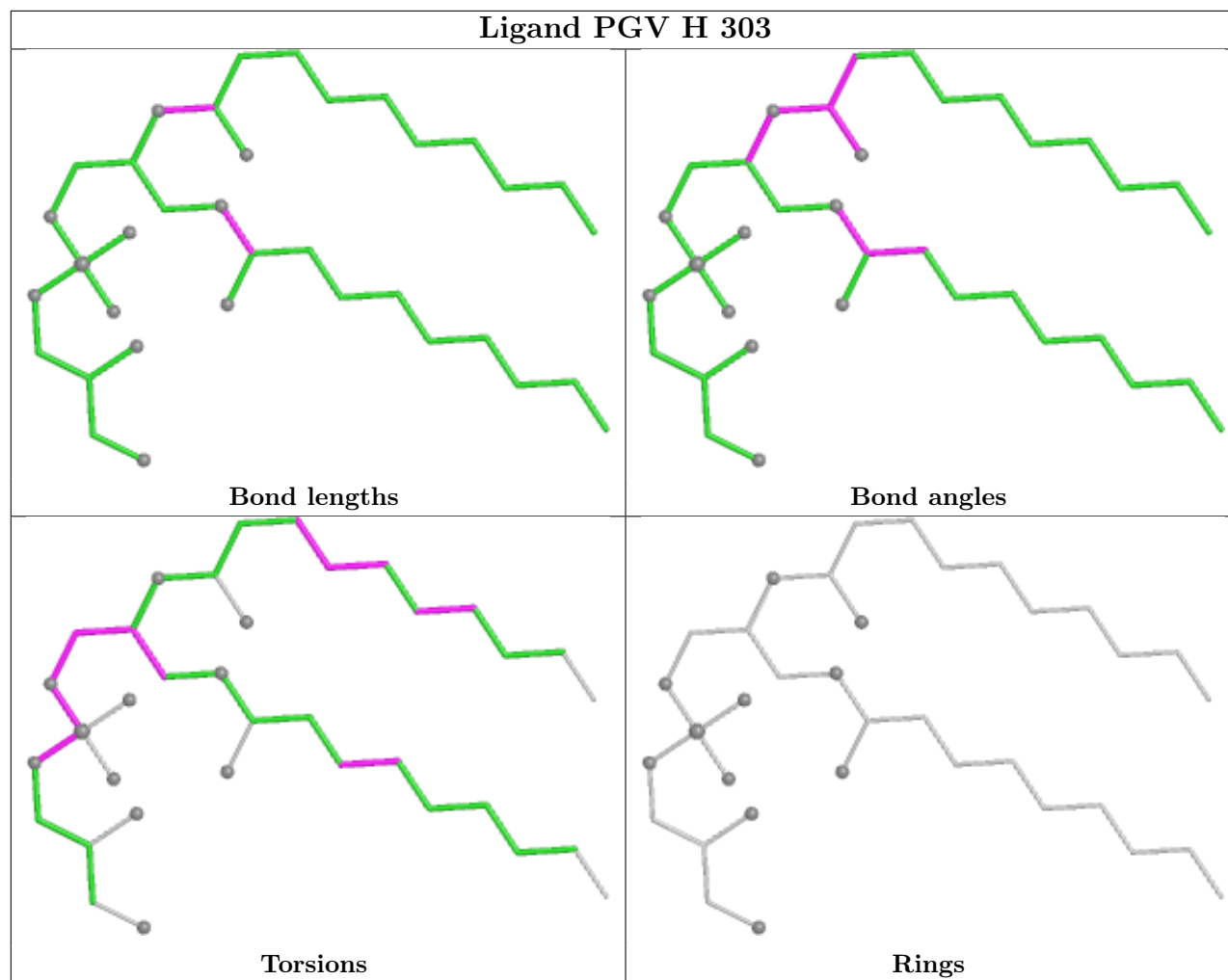


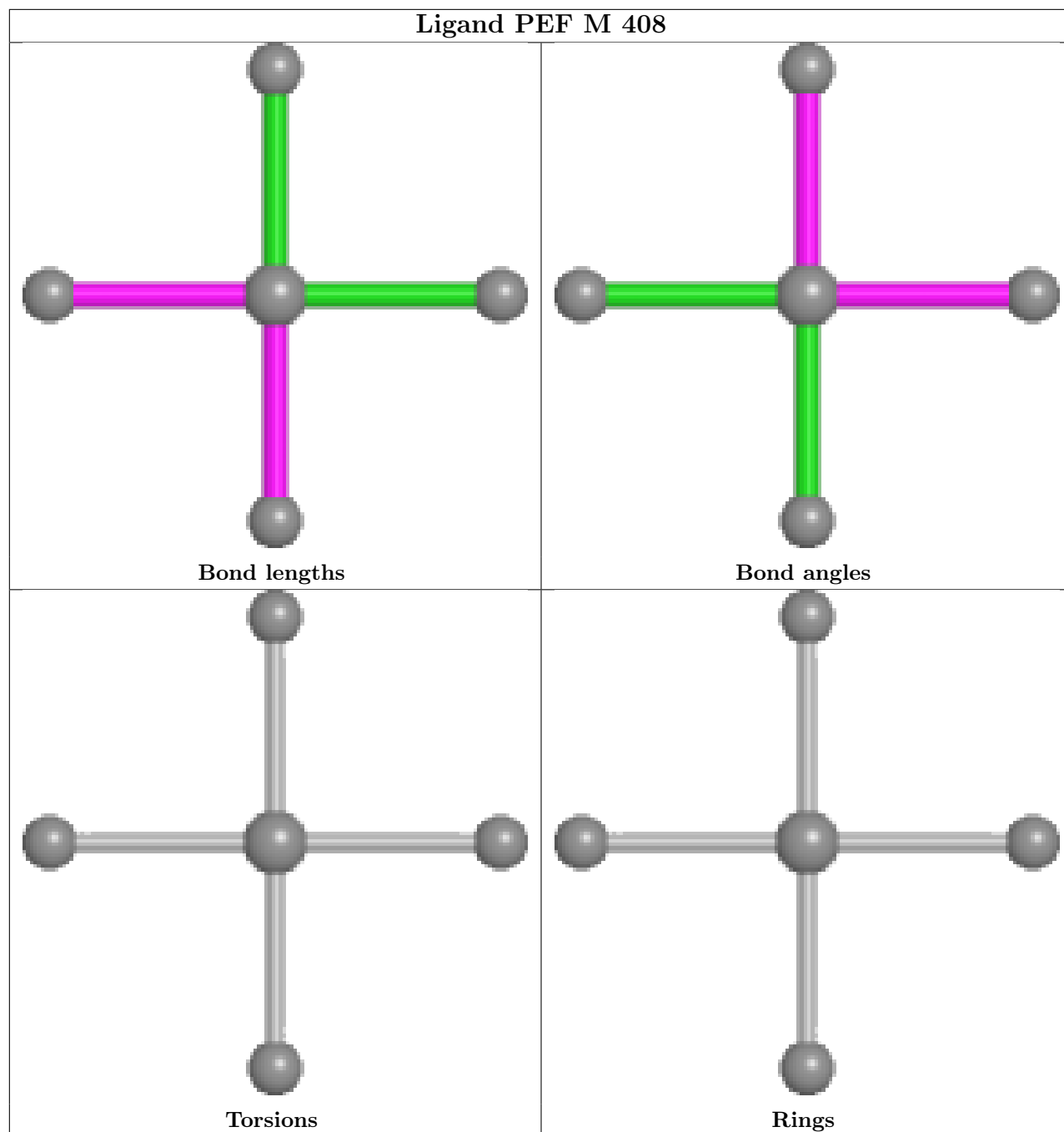
Ligand PGV 9 104

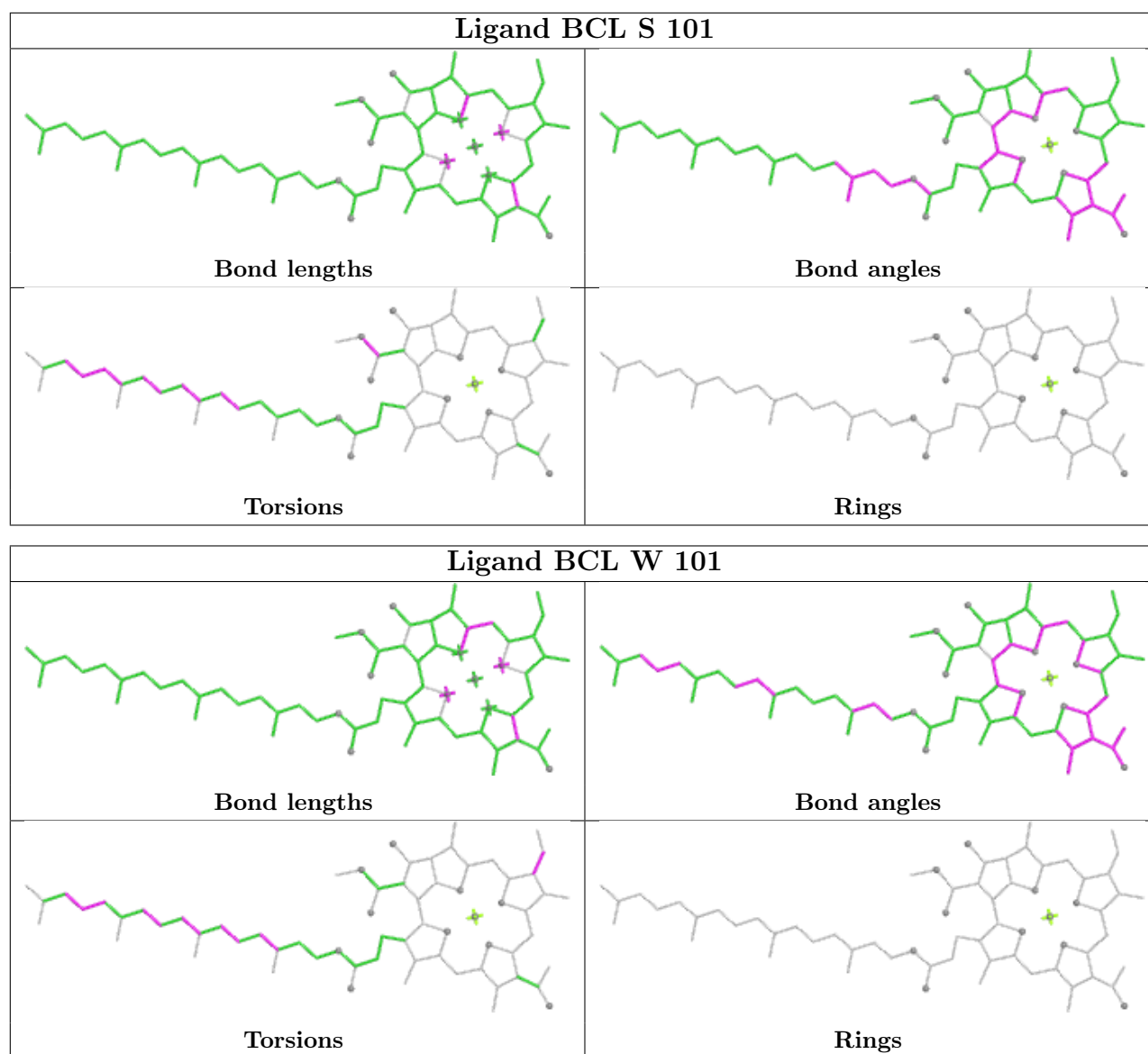




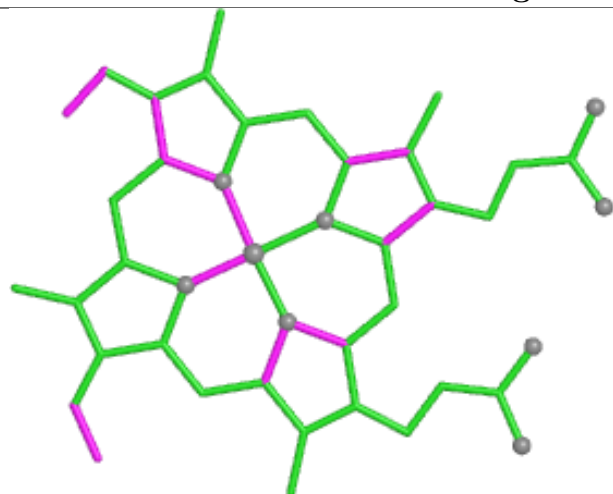




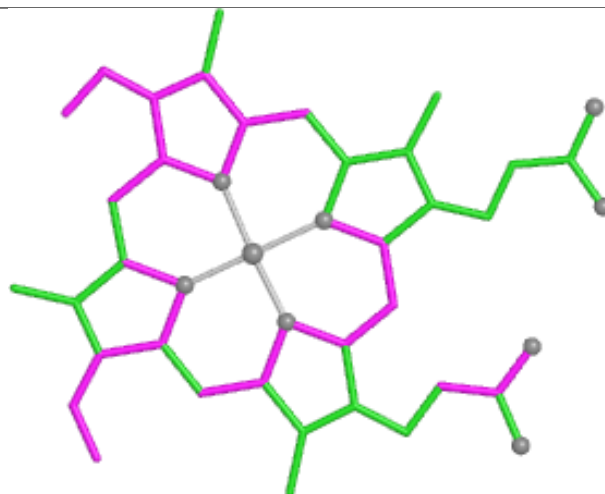




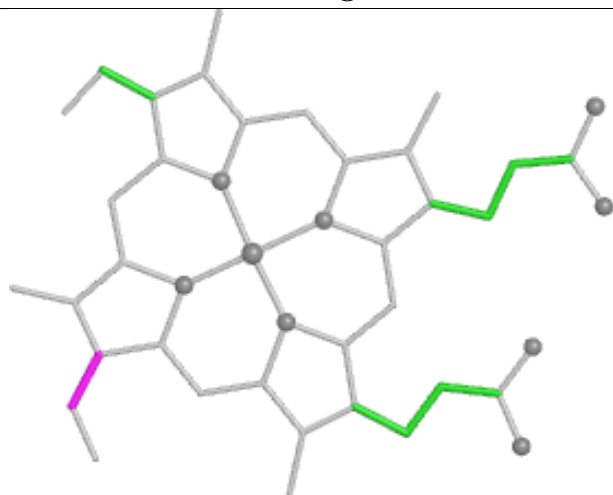
Ligand HEC C 503



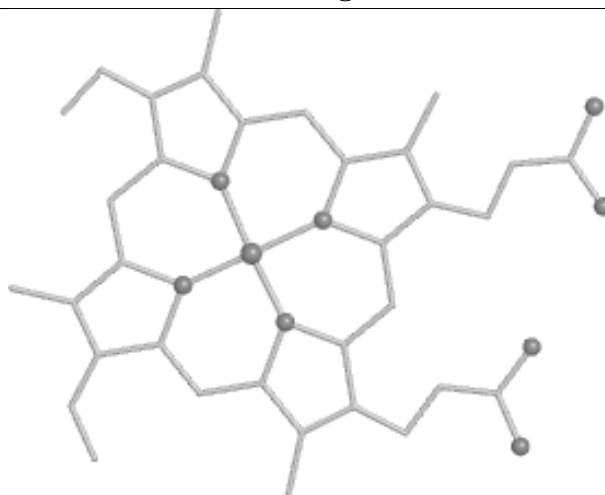
Bond lengths



Bond angles

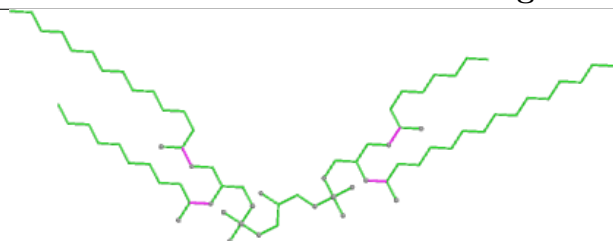


Torsions

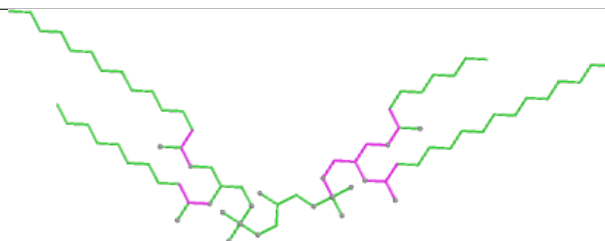


Rings

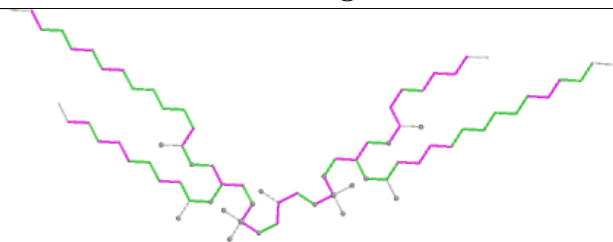
Ligand CDL S 104



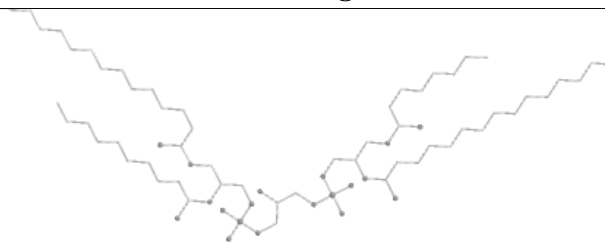
Bond lengths



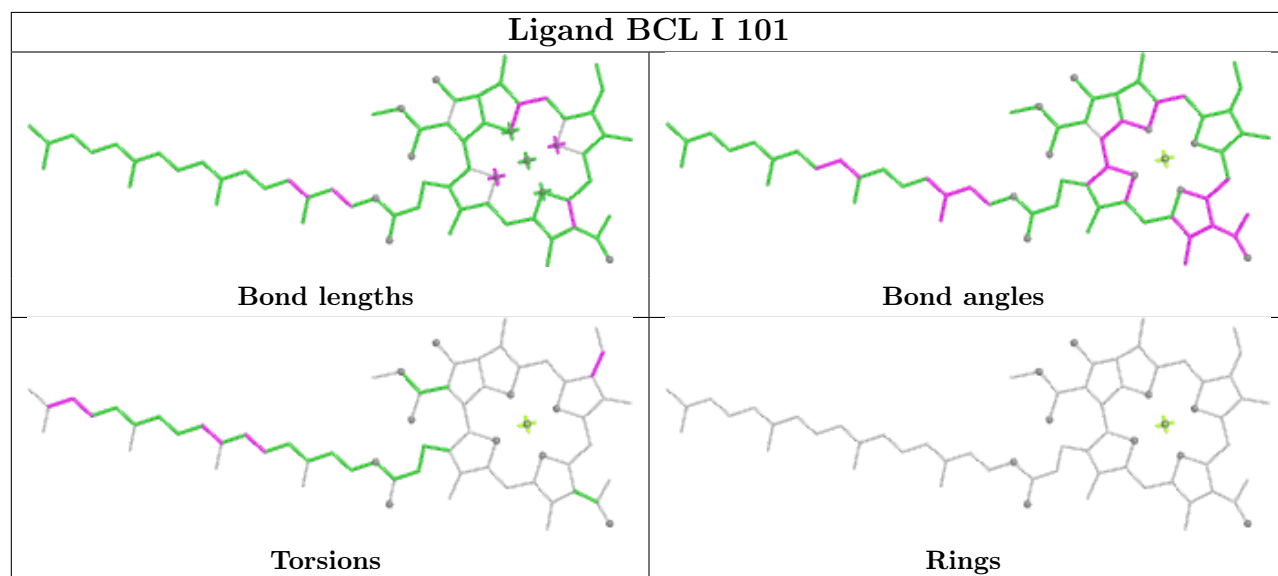
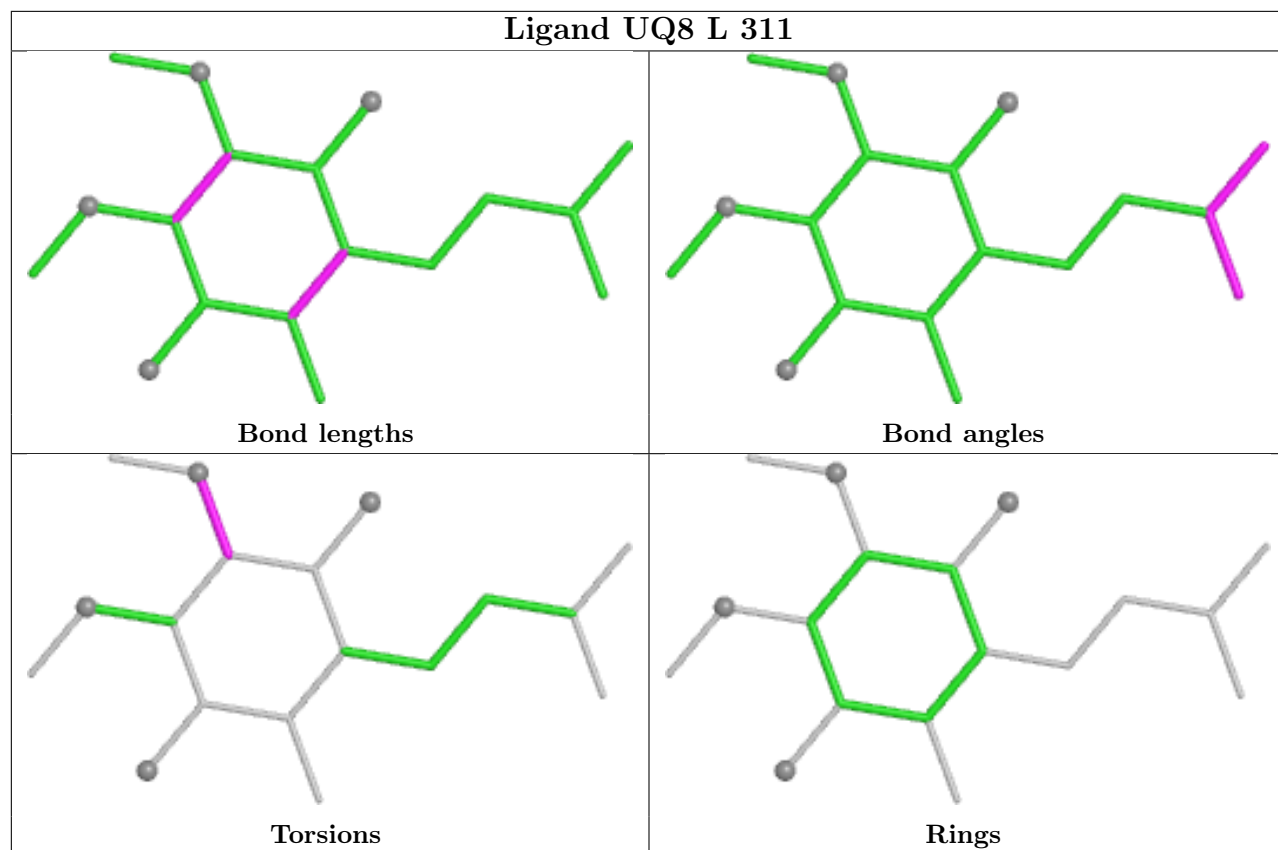
Bond angles

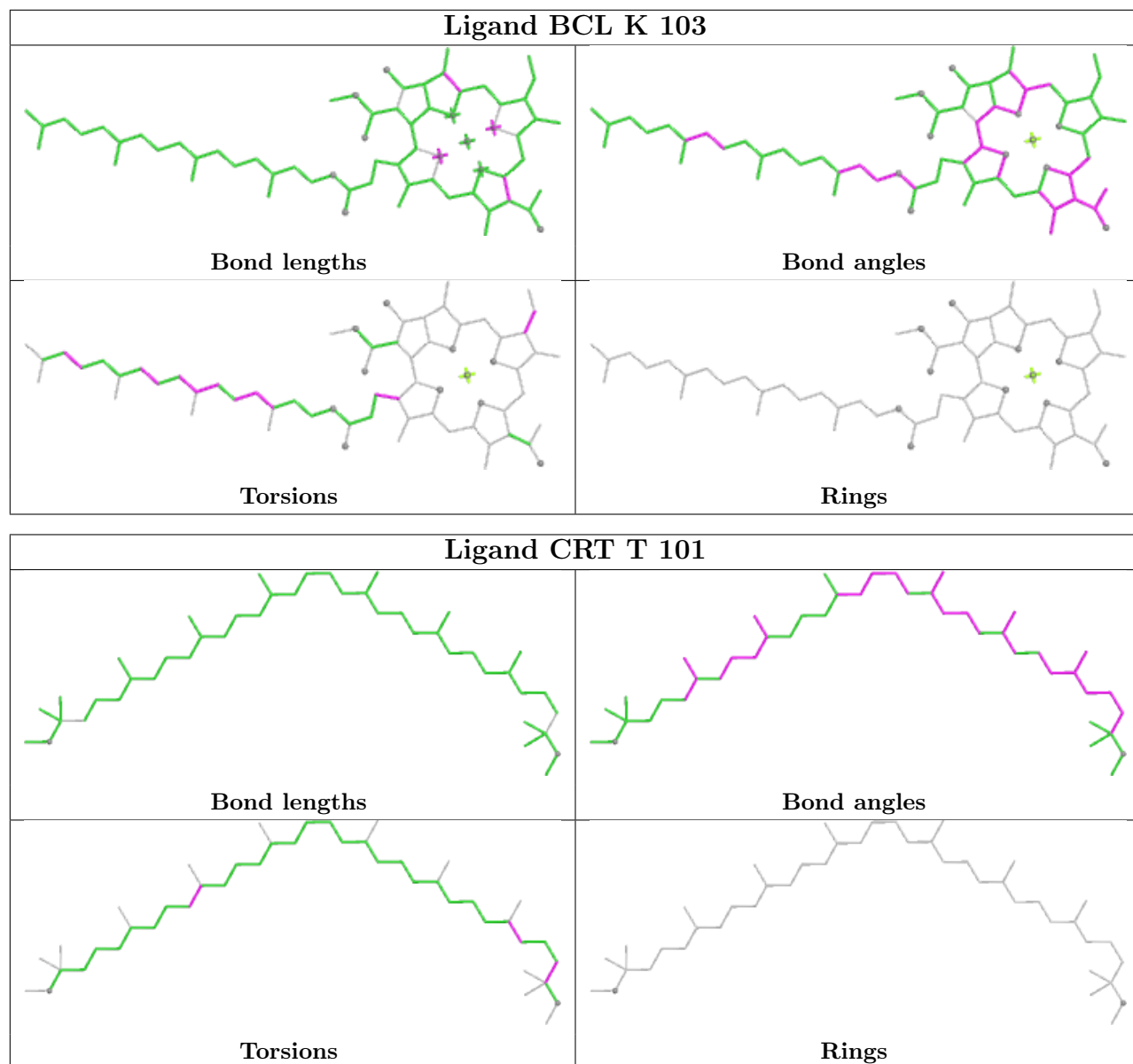


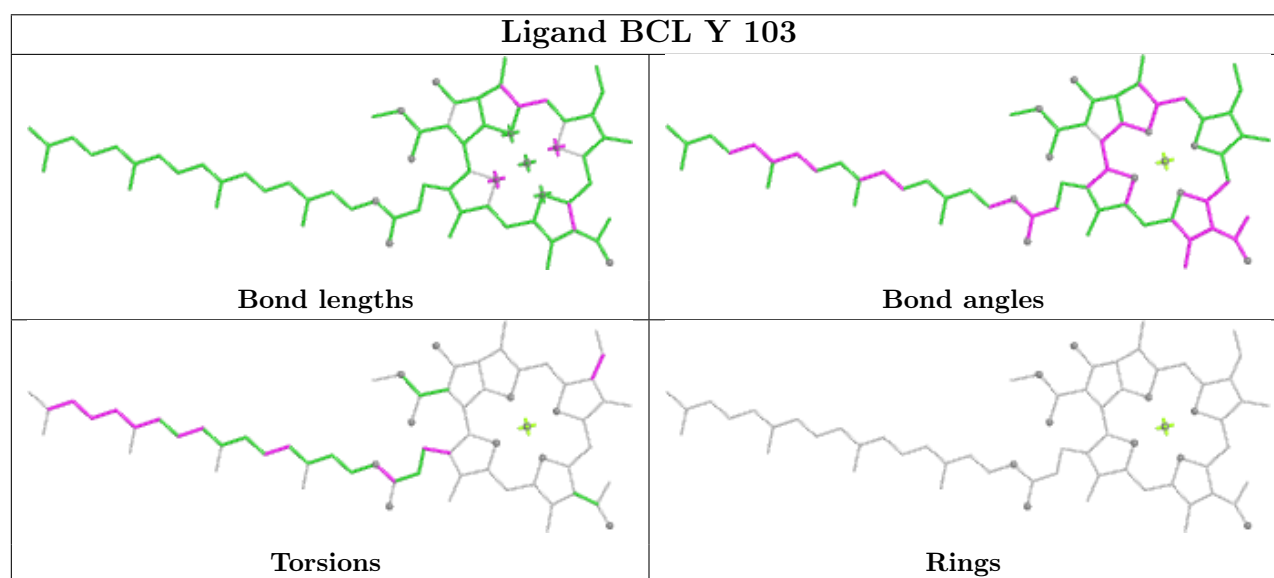
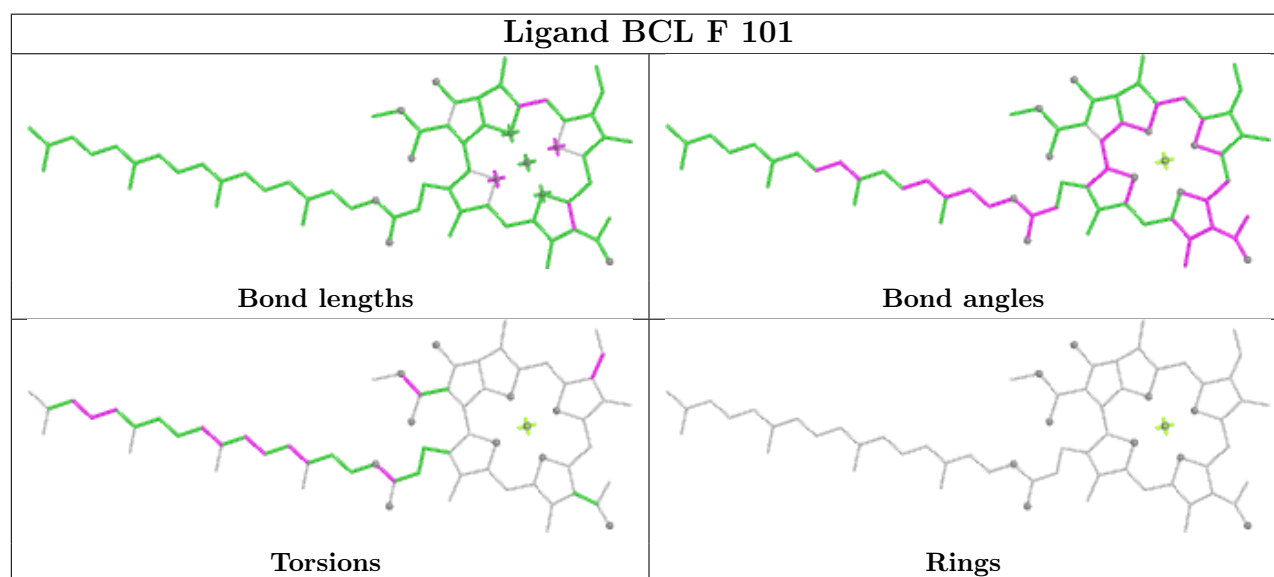
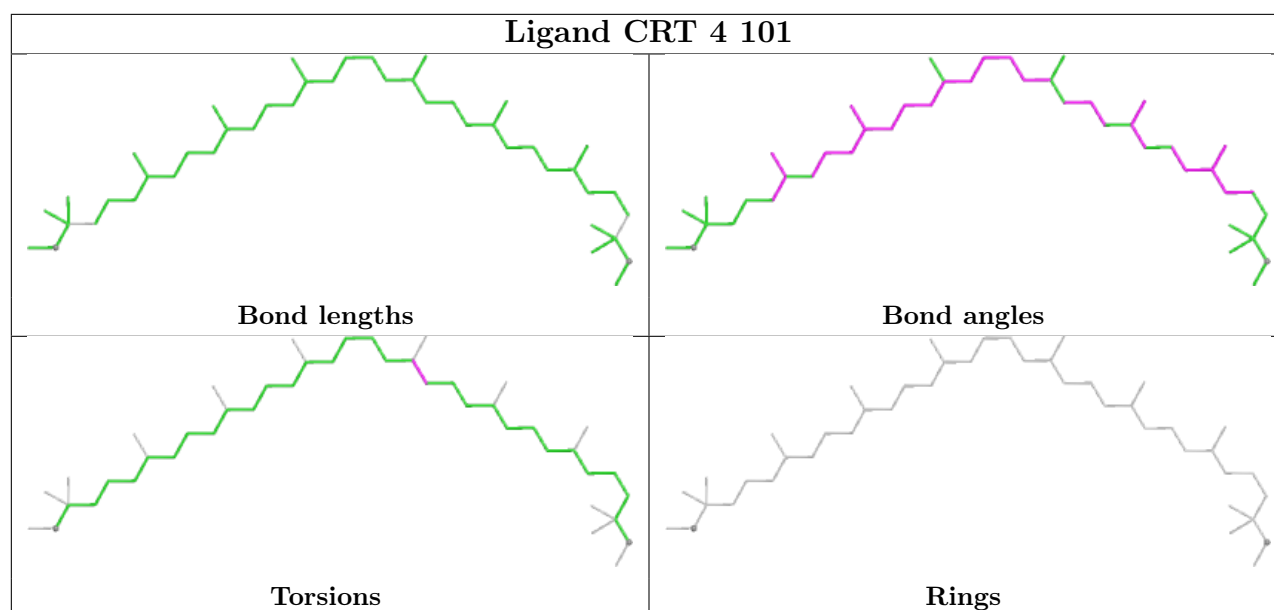
Torsions

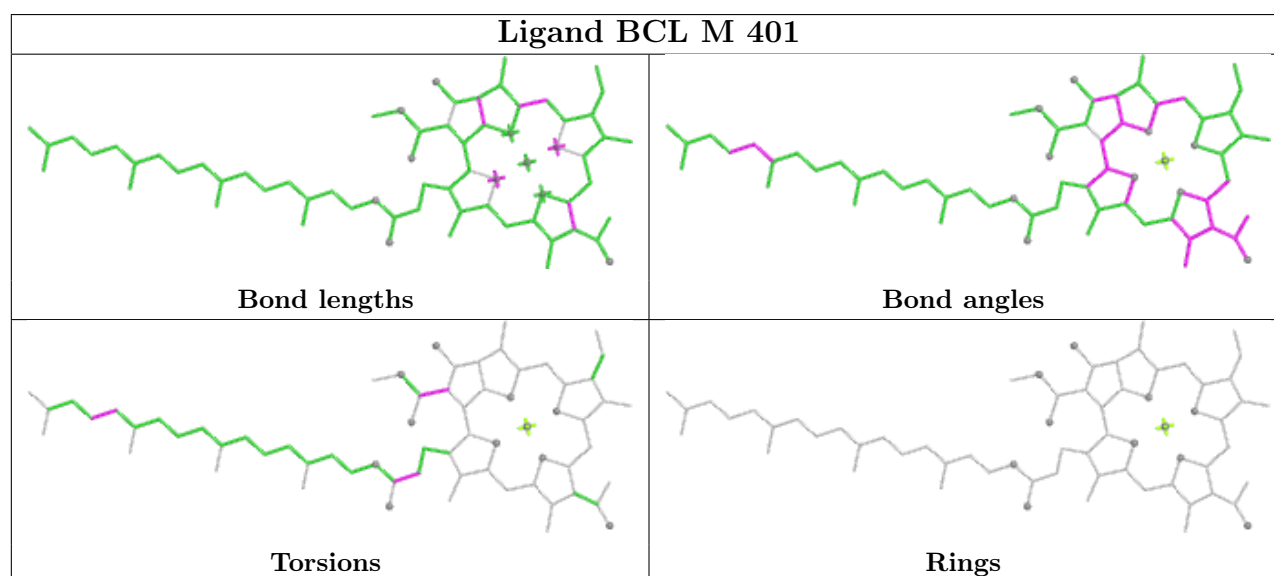
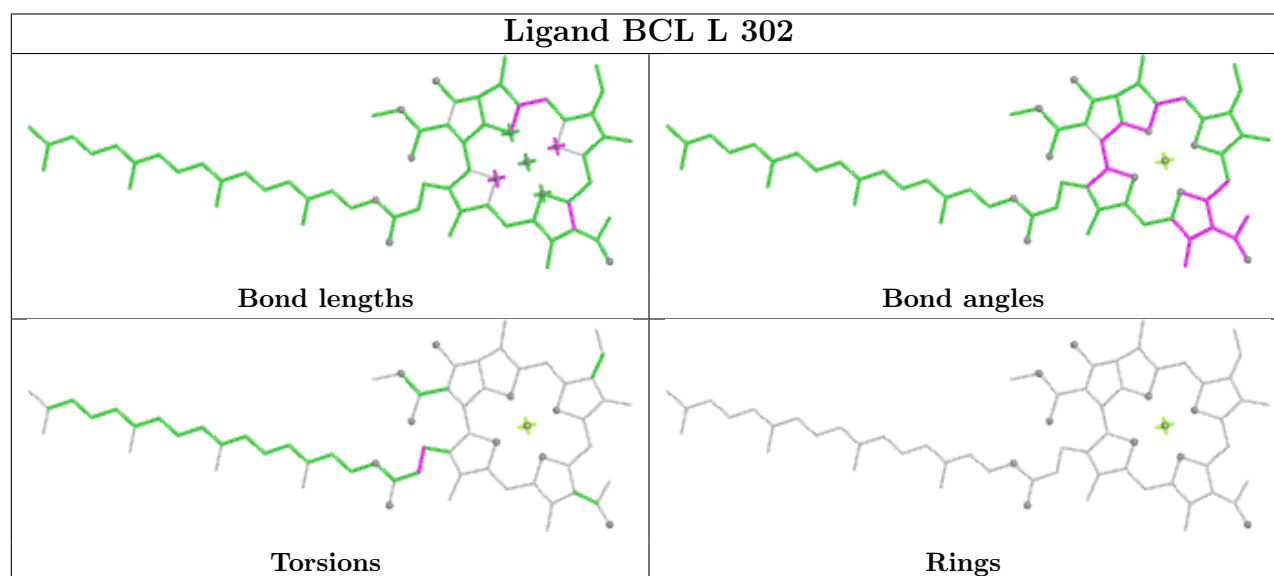
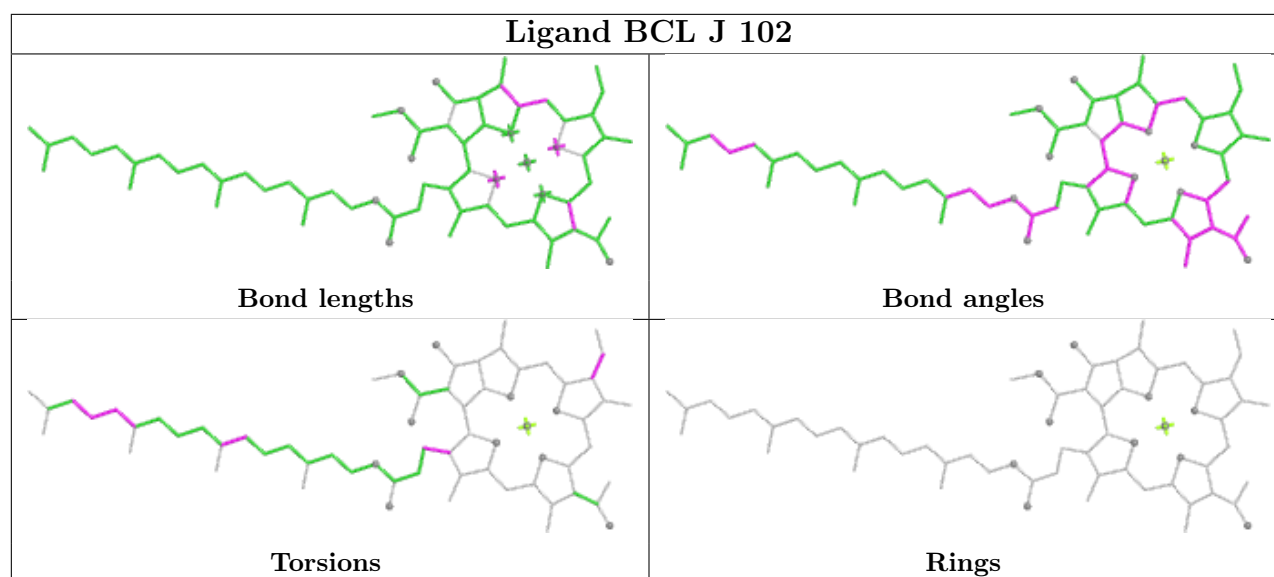


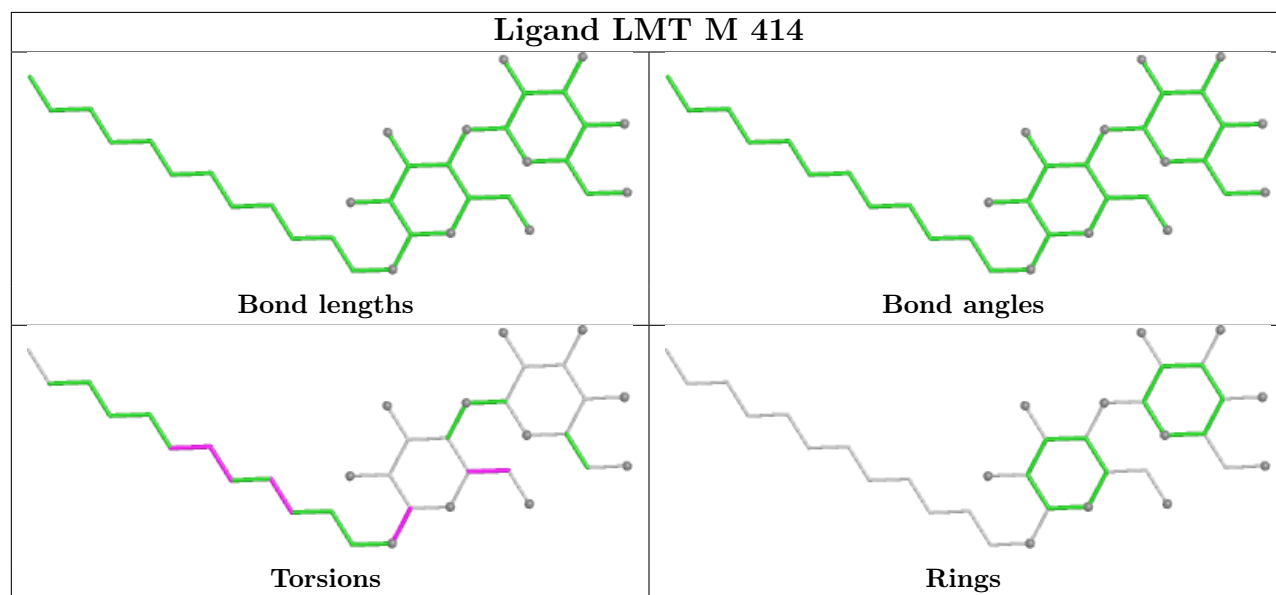
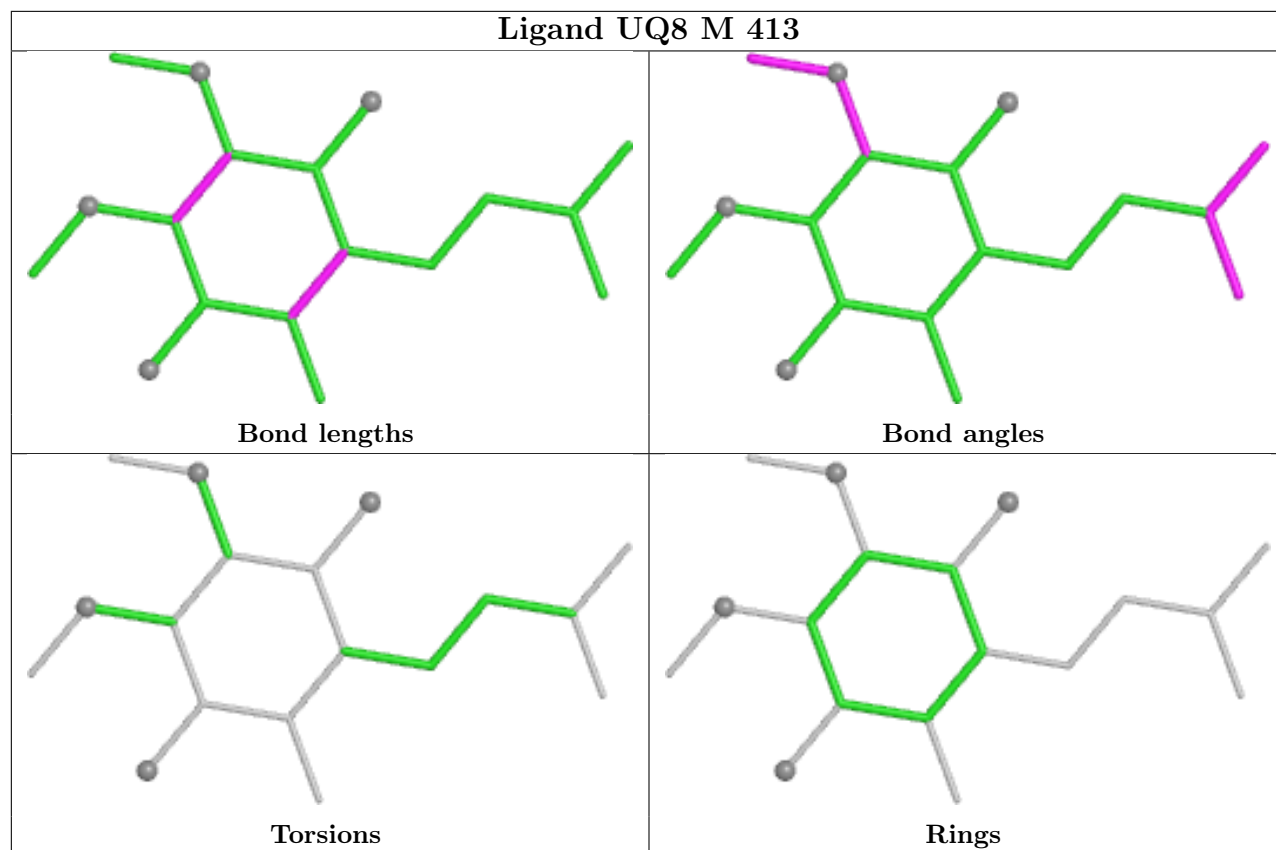
Rings

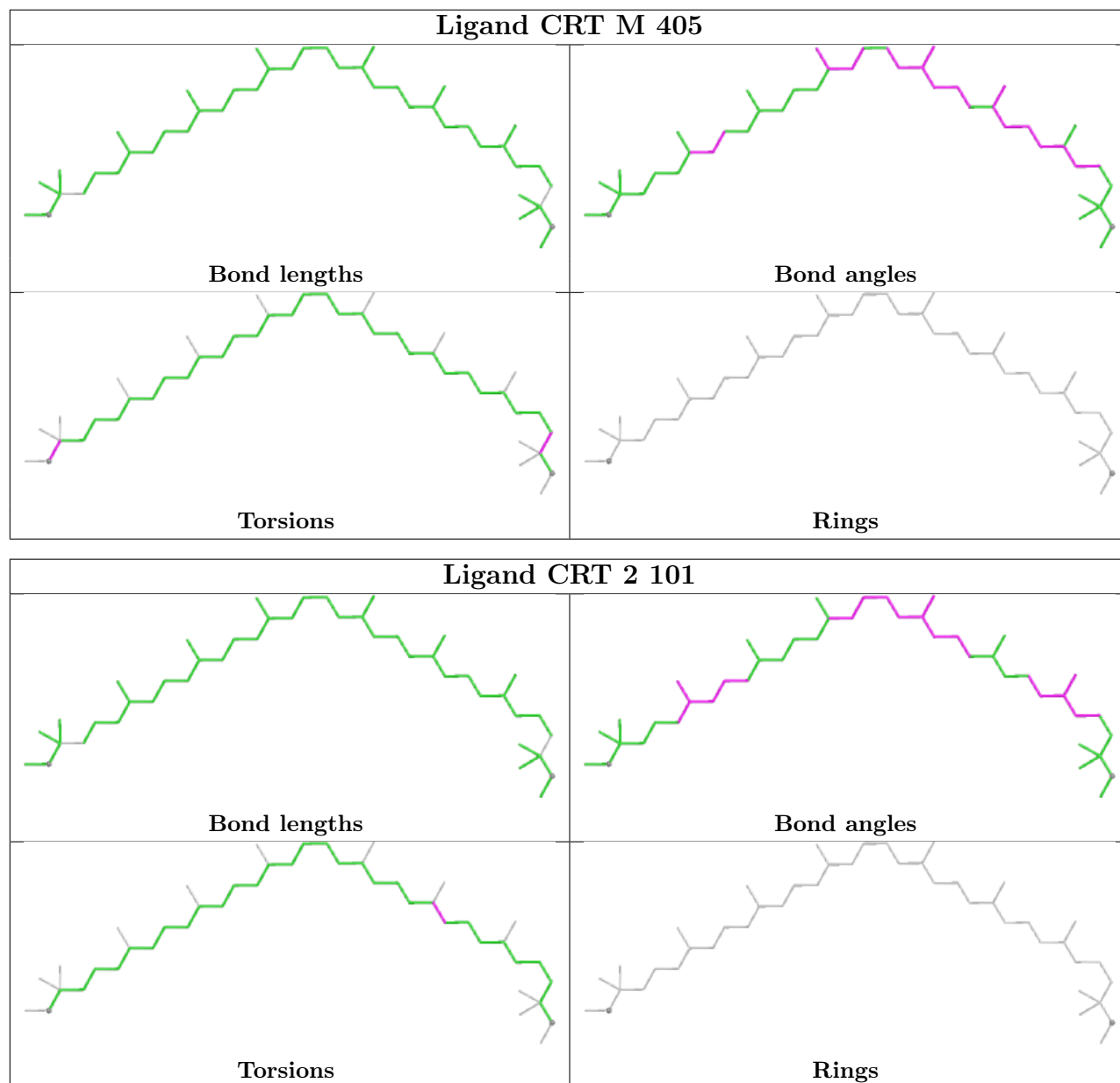


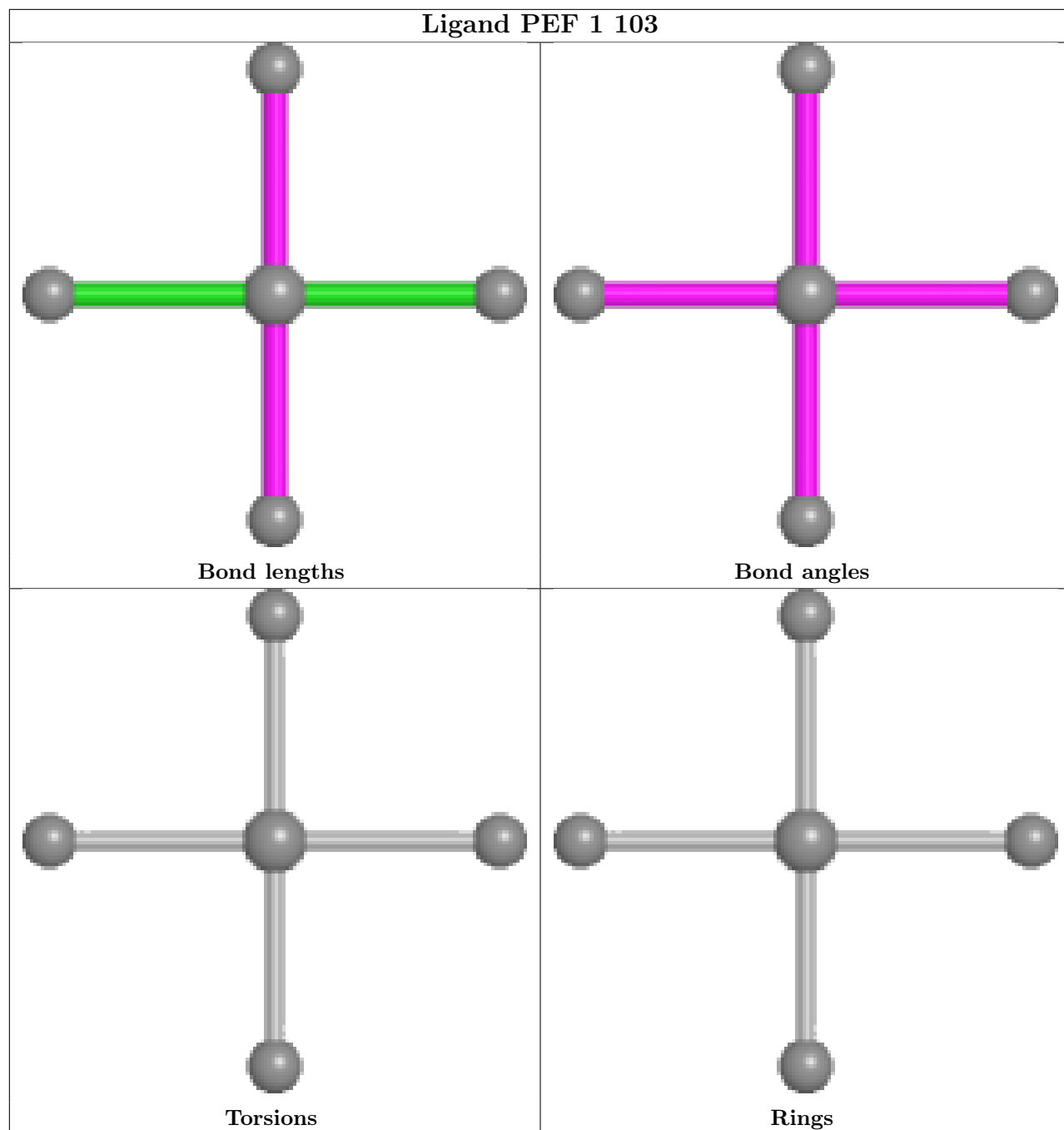


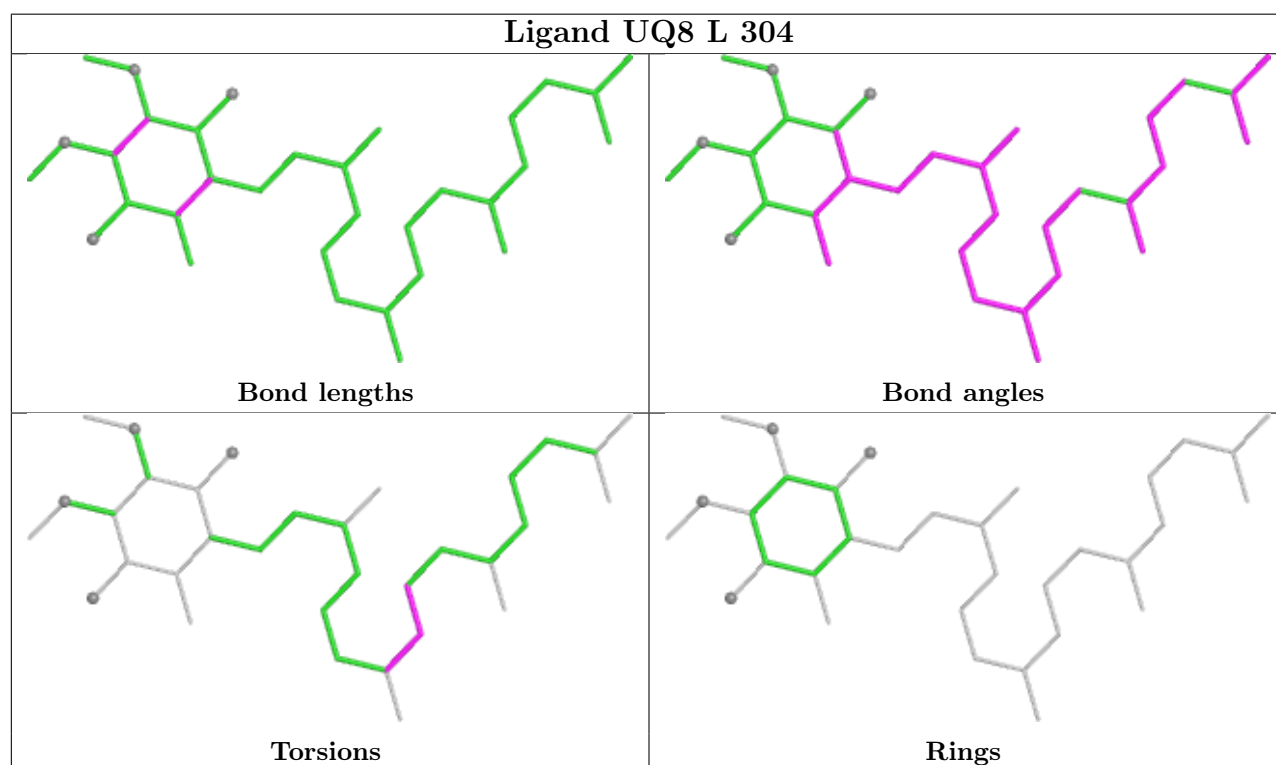
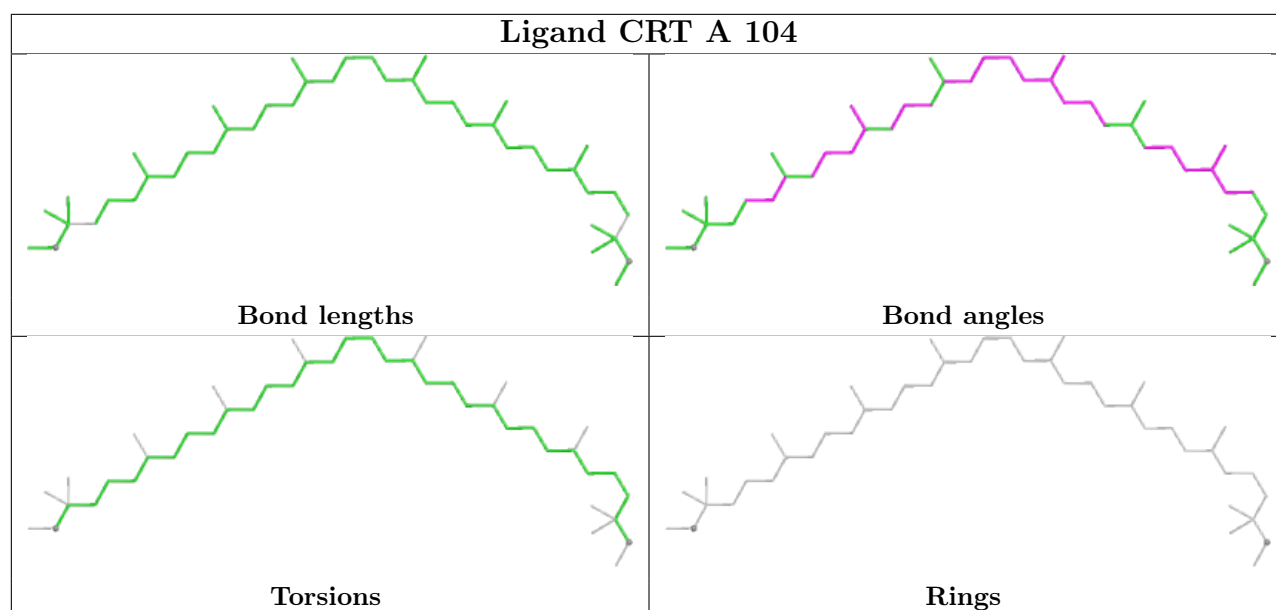


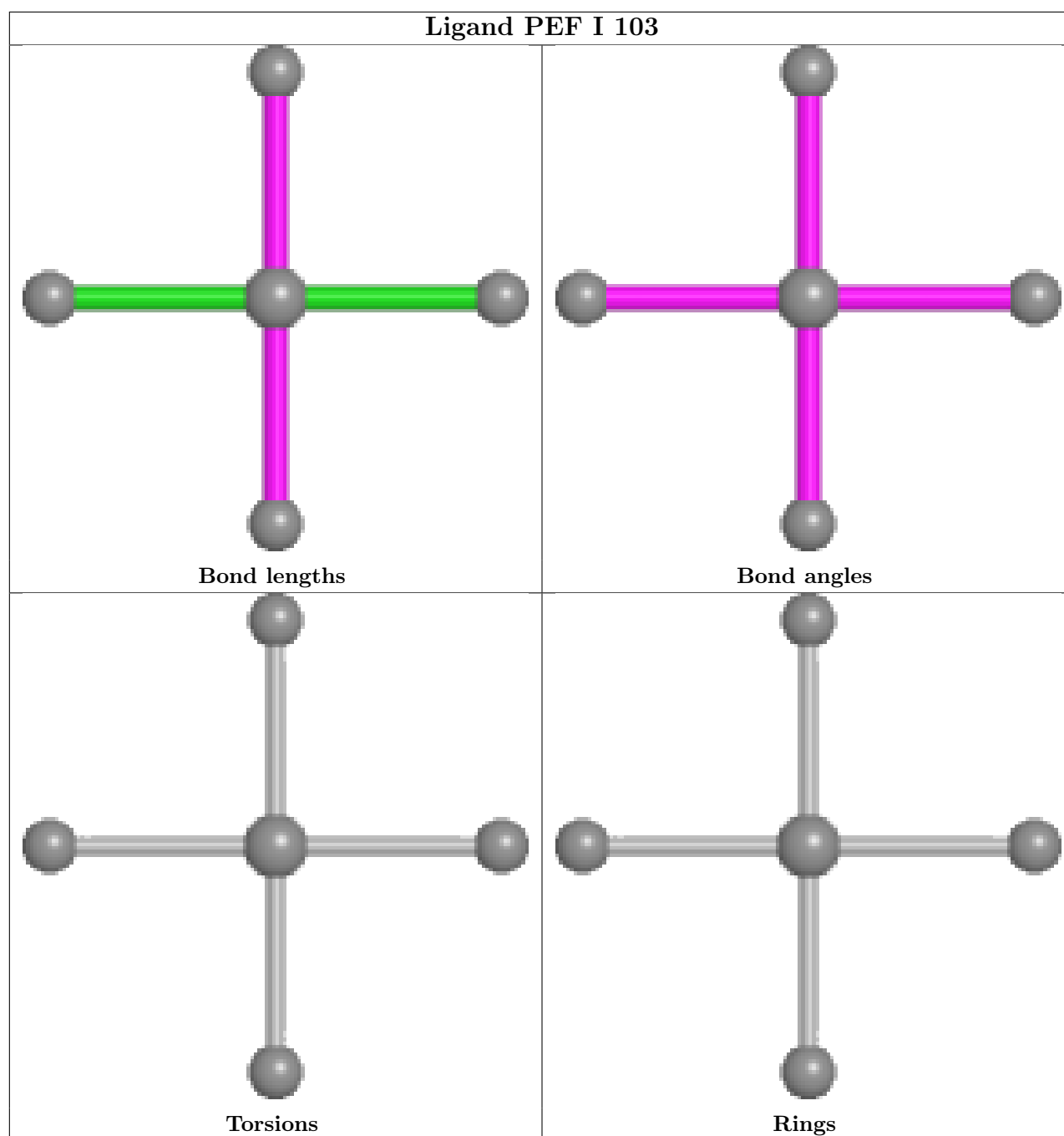


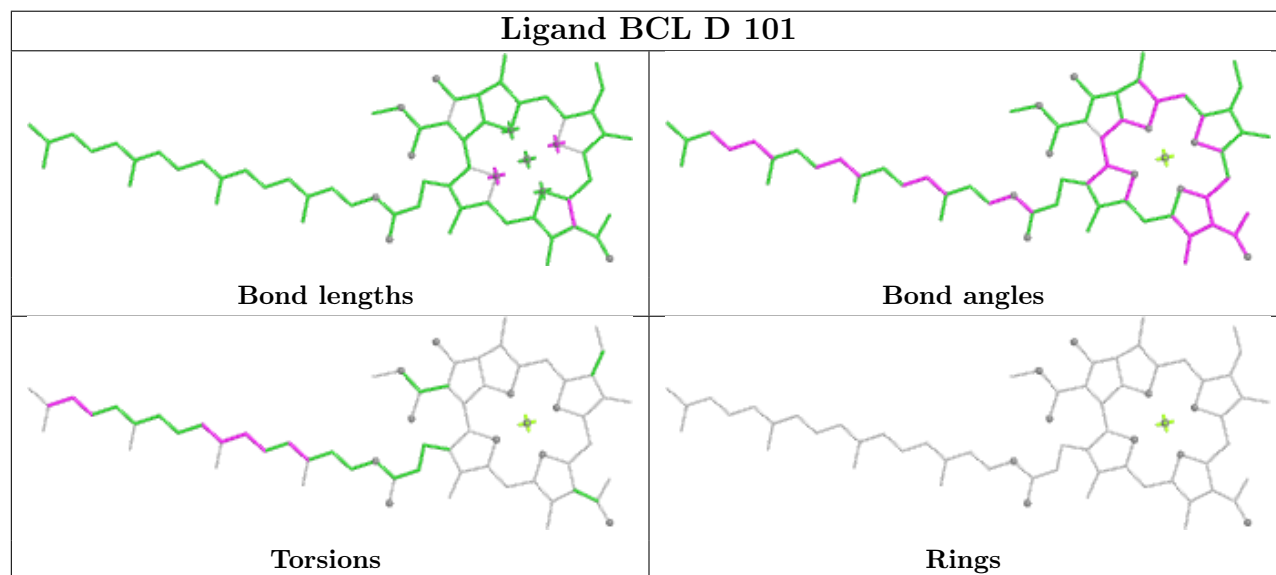
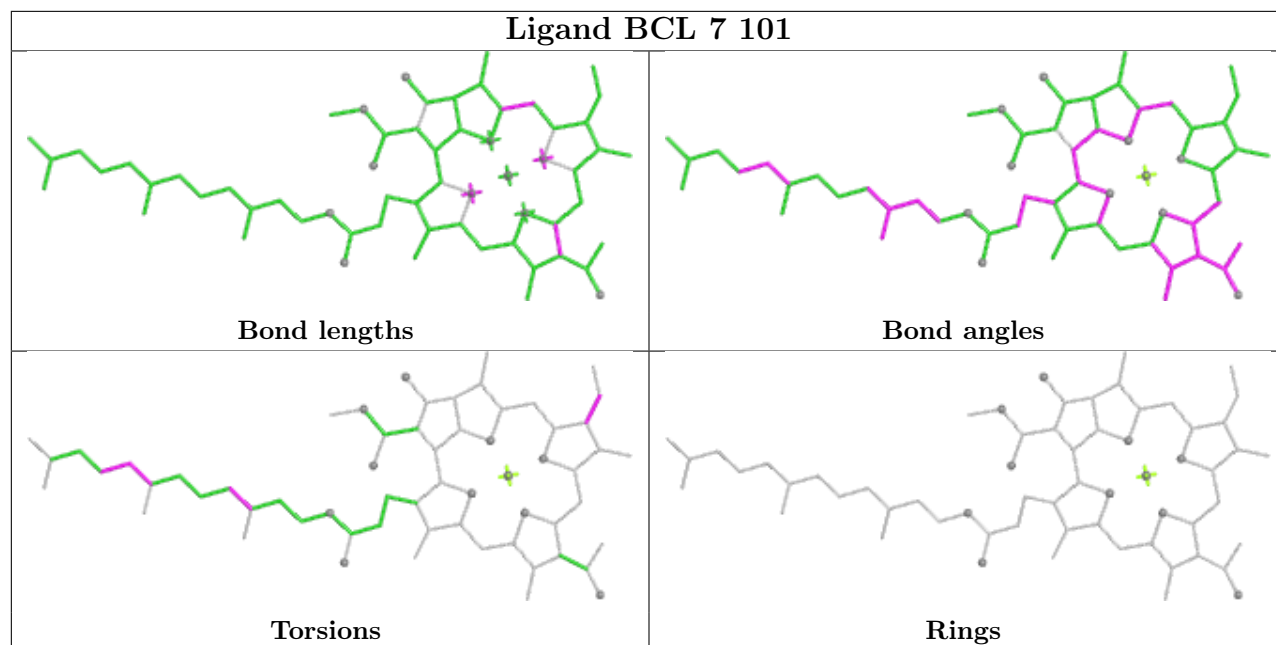


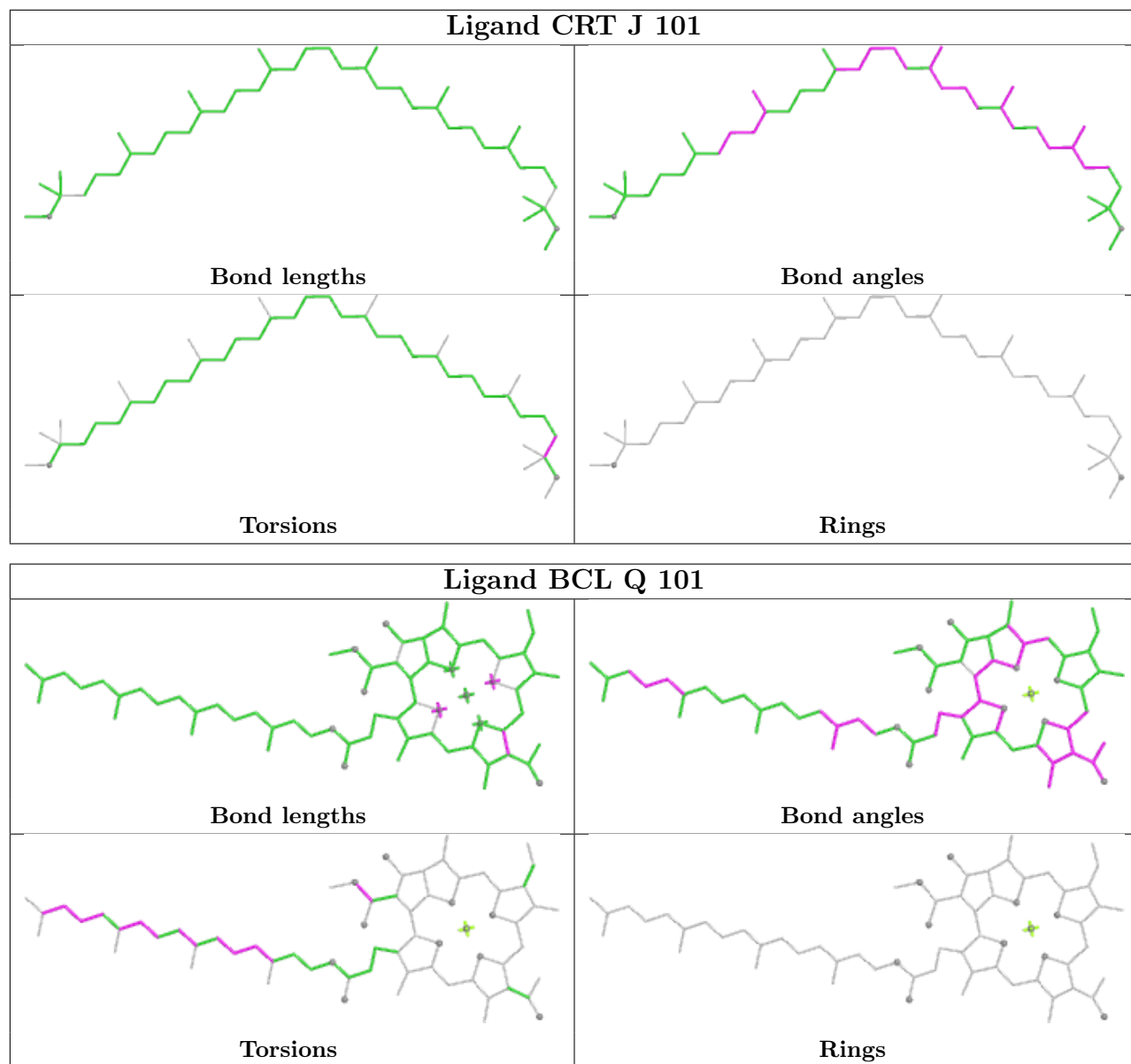


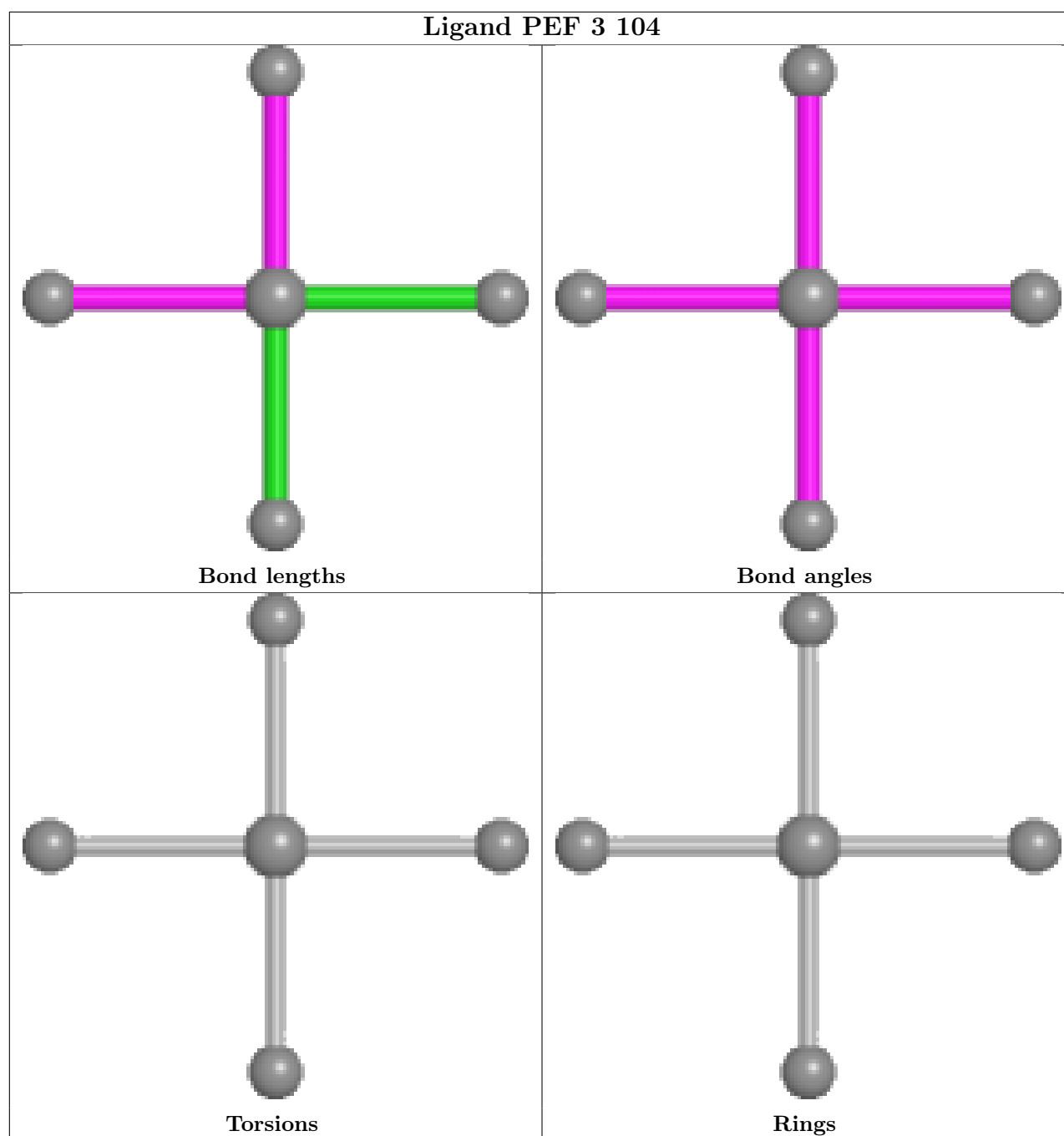


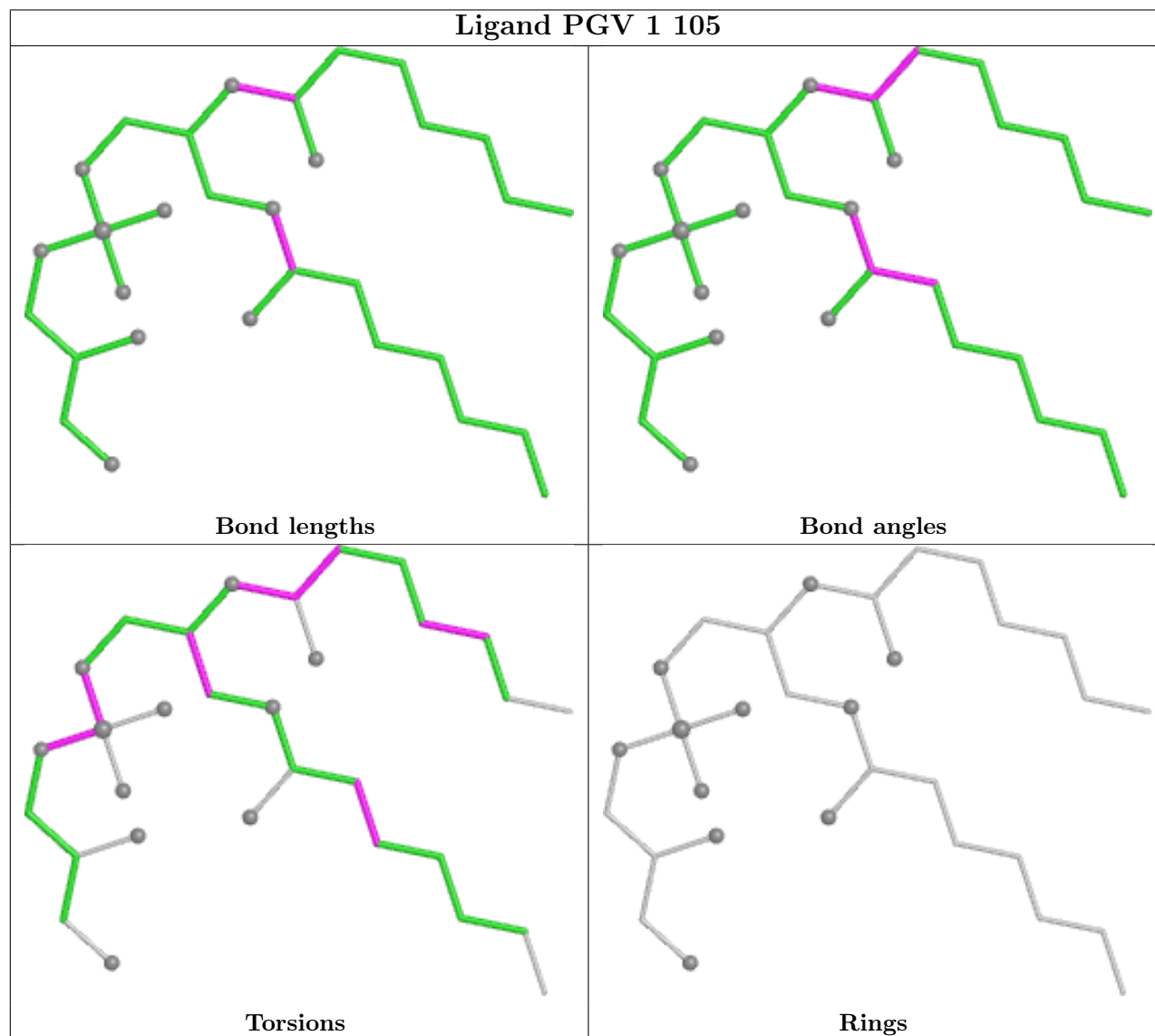
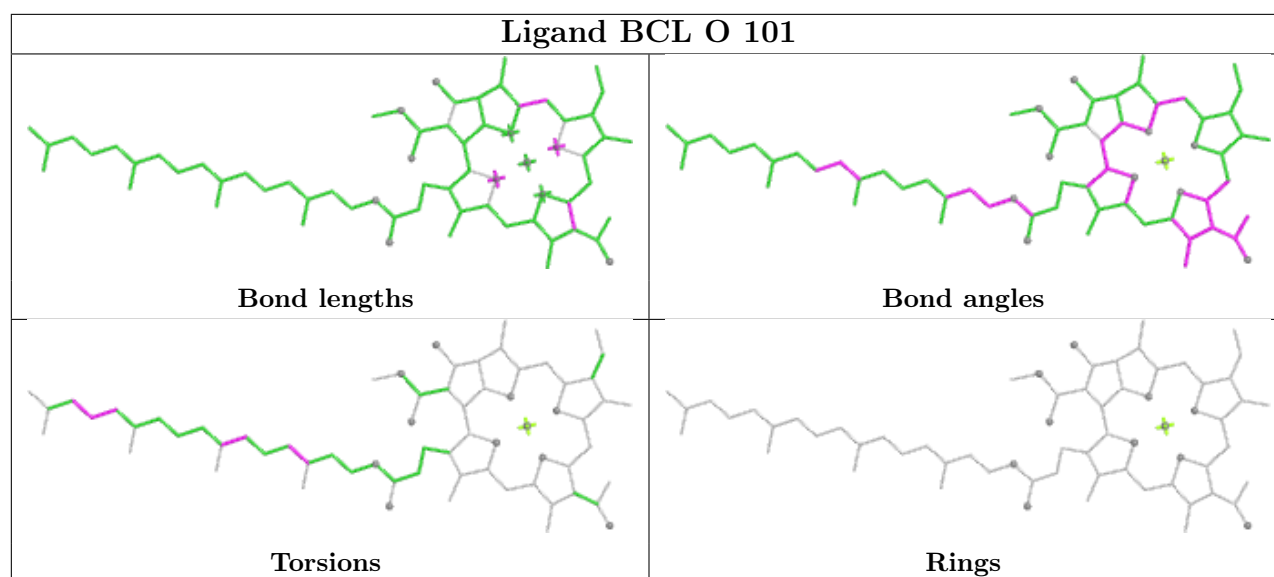


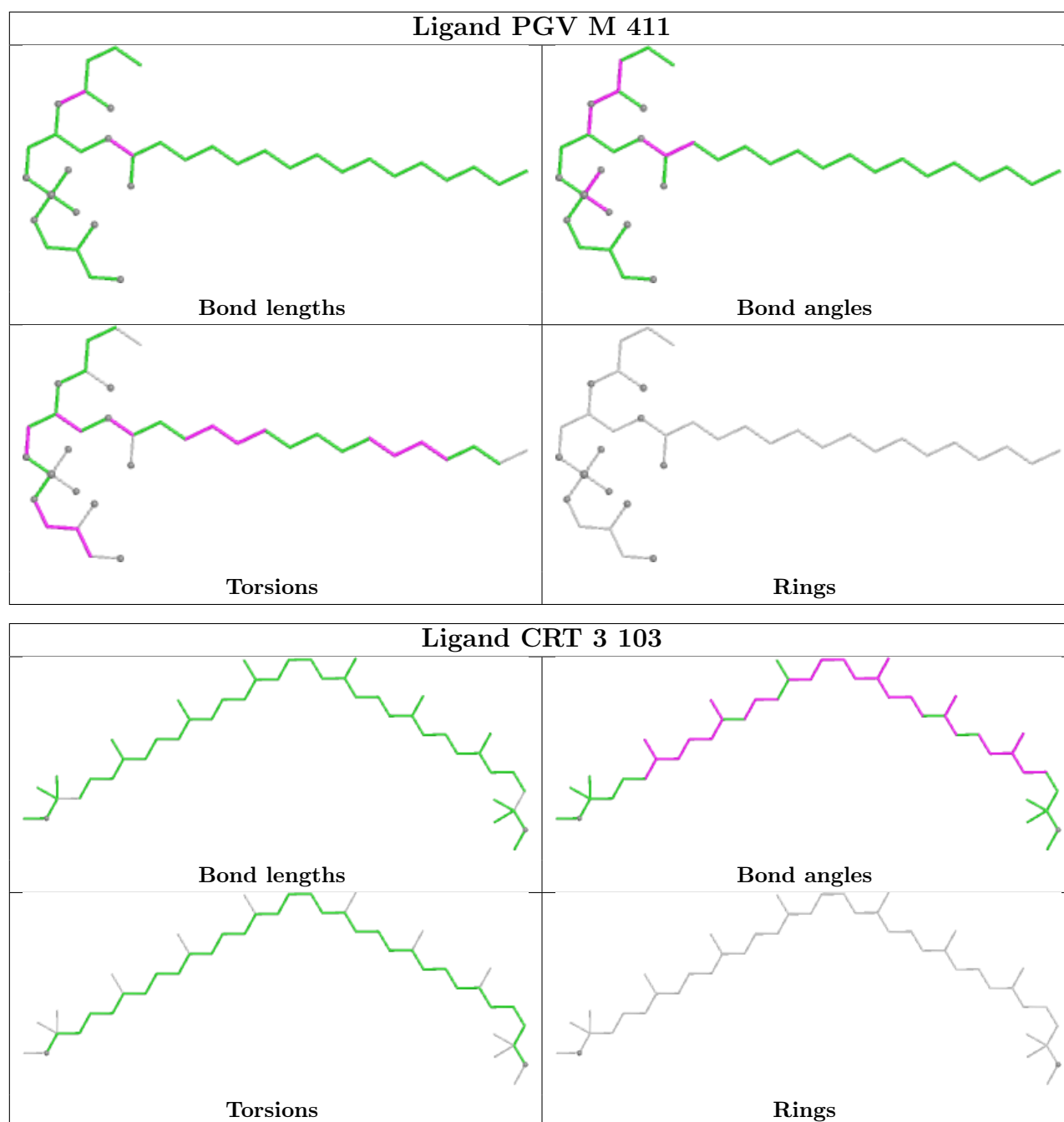


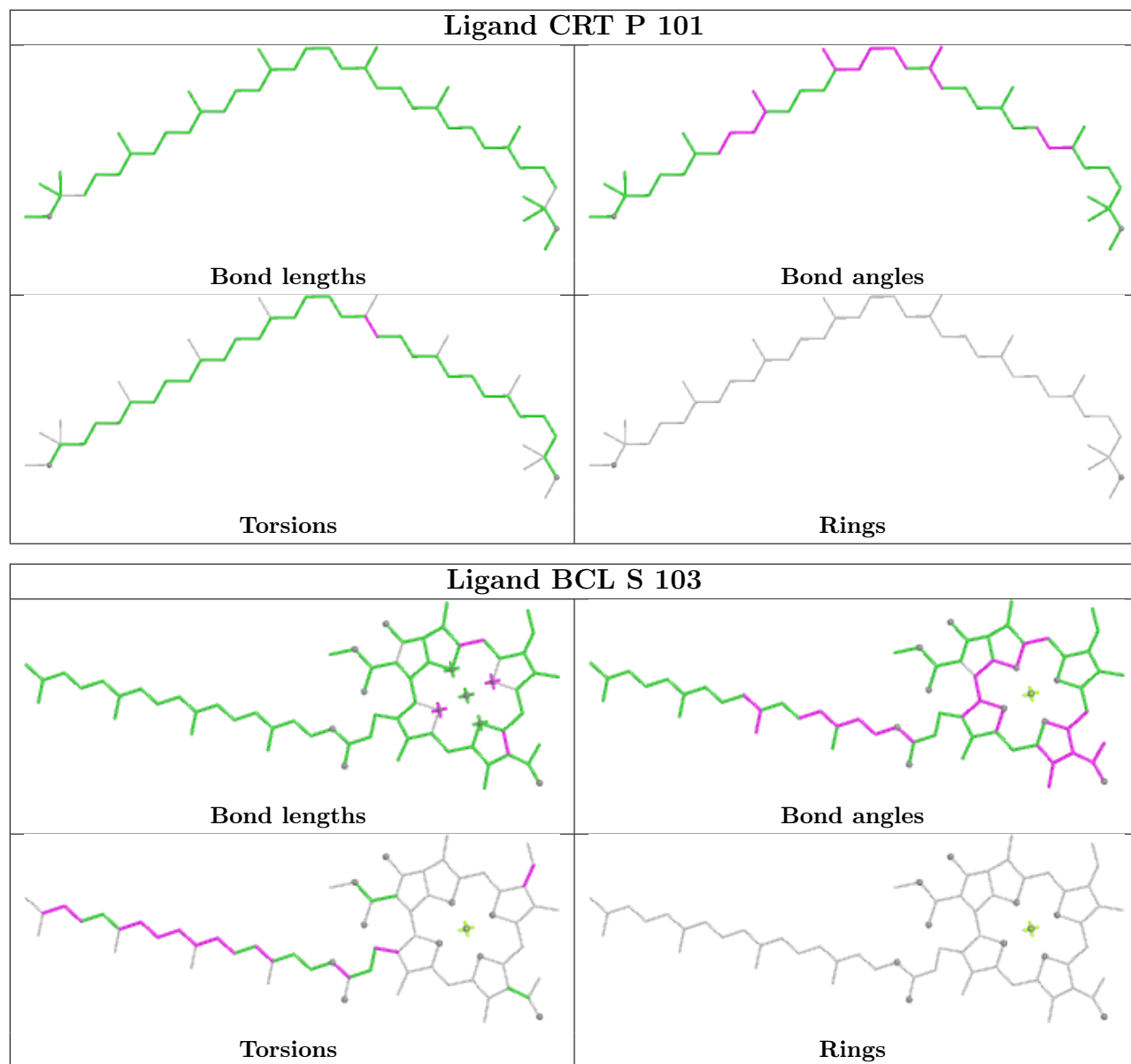


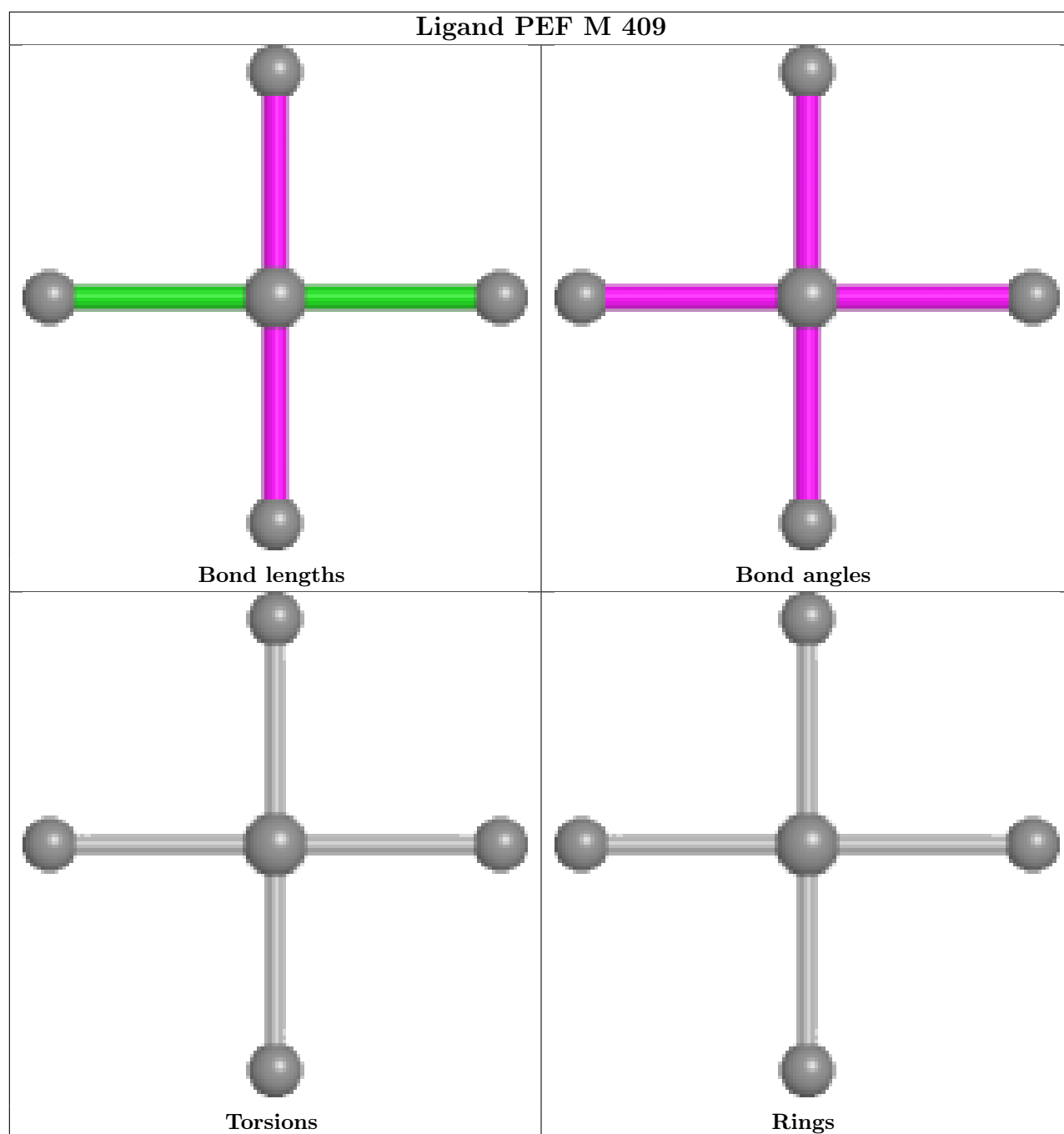


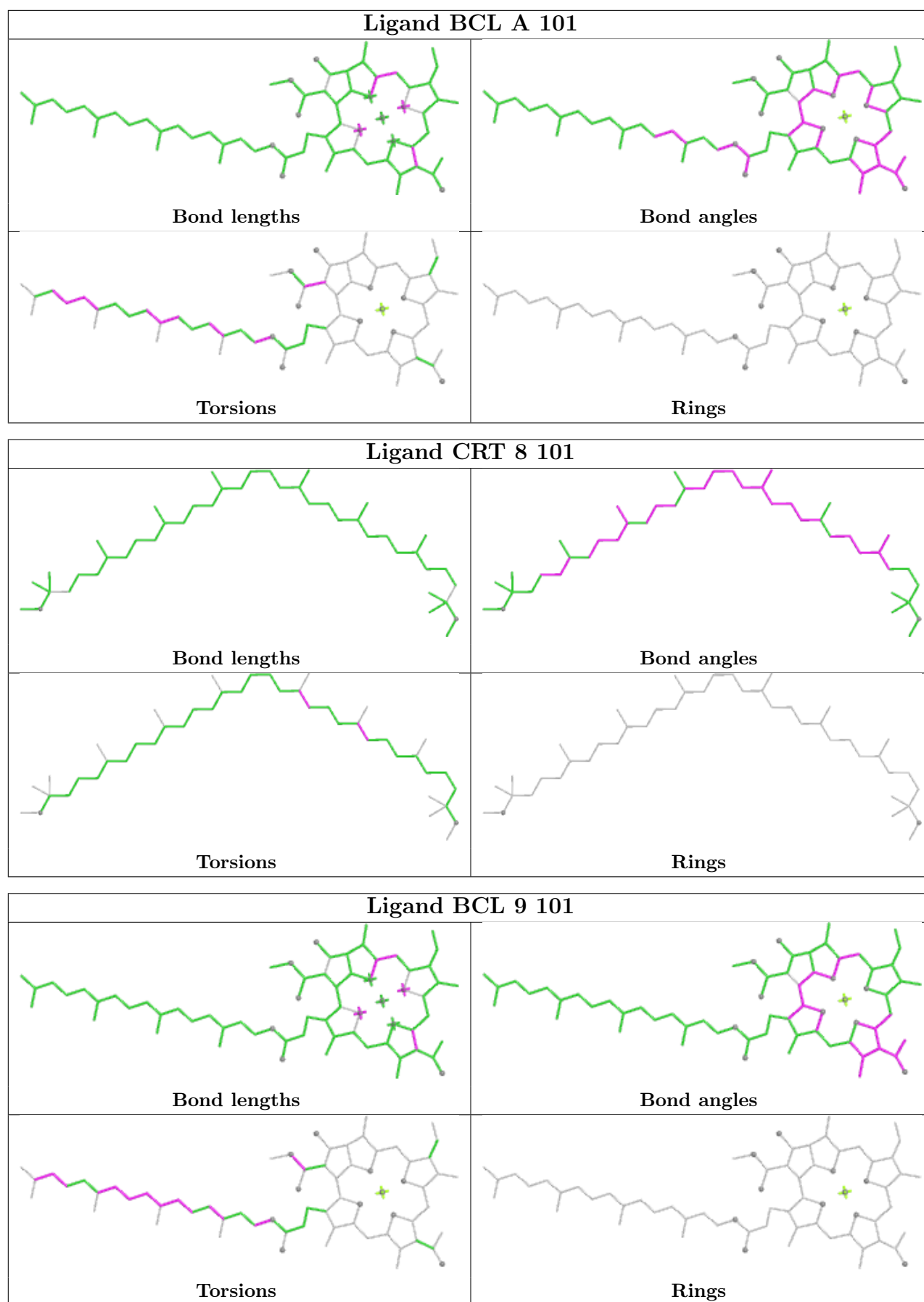


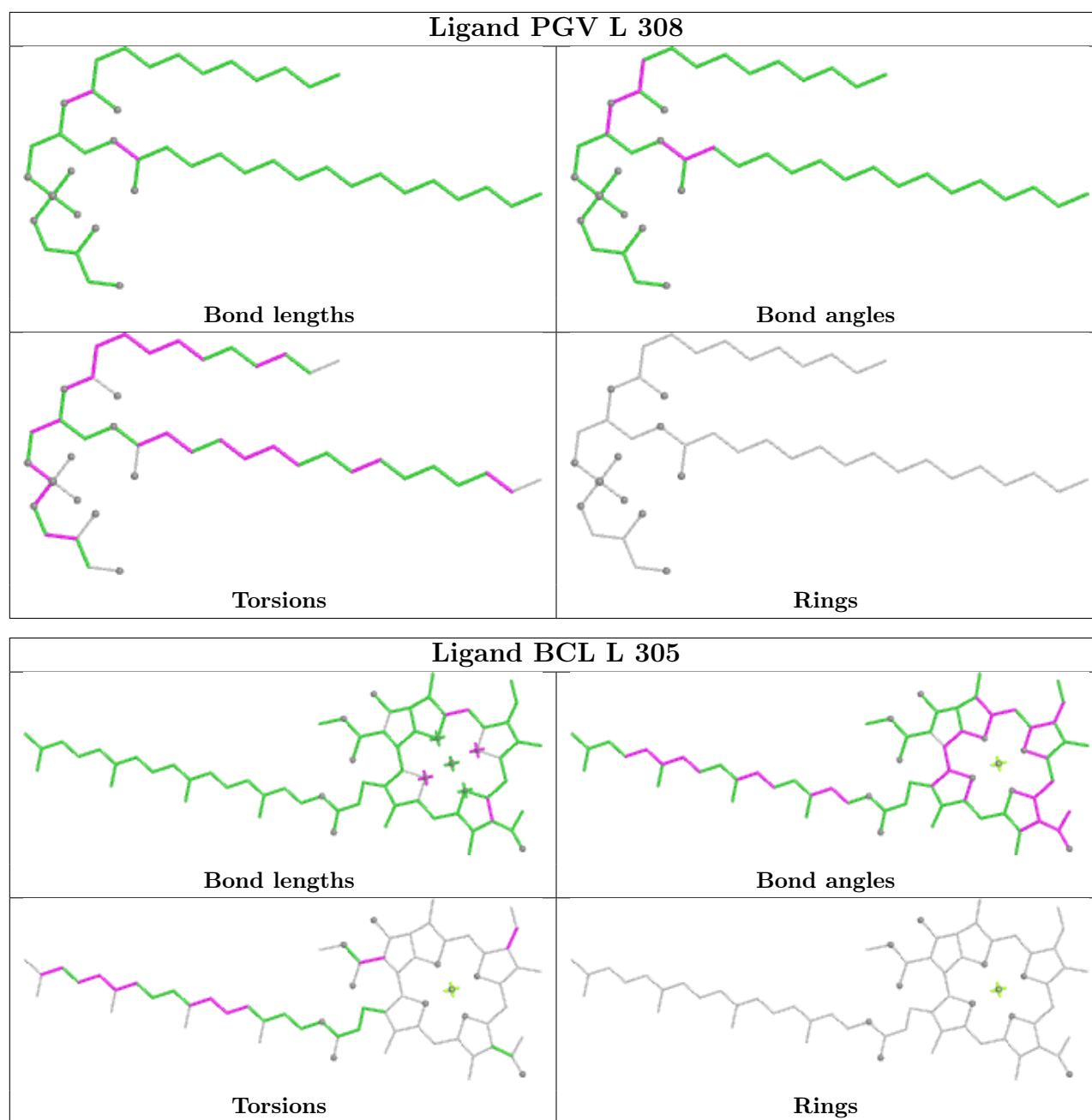


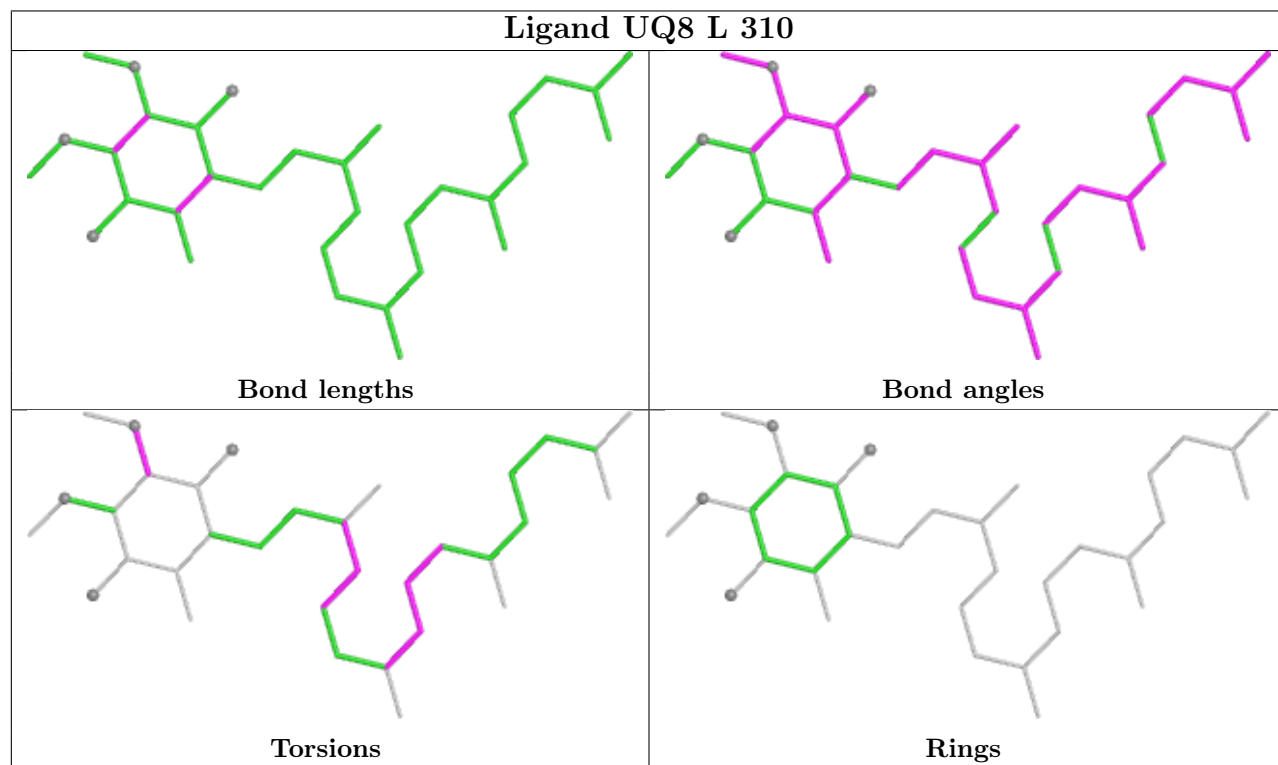
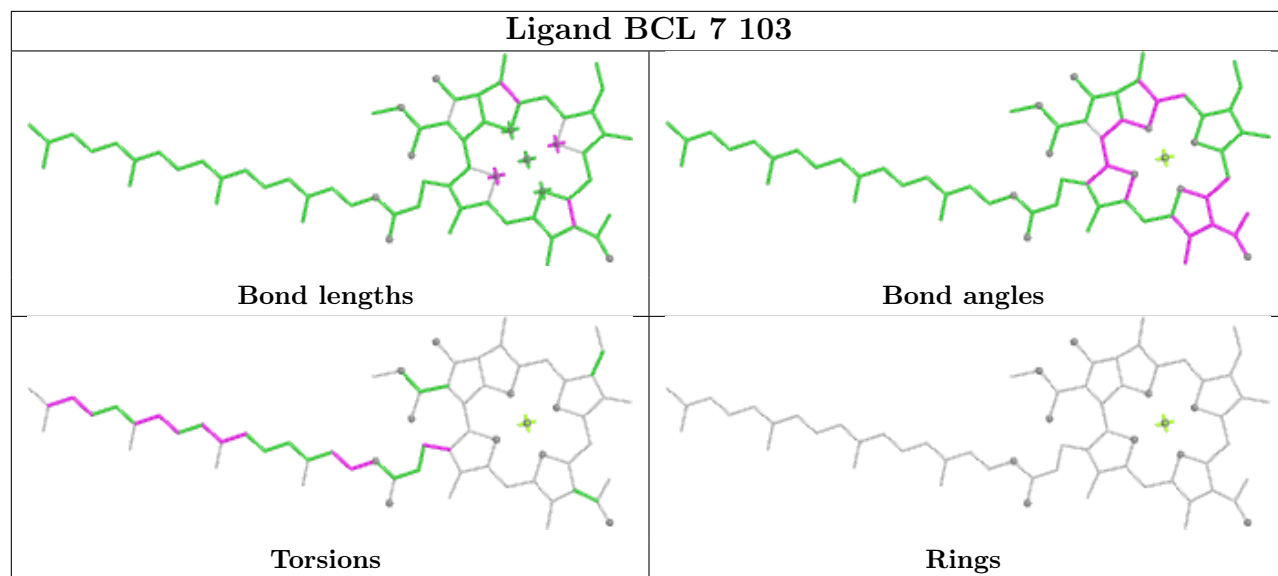


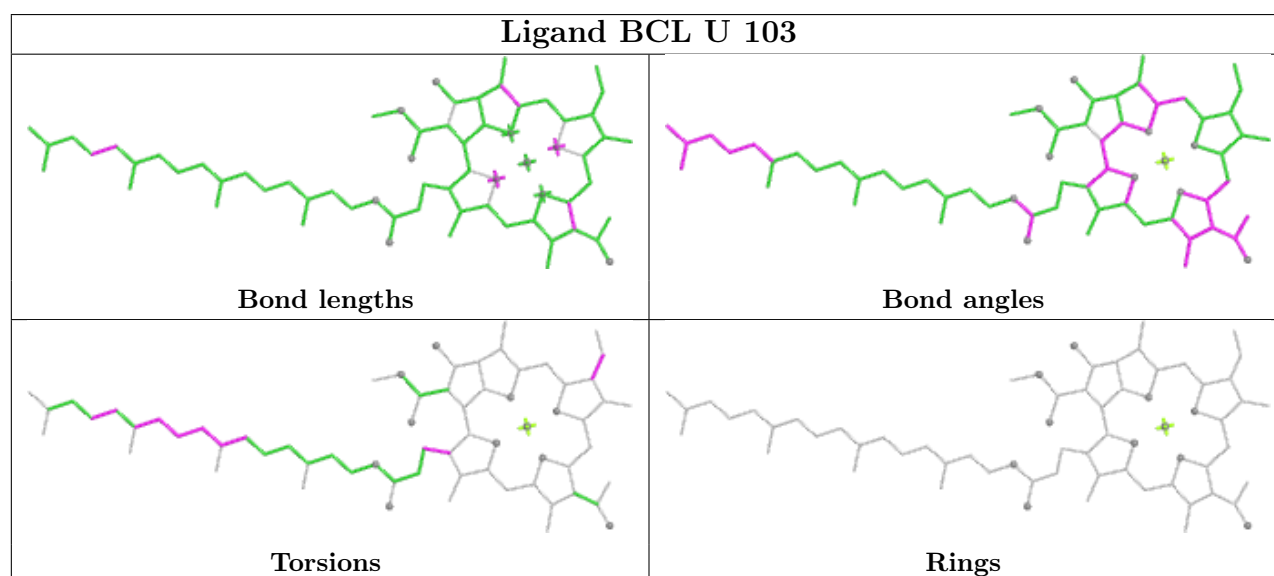
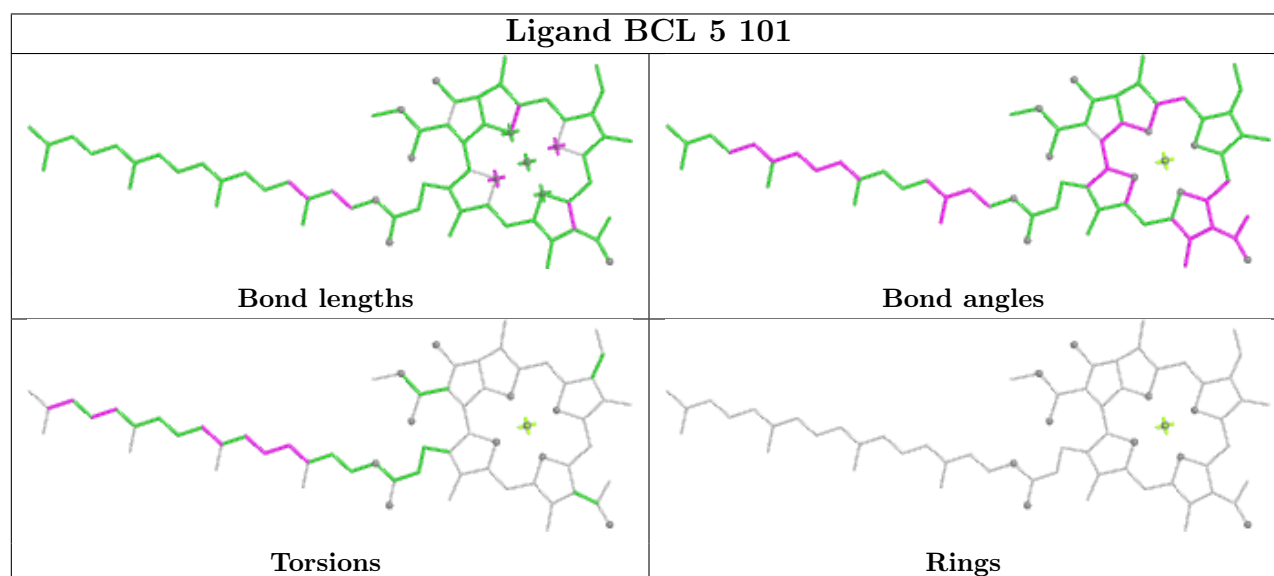
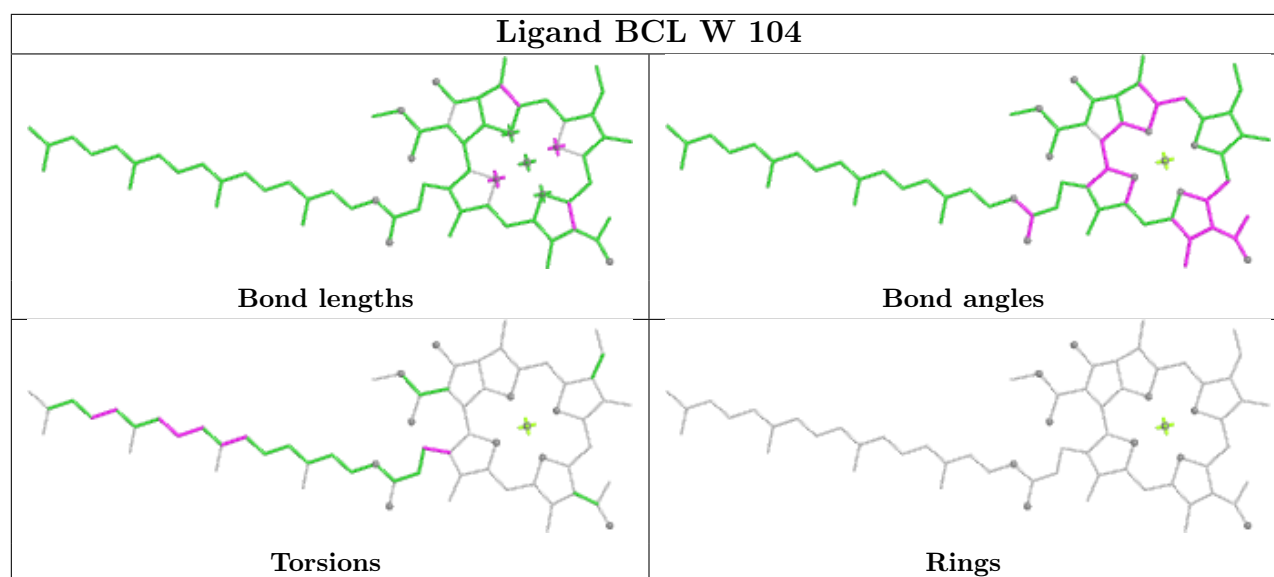


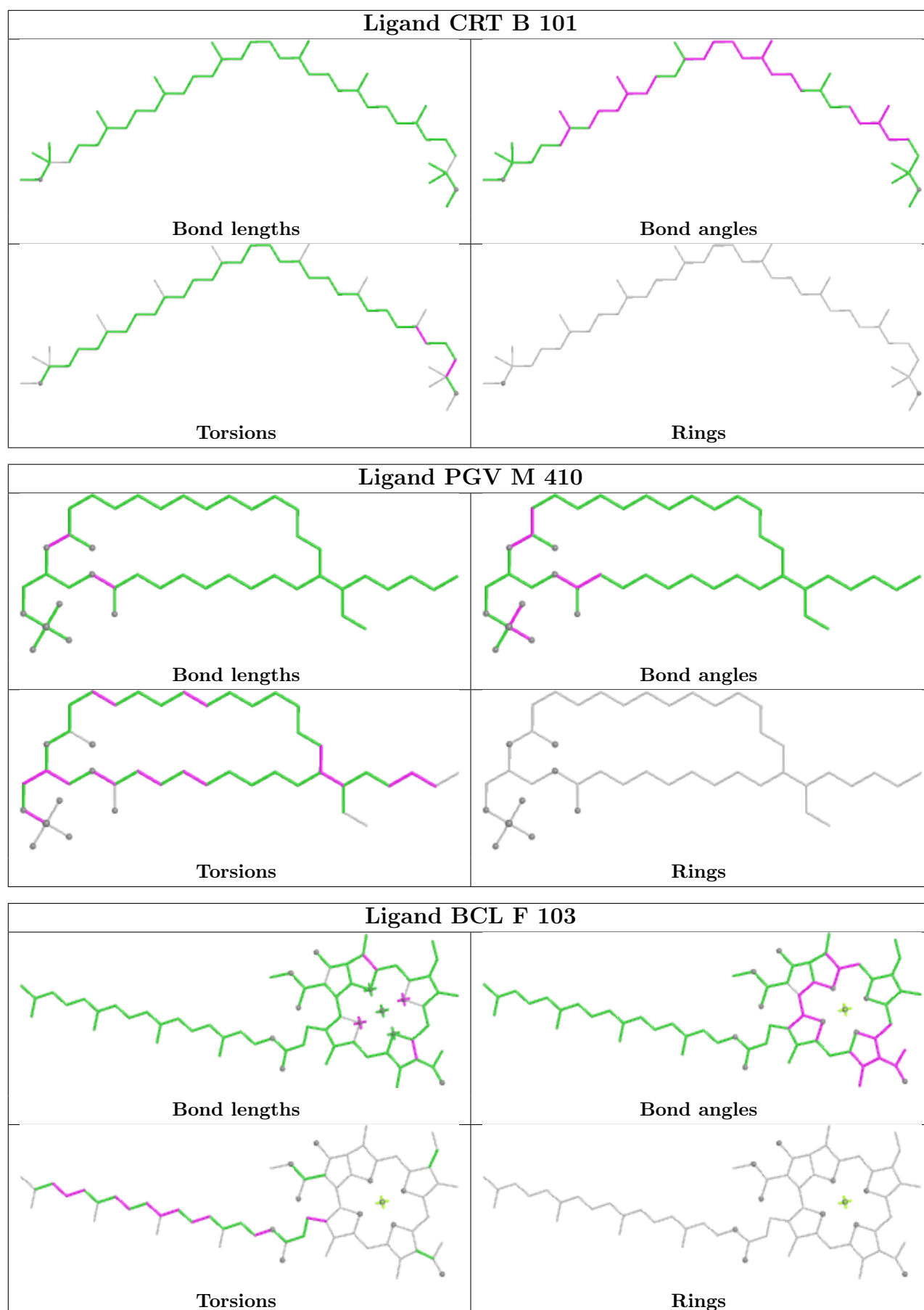




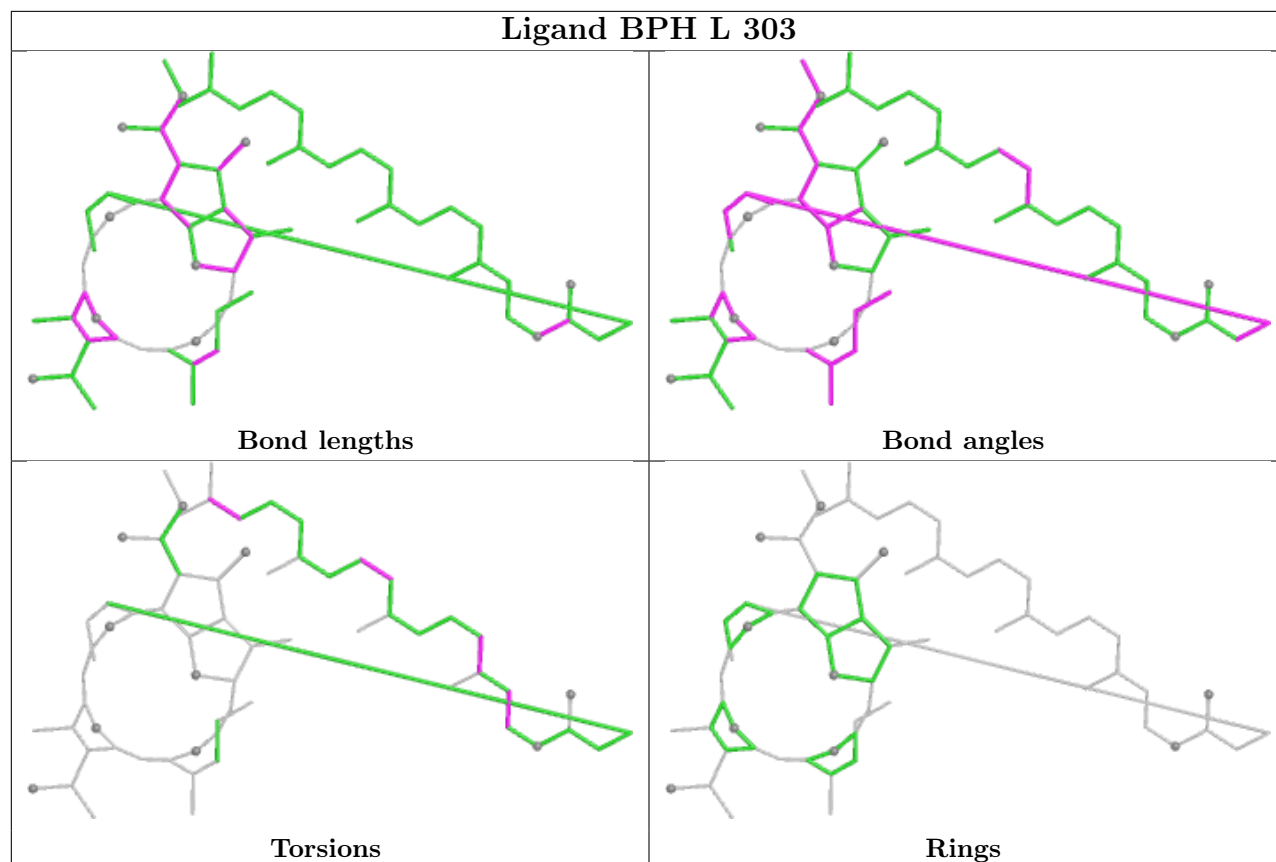




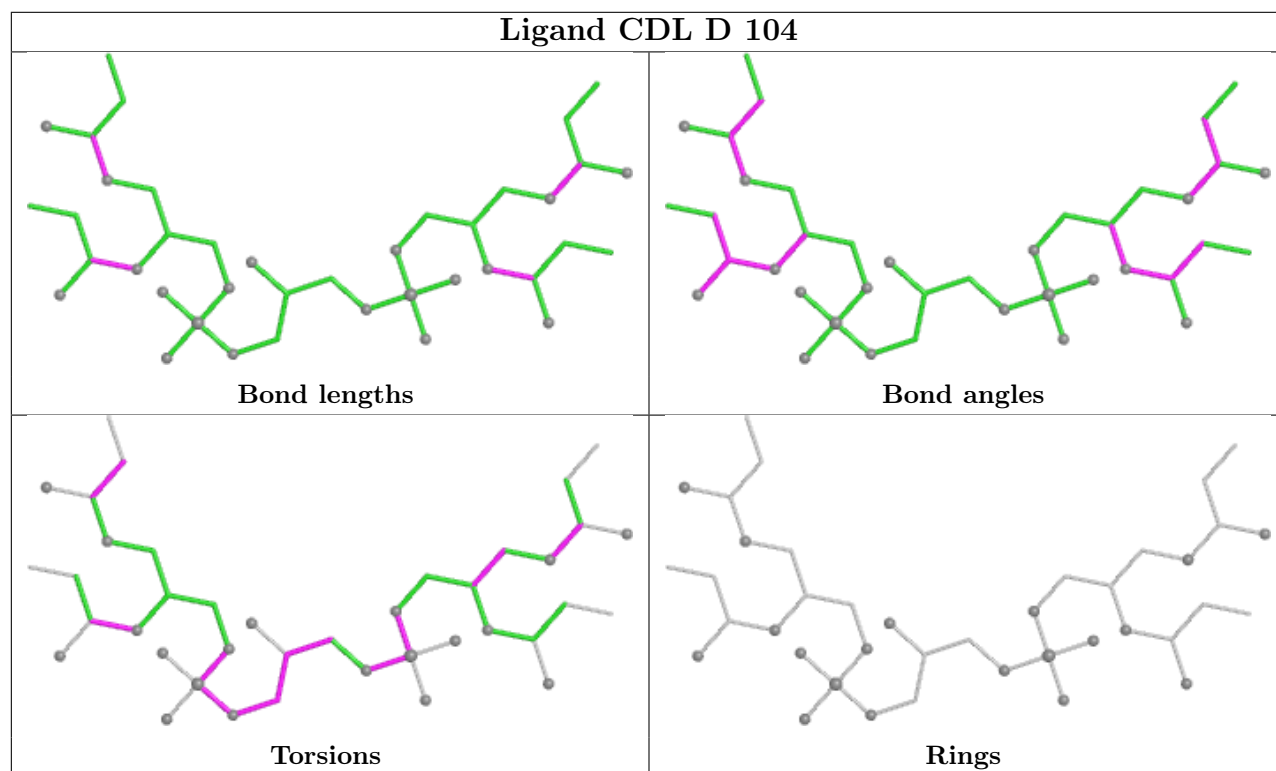


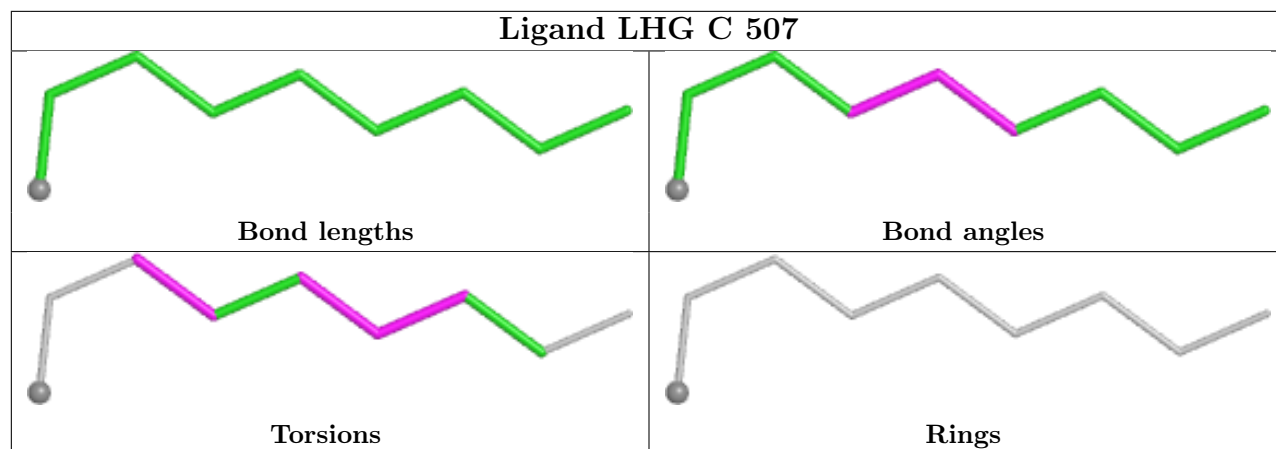


Ligand BPH L 303



Ligand CDL D 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	311/311 (100%)	-0.25	4 (1%) 75 67	71, 98, 140, 179	0
2	L	280/281 (99%)	-0.22	6 (2%) 63 54	64, 93, 123, 156	1 (0%)
3	M	318/325 (97%)	-0.33	4 (1%) 75 67	57, 94, 119, 178	2 (0%)
4	H	255/259 (98%)	-0.14	5 (1%) 65 56	62, 117, 153, 208	2 (0%)
5	1	56/61 (91%)	-0.29	2 (3%) 46 38	97, 126, 177, 195	0
5	3	56/61 (91%)	-0.29	0 100 100	82, 128, 177, 199	1 (1%)
5	5	54/61 (88%)	-0.16	3 (5%) 30 23	101, 132, 199, 226	0
5	7	57/61 (93%)	0.06	1 (1%) 67 59	101, 147, 221, 254	0
5	9	57/61 (93%)	-0.19	1 (1%) 67 59	108, 131, 219, 251	0
5	A	54/61 (88%)	-0.16	1 (1%) 66 58	110, 133, 174, 191	0
5	D	55/61 (90%)	-0.21	0 100 100	74, 129, 192, 206	1 (1%)
5	F	55/61 (90%)	-0.10	0 100 100	82, 135, 180, 190	1 (1%)
5	I	57/61 (93%)	-0.14	1 (1%) 67 59	72, 137, 191, 214	1 (1%)
5	K	57/61 (93%)	0.12	2 (3%) 47 38	108, 132, 181, 185	0
5	O	56/61 (91%)	-0.09	0 100 100	71, 136, 173, 188	1 (1%)
5	Q	57/61 (93%)	-0.15	1 (1%) 67 59	98, 125, 196, 238	0
5	S	56/61 (91%)	-0.05	1 (1%) 67 59	56, 129, 205, 221	3 (5%)
5	U	58/61 (95%)	-0.30	0 100 100	96, 126, 199, 214	0
5	W	56/61 (91%)	-0.30	2 (3%) 46 38	94, 131, 174, 211	0
5	Y	57/61 (93%)	-0.29	3 (5%) 32 25	93, 121, 215, 248	0
6	0	43/47 (91%)	-0.33	0 100 100	137, 155, 181, 190	0
6	2	41/47 (87%)	-0.47	0 100 100	121, 147, 174, 178	0
6	4	42/47 (89%)	-0.46	0 100 100	125, 153, 188, 200	0
6	6	42/47 (89%)	-0.22	0 100 100	134, 160, 235, 254	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
6	8	41/47 (87%)	-0.41	1 (2%) 59 50	124, 157, 227, 310	0
6	B	42/47 (89%)	-0.28	1 (2%) 59 50	132, 153, 177, 204	0
6	E	38/47 (80%)	-0.26	0 100 100	132, 150, 168, 170	0
6	G	42/47 (89%)	-0.38	0 100 100	132, 154, 180, 191	0
6	J	42/47 (89%)	-0.29	0 100 100	130, 152, 185, 201	0
6	N	42/47 (89%)	-0.19	1 (2%) 59 50	135, 147, 168, 180	0
6	P	42/47 (89%)	-0.33	0 100 100	126, 144, 170, 184	0
6	R	41/47 (87%)	-0.45	0 100 100	128, 141, 154, 158	0
6	T	43/47 (91%)	-0.26	1 (2%) 61 52	128, 151, 173, 185	0
6	V	42/47 (89%)	-0.35	0 100 100	122, 154, 203, 239	0
6	X	41/47 (87%)	-0.35	0 100 100	119, 146, 175, 186	0
6	Z	40/47 (85%)	-0.40	0 100 100	123, 146, 177, 192	0
7	b	83/83 (100%)	0.28	2 (2%) 59 50	116, 154, 194, 233	0
All	All	2809/2987 (94%)	-0.22	43 (1%) 72 64	56, 126, 182, 310	13 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	Y	17	PRO	3.7
5	7	21	LEU	3.6
1	C	120	ASP	3.5
4	H	61	LEU	3.2
5	5	47	LEU	3.2
5	Q	21	LEU	3.1
5	W	25	VAL	3.0
2	L	207	THR	3.0
7	b	14	ALA	2.9
3	M	55	LEU	2.8
4	H	138	VAL	2.8
5	Y	21	LEU	2.8
7	b	12	PRO	2.8
5	K	3	THR	2.7
1	C	140	ASP	2.7
5	I	47	LEU	2.6
5	5	58	LEU	2.6
4	H	146	GLU	2.6
1	C	162	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	5	21	LEU	2.6
5	A	13	LEU	2.5
2	L	169	VAL	2.5
6	N	21	PHE	2.5
2	L	166	VAL	2.4
1	C	313	ALA	2.4
2	L	206	VAL	2.3
6	T	34	ILE	2.3
5	Y	59	GLY	2.3
4	H	12	ALA	2.3
5	1	21	LEU	2.3
3	M	319	THR	2.3
5	K	30	VAL	2.3
4	H	194	LEU	2.2
5	S	39	VAL	2.2
3	M	23	LEU	2.2
5	9	21	LEU	2.2
6	B	10	THR	2.1
3	M	81	TRP	2.1
6	8	6	LEU	2.1
2	L	82	TYR	2.0
5	1	44	LEU	2.0
2	L	142	PHE	2.0
5	W	14	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
21	PEF	H	302	5/47	0.41	0.08	202,203,203,204	0
21	PEF	W	106	5/47	0.45	0.08	242,243,244,246	0
21	PEF	M	407	5/47	0.67	0.06	181,183,184,187	0
20	CDL	D	104	40/100	0.69	0.14	190,200,207,209	0
21	PEF	I	103	5/47	0.70	0.08	158,159,160,160	0
21	PEF	M	409	5/47	0.70	0.10	113,113,114,115	0
21	PEF	W	105	5/47	0.71	0.14	185,190,191,192	0
20	CDL	Y	104	40/100	0.73	0.13	187,196,210,210	0
12	PGV	1	105	31/51	0.75	0.15	105,145,149,155	0
20	CDL	1	104	13/100	0.75	0.11	153,157,163,166	0
15	UQ8	L	311	18/53	0.78	0.15	135,141,147,150	0
16	SO4	L	306	5/5	0.79	0.06	178,180,180,181	0
15	UQ8	M	413	18/53	0.81	0.13	154,157,166,170	0
21	PEF	3	104	5/47	0.81	0.10	207,209,211,213	0
22	LMT	H	304	35/35	0.81	0.11	95,142,151,155	0
21	PEF	K	104	27/47	0.82	0.15	119,140,143,145	0
21	PEF	1	103	5/47	0.82	0.07	175,175,177,179	0
10	GOL	C	506	6/6	0.83	0.10	139,143,147,148	0
20	CDL	U	104	62/100	0.83	0.13	146,181,209,216	0
12	PGV	9	104	33/51	0.84	0.15	136,155,166,169	0
21	PEF	M	408	5/47	0.85	0.07	131,134,135,137	0
12	PGV	L	308	44/51	0.86	0.13	100,135,148,149	0
20	CDL	D	105	64/100	0.86	0.11	130,142,153,159	0
20	CDL	S	104	75/100	0.87	0.15	120,157,196,209	0
12	PGV	D	106	35/51	0.87	0.10	115,135,159,167	0
22	LMT	M	414	35/35	0.87	0.10	128,162,179,183	0
12	PGV	L	307	43/51	0.87	0.14	98,150,173,178	0
19	CRT	G	101	44/44	0.88	0.16	113,138,160,162	0
19	CRT	0	101	44/44	0.88	0.17	109,135,168,170	0
12	PGV	H	303	36/51	0.88	0.10	86,123,130,131	0
12	PGV	3	105	51/51	0.88	0.14	99,130,187,191	0
12	PGV	C	508	21/51	0.88	0.14	103,127,138,143	0
15	UQ8	L	309	53/53	0.89	0.15	113,137,188,192	0
20	CDL	M	406	100/100	0.89	0.12	92,119,155,158	0
19	CRT	O	103	44/44	0.89	0.14	107,121,149,152	0
19	CRT	8	101	44/44	0.89	0.15	127,136,180,182	0
20	CDL	M	412	39/100	0.90	0.08	81,113,129,135	0
20	CDL	H	305	79/100	0.90	0.12	93,118,143,146	0
19	CRT	V	101	44/44	0.90	0.15	99,129,151,154	0
11	LHG	C	507	9/49	0.90	0.09	84,90,99,100	0
20	CDL	O	104	86/100	0.90	0.14	120,144,155,159	0
19	CRT	J	101	44/44	0.90	0.14	107,135,154,156	0
14	BPH	M	402	65/65	0.90	0.13	75,83,147,154	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
19	CRT	T	101	44/44	0.91	0.12	103,122,140,142	0
12	PGV	M	410	46/51	0.91	0.13	101,119,128,131	0
19	CRT	W	102	44/44	0.91	0.15	102,126,152,153	0
19	CRT	B	101	44/44	0.91	0.13	116,139,157,158	0
9	CA	I	102	1/1	0.91	0.06	139,139,139,139	0
9	CA	F	102	1/1	0.91	0.07	129,129,129,129	0
19	CRT	N	101	44/44	0.91	0.13	104,128,137,141	0
13	BCL	S	103	66/66	0.91	0.12	106,120,176,189	0
19	CRT	P	101	44/44	0.91	0.13	100,132,147,149	0
15	UQ8	L	304	33/53	0.92	0.15	75,85,129,131	0
12	PGV	M	411	37/51	0.92	0.10	120,151,194,196	0
19	CRT	M	405	44/44	0.92	0.11	72,88,127,129	0
13	BCL	S	101	66/66	0.92	0.11	111,123,163,167	0
13	BCL	A	101	66/66	0.93	0.11	130,139,162,170	0
13	BCL	U	103	66/66	0.93	0.11	113,131,174,185	0
13	BCL	5	103	66/66	0.93	0.11	116,136,163,167	0
13	BCL	9	103	66/66	0.93	0.09	113,129,177,186	0
9	CA	Y	102	1/1	0.93	0.06	115,115,115,115	0
19	CRT	2	101	44/44	0.93	0.13	113,129,154,157	0
19	CRT	3	103	44/44	0.93	0.13	116,127,160,162	0
19	CRT	4	101	44/44	0.93	0.12	101,131,161,164	0
13	BCL	F	101	66/66	0.94	0.10	119,131,162,173	0
13	BCL	9	101	66/66	0.94	0.10	126,133,177,179	0
13	BCL	Q	103	66/66	0.94	0.10	105,123,170,181	0
9	CA	9	102	1/1	0.94	0.09	120,120,120,120	0
9	CA	1	102	1/1	0.94	0.05	107,107,107,107	0
13	BCL	U	101	66/66	0.94	0.09	102,122,167,172	0
19	CRT	Z	101	44/44	0.94	0.13	91,133,166,169	0
15	UQ8	L	310	33/53	0.94	0.10	118,126,138,139	0
13	BCL	A	103	66/66	0.94	0.11	114,124,178,185	0
13	BCL	W	101	66/66	0.94	0.11	105,127,170,178	0
13	BCL	W	104	66/66	0.94	0.09	112,123,162,167	0
18	MQ8	M	404	53/53	0.94	0.11	84,88,161,163	0
13	BCL	Y	101	66/66	0.94	0.10	101,118,165,167	0
19	CRT	A	104	44/44	0.94	0.10	110,126,154,156	0
13	BCL	1	101	66/66	0.94	0.10	106,118,161,165	0
13	BCL	2	102	66/66	0.94	0.12	104,125,164,174	0
13	BCL	3	101	66/66	0.94	0.12	108,131,180,185	0
9	CA	3	102	1/1	0.95	0.05	121,121,121,121	0
13	BCL	M	401	66/66	0.95	0.10	61,80,89,92	0
9	CA	5	102	1/1	0.95	0.06	118,118,118,118	0
9	CA	Q	102	1/1	0.95	0.07	116,116,116,116	0

Continued on next page...

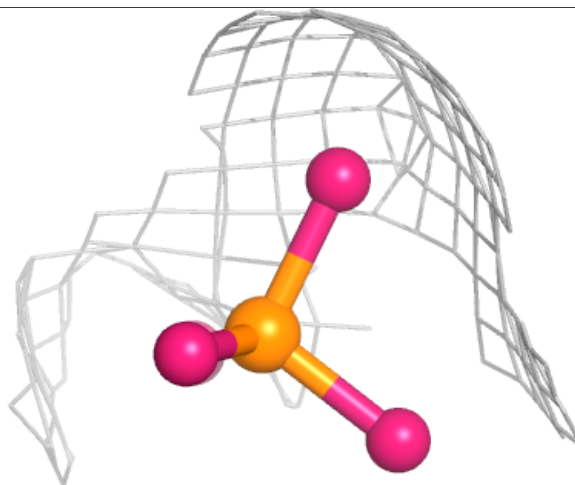
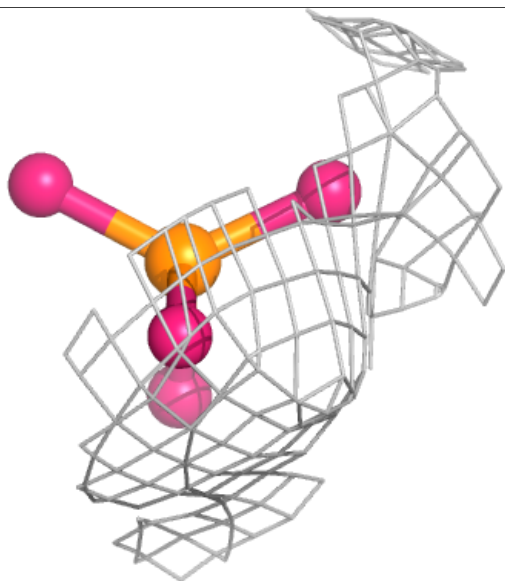
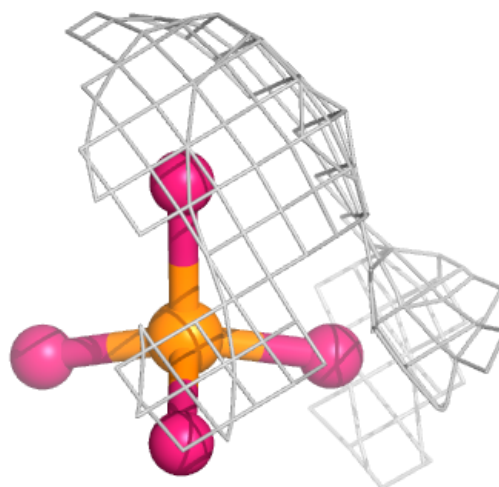
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	BCL	D	101	66/66	0.95	0.10	109,130,160,165	0
13	BCL	Y	103	66/66	0.95	0.09	109,120,159,166	0
9	CA	U	102	1/1	0.95	0.05	112,112,112,112	0
13	BCL	I	101	66/66	0.95	0.12	121,136,176,182	0
13	BCL	J	102	66/66	0.95	0.10	121,137,160,166	0
13	BCL	4	102	66/66	0.95	0.09	110,131,169,182	0
13	BCL	5	101	66/66	0.95	0.10	109,128,163,169	0
13	BCL	K	101	66/66	0.95	0.10	123,132,162,174	0
13	BCL	7	101	61/66	0.95	0.13	121,135,185,188	0
13	BCL	K	103	66/66	0.95	0.10	119,137,170,181	0
13	BCL	O	101	66/66	0.95	0.10	128,137,170,177	0
14	BPH	L	303	65/65	0.95	0.09	68,82,100,103	0
13	BCL	P	102	66/66	0.95	0.09	123,140,185,197	0
13	BCL	Q	101	66/66	0.95	0.10	110,128,174,181	0
9	CA	W	103	1/1	0.95	0.05	105,105,105,105	0
9	CA	C	505	1/1	0.95	0.14	103,103,103,103	0
9	CA	A	102	1/1	0.95	0.05	123,123,123,123	0
9	CA	D	102	1/1	0.96	0.05	127,127,127,127	0
13	BCL	D	103	66/66	0.96	0.09	118,126,164,173	0
13	BCL	L	301	66/66	0.96	0.08	64,80,101,108	0
13	BCL	F	103	66/66	0.96	0.10	123,135,177,188	0
13	BCL	L	302	66/66	0.96	0.07	59,68,90,98	0
13	BCL	L	305	66/66	0.96	0.09	69,80,135,143	0
10	GOL	H	301	6/6	0.96	0.14	107,113,116,117	0
9	CA	S	102	1/1	0.96	0.07	111,111,111,111	0
9	CA	K	102	1/1	0.96	0.04	120,120,120,120	0
13	BCL	7	103	66/66	0.96	0.10	124,136,182,184	0
9	CA	O	102	1/1	0.97	0.07	121,121,121,121	0
9	CA	7	102	1/1	0.97	0.04	115,115,115,115	0
23	SF4	b	101	8/8	0.97	0.04	123,152,192,194	0
8	HEC	C	504	43/43	0.98	0.08	74,79,89,92	0
8	HEC	C	501	43/43	0.98	0.07	97,107,117,120	0
8	HEC	C	502	43/43	0.98	0.09	71,88,104,106	0
17	FE	M	403	1/1	0.98	0.05	75,75,75,75	0
8	HEC	C	503	43/43	0.98	0.09	70,80,95,100	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.

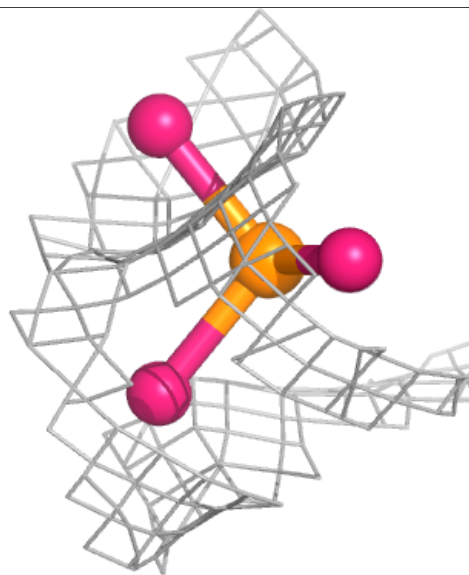
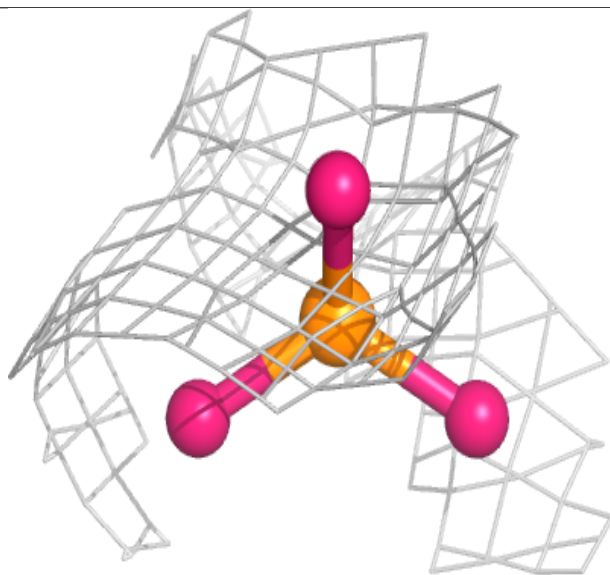
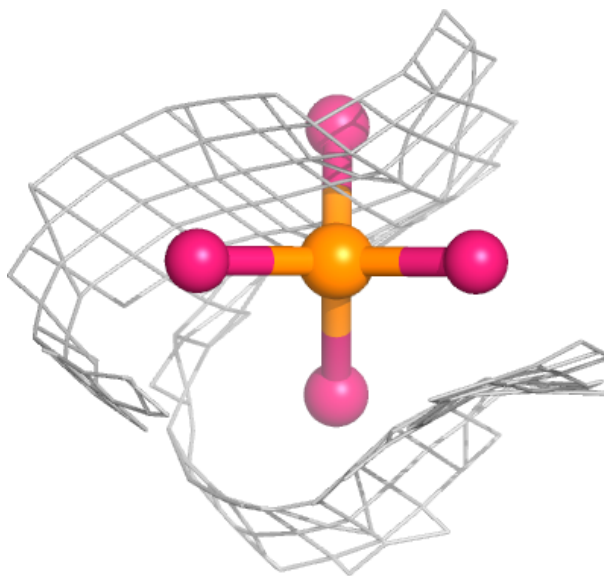
Electron density around PEF H 302:

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



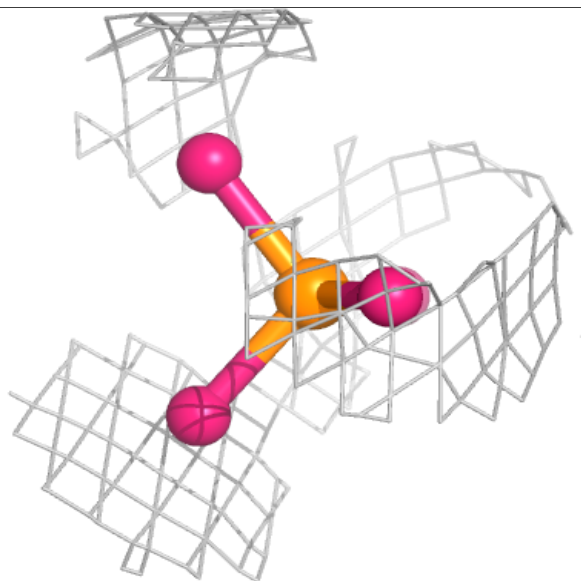
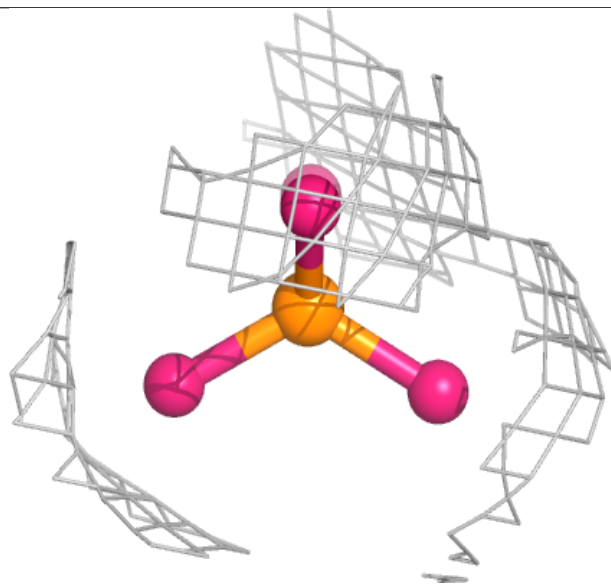
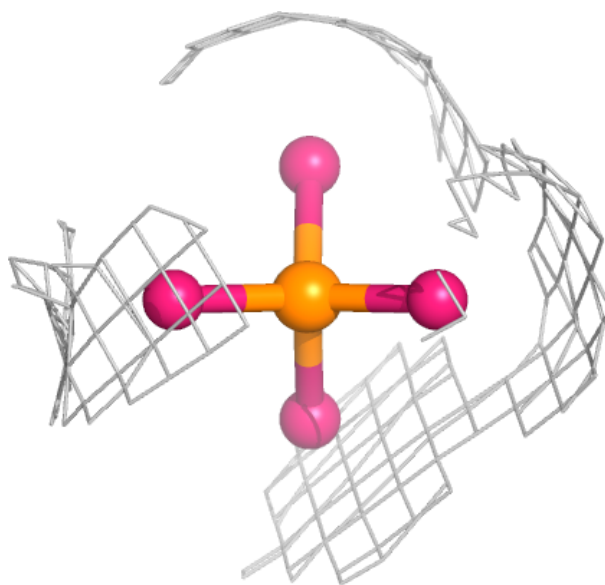
Electron density around PEF W 106:

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



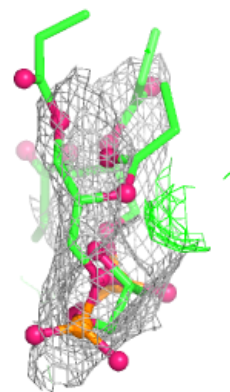
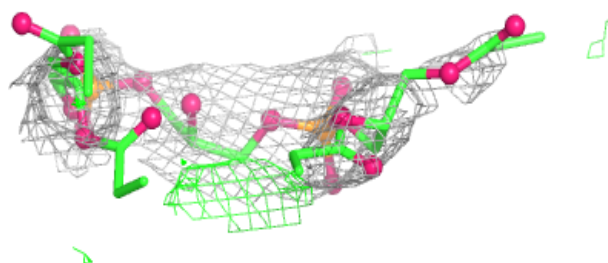
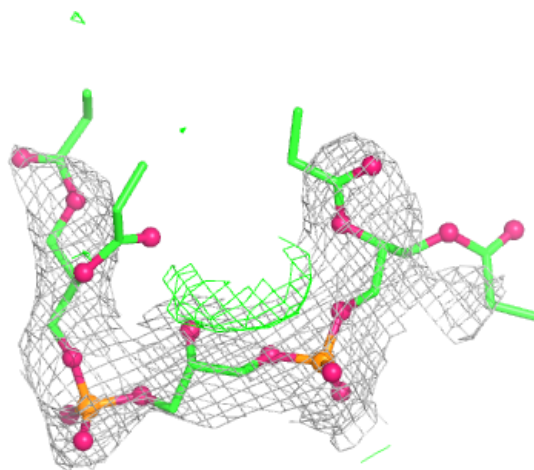
Electron density around PEF M 407:

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



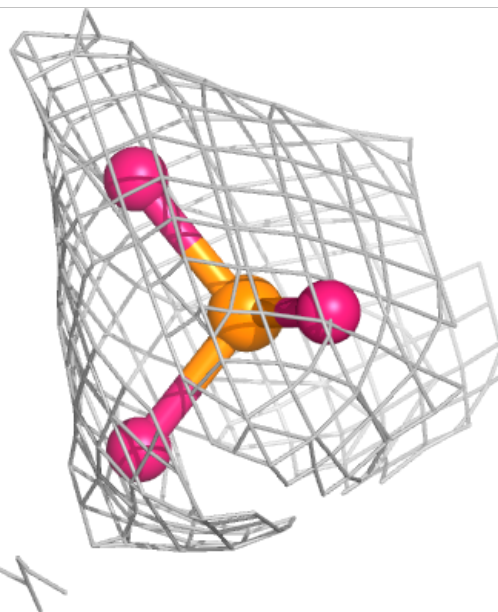
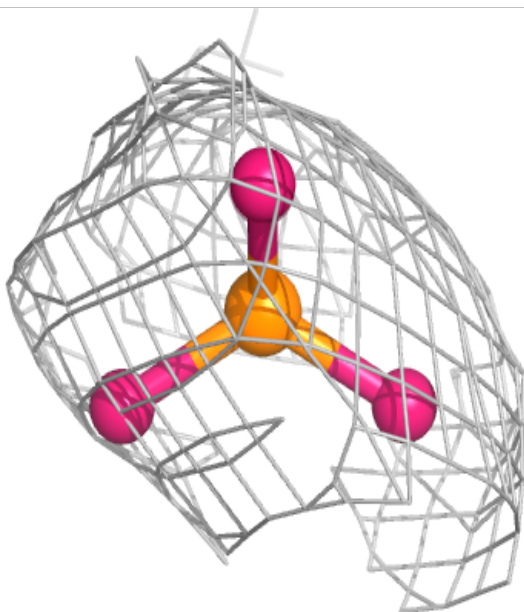
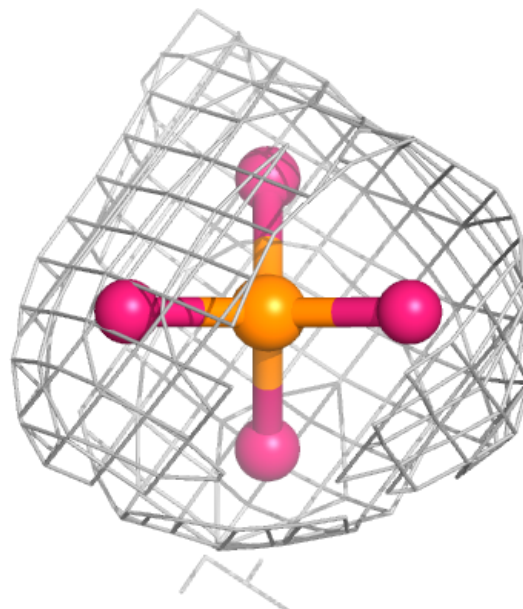
Electron density around CDL D 104:

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



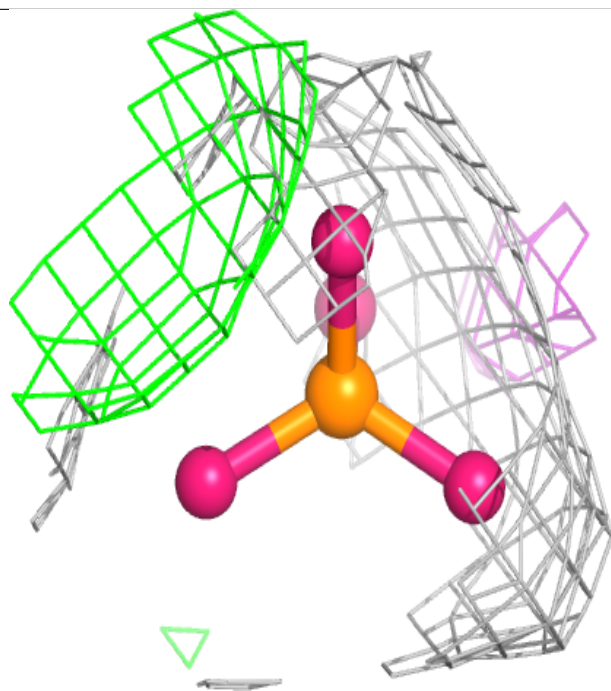
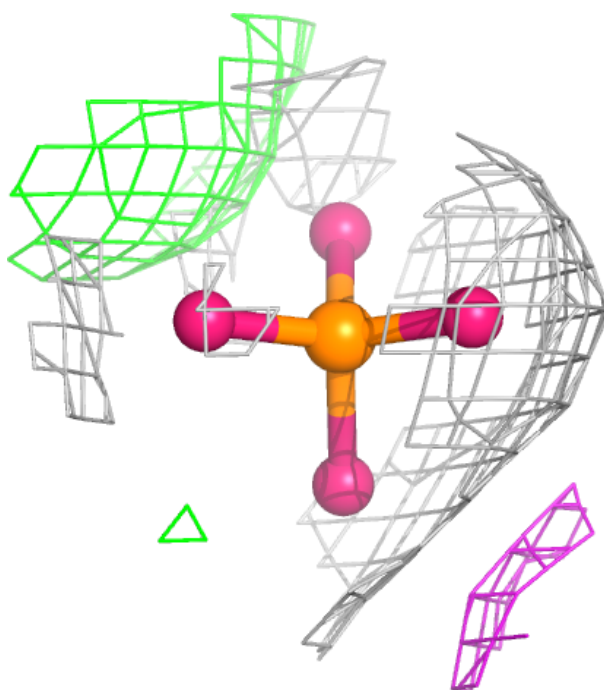
Electron density around PEF I 103:

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



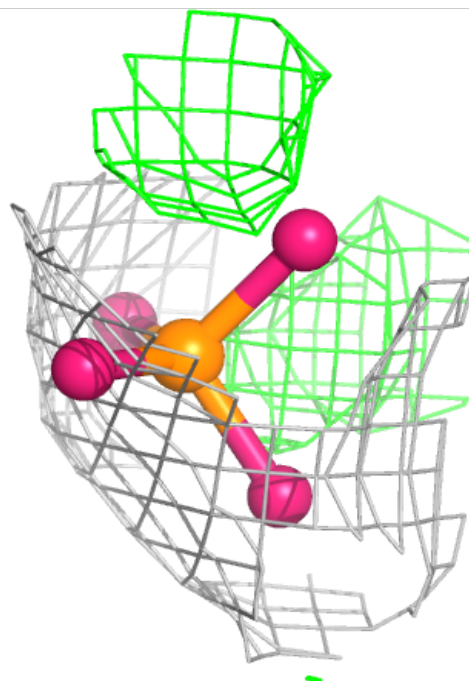
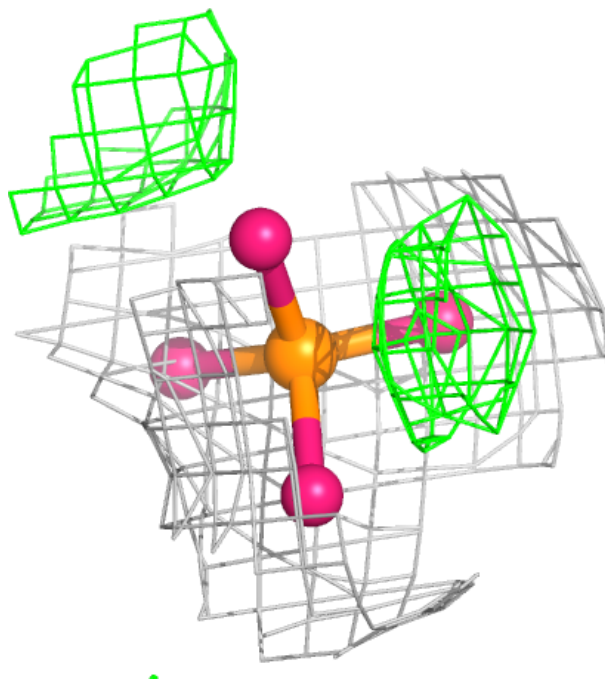
Electron density around PEF M 409:

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



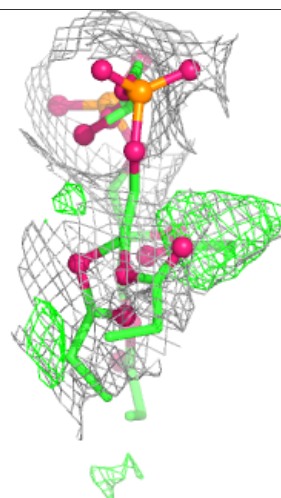
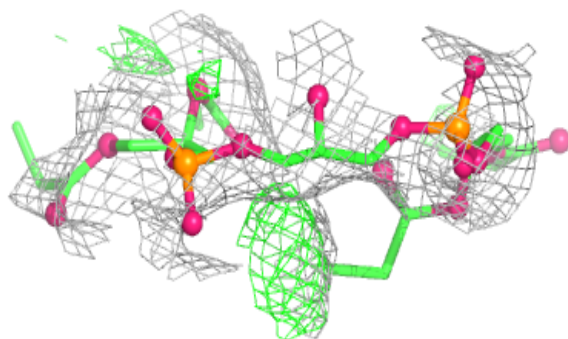
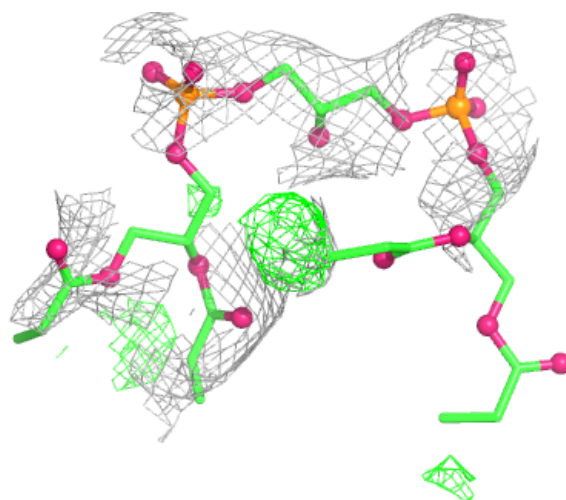
Electron density around PEF W 105:

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



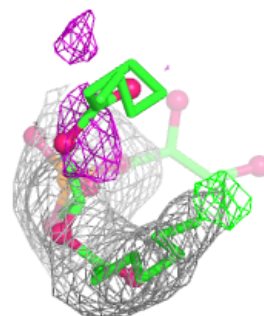
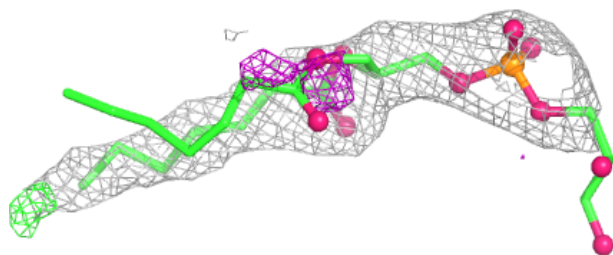
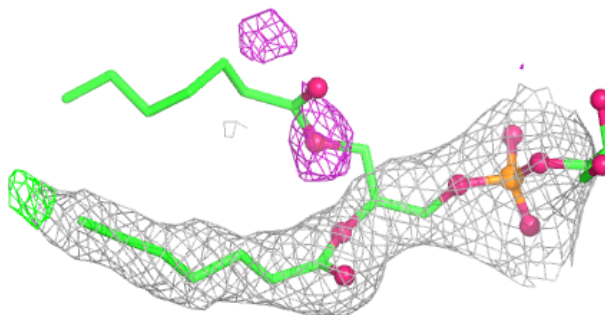
Electron density around CDL Y 104:

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



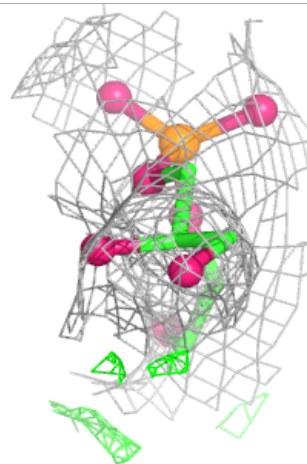
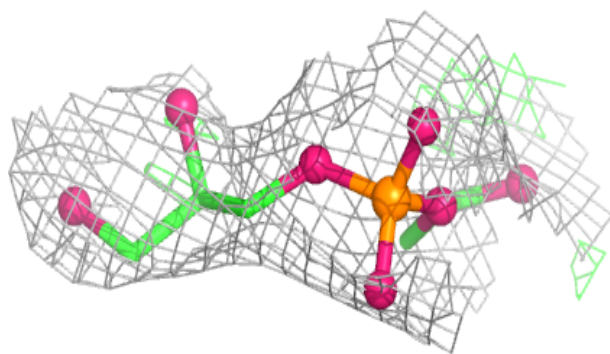
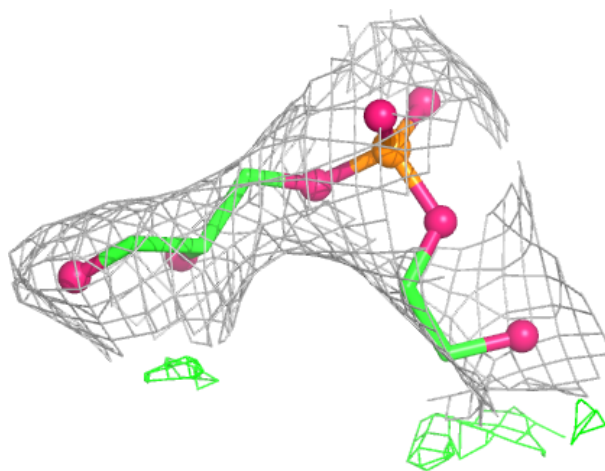
Electron density around PGV 1 105:

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



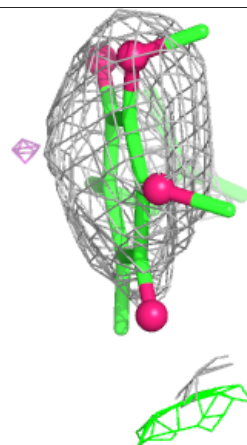
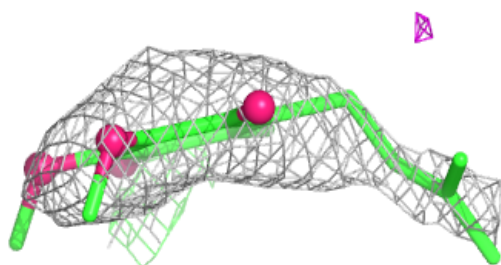
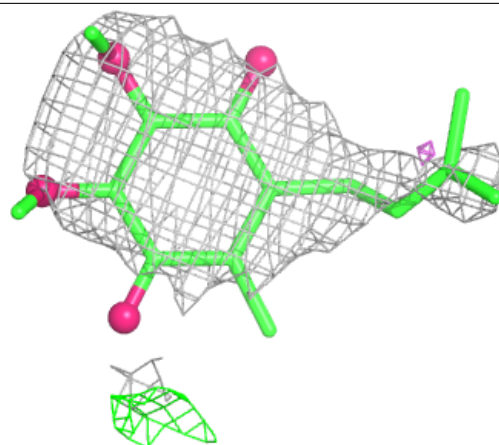
Electron density around CDL 1 104:

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



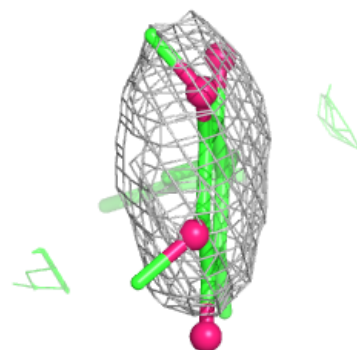
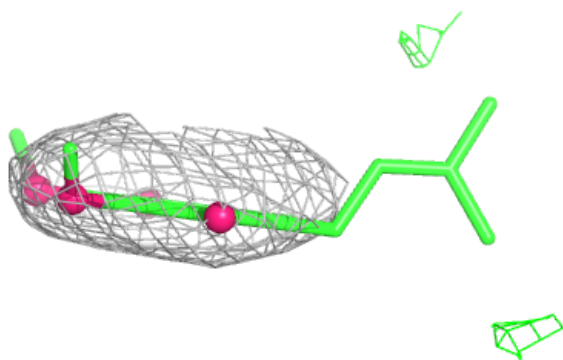
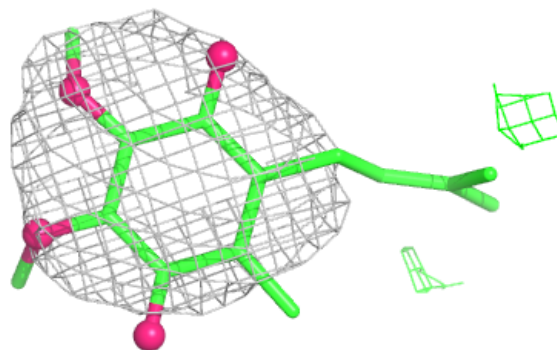
Electron density around UQ8 L 311:

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

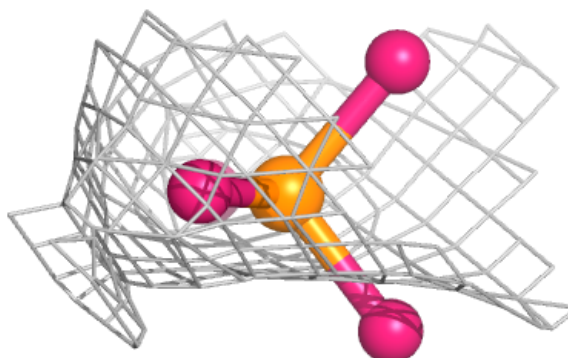
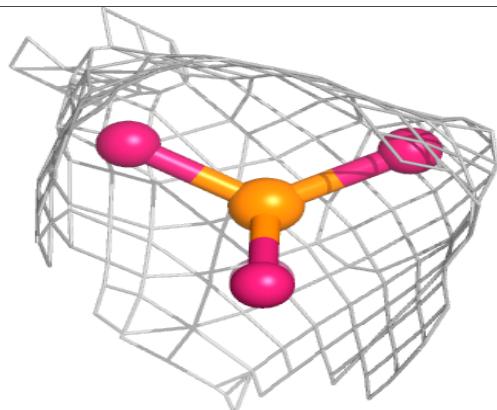
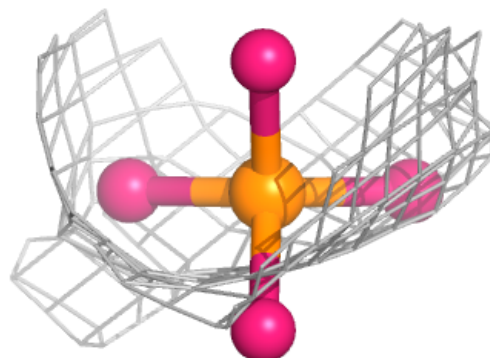


Electron density around UQ8 M 413:

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

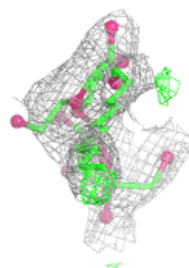
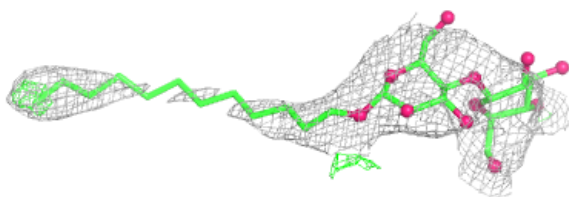
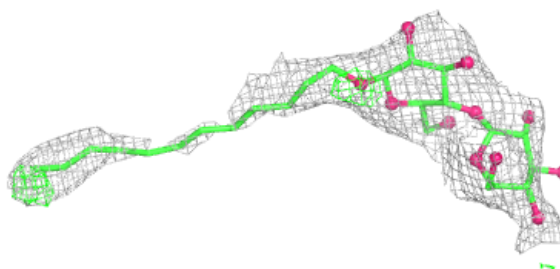
**Electron density around PEF 3 104:**

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

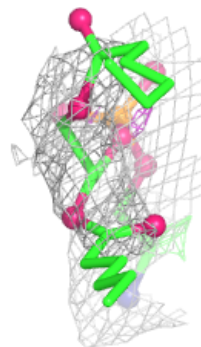
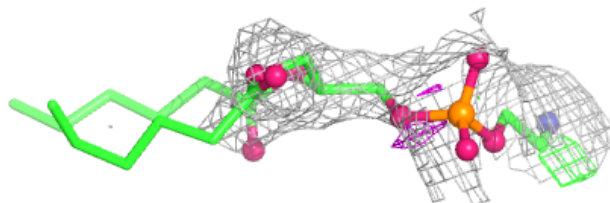
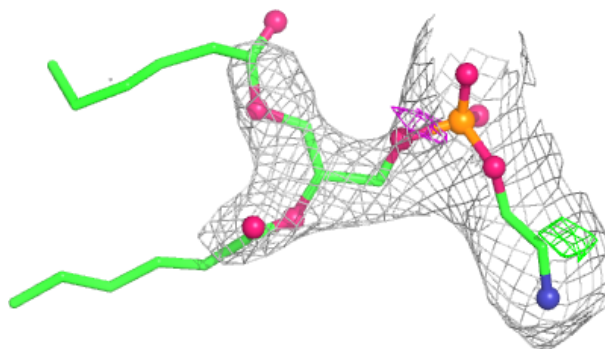


Electron density around LMT H 304:

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

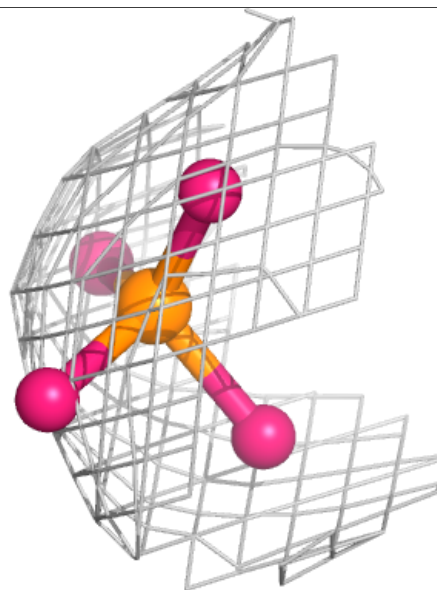
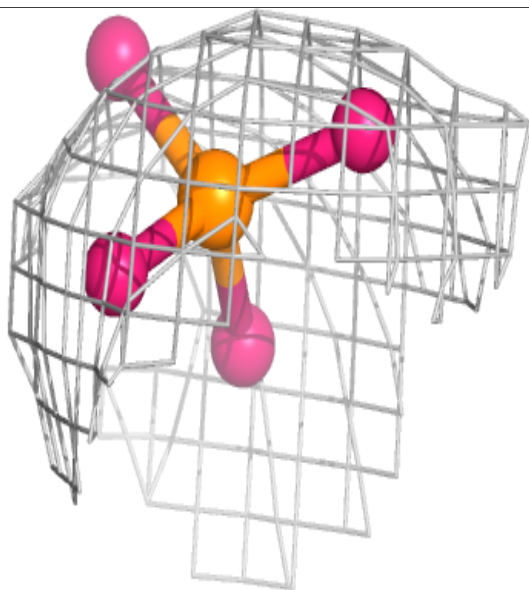
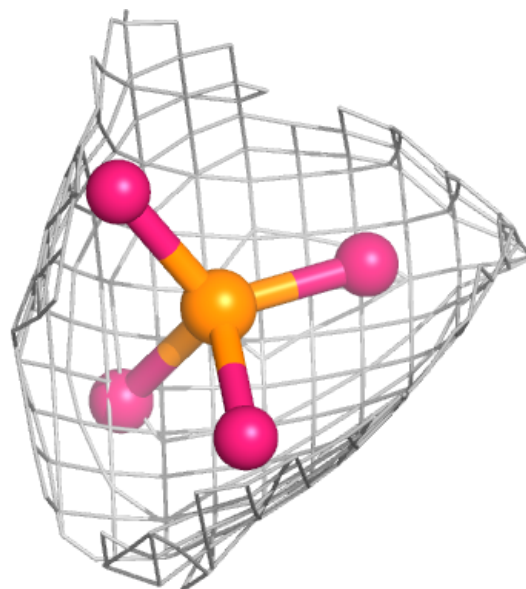
**Electron density around PEF K 104:**

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



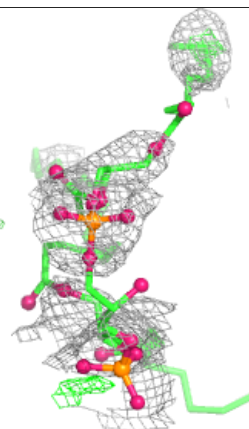
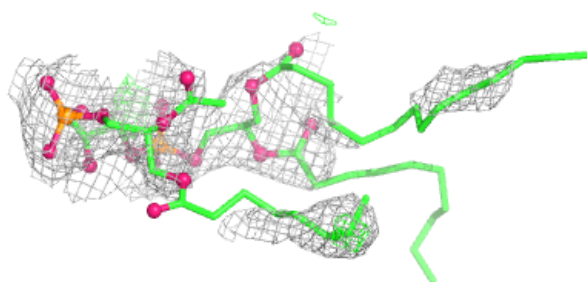
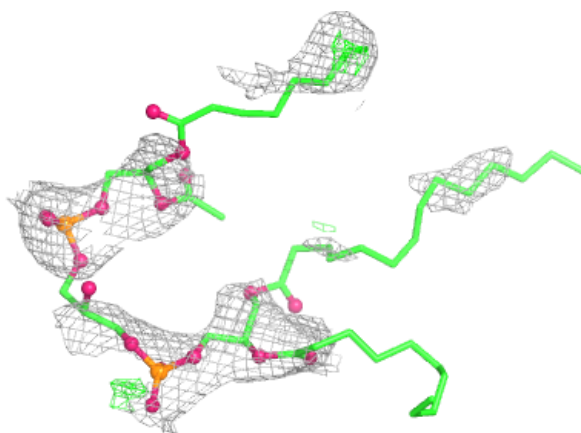
Electron density around PEF 1 103:

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

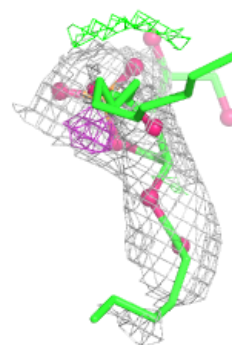
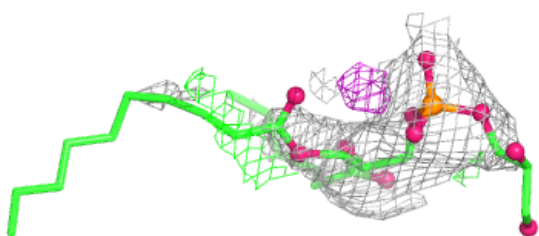
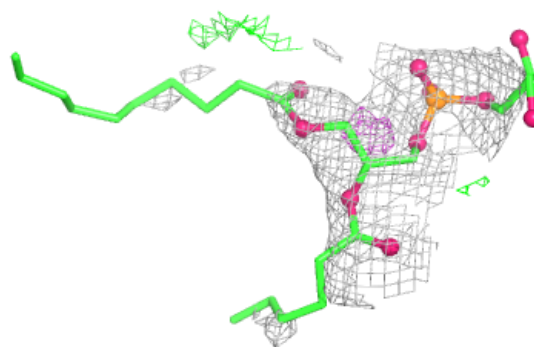


Electron density around CDL U 104:

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

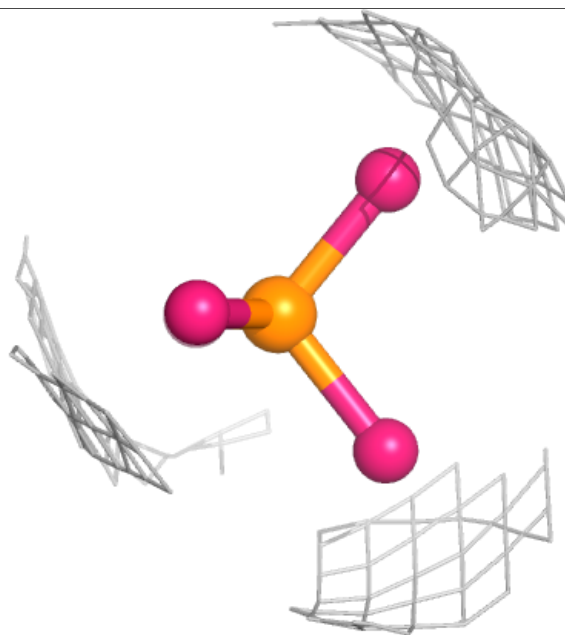
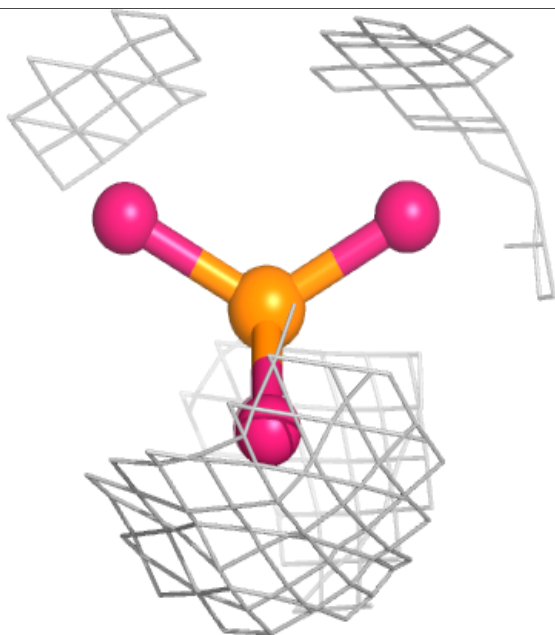
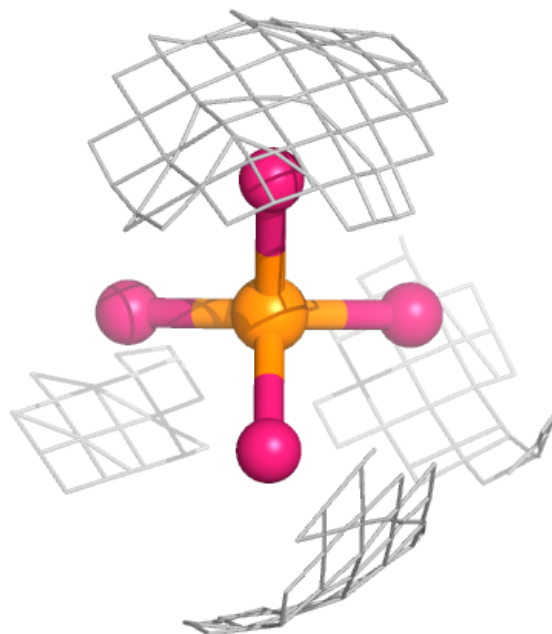
**Electron density around PGV 9 104:**

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



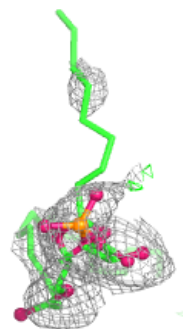
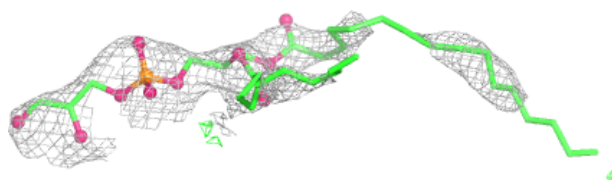
Electron density around PEF M 408:

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



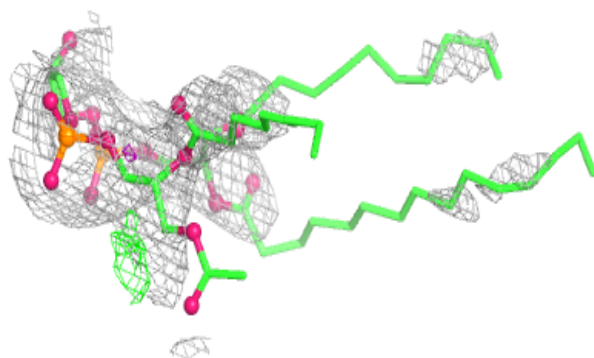
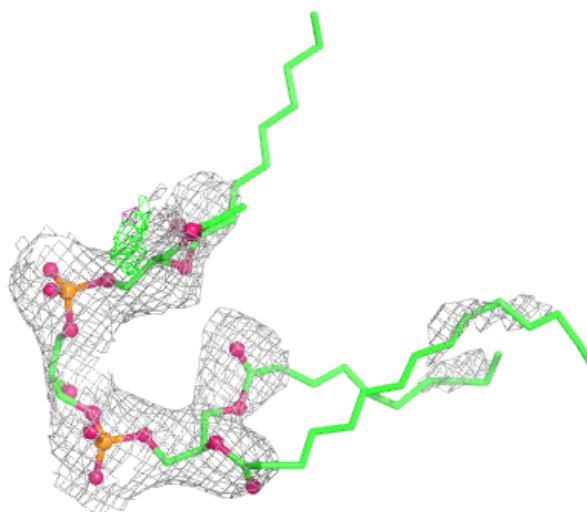
Electron density around PGV L 308:

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



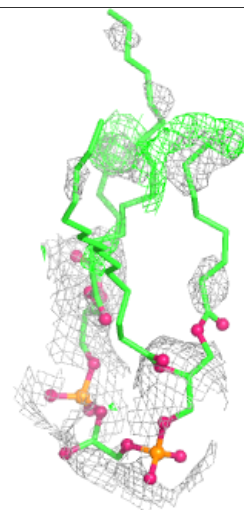
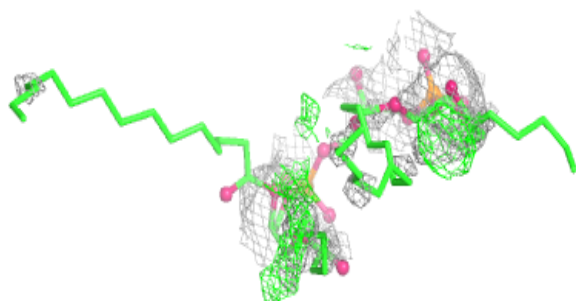
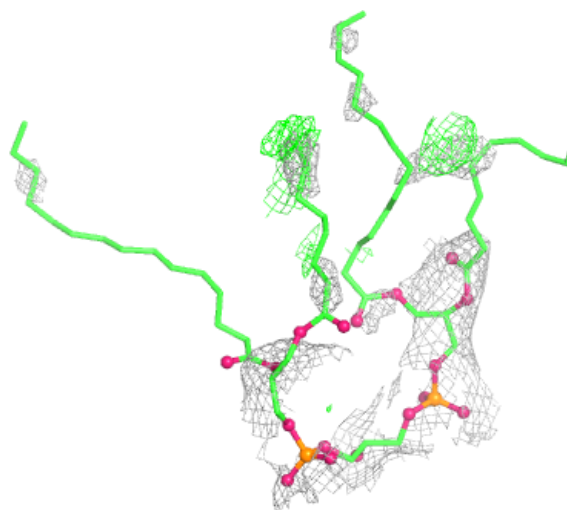
Electron density around CDL D 105:

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



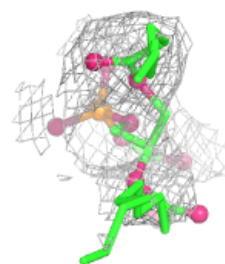
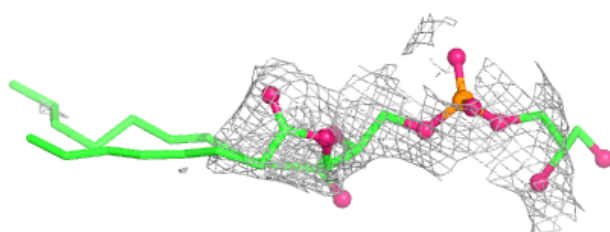
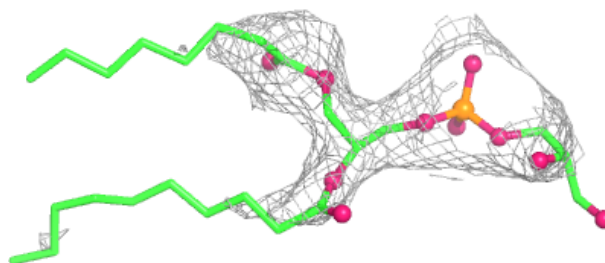
Electron density around CDL S 104:

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

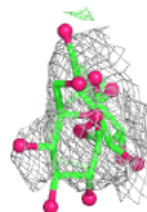
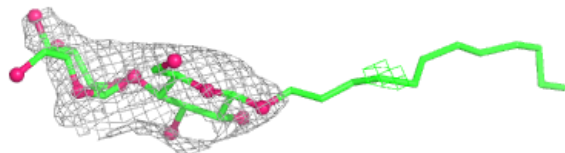
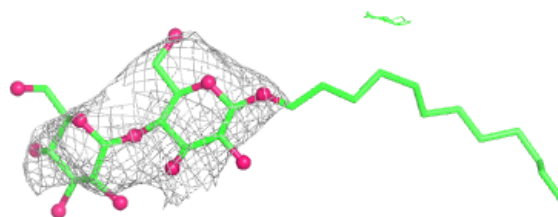


Electron density around PGV D 106:

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

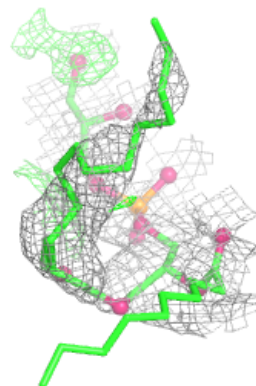
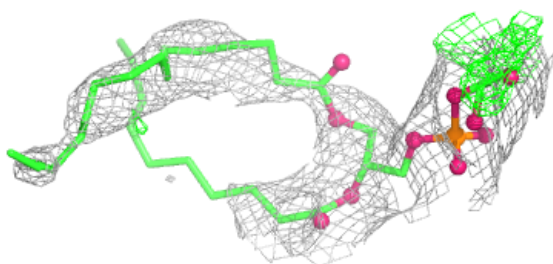
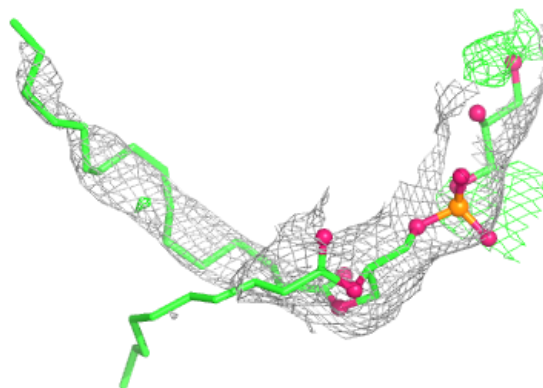
**Electron density around LMT M 414:**

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

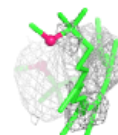
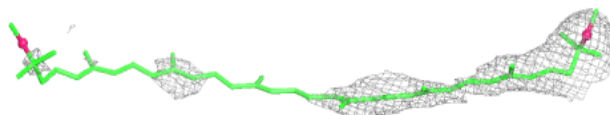
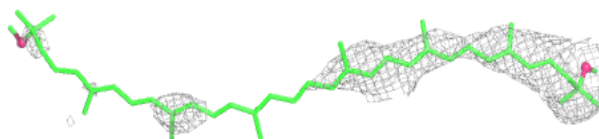


Electron density around PGV L 307:

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

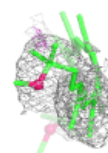
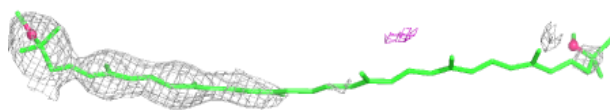
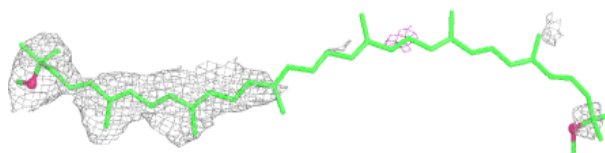
**Electron density around CRT G 101:**

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

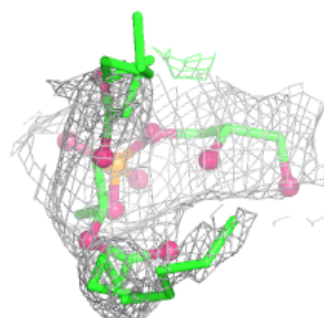
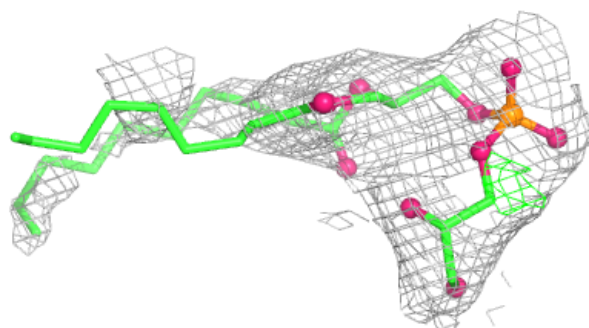
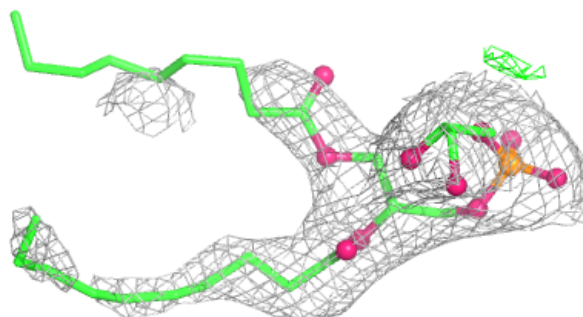


Electron density around CRT 0 101:

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

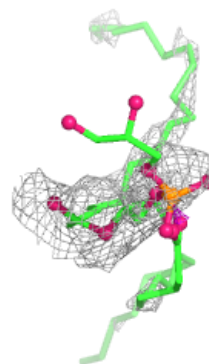
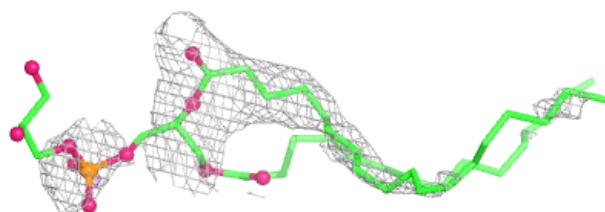
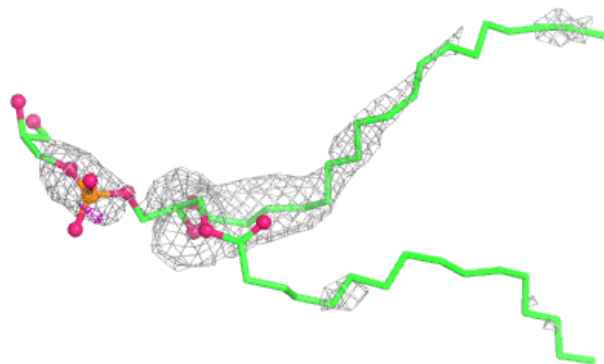
**Electron density around PGV H 303:**

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



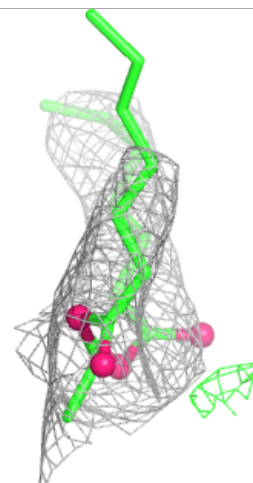
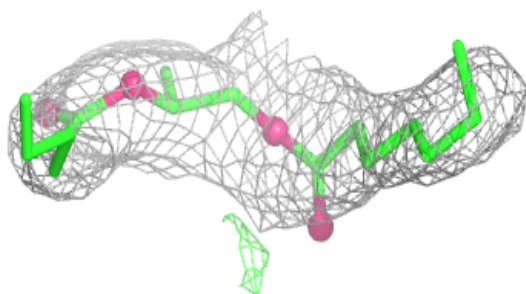
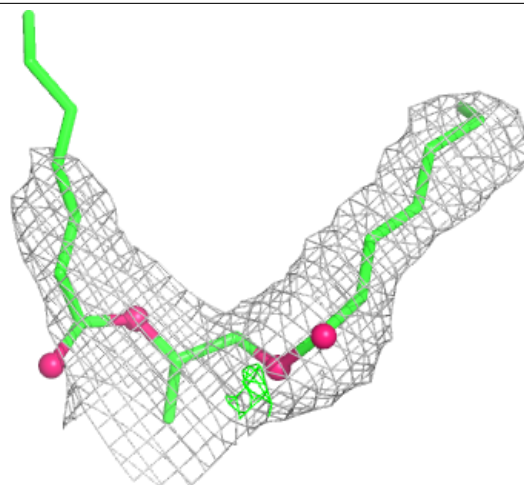
Electron density around PGV 3 105:

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



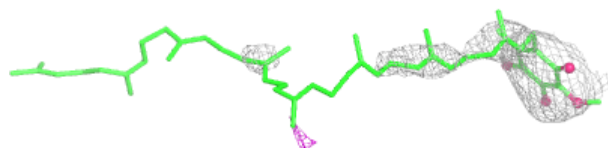
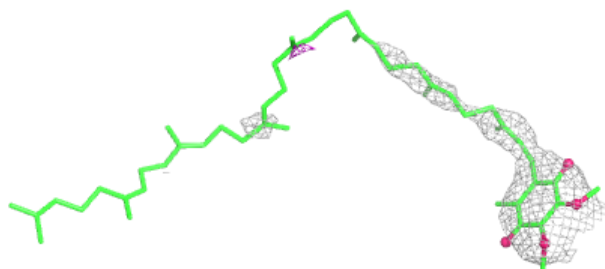
Electron density around PGV C 508:

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



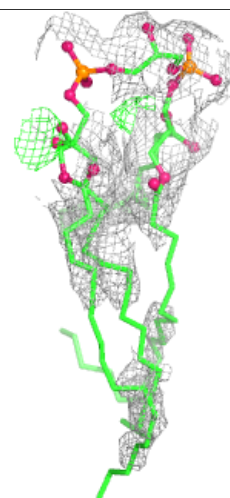
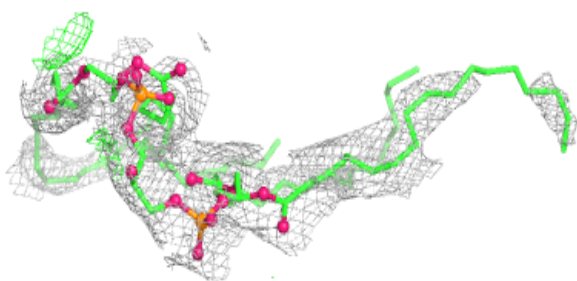
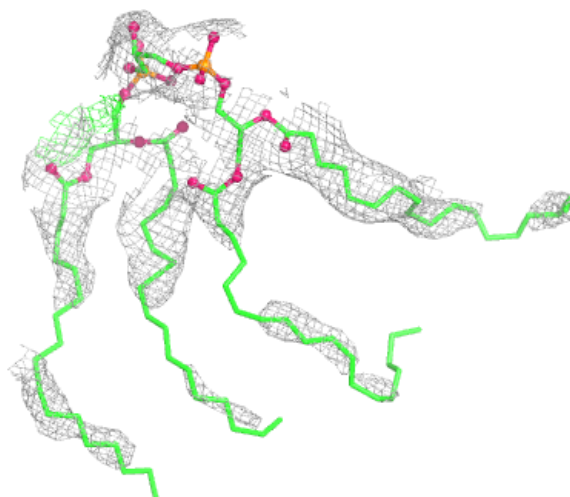
Electron density around UQ8 L 309:

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



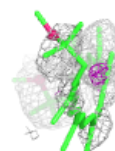
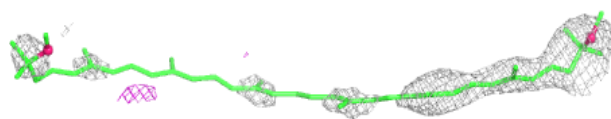
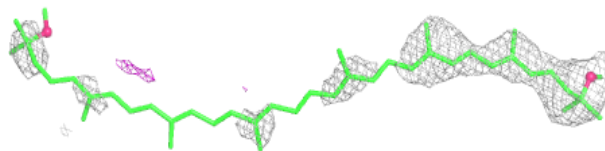
Electron density around CDL M 406:

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

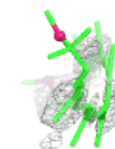
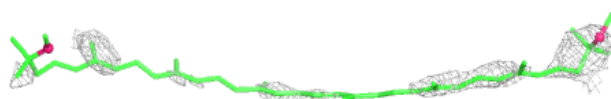
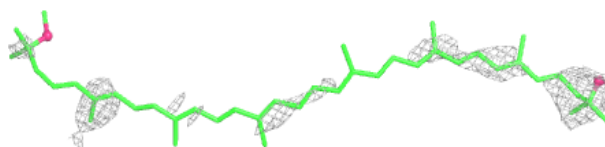


Electron density around CRT O 103:

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

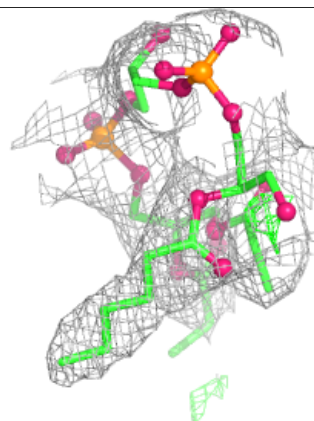
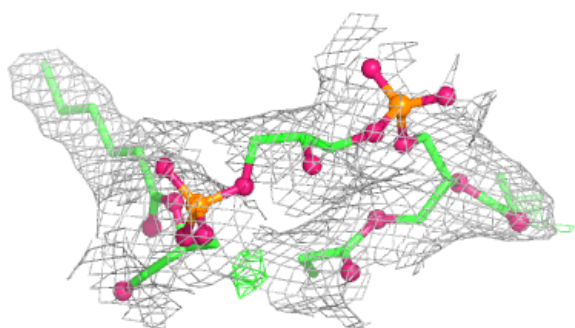
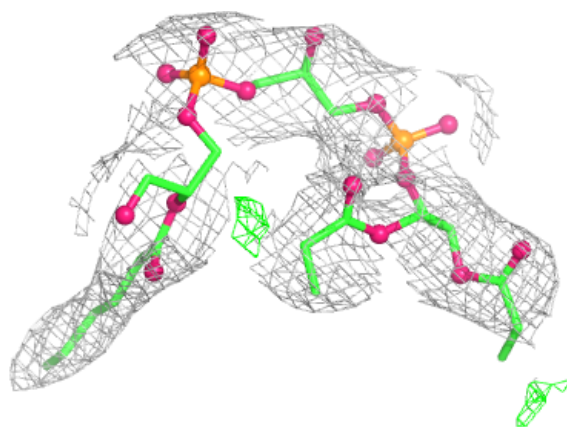
**Electron density around CRT 8 101:**

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



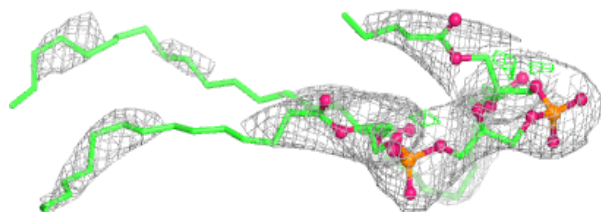
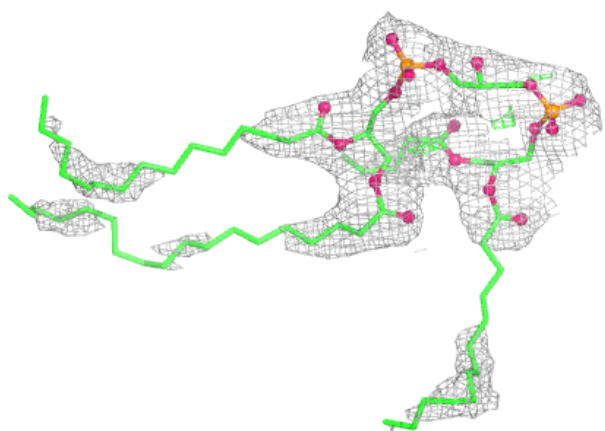
Electron density around CDL M 412:

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

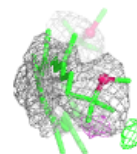
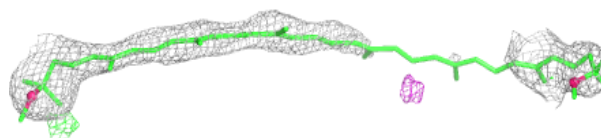
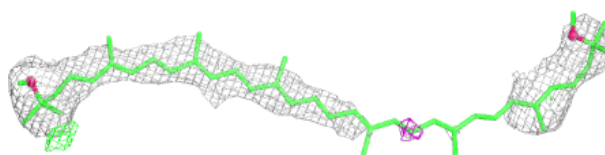


Electron density around CDL H 305:

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

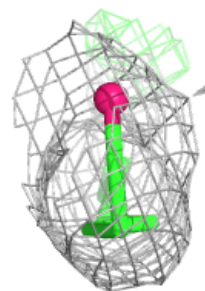
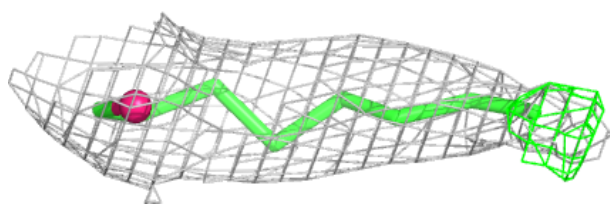
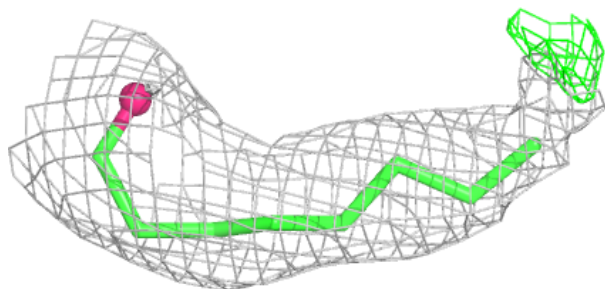
**Electron density around CRT V 101:**

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

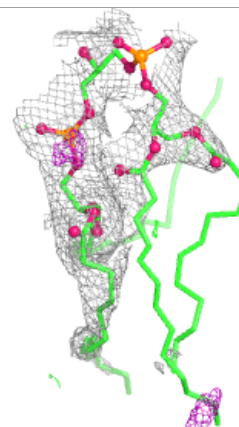
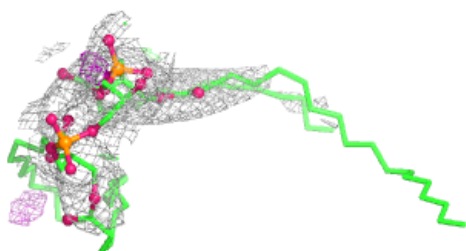


Electron density around LHG C 507:

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

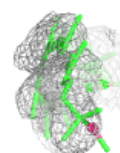
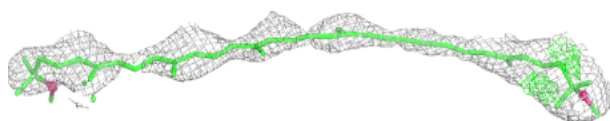
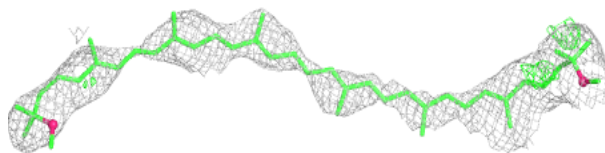
**Electron density around CDL O 104:**

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

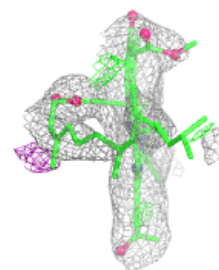
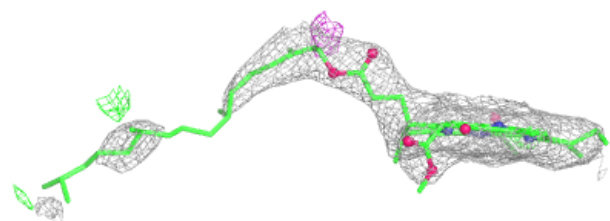
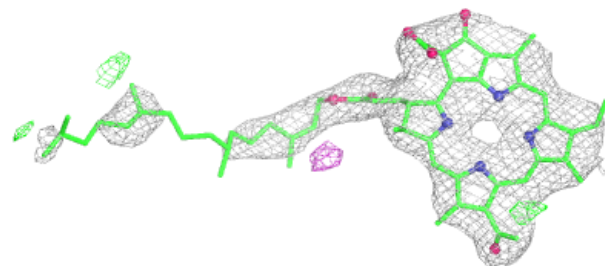


Electron density around CRT J 101:

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

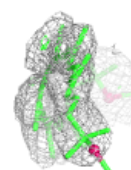
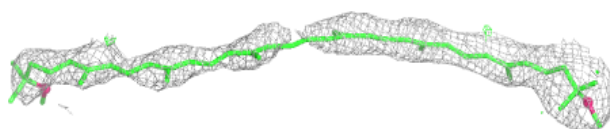
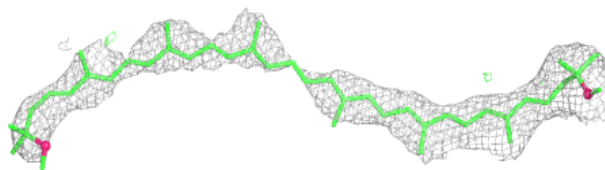
**Electron density around BPH M 402:**

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



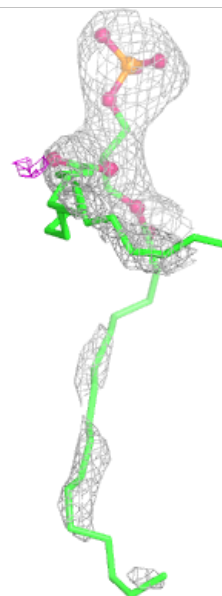
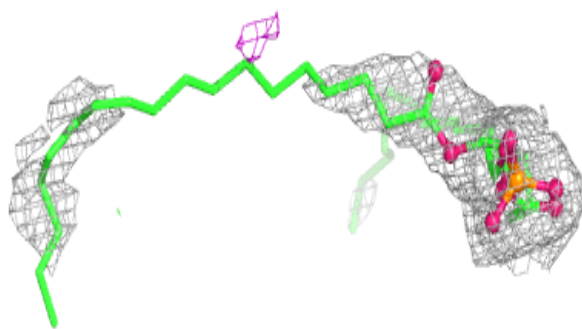
Electron density around CRT T 101:

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



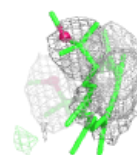
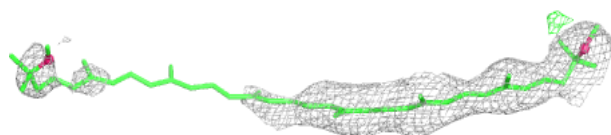
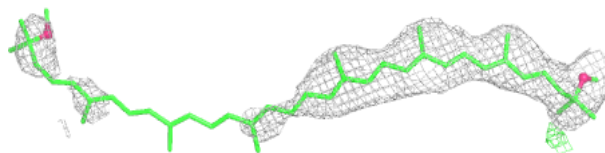
Electron density around PGV M 410:

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

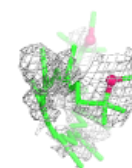
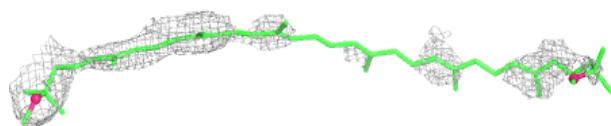
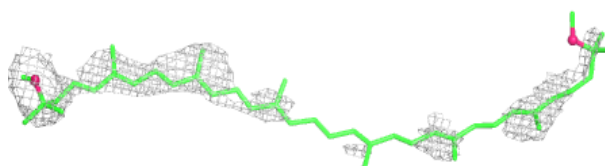


Electron density around CRT W 102:

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

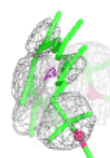
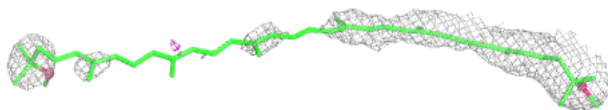
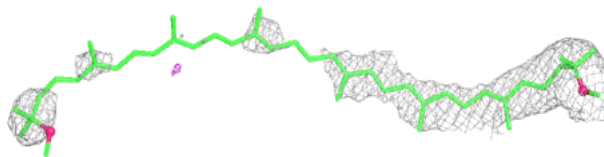
**Electron density around CRT B 101:**

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

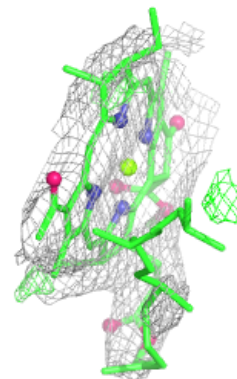
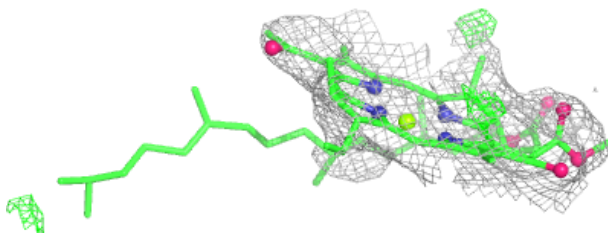
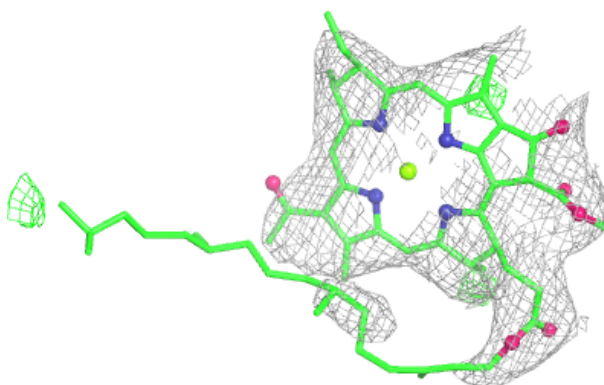


Electron density around CRT N 101:

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

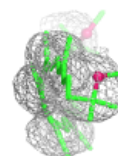
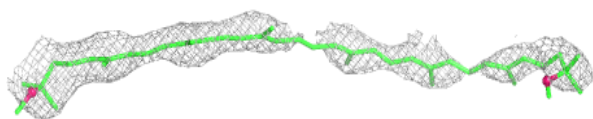
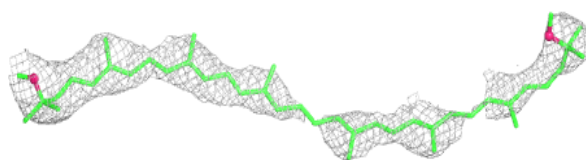
**Electron density around BCL S 103:**

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

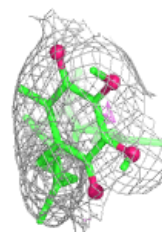
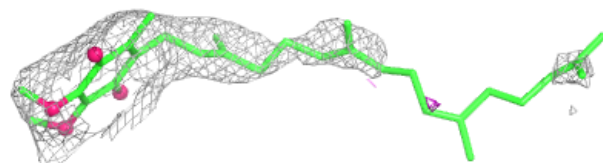
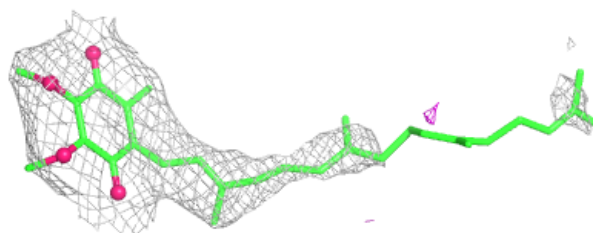


Electron density around CRT P 101:

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

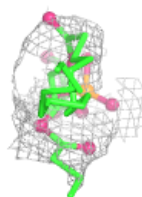
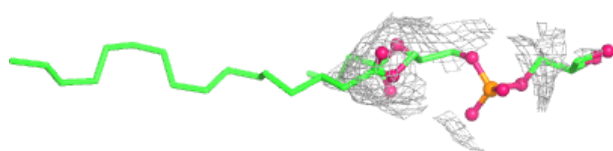
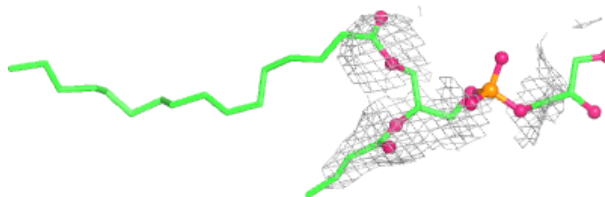
**Electron density around UQ8 L 304:**

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

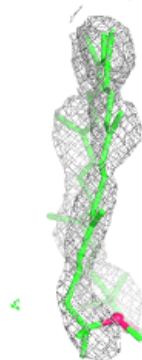
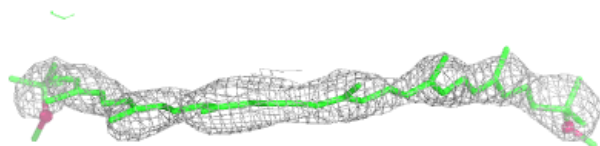
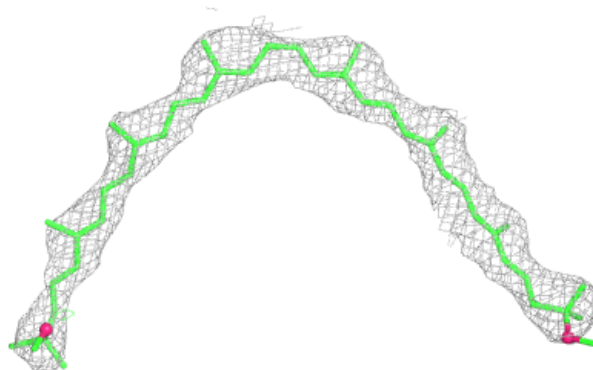


Electron density around PGV M 411:

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

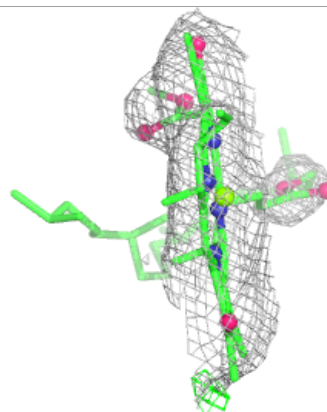
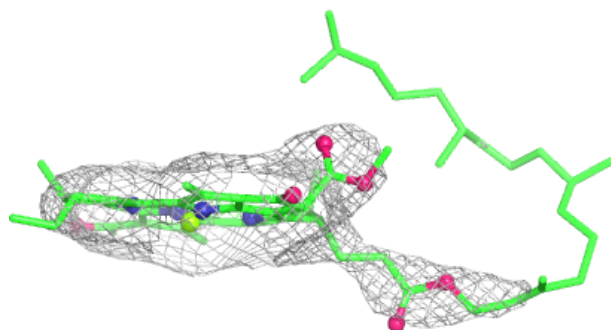
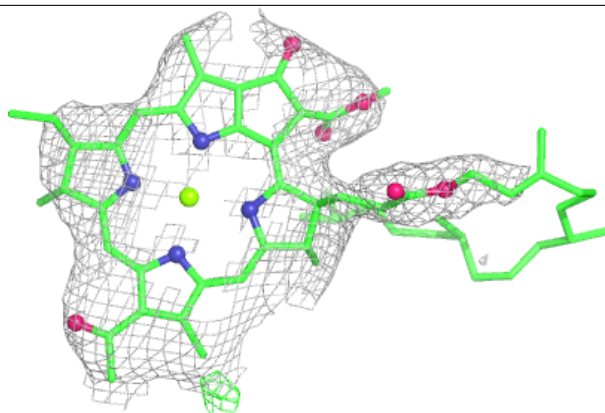
**Electron density around CRT M 405:**

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

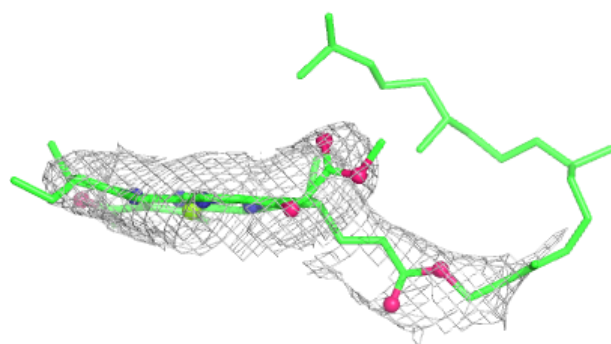
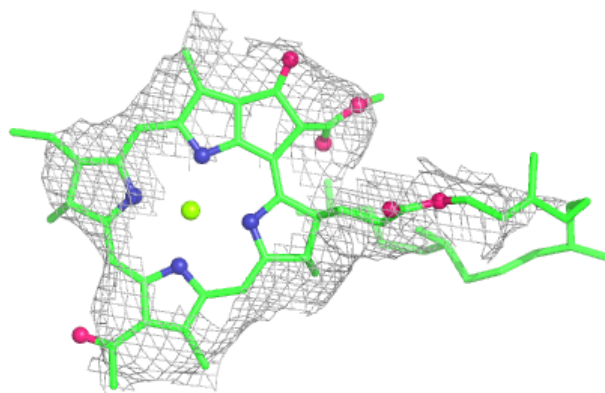


Electron density around BCL S 101:

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

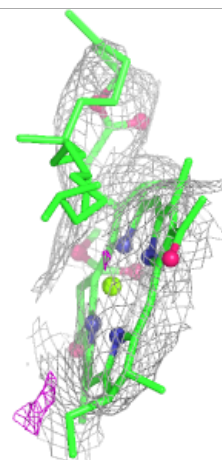
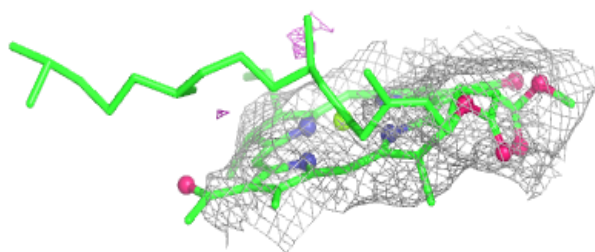
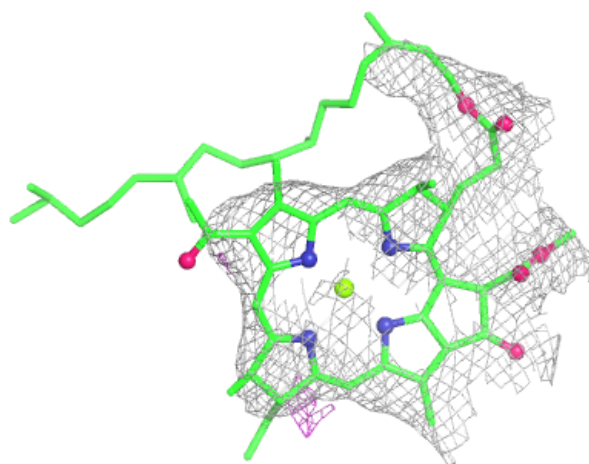
**Electron density around BCL A 101:**

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



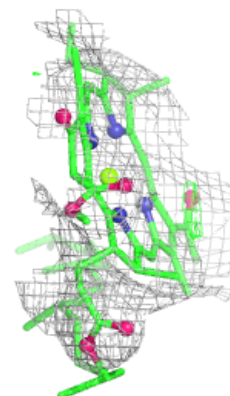
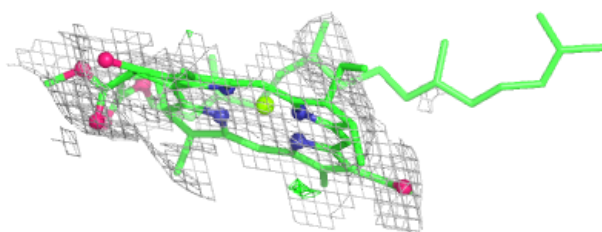
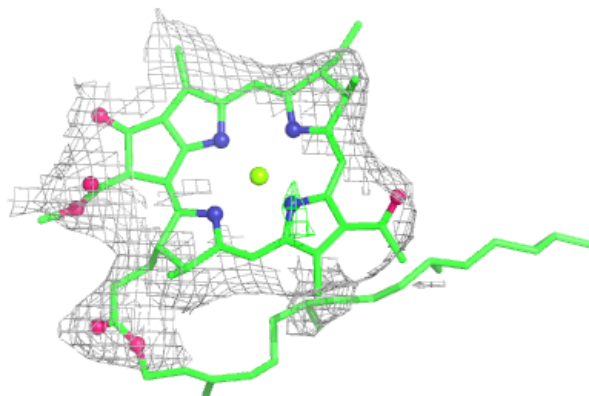
Electron density around BCL U 103:

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



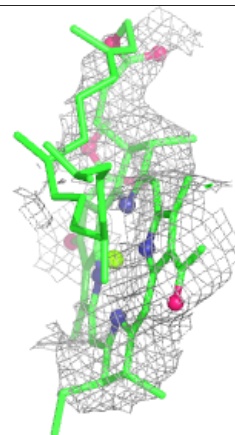
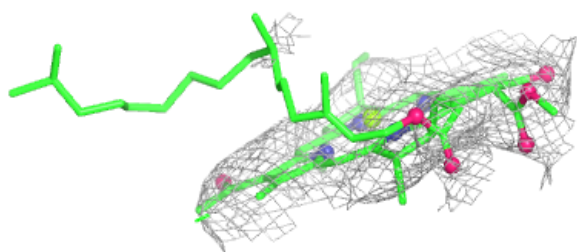
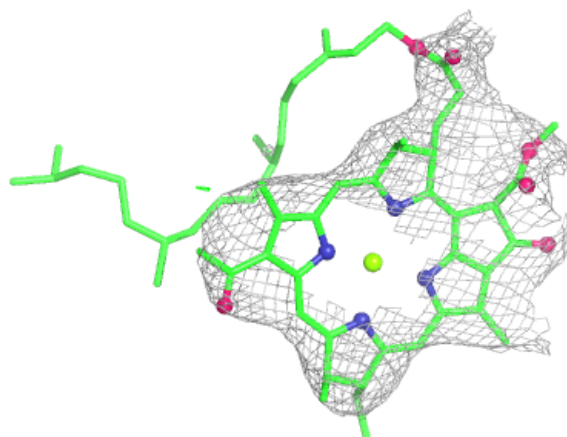
Electron density around BCL 5 103:

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

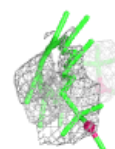
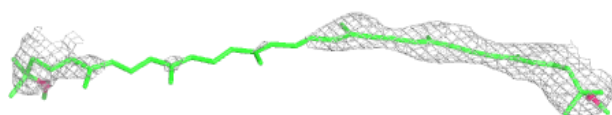
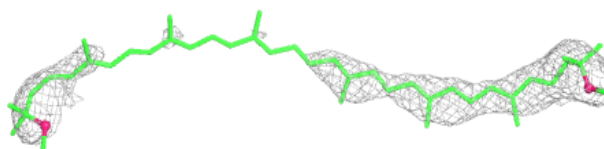


Electron density around BCL 9 103:

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

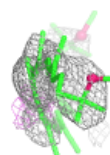
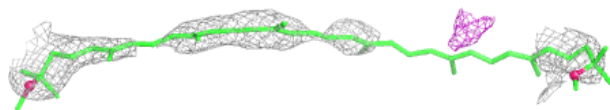
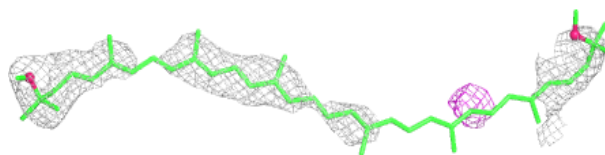
**Electron density around CRT 2 101:**

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

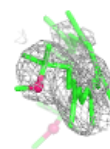
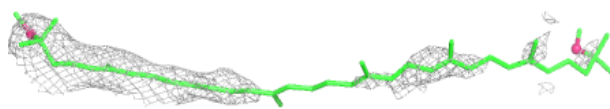
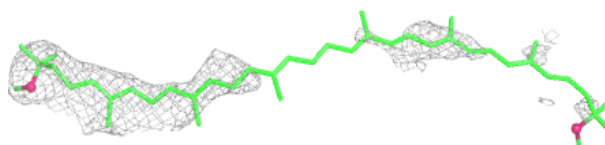


Electron density around CRT 3 103:

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

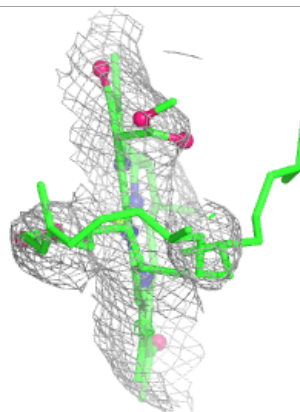
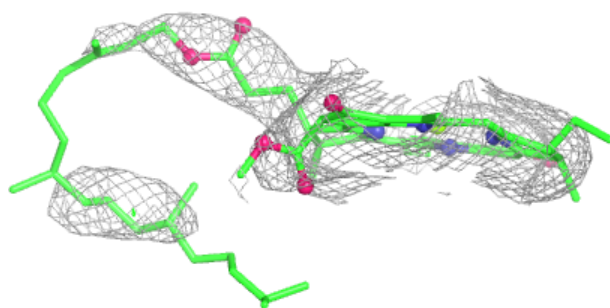
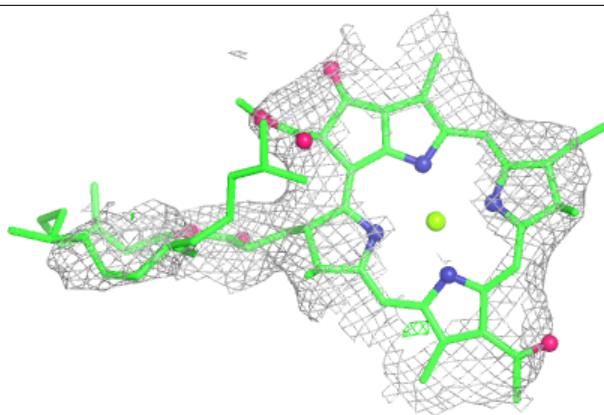
**Electron density around CRT 4 101:**

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

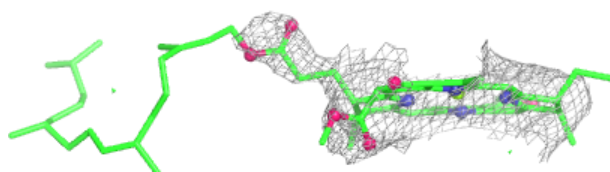
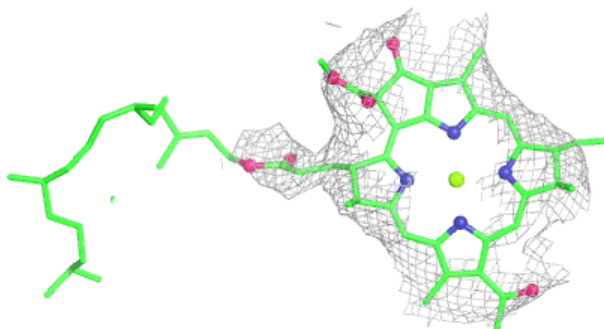


Electron density around BCL F 101:

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

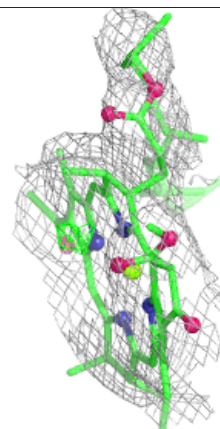
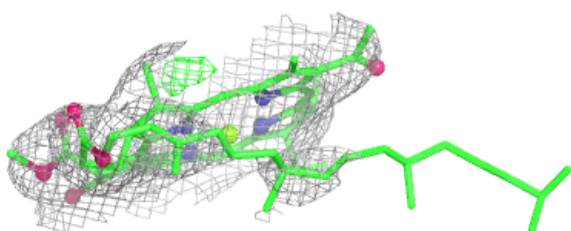
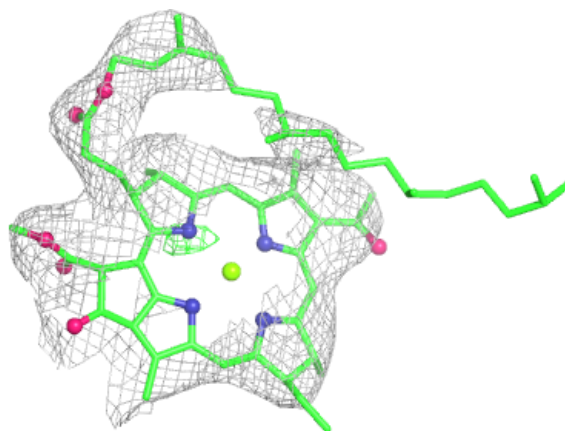
**Electron density around BCL 9 101:**

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

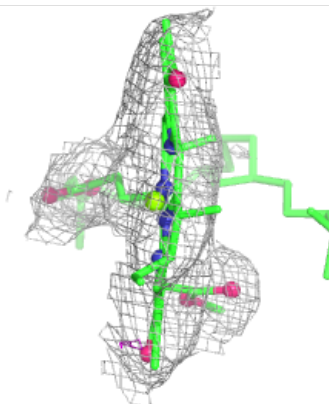
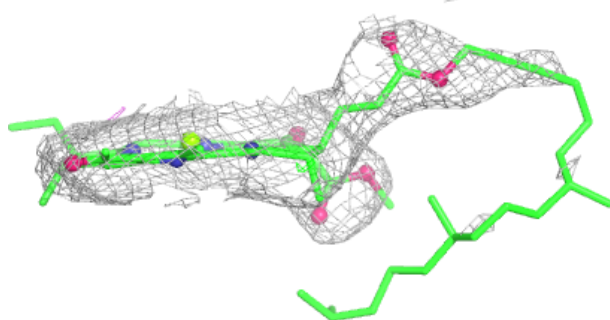
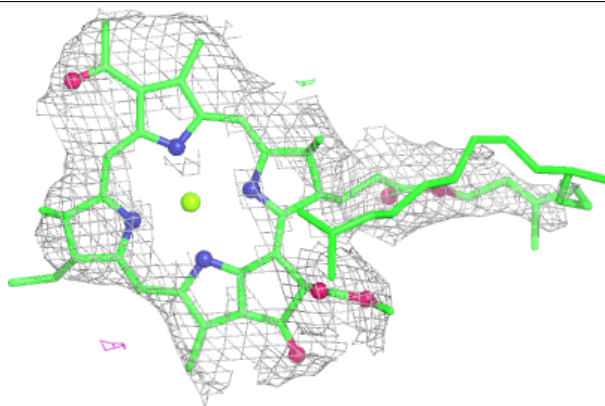


Electron density around BCL Q 103:

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

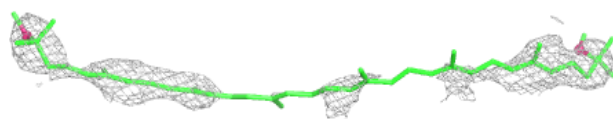
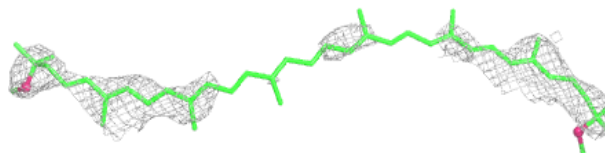
**Electron density around BCL U 101:**

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

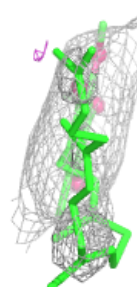
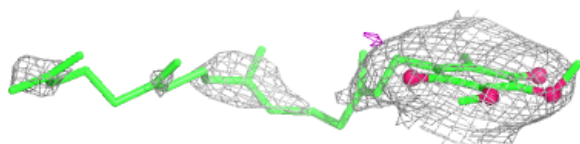


Electron density around CRT Z 101:

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

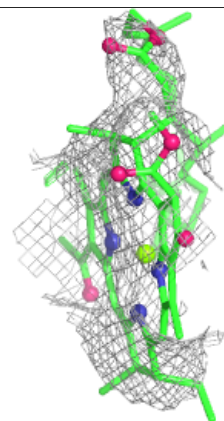
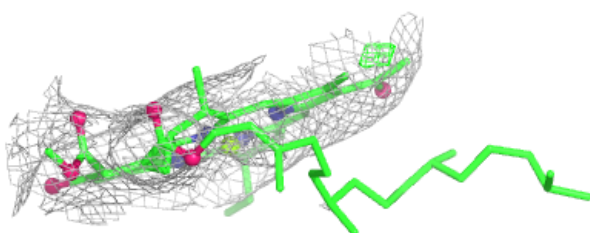
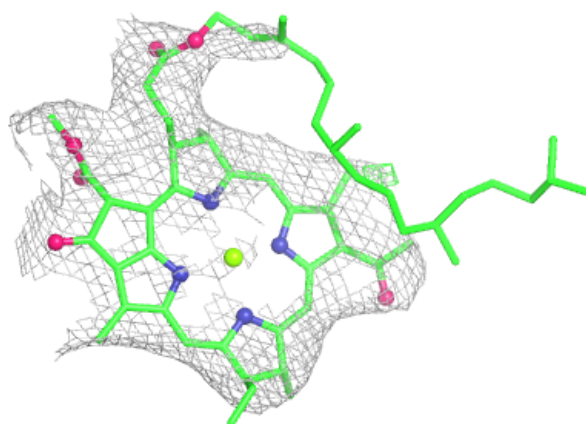
**Electron density around UQ8 L 310:**

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

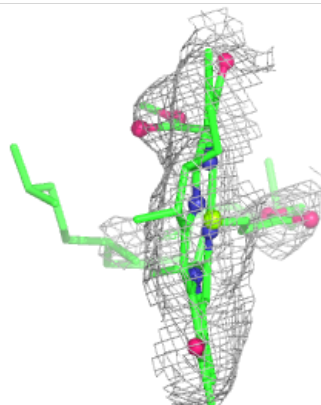
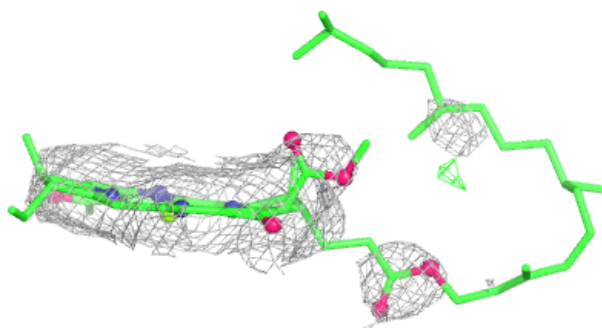
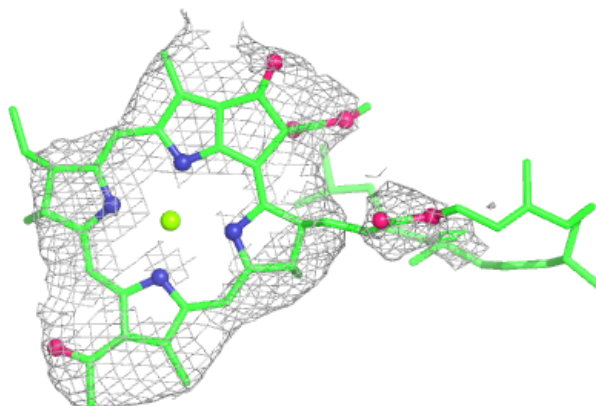


Electron density around BCL A 103:

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

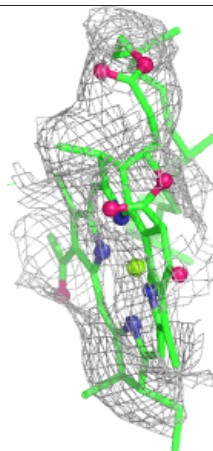
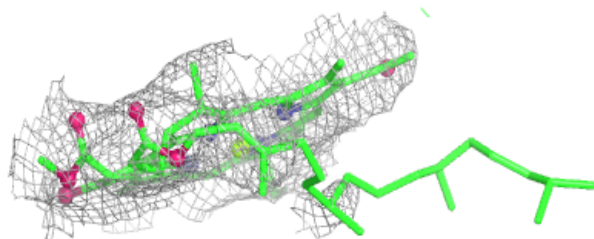
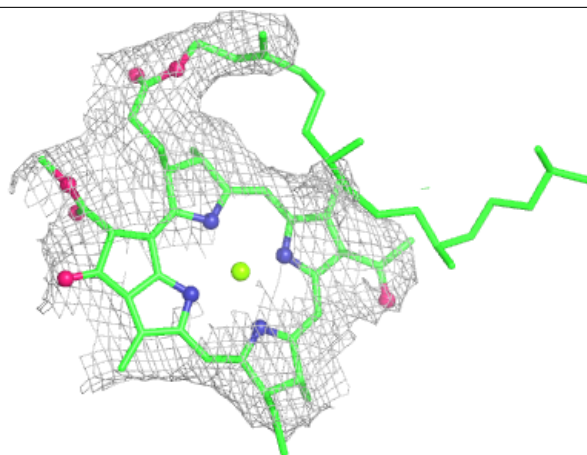
**Electron density around BCL W 101:**

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

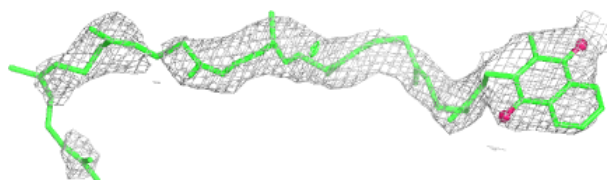
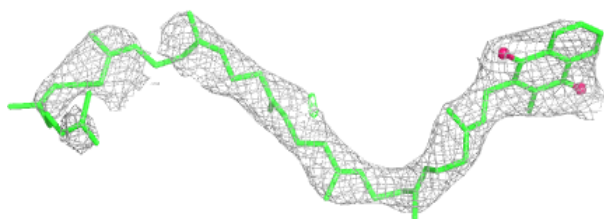


Electron density around BCL W 104:

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

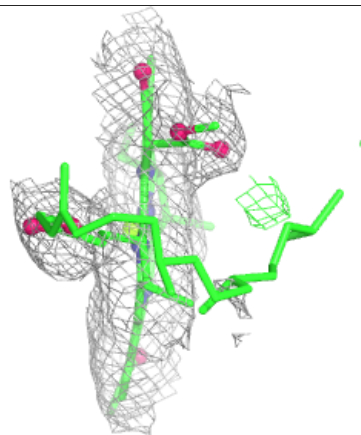
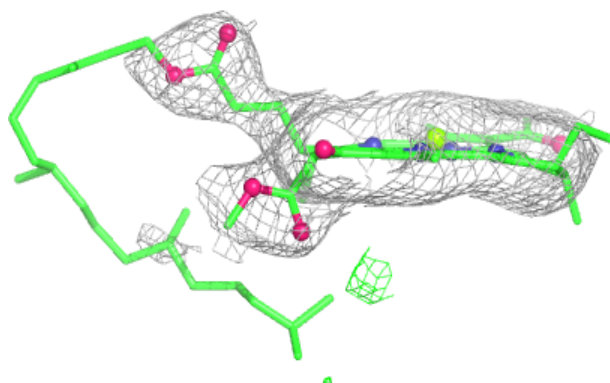
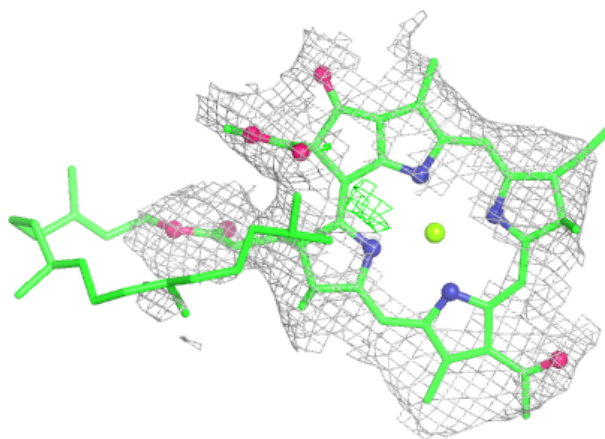
**Electron density around MQ8 M 404:**

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

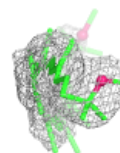
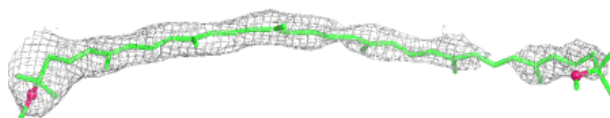


Electron density around BCL Y 101:

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

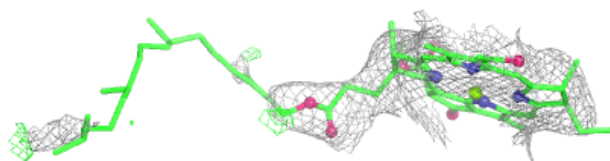
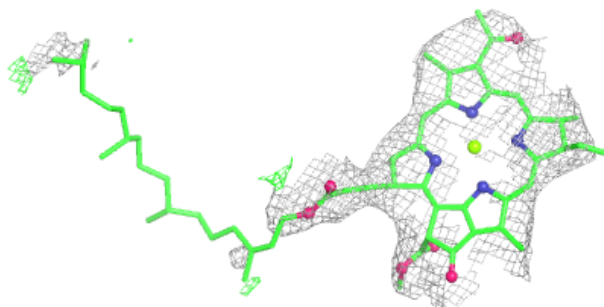
**Electron density around CRT A 104:**

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

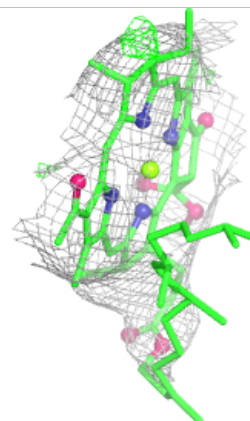
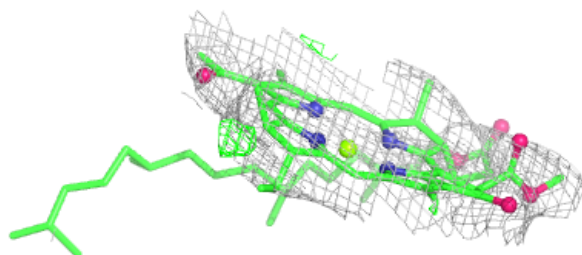
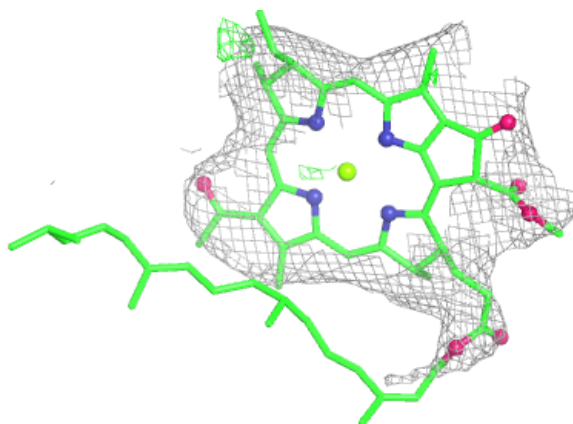


Electron density around BCL 1 101:

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

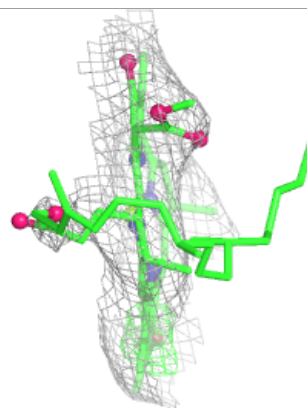
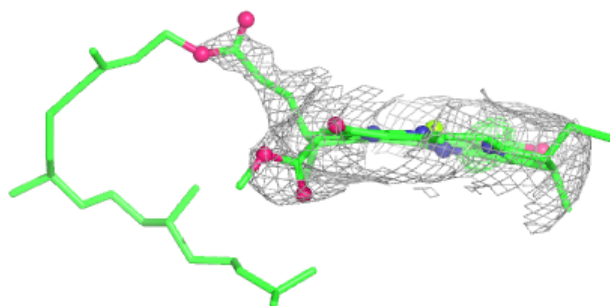
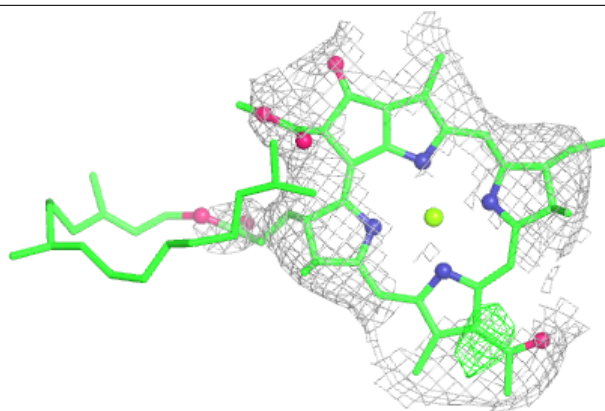
**Electron density around BCL 2 102:**

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

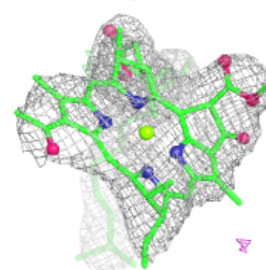
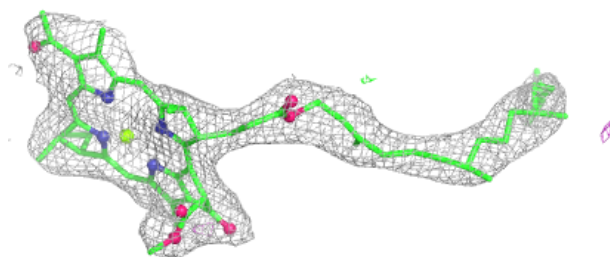
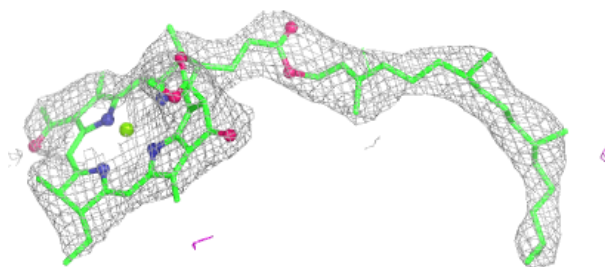


Electron density around BCL 3 101:

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

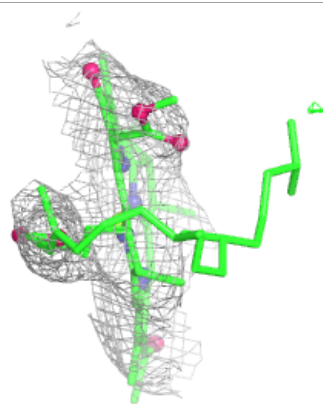
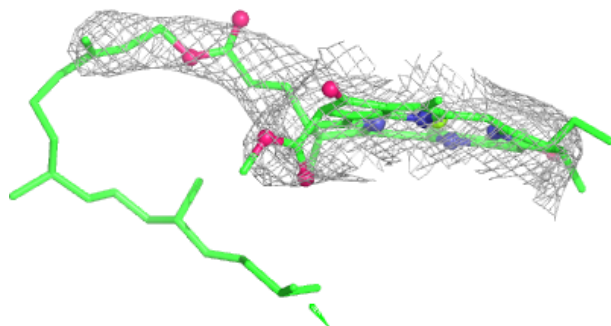
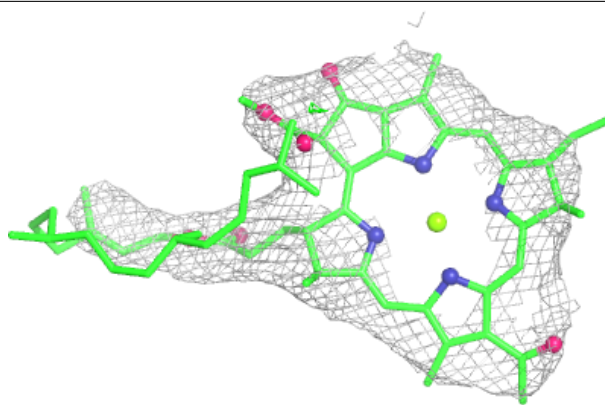
**Electron density around BCL M 401:**

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



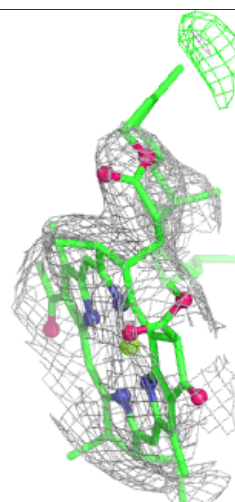
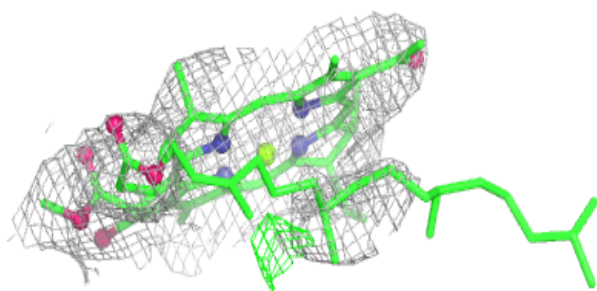
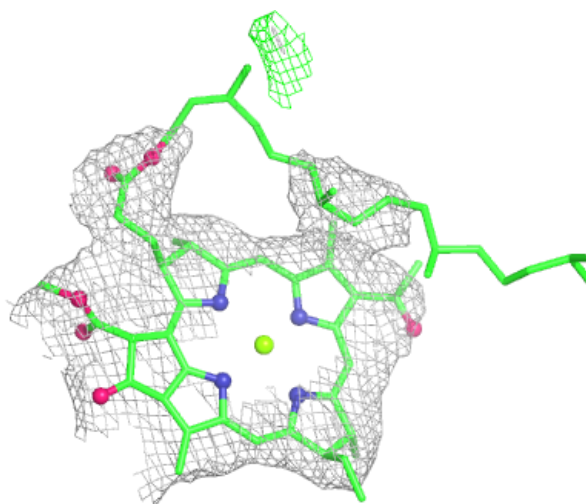
Electron density around BCL D 101:

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



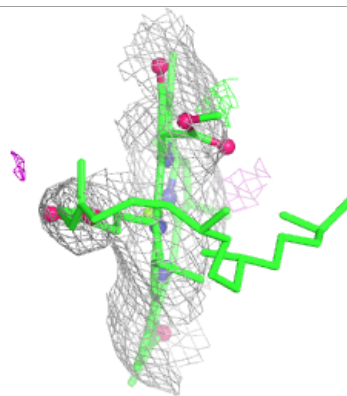
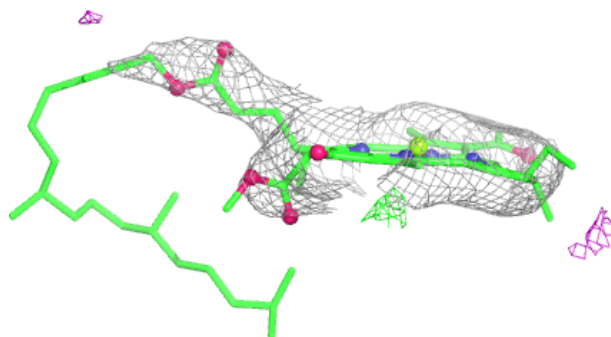
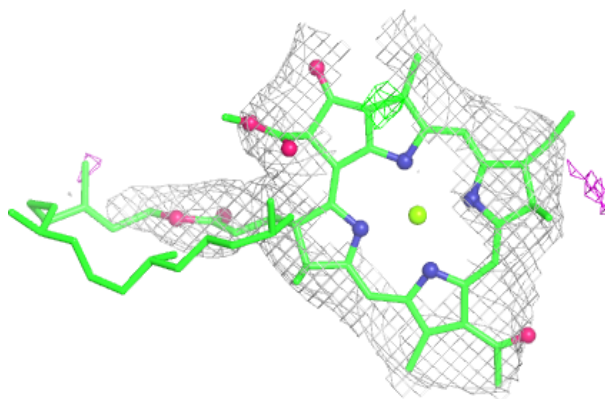
Electron density around BCL Y 103:

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

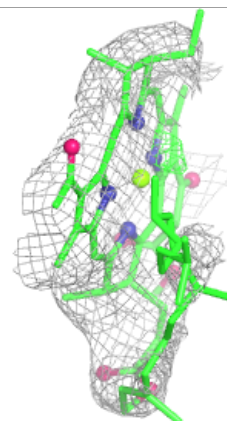
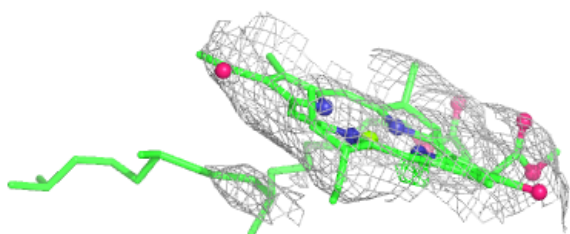
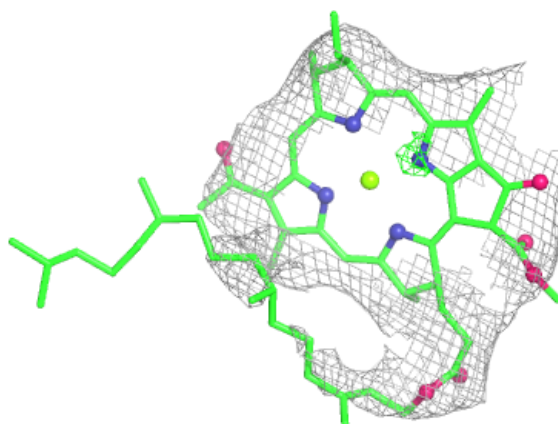


Electron density around BCL I 101:

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

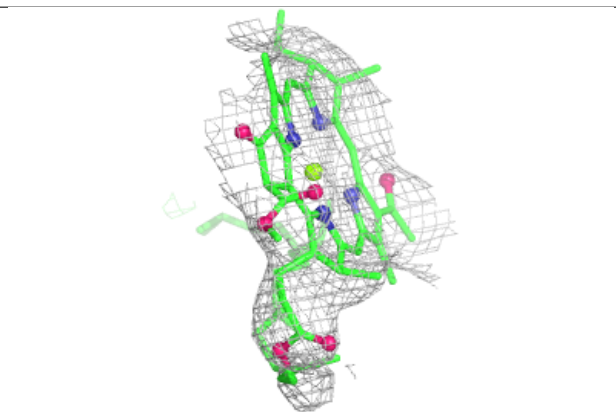
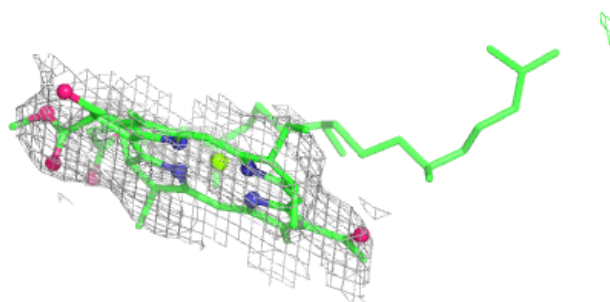
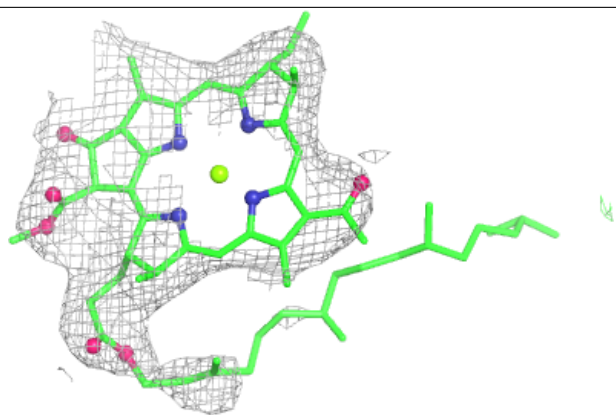
**Electron density around BCL J 102:**

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

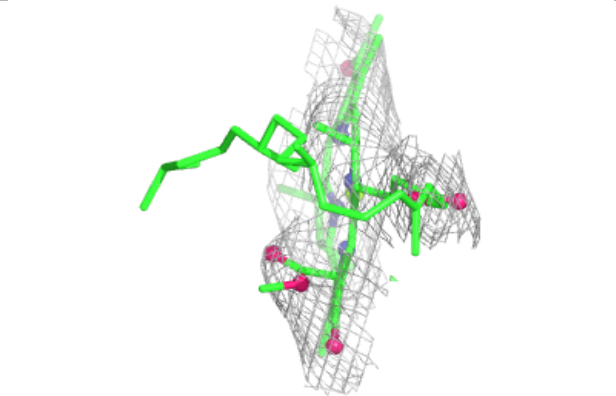
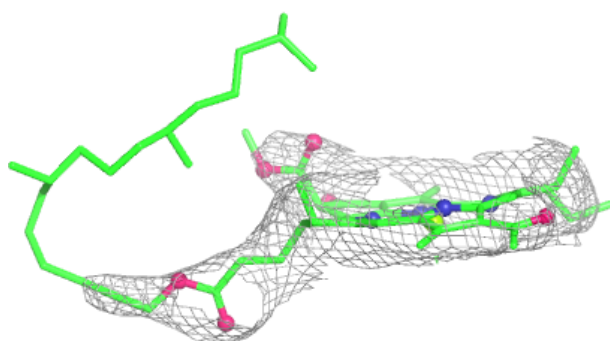
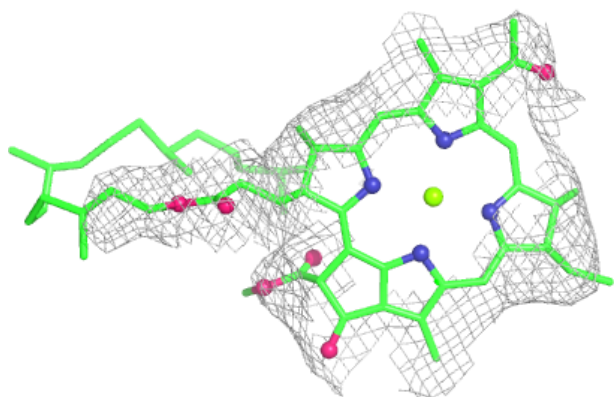


Electron density around BCL 4 102:

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

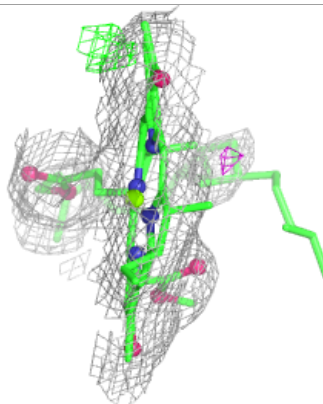
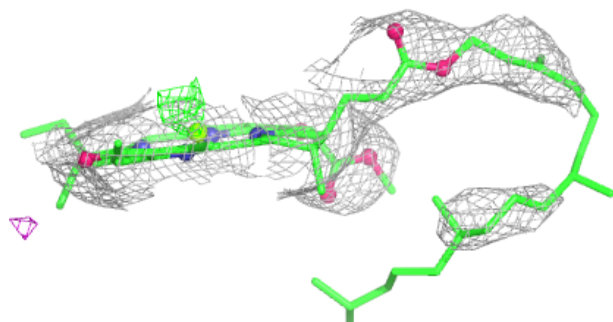
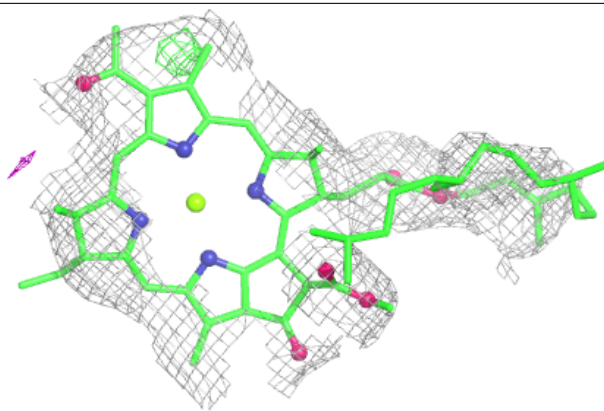
**Electron density around BCL 5 101:**

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

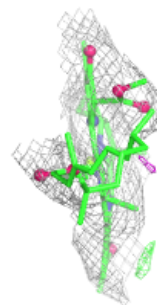
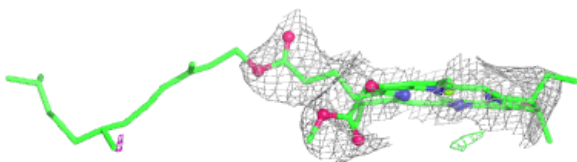
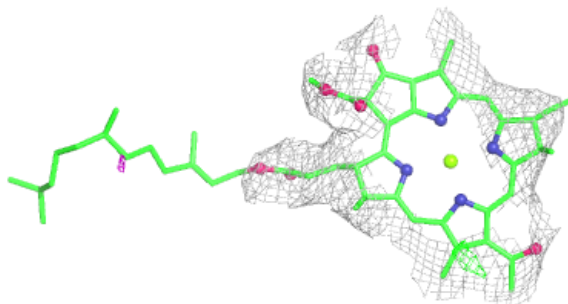


Electron density around BCL K 101:

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

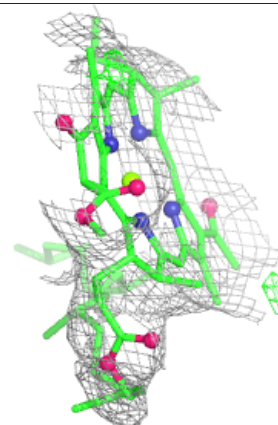
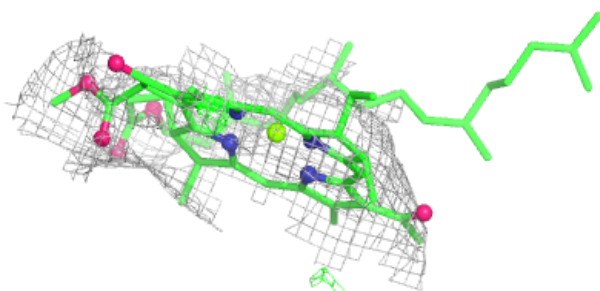
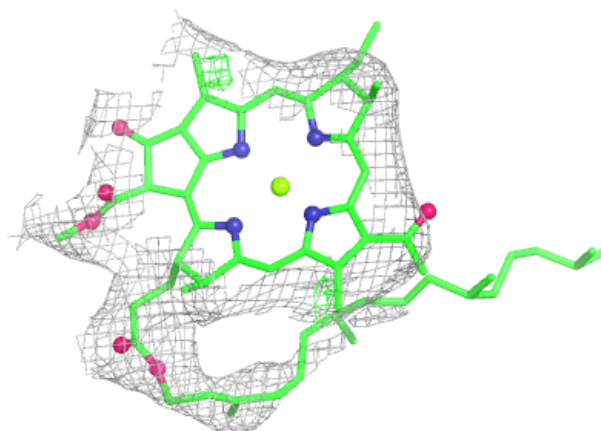
**Electron density around BCL 7 101:**

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

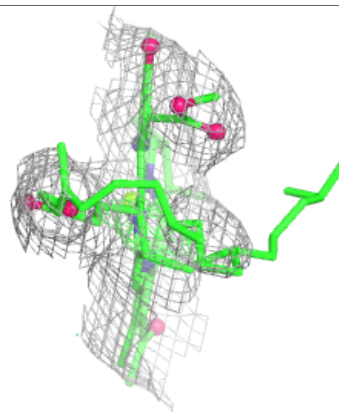
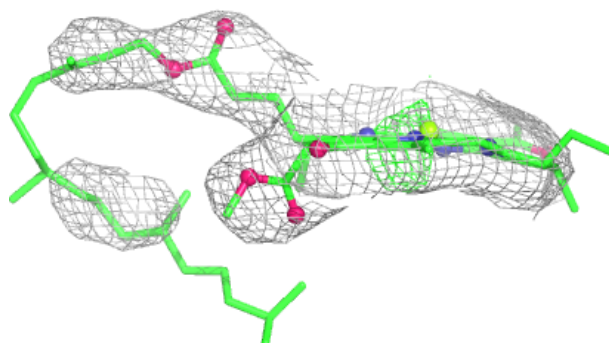
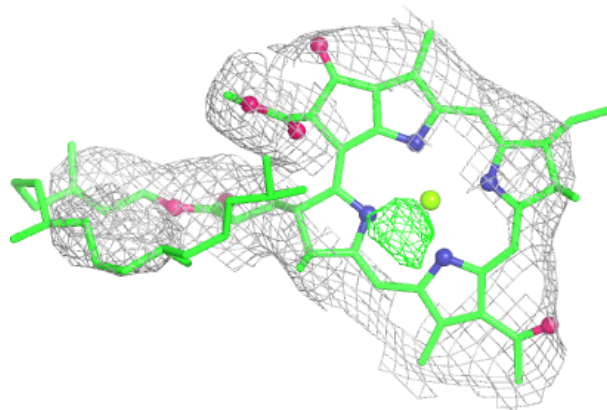


Electron density around BCL K 103:

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

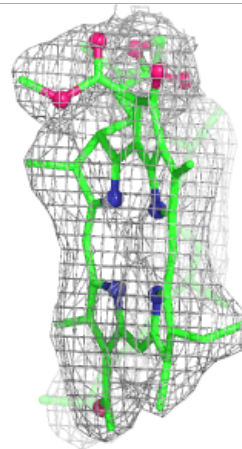
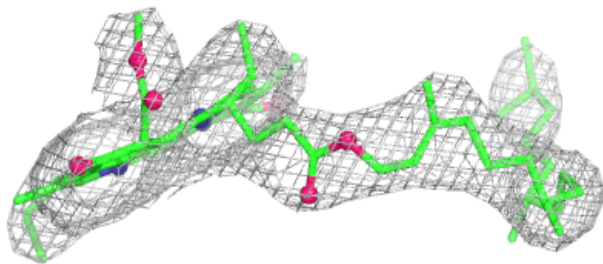
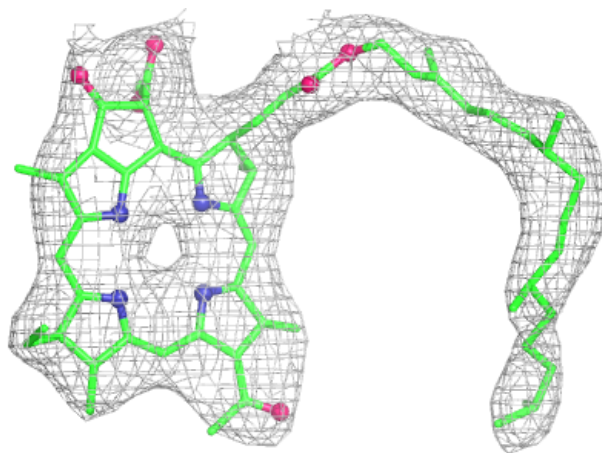
**Electron density around BCL O 101:**

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



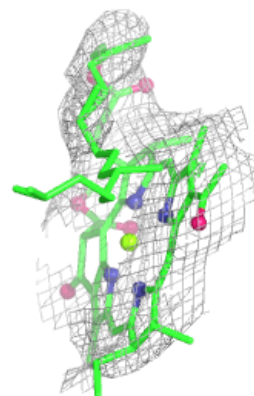
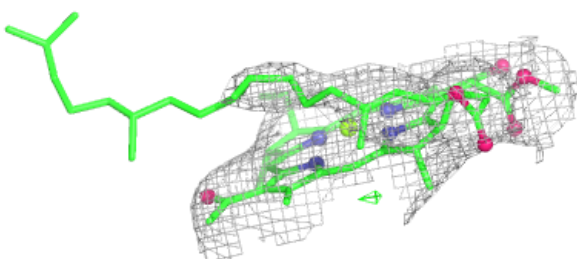
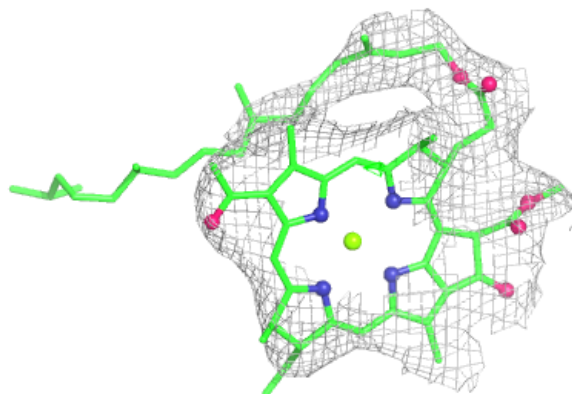
Electron density around BPH L 303:

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

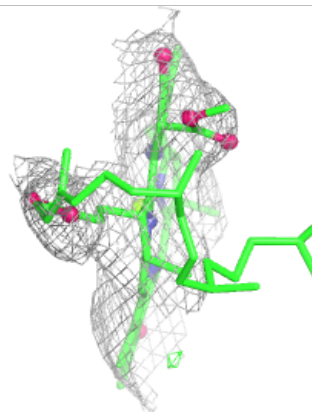
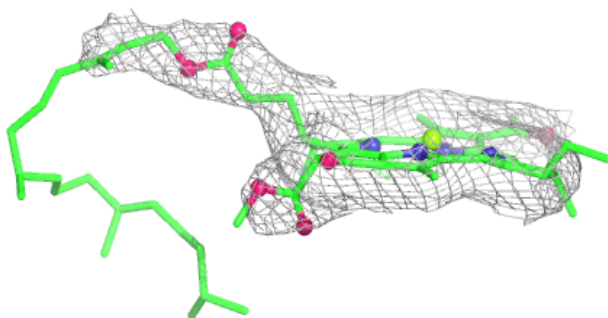
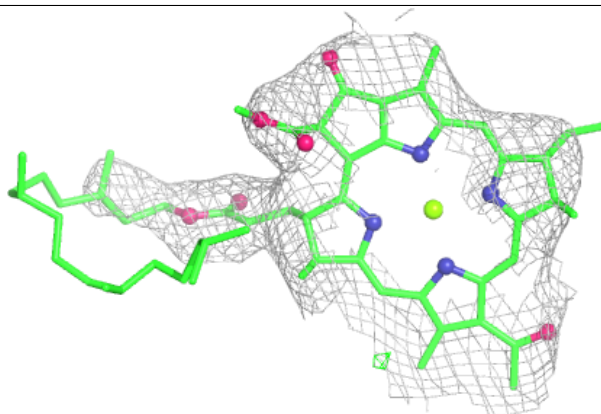


Electron density around BCL P 102:

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

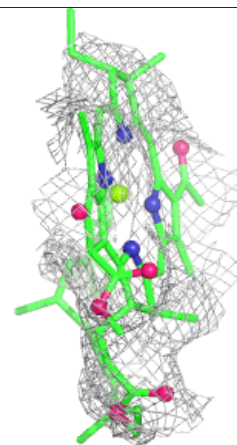
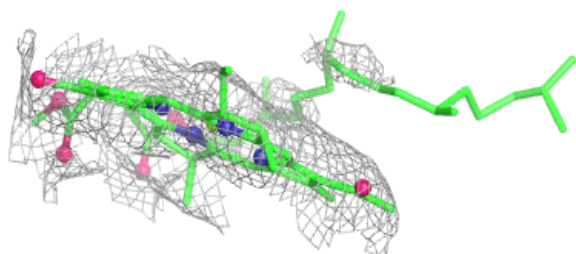
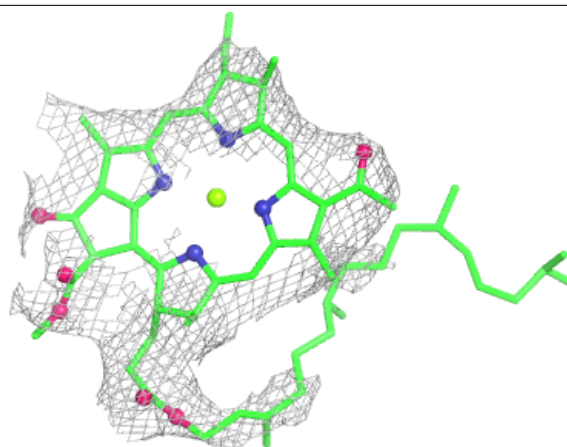
**Electron density around BCL Q 101:**

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



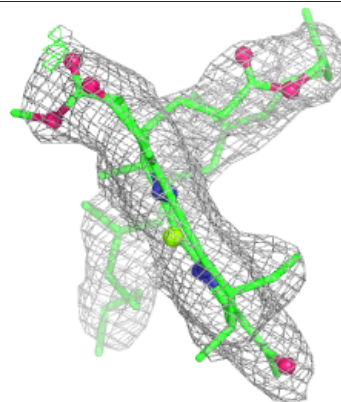
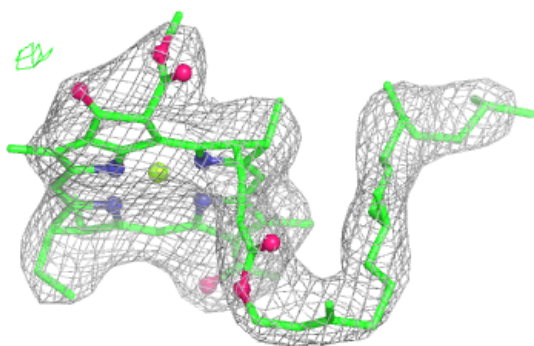
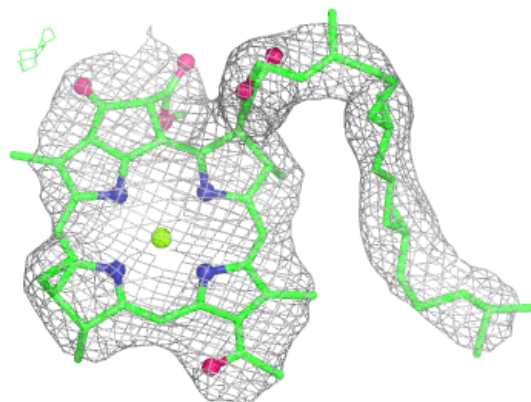
Electron density around BCL D 103:

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



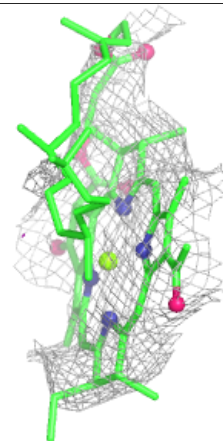
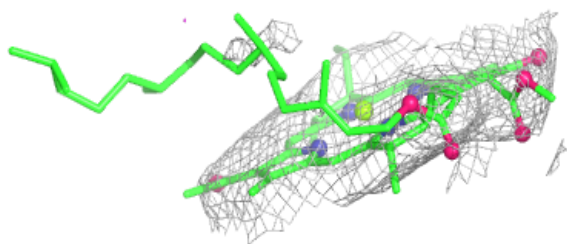
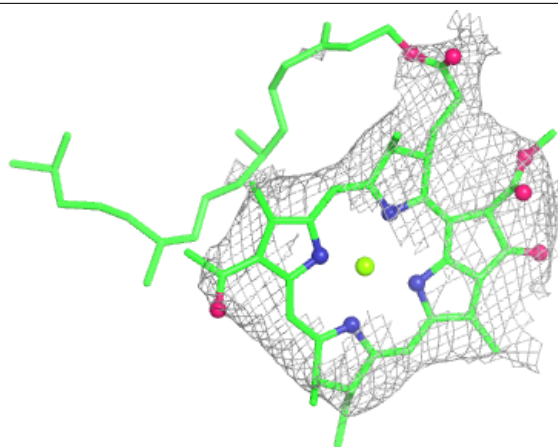
Electron density around BCL L 301:

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



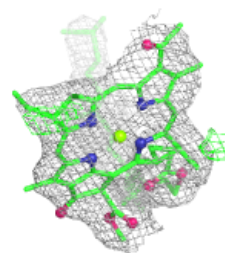
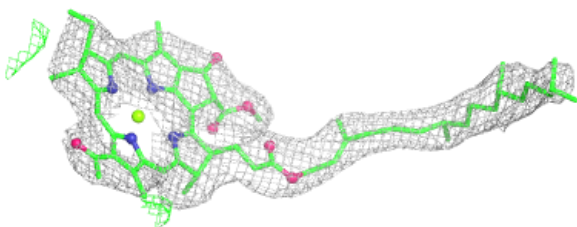
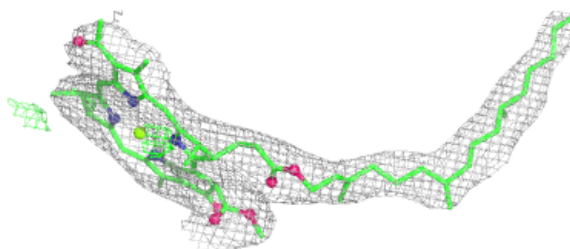
Electron density around BCL F 103:

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



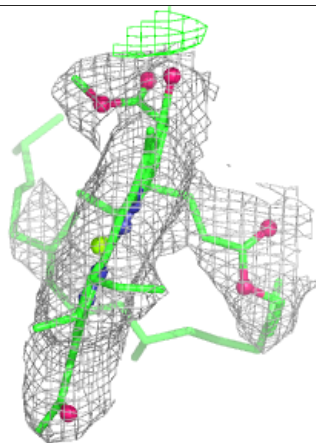
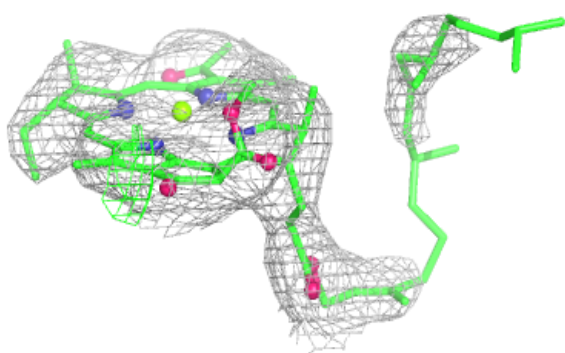
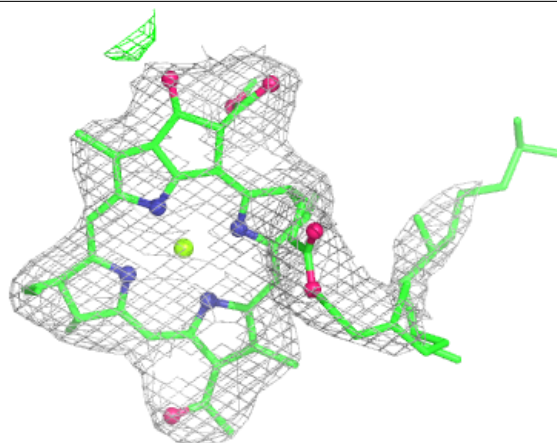
Electron density around BCL L 302:

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



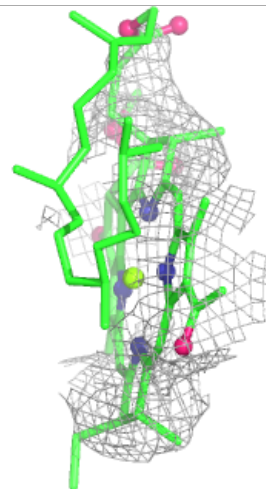
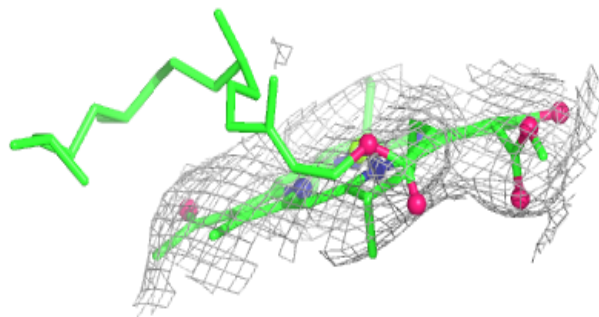
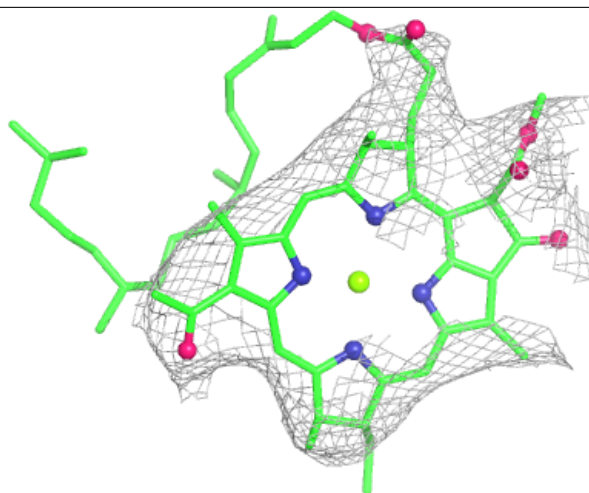
Electron density around BCL L 305:

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



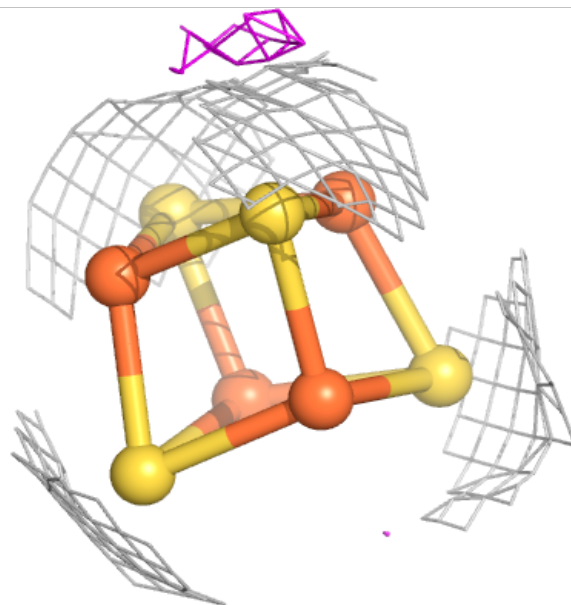
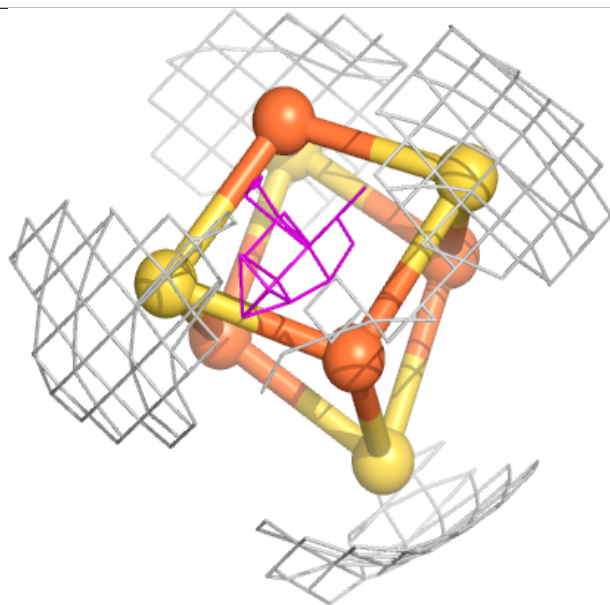
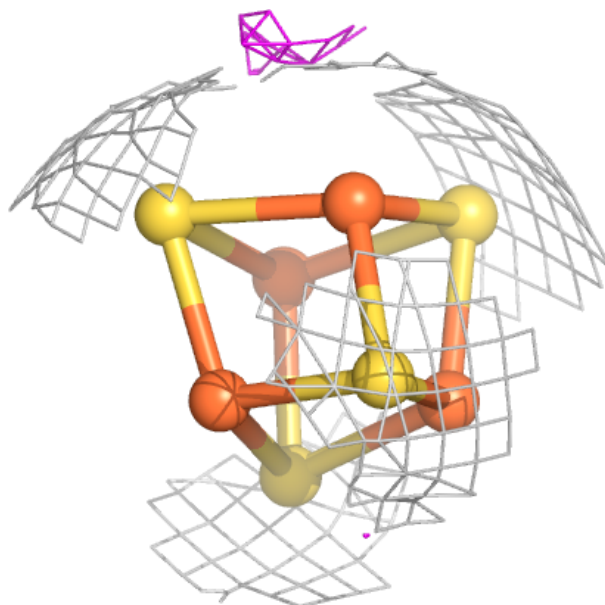
Electron density around BCL 7 103:

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



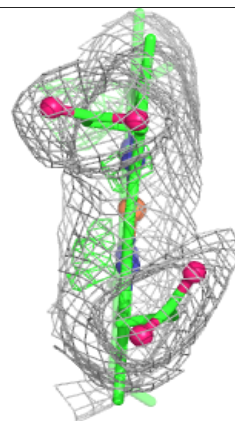
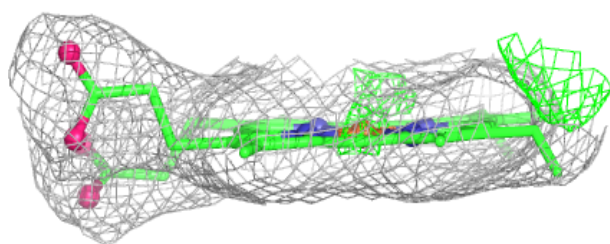
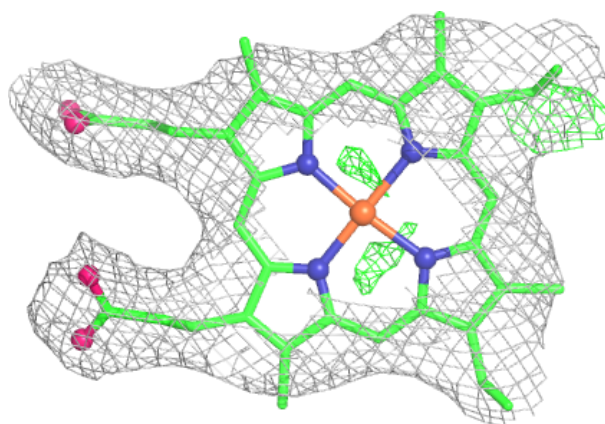
Electron density around SF4 b 101:

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



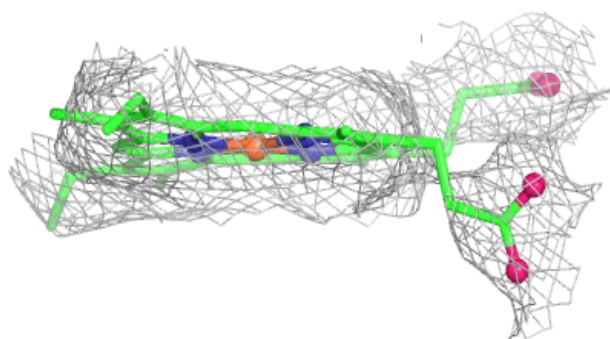
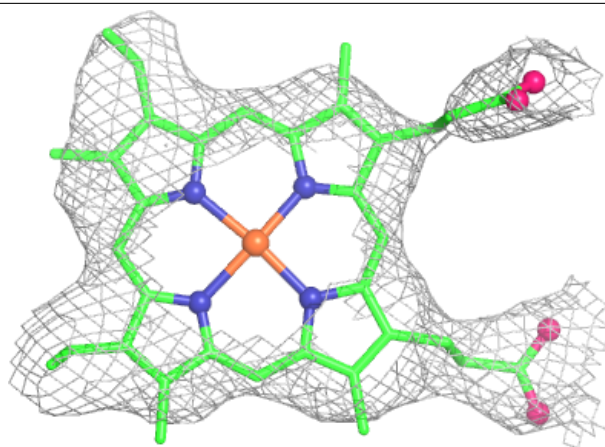
Electron density around HEC C 504:

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



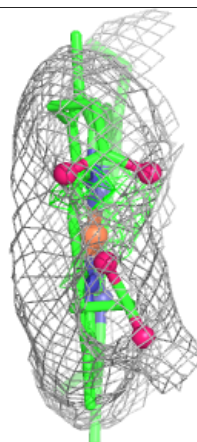
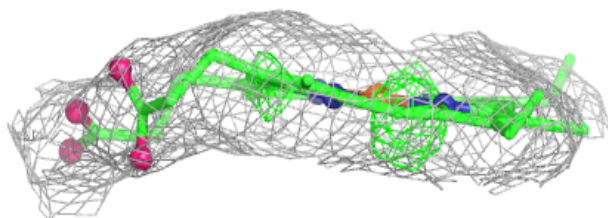
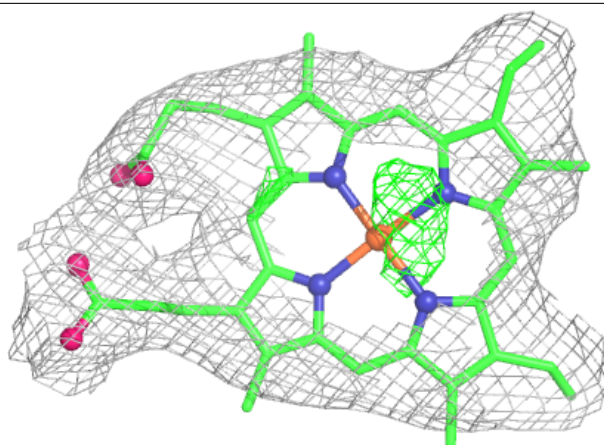
Electron density around HEC C 501:

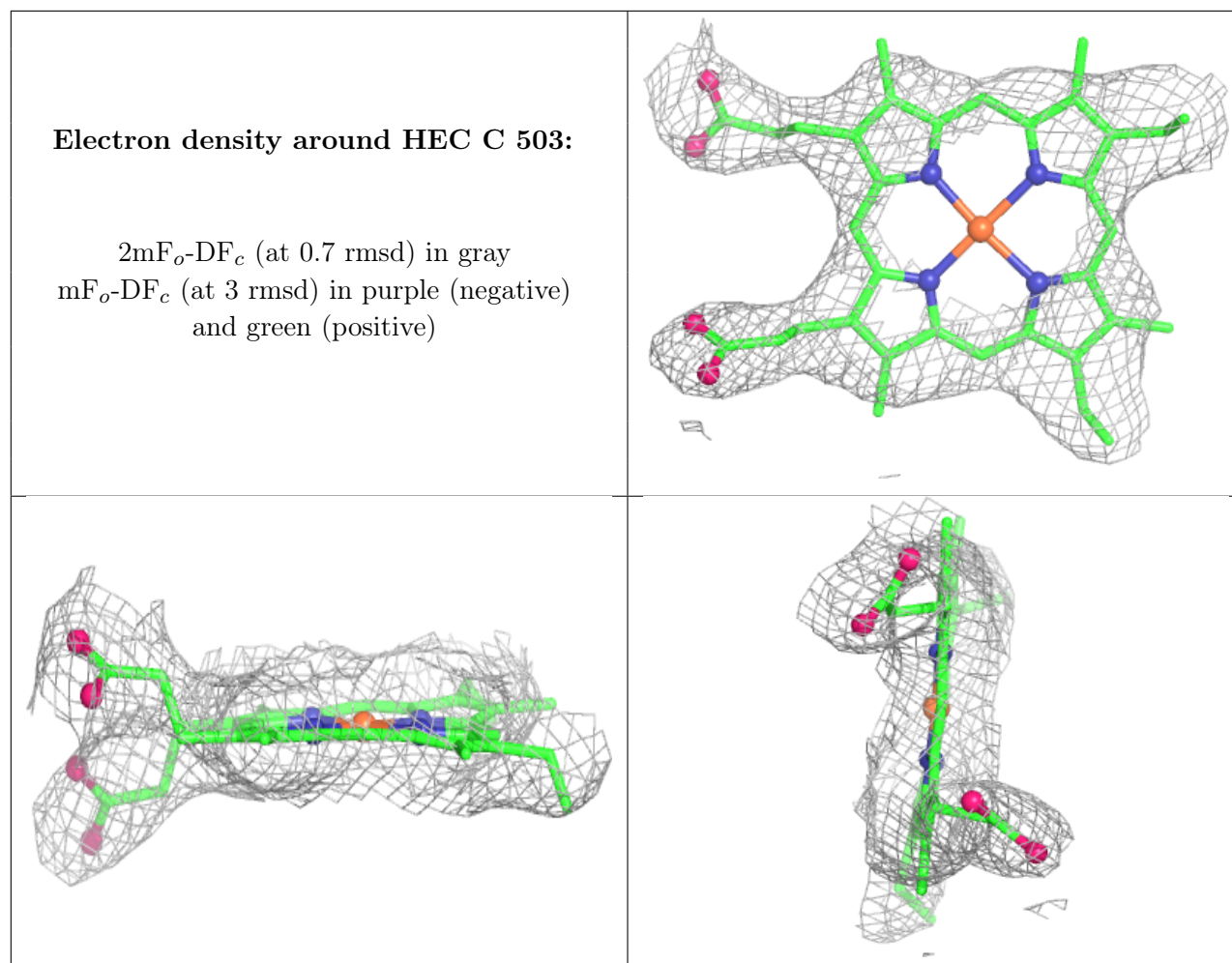
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.