wwPDB X-ray Structure Validation Summary Report (i)

Nov 19, 2023 – 11:50 PM JST

PDB ID	:	7C52
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 wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

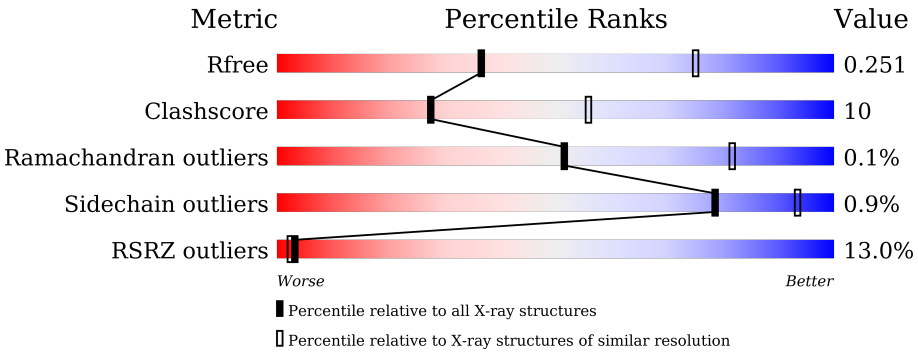
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 <=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	5% 93% 7%
2	L	281	3% 89% 10%
3	M	325	2% 83% 14%
4	H	259	17% 87% 11%
5	1	61	18% 77% 13% 8%
5	3	61	2% 82% 10% 8%

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Mol	Chain	Length	Quality of chain
5	5	61	11% 66% 20% 11%
5	7	61	16% 70% 21% 7%
5	9	61	8% 74% 16% 7%
5	A	61	8% 69% 20% 11%
5	D	61	8% 77% 11% 10%
5	F	61	15% 72% 18% 10%
5	I	61	18% 79% 15% 7%
5	K	61	16% 77% 16% 7%
5	O	61	13% 62% 28% 8%
5	Q	61	13% 80% 11% 7%
5	S	61	11% 72% 16% 8%
5	U	61	33% 79% 15% 5%
5	W	61	13% 82% 10% 8%
5	Y	61	15% 74% 18% 7%
6	0	47	6% 77% 13% 9%
6	2	47	9% 60% 28% 13%
6	4	47	13% 72% 17% 11%
6	6	47	38% 74% 13% 11%
6	8	47	15% 74% 13% 13%
6	B	47	13% 77% 13% 11%
6	E	47	13% 77% 19%
6	G	47	21% 79% 11% 11%
6	J	47	23% 79% 11% 11%
6	N	47	9% 66% 23% 11%
6	P	47	6% 72% 17% 11%

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Mol	Chain	Length	Quality of chain
6	R	47	2% 77% 11% 13%
6	T	47	15% 83% 9% 9%
6	V	47	17% 81% 9% 11%
6	X	47	19% 77% 11% 13%
6	Z	47	15% 66% 19% 15%
7	b	83	57% 99%

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
10	GOL	C	506	-	-	-	X
12	PGV	3	105	-	-	-	X
12	PGV	L	308	-	-	-	X
12	PGV	M	410	-	-	-	X
15	UQ8	L	309	-	-	-	X
19	CRT	0	101	-	-	-	X
19	CRT	2	101	-	-	-	X
19	CRT	3	103	-	-	-	X
19	CRT	4	101	-	-	-	X
19	CRT	8	101	-	-	-	X
19	CRT	B	101	-	-	-	X
19	CRT	G	101	-	-	-	X
19	CRT	J	101	-	-	-	X
19	CRT	N	101	-	-	-	X
19	CRT	O	103	-	-	-	X
19	CRT	P	101	-	-	-	X
19	CRT	V	101	-	-	-	X
19	CRT	W	102	-	-	-	X
21	PEF	1	103	-	X	-	-
21	PEF	3	104	-	X	-	X
21	PEF	H	302	-	-	-	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	-	-

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			

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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			

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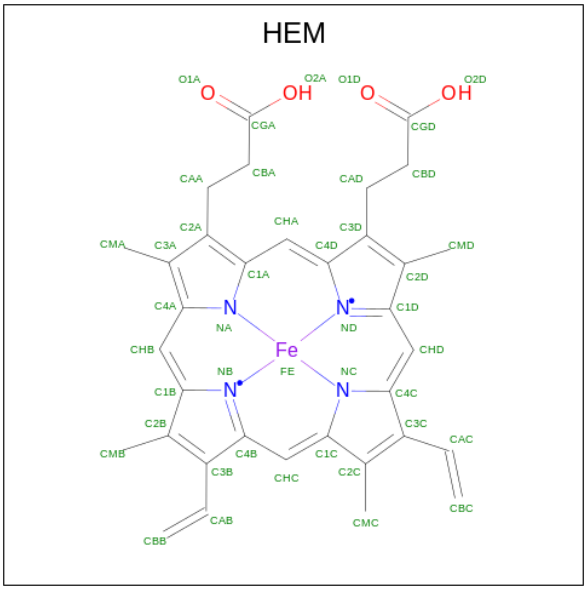
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	T	43	Total	C	N	O	S	0	0	0
			360	243	56	59	2			
6	V	42	Total	C	N	O	S	0	0	0
			351	237	54	58	2			
6	X	41	Total	C	N	O	S	0	0	0
			345	234	53	56	2			
6	Z	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	2	41	Total	C	N	O	S	0	0	0
			345	234	53	56	2			
6	4	42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

- Molecule 7 is a protein called High-potential iron-sulfur protein.

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

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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 (three-letter code: 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

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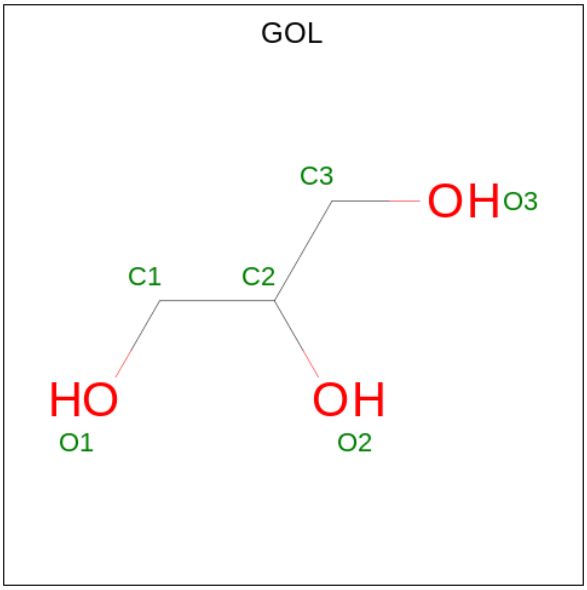
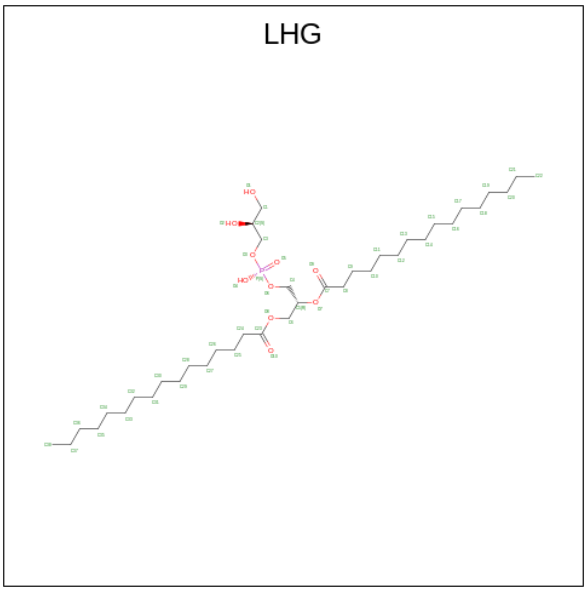
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	9	1	Total Ca 1 1	0	0

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



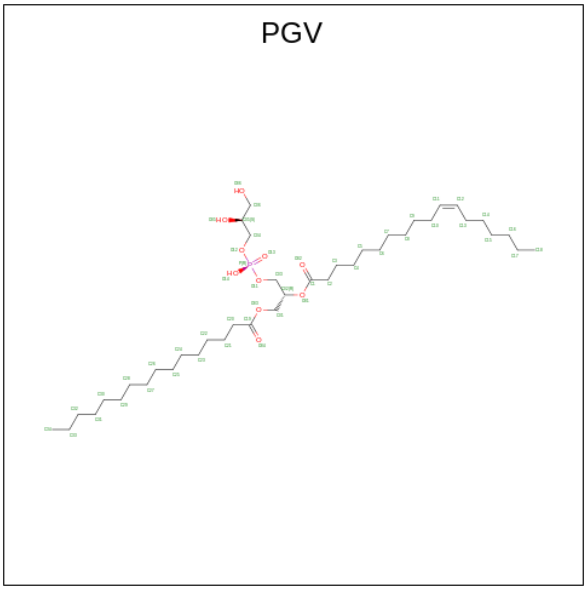
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total C O 6 3 3	0	0
10	H	1	Total C O 6 3 3	0	0

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



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

- Molecule 12 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



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

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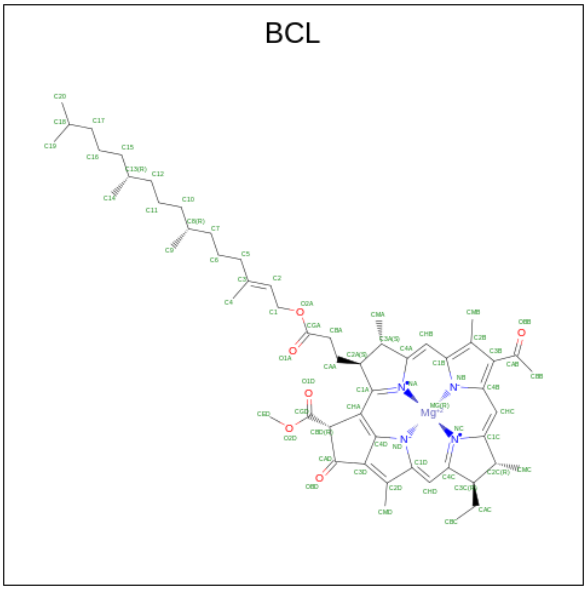
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	L	1	Total C O P 44 33 10 1	0	0
12	M	1	Total C O P 46 37 8 1	0	0
12	M	1	Total C O P 37 26 10 1	0	0
12	H	1	Total C O P 36 25 10 1	0	0
12	D	1	Total C O P 35 24 10 1	0	0
12	1	1	Total C O P 31 20 10 1	0	0
12	3	1	Total C O P 51 40 10 1	0	0
12	9	1	Total C O P 33 22 10 1	0	0

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



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

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

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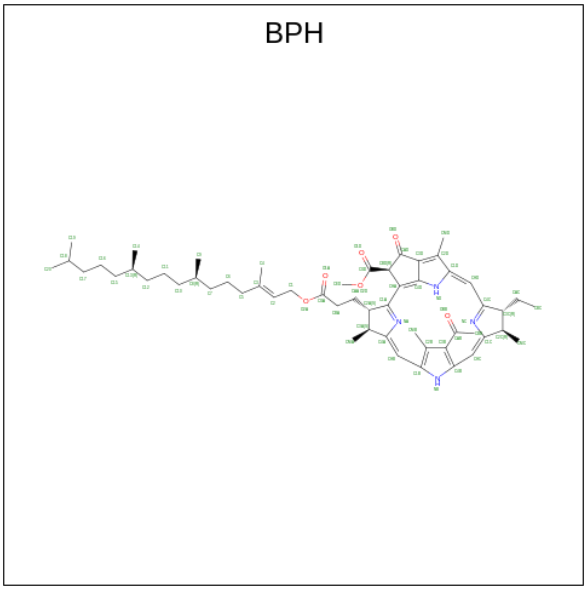
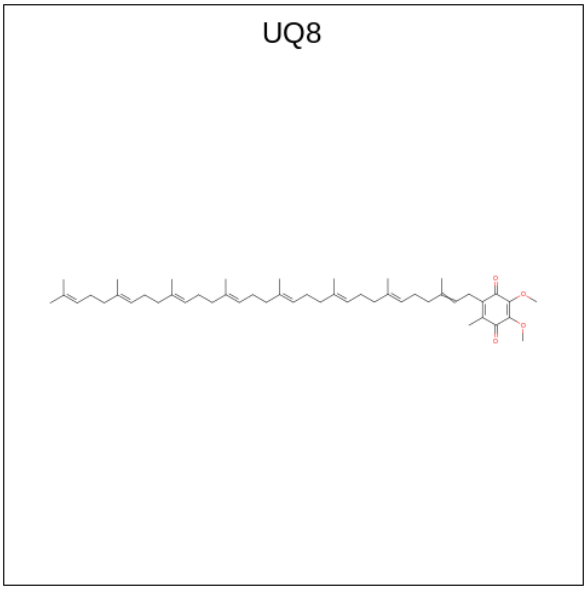
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	Y	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
13	Y	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
13	1	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
13	2	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
13	3	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
13	4	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
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 (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



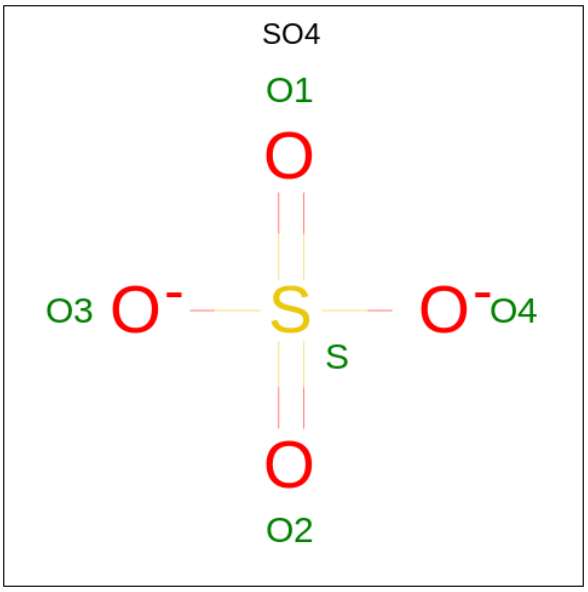
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	L	1	Total C N O 65 55 4 6	0	0
14	M	1	Total C N O 65 55 4 6	0	0

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



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

- Molecule 16 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

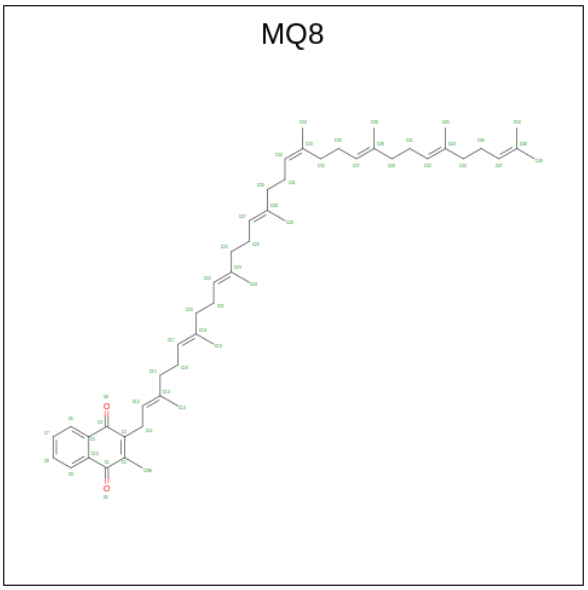


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	L	1	Total O S 5 4 1	0	0

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

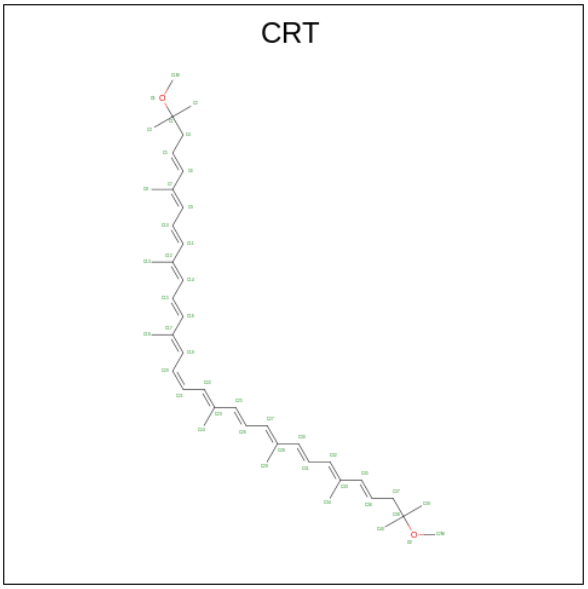
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	M	1	Total Fe 1 1	0	0

- Molecule 18 is MENAQUINONE 8 (three-letter code: MQ8) (formula: $C_{51}H_{72}O_2$).



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

- Molecule 19 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: $C_{42}H_{60}O_2$).



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

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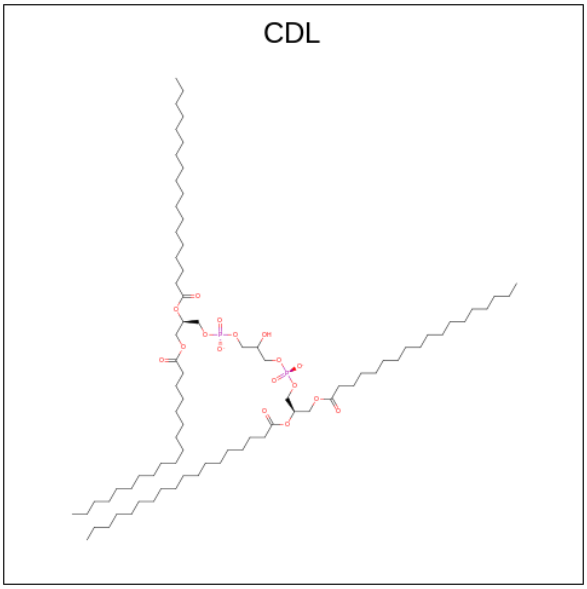
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	Z	1	Total C O 44 42 2	0	0
19	2	1	Total C O 44 42 2	0	0
19	3	1	Total C O 44 42 2	0	0
19	4	1	Total C O 44 42 2	0	0
19	8	1	Total C O 44 42 2	0	0
19	0	1	Total C O 44 42 2	0	0

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



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

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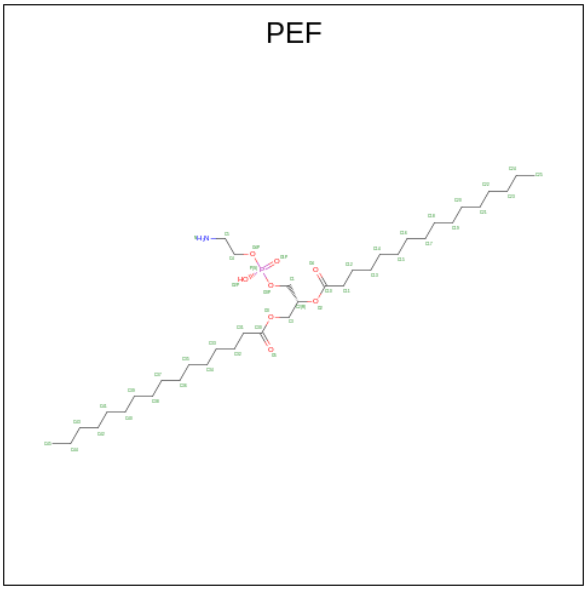
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	O	1	Total C O P 86 67 17 2	0	0
20	S	1	Total C O P 75 56 17 2	0	0
20	U	1	Total C O P 62 43 17 2	0	0
20	Y	1	Total C O P 40 21 17 2	0	0
20	1	1	Total C O P 13 5 7 1	0	0

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



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

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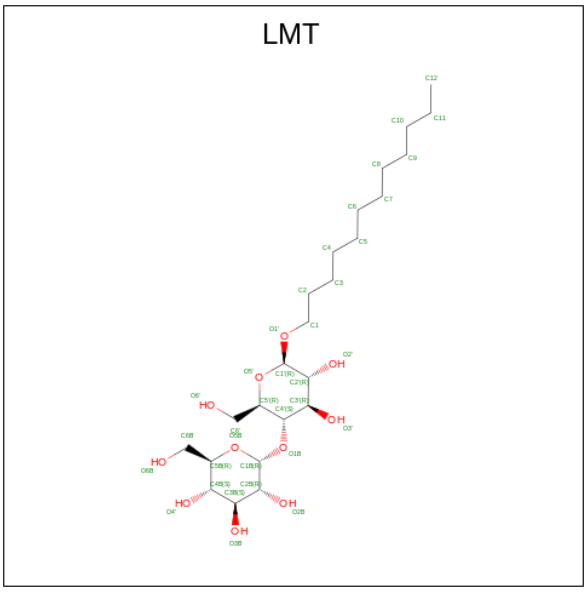
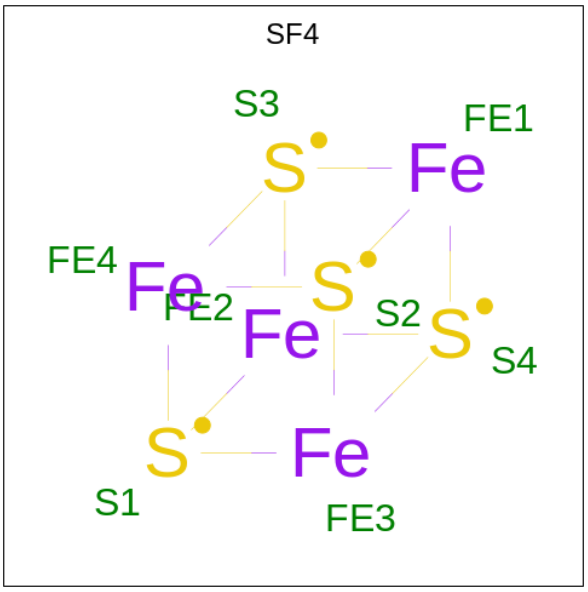
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	W	1	Total O P 5 4 1	0	0
21	W	1	Total O P 5 4 1	0	0
21	1	1	Total O P 5 4 1	0	0
21	3	1	Total O P 5 4 1	0	0

- Molecule 22 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

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



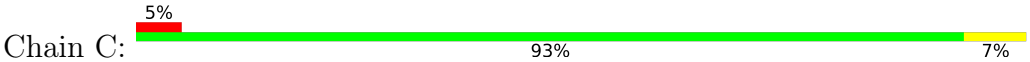
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	b	1	Total	Fe	S	0	0
			8	4	4		

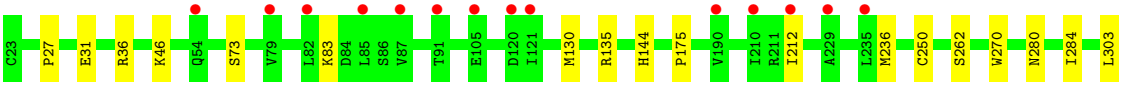
3 Residue-property plots (i)

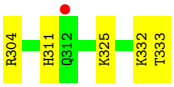
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

Chain C:

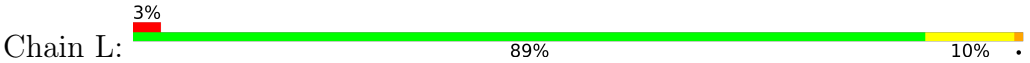


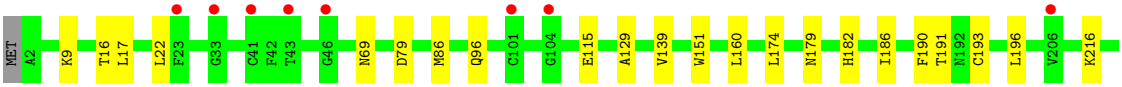




• Molecule 2: Photosynthetic reaction center L subunit

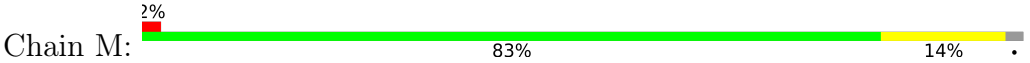
Chain L:

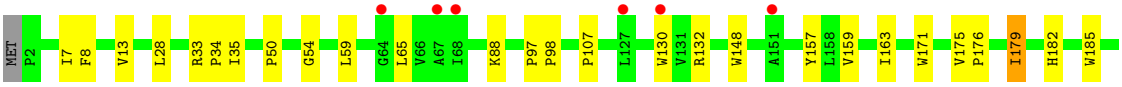


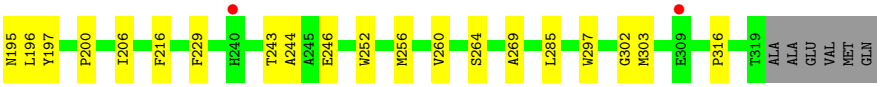


• Molecule 3: Photosynthetic reaction center M subunit

Chain M:

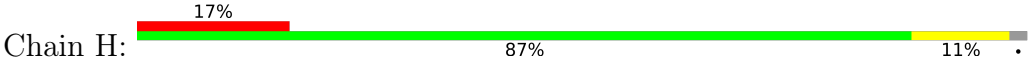


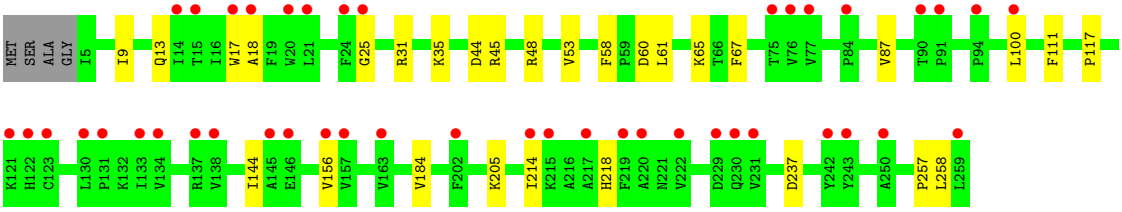




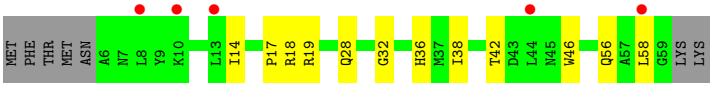
• Molecule 4: Photosynthetic reaction center H subunit

Chain H:

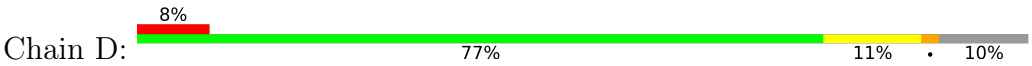




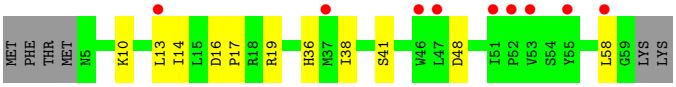
• Molecule 5: LH1 alpha polypeptide



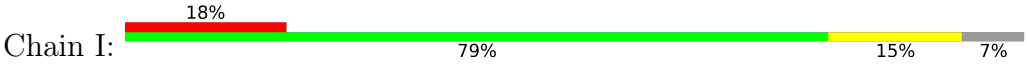
• Molecule 5: LH1 alpha polypeptide

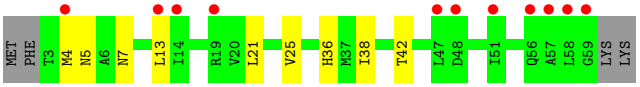


• Molecule 5: LH1 alpha polypeptide

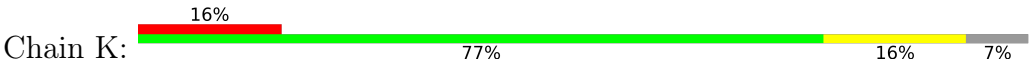


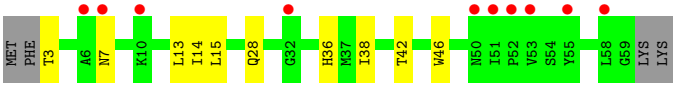
• Molecule 5: LH1 alpha polypeptide



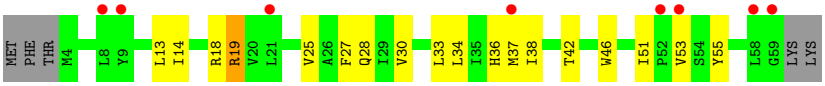


• Molecule 5: LH1 alpha polypeptide



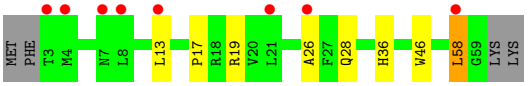


• Molecule 5: LH1 alpha polypeptide



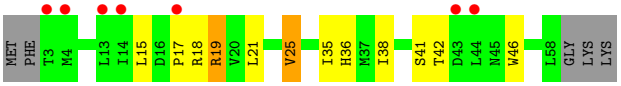
• Molecule 5: LH1 alpha polypeptide

Chain Q:



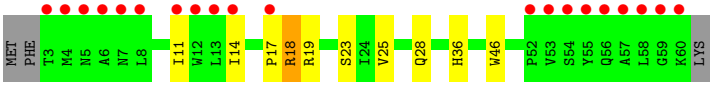
• Molecule 5: LH1 alpha polypeptide

Chain S:



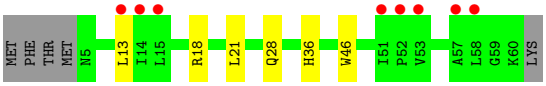
• Molecule 5: LH1 alpha polypeptide

Chain U:



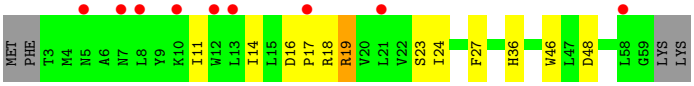
• Molecule 5: LH1 alpha polypeptide

Chain W:



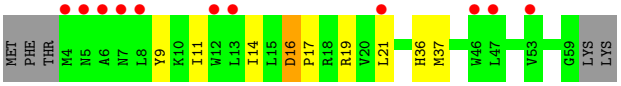
• Molecule 5: LH1 alpha polypeptide

Chain Y:



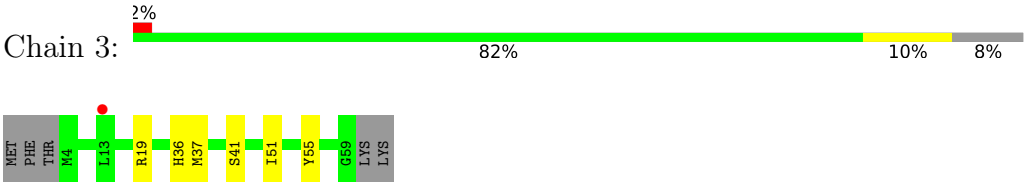
• Molecule 5: LH1 alpha polypeptide

Chain 1:



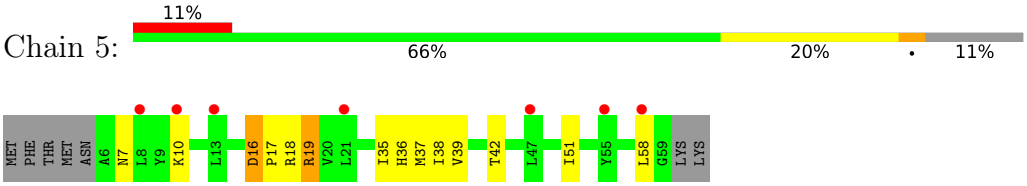
• Molecule 5: LH1 alpha polypeptide

Chain 3:



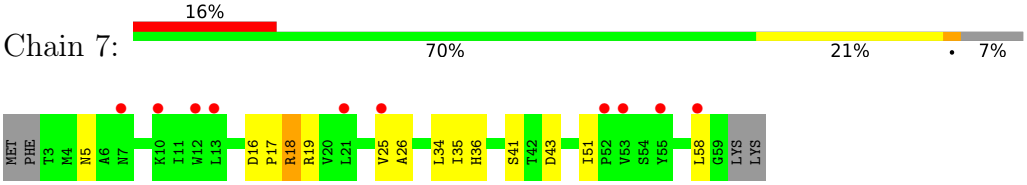
• Molecule 5: LH1 alpha polypeptide

Chain 5:



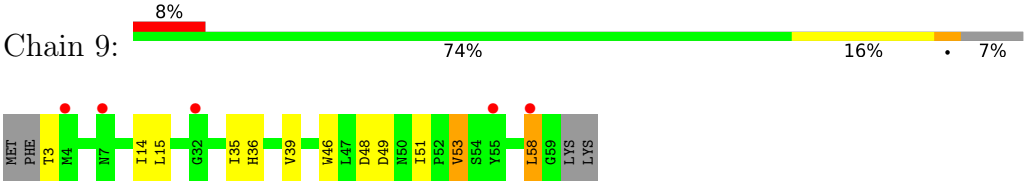
• Molecule 5: LH1 alpha polypeptide

Chain 7:



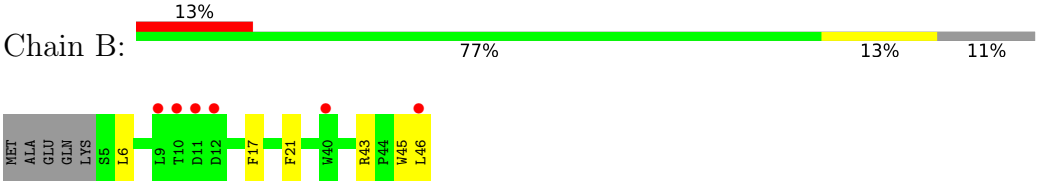
• Molecule 5: LH1 alpha polypeptide

Chain 9:



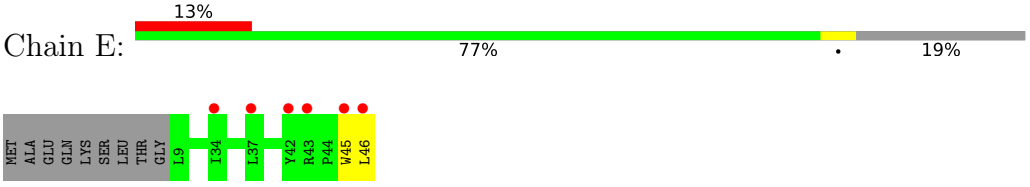
• Molecule 6: LH1 beta polypeptide

Chain B:



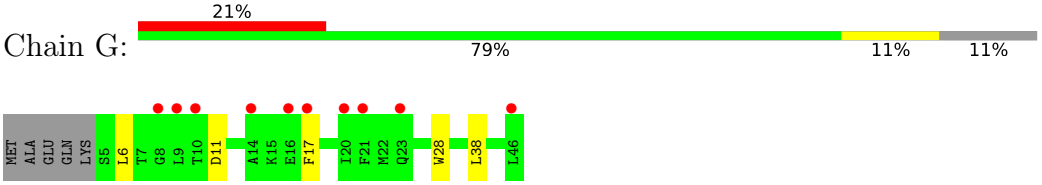
• Molecule 6: LH1 beta polypeptide

Chain E:



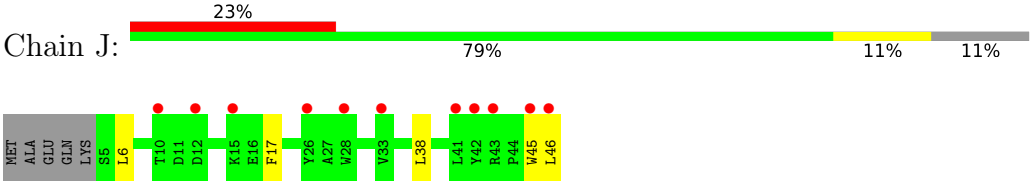
• Molecule 6: LH1 beta polypeptide

Chain G:



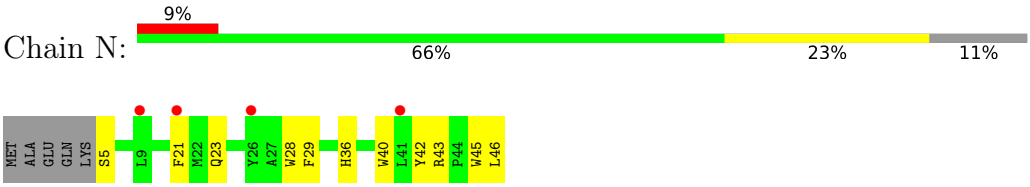
• Molecule 6: LH1 beta polypeptide

Chain J:



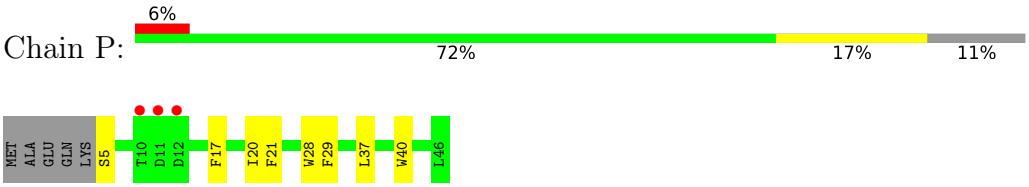
• Molecule 6: LH1 beta polypeptide

Chain N:



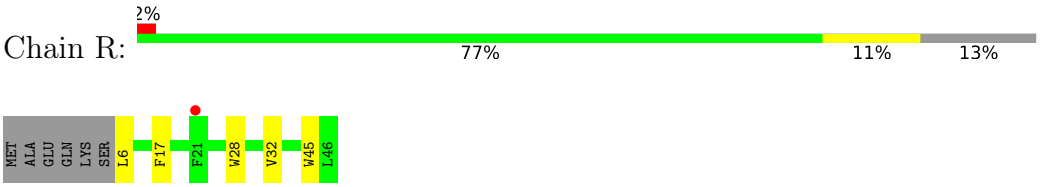
• Molecule 6: LH1 beta polypeptide

Chain P:



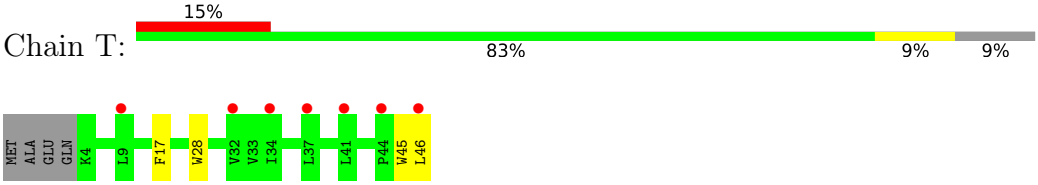
• Molecule 6: LH1 beta polypeptide

Chain R:



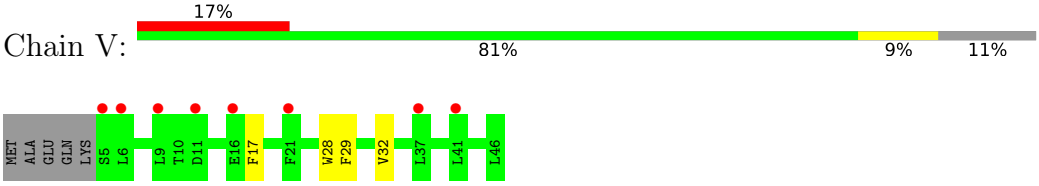
• Molecule 6: LH1 beta polypeptide

Chain T:



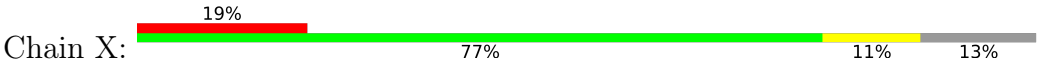
• Molecule 6: LH1 beta polypeptide

Chain V:



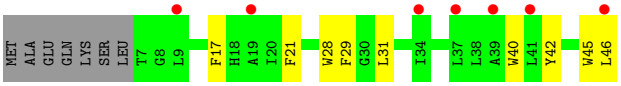
• Molecule 6: LH1 beta polypeptide

Chain X:



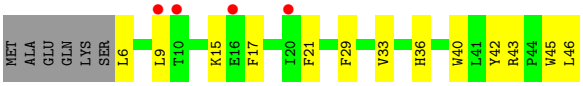
• Molecule 6: LH1 beta polypeptide

Chain Z:



• Molecule 6: LH1 beta polypeptide

Chain 2:

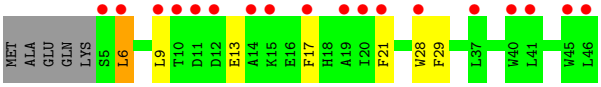


• Molecule 6: LH1 beta polypeptide

Chain 4:

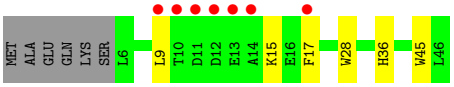
• Molecule 6: LH1 beta polypeptide

Chain 6:



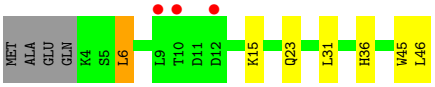
• Molecule 6: LH1 beta polypeptide

Chain 8:



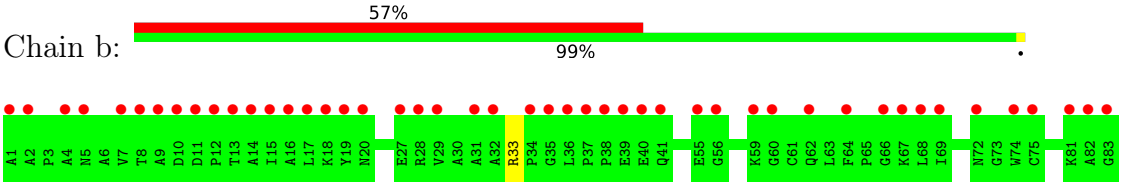
• Molecule 6: LH1 beta polypeptide

Chain 0:



• Molecule 7: High-potential iron-sulfur protein

Chain b:


57%
99%
A1 A2 P3 A4 N5 A6 V7 T8 A9 D10 D11 P12 T13 A14 I15 A16 L17 K18 Y19 N20 E27 R28 V29 A30 A31 A32 R33 P34 G35 L36 P37 P38 E39 E40 Q41 E55 G56 K59 G60 C61 Q62 L63 F64 P65 G66 K67 L68 I69 N72 G73 W74 C75 K81 A82 G83

4 Data and refinement statistics (i)

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 48.22 – 2.89	Depositor EDS
% Data completeness (in resolution range)	97.6 (29.99-2.89) 97.6 (48.22-2.89)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.219 , 0.248 0.222 , 0.251	Depositor DCC
R_{free} test set	4316 reflections (5.00%)	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)	0.27 , 76.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, LHG, CA, CDL, BPH, SF4, MQ8, UQ8, HEM, PEF, PGV, FE, LMT, SO4, CRT, BCL

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	0.27	0/2487	0.53	0/3396
2	L	0.28	0/2326	0.51	1/3177 (0.0%)
3	M	0.28	0/2658	0.50	0/3637
4	H	0.29	0/2031	0.55	0/2769
5	1	0.36	0/456	0.63	1/625 (0.2%)
5	3	0.26	0/467	0.51	0/638
5	5	0.49	1/443 (0.2%)	0.98	4/607 (0.7%)
5	7	0.60	1/466 (0.2%)	0.91	4/638 (0.6%)
5	9	0.28	0/466	0.58	1/638 (0.2%)
5	A	0.24	0/443	0.49	0/607
5	D	0.30	0/457	0.66	2/626 (0.3%)
5	F	0.29	0/457	0.61	0/626
5	I	0.26	0/472	0.55	0/646
5	K	0.24	0/463	0.48	0/635
5	O	0.28	0/467	0.64	1/638 (0.2%)
5	Q	0.24	0/466	0.59	0/638
5	S	0.33	0/480	0.60	1/658 (0.2%)
5	U	0.34	0/475	0.65	2/649 (0.3%)
5	W	0.28	0/460	0.66	1/629 (0.2%)
5	Y	0.63	2/466 (0.4%)	0.84	3/638 (0.5%)
6	0	0.26	0/373	0.43	0/506
6	2	0.25	0/358	0.43	0/487
6	4	0.25	0/364	0.46	0/495
6	6	0.28	0/364	0.59	2/495 (0.4%)
6	8	0.26	0/358	0.54	1/487 (0.2%)
6	B	0.25	0/364	0.46	0/495
6	E	0.27	0/339	0.49	0/461
6	G	0.26	0/364	0.45	0/495
6	J	0.26	0/364	0.48	0/495
6	N	0.27	0/364	0.43	0/495
6	P	0.24	0/364	0.41	0/495
6	R	0.25	0/358	0.42	0/487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
6	T	0.25	0/373	0.44	0/506
6	V	0.26	0/364	0.42	0/495
6	X	0.25	0/358	0.42	0/487
6	Z	0.25	0/350	0.40	0/476
7	b	0.26	0/631	0.52	0/859
All	All	0.30	4/23316 (0.0%)	0.56	24/31831 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	7	18	ARG	CG-CD	-10.38	1.25	1.51
5	Y	19	ARG	CG-CD	-9.51	1.28	1.51
5	5	19	ARG	CZ-NH1	6.11	1.41	1.33
5	Y	19	ARG	CB-CG	-6.08	1.36	1.52

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	7	18	ARG	NE-CZ-NH2	-12.70	113.95	120.30
5	7	18	ARG	NE-CZ-NH1	11.88	126.24	120.30
5	5	19	ARG	NE-CZ-NH2	-11.87	114.36	120.30
5	Y	19	ARG	NE-CZ-NH2	-10.70	114.95	120.30
5	Y	19	ARG	NE-CZ-NH1	10.10	125.35	120.30

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	17	0
2	L	2236	0	2201	30	0
3	M	2555	0	2528	40	0
4	H	1973	0	1968	36	0
5	1	447	0	468	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	3	455	0	484	7	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	15	0
5	D	445	0	471	11	0
5	F	445	0	471	12	0
5	I	460	0	487	8	0
5	K	454	0	475	9	0
5	O	455	0	484	19	0
5	Q	457	0	482	9	0
5	S	465	0	494	18	0
5	U	466	0	495	19	0
5	W	451	0	479	5	0
5	Y	457	0	482	13	0
6	0	360	0	352	9	0
6	2	345	0	334	16	0
6	4	351	0	339	8	0
6	6	351	0	339	9	0
6	8	345	0	334	6	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	5	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	0	0
8	C	172	0	120	6	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	10	0
12	M	83	0	116	8	0
13	1	66	0	74	7	0
13	2	66	0	74	12	0
13	3	66	0	74	4	0
13	4	66	0	74	7	0
13	5	132	0	148	9	0
13	7	127	0	135	13	0
13	9	132	0	148	9	0
13	A	132	0	148	10	0
13	D	132	0	148	6	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	10	0
13	L	198	0	222	15	0
13	M	66	0	74	2	0
13	O	66	0	74	7	0
13	P	66	0	74	6	0
13	Q	132	0	148	12	0
13	S	132	0	148	12	0
13	U	132	0	148	15	0
13	W	132	0	148	11	0
13	Y	132	0	148	15	0
14	L	65	0	74	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	M	65	0	74	8	0
15	L	137	0	167	18	0
15	M	18	0	15	0	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	7	0
19	3	44	0	60	2	0
19	4	44	0	60	7	0
19	8	44	0	60	5	0
19	A	44	0	60	8	0
19	B	44	0	60	7	0
19	G	44	0	60	4	0
19	J	44	0	60	3	0
19	M	44	0	60	6	0
19	N	44	0	60	5	0
19	O	44	0	60	0	0
19	P	44	0	60	5	0
19	T	44	0	60	4	0
19	V	44	0	60	3	0
19	W	44	0	60	1	0
19	Z	44	0	60	6	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
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	547	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.

The worst 5 of 547 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

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%)	25 58
4	H	255/259 (98%)	254 (100%)	1 (0%)	0	100 100
5	1	54/61 (88%)	54 (100%)	0	0	100 100
5	3	55/61 (90%)	54 (98%)	1 (2%)	0	100 100
5	5	52/61 (85%)	50 (96%)	2 (4%)	0	100 100
5	7	55/61 (90%)	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%)	8 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	51	82

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 (i)

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%)	257 (99%)	3 (1%)	71 91
2	L	229/229 (100%)	226 (99%)	3 (1%)	69 90
3	M	258/261 (99%)	257 (100%)	1 (0%)	91 97
4	H	210/211 (100%)	209 (100%)	1 (0%)	88 96
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%)	33 67
5	A	49/56 (88%)	49 (100%)	0	100 100
5	D	51/56 (91%)	51 (100%)	0	100 100
5	F	51/56 (91%)	50 (98%)	1 (2%)	55 82
5	I	53/56 (95%)	52 (98%)	1 (2%)	57 84
5	K	51/56 (91%)	50 (98%)	1 (2%)	55 82
5	O	52/56 (93%)	50 (96%)	2 (4%)	33 67
5	Q	52/56 (93%)	51 (98%)	1 (2%)	57 84
5	S	54/56 (96%)	53 (98%)	1 (2%)	57 84
5	U	53/56 (95%)	53 (100%)	0	100 100
5	W	51/56 (91%)	51 (100%)	0	100 100
5	Y	52/56 (93%)	51 (98%)	1 (2%)	57 84
6	0	36/39 (92%)	34 (94%)	2 (6%)	21 52
6	2	34/39 (87%)	33 (97%)	1 (3%)	42 76
6	4	35/39 (90%)	35 (100%)	0	100 100
6	6	35/39 (90%)	35 (100%)	0	100 100
6	8	34/39 (87%)	34 (100%)	0	100 100
6	B	35/39 (90%)	35 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	E	32/39 (82%)	32 (100%)	0	100 100
6	G	35/39 (90%)	35 (100%)	0	100 100
6	J	35/39 (90%)	35 (100%)	0	100 100
6	N	35/39 (90%)	35 (100%)	0	100 100
6	P	35/39 (90%)	35 (100%)	0	100 100
6	R	34/39 (87%)	34 (100%)	0	100 100
6	T	36/39 (92%)	36 (100%)	0	100 100
6	V	35/39 (90%)	35 (100%)	0	100 100
6	X	34/39 (87%)	34 (100%)	0	100 100
6	Z	33/39 (85%)	33 (100%)	0	100 100
7	b	61/61 (100%)	60 (98%)	1 (2%)	62 86
All	All	2395/2542 (94%)	2373 (99%)	22 (1%)	78 93

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	S	25	VAL
5	9	3	THR
6	2	6	LEU
5	9	53	VAL
3	M	216	PHE

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
20	CDL	D	104	-	39,39,99	1.45	4 (10%)	45,51,111	1.40	7 (15%)
13	BCL	F	101	-	64,74,74	1.27	5 (7%)	78,115,115	1.81	17 (21%)
19	CRT	J	101	-	41,43,43	0.80	0	50,54,54	1.50	10 (20%)
20	CDL	D	105	-	63,63,99	1.08	4 (6%)	69,75,111	1.27	6 (8%)
20	CDL	M	406	-	99,99,99	0.93	4 (4%)	105,111,111	1.14	7 (6%)
13	BCL	K	101	-	64,74,74	1.31	6 (9%)	78,115,115	1.71	15 (19%)
13	BCL	D	103	-	64,74,74	1.29	5 (7%)	78,115,115	1.57	14 (17%)
19	CRT	A	104	-	41,43,43	0.71	0	50,54,54	1.67	13 (26%)
13	BCL	2	102	-	64,74,74	1.41	8 (12%)	78,115,115	1.79	12 (15%)
10	GOL	H	301	-	5,5,5	0.93	0	5,5,5	0.94	0
20	CDL	U	104	-	61,61,99	1.17	4 (6%)	67,73,111	1.62	14 (20%)
12	PGV	L	307	-	42,42,50	0.99	2 (4%)	45,48,56	1.22	4 (8%)
13	BCL	L	305	-	64,74,74	1.29	4 (6%)	78,115,115	1.76	17 (21%)
13	BCL	J	102	-	64,74,74	1.25	6 (9%)	78,115,115	1.62	15 (19%)
12	PGV	9	104	-	32,32,50	1.16	2 (6%)	35,38,56	1.31	6 (17%)
19	CRT	G	101	-	41,43,43	0.71	0	50,54,54	1.56	11 (22%)
11	LHG	C	507	1	8,8,48	0.29	0	7,7,54	1.04	1 (14%)
16	SO4	L	306	-	4,4,4	0.14	0	6,6,6	0.05	0
18	MQ8	M	404	-	54,54,54	1.36	2 (3%)	66,69,69	1.50	14 (21%)
8	HEM	C	503	1	41,50,50	1.27	5 (12%)	45,82,82	1.83	8 (17%)
8	HEM	C	502	1	41,50,50	1.34	5 (12%)	45,82,82	1.87	9 (20%)
13	BCL	3	101	-	64,74,74	1.34	4 (6%)	78,115,115	2.01	17 (21%)
13	BCL	K	103	-	64,74,74	1.27	5 (7%)	78,115,115	1.66	13 (16%)
12	PGV	M	411	-	36,36,50	1.06	2 (5%)	39,42,56	1.24	4 (10%)
13	BCL	5	103	-	64,74,74	1.30	6 (9%)	78,115,115	1.68	14 (17%)
13	BCL	M	401	-	64,74,74	1.29	6 (9%)	78,115,115	1.60	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CRT	M	405	-	41,43,43	0.74	0	50,54,54	1.57	10 (20%)
23	SF4	b	101	7	0,12,12	-	-	-		
19	CRT	T	101	-	41,43,43	0.76	0	50,54,54	1.66	13 (26%)
13	BCL	S	101	-	64,74,74	1.34	5 (7%)	78,115,115	1.59	12 (15%)
21	PEF	W	106	-	4,4,46	2.63	2 (50%)	6,6,51	1.83	2 (33%)
12	PGV	L	308	-	43,43,50	0.98	2 (4%)	46,49,56	1.13	3 (6%)
12	PGV	H	303	-	35,35,50	1.10	2 (5%)	38,41,56	1.19	4 (10%)
15	UQ8	L	309	-	53,53,53	1.18	2 (3%)	64,67,67	1.77	18 (28%)
13	BCL	D	101	-	64,74,74	1.30	4 (6%)	78,115,115	1.74	17 (21%)
13	BCL	7	103	-	64,74,74	1.32	5 (7%)	78,115,115	1.50	10 (12%)
8	HEM	C	501	1	41,50,50	1.52	3 (7%)	45,82,82	2.17	15 (33%)
13	BCL	L	302	-	64,74,74	1.27	5 (7%)	78,115,115	1.49	9 (11%)
12	PGV	3	105	-	50,50,50	0.94	2 (4%)	53,56,56	0.97	2 (3%)
13	BCL	7	101	-	59,69,74	1.35	5 (8%)	72,109,115	1.79	13 (18%)
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%)
15	UQ8	L	311	-	18,18,53	2.10	2 (11%)	22,25,67	1.05	1 (4%)
19	CRT	0	101	-	41,43,43	0.75	0	50,54,54	1.49	9 (18%)
14	BPH	M	402	-	51,70,70	1.80	8 (15%)	52,101,101	2.13	15 (28%)
20	CDL	O	104	-	85,85,99	1.00	4 (4%)	91,97,111	1.26	11 (12%)
21	PEF	H	302	-	4,4,46	2.48	1 (25%)	6,6,51	2.44	2 (33%)
20	CDL	H	305	-	78,78,99	1.05	4 (5%)	84,90,111	1.05	5 (5%)
21	PEF	M	407	-	4,4,46	2.63	2 (50%)	6,6,51	1.84	2 (33%)
8	HEM	C	504	1	41,50,50	1.32	5 (12%)	45,82,82	1.81	9 (20%)
20	CDL	Y	104	-	39,39,99	1.48	5 (12%)	45,51,111	2.00	14 (31%)
13	BCL	I	101	-	64,74,74	1.33	8 (12%)	78,115,115	1.64	13 (16%)
19	CRT	8	101	-	41,43,43	0.73	0	50,54,54	1.57	13 (26%)
22	LMT	H	304	-	36,36,36	0.52	0	47,47,47	1.31	8 (17%)
15	UQ8	L	304	-	33,33,53	1.48	2 (6%)	40,43,67	1.86	12 (30%)
13	BCL	P	102	-	64,74,74	1.35	4 (6%)	78,115,115	1.78	15 (19%)
19	CRT	O	103	-	41,43,43	0.71	0	50,54,54	1.52	9 (18%)
13	BCL	1	101	-	64,74,74	1.29	6 (9%)	78,115,115	1.66	11 (14%)
13	BCL	W	104	-	64,74,74	1.30	5 (7%)	78,115,115	1.56	12 (15%)
13	BCL	W	101	-	64,74,74	1.29	6 (9%)	78,115,115	1.62	13 (16%)
19	CRT	3	103	-	41,43,43	0.71	0	50,54,54	1.69	14 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	BCL	9	103	-	64,74,74	1.31	4 (6%)	78,115,115	1.65	12 (15%)
12	PGV	1	105	-	30,30,50	1.22	2 (6%)	33,36,56	1.17	2 (6%)
19	CRT	V	101	-	41,43,43	0.70	0	50,54,54	1.62	12 (24%)
19	CRT	P	101	-	41,43,43	0.74	0	50,54,54	1.59	7 (14%)
13	BCL	4	102	-	64,74,74	1.28	6 (9%)	78,115,115	1.64	12 (15%)
13	BCL	Q	103	-	64,74,74	1.32	5 (7%)	78,115,115	1.67	13 (16%)
12	PGV	C	508	1	20,20,50	1.45	3 (15%)	22,22,56	1.56	3 (13%)
21	PEF	K	104	-	26,26,46	1.31	2 (7%)	29,31,51	1.27	2 (6%)
13	BCL	L	301	-	64,74,74	1.28	5 (7%)	78,115,115	1.60	12 (15%)
15	UQ8	L	310	-	33,33,53	1.47	2 (6%)	40,43,67	1.82	13 (32%)
21	PEF	I	103	-	4,4,46	2.63	2 (50%)	6,6,51	1.83	2 (33%)
19	CRT	4	101	-	41,43,43	0.70	0	50,54,54	1.64	13 (26%)
13	BCL	A	103	-	64,74,74	1.27	6 (9%)	78,115,115	1.53	11 (14%)
13	BCL	U	103	-	64,74,74	1.37	6 (9%)	78,115,115	1.68	16 (20%)
10	GOL	C	506	-	5,5,5	0.90	0	5,5,5	1.00	0
13	BCL	O	101	-	64,74,74	1.27	5 (7%)	78,115,115	1.69	13 (16%)
15	UQ8	M	413	-	18,18,53	2.13	2 (11%)	22,25,67	1.27	2 (9%)
21	PEF	M	408	-	4,4,46	1.71	2 (50%)	6,6,51	1.28	1 (16%)
13	BCL	A	101	-	64,74,74	1.29	6 (9%)	78,115,115	1.69	14 (17%)
12	PGV	D	106	-	34,34,50	1.12	2 (5%)	37,40,56	1.05	3 (8%)
14	BPH	L	303	-	51,70,70	1.84	8 (15%)	52,101,101	1.90	10 (19%)
12	PGV	M	410	-	45,45,50	1.05	2 (4%)	49,50,56	0.95	3 (6%)
22	LMT	M	414	-	36,36,36	0.42	0	47,47,47	0.77	0
13	BCL	U	101	-	64,74,74	1.31	4 (6%)	78,115,115	1.66	15 (19%)
19	CRT	N	101	-	41,43,43	0.75	0	50,54,54	1.83	14 (28%)
13	BCL	Y	101	-	64,74,74	1.30	6 (9%)	78,115,115	1.58	10 (12%)
21	PEF	W	105	-	4,4,46	2.68	2 (50%)	6,6,51	1.65	2 (33%)
21	PEF	M	409	-	4,4,46	2.64	2 (50%)	6,6,51	1.85	2 (33%)
20	CDL	1	104	-	12,12,99	0.44	0	13,15,111	0.58	0
20	CDL	M	412	3	38,38,99	1.31	3 (7%)	43,49,111	1.34	5 (11%)
13	BCL	9	101	-	64,74,74	1.28	6 (9%)	78,115,115	1.53	10 (12%)
19	CRT	W	102	-	41,43,43	0.74	0	50,54,54	1.59	13 (26%)
13	BCL	Y	103	-	64,74,74	1.31	6 (9%)	78,115,115	1.68	17 (21%)
13	BCL	Q	101	-	64,74,74	1.30	4 (6%)	78,115,115	1.80	15 (19%)
19	CRT	Z	101	-	41,43,43	0.72	0	50,54,54	1.74	14 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CDL	S	104	-	74,74,99	1.18	4 (5%)	80,86,111	1.34	9 (11%)
19	CRT	B	101	-	41,43,43	0.73	0	50,54,54	1.62	12 (24%)
13	BCL	F	103	-	64,74,74	1.29	5 (7%)	78,115,115	1.53	11 (14%)
21	PEF	3	104	-	4,4,46	2.63	2 (50%)	6,6,51	1.84	2 (33%)
13	BCL	S	103	-	64,74,74	1.38	5 (7%)	78,115,115	1.83	13 (16%)
13	BCL	5	101	-	64,74,74	1.32	7 (10%)	78,115,115	1.77	16 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CDL	D	104	-	-	23/50/50/110	-
13	BCL	F	101	-	-	12/37/137/137	-
19	CRT	J	101	-	-	2/51/51/51	-
20	CDL	D	105	-	-	26/73/73/110	-
20	CDL	M	406	-	-	47/110/110/110	-
13	BCL	K	101	-	-	10/37/137/137	-
13	BCL	D	103	-	-	7/37/137/137	-
19	CRT	A	104	-	-	0/51/51/51	-
13	BCL	2	102	-	-	14/37/137/137	-
10	GOL	H	301	-	-	2/4/4/4	-
20	CDL	U	104	-	-	33/71/71/110	-
12	PGV	L	307	-	-	22/47/47/55	-
13	BCL	L	305	-	-	15/37/137/137	-
13	BCL	J	102	-	-	10/37/137/137	-
12	PGV	9	104	-	-	14/37/37/55	-
19	CRT	G	101	-	-	2/51/51/51	-
11	LHG	C	507	1	-	3/5/6/53	-
18	MQ8	M	404	-	-	2/47/67/67	0/2/2/2
8	HEM	C	503	1	-	2/12/54/54	-
8	HEM	C	502	1	-	7/12/54/54	-
13	BCL	3	101	-	-	19/37/137/137	-
13	BCL	K	103	-	-	13/37/137/137	-
12	PGV	M	411	-	-	15/41/41/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCL	5	103	-	-	14/37/137/137	-
13	BCL	M	401	-	-	6/37/137/137	-
19	CRT	M	405	-	-	5/51/51/51	-
23	SF4	b	101	7	-	-	0/6/5/5
19	CRT	T	101	-	-	3/51/51/51	-
13	BCL	S	101	-	-	10/37/137/137	-
12	PGV	L	308	-	-	25/48/48/55	-
12	PGV	H	303	-	-	11/40/40/55	-
15	UQ8	L	309	-	-	16/51/75/75	0/1/1/1
13	BCL	D	101	-	-	8/37/137/137	-
13	BCL	7	103	-	-	12/37/137/137	-
8	HEM	C	501	1	-	4/12/54/54	-
13	BCL	L	302	-	-	1/37/137/137	-
12	PGV	3	105	-	-	17/55/55/55	-
13	BCL	7	101	-	-	6/31/131/137	-
19	CRT	2	101	-	-	1/51/51/51	-
15	UQ8	L	311	-	-	2/9/33/75	0/1/1/1
19	CRT	0	101	-	-	4/51/51/51	-
14	BPH	M	402	-	-	8/37/105/105	0/5/6/6
20	CDL	O	104	-	-	35/96/96/110	-
20	CDL	H	305	-	-	29/89/89/110	-
8	HEM	C	504	1	-	6/12/54/54	-
20	CDL	Y	104	-	-	20/50/50/110	-
13	BCL	I	101	-	-	8/37/137/137	-
19	CRT	8	101	-	-	4/51/51/51	-
22	LMT	H	304	-	-	9/21/61/61	0/2/2/2
15	UQ8	L	304	-	-	3/27/51/75	0/1/1/1
13	BCL	P	102	-	-	13/37/137/137	-
19	CRT	O	103	-	-	1/51/51/51	-
13	BCL	1	101	-	-	14/37/137/137	-
13	BCL	W	104	-	-	7/37/137/137	-
13	BCL	W	101	-	-	10/37/137/137	-
19	CRT	3	103	-	-	0/51/51/51	-
13	BCL	9	103	-	-	11/37/137/137	-
12	PGV	1	105	-	-	11/35/35/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CRT	V	101	-	-	5/51/51/51	-
19	CRT	P	101	-	-	1/51/51/51	-
13	BCL	4	102	-	-	14/37/137/137	-
13	BCL	Q	103	-	-	8/37/137/137	-
12	PGV	C	508	1	-	6/21/21/55	-
21	PEF	K	104	-	-	6/30/30/50	-
13	BCL	L	301	-	-	3/37/137/137	-
15	UQ8	L	310	-	-	9/27/51/75	0/1/1/1
19	CRT	4	101	-	-	1/51/51/51	-
13	BCL	A	103	-	-	11/37/137/137	-
13	BCL	U	103	-	-	13/37/137/137	-
10	GOL	C	506	-	-	2/4/4/4	-
13	BCL	O	101	-	-	6/37/137/137	-
15	UQ8	M	413	-	-	0/9/33/75	0/1/1/1
13	BCL	A	101	-	-	11/37/137/137	-
12	PGV	D	106	-	-	16/39/39/55	-
14	BPH	L	303	-	-	6/37/105/105	0/5/6/6
12	PGV	M	410	-	-	15/47/47/55	-
22	LMT	M	414	-	-	6/21/61/61	0/2/2/2
13	BCL	U	101	-	-	4/37/137/137	-
19	CRT	N	101	-	-	0/51/51/51	-
13	BCL	Y	101	-	-	8/37/137/137	-
20	CDL	1	104	-	-	8/13/13/110	-
20	CDL	M	412	3	-	7/48/48/110	-
13	BCL	9	101	-	-	16/37/137/137	-
19	CRT	W	102	-	-	3/51/51/51	-
13	BCL	Y	103	-	-	14/37/137/137	-
13	BCL	Q	101	-	-	15/37/137/137	-
19	CRT	Z	101	-	-	0/51/51/51	-
20	CDL	S	104	-	-	40/85/85/110	-
19	CRT	B	101	-	-	5/51/51/51	-
13	BCL	F	103	-	-	10/37/137/137	-
13	BCL	S	103	-	-	18/37/137/137	-
13	BCL	5	101	-	-	9/37/137/137	-

The worst 5 of 316 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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

The worst 5 of 945 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
19	N	101	CRT	C21-C22-C23	-6.08	118.63	127.31

There are no chirality outliers.

5 of 930 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	503	HEM	C2B-C3B-CAB-CBB
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

There are no ring outliers.

84 monomers are involved in 368 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	D	104	CDL	1	0
13	F	101	BCL	4	0
19	J	101	CRT	3	0
20	D	105	CDL	9	0
20	M	406	CDL	5	0
13	K	101	BCL	6	0
13	D	103	BCL	5	0
19	A	104	CRT	8	0
13	2	102	BCL	12	0
20	U	104	CDL	9	0
12	L	307	PGV	5	0
13	L	305	BCL	7	0
13	J	102	BCL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	9	104	PGV	5	0
19	G	101	CRT	4	0
18	M	404	MQ8	5	0
8	C	503	HEM	2	0
8	C	502	HEM	2	0
13	3	101	BCL	4	0
13	K	103	BCL	4	0
12	M	411	PGV	4	0
13	5	103	BCL	5	0
13	M	401	BCL	2	0
19	M	405	CRT	6	0
19	T	101	CRT	4	0
13	S	101	BCL	6	0
12	L	308	PGV	5	0
12	H	303	PGV	2	0
15	L	309	UQ8	10	0
13	D	101	BCL	1	0
13	7	103	BCL	6	0
13	L	302	BCL	3	0
12	3	105	PGV	6	0
13	7	101	BCL	7	0
19	2	101	CRT	7	0
21	1	103	PEF	2	0
15	L	311	UQ8	2	0
19	0	101	CRT	5	0
14	M	402	BPH	8	0
20	O	104	CDL	13	0
20	H	305	CDL	6	0
8	C	504	HEM	2	0
20	Y	104	CDL	3	0
13	I	101	BCL	3	0
19	8	101	CRT	5	0
22	H	304	LMT	8	0
15	L	304	UQ8	1	0
13	P	102	BCL	6	0
13	1	101	BCL	7	0
13	W	104	BCL	6	0
13	W	101	BCL	5	0
19	3	103	CRT	2	0
13	9	103	BCL	5	0
12	1	105	PGV	1	0
19	V	101	CRT	3	0

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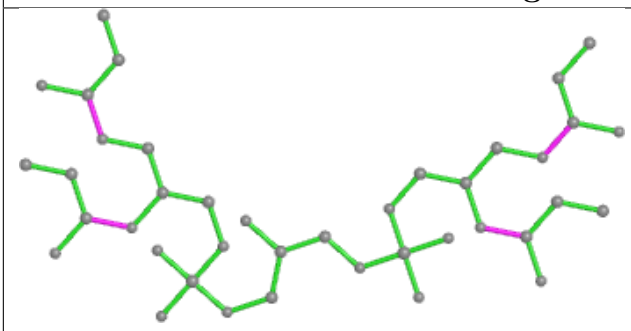
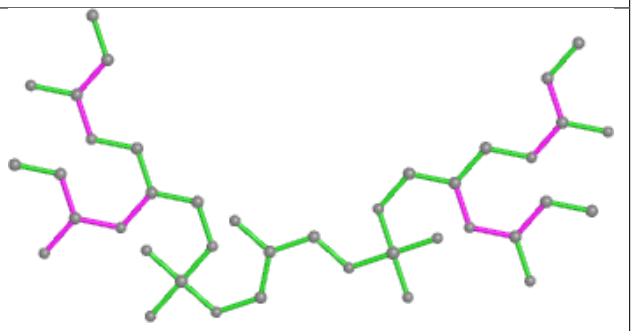
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	P	101	CRT	5	0
13	4	102	BCL	7	0
13	Q	103	BCL	4	0
21	K	104	PEF	2	0
13	L	301	BCL	5	0
15	L	310	UQ8	5	0
19	4	101	CRT	7	0
13	A	103	BCL	5	0
13	U	103	BCL	7	0
10	C	506	GOL	1	0
13	O	101	BCL	7	0
13	A	101	BCL	5	0
12	D	106	PGV	2	0
14	L	303	BPH	4	0
12	M	410	PGV	4	0
13	U	101	BCL	8	0
19	N	101	CRT	5	0
13	Y	101	BCL	5	0
20	M	412	CDL	2	0
13	9	101	BCL	4	0
19	W	102	CRT	1	0
13	Y	103	BCL	10	0
13	Q	101	BCL	8	0
19	Z	101	CRT	6	0
20	S	104	CDL	12	0
19	B	101	CRT	7	0
13	F	103	BCL	7	0
13	S	103	BCL	6	0
13	5	101	BCL	4	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 then 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.

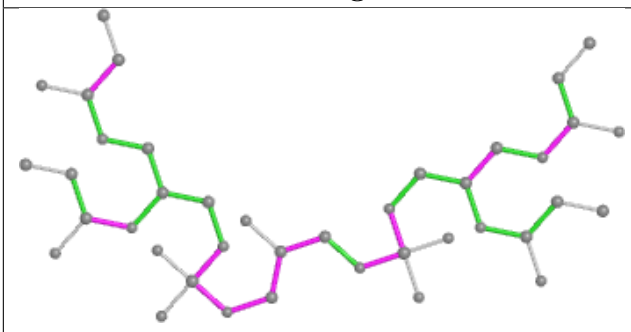
Ligand CDL D 104



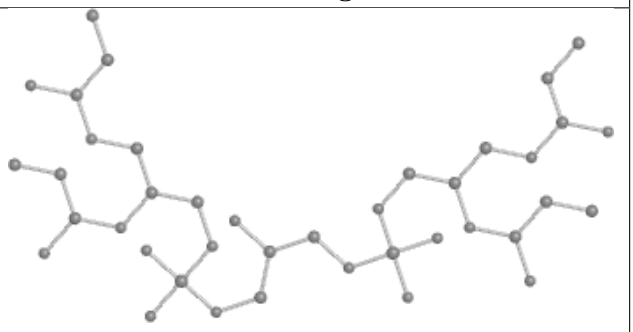
Bond lengths



Bond angles

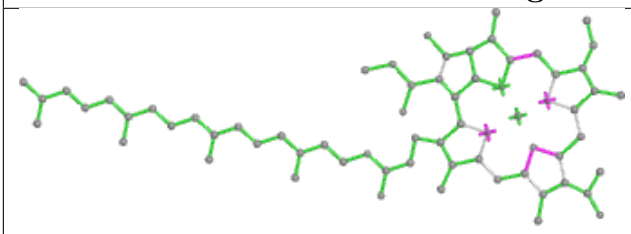


Torsions

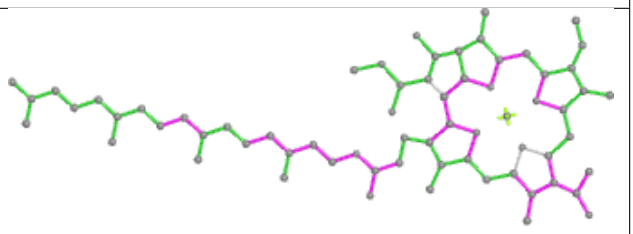


Rings

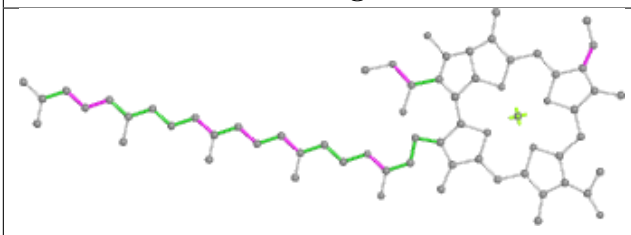
Ligand BCL F 101



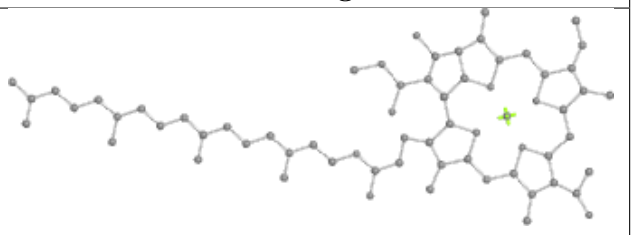
Bond lengths



Bond angles

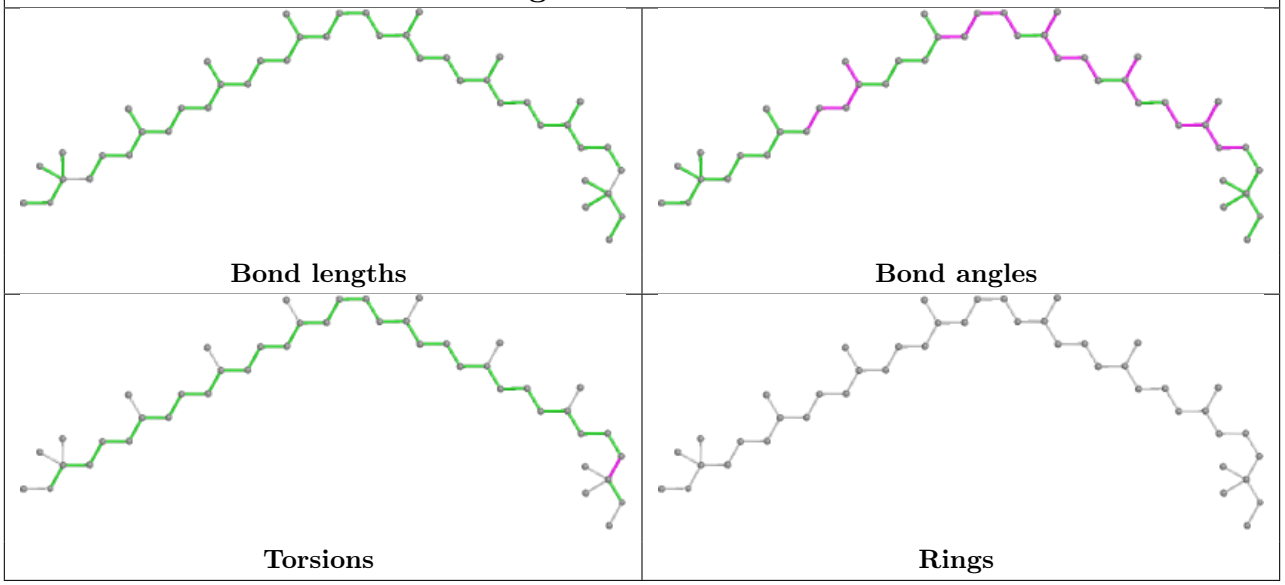


Torsions

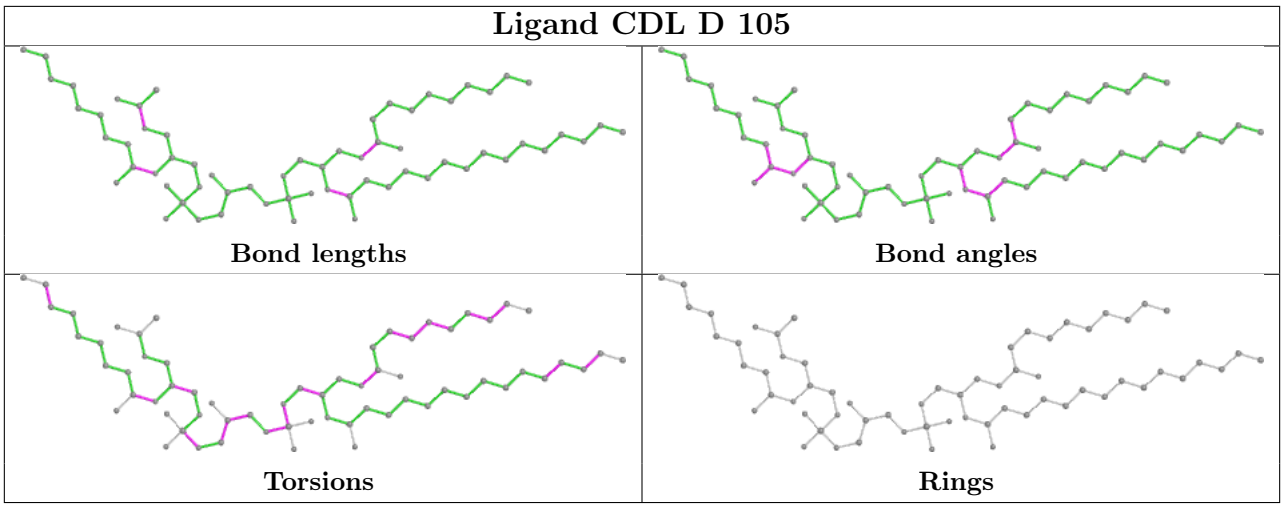


Rings

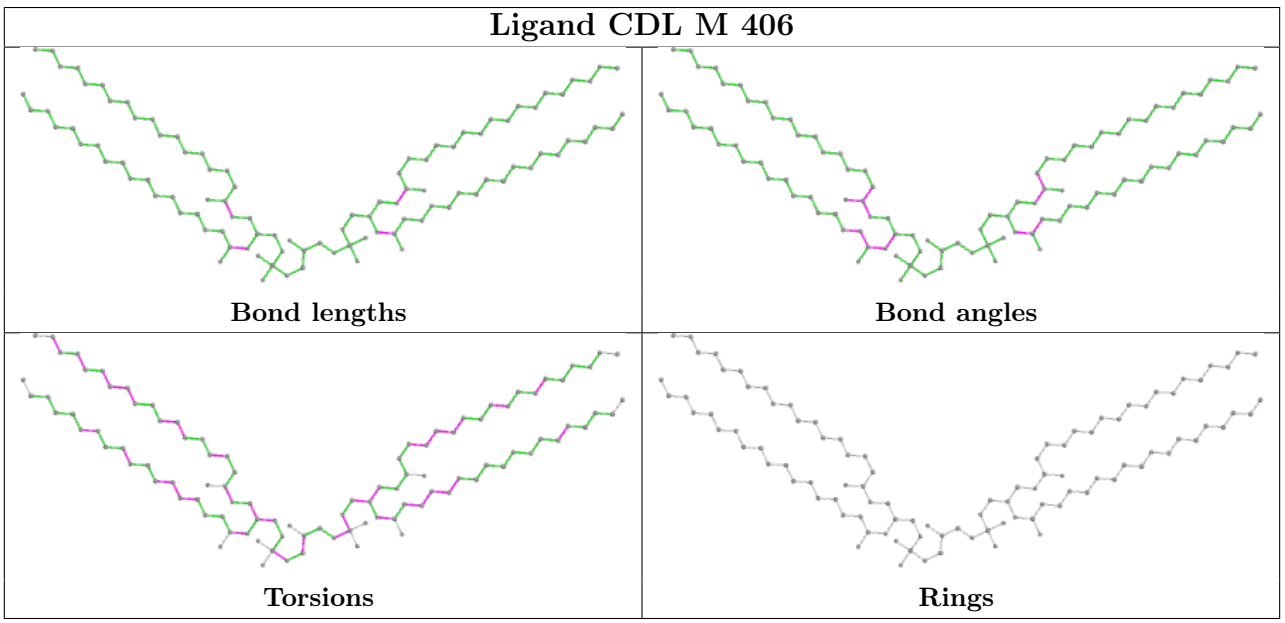
Ligand CRT J 101



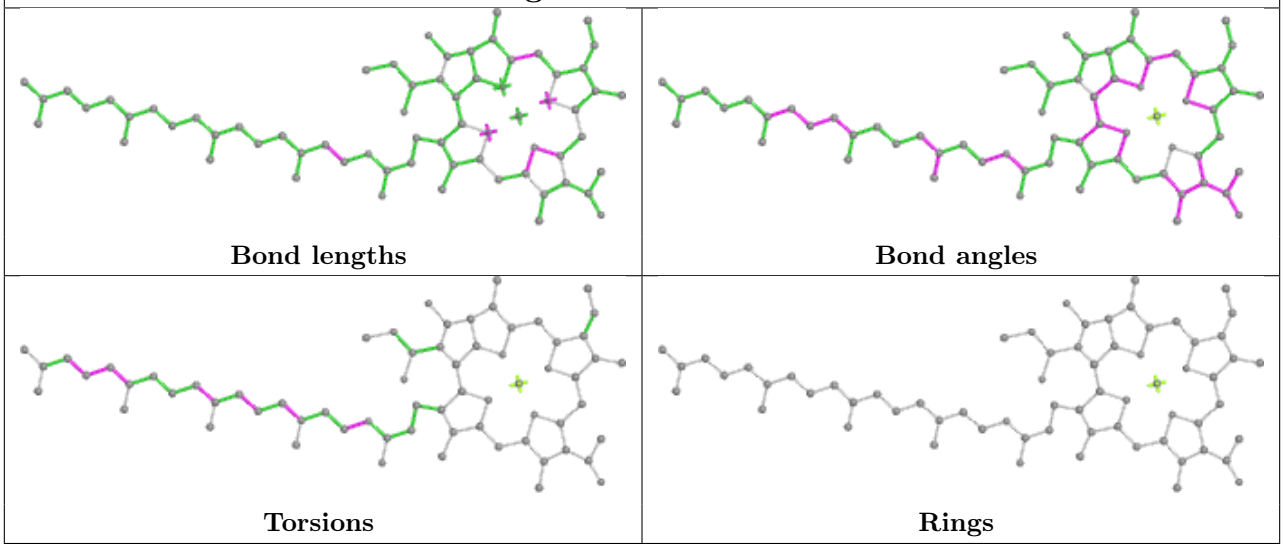
Ligand CDL D 105



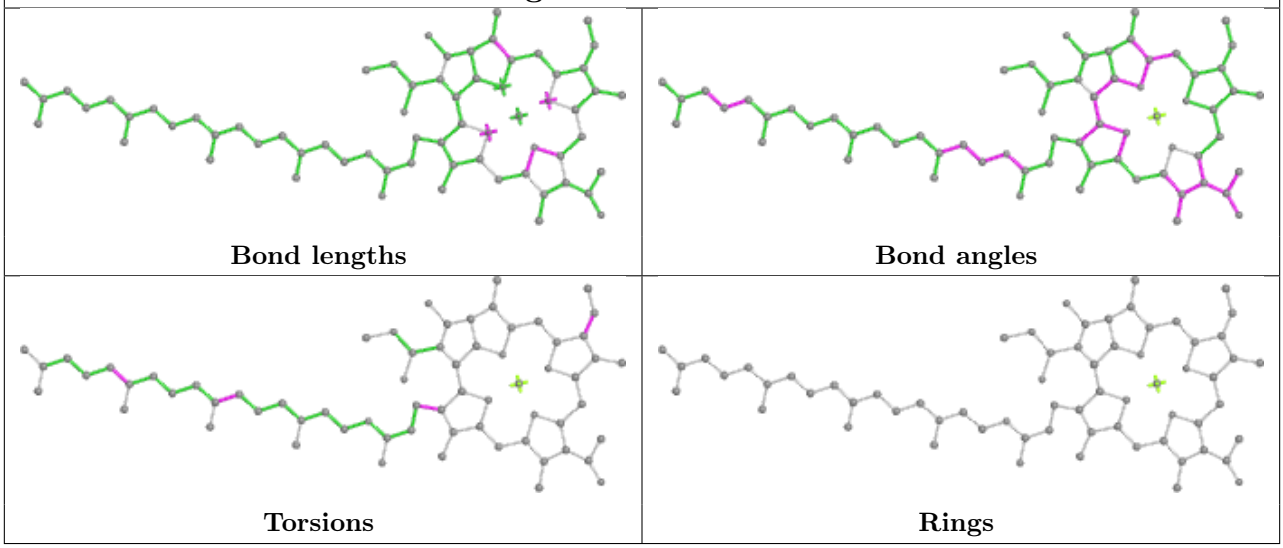
Ligand CDL M 406



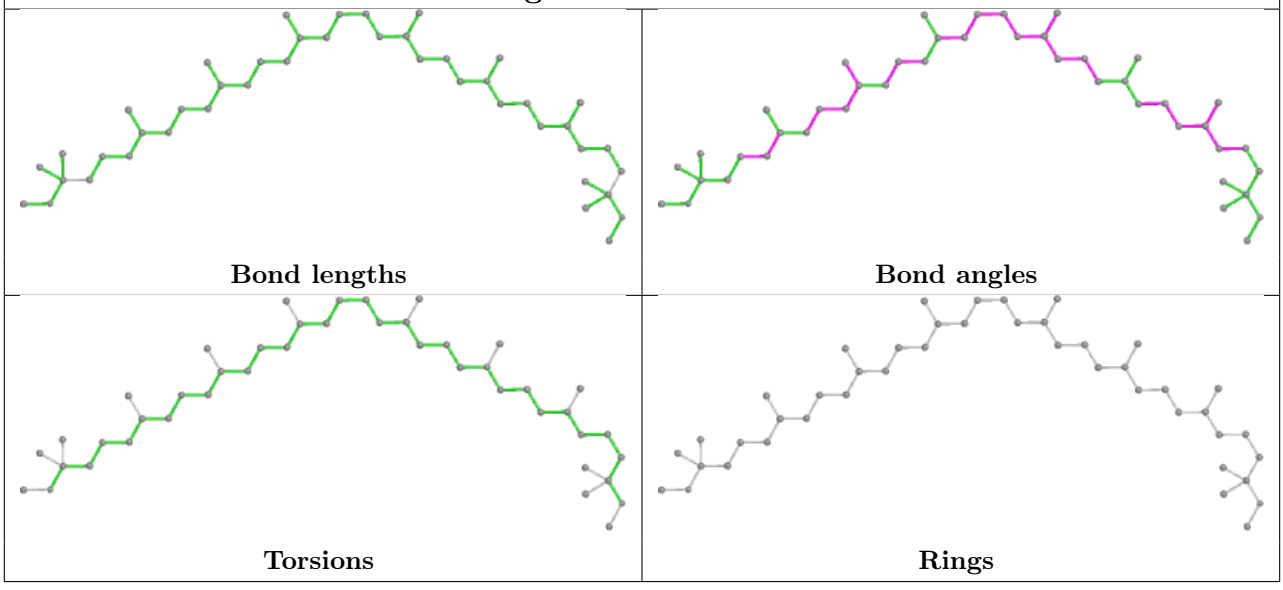
Ligand BCL K 101



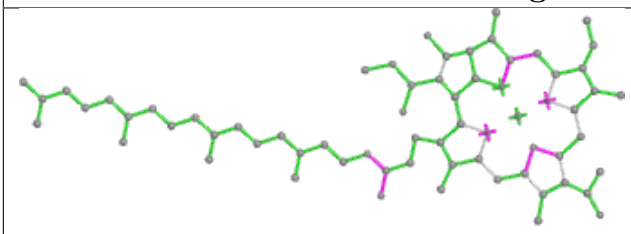
Ligand BCL D 103



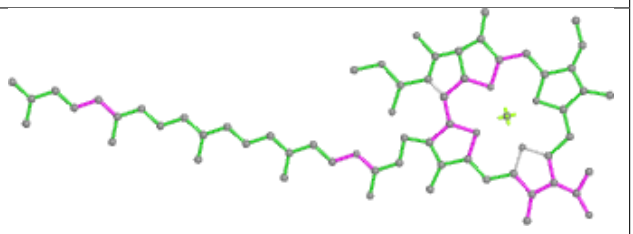
Ligand CRT A 104



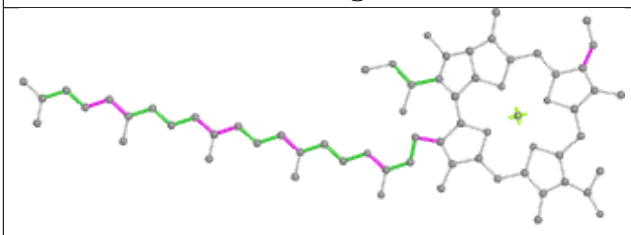
Ligand BCL 2 102



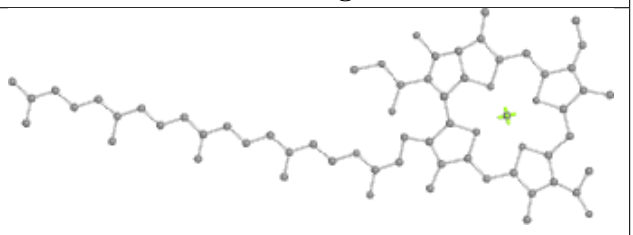
Bond lengths



Bond angles

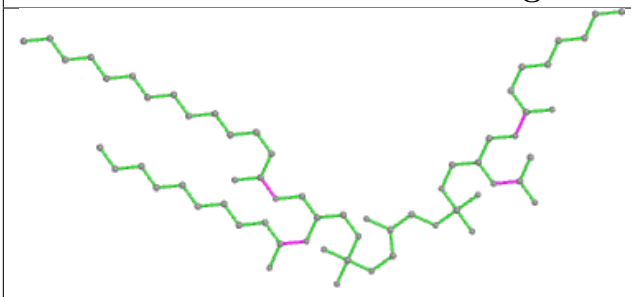


Torsions



Rings

Ligand CDL U 104



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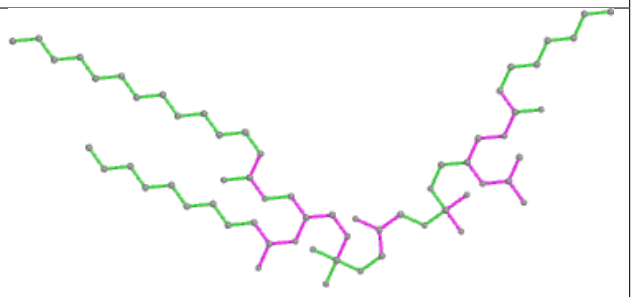
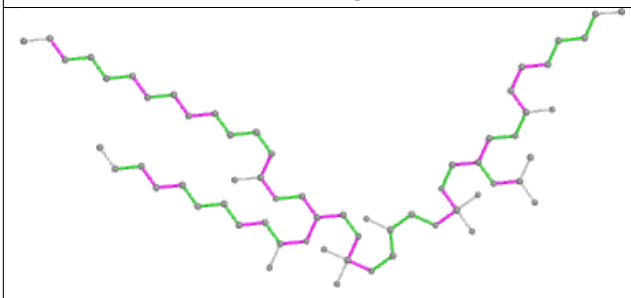
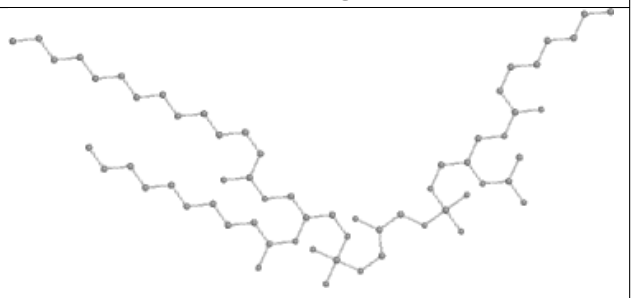


Bond angles

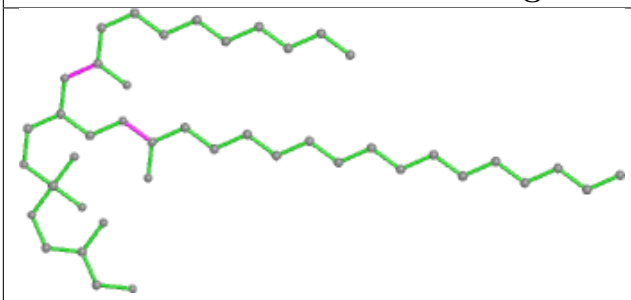


Torsions

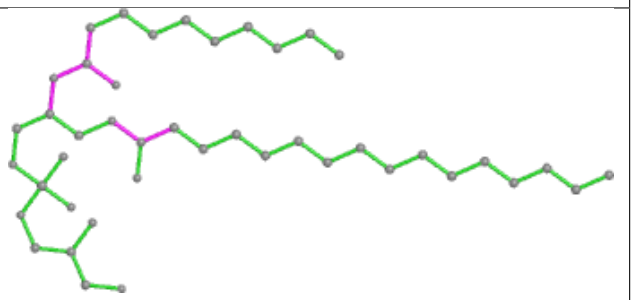


Rings

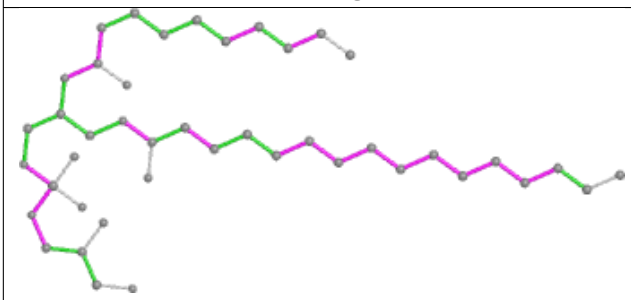
Ligand PGV L 307



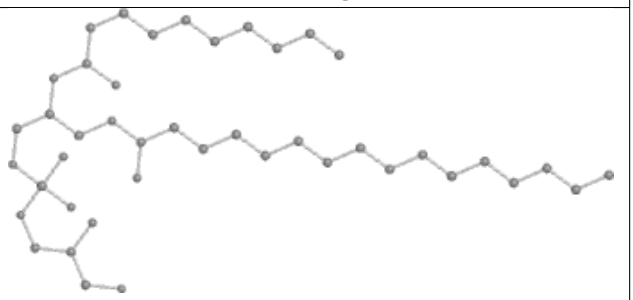
Bond lengths



Bond angles

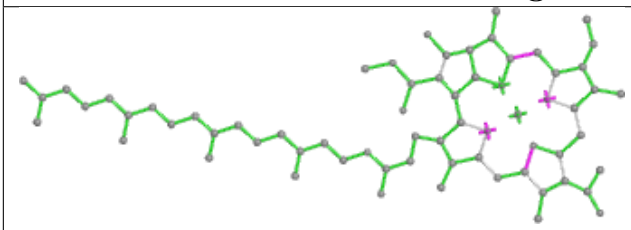


Torsions

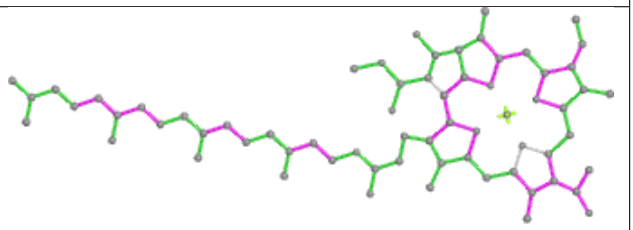


Rings

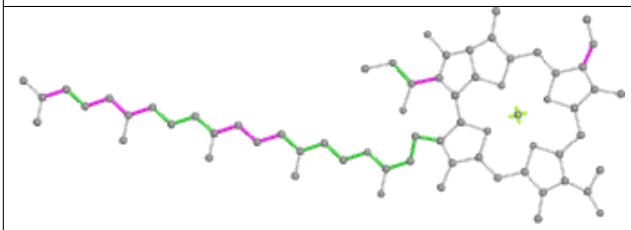
Ligand BCL L 305



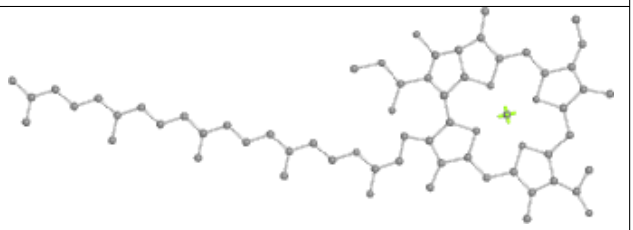
Bond lengths



Bond angles

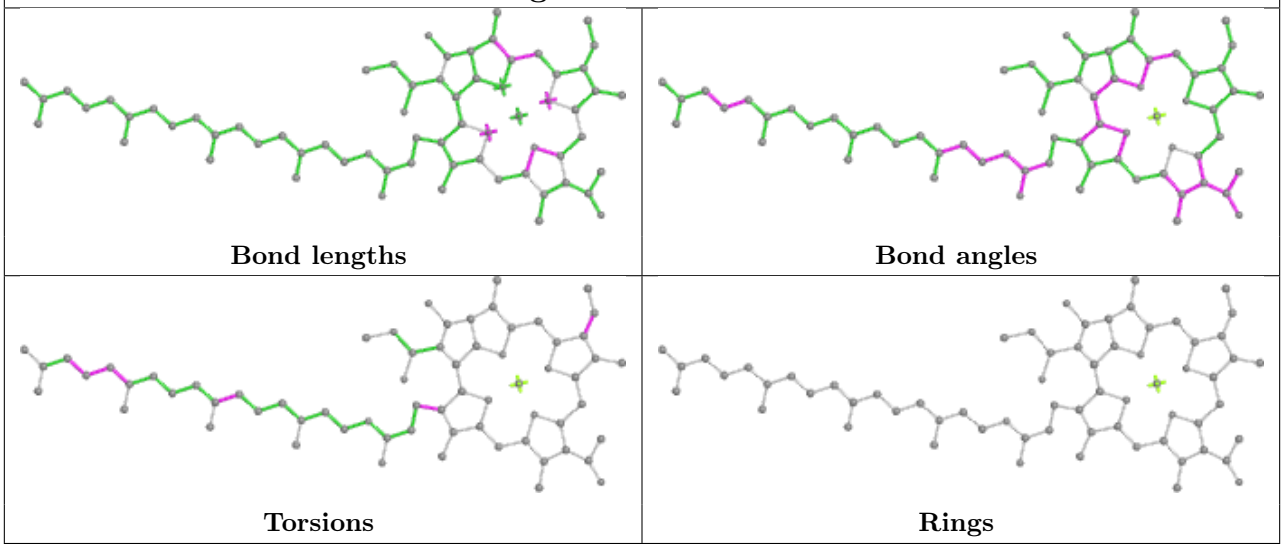


Torsions

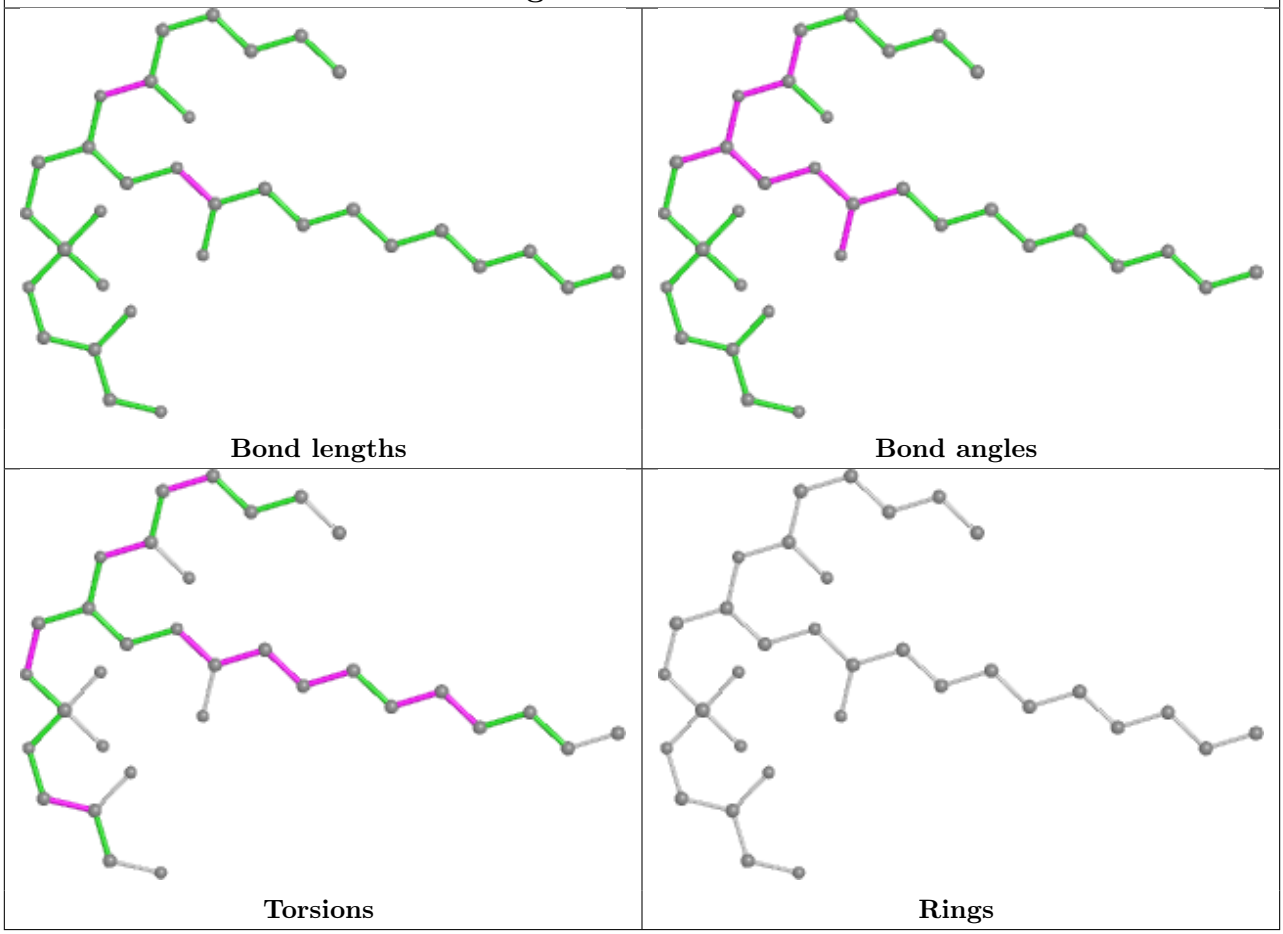


Rings

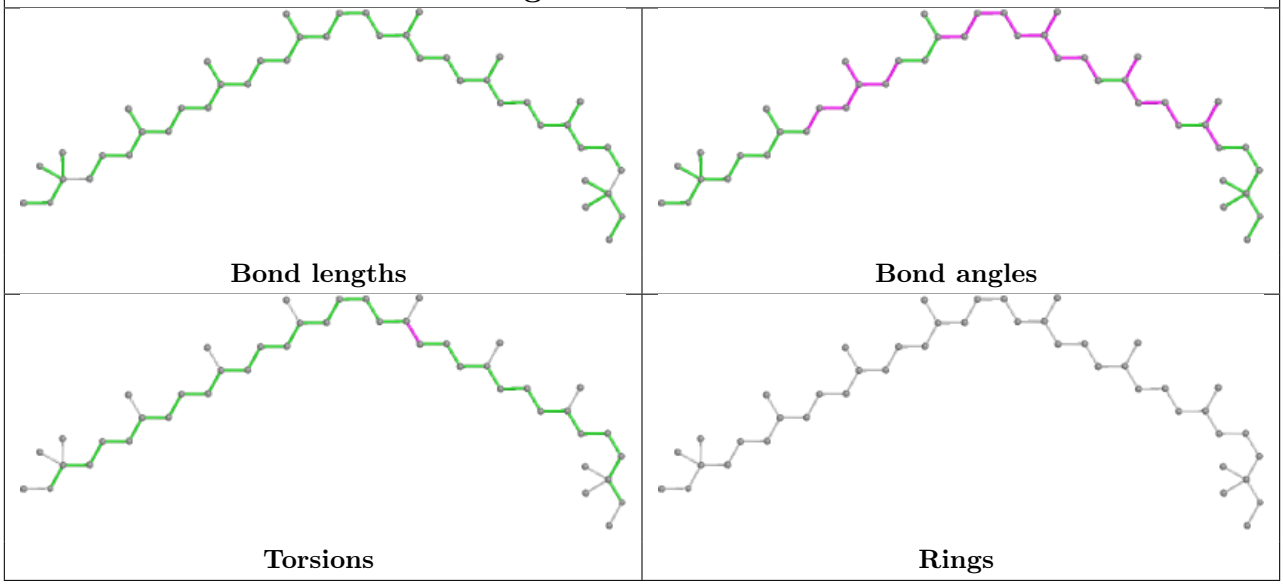
Ligand BCL J 102



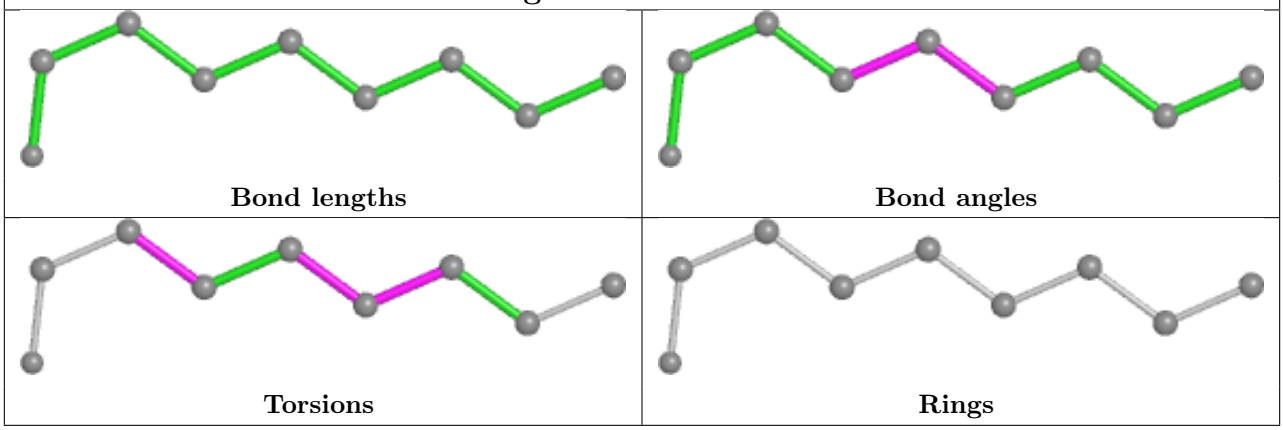
Ligand PGV 9 104



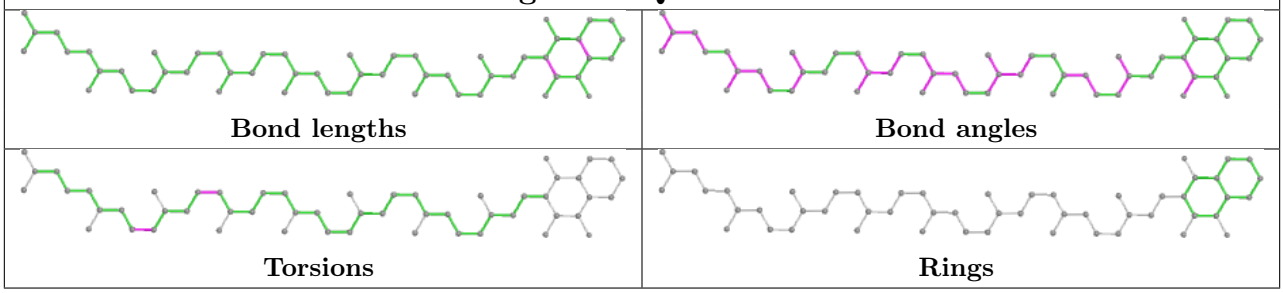
Ligand CRT G 101



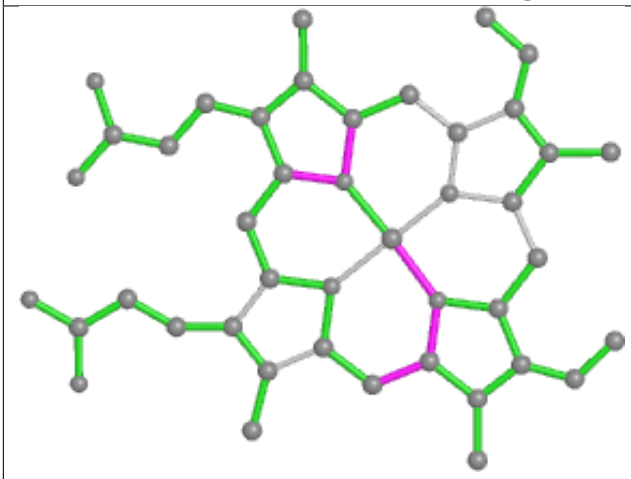
Ligand LHG C 507



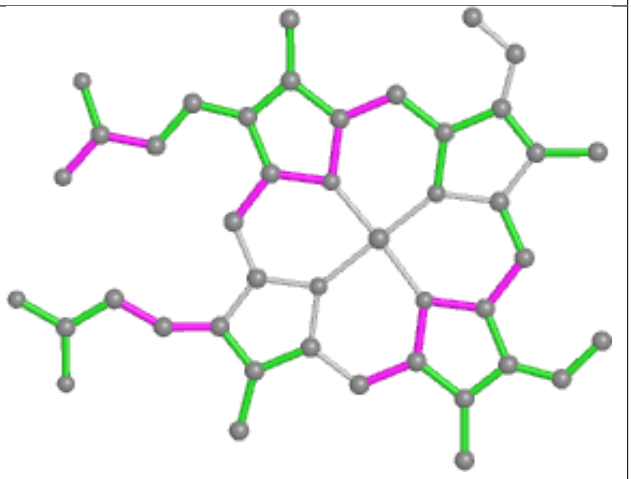
Ligand MQ8 M 404



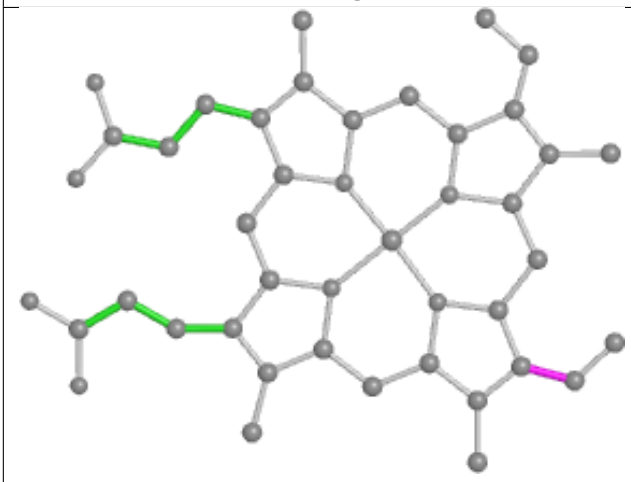
Ligand HEM C 503



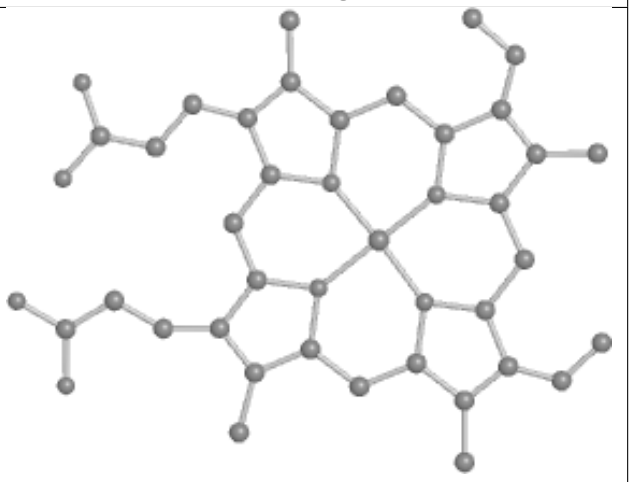
Bond lengths



Bond angles

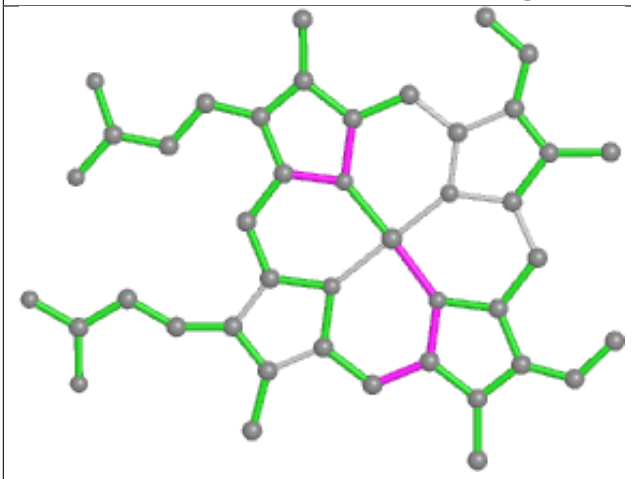


Torsions

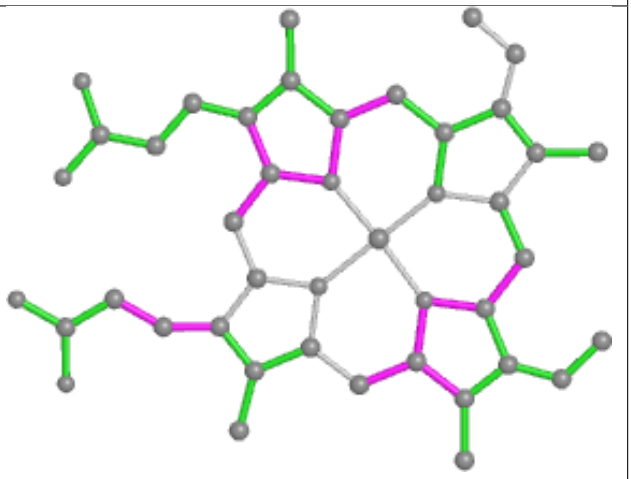


Rings

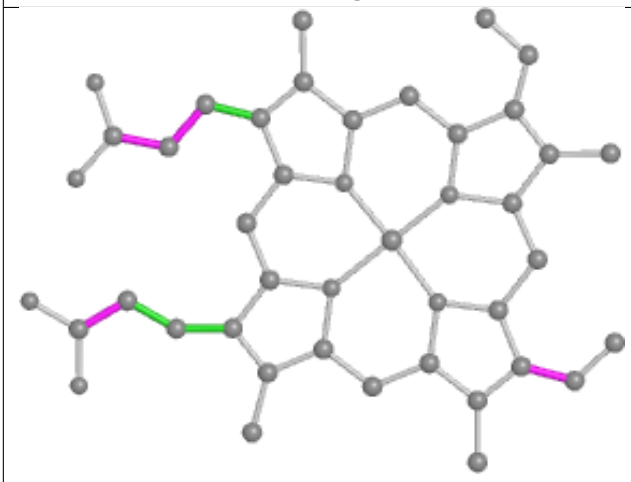
Ligand HEM C 502



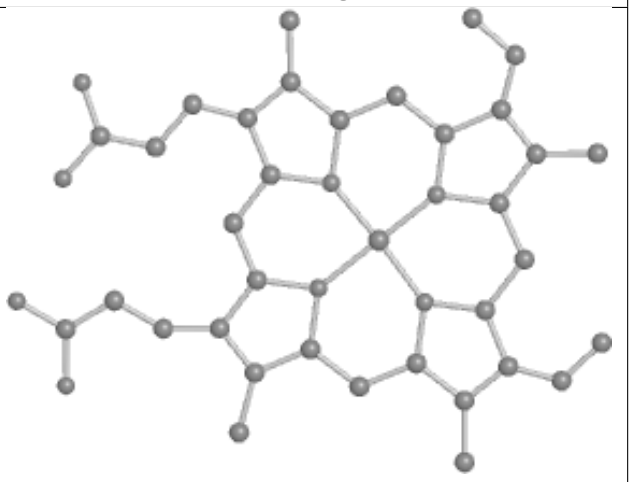
Bond lengths



Bond angles

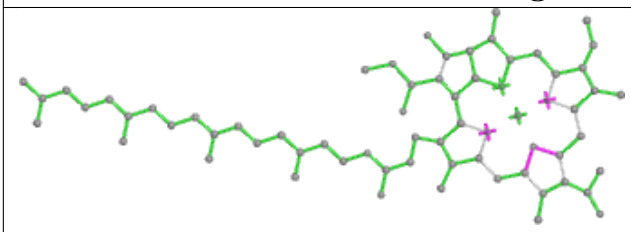


Torsions

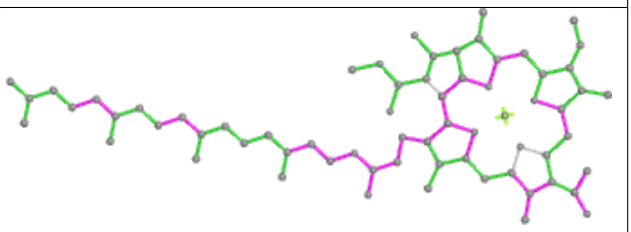


Rings

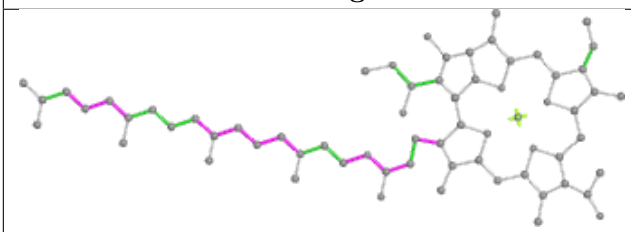
Ligand BCL 3 101



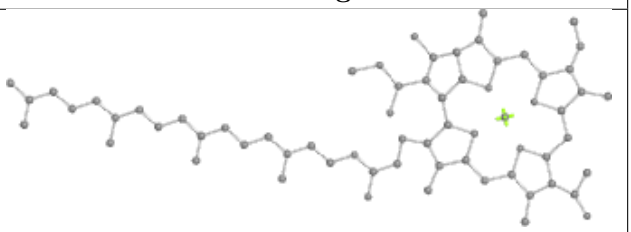
Bond lengths



Bond angles

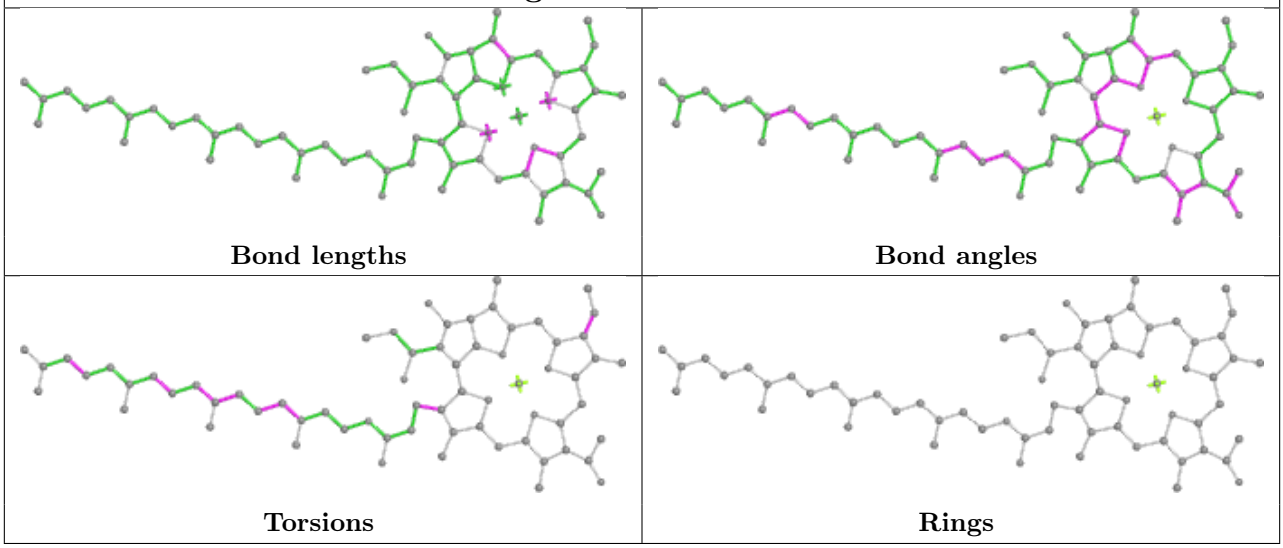


Torsions

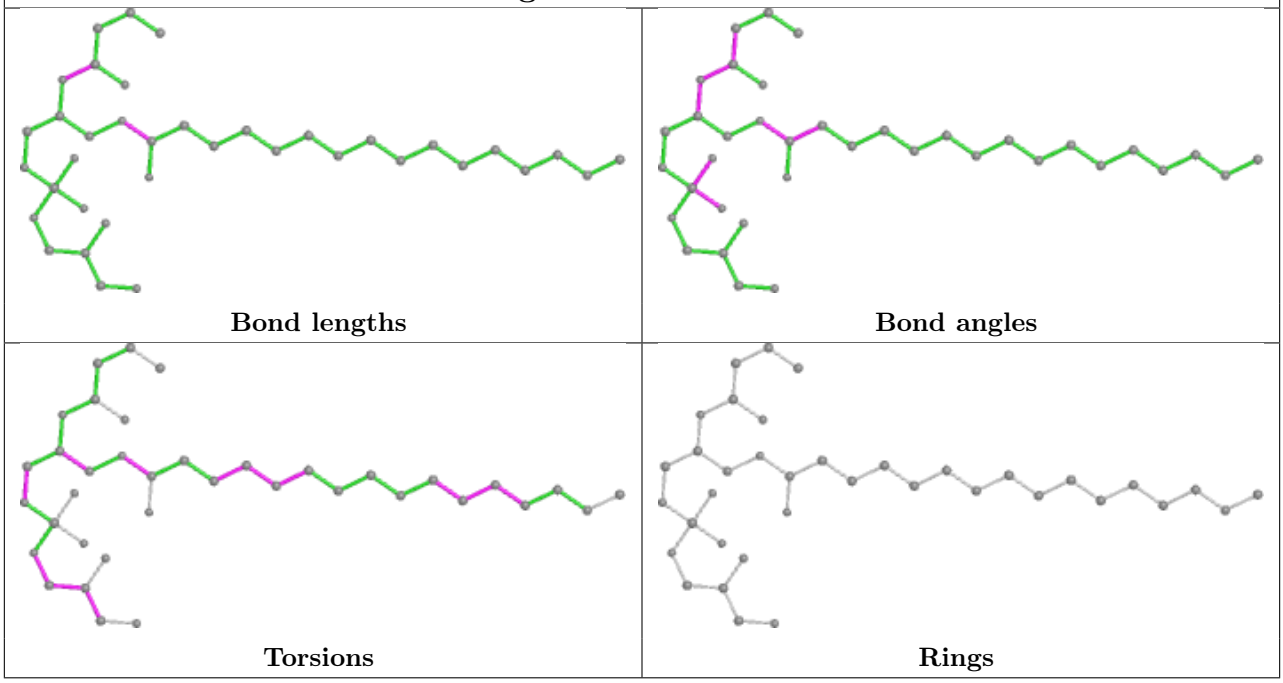


Rings

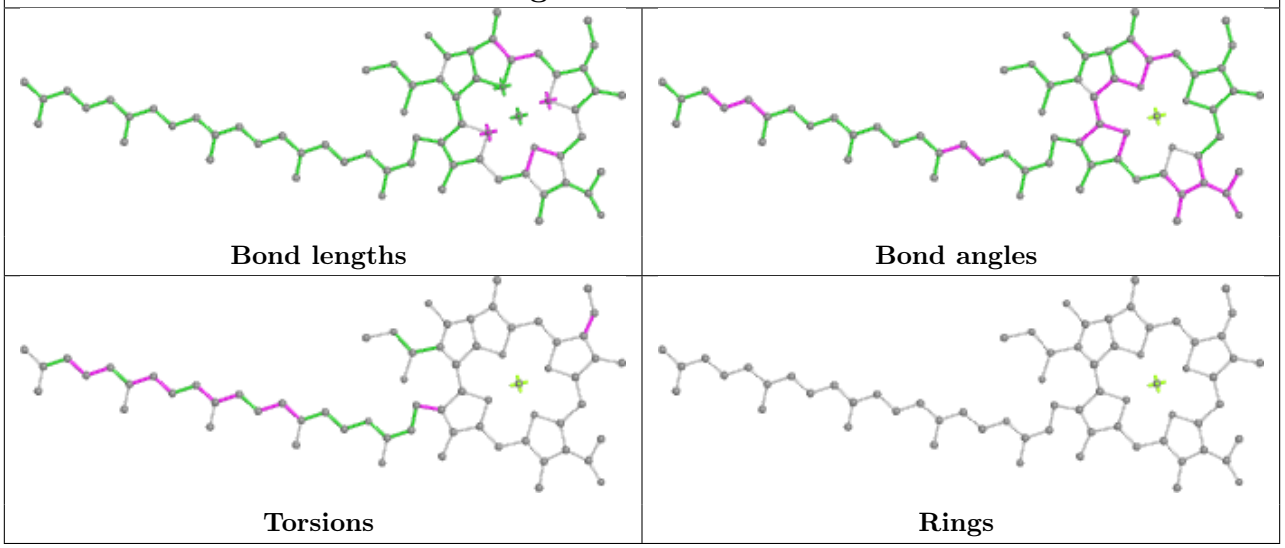
Ligand BCL K 103



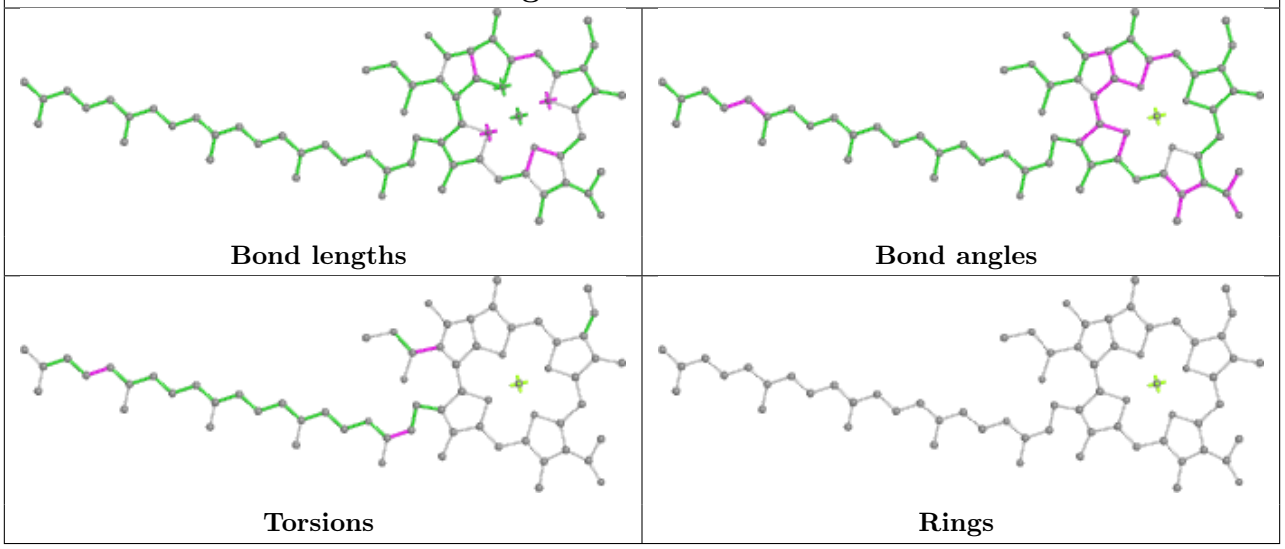
Ligand PGV M 411



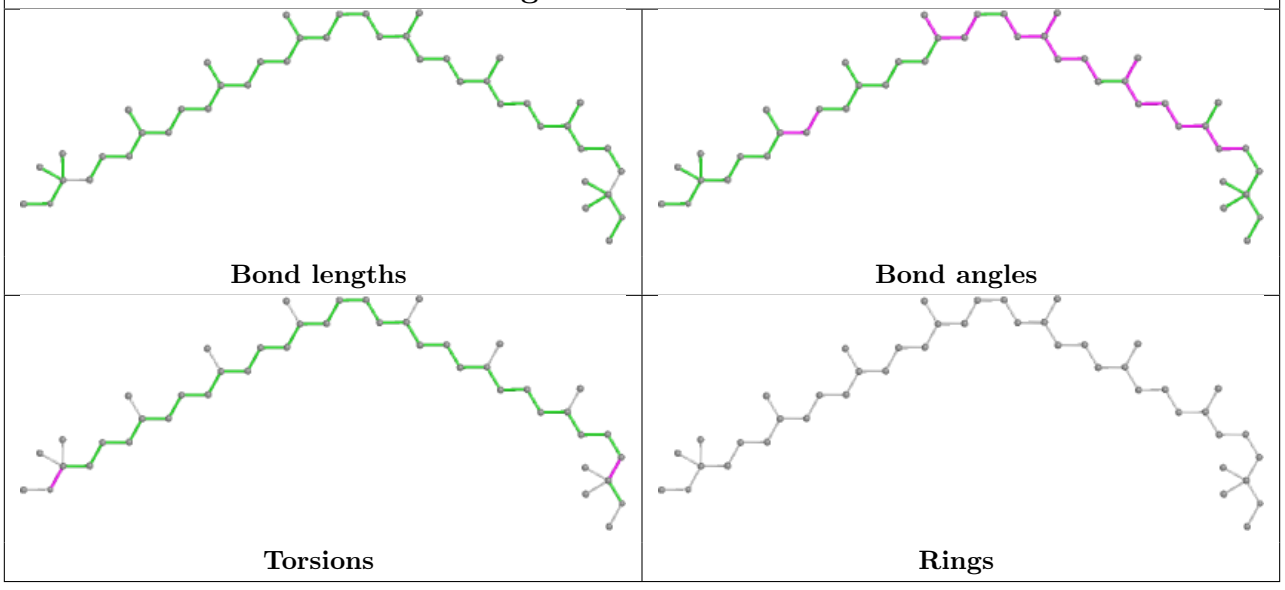
Ligand BCL 5 103



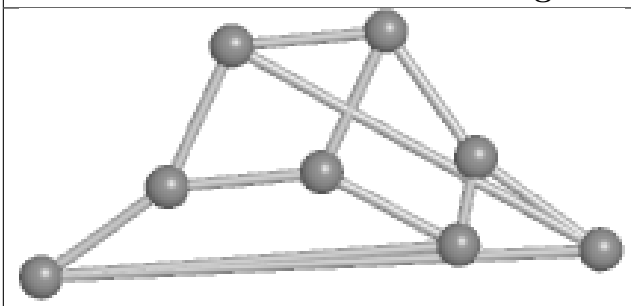
Ligand BCL M 401



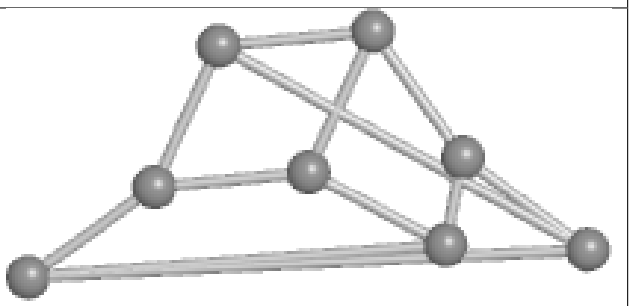
Ligand CRT M 405



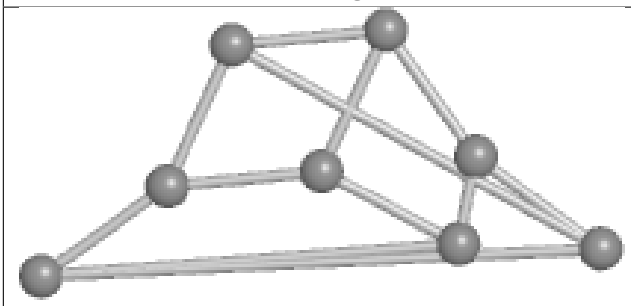
Ligand SF4 b 101



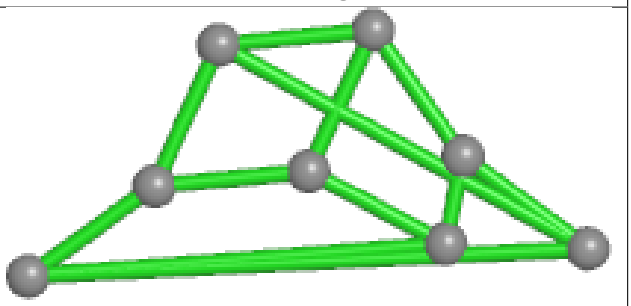
Bond lengths



Bond angles

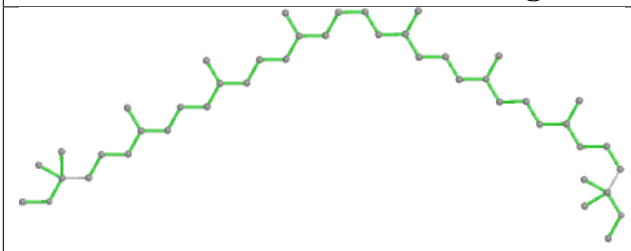


Torsions



Rings

Ligand CRT T 101



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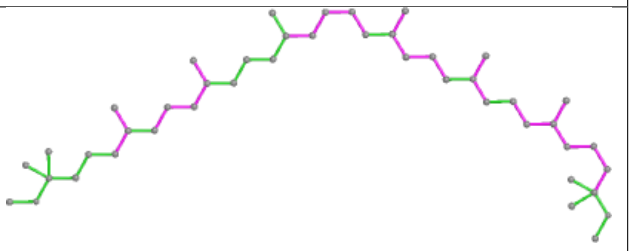
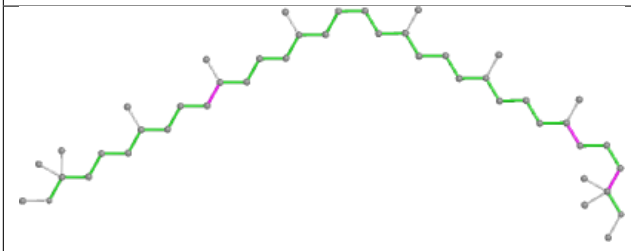
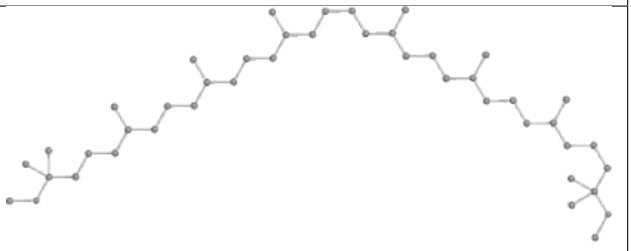


Bond angles

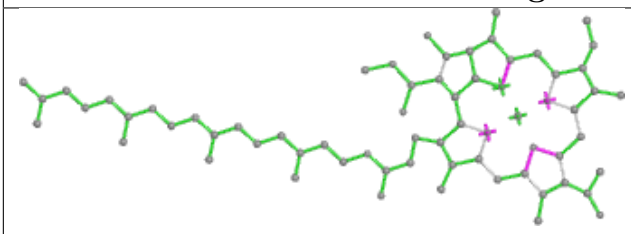


Torsions



Rings

Ligand BCL S 101



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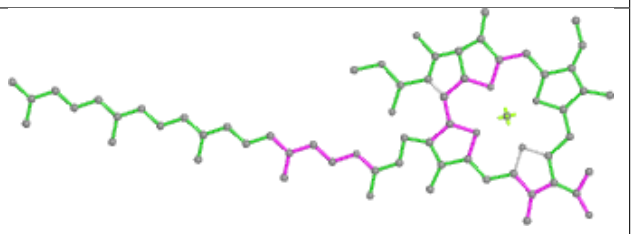
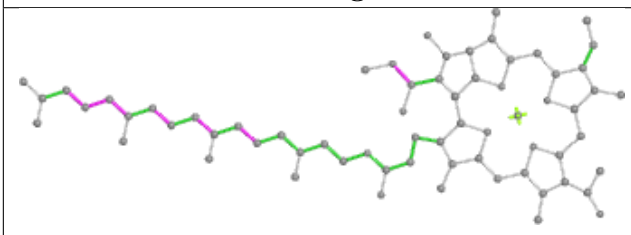
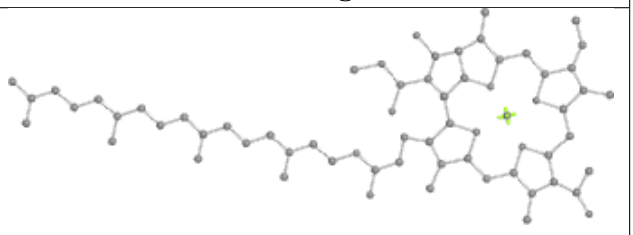


Bond angles

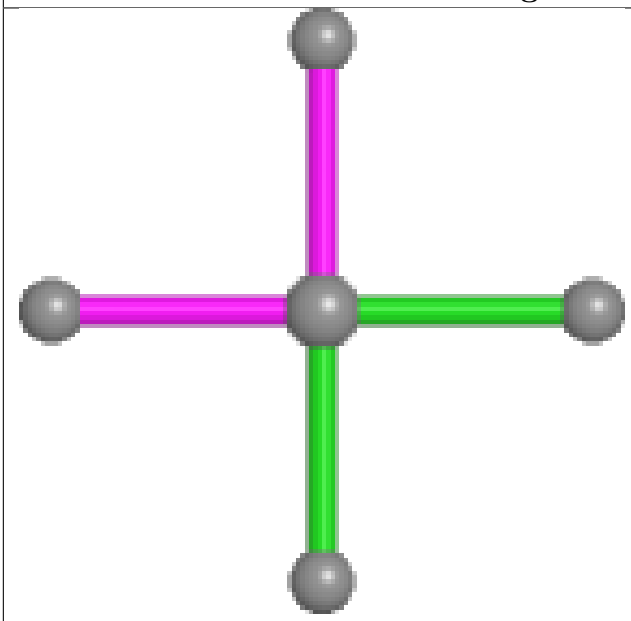


Torsions

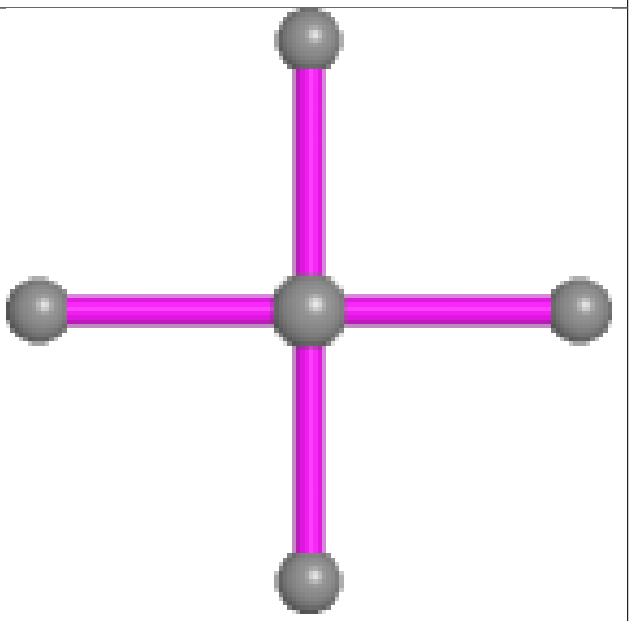


Rings

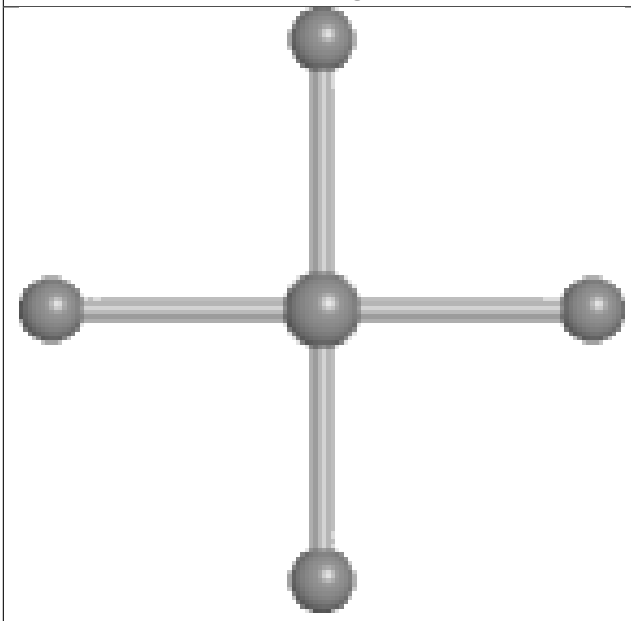
Ligand PEF W 106



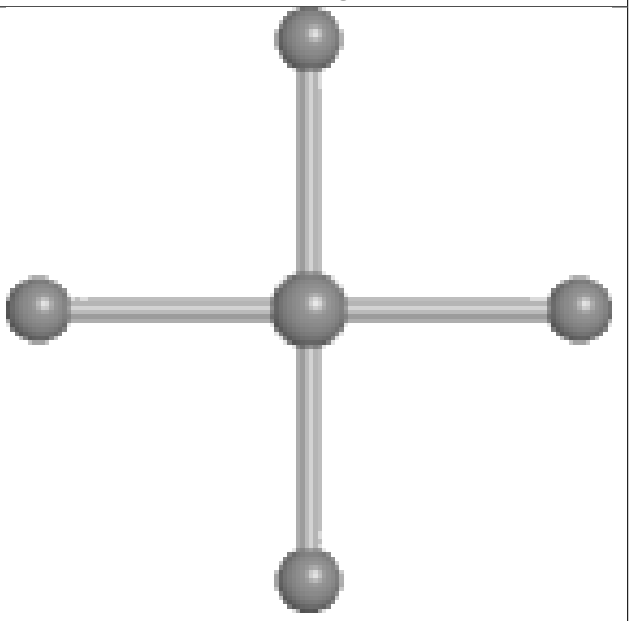
Bond lengths



Bond angles

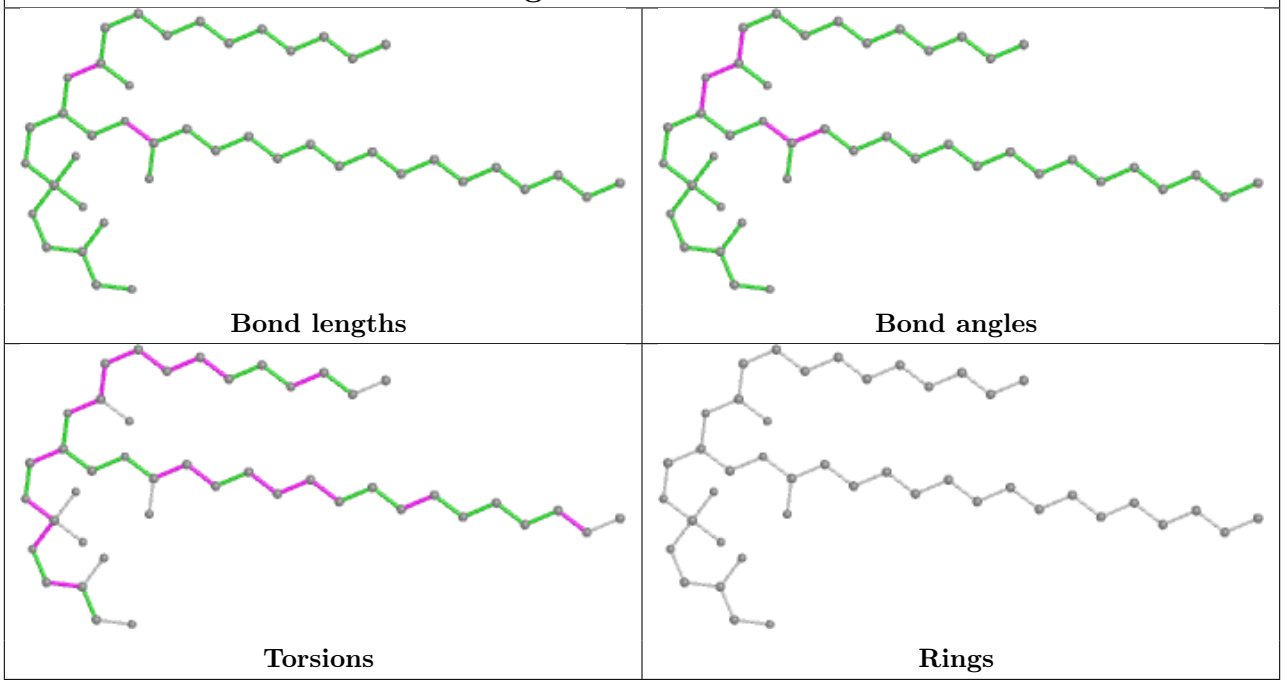


Torsions

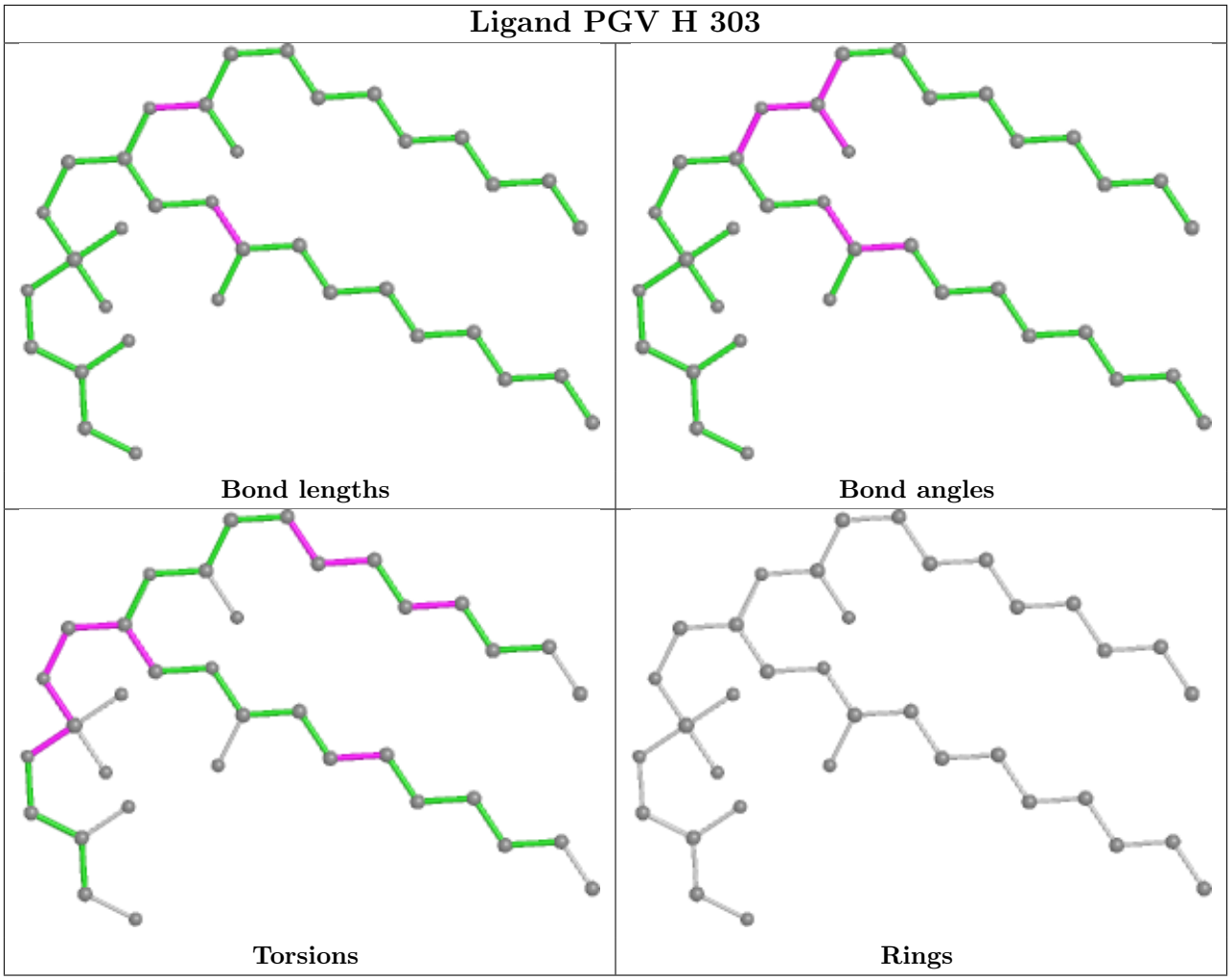


Rings

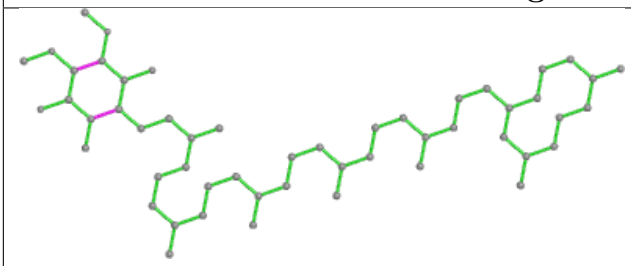
Ligand PGV L 308



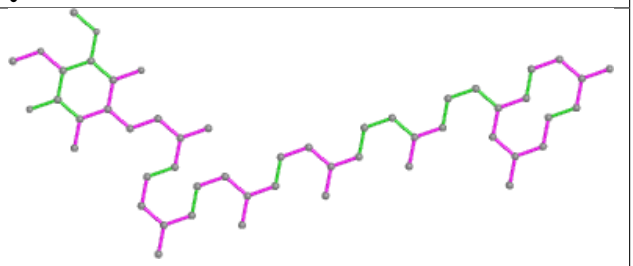
Ligand PGV H 303



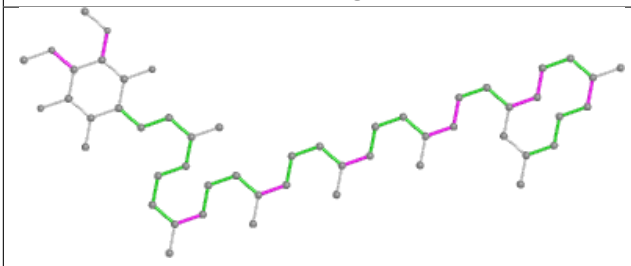
Ligand UQ8 L 309



Bond lengths



Bond angles



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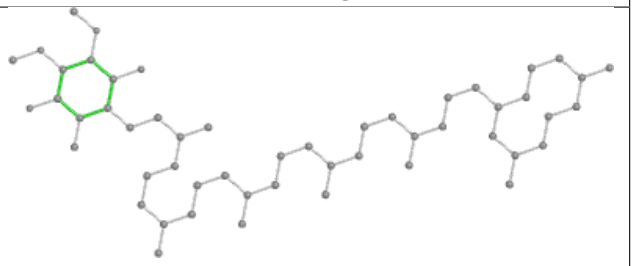
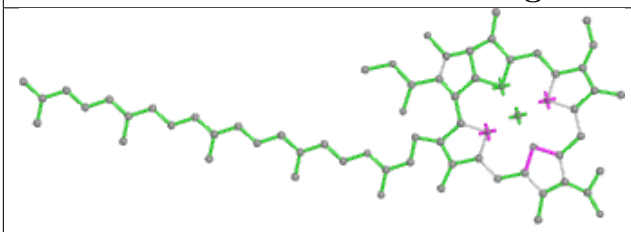


Rings

Ligand BCL D 101



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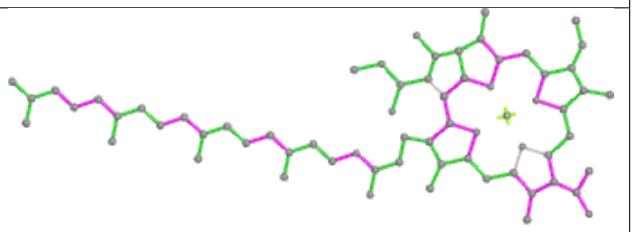
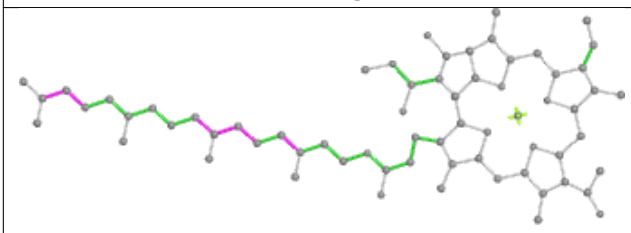
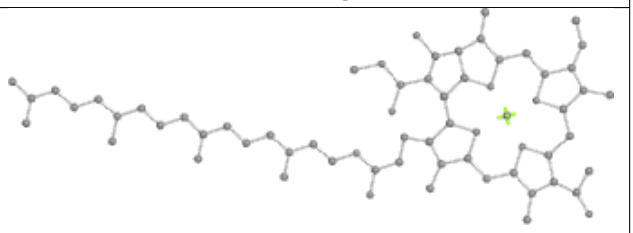


Bond angles

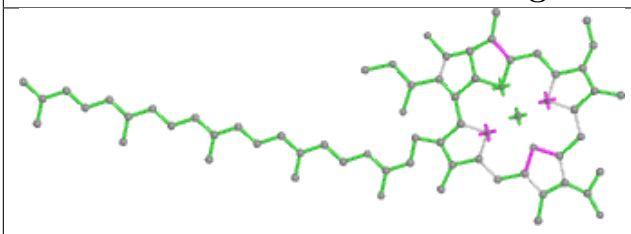


Torsions

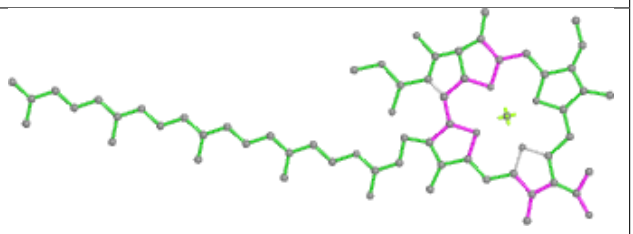


Rings

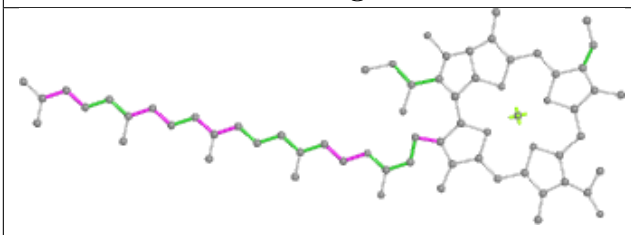
Ligand BCL 7 103



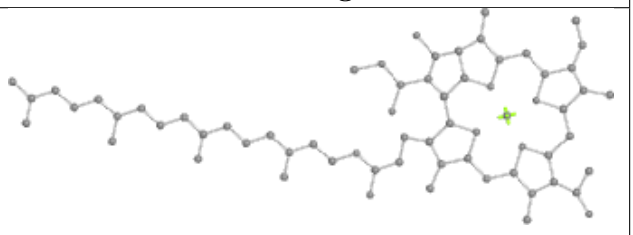
Bond lengths



Bond angles

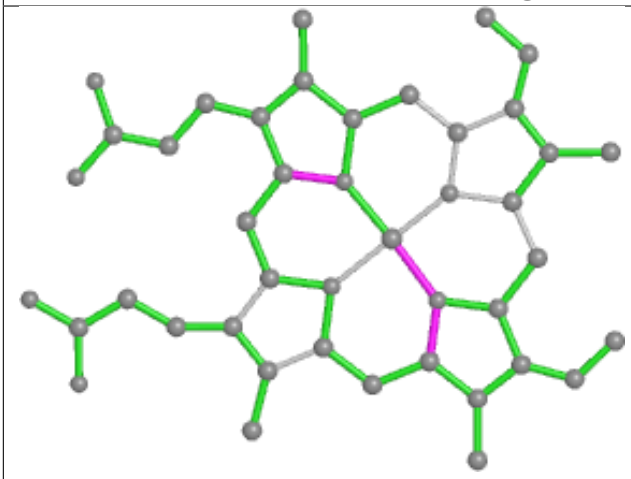


Torsions

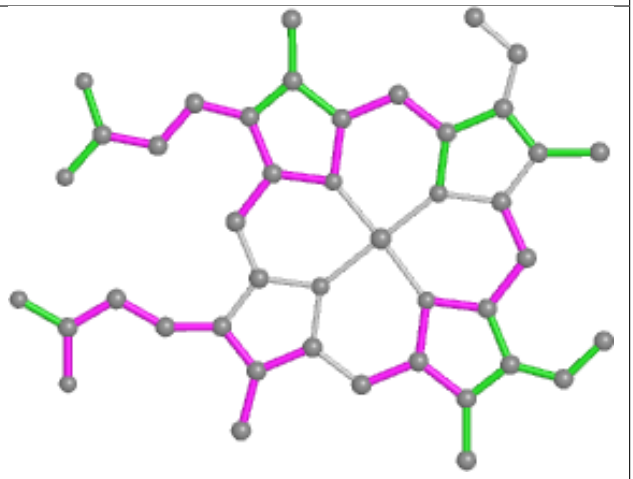


Rings

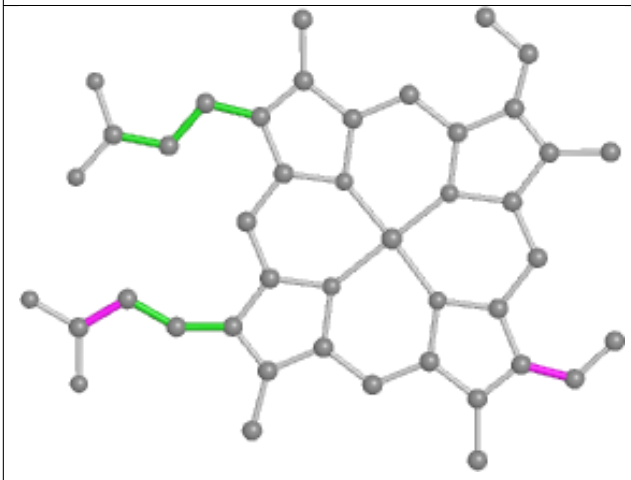
Ligand HEM C 501



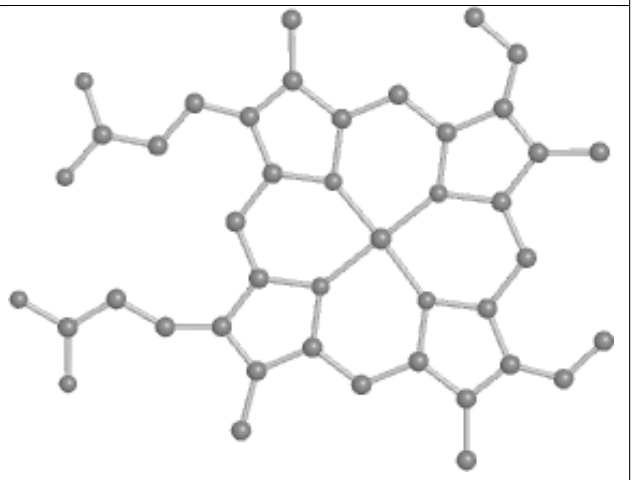
Bond lengths



Bond angles

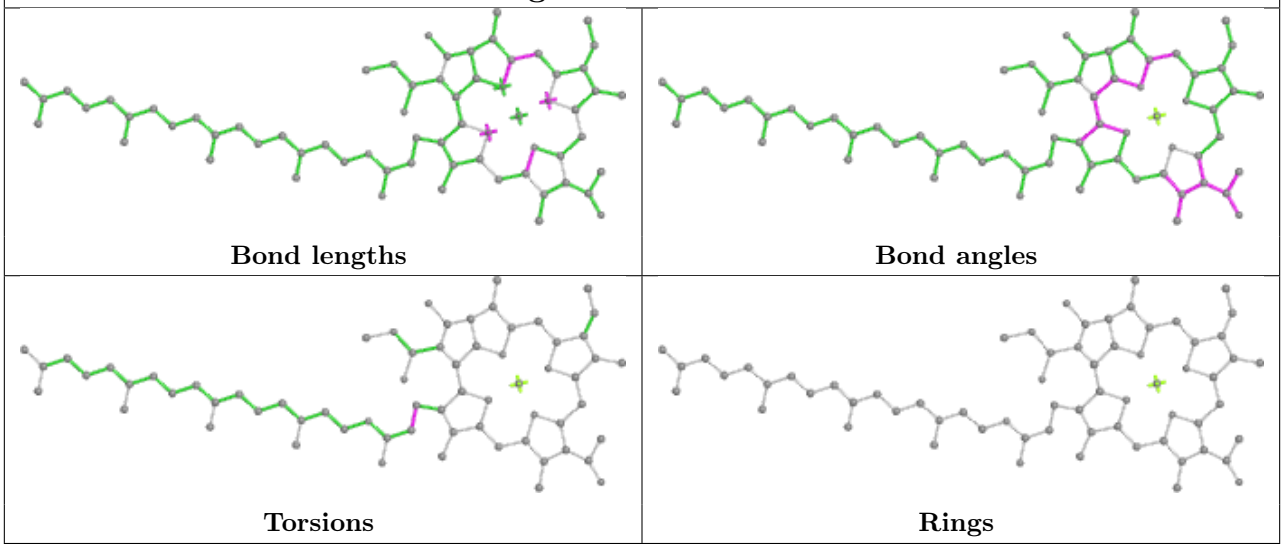


Torsions

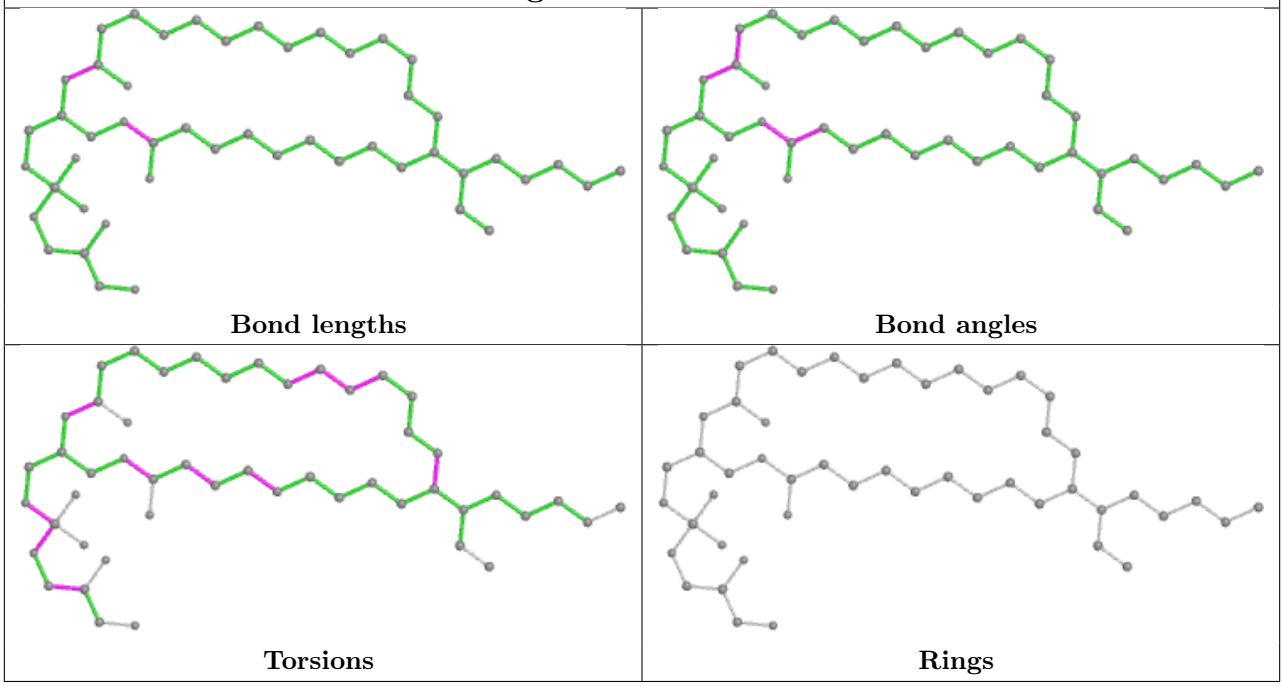


Rings

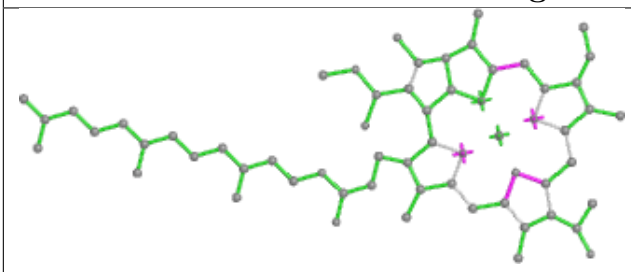
Ligand BCL L 302



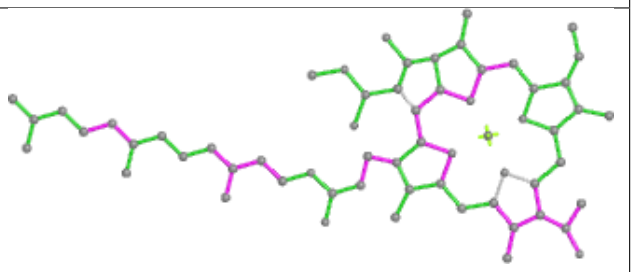
Ligand PGV 3 105



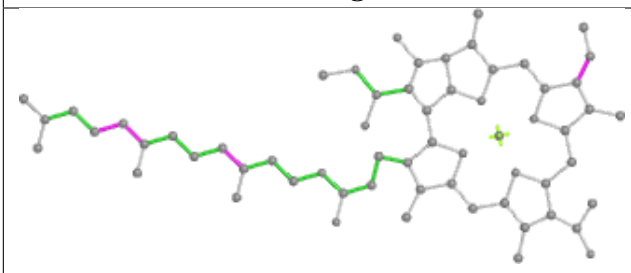
Ligand BCL 7 101



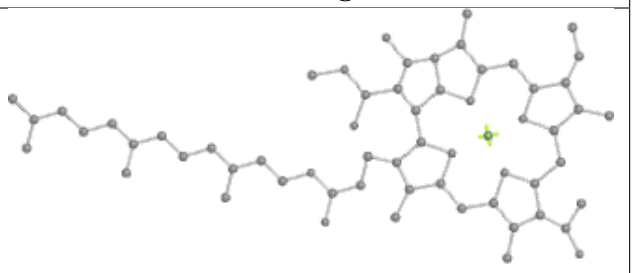
Bond lengths



Bond angles

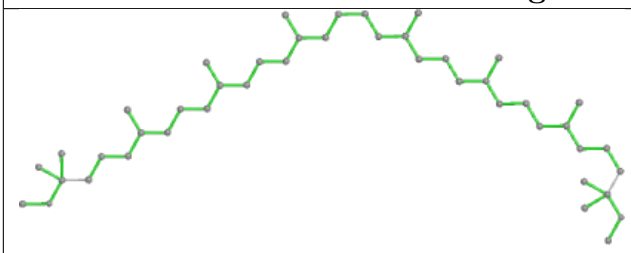


Torsions



Rings

Ligand CRT 2 101



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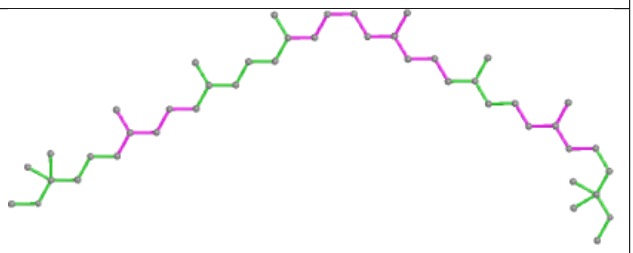
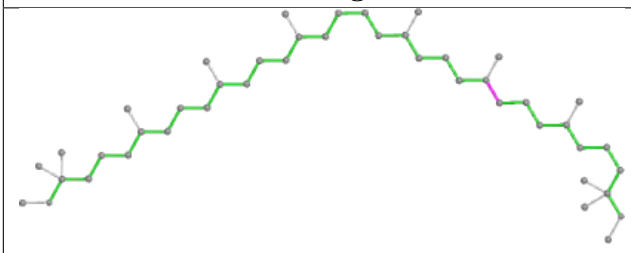


Bond angles



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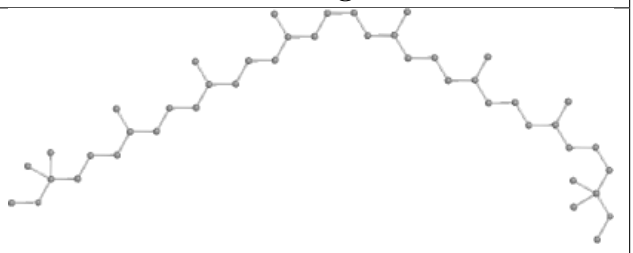
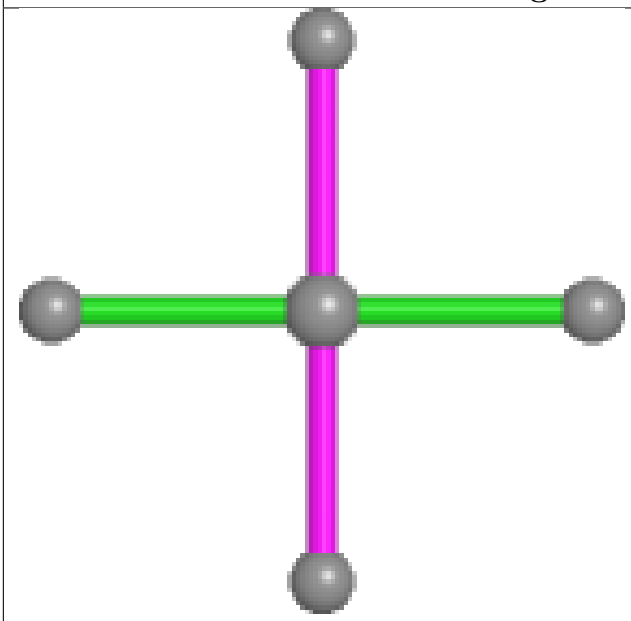
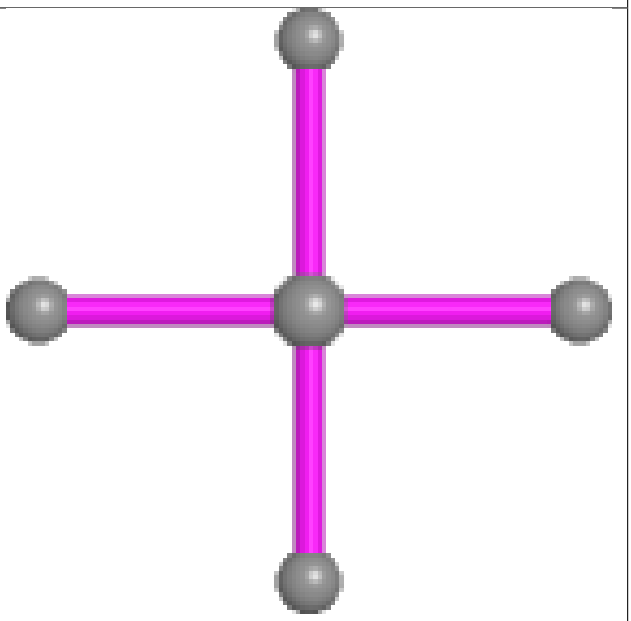


Rings

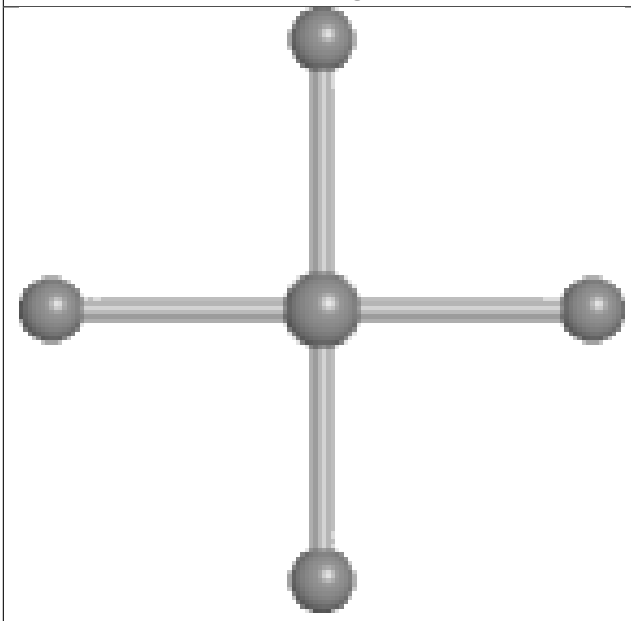
Ligand PEF 1 103



Bond lengths



Bond angles



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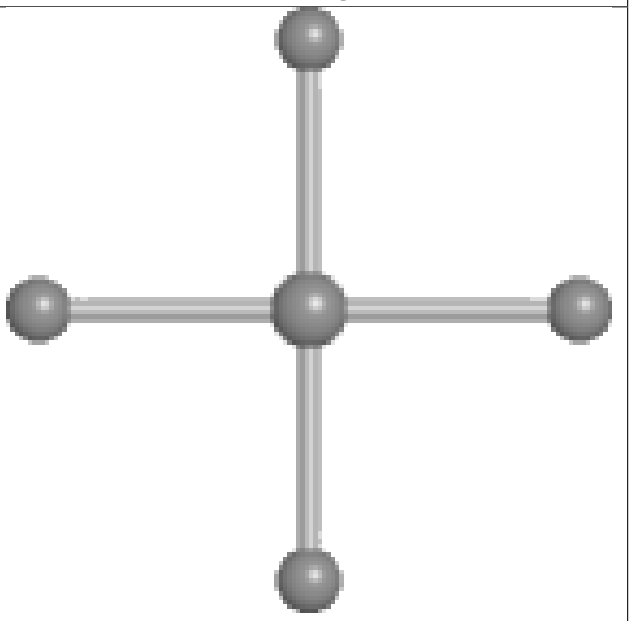
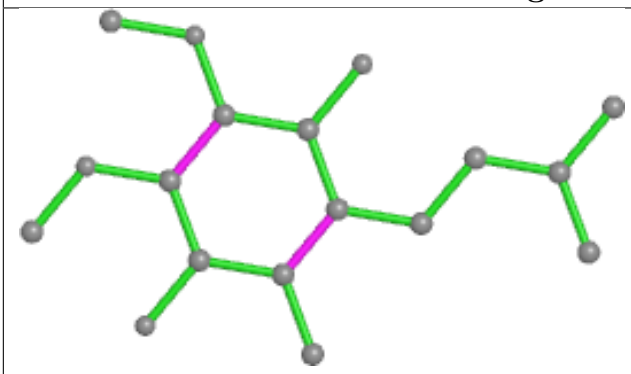
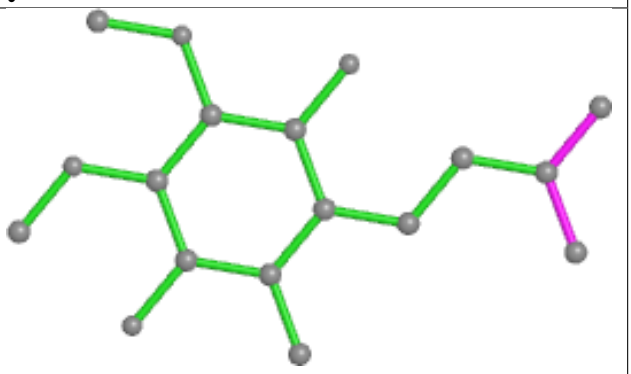


Rings

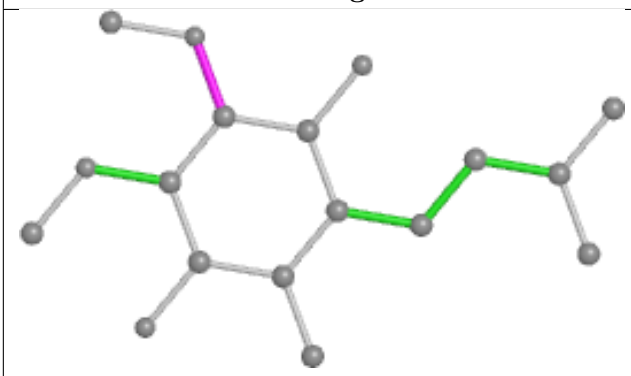
Ligand UQ8 L 311



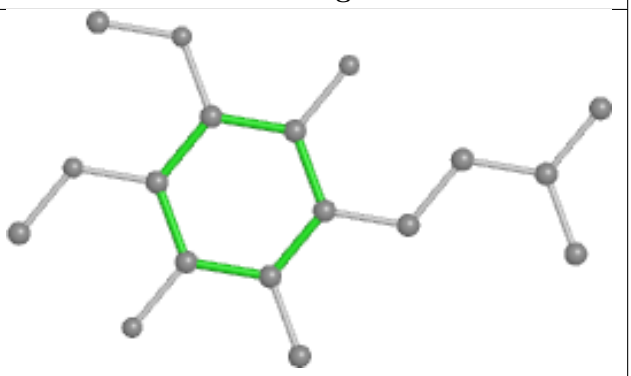
Bond lengths



Bond angles

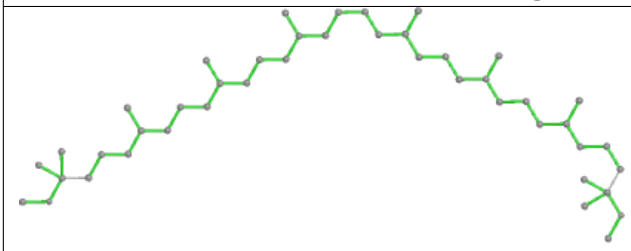


Torsions

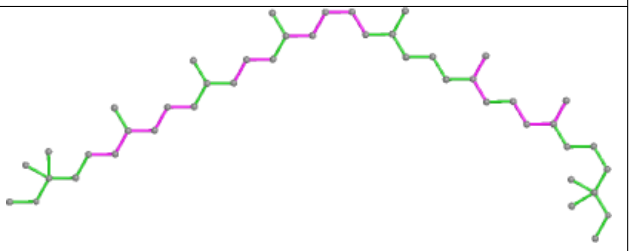


Rings

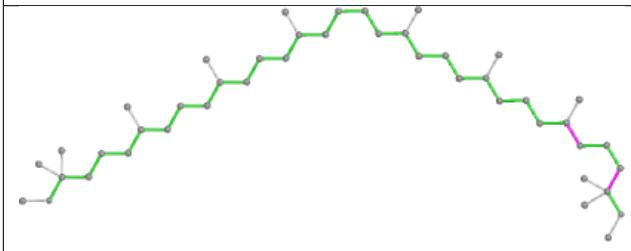
Ligand CRT 0 101



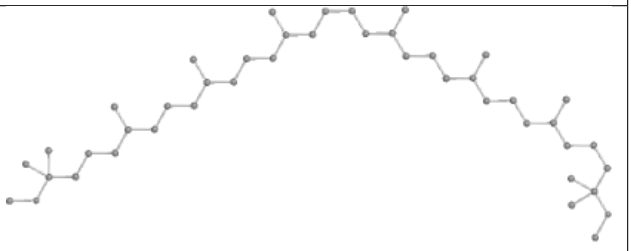
Bond lengths



Bond angles

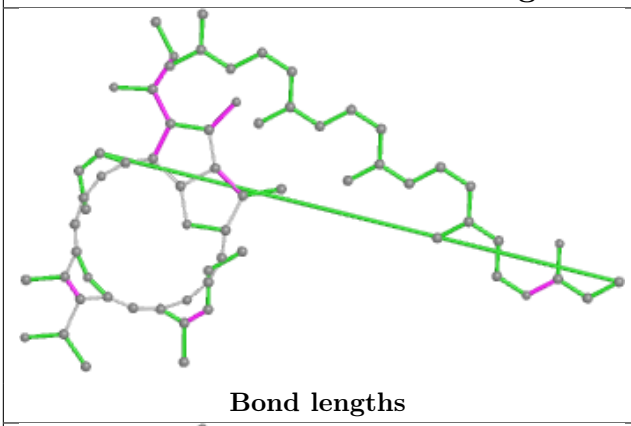


Torsions

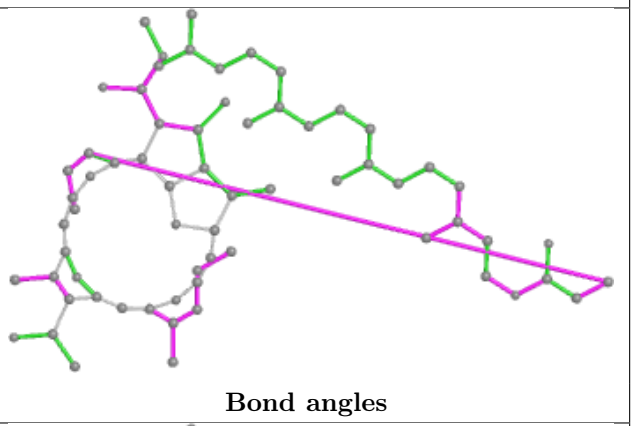


Rings

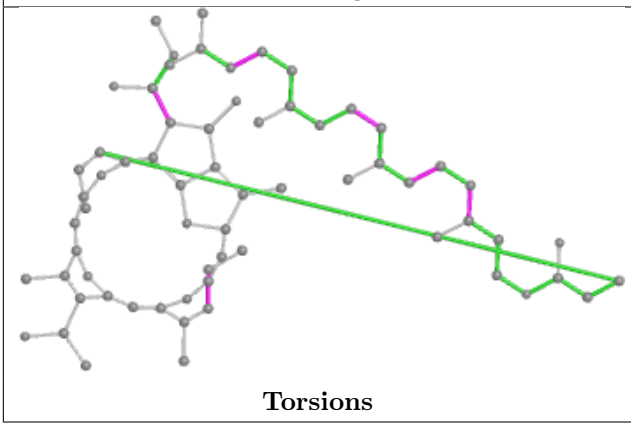
Ligand BPH M 402



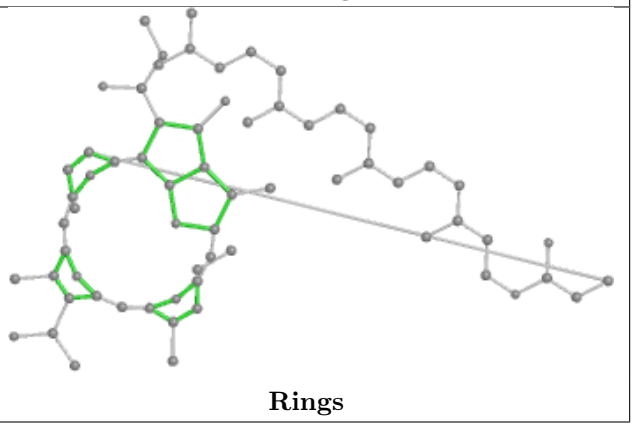
Bond lengths



Bond angles

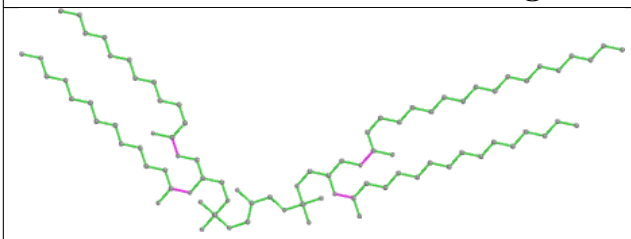


Torsions



Rings

Ligand CDL O 104



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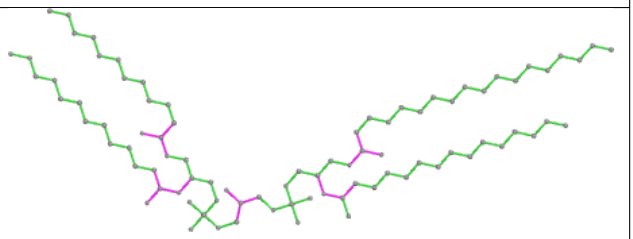
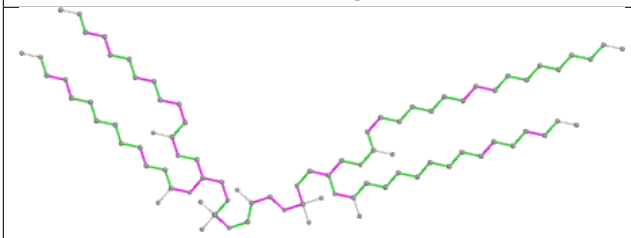
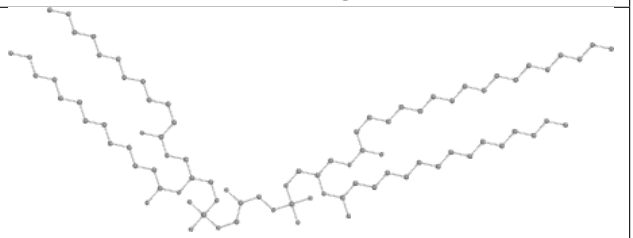


Bond angles

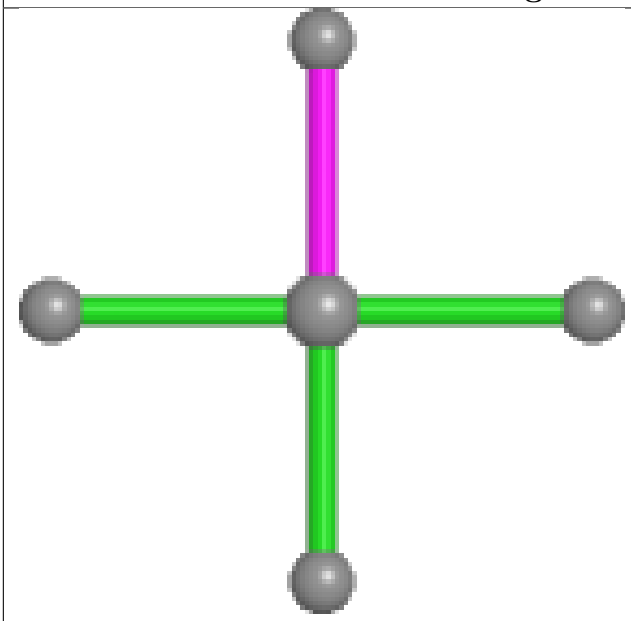


Torsions



Rings

Ligand PEF H 302



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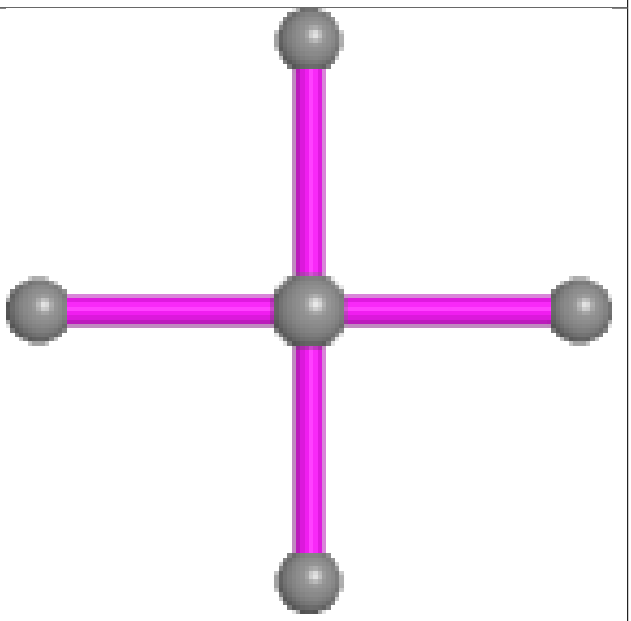
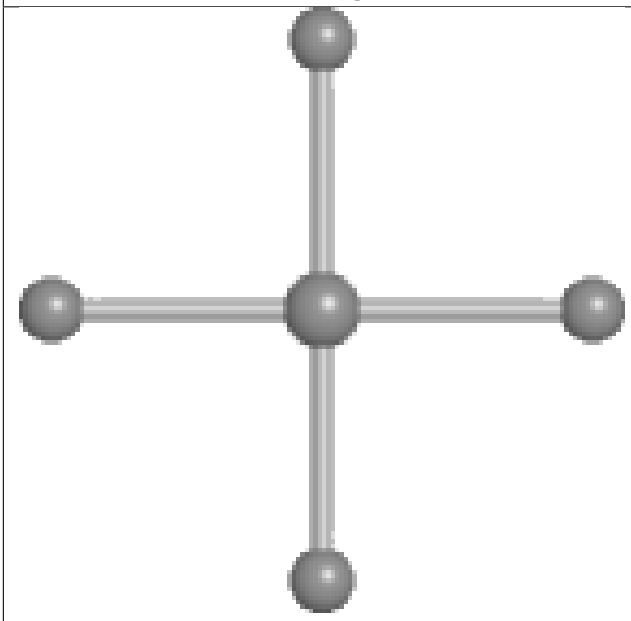
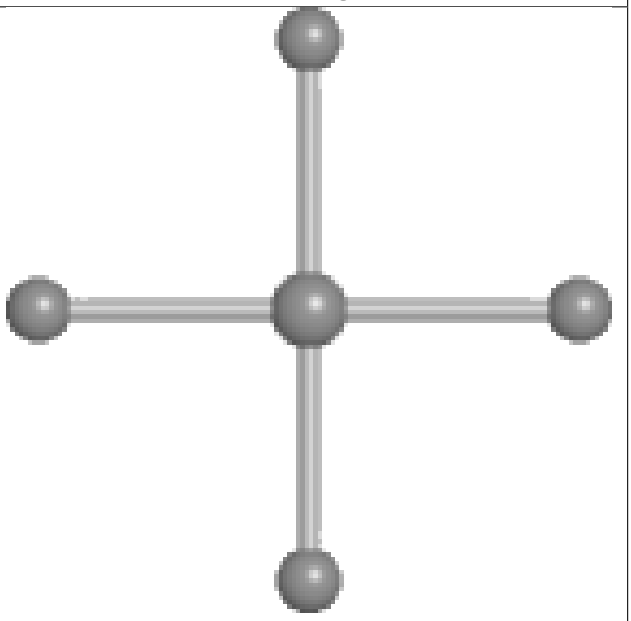


Bond angles

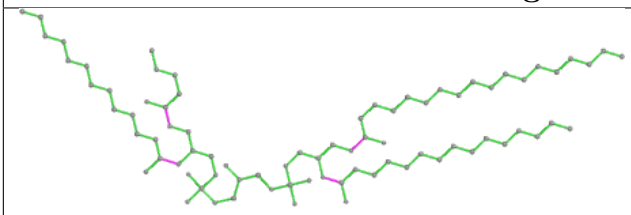


Torsions



Rings

Ligand CDL H 305



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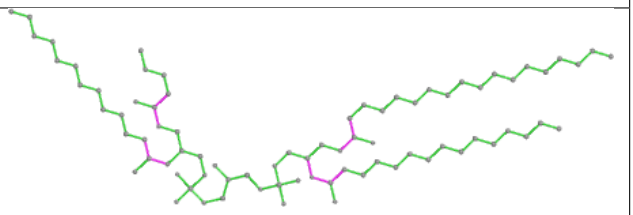
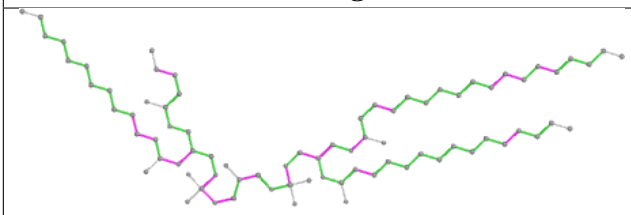
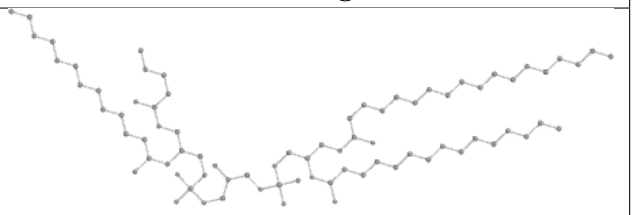


Bond angles

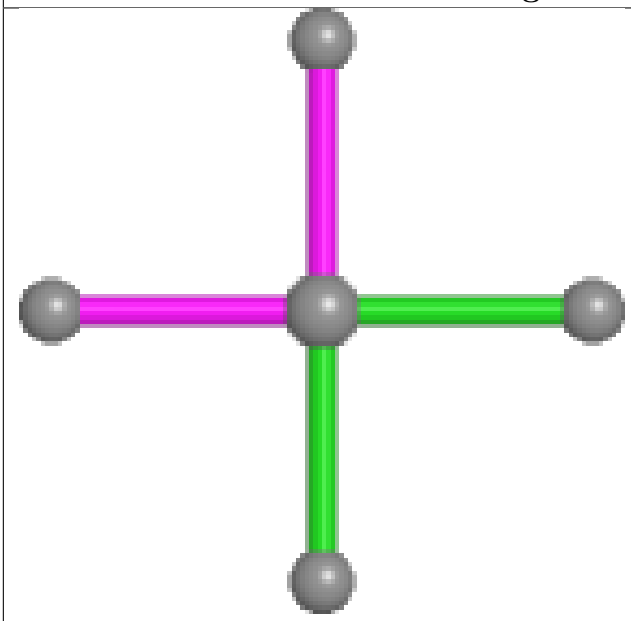


Torsions

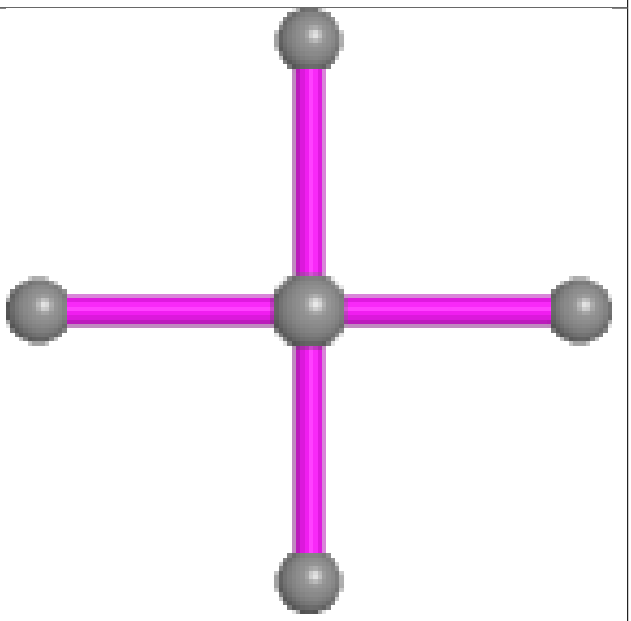


Rings

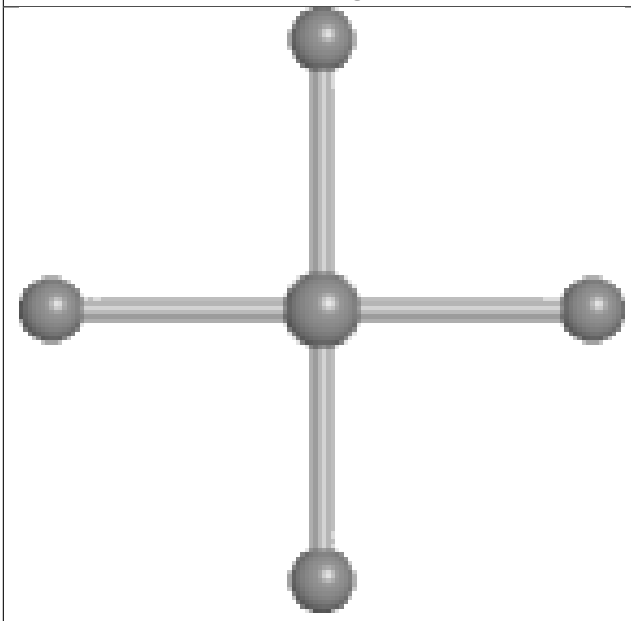
Ligand PEF M 407



Bond lengths



Bond angles



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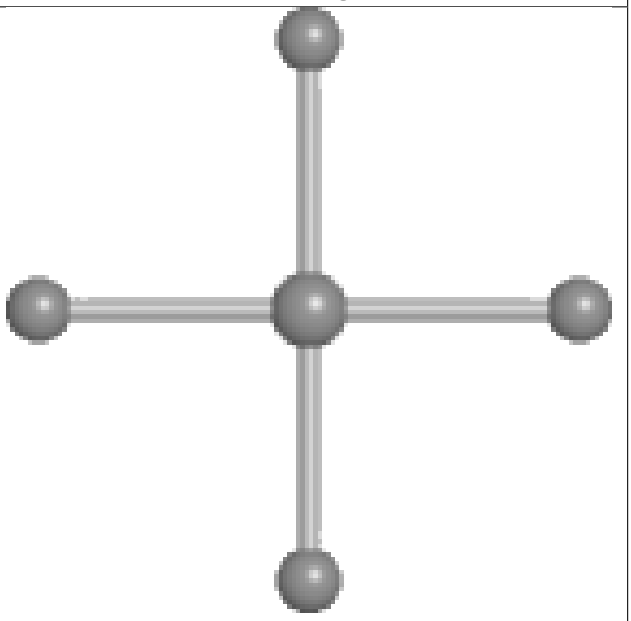
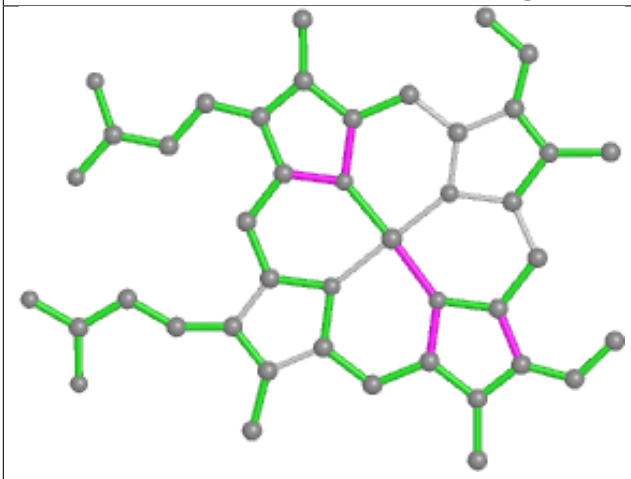
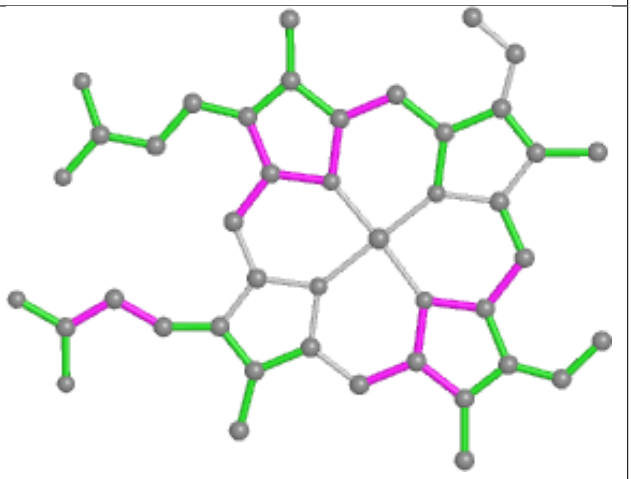


Rings

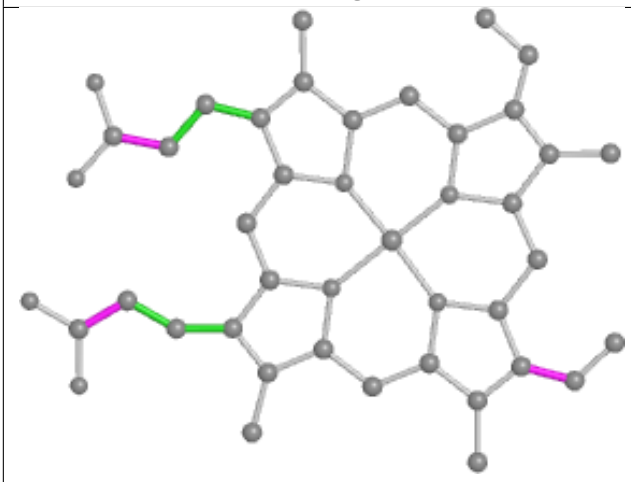
Ligand HEM C 504



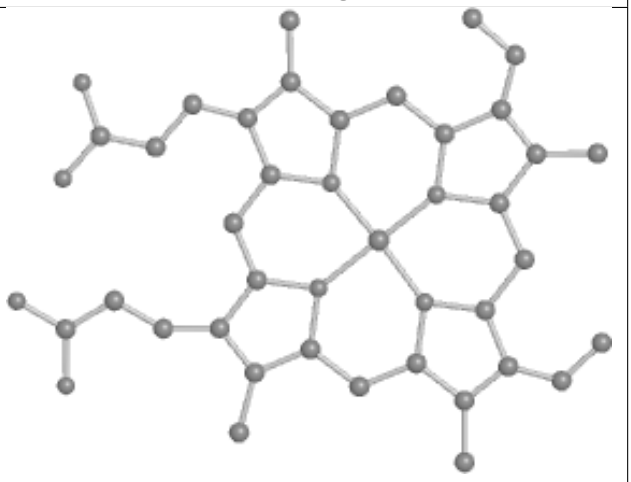
Bond lengths



Bond angles

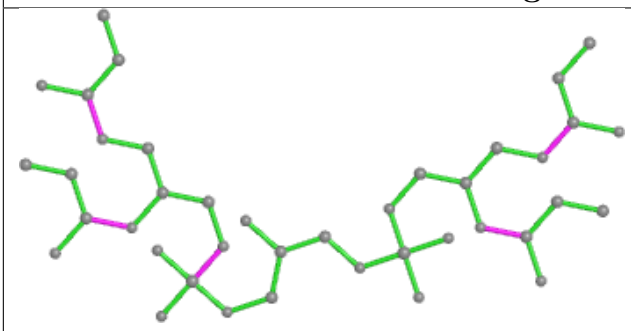


Torsions

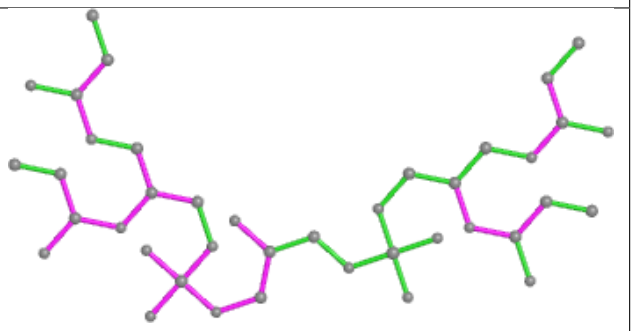


Rings

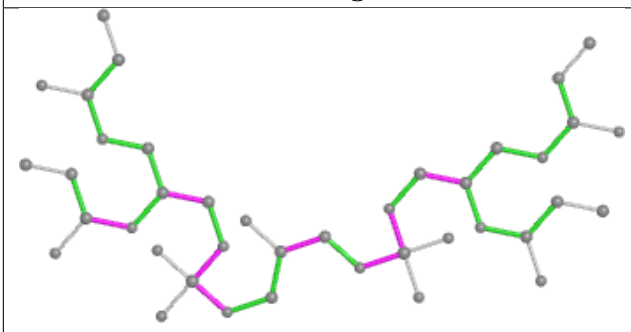
Ligand CDL Y 104



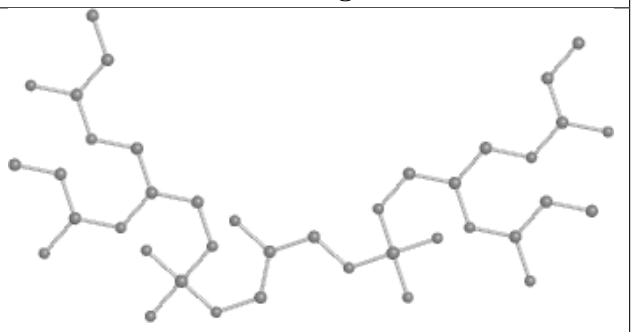
Bond lengths



Bond angles

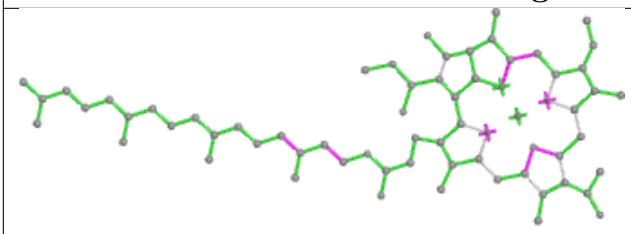


Torsions

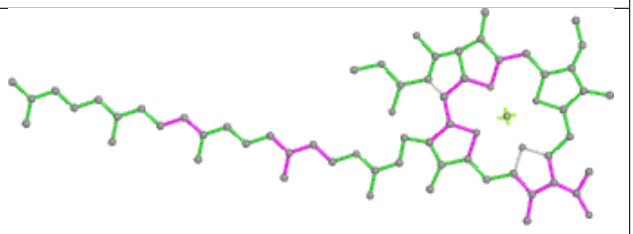


Rings

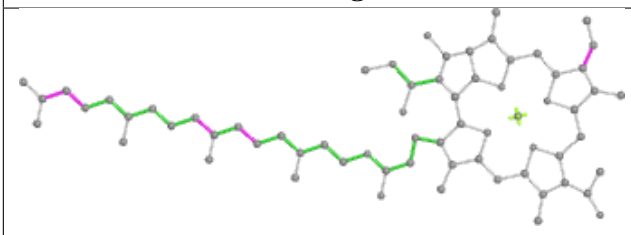
Ligand BCL I 101



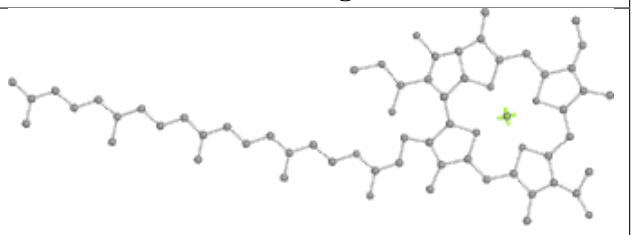
Bond lengths



Bond angles

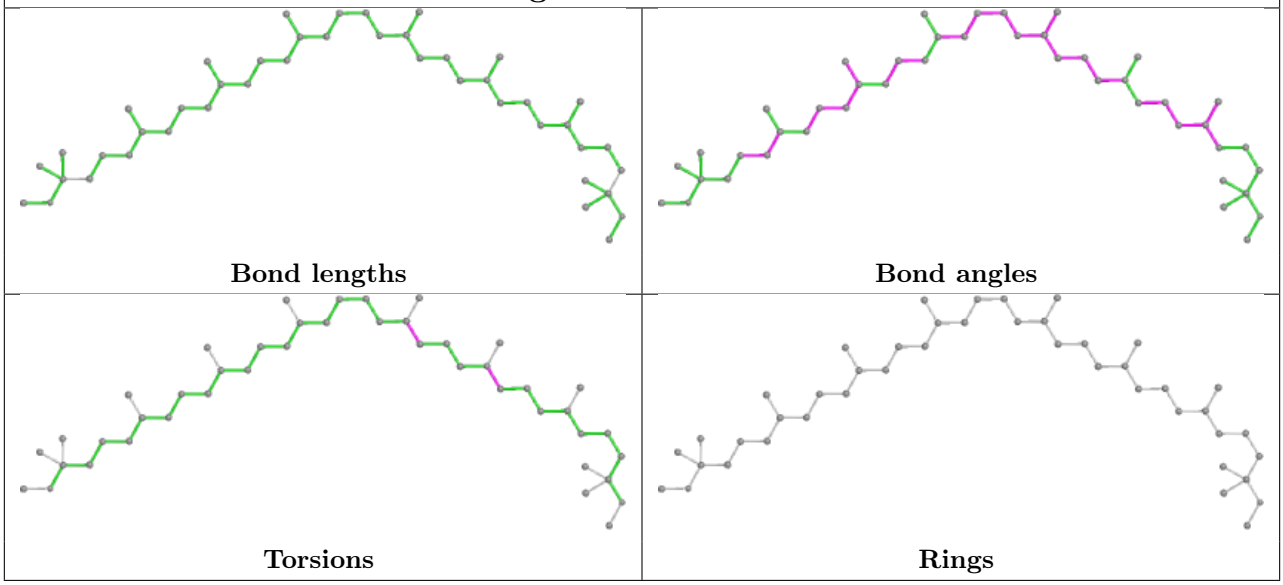


Torsions

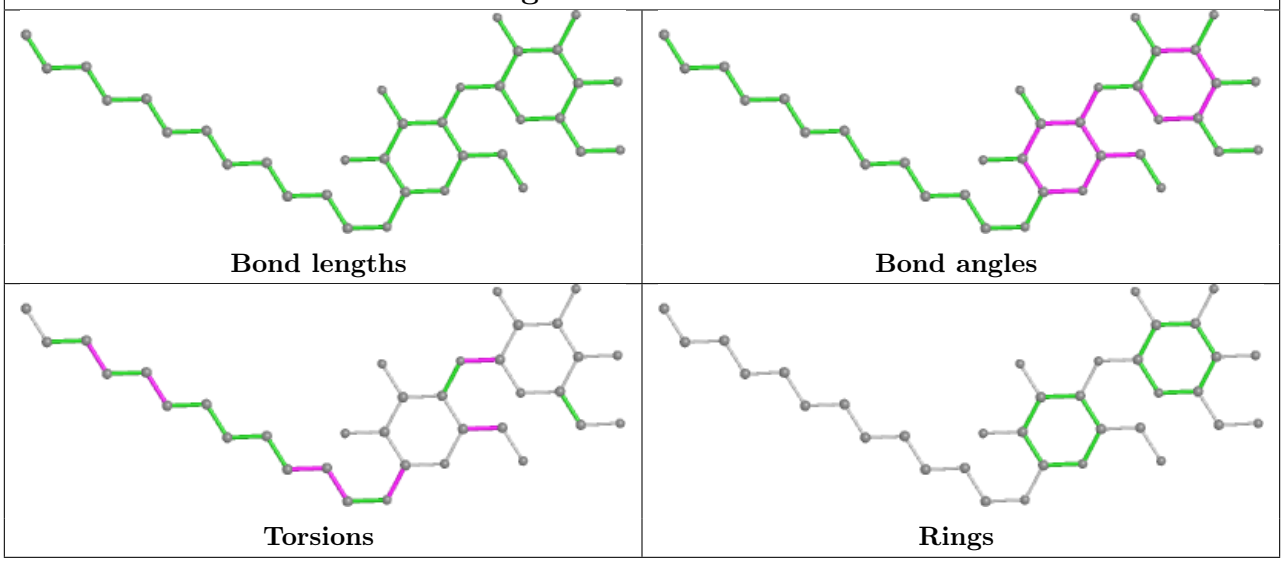


Rings

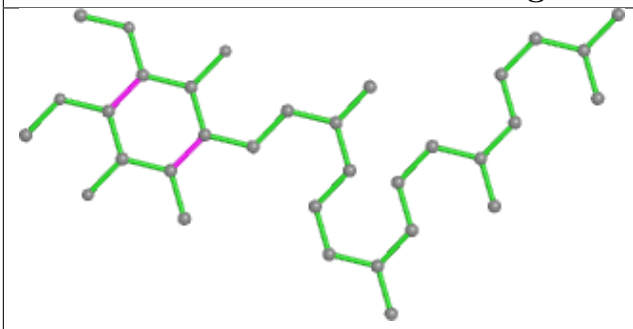
Ligand CRT 8 101



Ligand LMT H 304



Ligand UQ8 L 304



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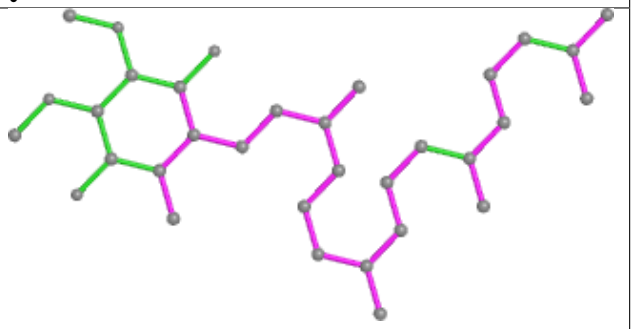
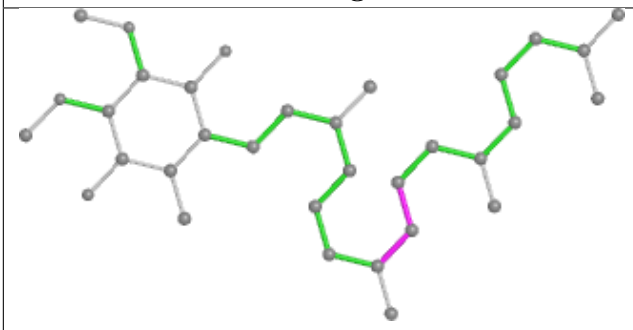
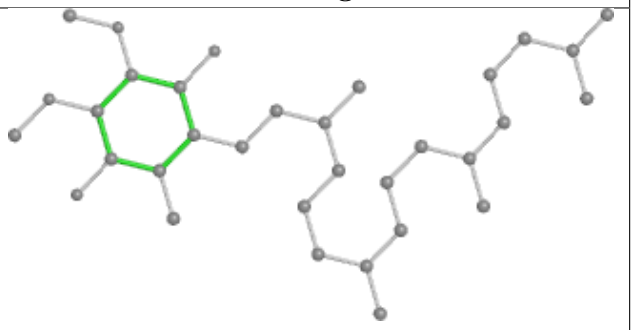


Bond angles

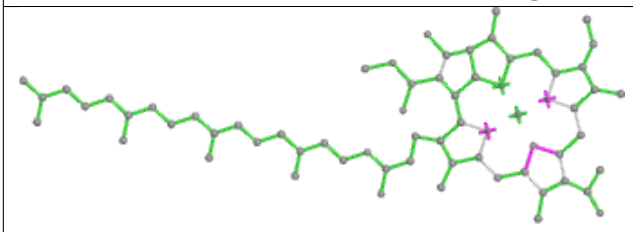


Torsions

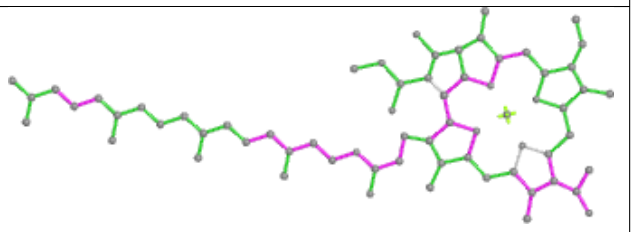


Rings

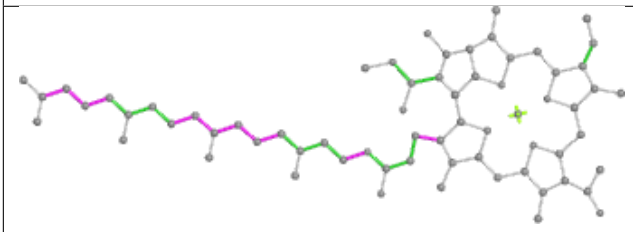
Ligand BCL P 102



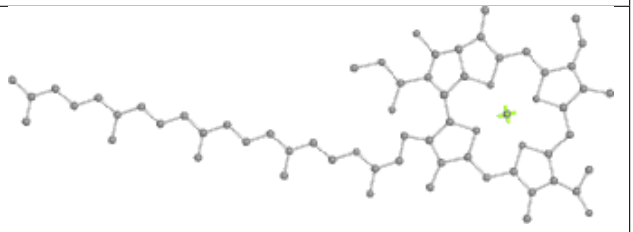
Bond lengths



Bond angles

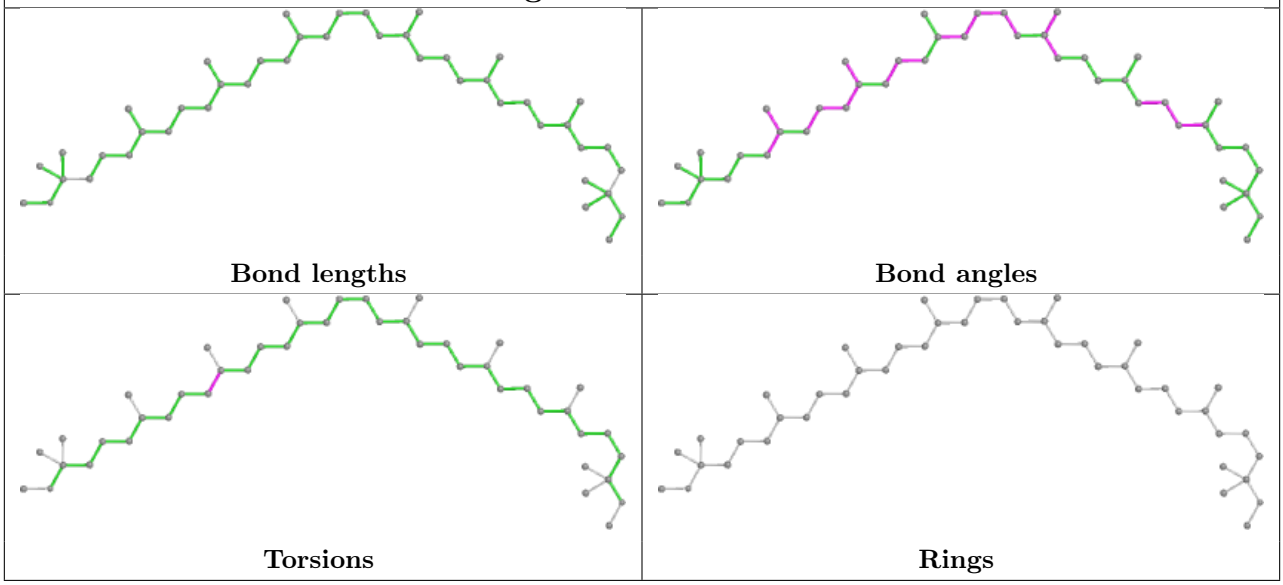


Torsions

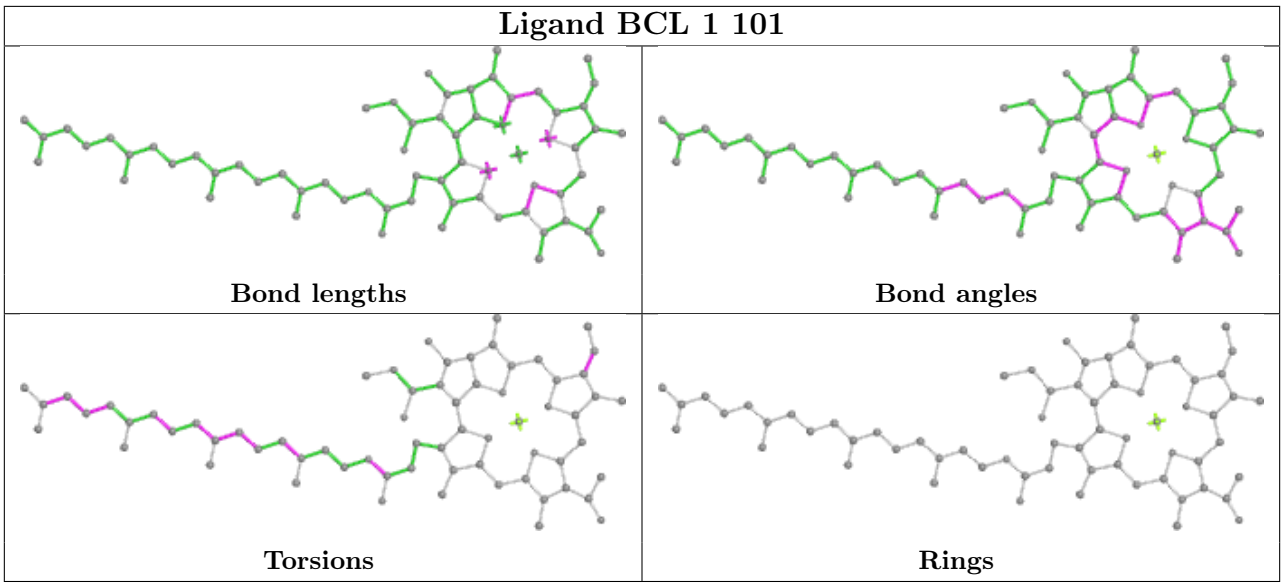


Rings

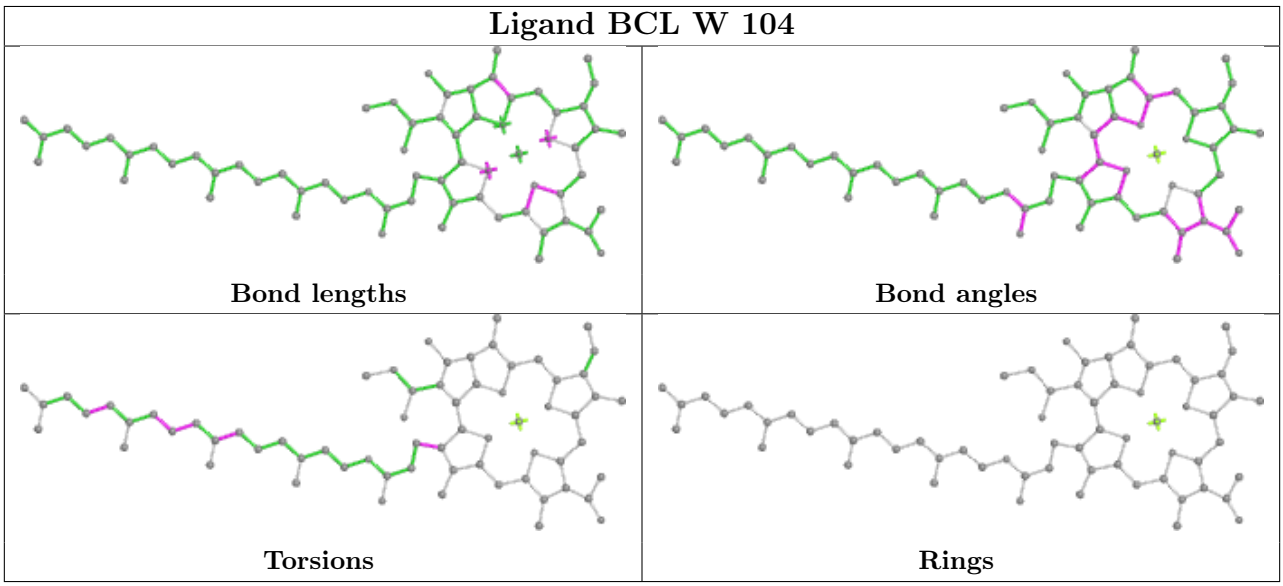
Ligand CRT O 103



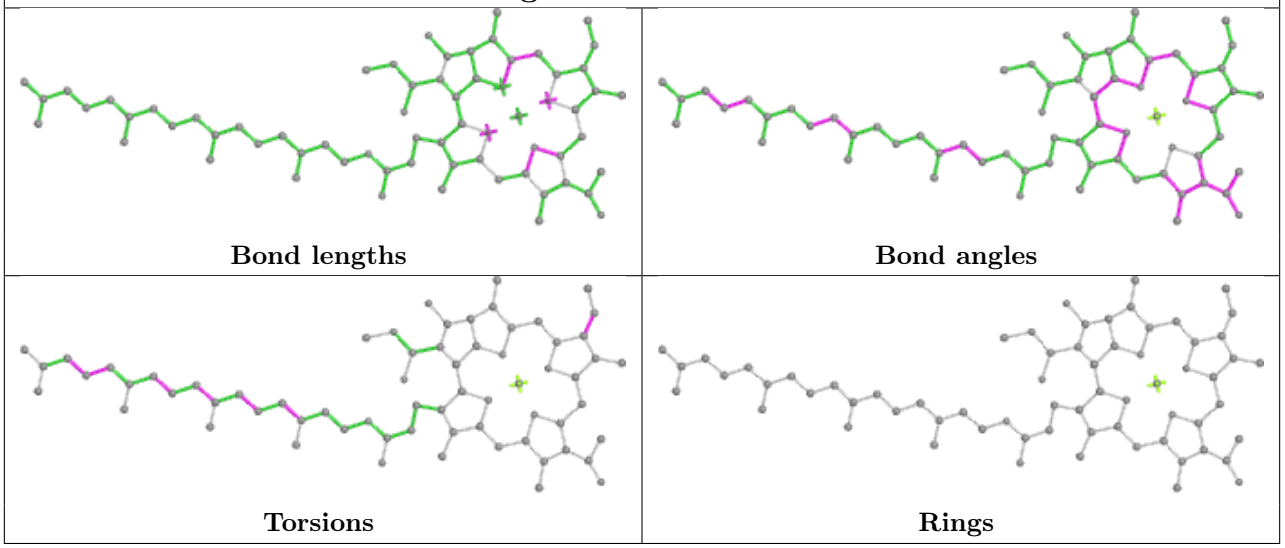
Ligand BCL 1 101



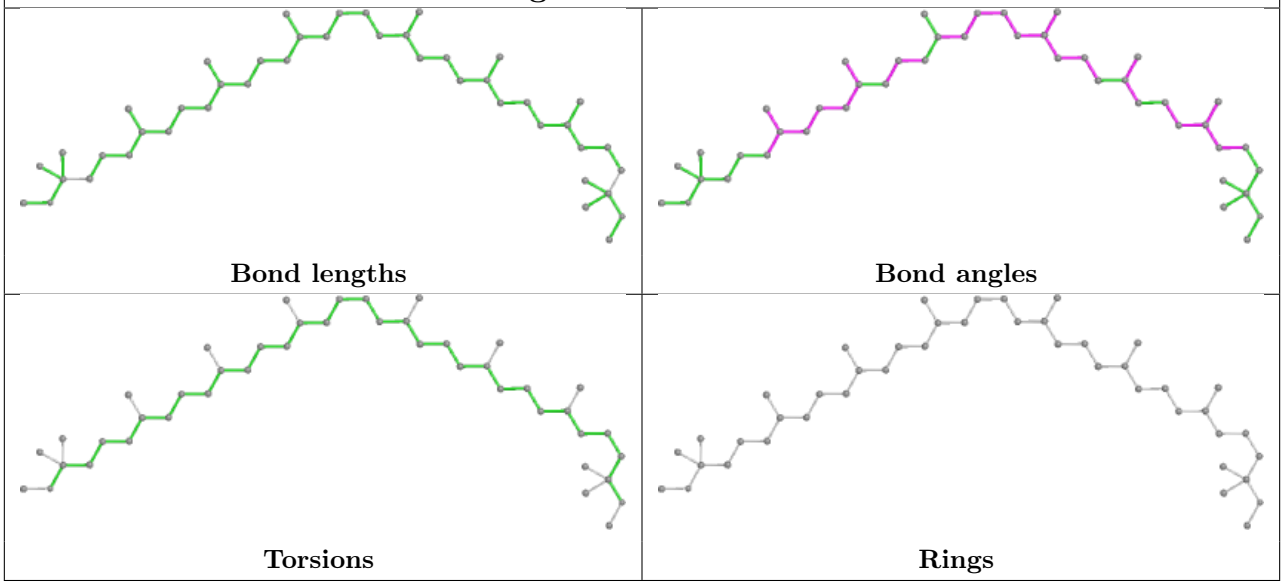
Ligand BCL W 104



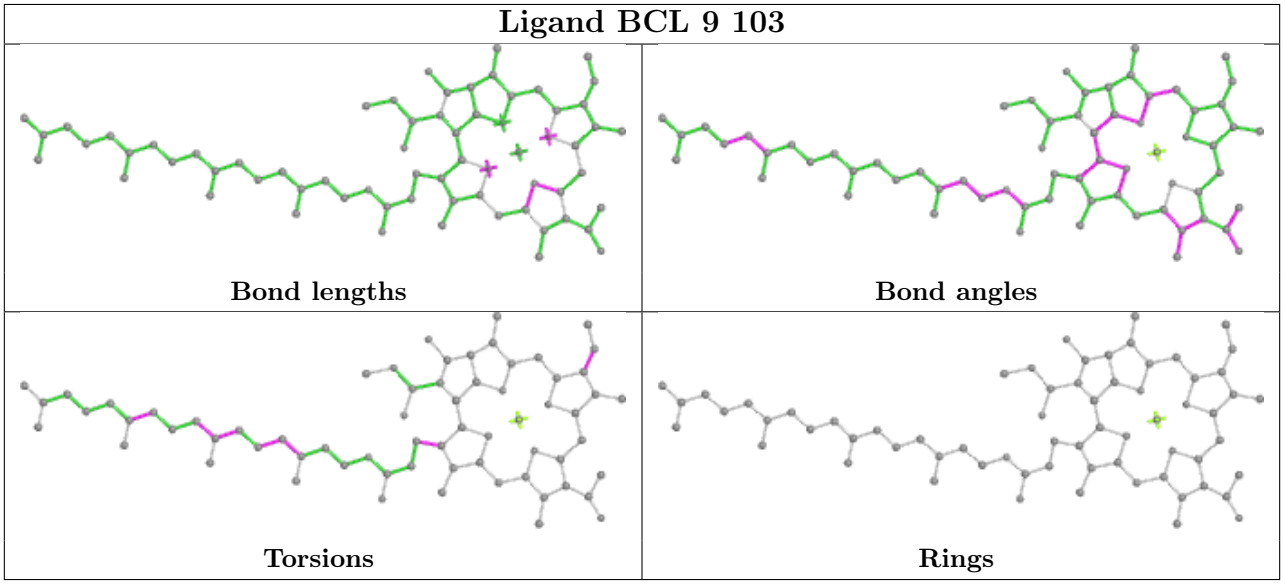
Ligand BCL W 101



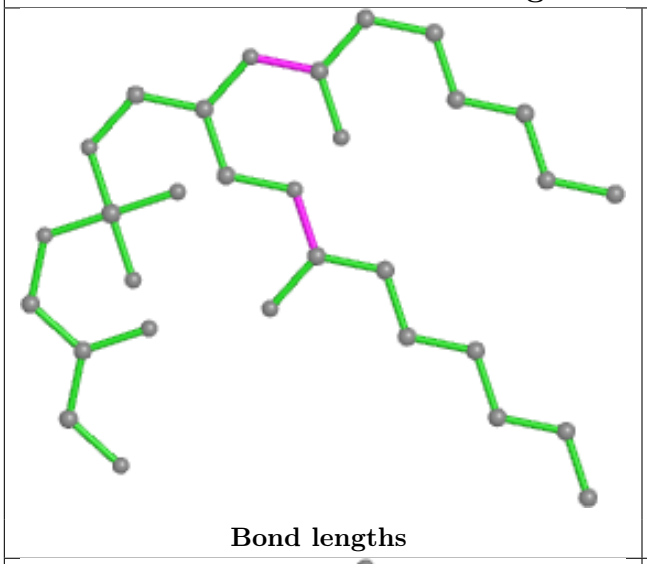
Ligand CRT 3 103



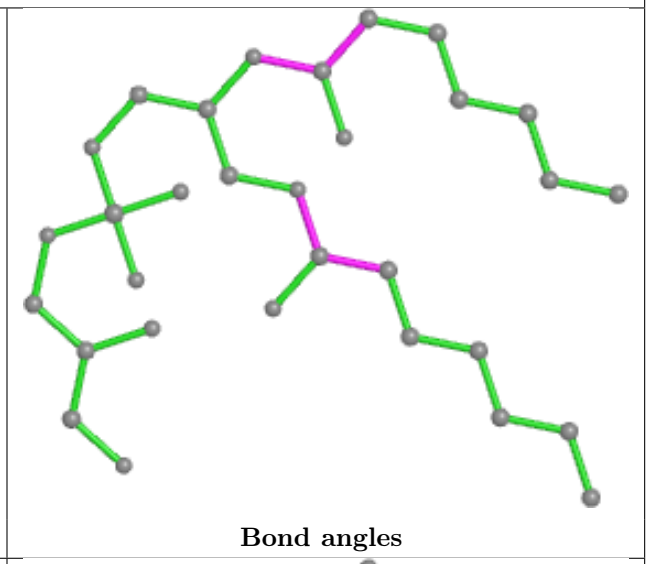
Ligand BCL 9 103



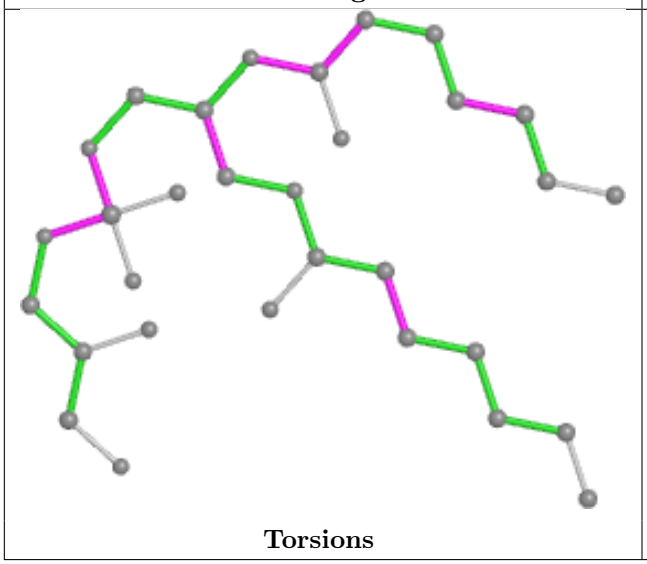
Ligand PGV 1 105



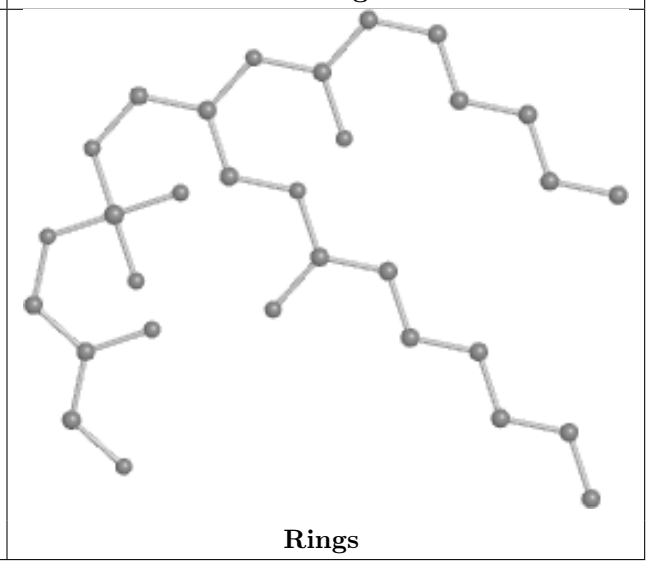
Bond lengths



Bond angles

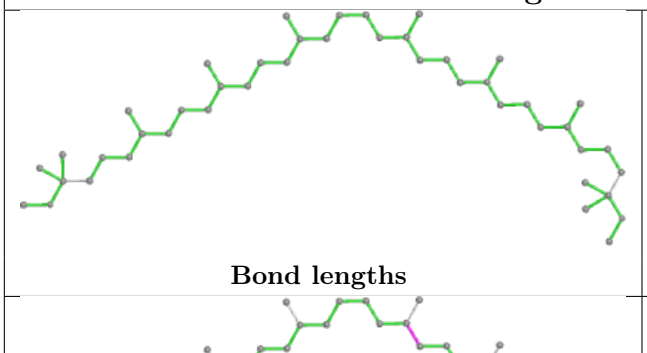


Torsions

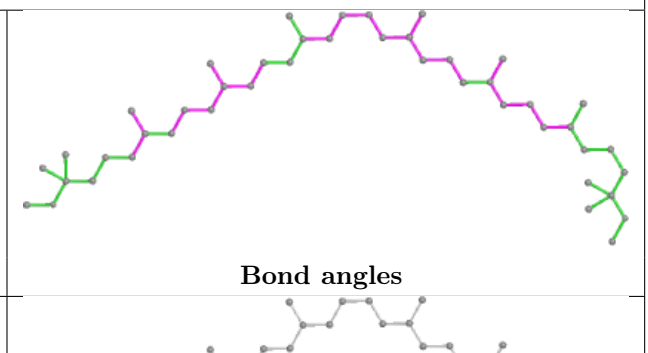


Rings

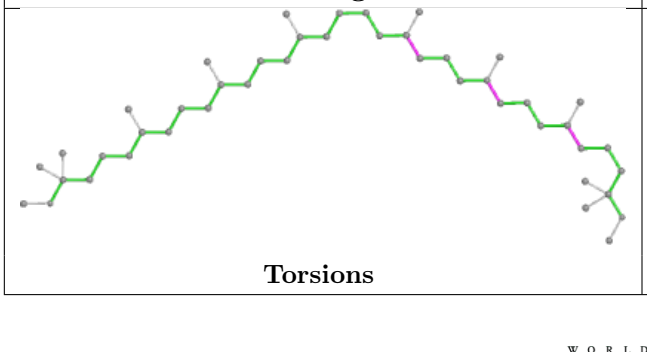
Ligand CRT V 101



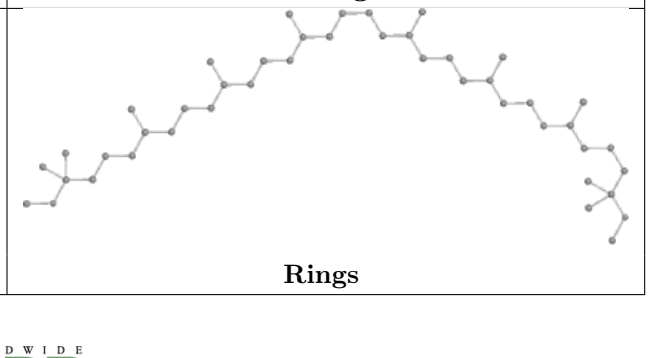
Bond lengths



Bond angles

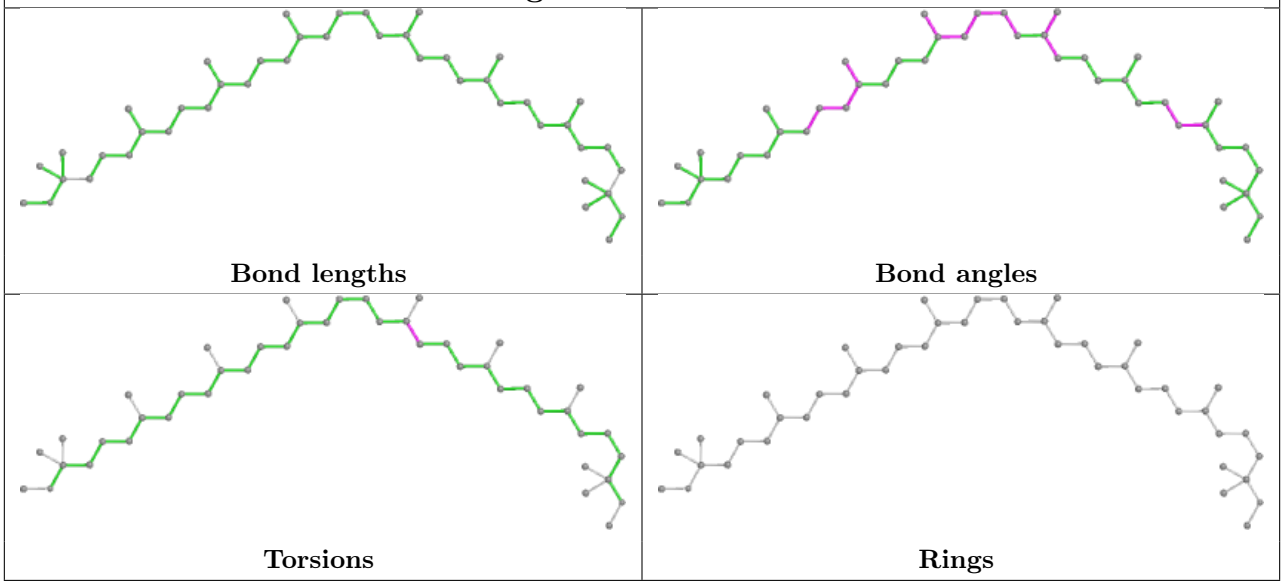


Torsions

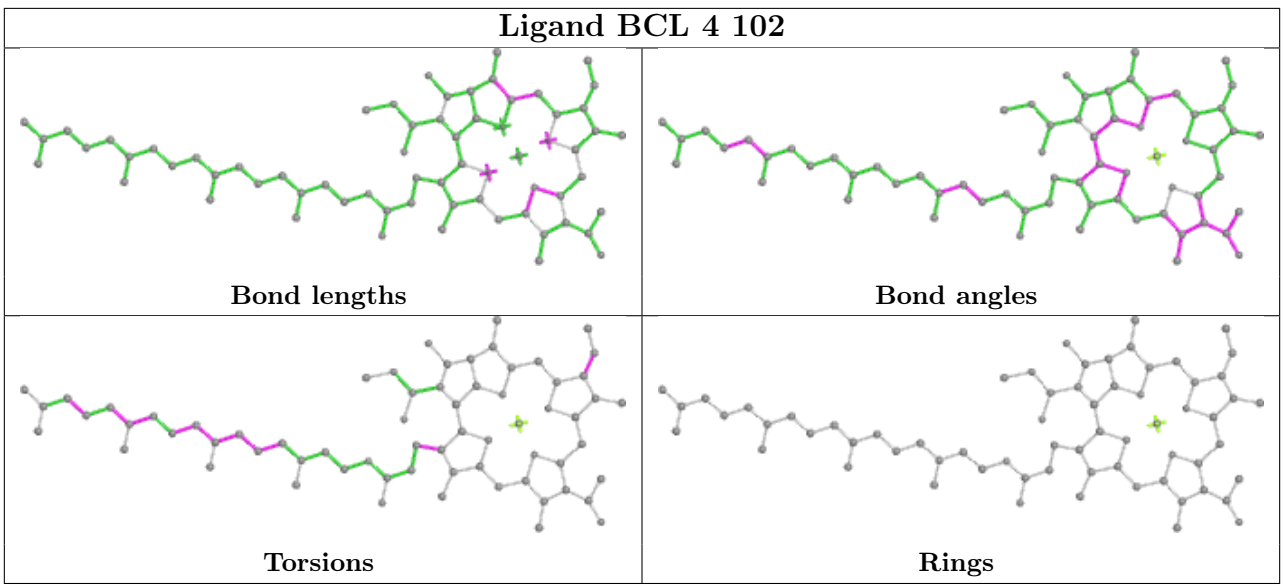


Rings

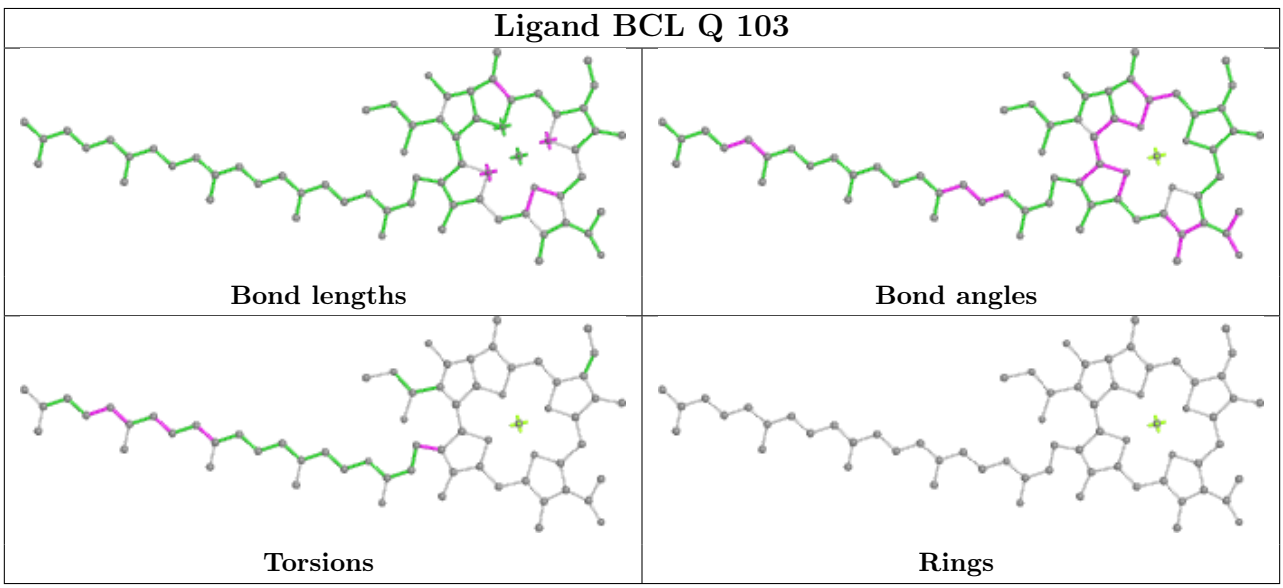
Ligand CRT P 101



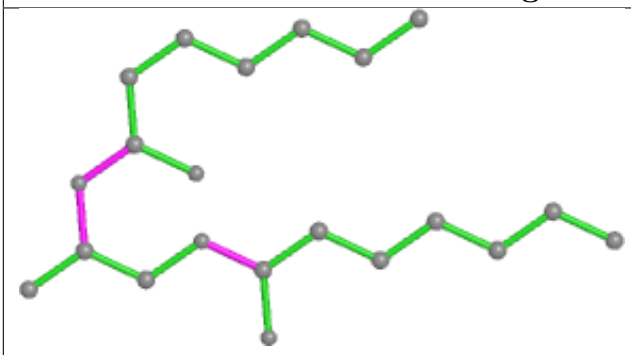
Ligand BCL 4 102



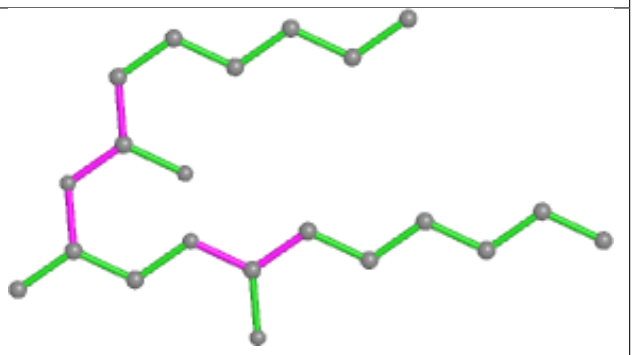
Ligand BCL Q 103



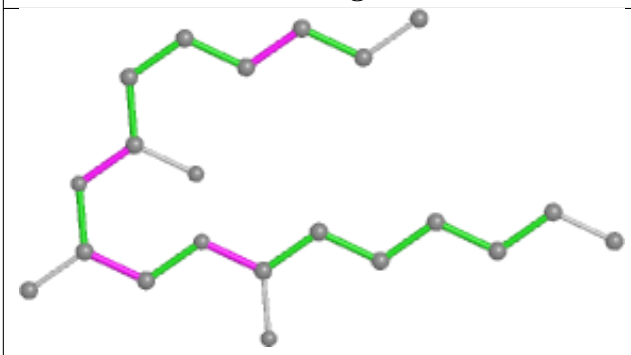
Ligand PGV C 508



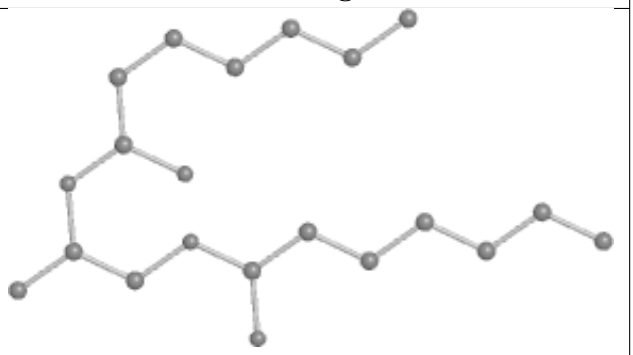
Bond lengths



Bond angles

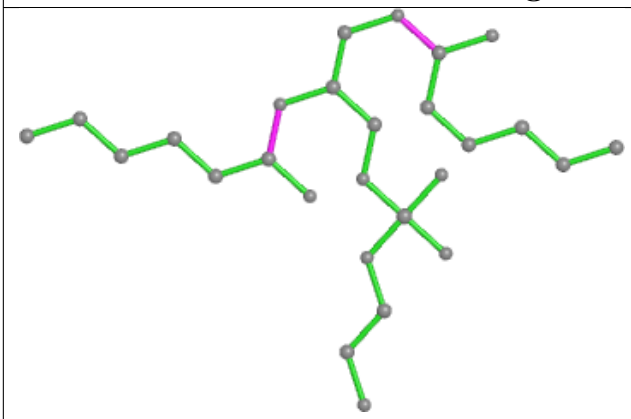


Torsions

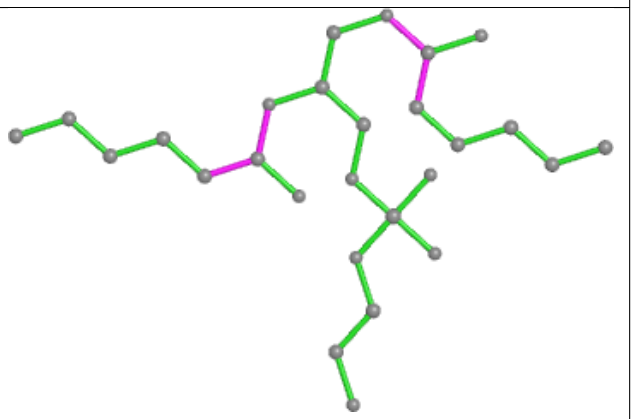


Rings

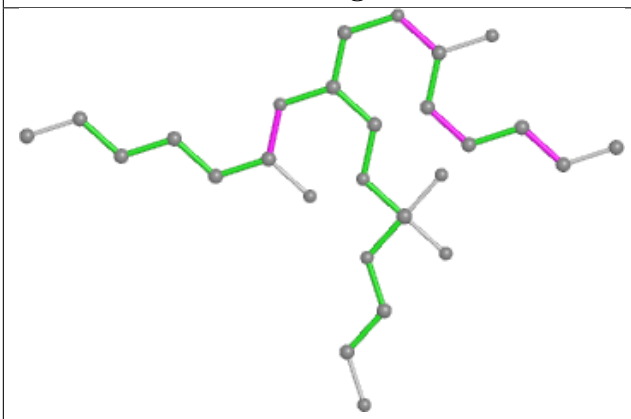
Ligand PEF K 104



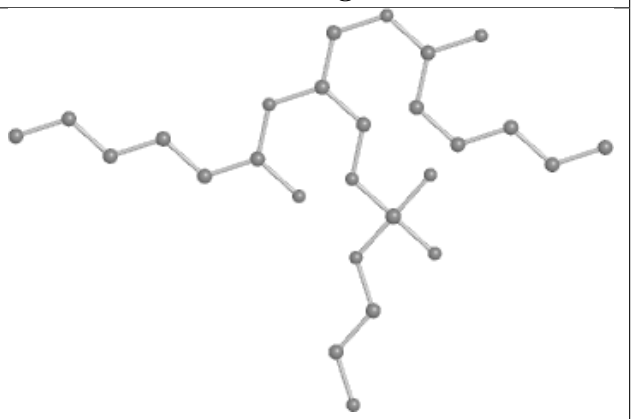
Bond lengths



Bond angles

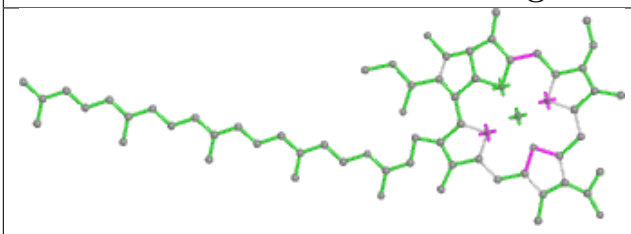


Torsions

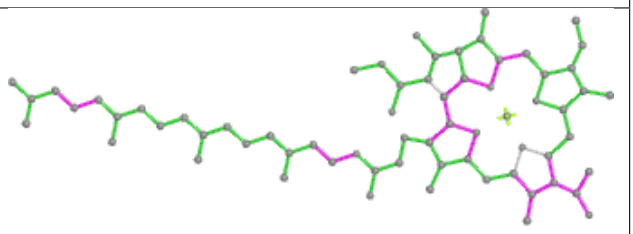


Rings

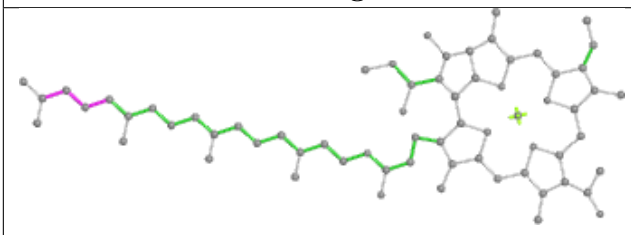
Ligand BCL L 301



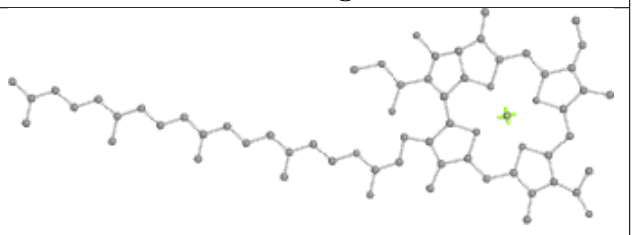
Bond lengths



Bond angles

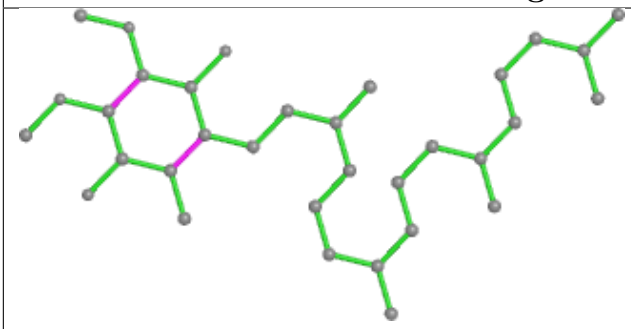


Torsions

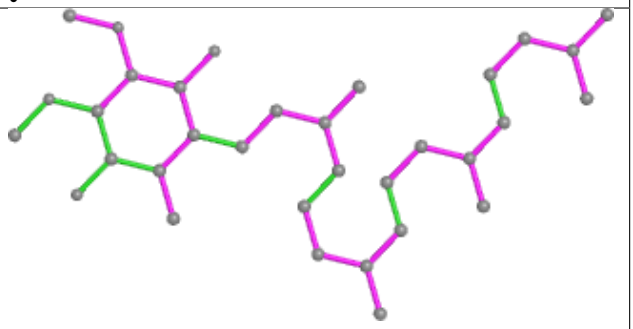


Rings

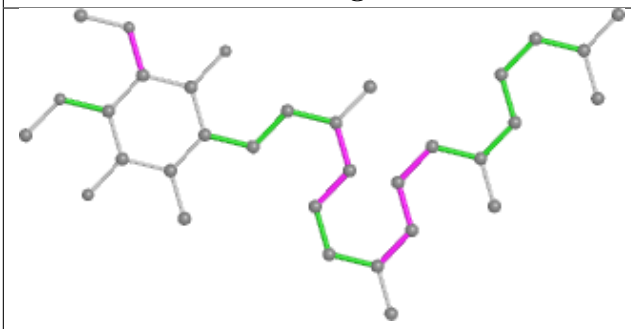
Ligand UQ8 L 310



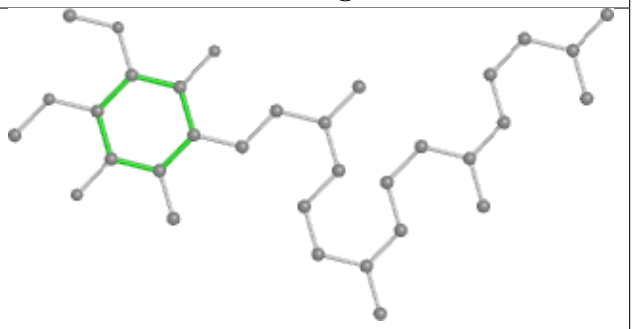
Bond lengths



Bond angles

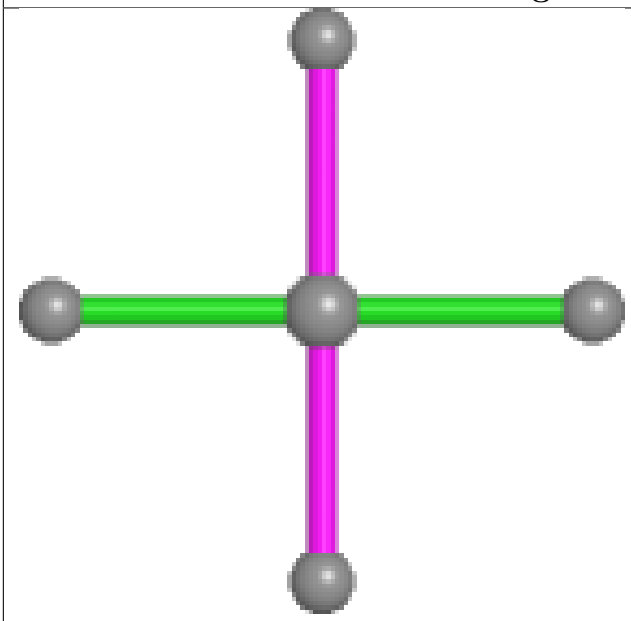


Torsions

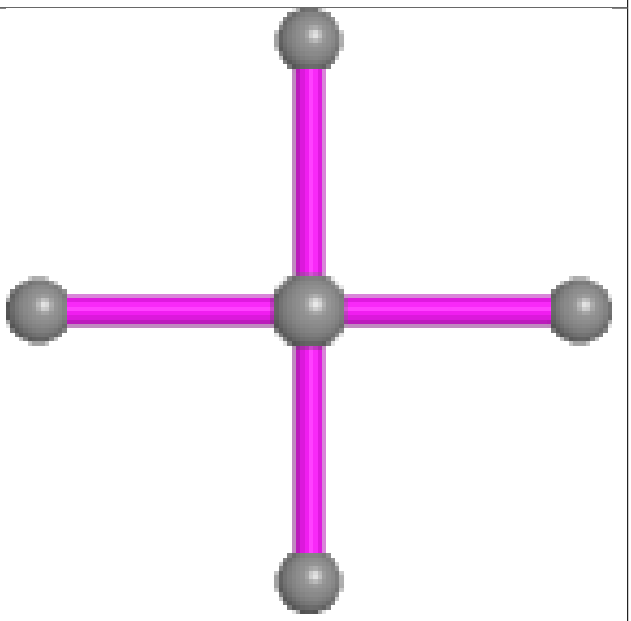


Rings

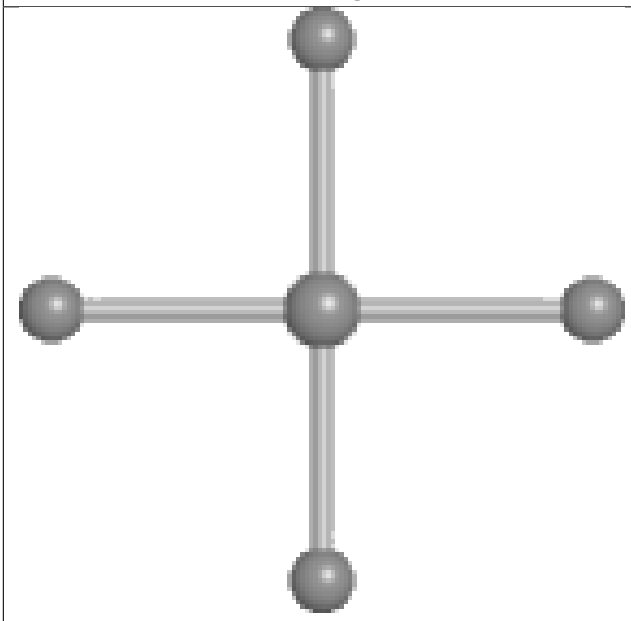
Ligand PEF I 103



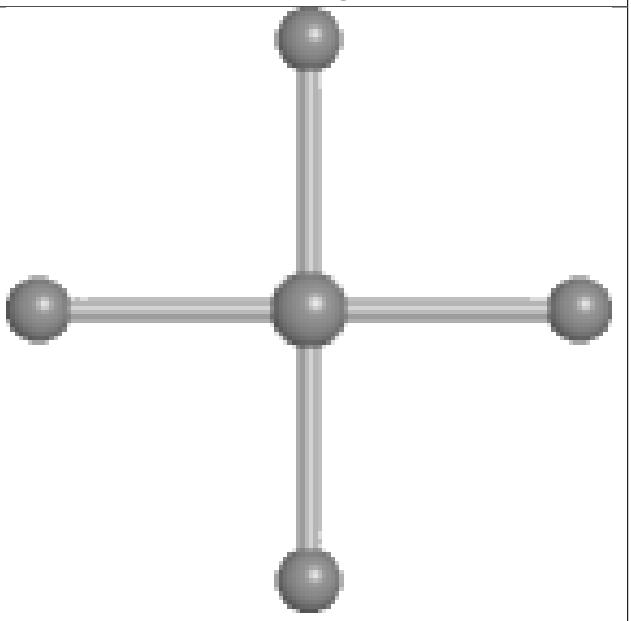
Bond lengths



Bond angles

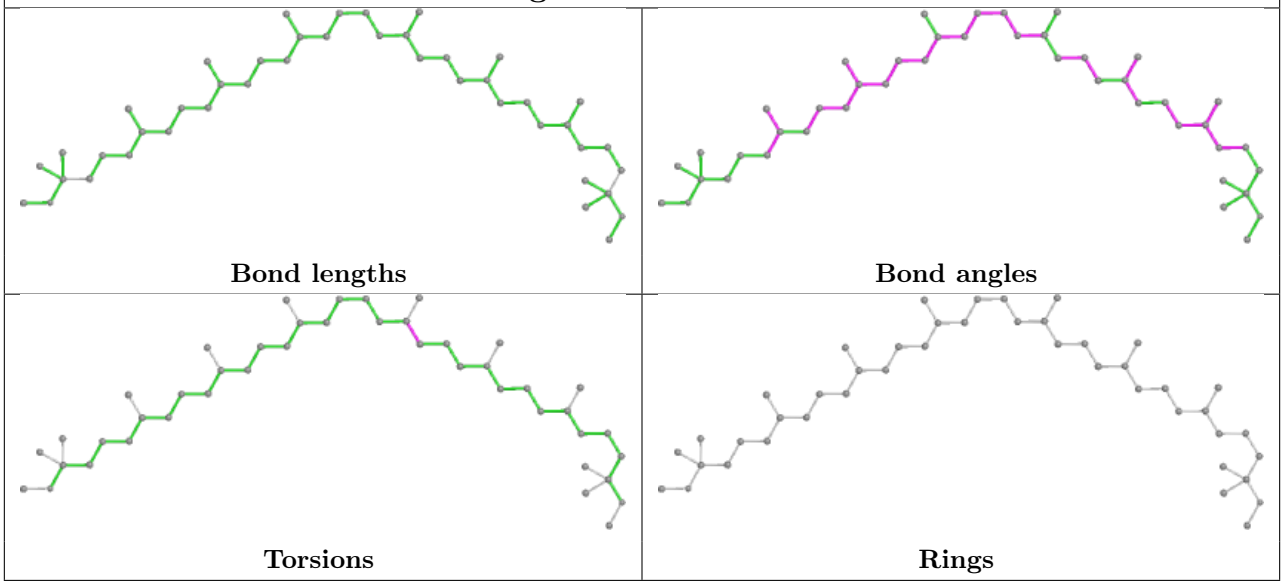


Torsions

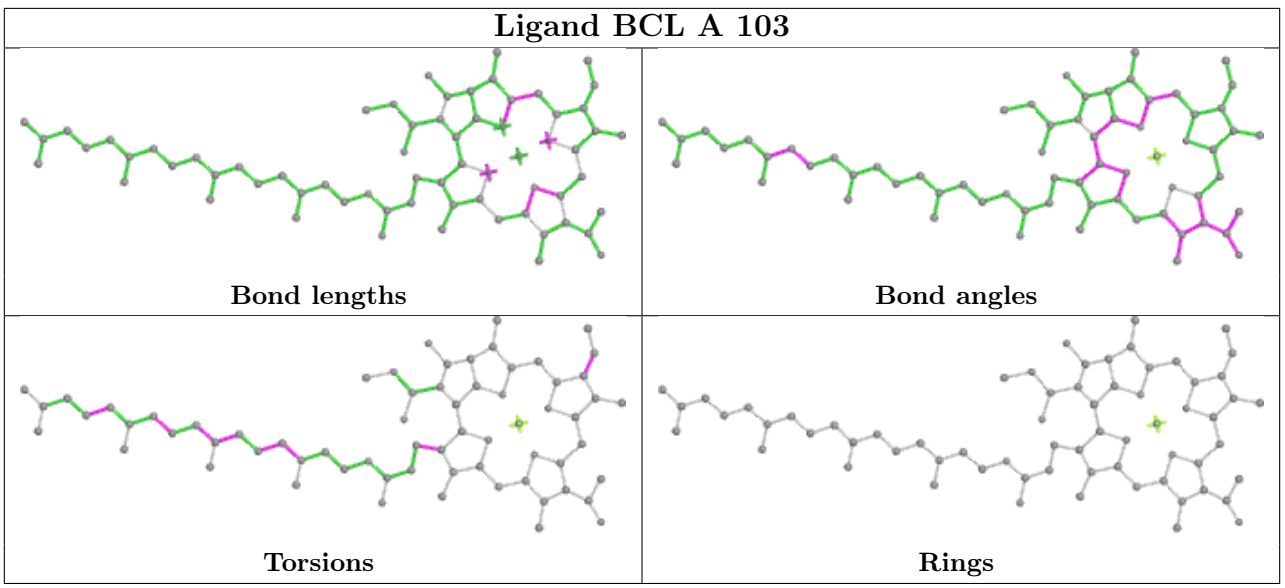


Rings

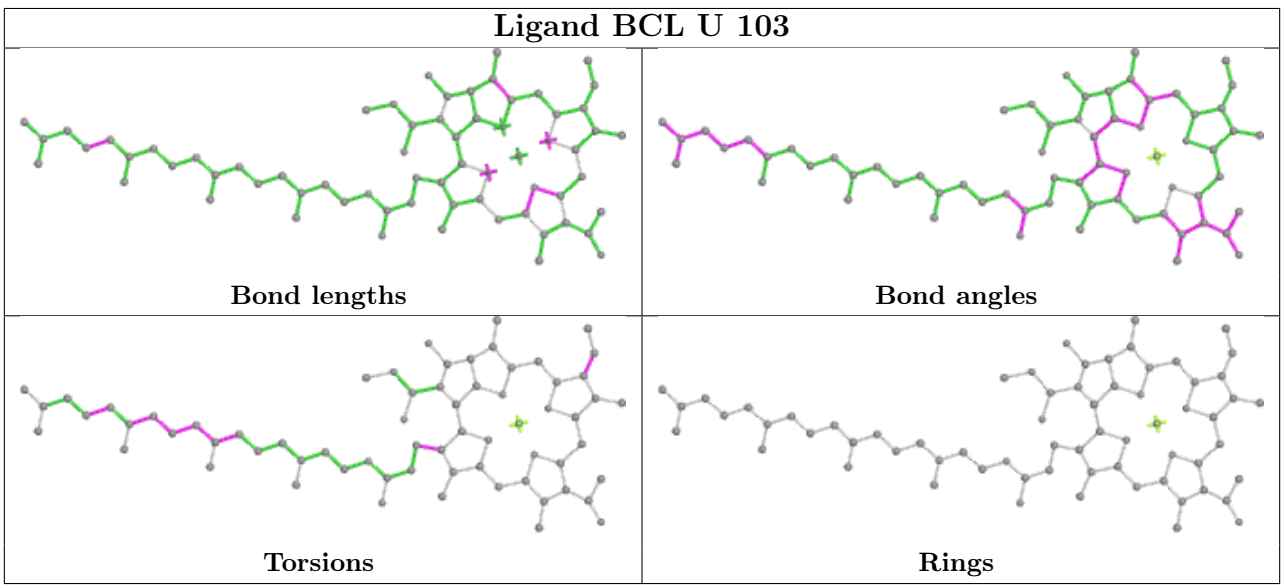
Ligand CRT 4 101



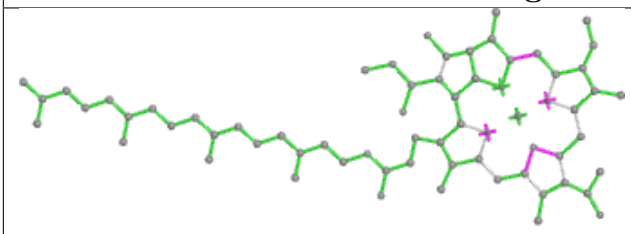
Ligand BCL A 103



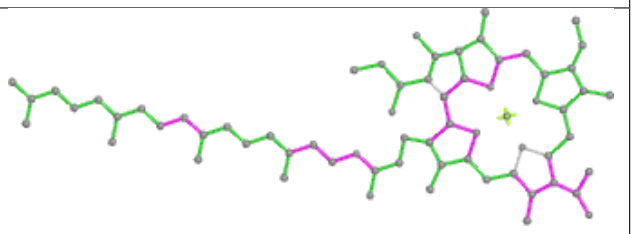
Ligand BCL U 103



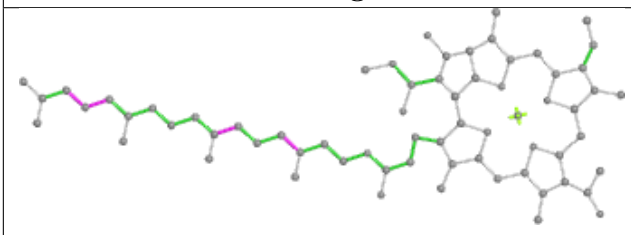
Ligand BCL O 101



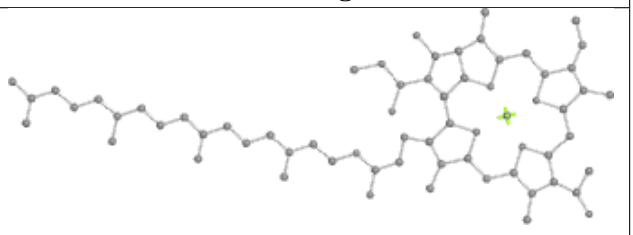
Bond lengths



Bond angles

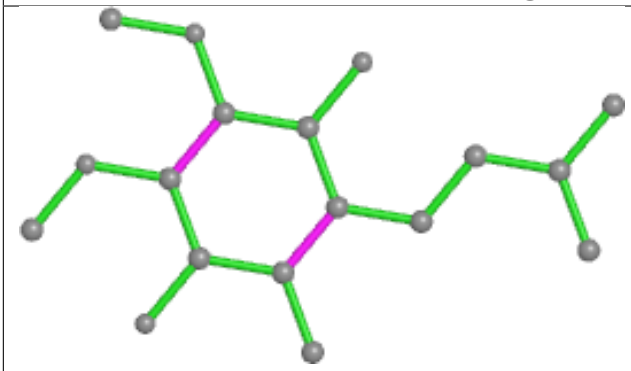


Torsions

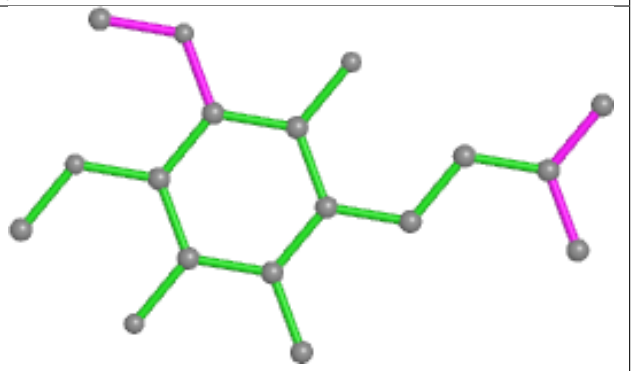


Rings

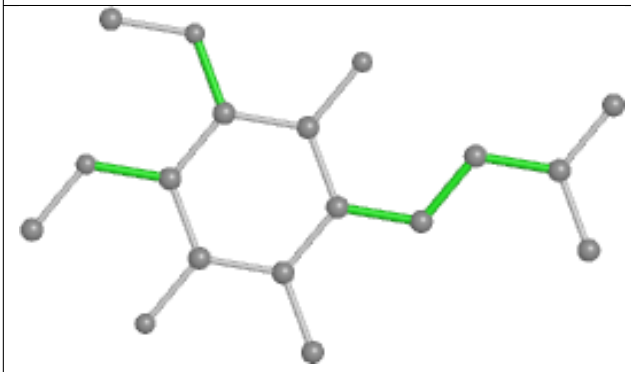
Ligand UQ8 M 413



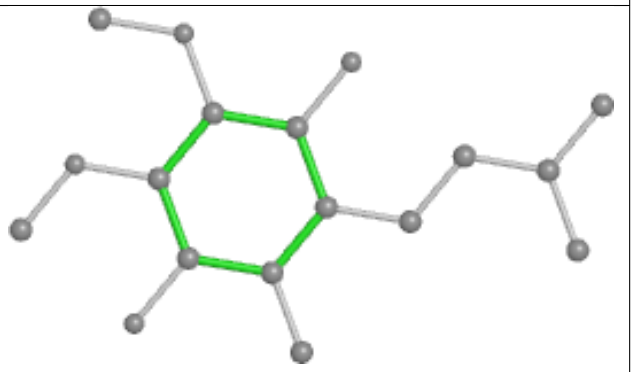
Bond lengths



Bond angles

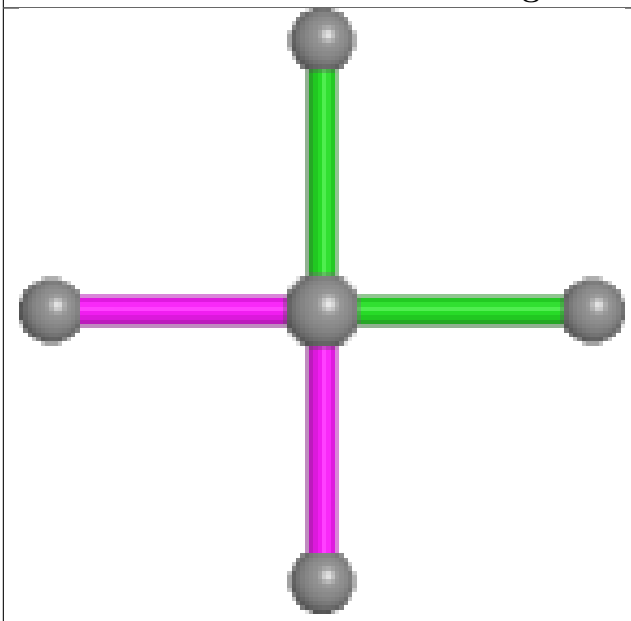


Torsions

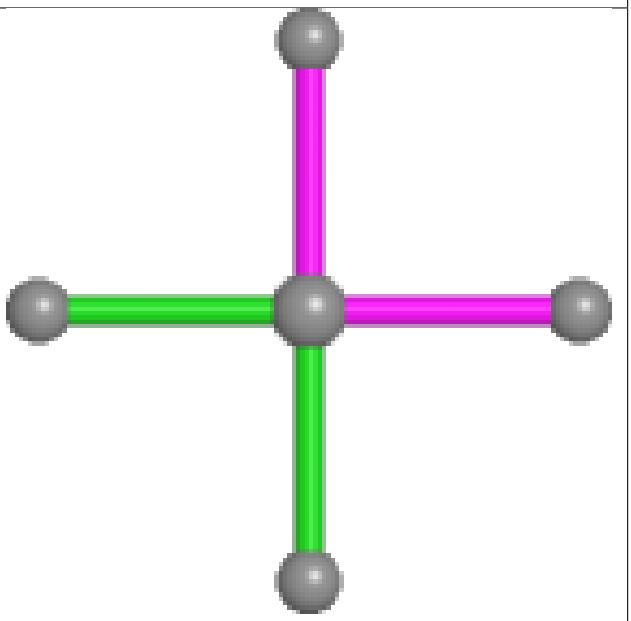


Rings

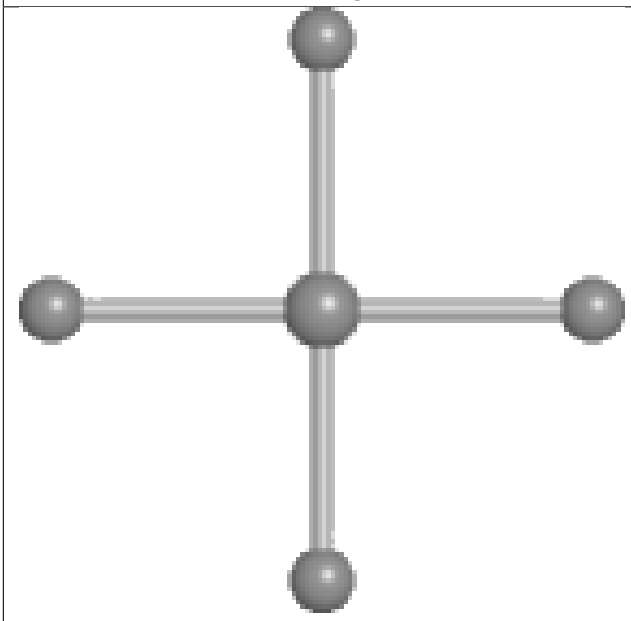
Ligand PEF M 408



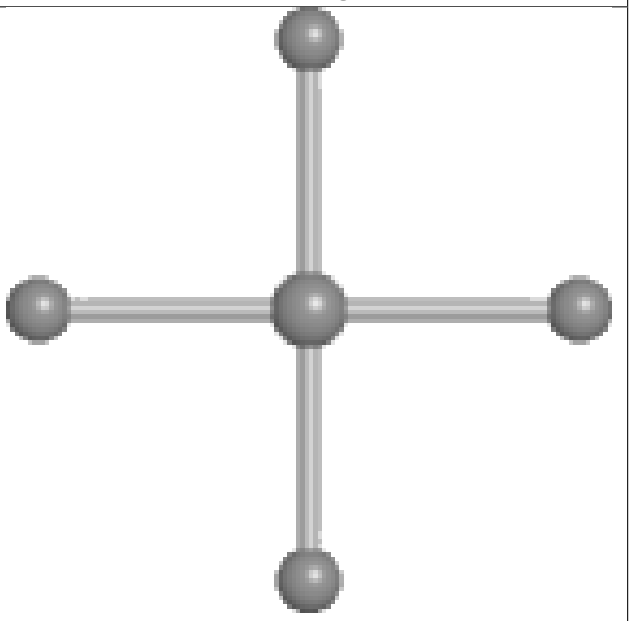
Bond lengths



Bond angles

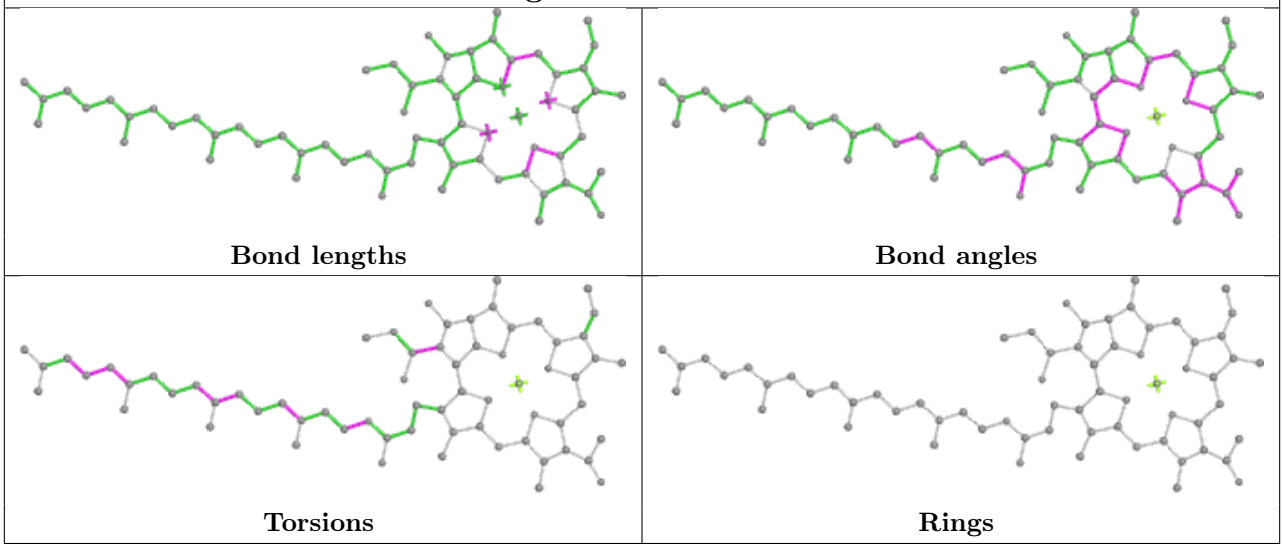


Torsions

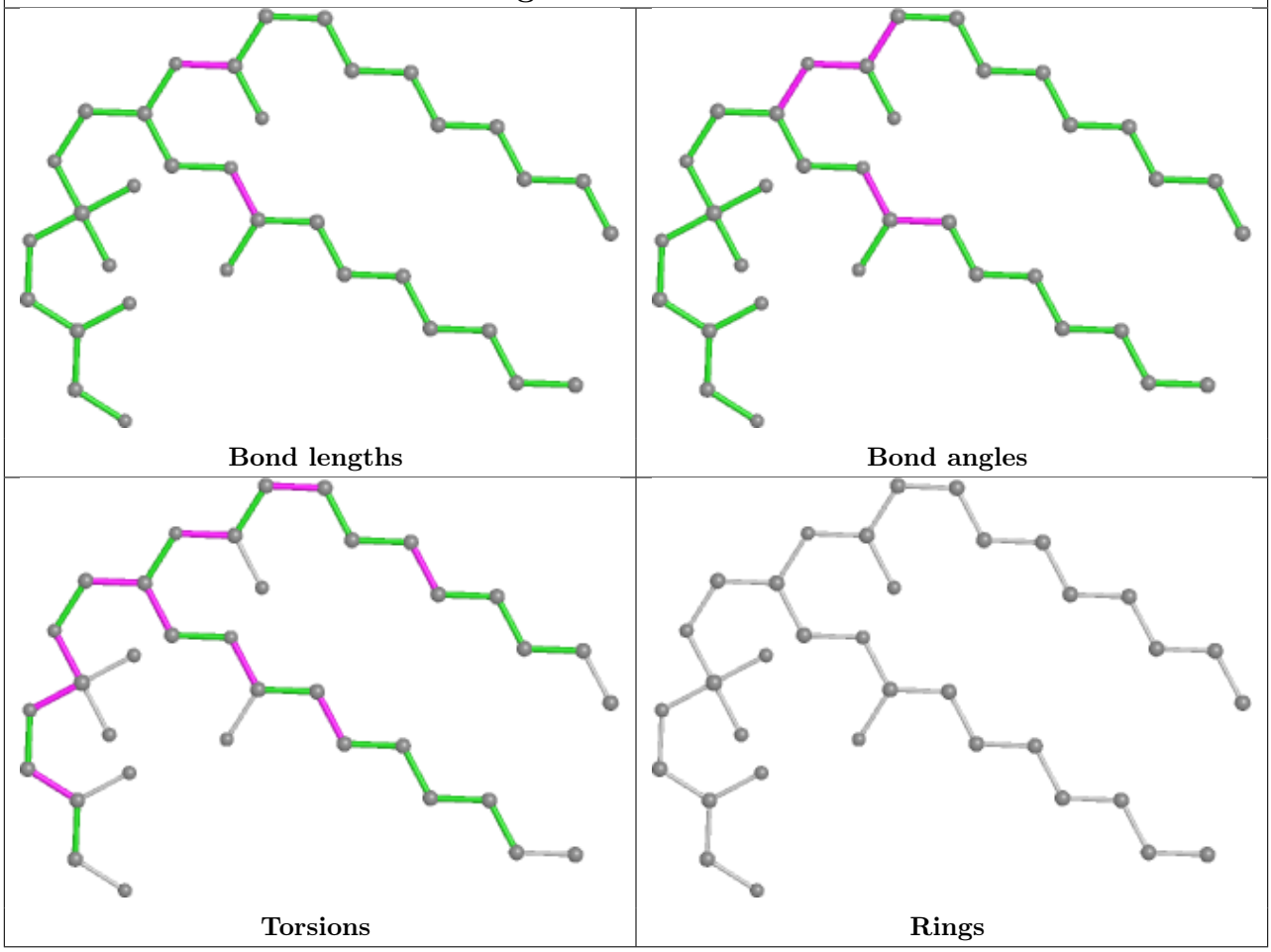


Rings

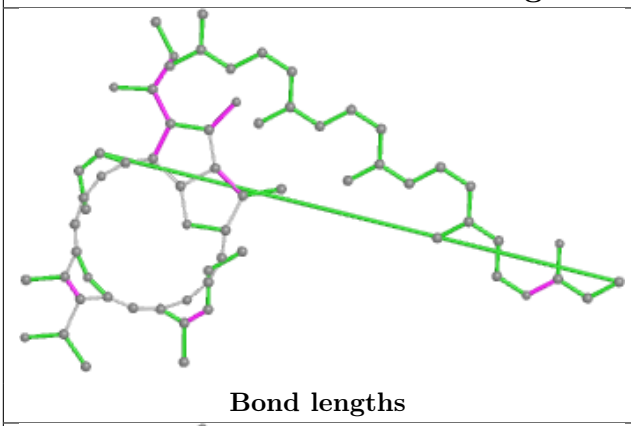
Ligand BCL A 101



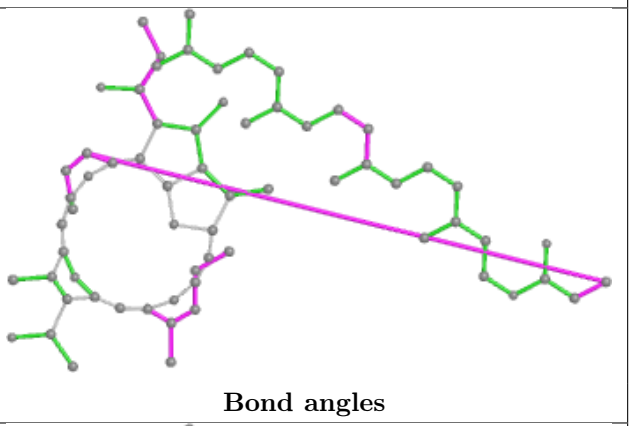
Ligand PGV D 106



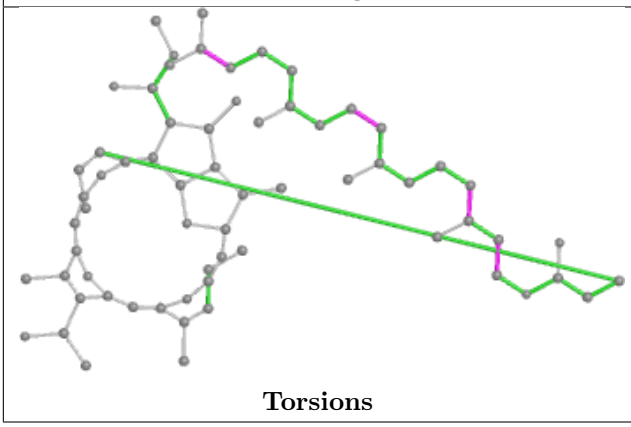
Ligand BPH L 303



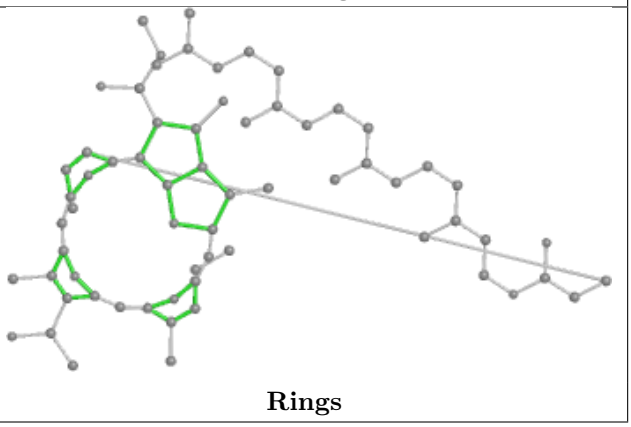
Bond lengths



Bond angles

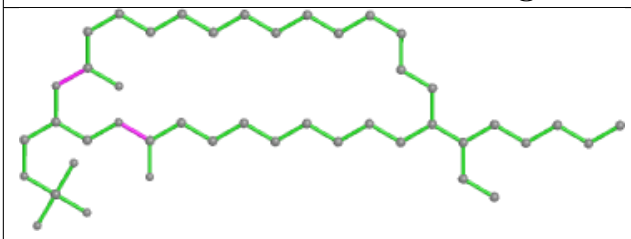


Torsions

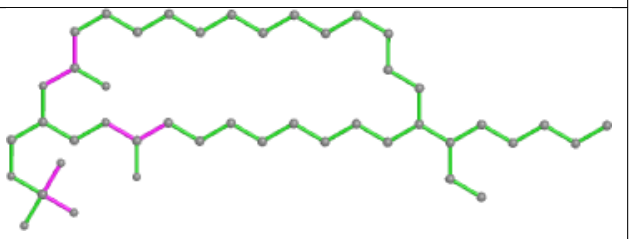


Rings

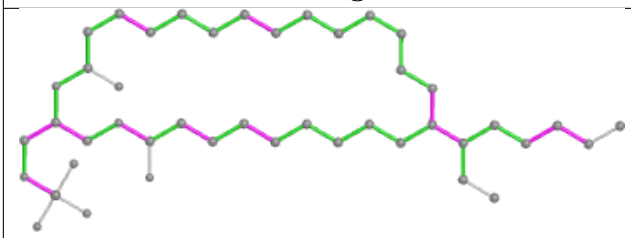
Ligand PGV M 410



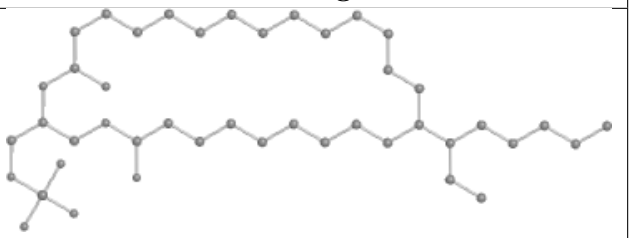
Bond lengths



Bond angles

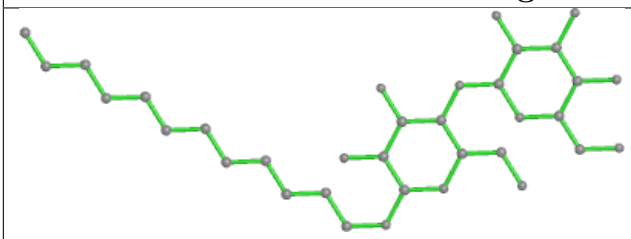


Torsions

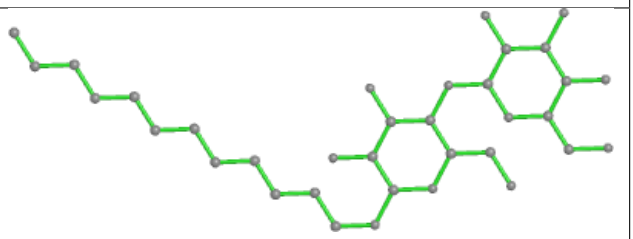


Rings

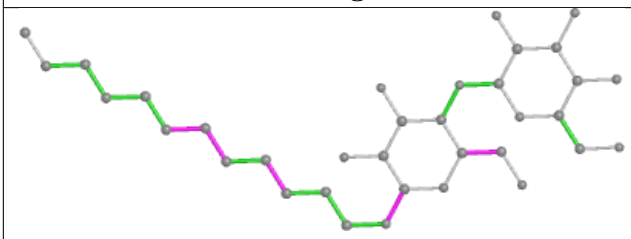
Ligand LMT M 414



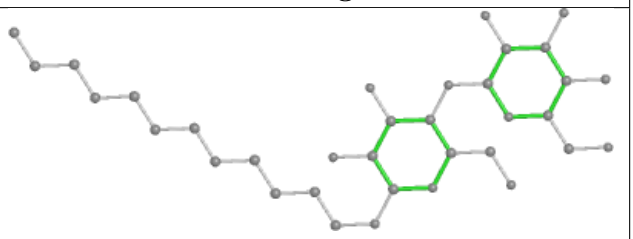
Bond lengths



Bond angles

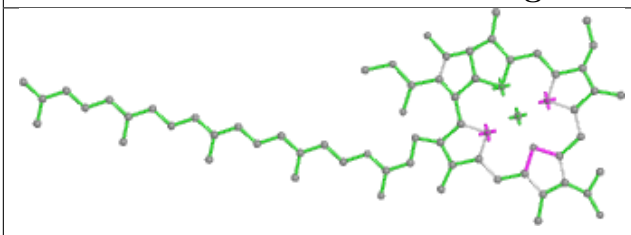


Torsions

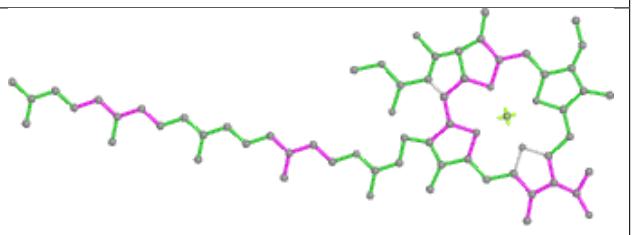


Rings

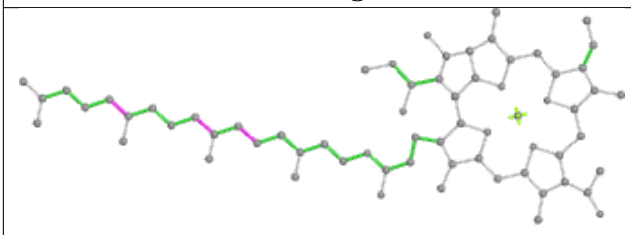
Ligand BCL U 101



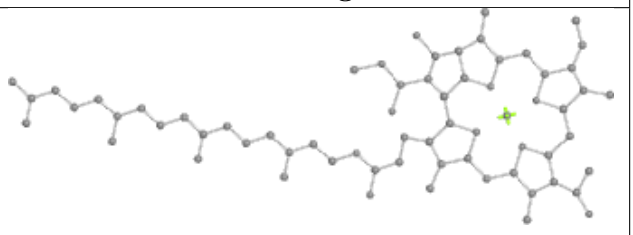
Bond lengths



Bond angles

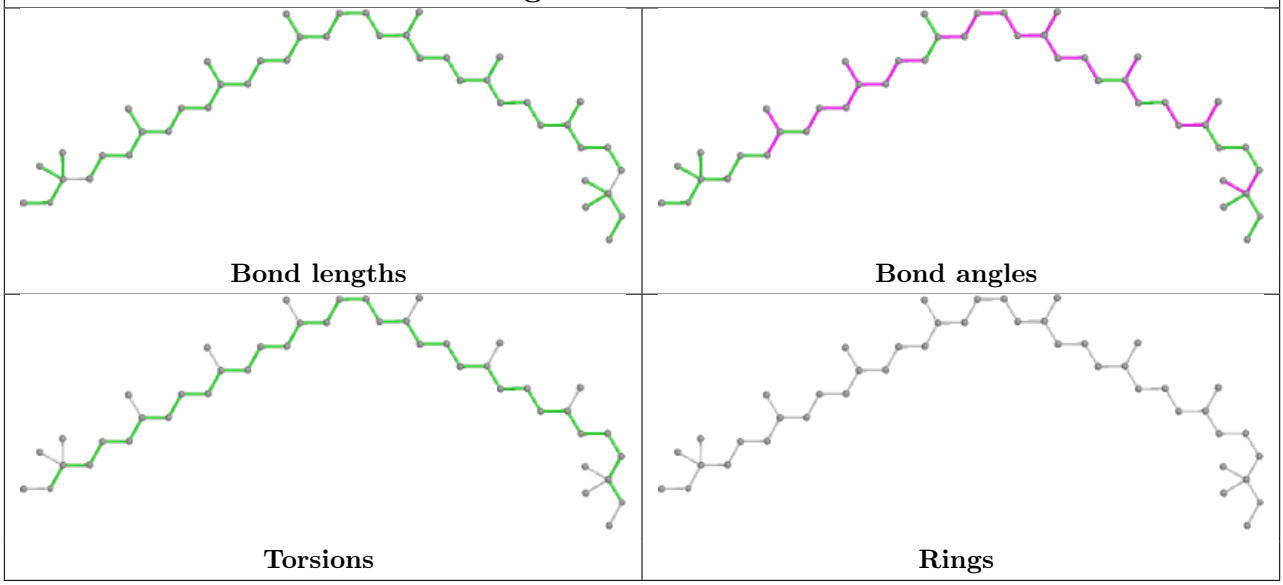


Torsions

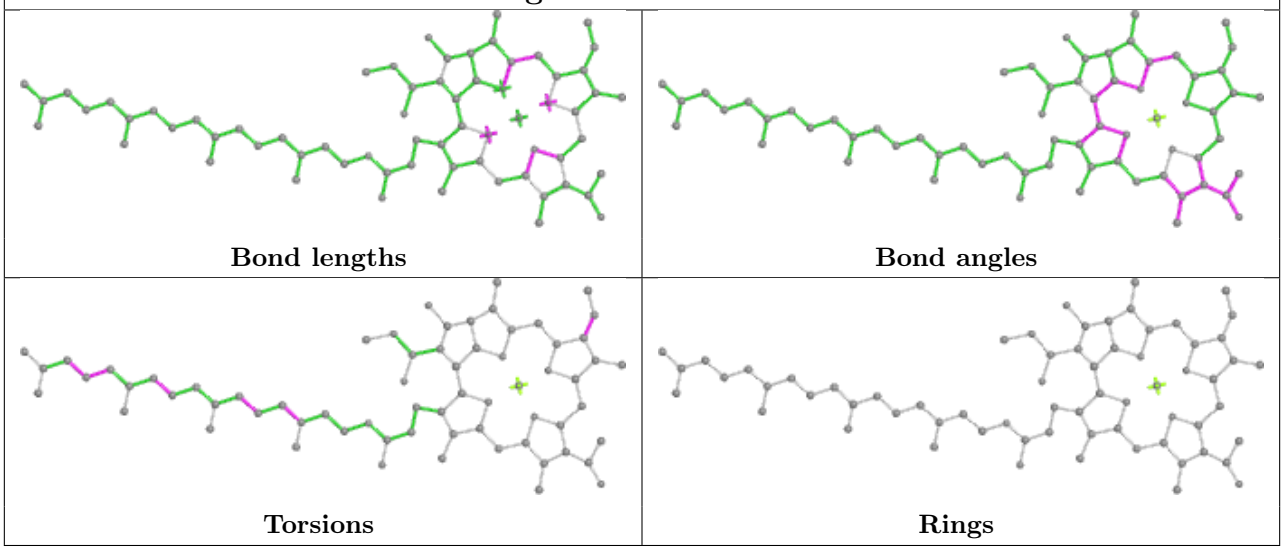


Rings

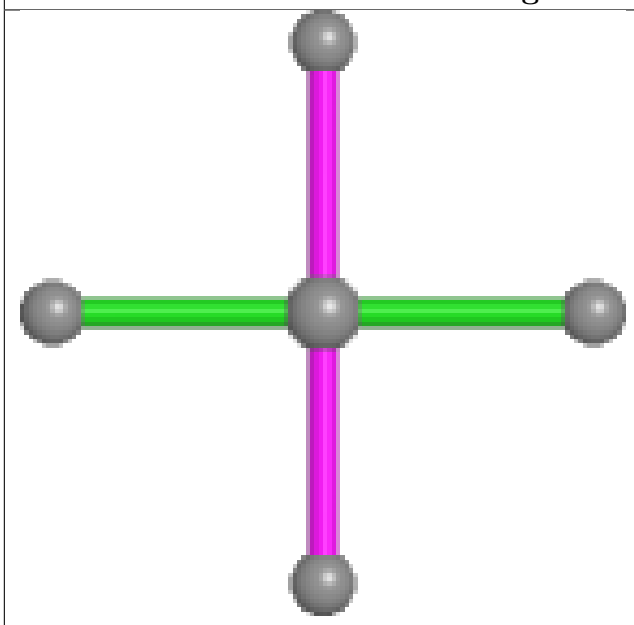
Ligand CRT N 101



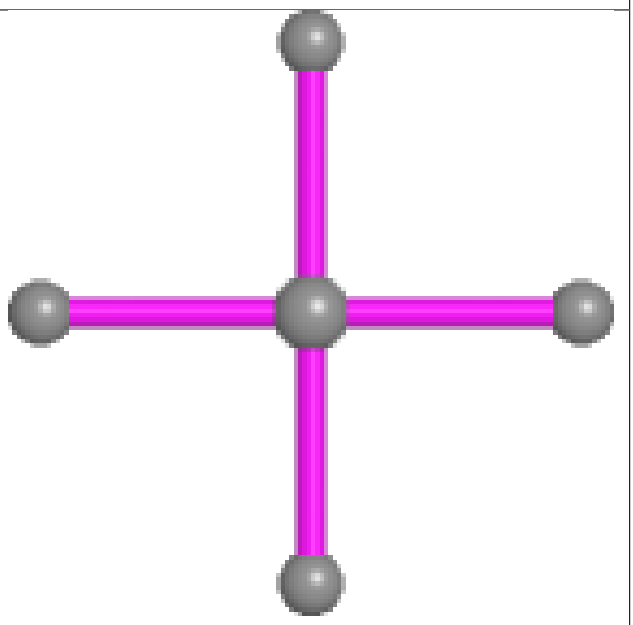
Ligand BCL Y 101



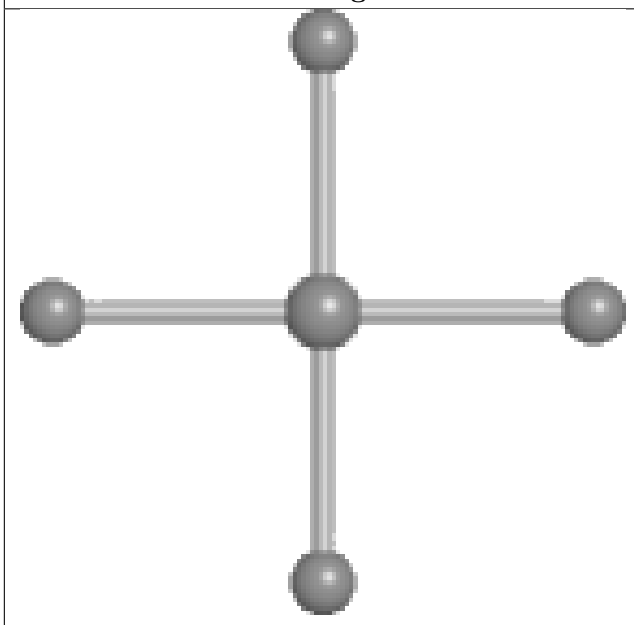
Ligand PEF W 105



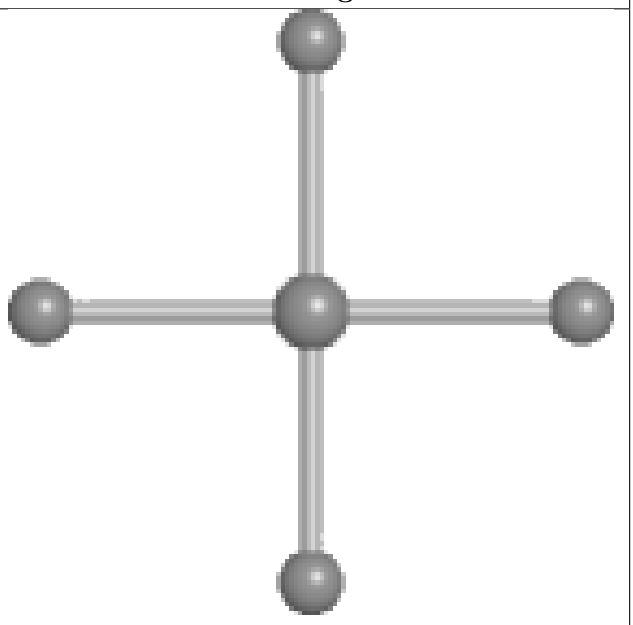
Bond lengths



Bond angles

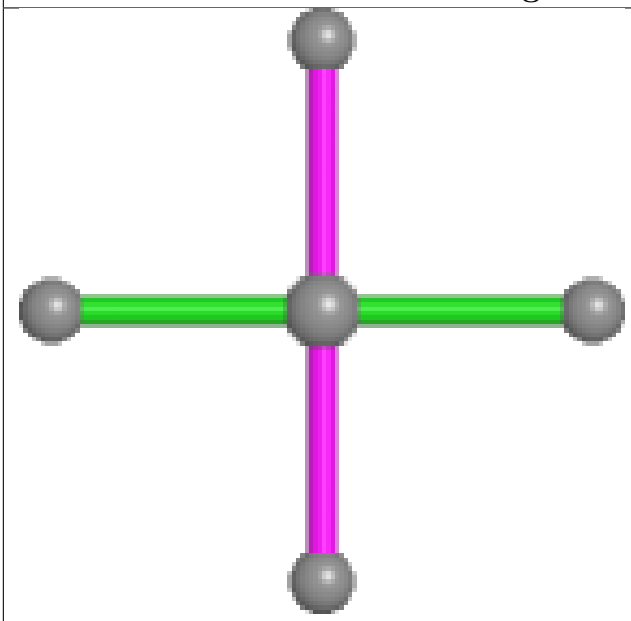


Torsions

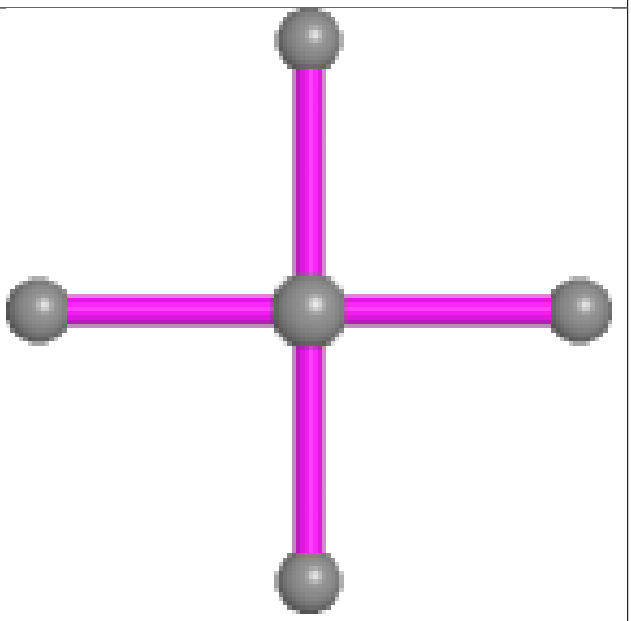


Rings

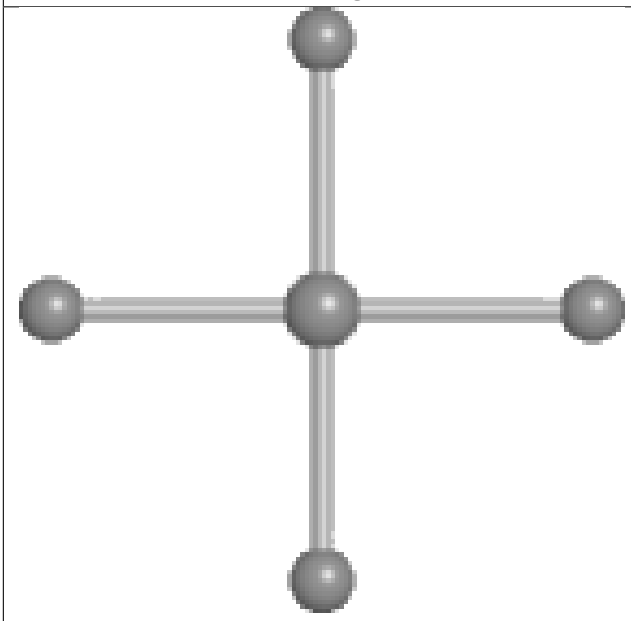
Ligand PEF M 409



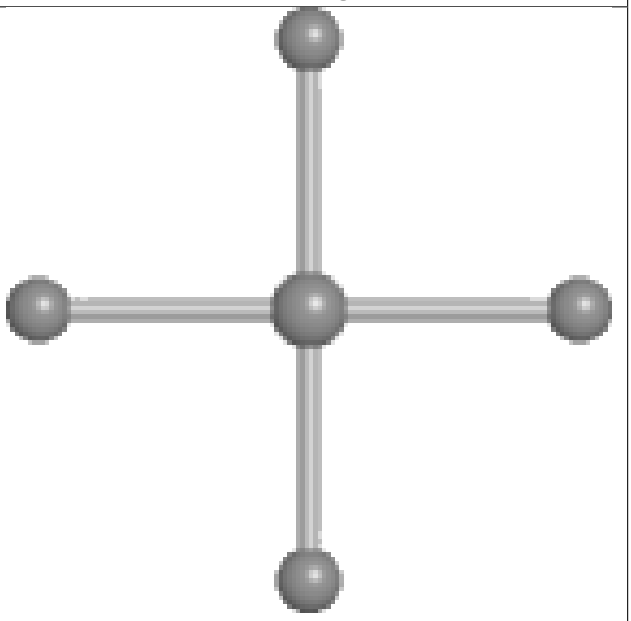
Bond lengths



Bond angles

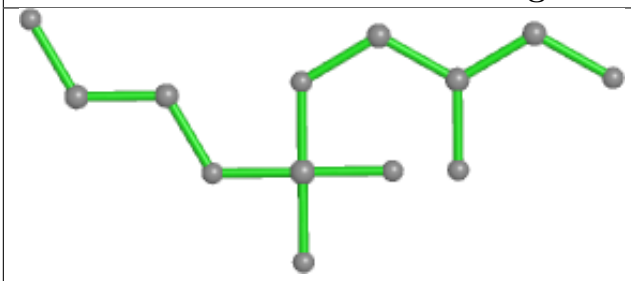


Torsions

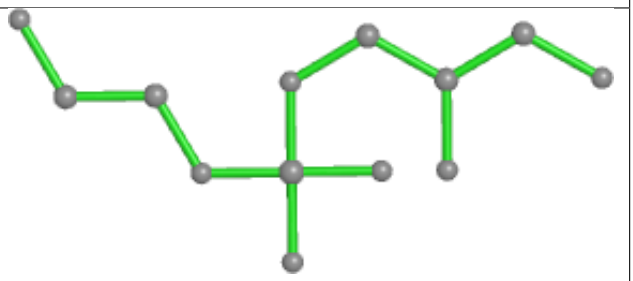


Rings

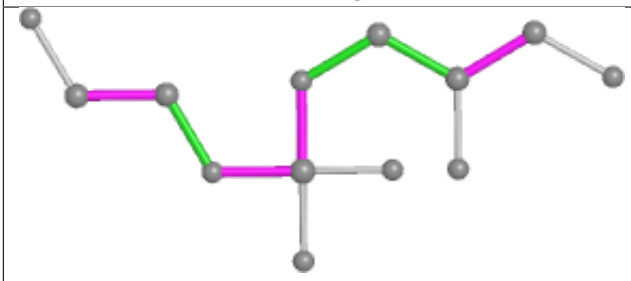
Ligand CDL 1 104



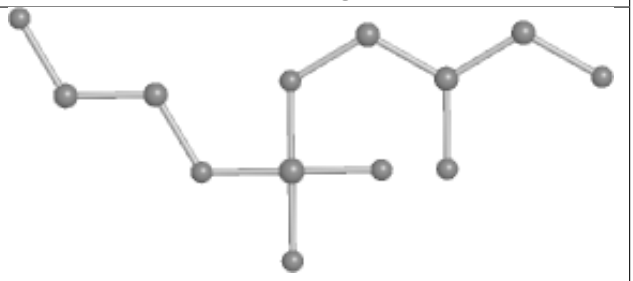
Bond lengths



Bond angles

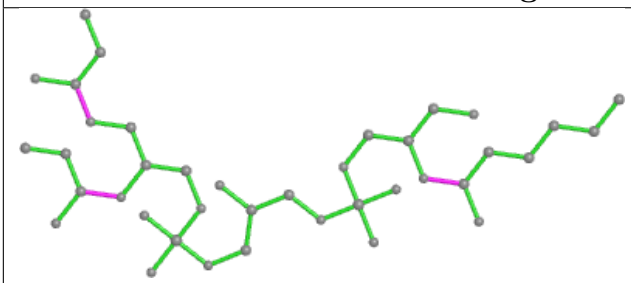


Torsions

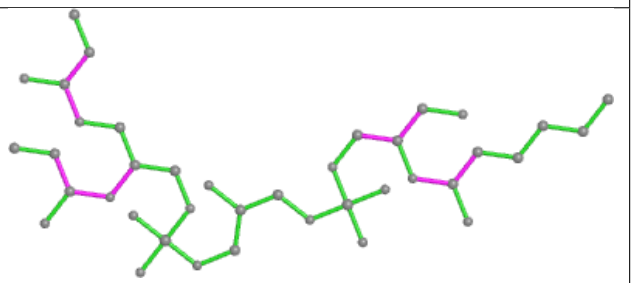


Rings

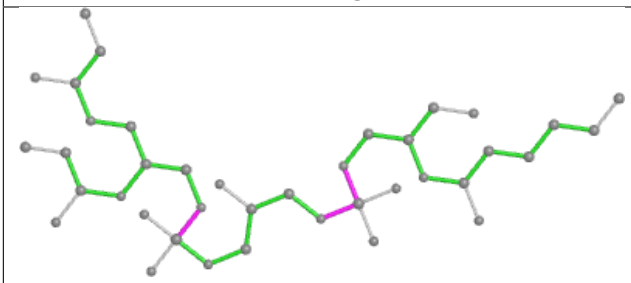
Ligand CDL M 412



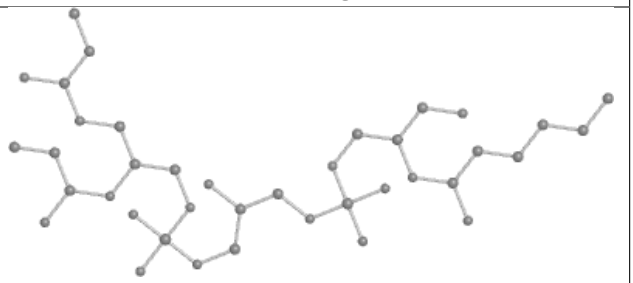
Bond lengths



Bond angles

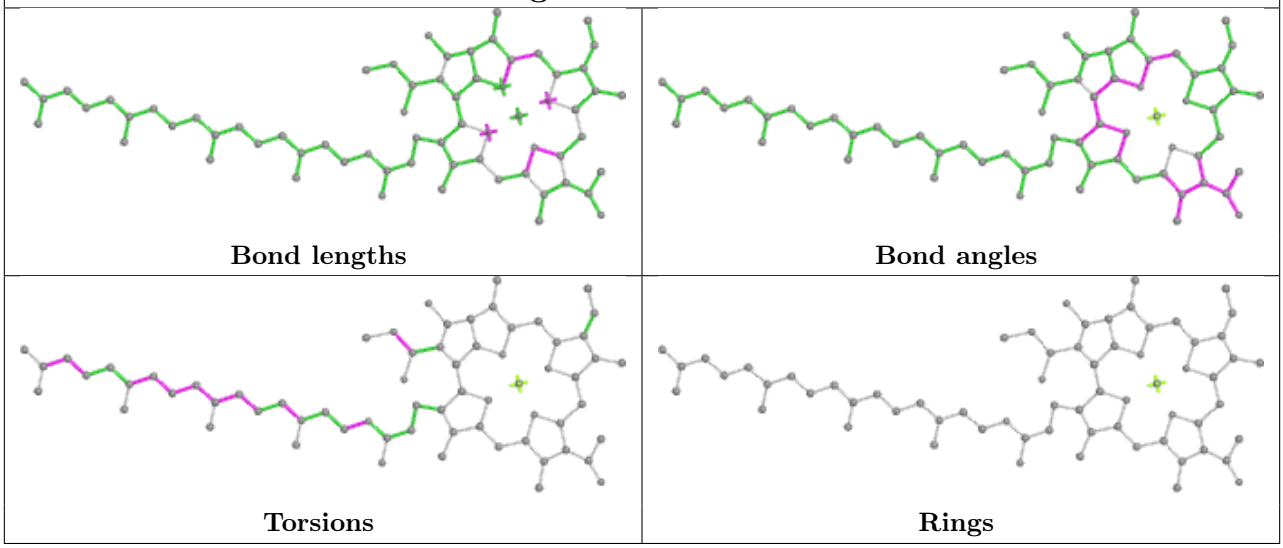


Torsions

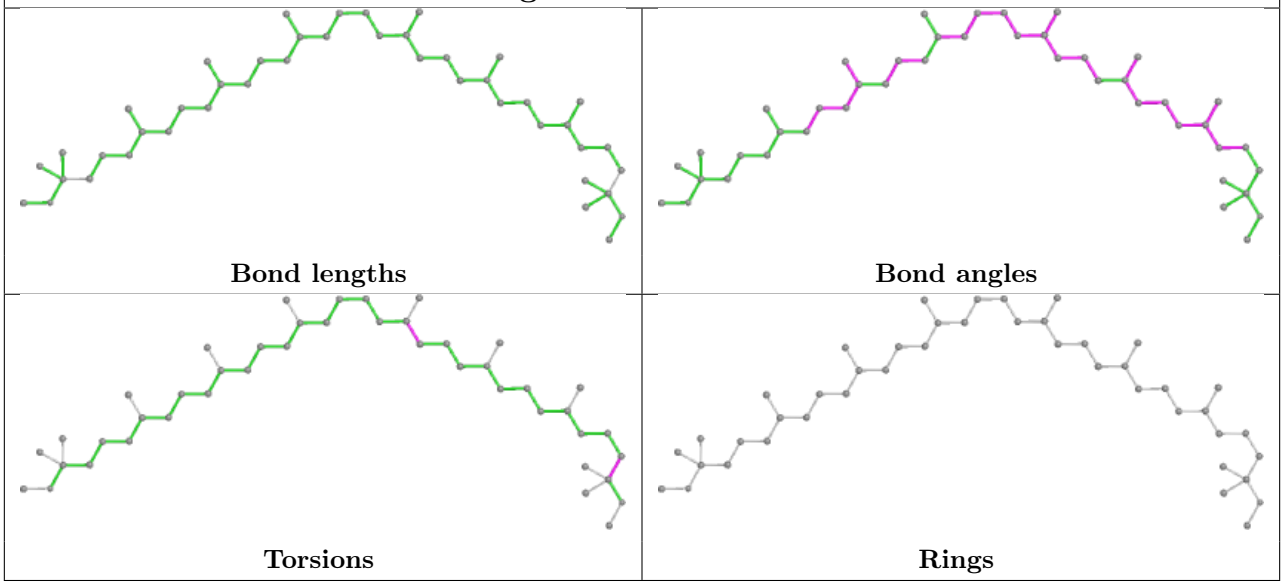


Rings

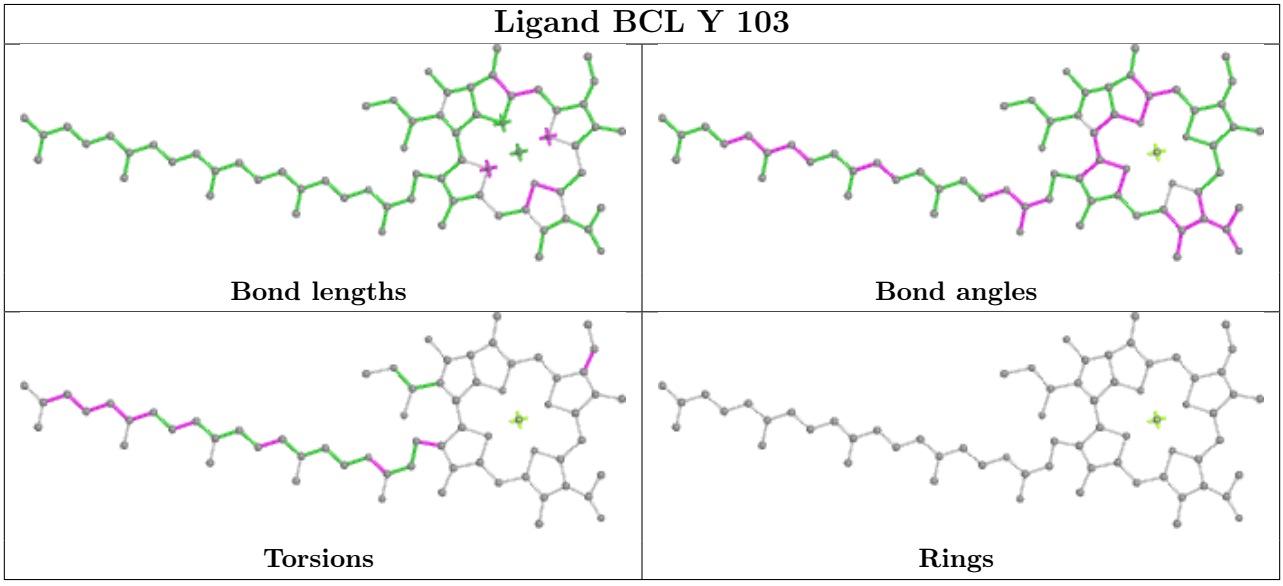
Ligand BCL 9 101



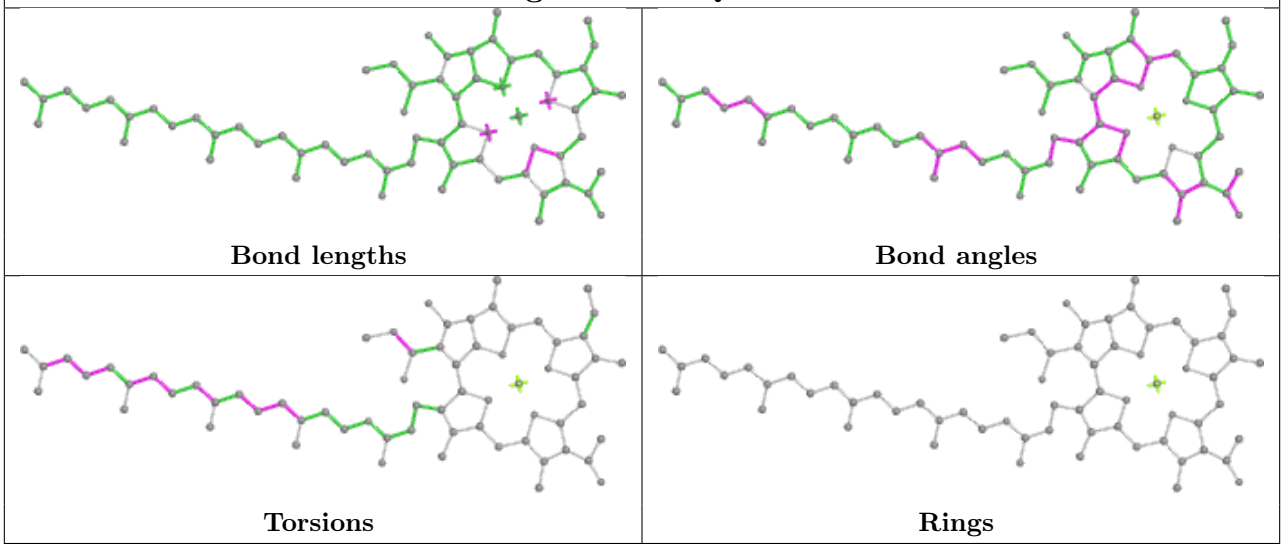
Ligand CRT W 102



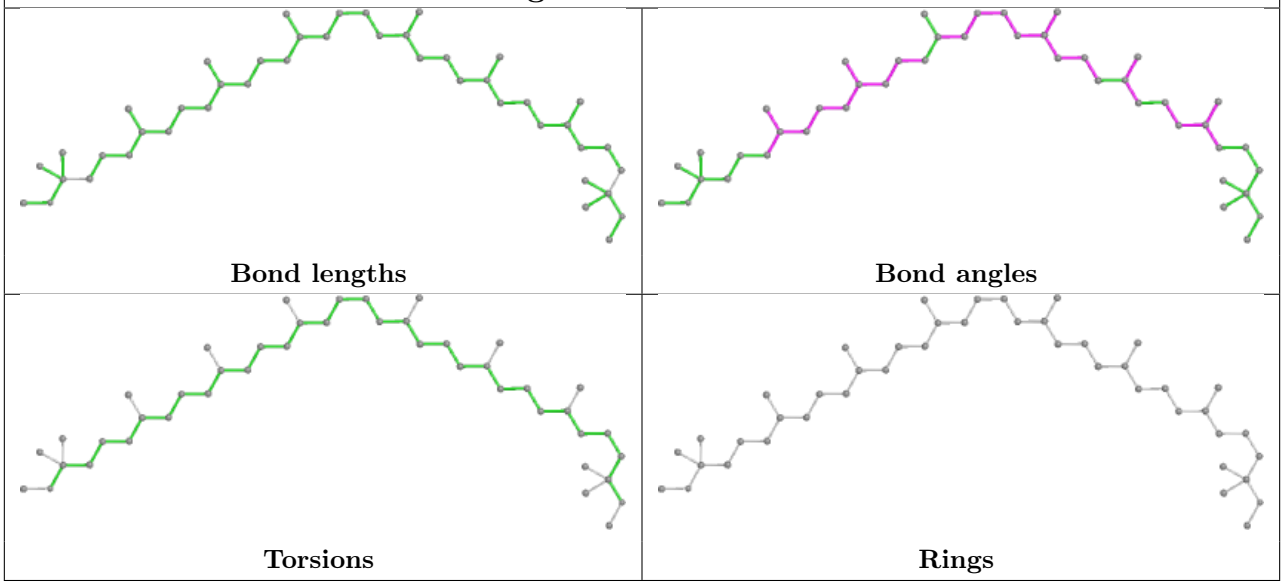
Ligand BCL Y 103



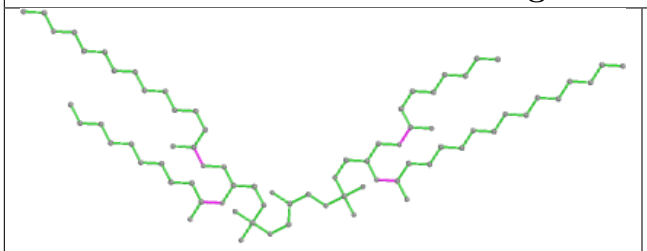
Ligand BCL Q 101



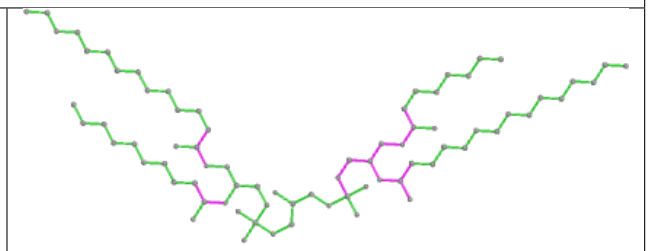
Ligand CRT Z 101



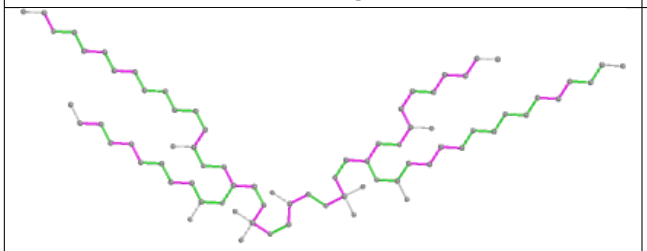
Ligand CDL S 104



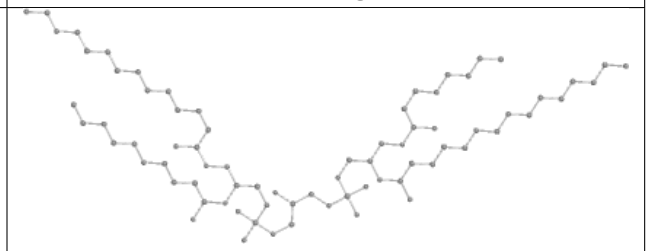
Bond lengths



Bond angles

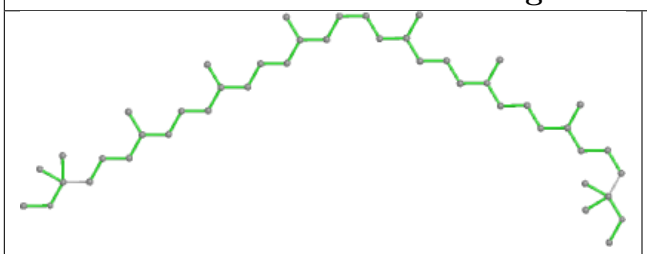


Torsions

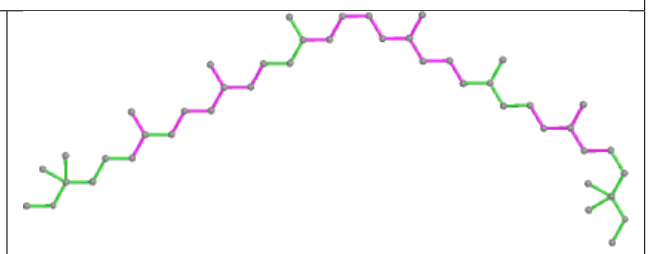


Rings

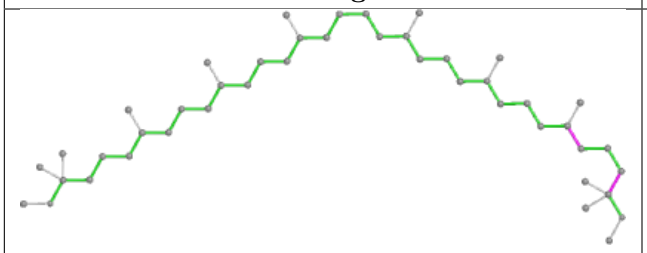
Ligand CRT B 101



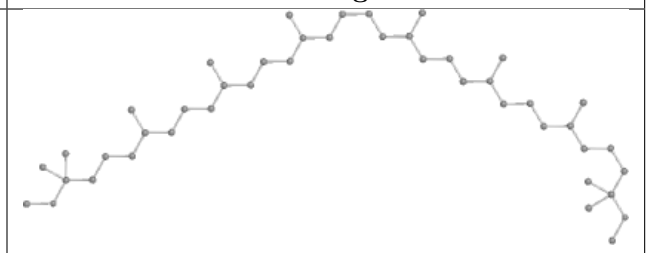
Bond lengths



Bond angles

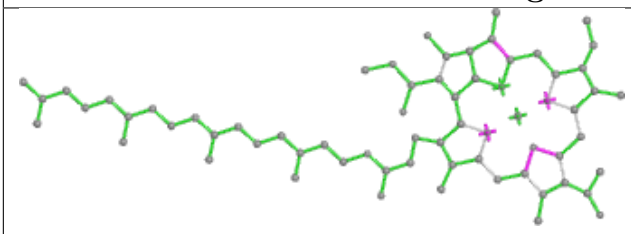


Torsions

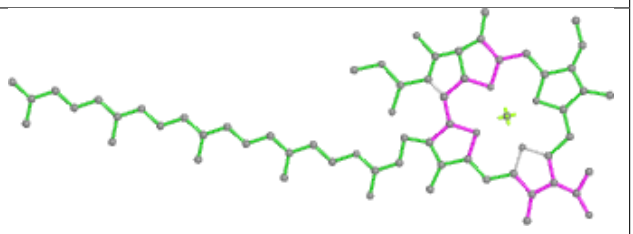


Rings

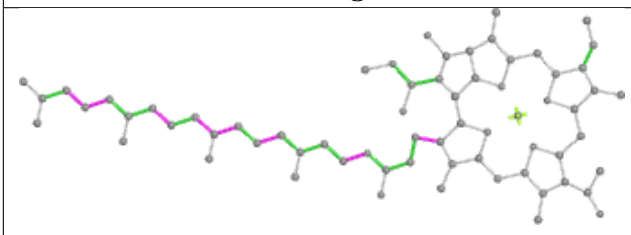
Ligand BCL F 103



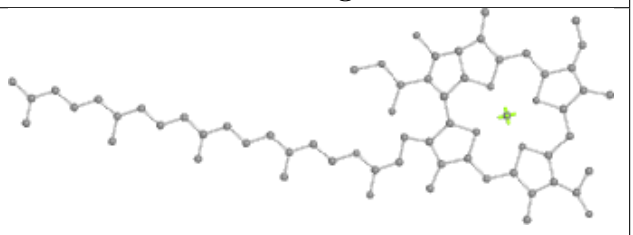
Bond lengths



Bond angles

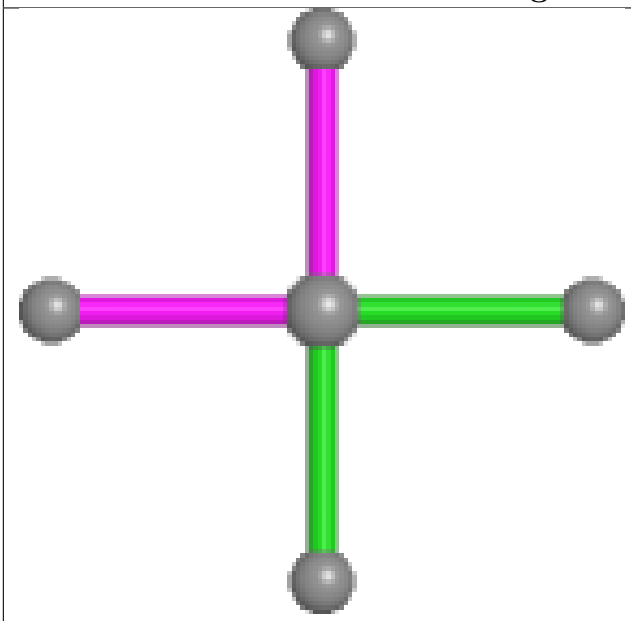


Torsions

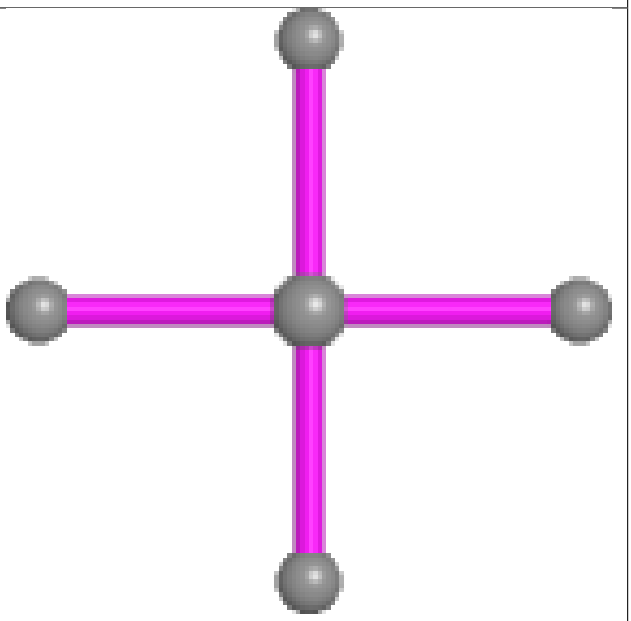


Rings

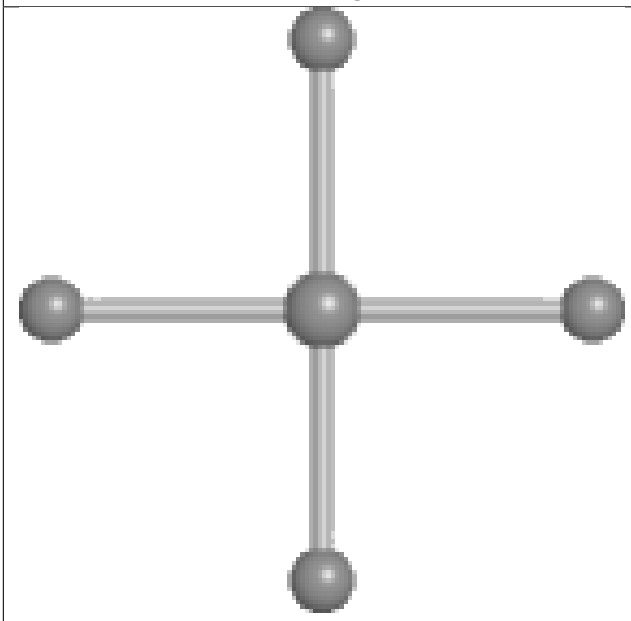
Ligand PEF 3 104



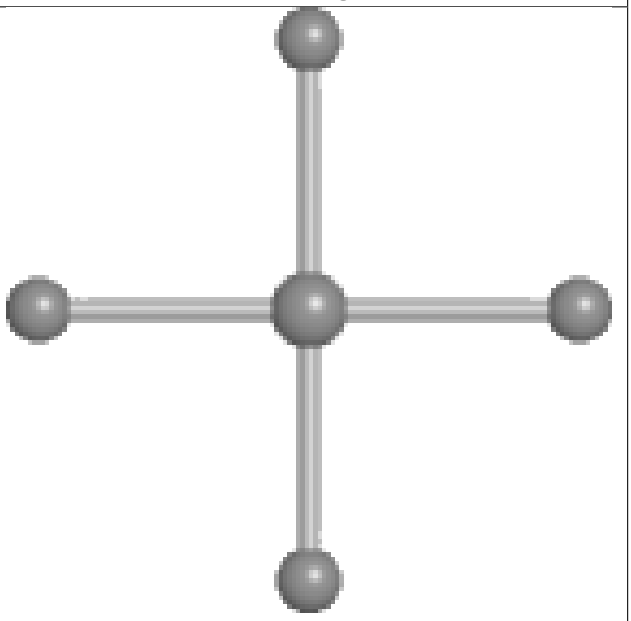
Bond lengths



Bond angles

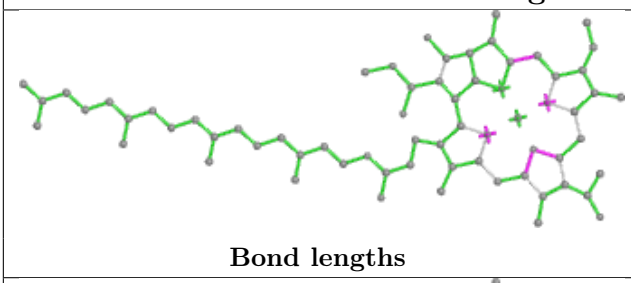


Torsions

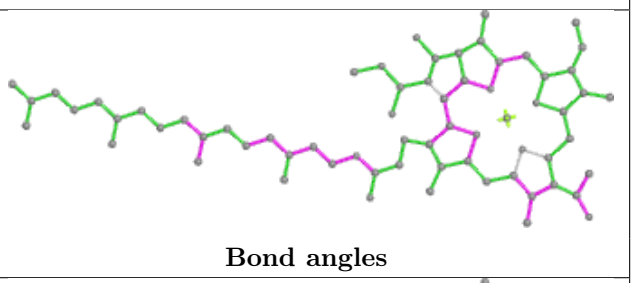


Rings

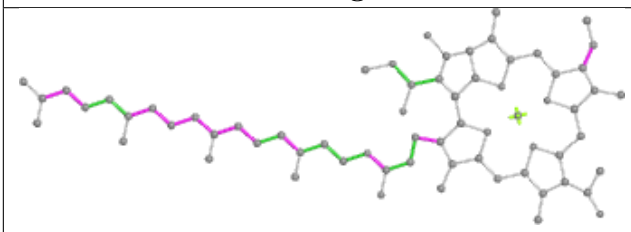
Ligand BCL S 103



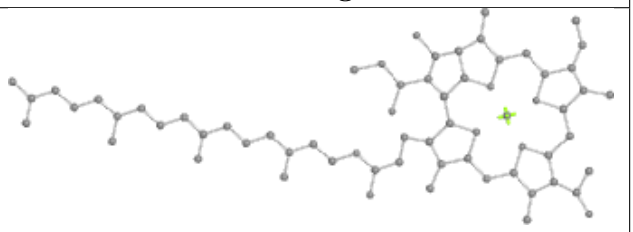
Bond lengths



Bond angles

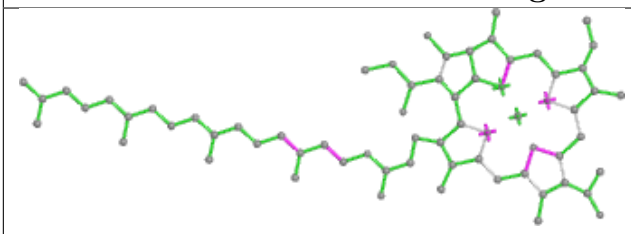


Torsions

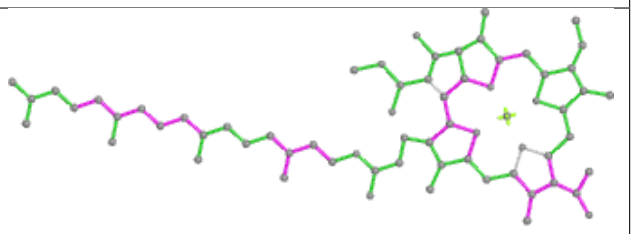


Rings

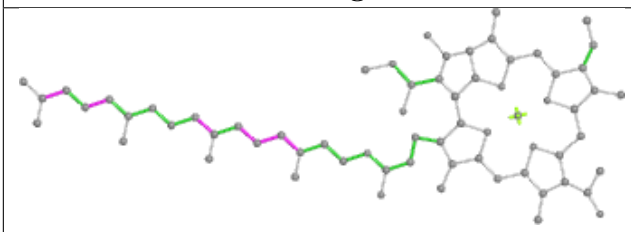
Ligand BCL 5 101



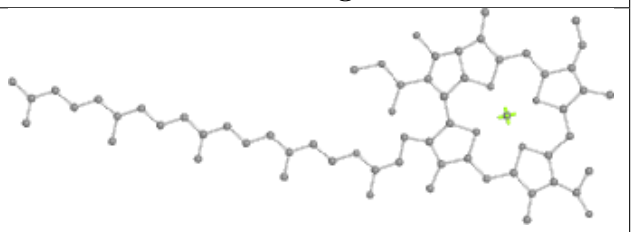
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.15	15 (4%) 30 27	71, 98, 140, 179	0
2	L	280/281 (99%)	0.22	8 (2%) 51 47	64, 93, 123, 156	0
3	M	318/325 (97%)	0.28	8 (2%) 57 55	71, 94, 119, 178	0
4	H	255/259 (98%)	0.79	44 (17%) 1 1	87, 117, 153, 208	0
5	1	56/61 (91%)	0.68	11 (19%) 1 0	97, 126, 177, 195	0
5	3	56/61 (91%)	0.34	1 (1%) 68 67	99, 129, 177, 199	0
5	5	54/61 (88%)	0.73	7 (12%) 3 2	101, 132, 199, 226	0
5	7	57/61 (93%)	1.06	10 (17%) 1 1	101, 147, 221, 254	0
5	9	57/61 (93%)	0.48	5 (8%) 10 7	108, 131, 219, 251	0
5	A	54/61 (88%)	0.42	5 (9%) 8 6	110, 133, 174, 191	0
5	D	55/61 (90%)	0.43	5 (9%) 9 6	105, 129, 192, 206	0
5	F	55/61 (90%)	0.83	9 (16%) 1 1	103, 135, 180, 190	0
5	I	57/61 (93%)	1.11	11 (19%) 1 0	102, 137, 191, 214	0
5	K	57/61 (93%)	1.00	10 (17%) 1 1	108, 132, 181, 185	0
5	O	56/61 (91%)	0.91	8 (14%) 2 2	100, 136, 173, 188	0
5	Q	57/61 (93%)	0.61	8 (14%) 2 2	98, 125, 196, 238	0
5	S	56/61 (91%)	0.61	7 (12%) 3 3	97, 129, 205, 221	0
5	U	58/61 (95%)	1.62	20 (34%) 0 0	96, 126, 199, 214	0
5	W	56/61 (91%)	0.44	8 (14%) 2 2	94, 131, 174, 211	0
5	Y	57/61 (93%)	0.52	9 (15%) 2 1	93, 121, 215, 248	0
6	0	43/47 (91%)	0.16	3 (6%) 16 12	137, 155, 181, 190	0
6	2	41/47 (87%)	0.46	4 (9%) 7 5	121, 147, 174, 178	0
6	4	42/47 (89%)	0.59	6 (14%) 2 2	125, 153, 188, 200	0
6	6	42/47 (89%)	1.77	18 (42%) 0 0	134, 160, 235, 254	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
6	8	41/47 (87%)	0.84	7 (17%) 1 1	124, 157, 227, 310	0
6	B	42/47 (89%)	0.30	6 (14%) 2 2	132, 153, 177, 204	0
6	E	38/47 (80%)	0.65	6 (15%) 2 1	132, 150, 168, 170	0
6	G	42/47 (89%)	0.88	10 (23%) 0 0	132, 154, 180, 191	0
6	J	42/47 (89%)	0.98	11 (26%) 0 0	130, 152, 185, 201	0
6	N	42/47 (89%)	0.33	4 (9%) 8 6	135, 147, 168, 180	0
6	P	42/47 (89%)	0.24	3 (7%) 16 12	126, 144, 170, 184	0
6	R	41/47 (87%)	-0.10	1 (2%) 59 56	128, 141, 154, 158	0
6	T	43/47 (91%)	0.58	7 (16%) 1 1	128, 151, 173, 185	0
6	V	42/47 (89%)	0.64	8 (19%) 1 0	122, 154, 203, 239	0
6	X	41/47 (87%)	0.92	9 (21%) 0 0	119, 146, 175, 186	0
6	Z	40/47 (85%)	0.61	7 (17%) 1 1	123, 146, 177, 192	0
7	b	83/83 (100%)	2.78	47 (56%) 0 0	128, 171, 216, 259	0
All	All	2809/2987 (94%)	0.61	366 (13%) 3 2	64, 126, 184, 310	0

The worst 5 of 366 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	b	83	GLY	15.8
6	8	10	THR	8.9
5	U	58	LEU	8.1
6	6	12	ASP	7.9
6	8	9	LEU	7.9

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 monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	PEF	3	104	5/47	0.23	0.54	207,209,211,213	0
21	PEF	W	105	5/47	0.48	0.26	185,190,191,192	0
21	PEF	W	106	5/47	0.51	0.24	242,243,244,246	0
19	CRT	G	101	44/44	0.52	0.71	113,138,160,162	0
19	CRT	8	101	44/44	0.55	0.74	127,136,180,182	0
19	CRT	J	101	44/44	0.55	0.49	107,135,154,156	0
19	CRT	0	101	44/44	0.57	0.66	109,135,168,170	0
19	CRT	O	103	44/44	0.63	0.60	107,121,149,152	0
19	CRT	W	102	44/44	0.66	0.44	102,126,152,153	0
19	CRT	P	101	44/44	0.71	0.46	100,132,147,149	0
21	PEF	H	302	5/47	0.72	0.94	202,203,203,204	0
19	CRT	V	101	44/44	0.73	0.44	99,129,151,154	0
19	CRT	N	101	44/44	0.73	0.54	104,128,137,141	0
19	CRT	B	101	44/44	0.75	0.59	116,139,157,158	0
12	PGV	M	410	46/51	0.75	0.49	101,119,128,131	0
20	CDL	U	104	62/100	0.76	0.37	146,181,209,216	0
20	CDL	Y	104	40/100	0.76	0.25	187,196,210,210	0
10	GOL	C	506	6/6	0.76	1.02	139,143,147,148	0
12	PGV	3	105	51/51	0.77	0.41	99,130,187,191	0
21	PEF	1	103	5/47	0.77	0.23	175,175,177,179	0
19	CRT	2	101	44/44	0.77	0.55	113,129,154,157	0
12	PGV	1	105	31/51	0.78	0.38	105,145,149,155	0
12	PGV	L	308	44/51	0.78	0.41	100,135,148,149	0
20	CDL	D	104	40/100	0.78	0.31	190,200,207,209	0
15	UQ8	L	309	53/53	0.78	0.51	113,137,188,192	0
19	CRT	4	101	44/44	0.78	0.55	101,131,161,164	0
19	CRT	3	103	44/44	0.79	0.72	116,127,160,162	0
19	CRT	T	101	44/44	0.79	0.33	103,122,140,142	0
20	CDL	1	104	13/100	0.80	0.20	153,157,163,166	0
19	CRT	A	104	44/44	0.80	0.46	110,126,154,156	0
12	PGV	9	104	33/51	0.82	0.30	136,155,166,169	0
10	GOL	H	301	6/6	0.83	0.44	107,113,116,117	0
21	PEF	I	103	5/47	0.83	0.28	158,159,160,160	0
20	CDL	S	104	75/100	0.84	0.33	120,157,196,209	0
21	PEF	M	407	5/47	0.84	0.14	181,183,184,187	0
12	PGV	L	307	43/51	0.84	0.34	98,150,173,178	0
15	UQ8	L	311	18/53	0.84	0.75	135,141,147,150	0
22	LMT	M	414	35/35	0.84	0.29	128,162,179,183	0
21	PEF	K	104	27/47	0.85	0.37	119,140,143,145	0
12	PGV	M	411	37/51	0.85	0.44	120,151,194,196	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CDL	O	104	86/100	0.86	0.34	120,144,155,159	0
15	UQ8	M	413	18/53	0.86	0.28	154,157,166,170	0
22	LMT	H	304	35/35	0.86	0.28	95,142,151,155	0
18	MQ8	M	404	53/53	0.88	0.31	84,88,161,163	0
13	BCL	K	103	66/66	0.89	0.34	119,137,170,181	0
19	CRT	Z	101	44/44	0.89	0.55	91,133,166,169	0
13	BCL	S	103	66/66	0.89	0.36	106,120,176,189	0
20	CDL	M	406	100/100	0.89	0.42	92,119,155,158	0
19	CRT	M	405	44/44	0.89	0.26	72,88,127,129	0
9	CA	1	102	1/1	0.90	0.05	107,107,107,107	0
12	PGV	C	508	21/51	0.90	0.27	103,127,138,143	0
20	CDL	M	412	39/100	0.90	0.21	81,113,129,135	0
20	CDL	H	305	79/100	0.90	0.31	93,118,143,146	0
16	SO4	L	306	5/5	0.90	0.42	178,180,180,181	0
20	CDL	D	105	64/100	0.90	0.28	130,142,153,159	0
12	PGV	D	106	35/51	0.90	0.27	115,135,159,167	0
12	PGV	H	303	36/51	0.91	0.28	86,123,130,131	0
13	BCL	U	103	66/66	0.91	0.37	113,131,174,185	0
15	UQ8	L	304	33/53	0.91	0.41	75,85,129,131	0
9	CA	D	102	1/1	0.91	0.05	127,127,127,127	0
9	CA	U	102	1/1	0.91	0.06	112,112,112,112	0
13	BCL	5	103	66/66	0.92	0.34	116,136,163,167	0
13	BCL	J	102	66/66	0.92	0.37	121,137,160,166	0
13	BCL	K	101	66/66	0.92	0.30	123,132,162,174	0
15	UQ8	L	310	33/53	0.92	0.28	118,126,138,139	0
9	CA	5	102	1/1	0.92	0.07	118,118,118,118	0
13	BCL	Q	103	66/66	0.92	0.25	105,123,170,181	0
13	BCL	S	101	66/66	0.92	0.29	111,123,163,167	0
13	BCL	A	101	66/66	0.92	0.27	130,139,162,170	0
13	BCL	A	103	66/66	0.92	0.34	114,124,178,185	0
9	CA	F	102	1/1	0.93	0.05	129,129,129,129	0
13	BCL	W	101	66/66	0.93	0.33	105,127,170,178	0
13	BCL	O	101	66/66	0.93	0.32	128,137,170,177	0
13	BCL	9	103	66/66	0.93	0.31	113,129,177,186	0
13	BCL	P	102	66/66	0.93	0.27	123,140,185,197	0
13	BCL	U	101	66/66	0.93	0.26	102,122,167,172	0
13	BCL	D	103	66/66	0.94	0.34	118,126,164,173	0
13	BCL	F	101	66/66	0.94	0.29	119,131,162,173	0
21	PEF	M	408	5/47	0.94	0.17	131,134,135,137	0
13	BCL	I	101	66/66	0.94	0.36	121,136,176,182	0
13	BCL	Q	101	66/66	0.94	0.30	110,128,174,181	0
13	BCL	W	104	66/66	0.94	0.26	112,123,162,167	0

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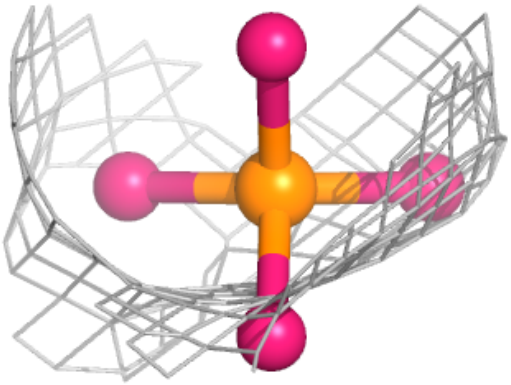
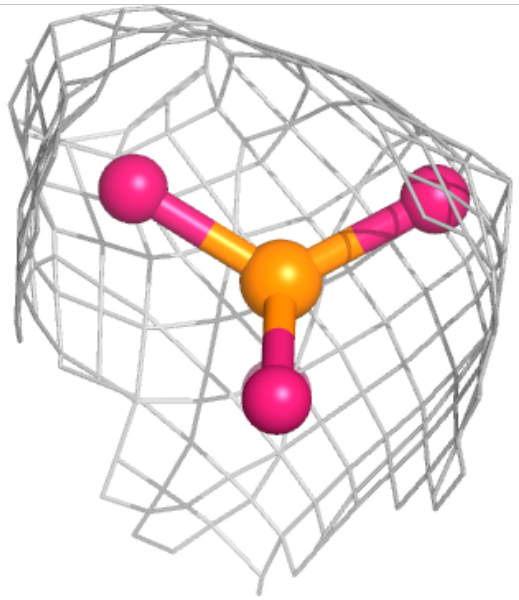
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	BCL	5	101	66/66	0.94	0.28	109,128,163,169	0
9	CA	O	102	1/1	0.94	0.09	121,121,121,121	0
13	BCL	7	101	61/66	0.94	0.33	121,135,185,188	0
13	BCL	7	103	66/66	0.94	0.29	124,136,182,184	0
13	BCL	D	101	66/66	0.94	0.33	109,130,160,165	0
14	BPH	M	402	65/65	0.94	0.26	75,83,147,154	0
9	CA	C	505	1/1	0.95	0.28	103,103,103,103	0
21	PEF	M	409	5/47	0.95	0.36	113,113,114,115	0
9	CA	7	102	1/1	0.95	0.04	115,115,115,115	0
13	BCL	9	101	66/66	0.95	0.25	126,133,177,179	0
13	BCL	Y	101	66/66	0.95	0.30	101,118,165,167	0
13	BCL	1	101	66/66	0.95	0.25	106,118,161,165	0
13	BCL	2	102	66/66	0.95	0.35	104,125,164,174	0
13	BCL	3	101	66/66	0.95	0.32	108,131,180,185	0
13	BCL	4	102	66/66	0.95	0.31	110,131,169,182	0
9	CA	9	102	1/1	0.95	0.14	120,120,120,120	0
9	CA	3	102	1/1	0.95	0.07	121,121,121,121	0
13	BCL	F	103	66/66	0.96	0.32	123,135,177,188	0
9	CA	Q	102	1/1	0.96	0.10	116,116,116,116	0
9	CA	S	102	1/1	0.96	0.04	111,111,111,111	0
13	BCL	L	301	66/66	0.96	0.20	64,80,101,108	0
14	BPH	L	303	65/65	0.96	0.24	68,82,100,103	0
13	BCL	L	305	66/66	0.96	0.24	69,80,135,143	0
13	BCL	Y	103	66/66	0.96	0.32	109,120,159,166	0
13	BCL	M	401	66/66	0.96	0.20	61,80,89,92	0
9	CA	I	102	1/1	0.96	0.11	139,139,139,139	0
9	CA	Y	102	1/1	0.96	0.07	115,115,115,115	0
9	CA	K	102	1/1	0.96	0.06	120,120,120,120	0
11	LHG	C	507	9/49	0.96	0.19	84,90,99,100	0
9	CA	A	102	1/1	0.96	0.10	123,123,123,123	0
13	BCL	L	302	66/66	0.97	0.16	59,68,90,98	0
17	FE	M	403	1/1	0.97	0.21	75,75,75,75	0
9	CA	W	103	1/1	0.98	0.06	105,105,105,105	0
8	HEM	C	503	43/43	0.98	0.23	70,80,95,100	0
8	HEM	C	504	43/43	0.98	0.21	74,79,89,92	0
8	HEM	C	501	43/43	0.98	0.22	97,107,117,120	0
8	HEM	C	502	43/43	0.98	0.22	71,88,104,106	0
23	SF4	b	101	8/8	0.99	0.08	123,152,192,194	0

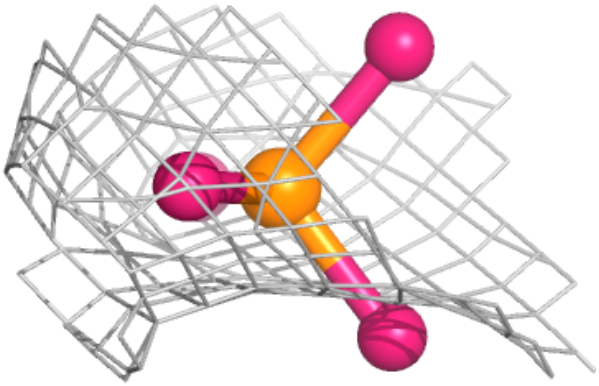
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PEF 3 104:

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

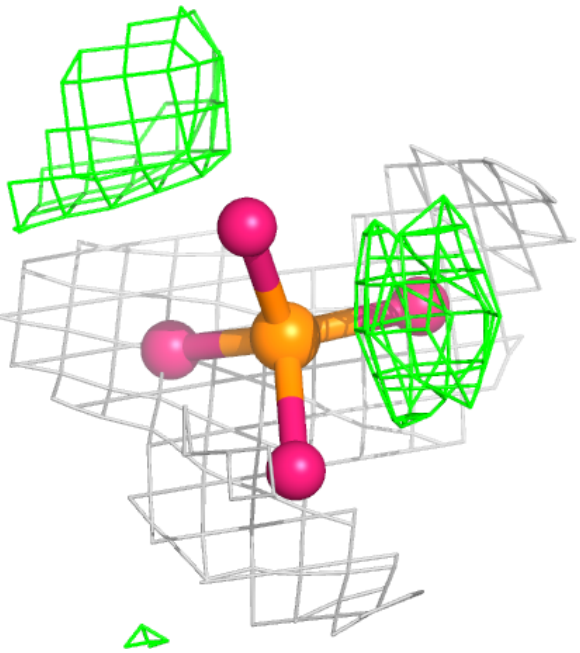


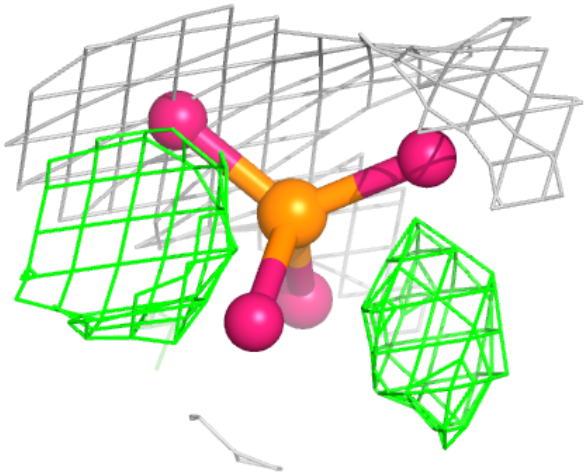


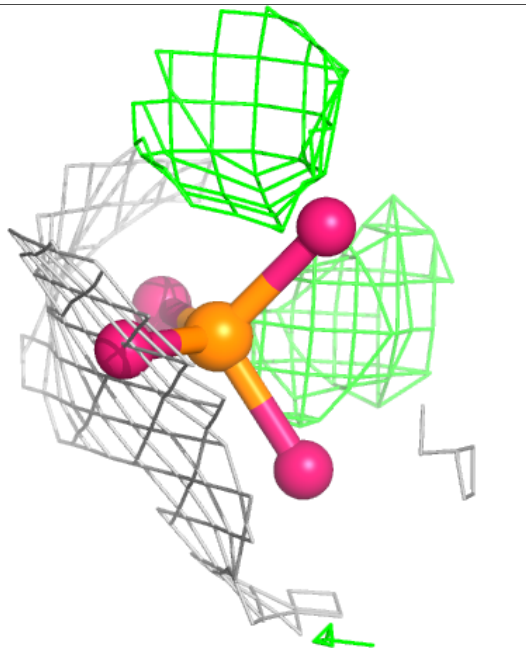


Electron density around PEF W 105:

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

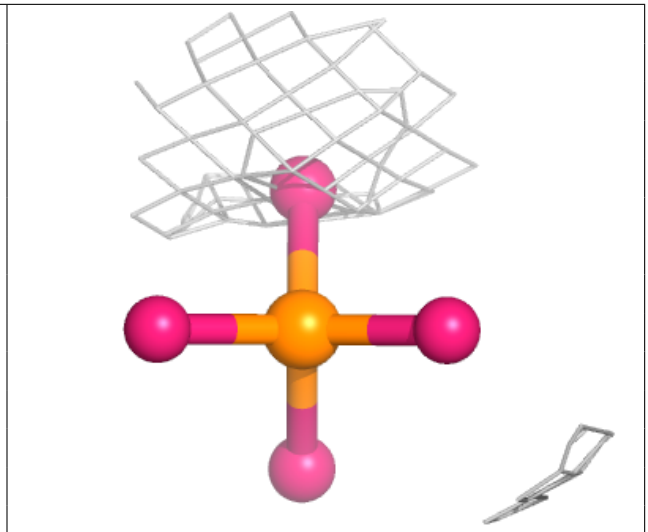


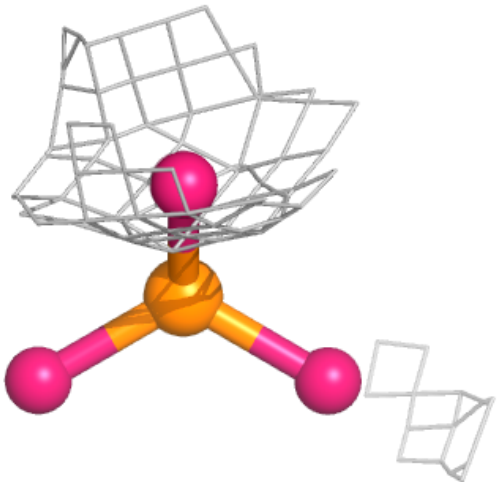


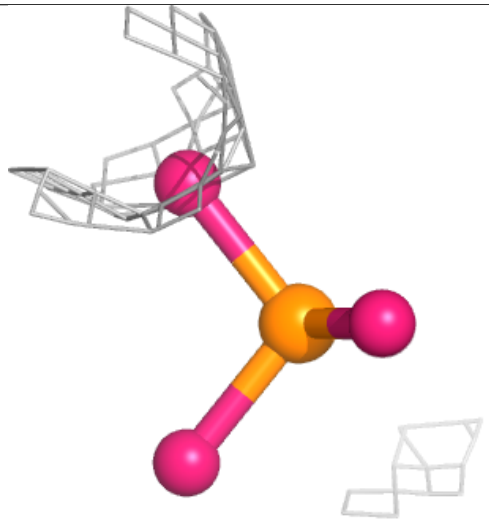


Electron density around PEF W 106:

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

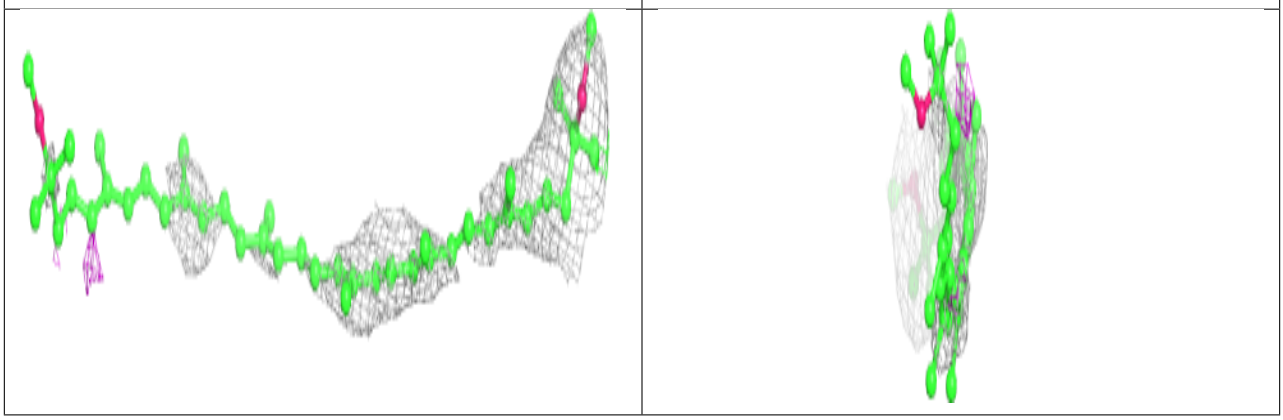






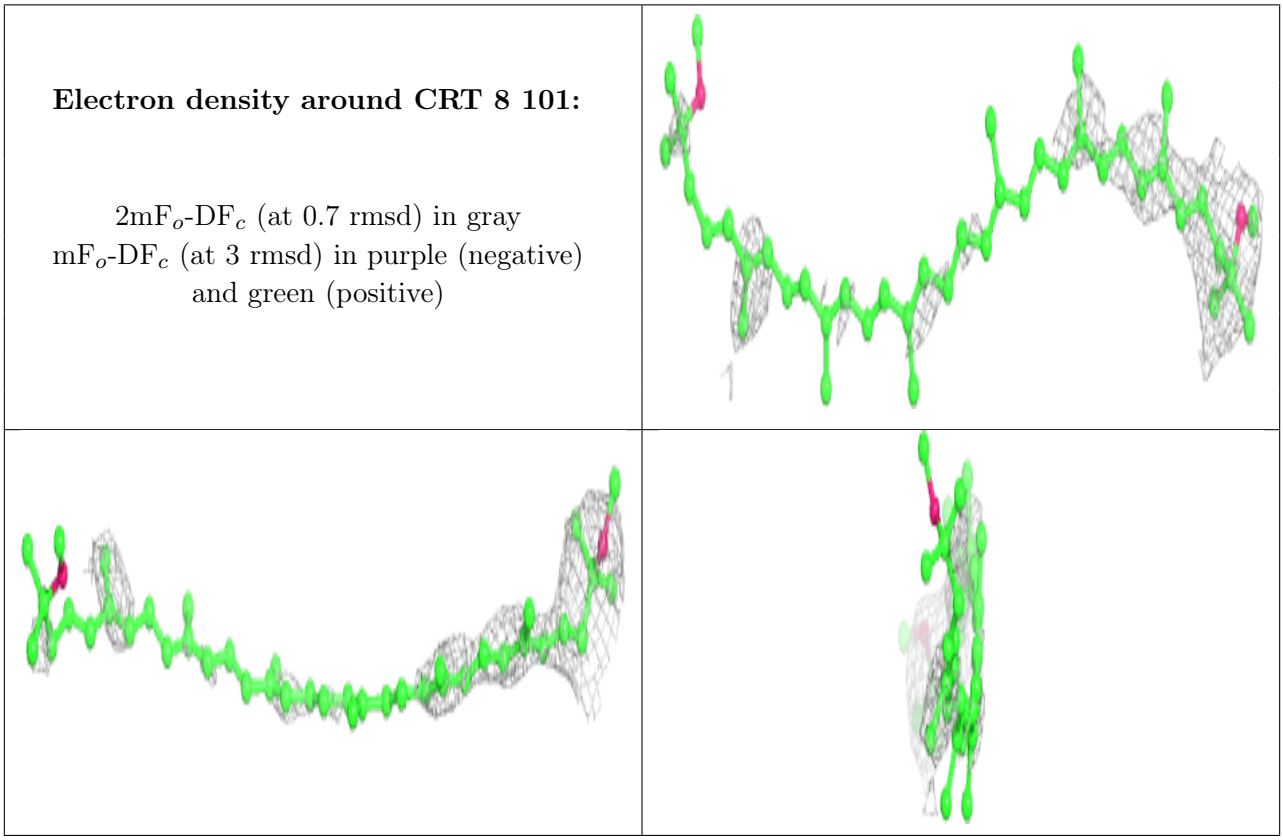
Electron density around CRT G 101:

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



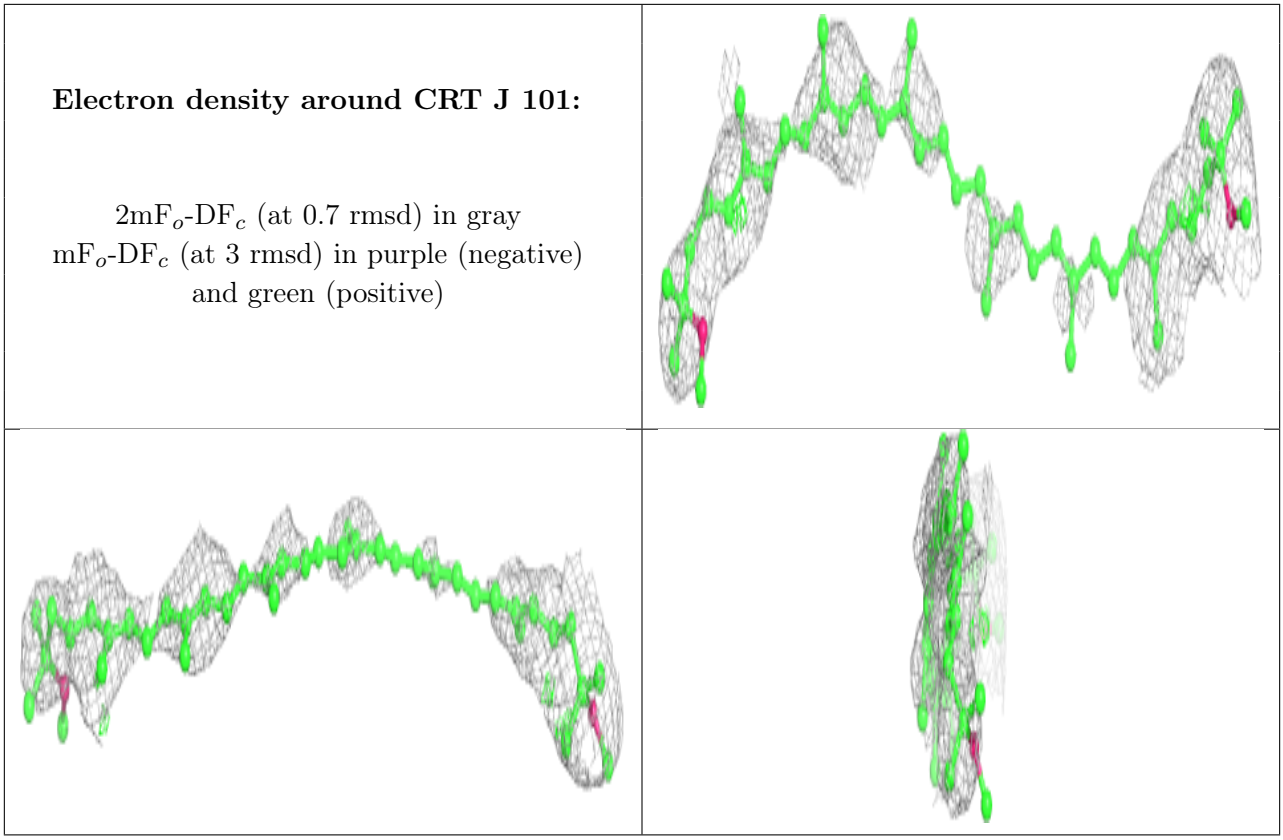
Electron density around CRT 8 101:

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



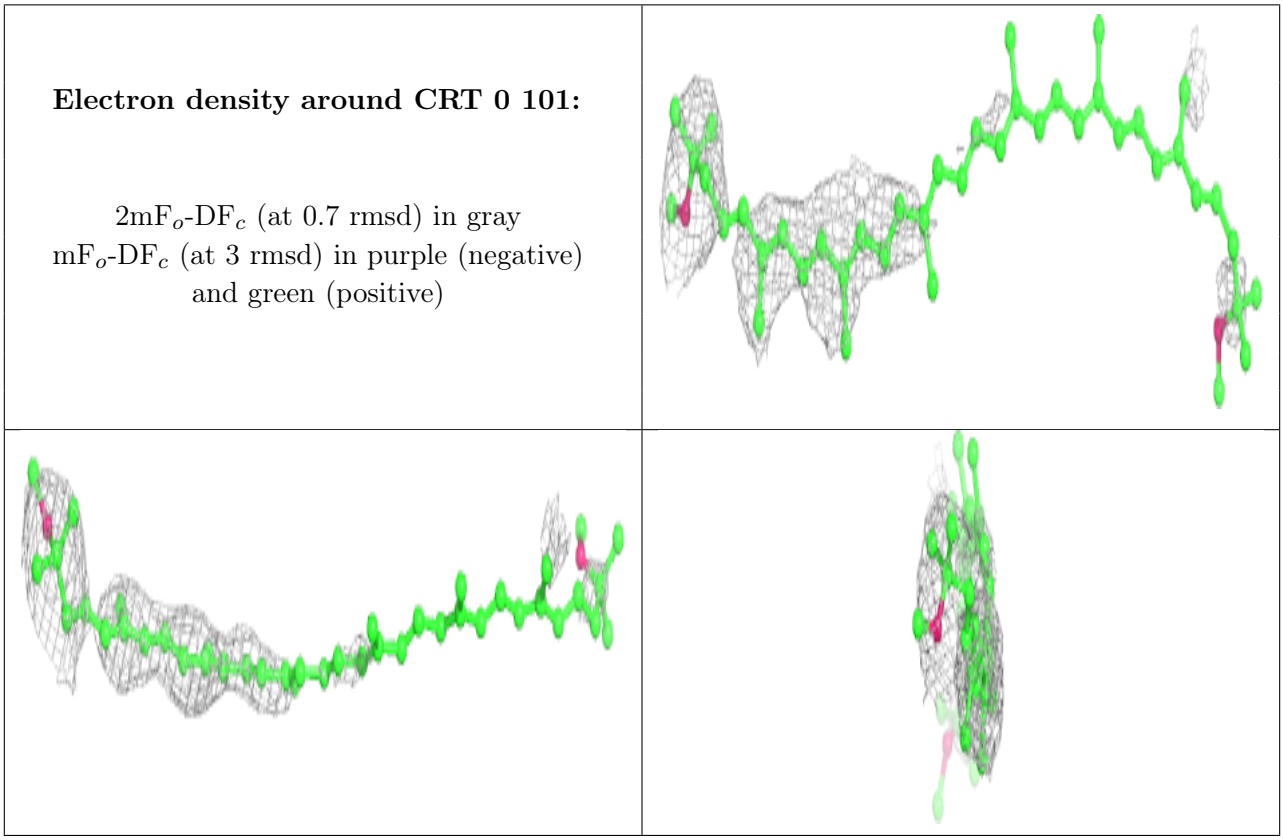
Electron density around CRT J 101:

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



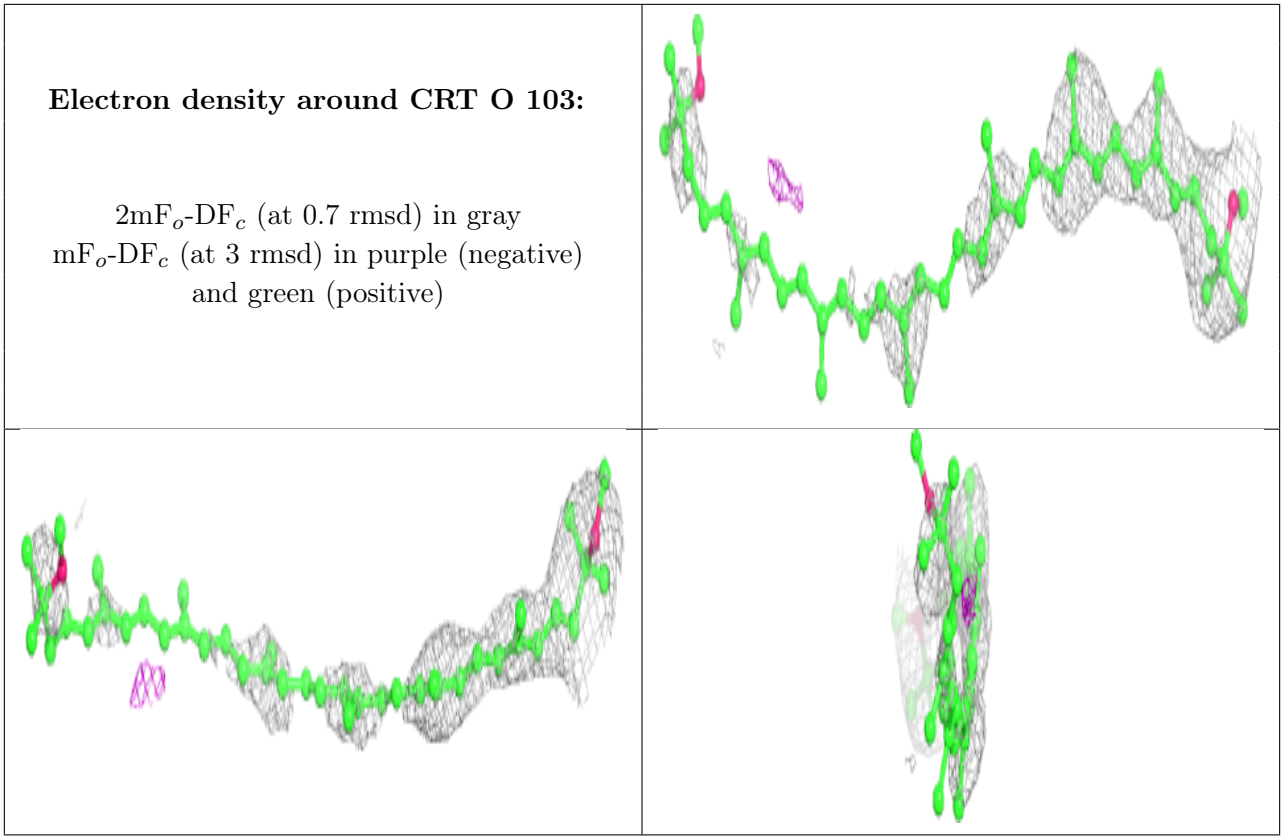
Electron density around CRT 0 101:

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



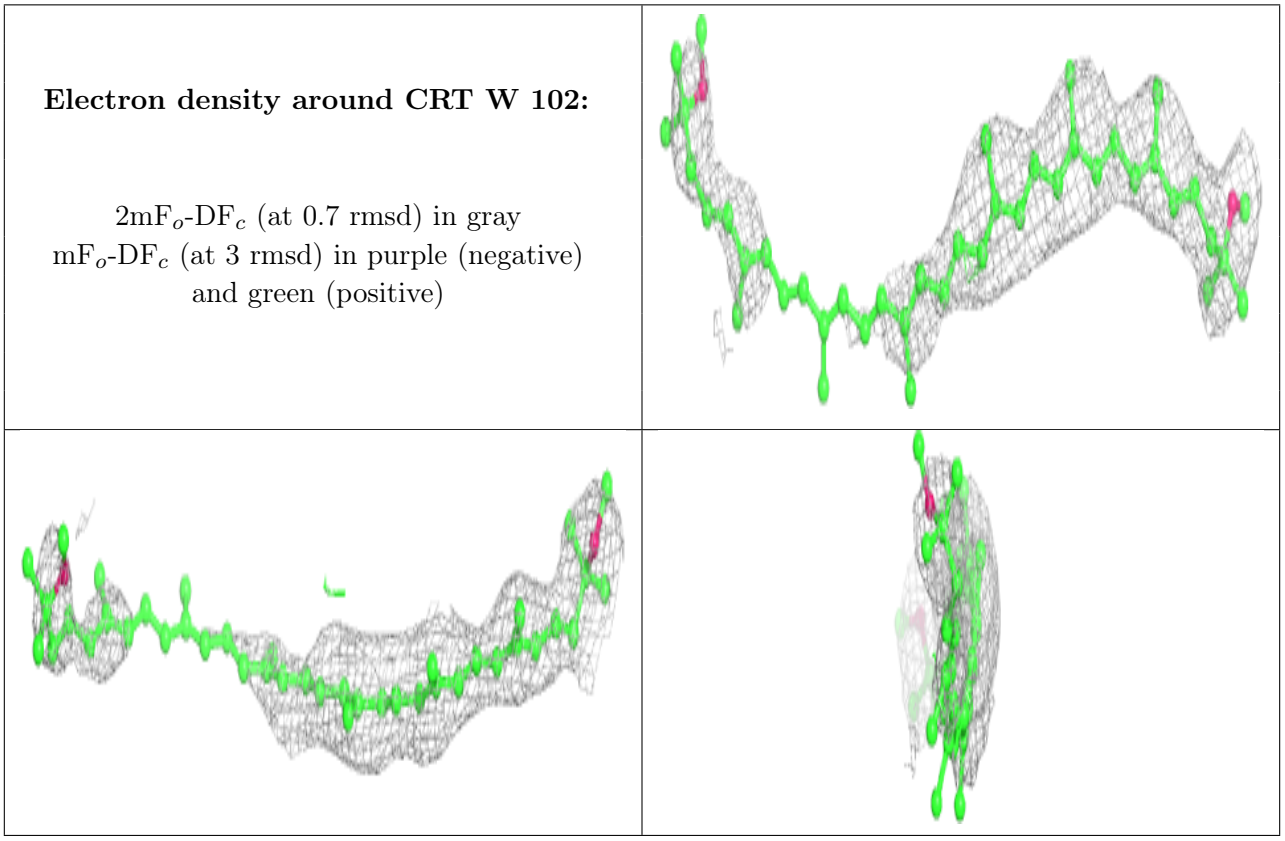
Electron density around CRT O 103:

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



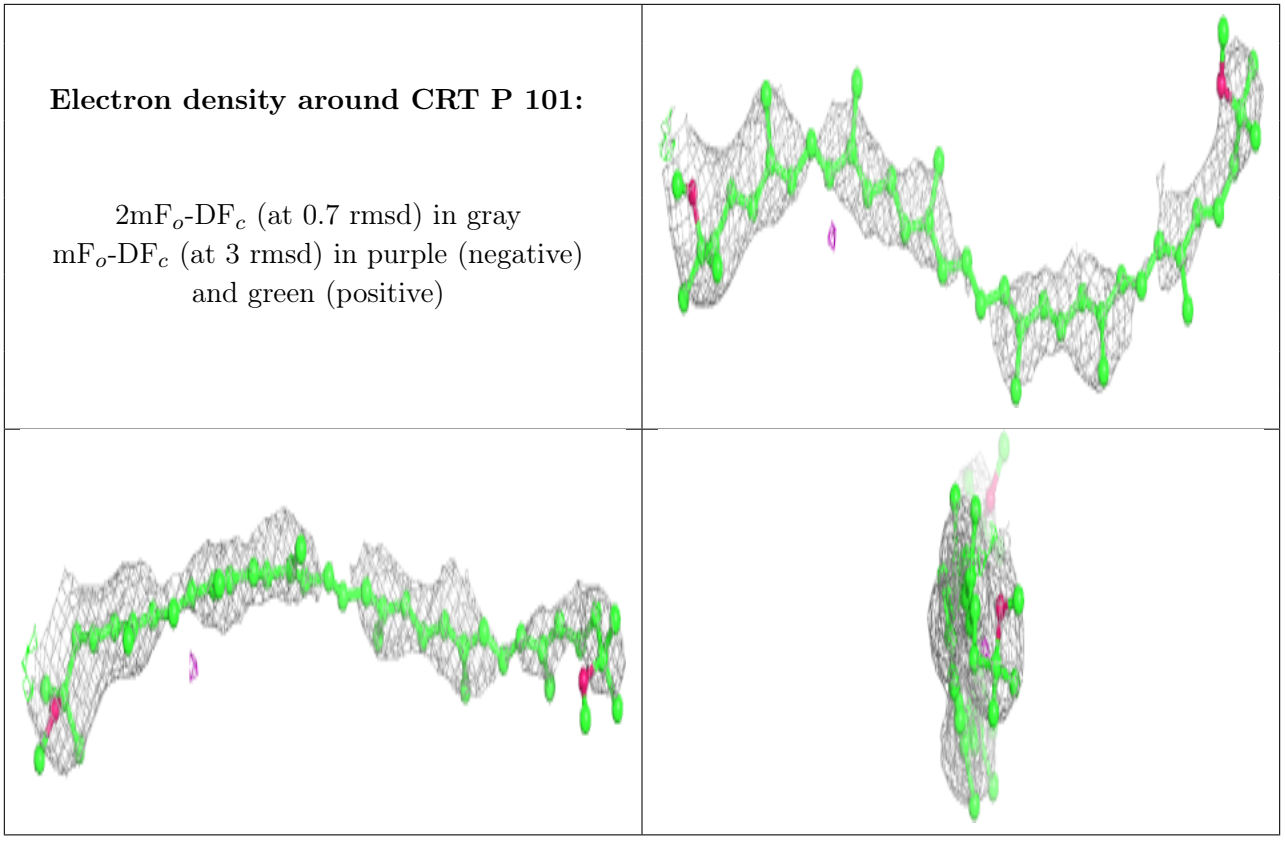
Electron density around CRT W 102:

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



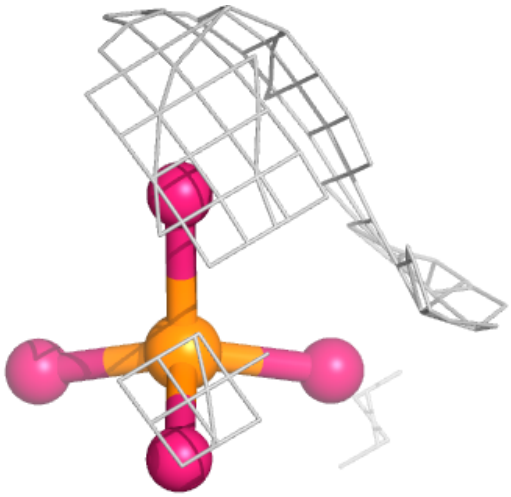
Electron density around CRT P 101:

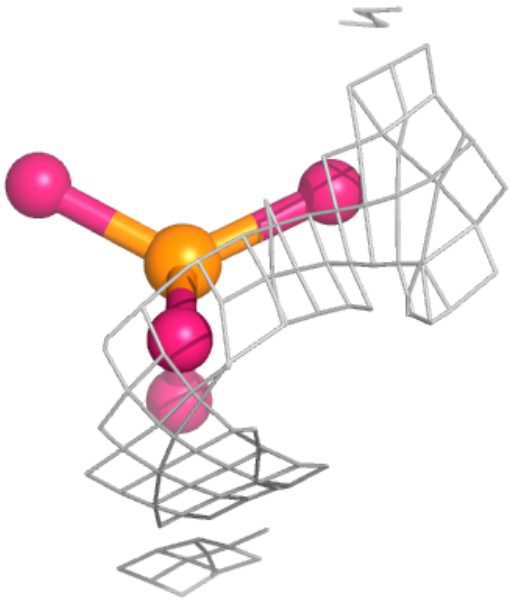
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

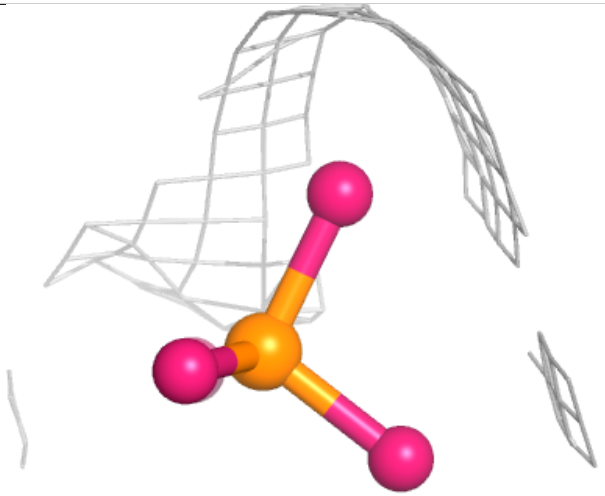


Electron density around PEF H 302:

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

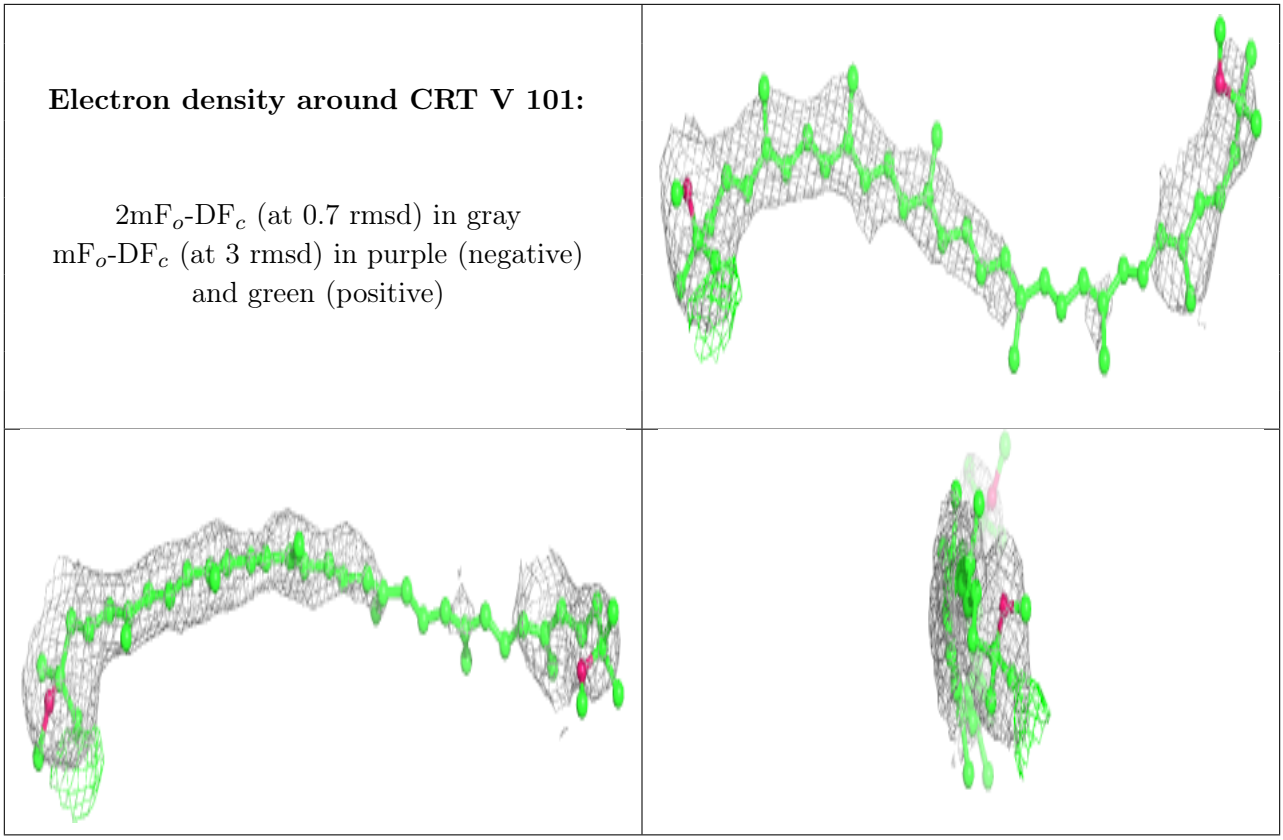






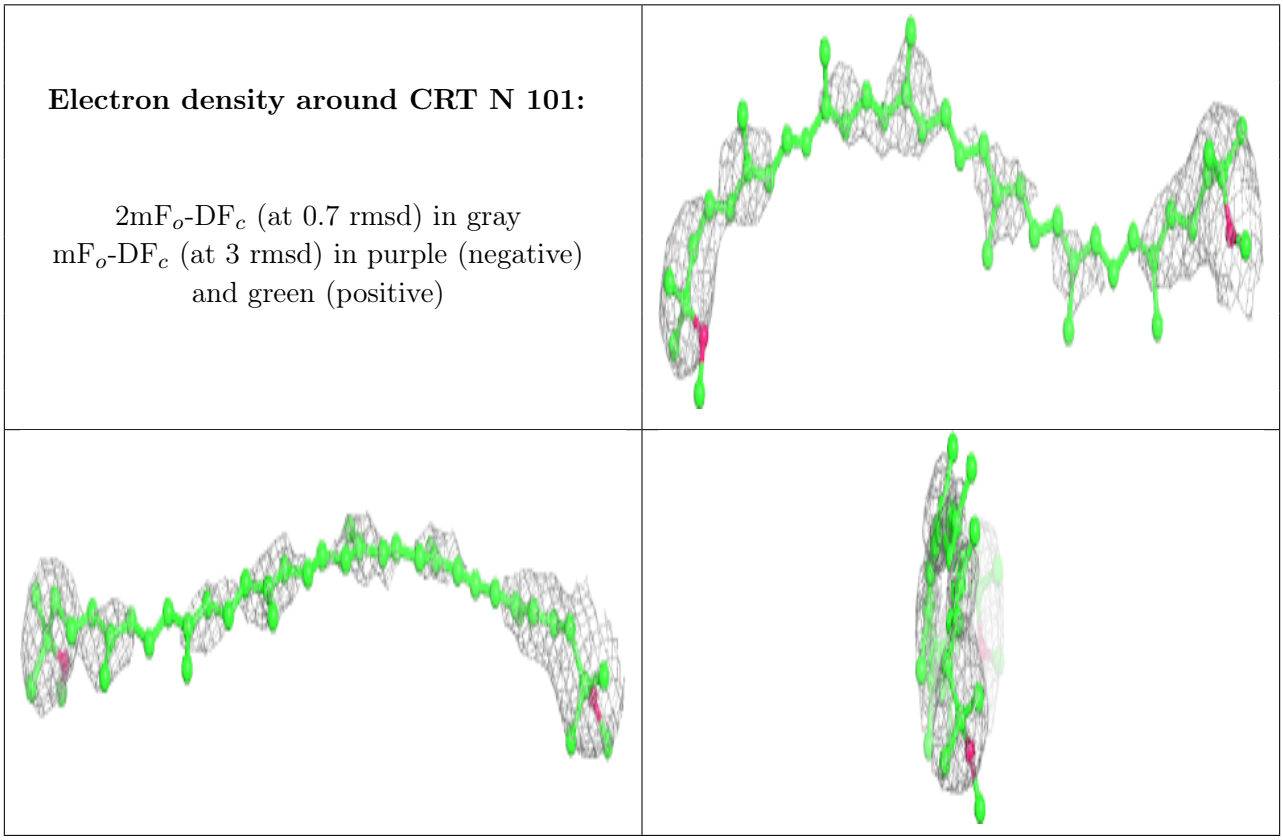
Electron density around CRT V 101:

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



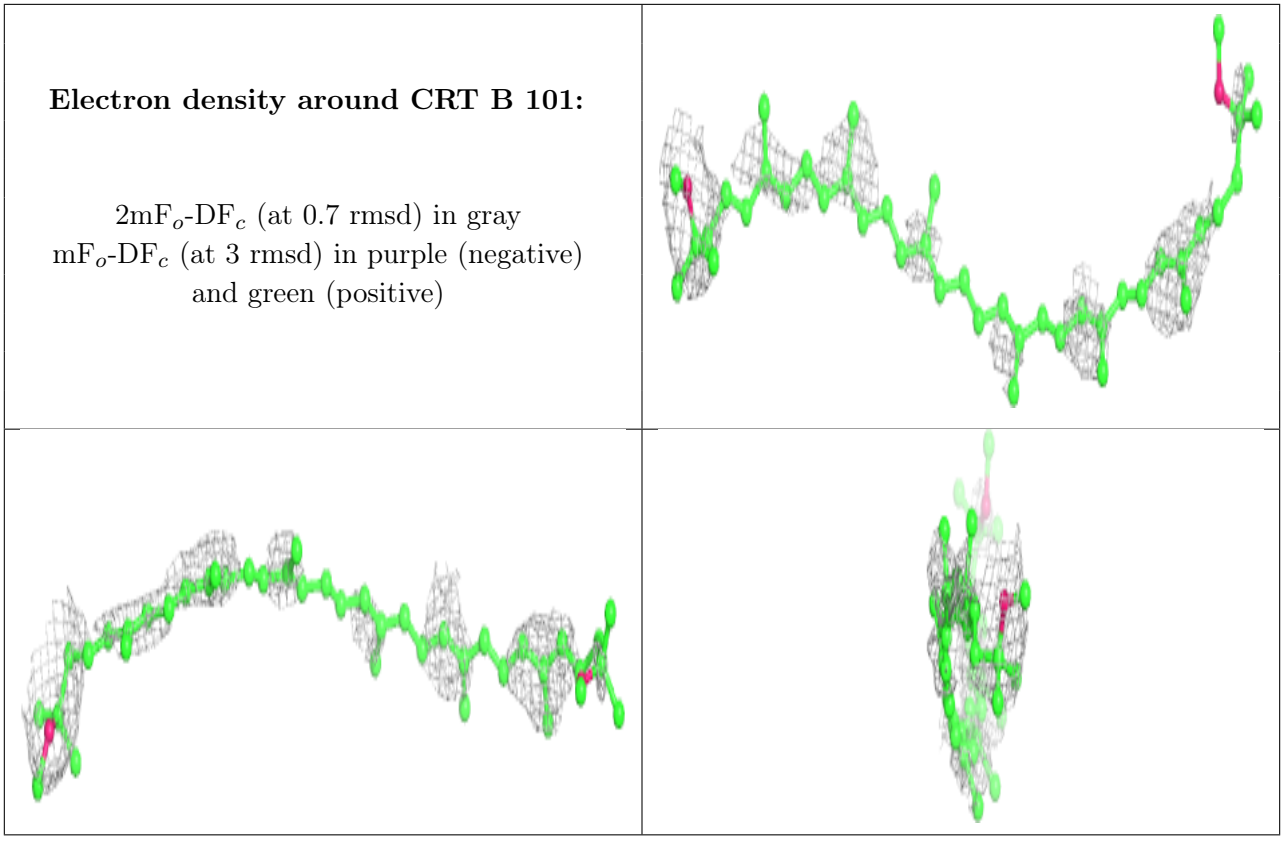
Electron density around CRT N 101:

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



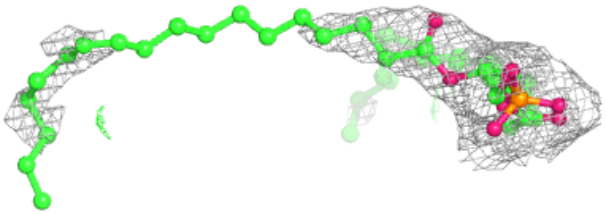
Electron density around CRT B 101:

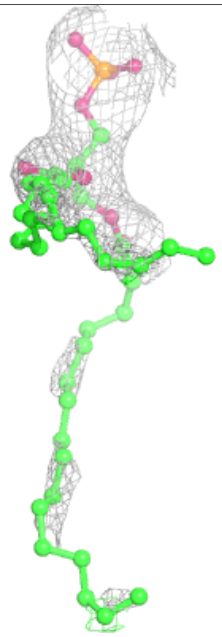
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PGV M 410:

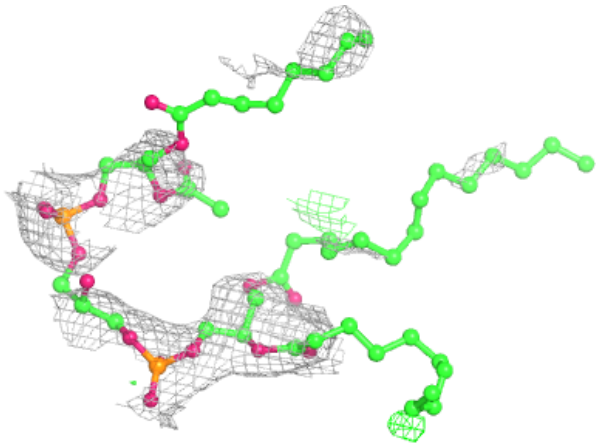
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

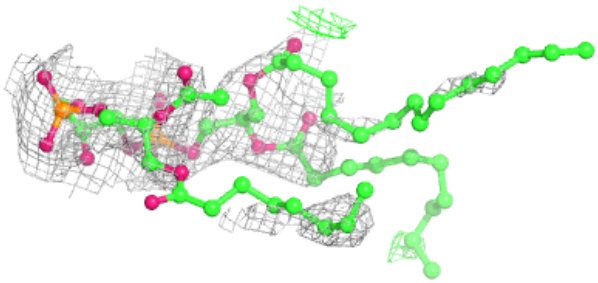


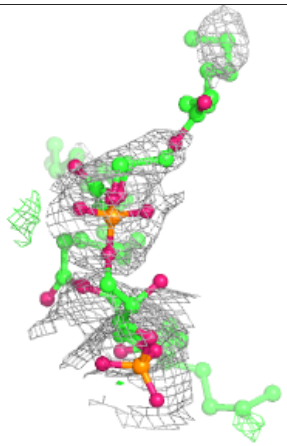


Electron density around CDL U 104:

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

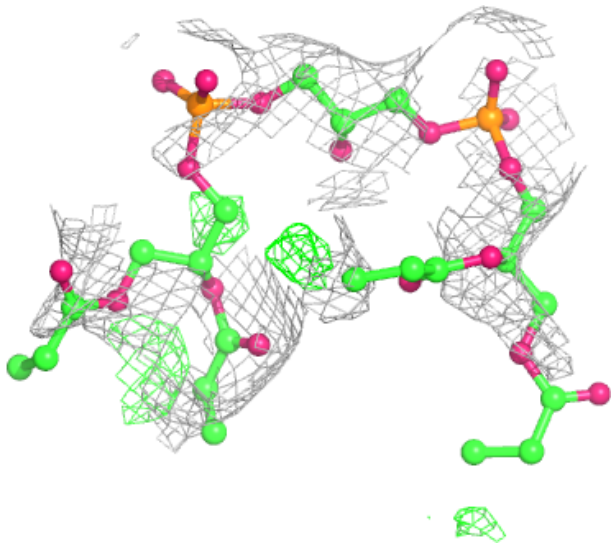


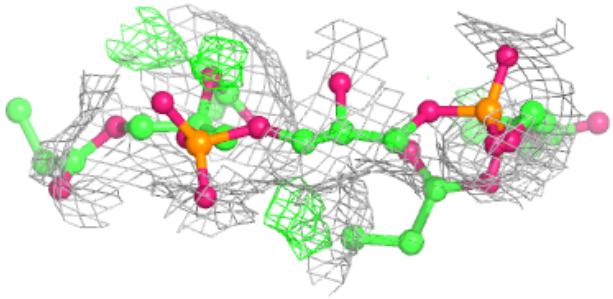


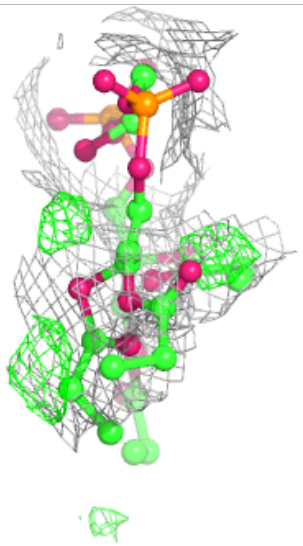


Electron density around CDL Y 104:

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

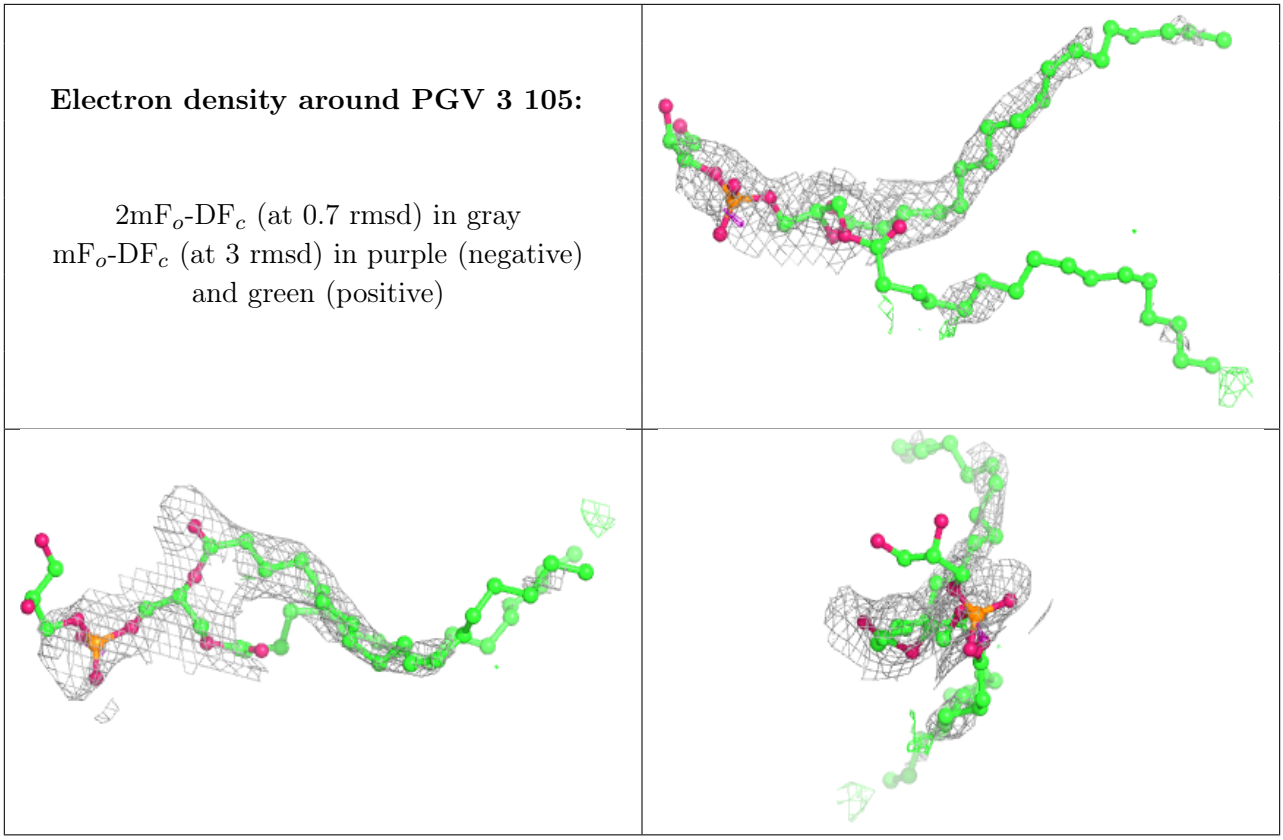






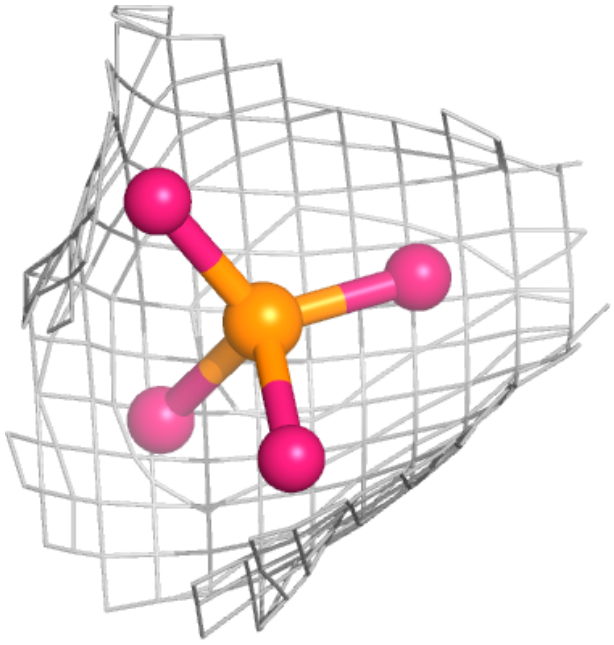
Electron density around PGV 3 105:

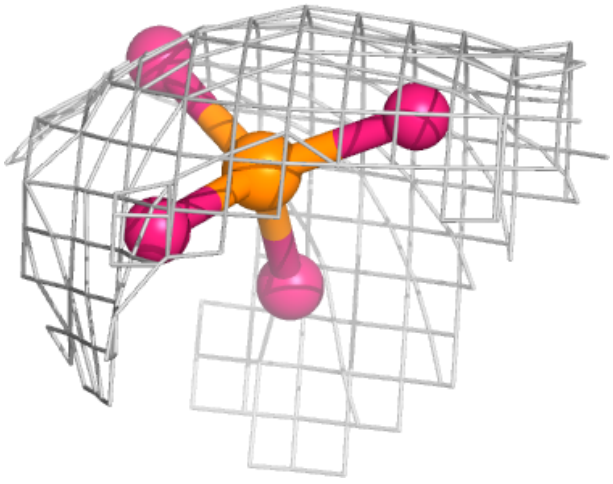
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

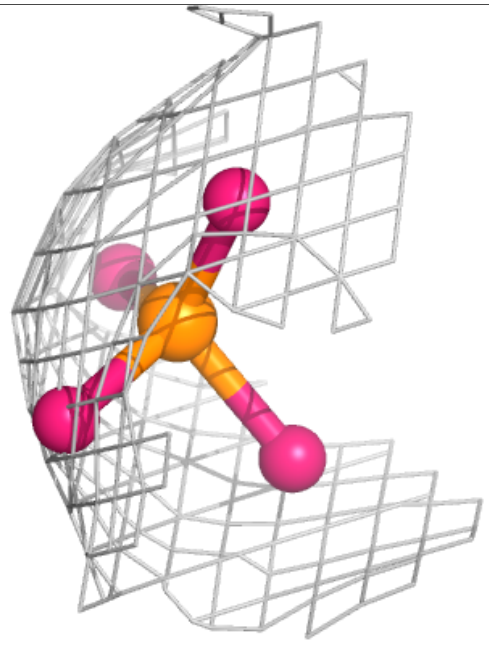


Electron density around PEF 1 103:

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

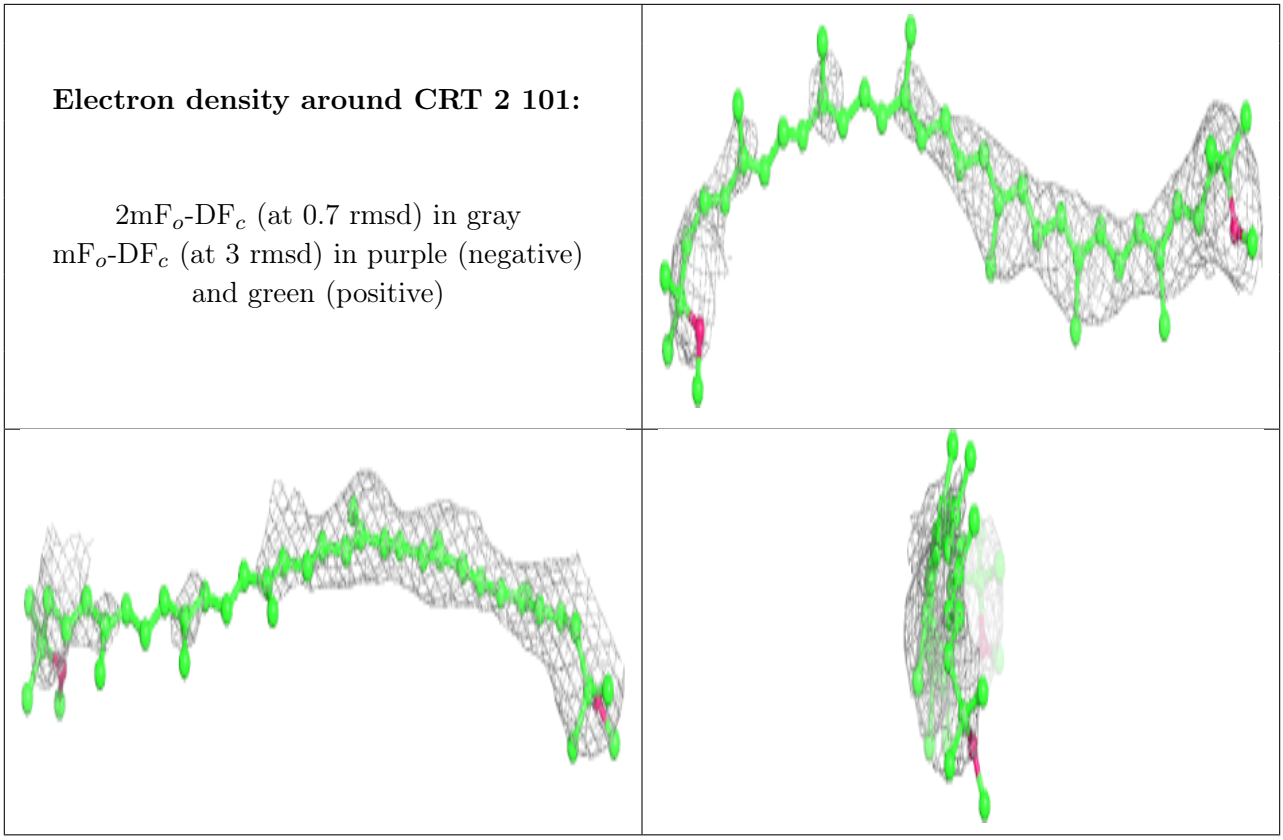






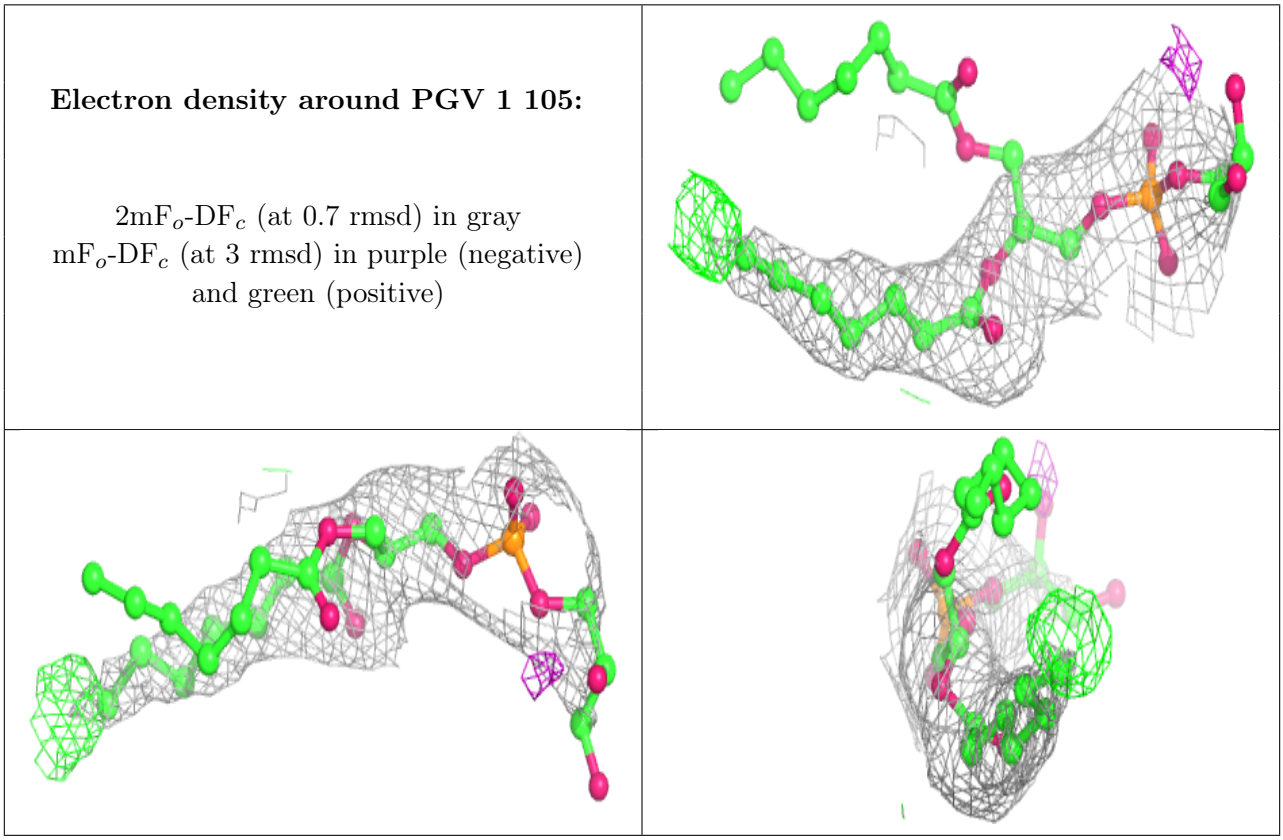
Electron density around CRT 2 101:

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



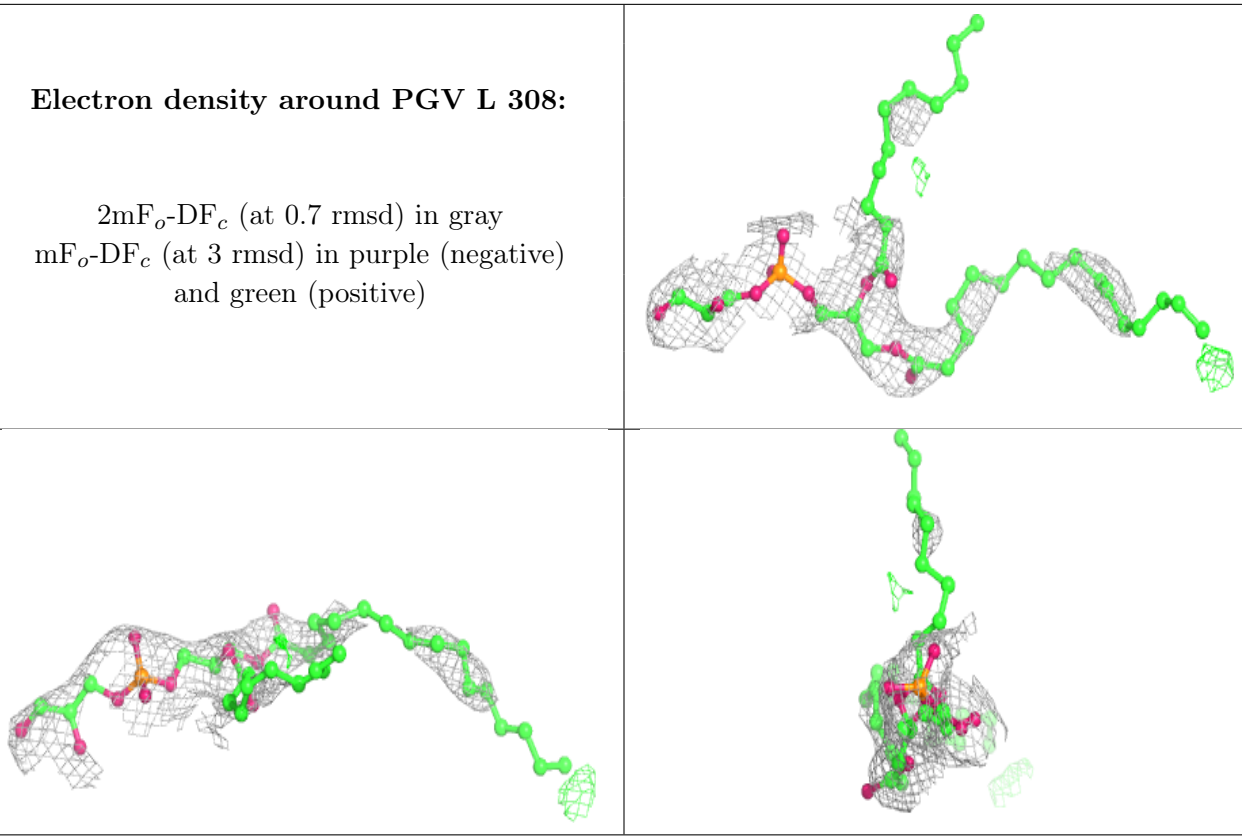
Electron density around PGV 1 105:

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



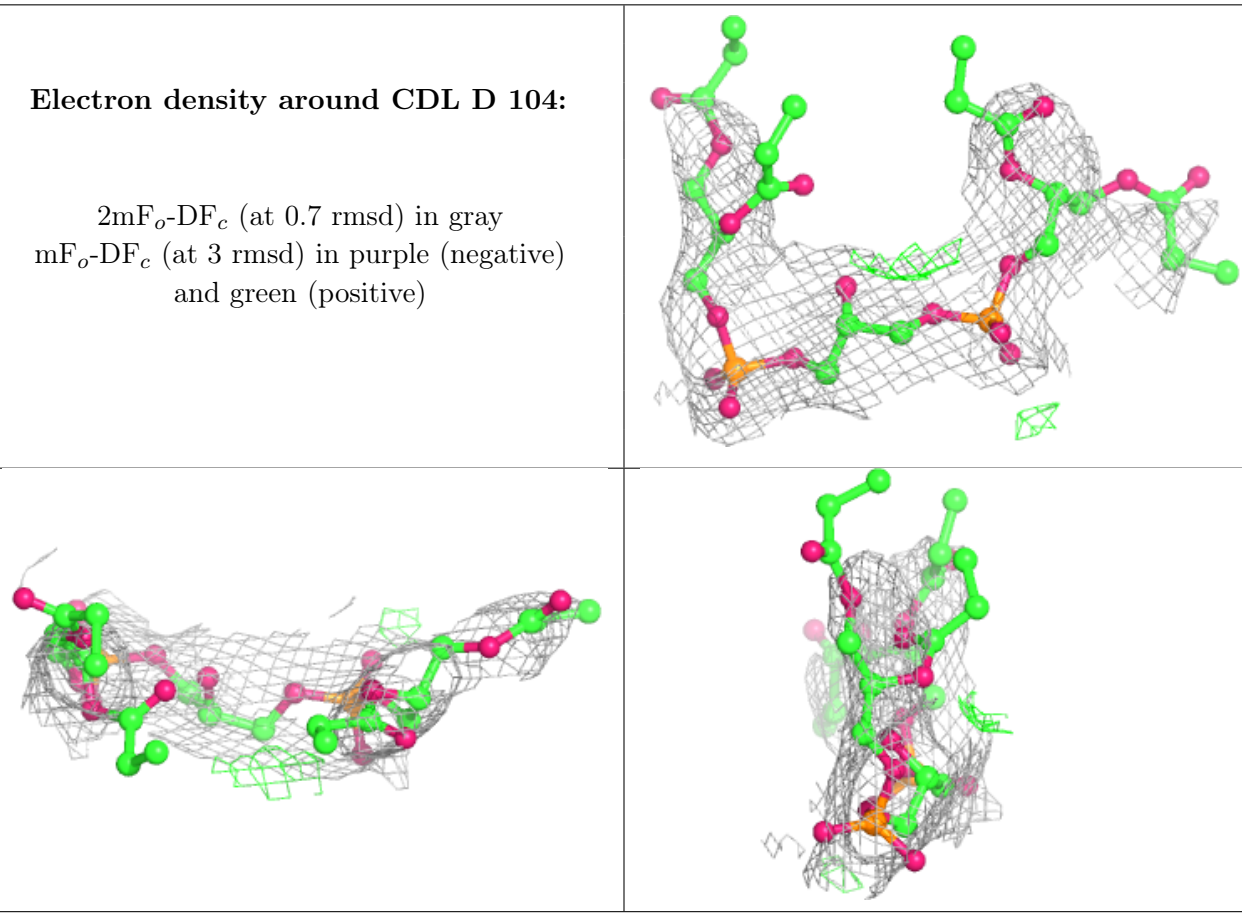
Electron density around PGV L 308:

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



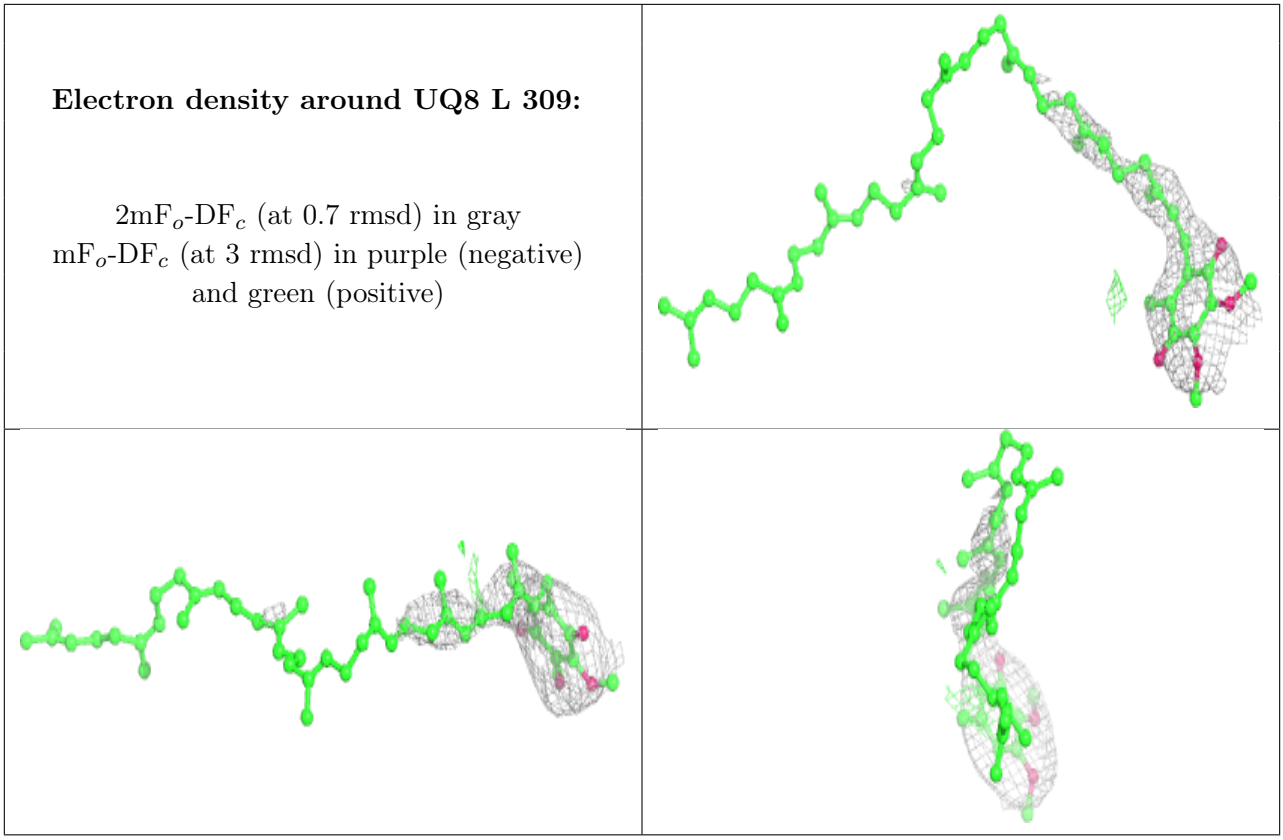
Electron density around CDL D 104:

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



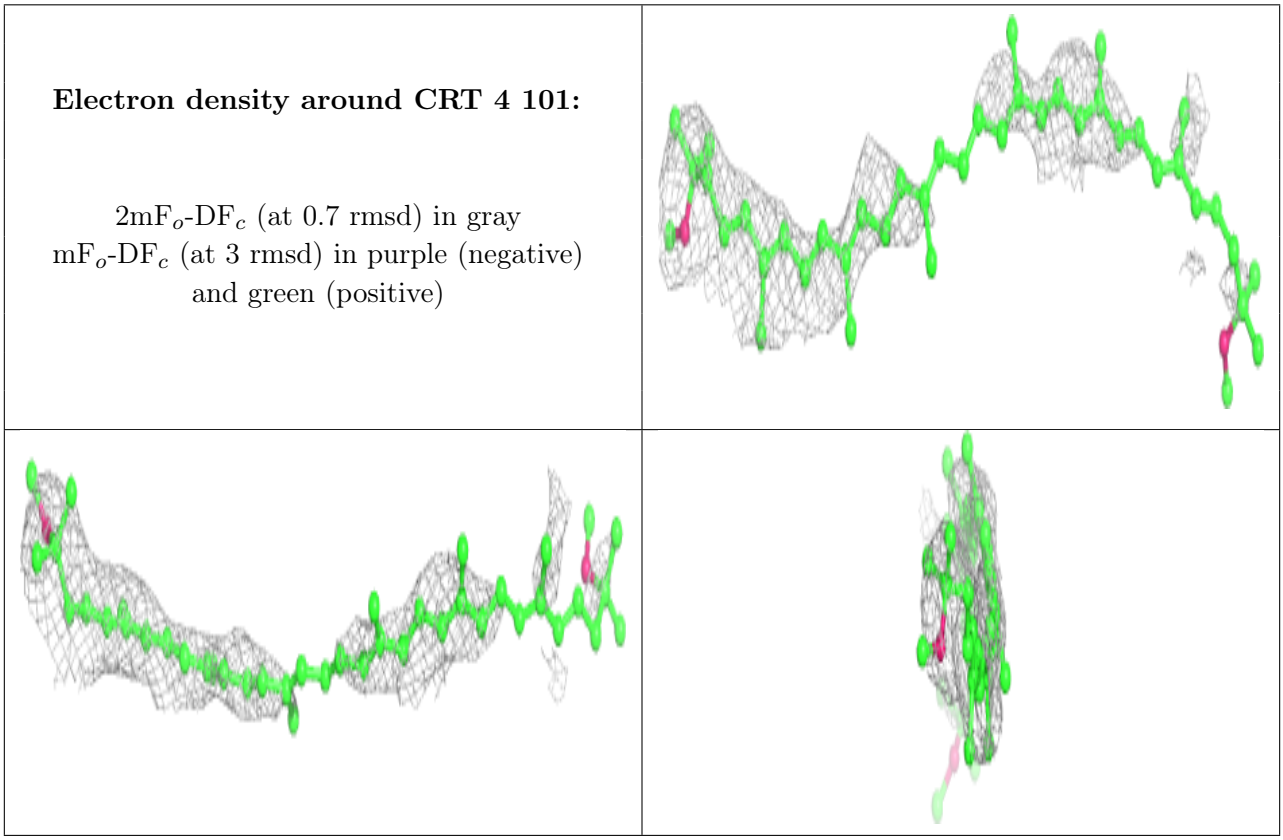
Electron density around UQ8 L 309:

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



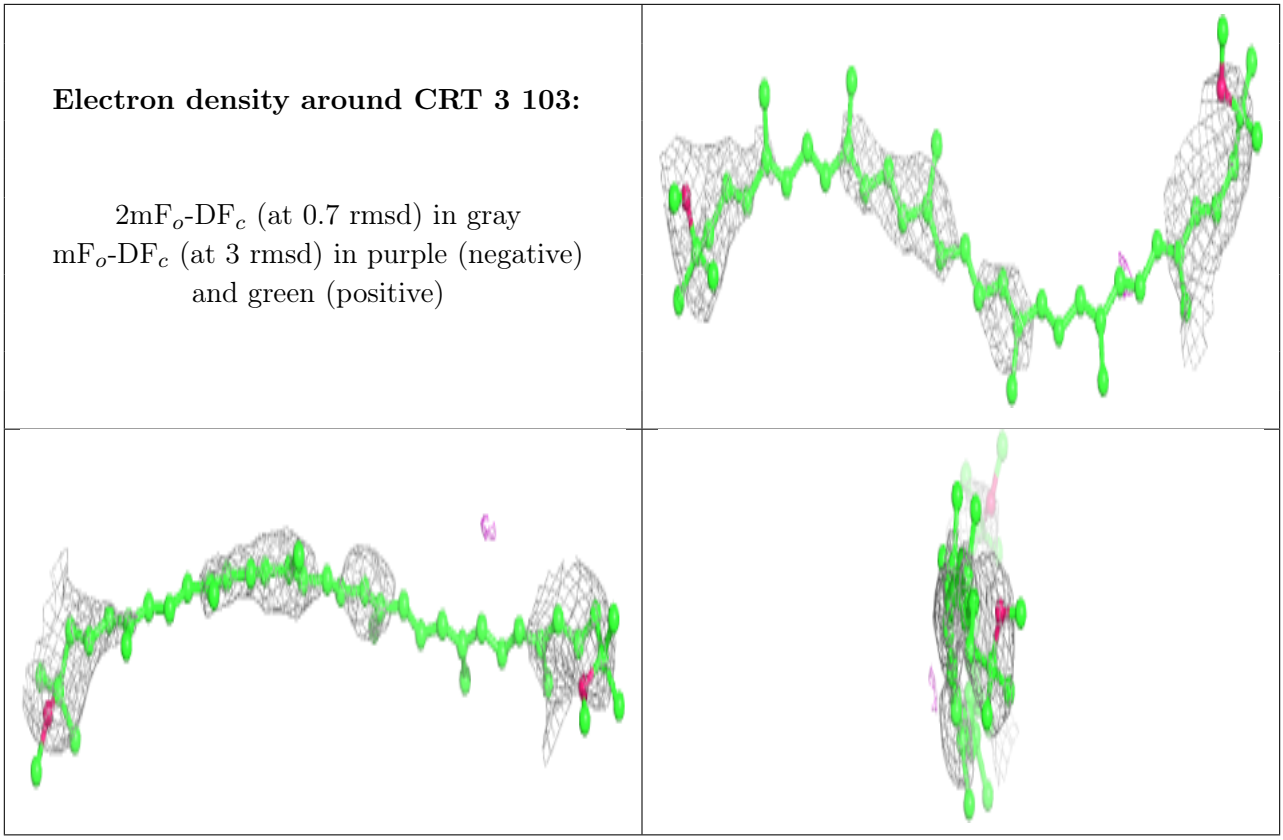
Electron density around CRT 4 101:

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



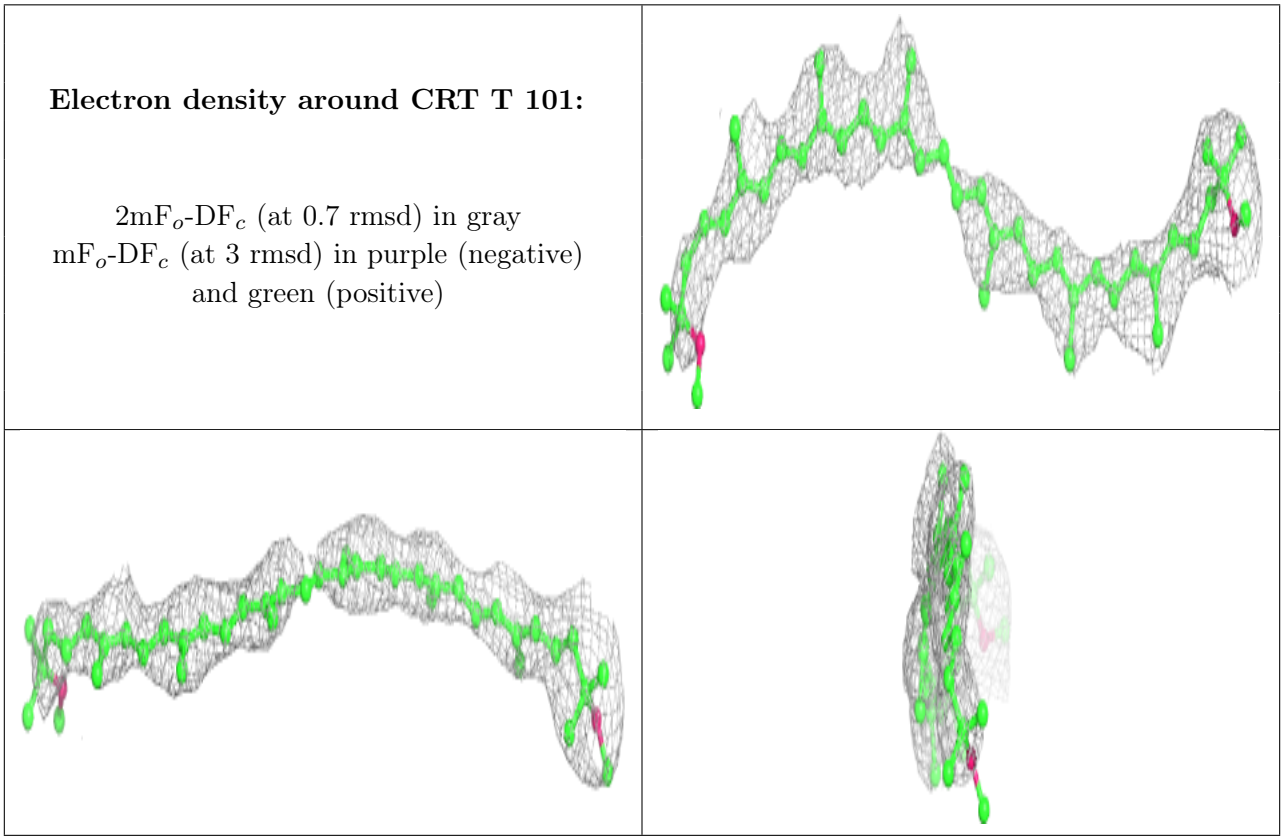
Electron density around CRT 3 103:

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



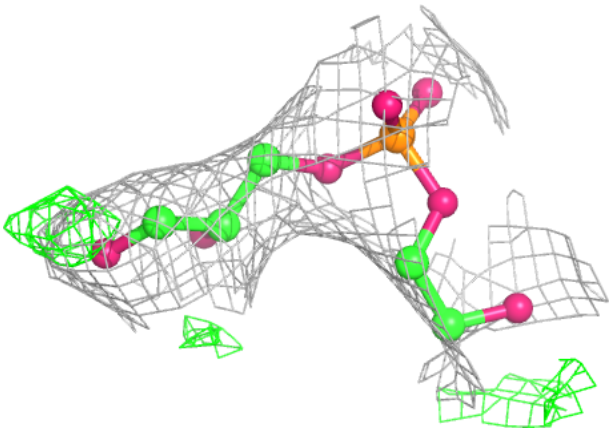
Electron density around CRT T 101:

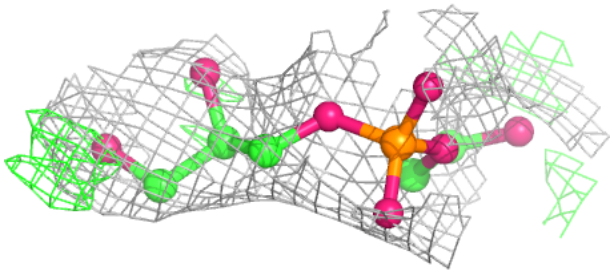
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

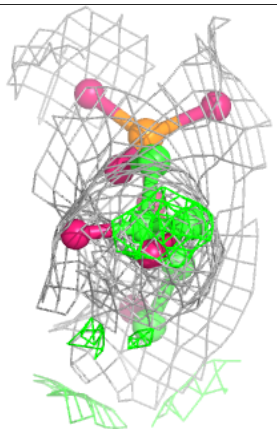


Electron density around CDL 1 104:

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

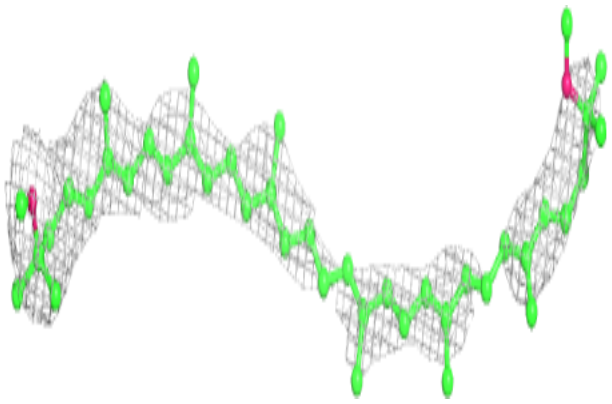


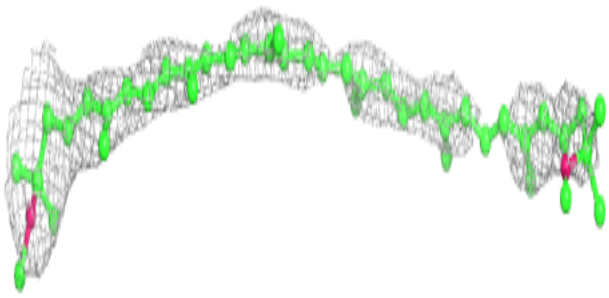


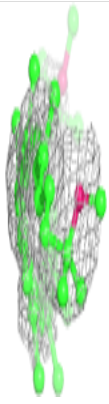


Electron density around CRT A 104:

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

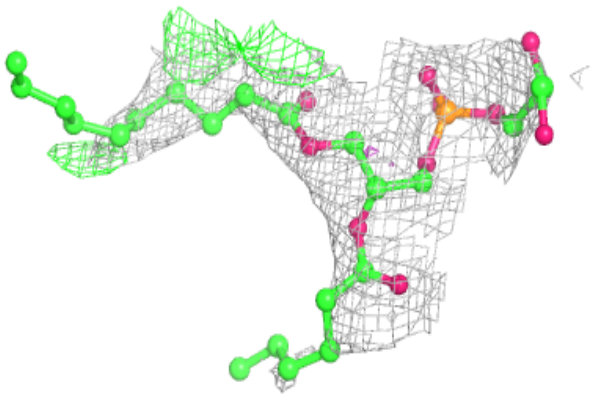


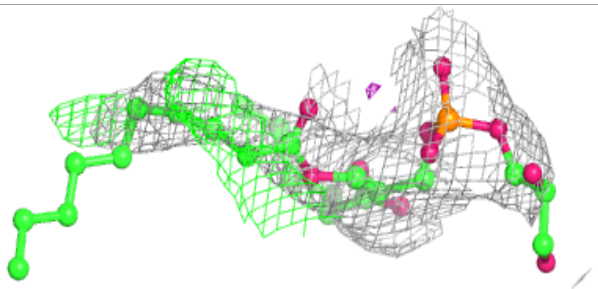


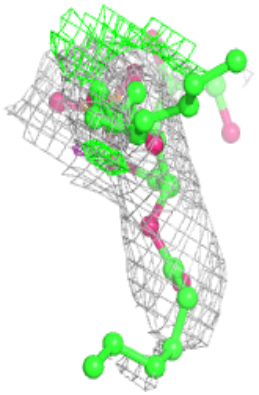


Electron density around PGV 9 104:

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

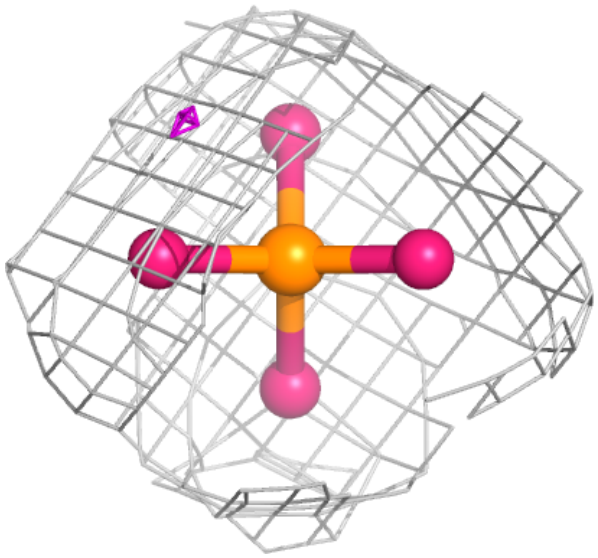


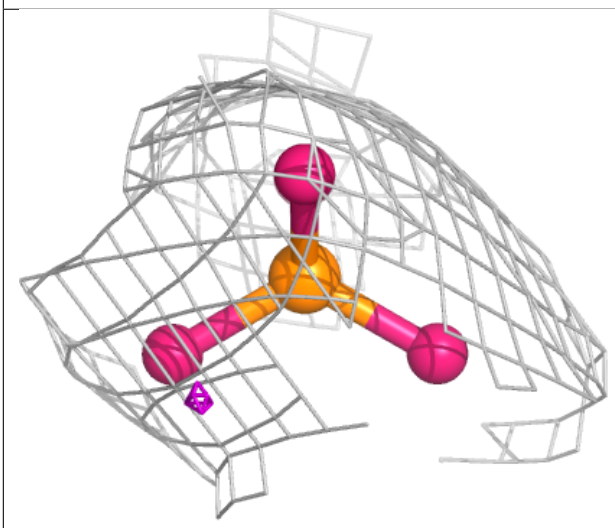


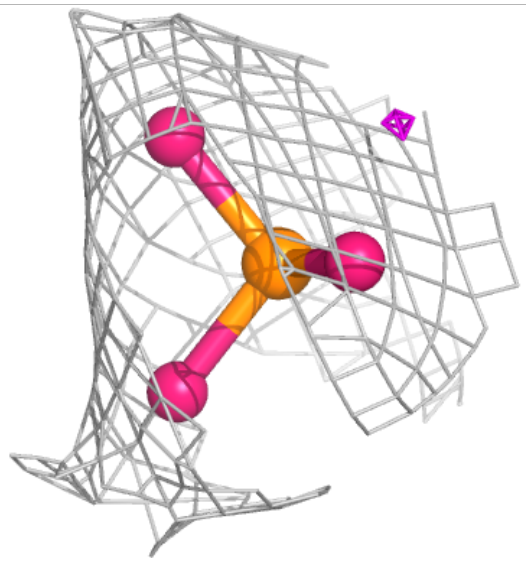


Electron density around PEF I 103:

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

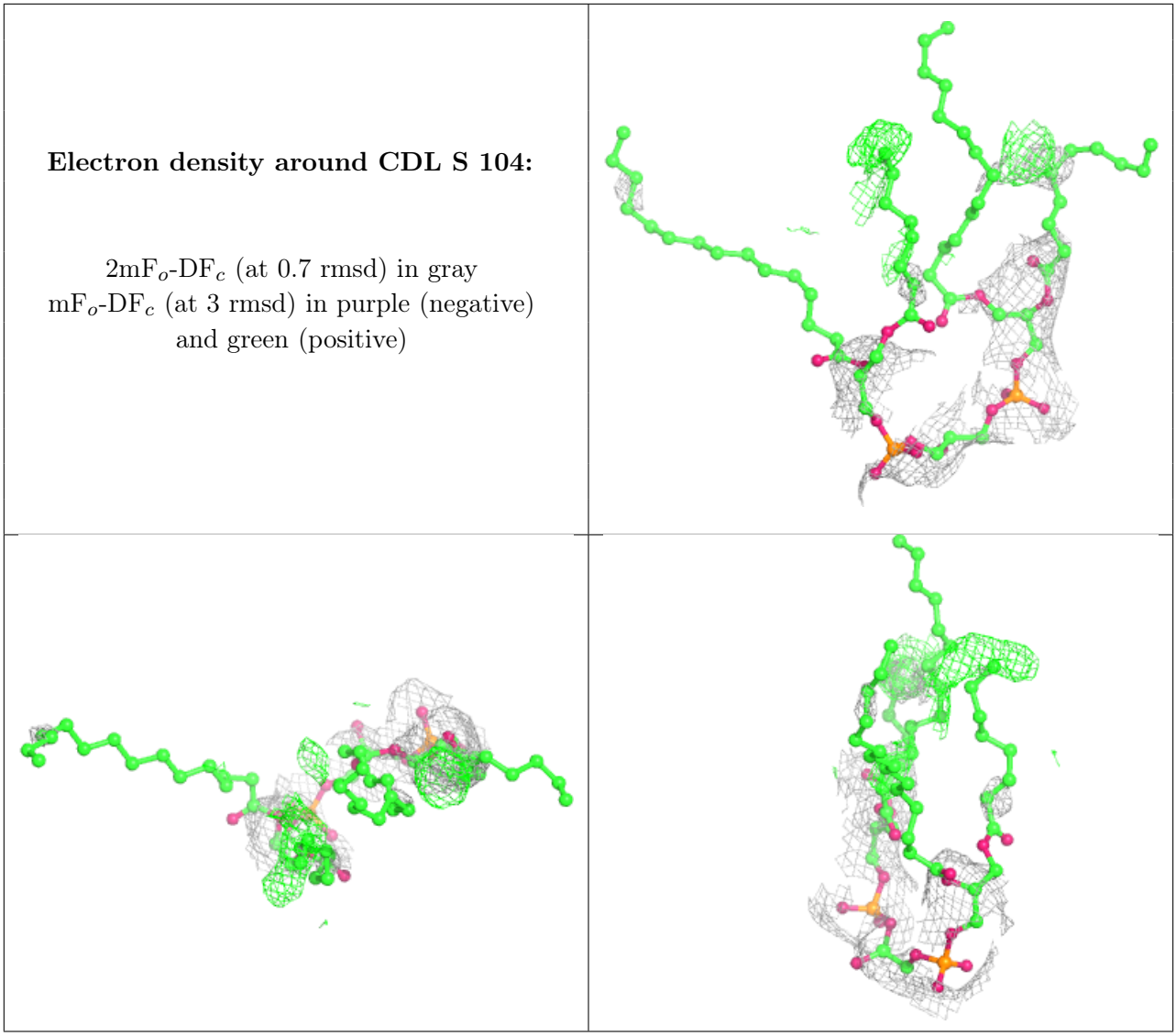






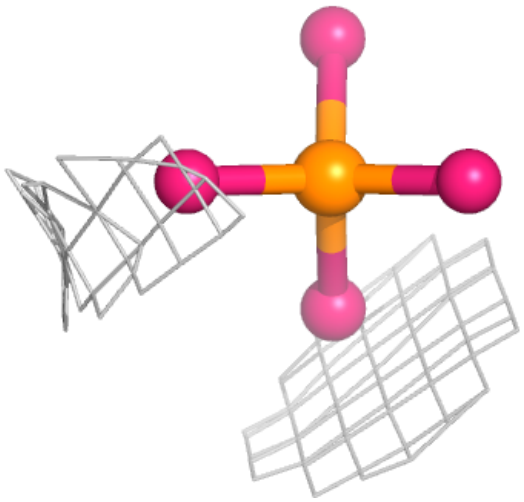
Electron density around CDL S 104:

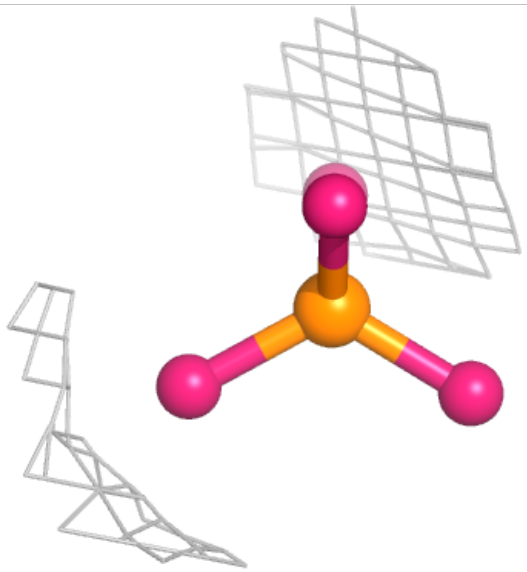
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

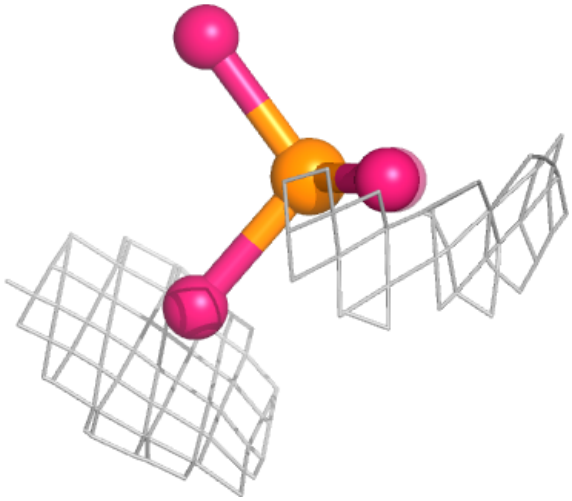


Electron density around PEF M 407:

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

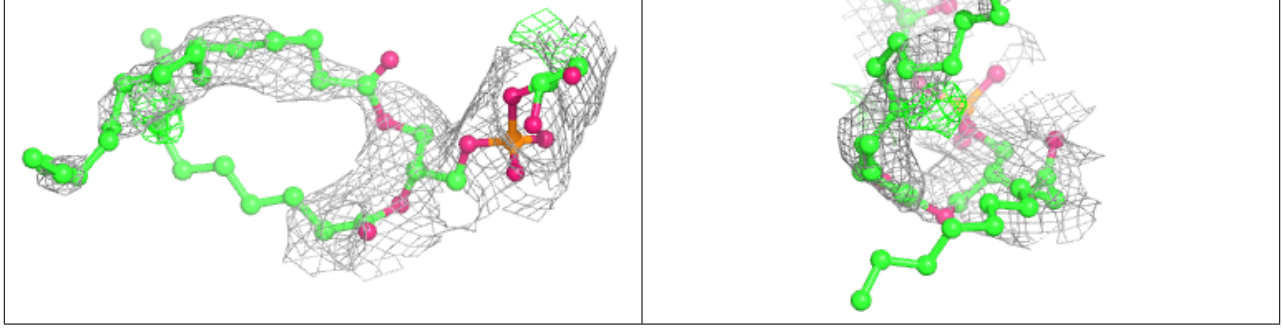






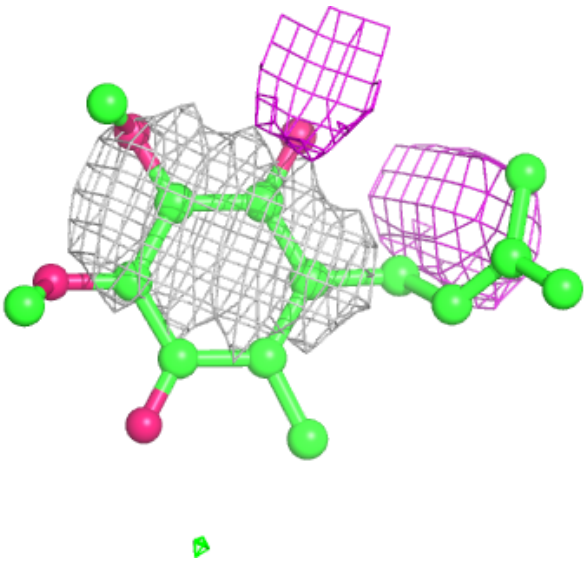
Electron density around PGV L 307:

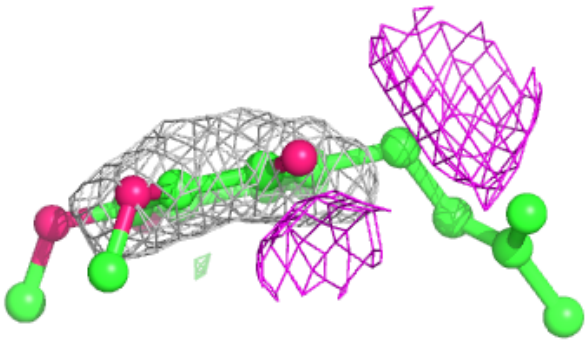
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

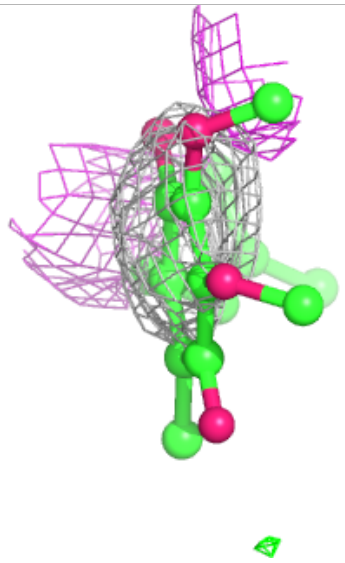


Electron density around UQ8 L 311:

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

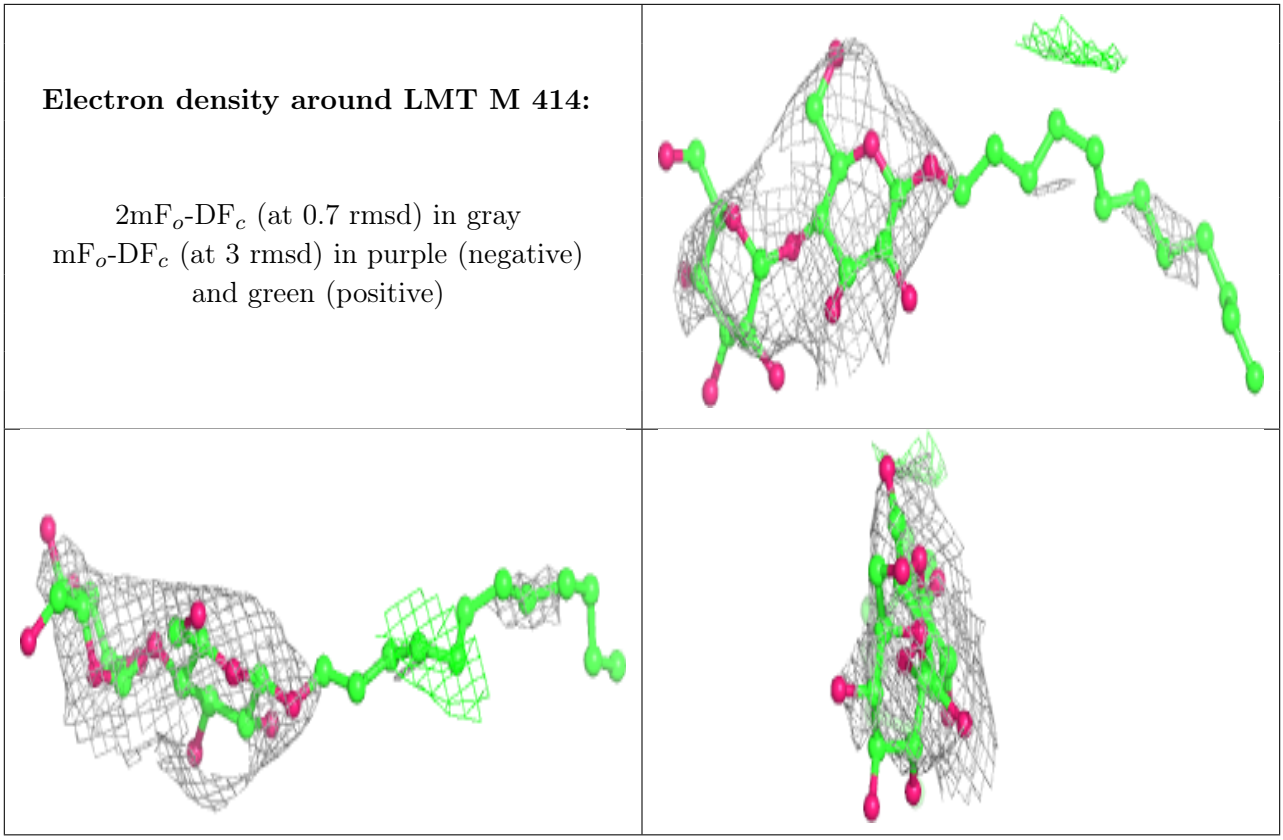






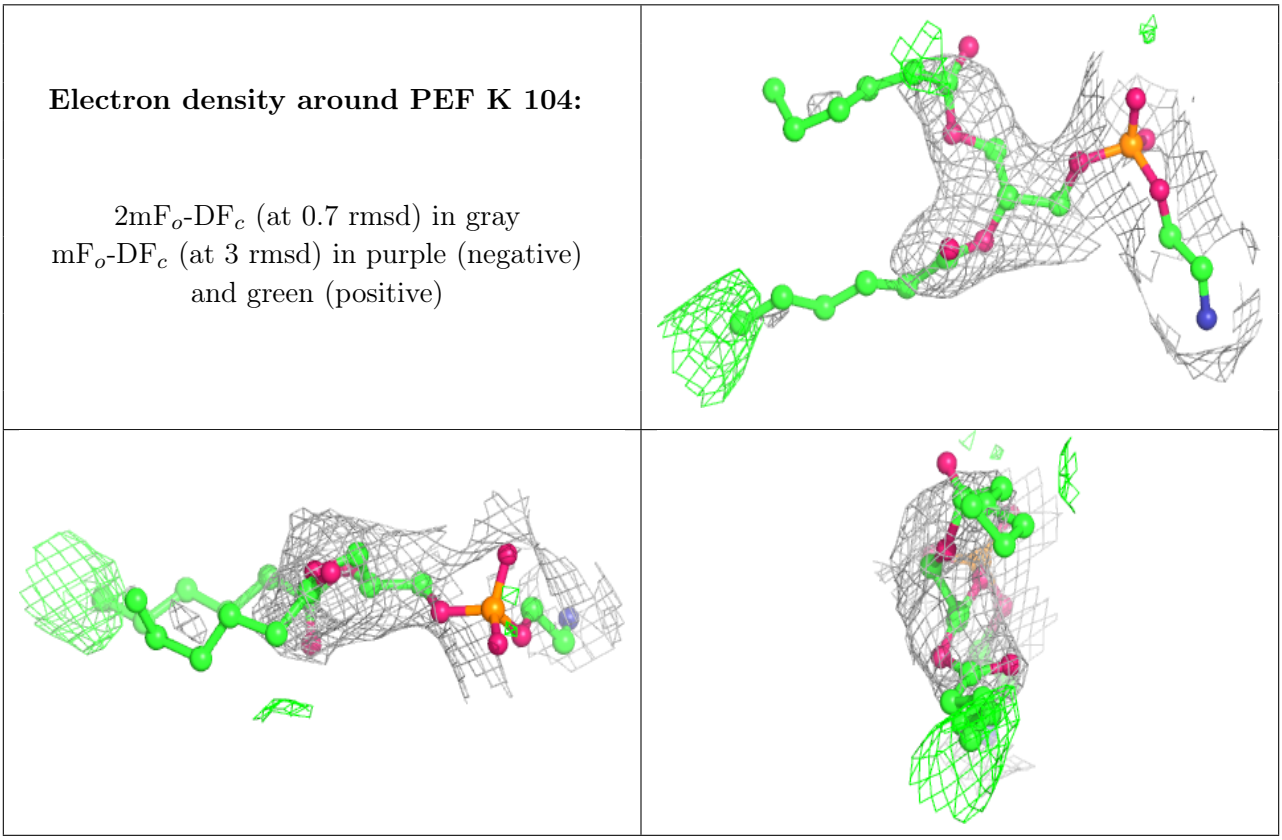
Electron density around LMT M 414:

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



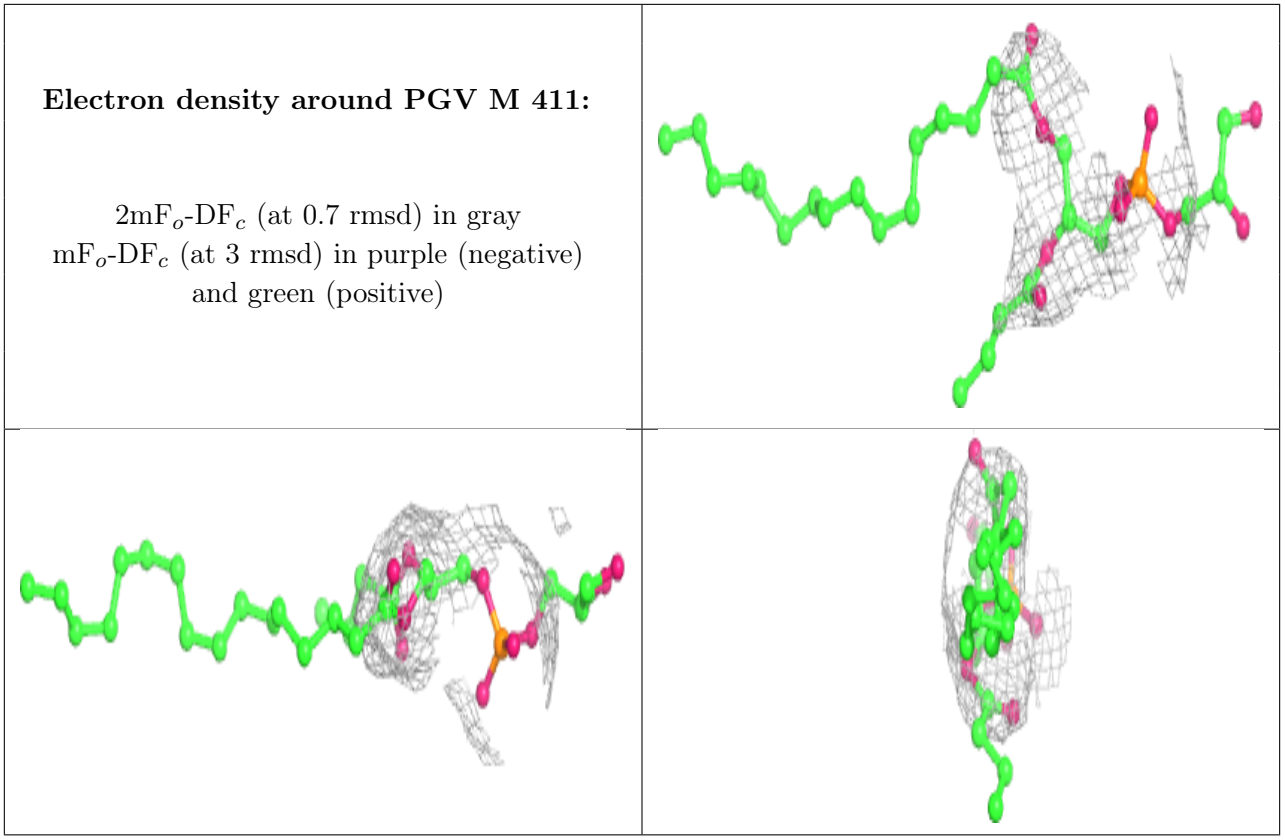
Electron density around PEF K 104:

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



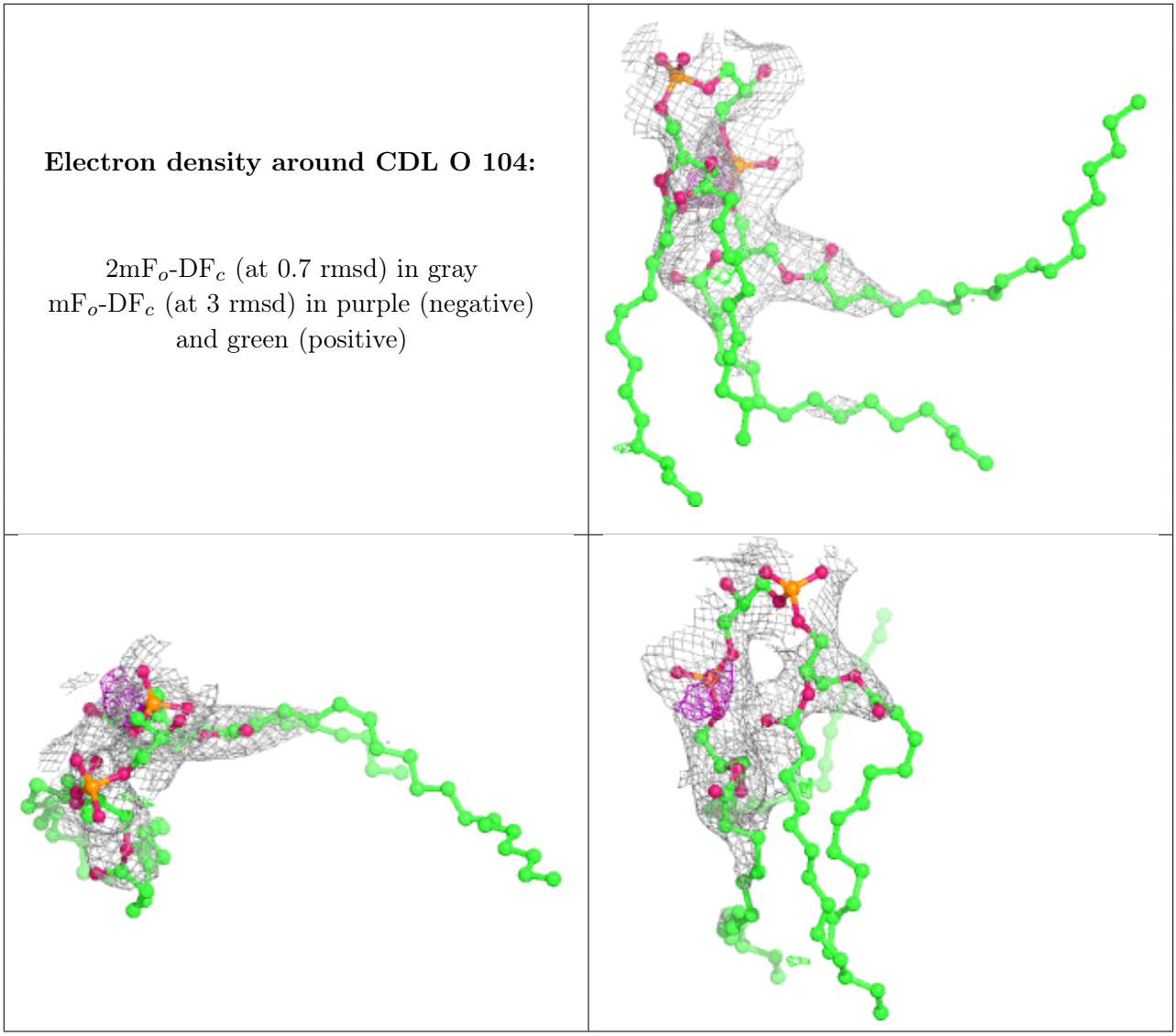
Electron density around PGV M 411:

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



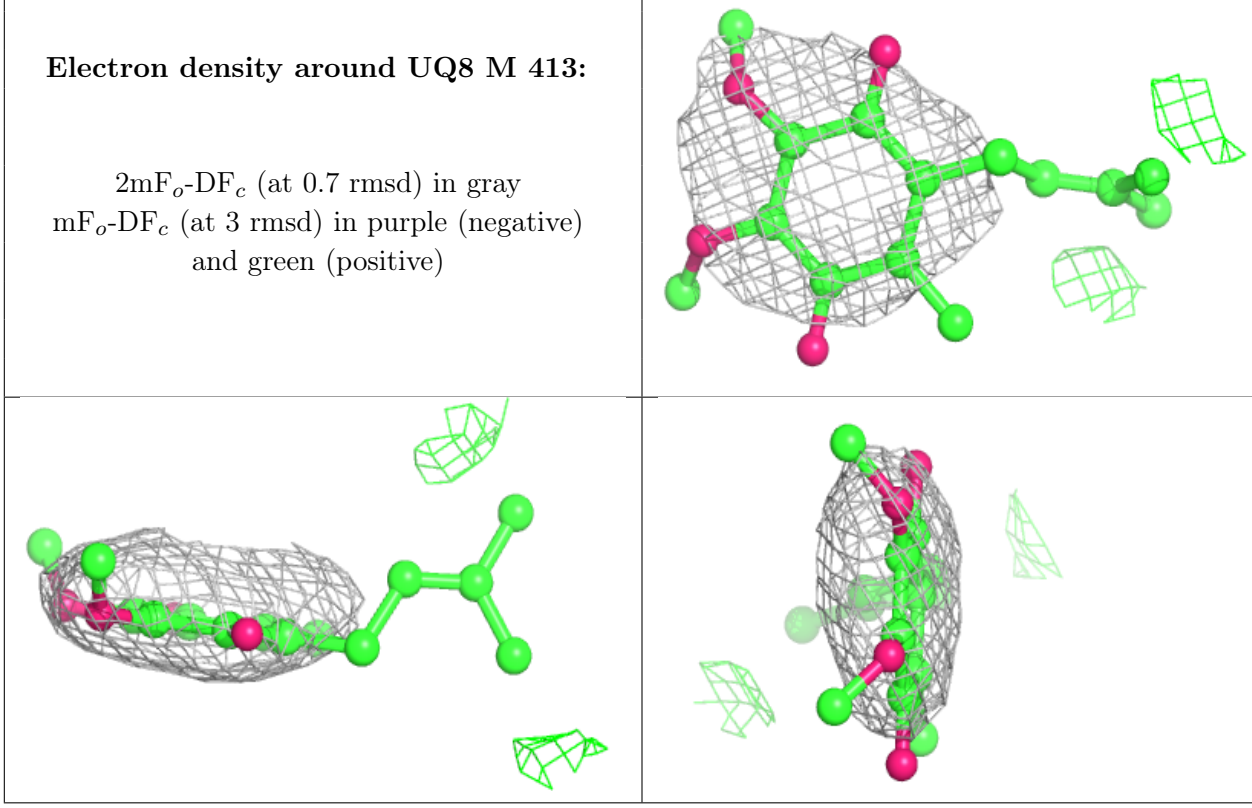
Electron density around CDL O 104:

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



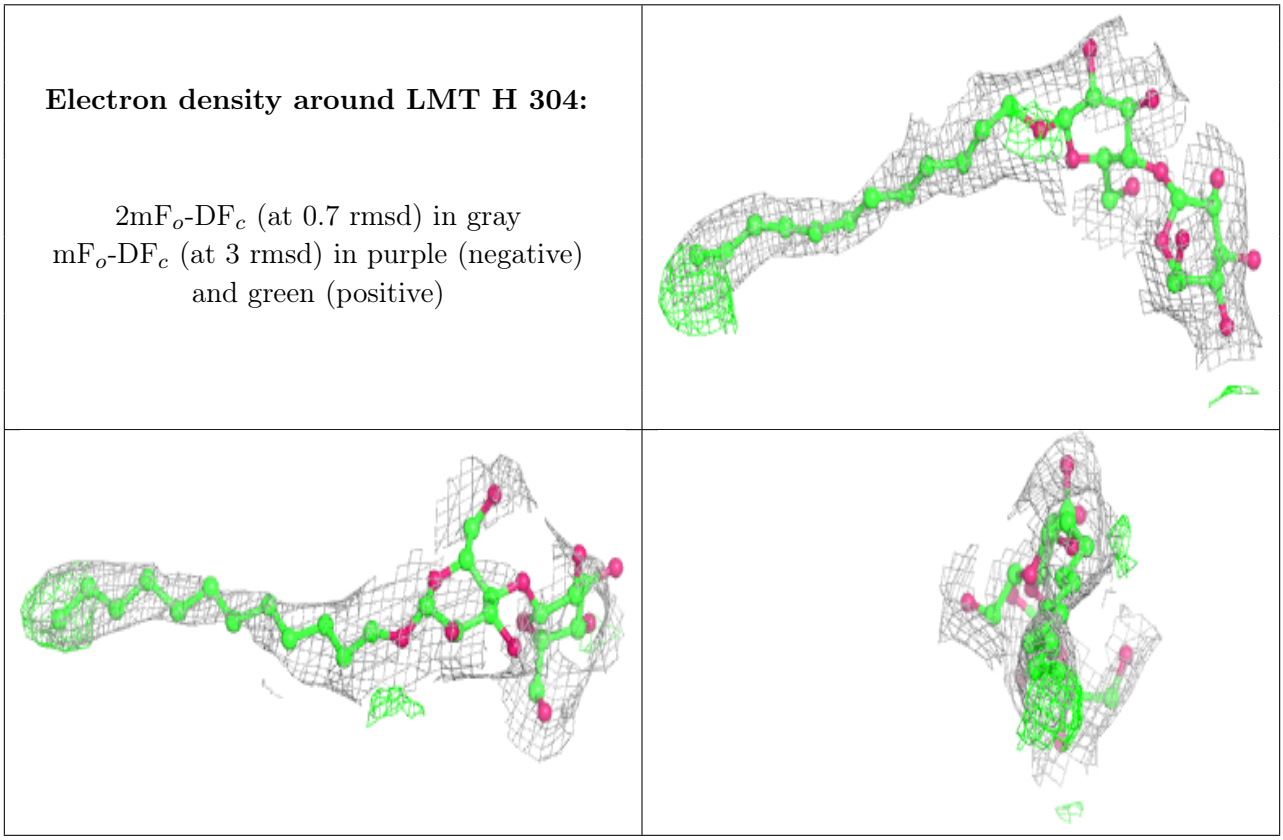
Electron density around UQ8 M 413:

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



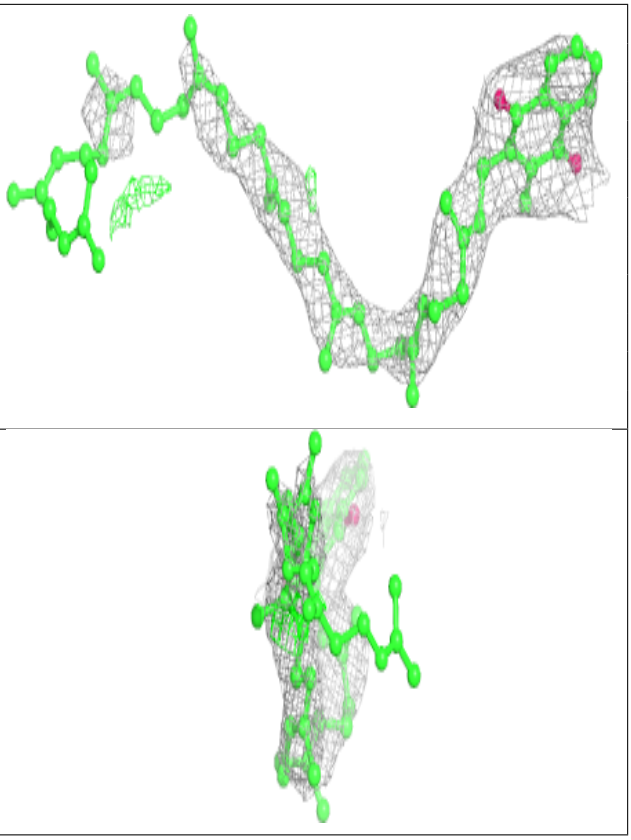
Electron density around LMT H 304:

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



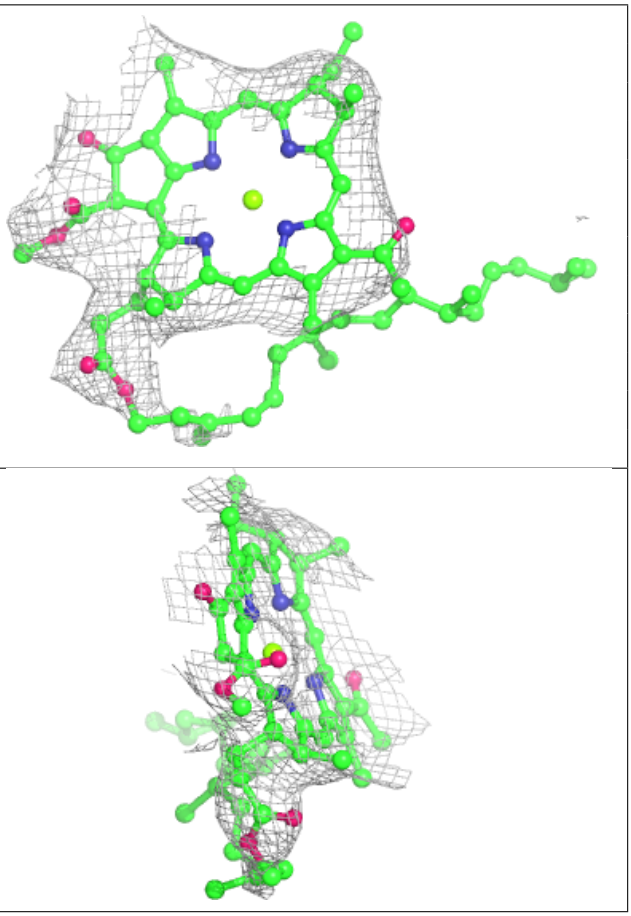
Electron density around MQ8 M 404:

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



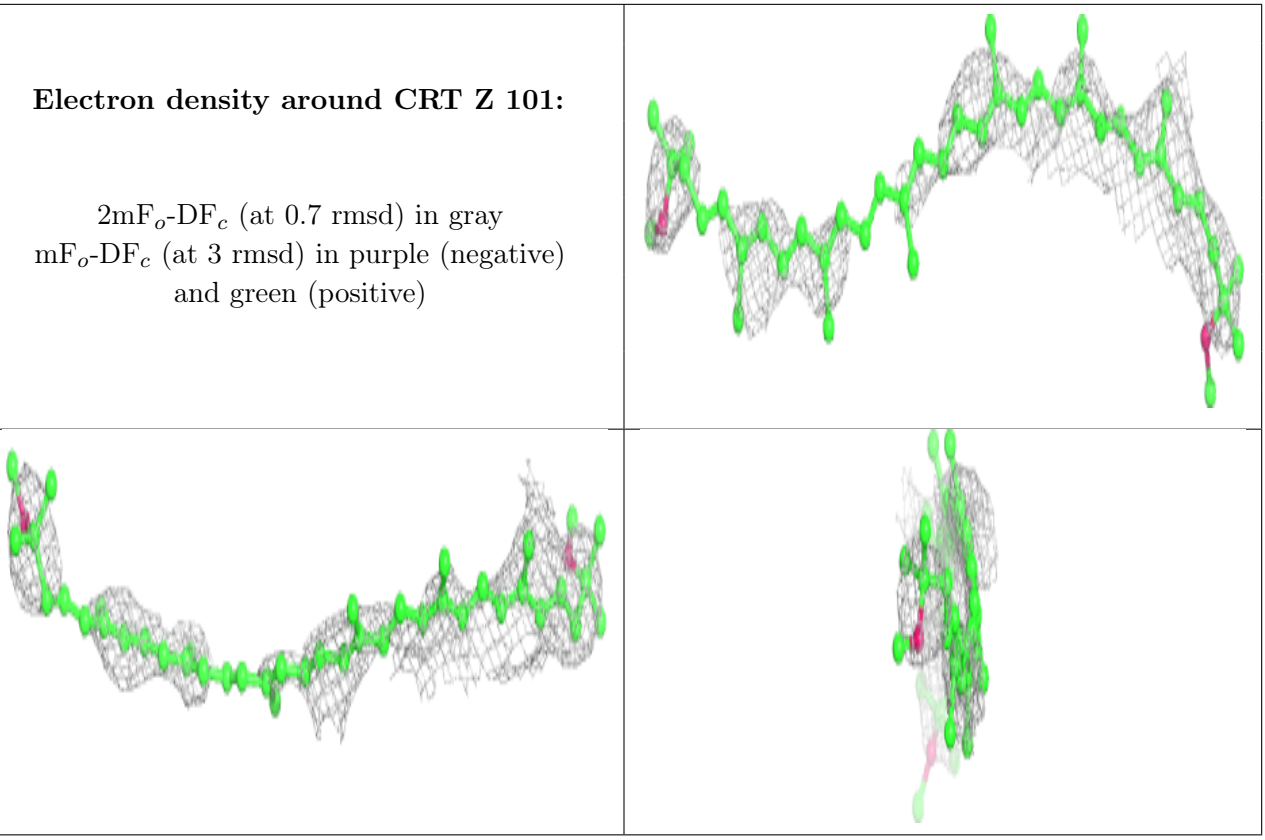
Electron density around BCL K 103:

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



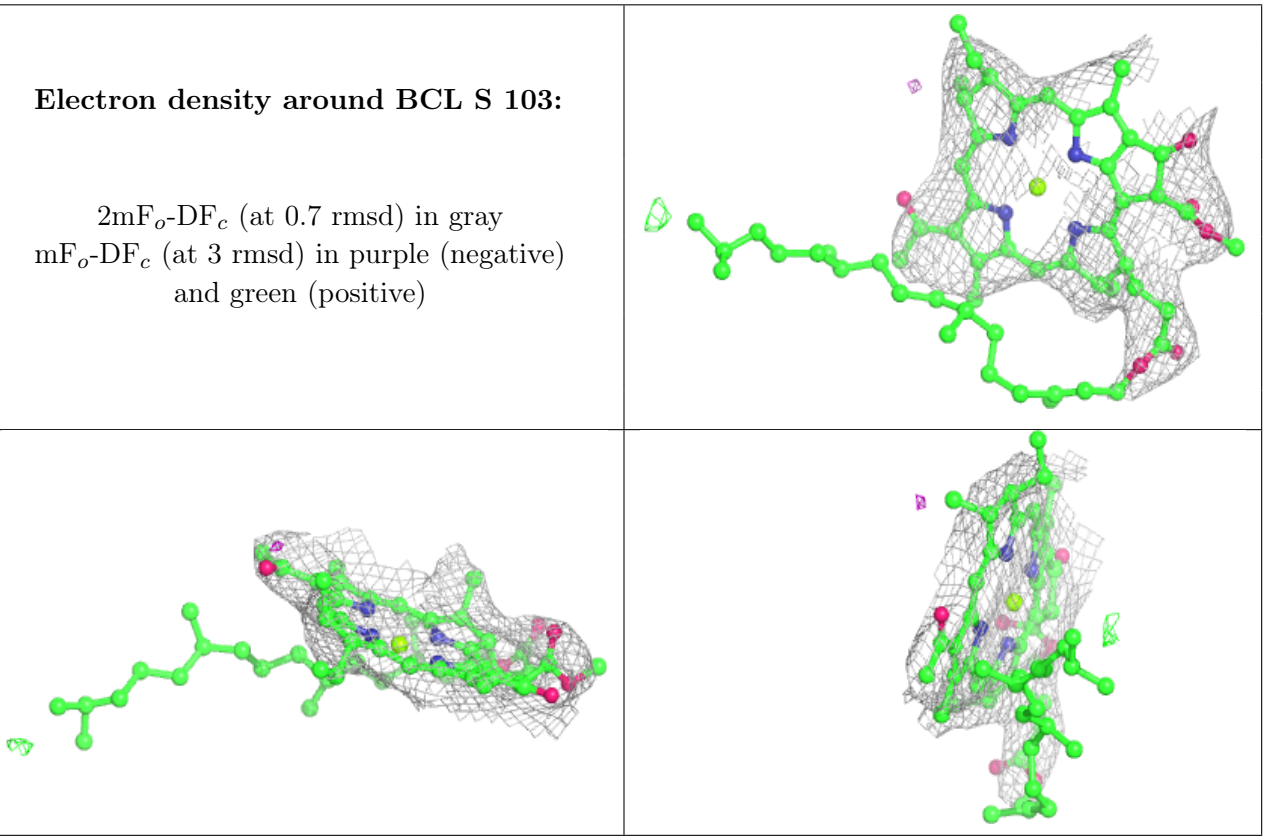
Electron density around CRT Z 101:

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



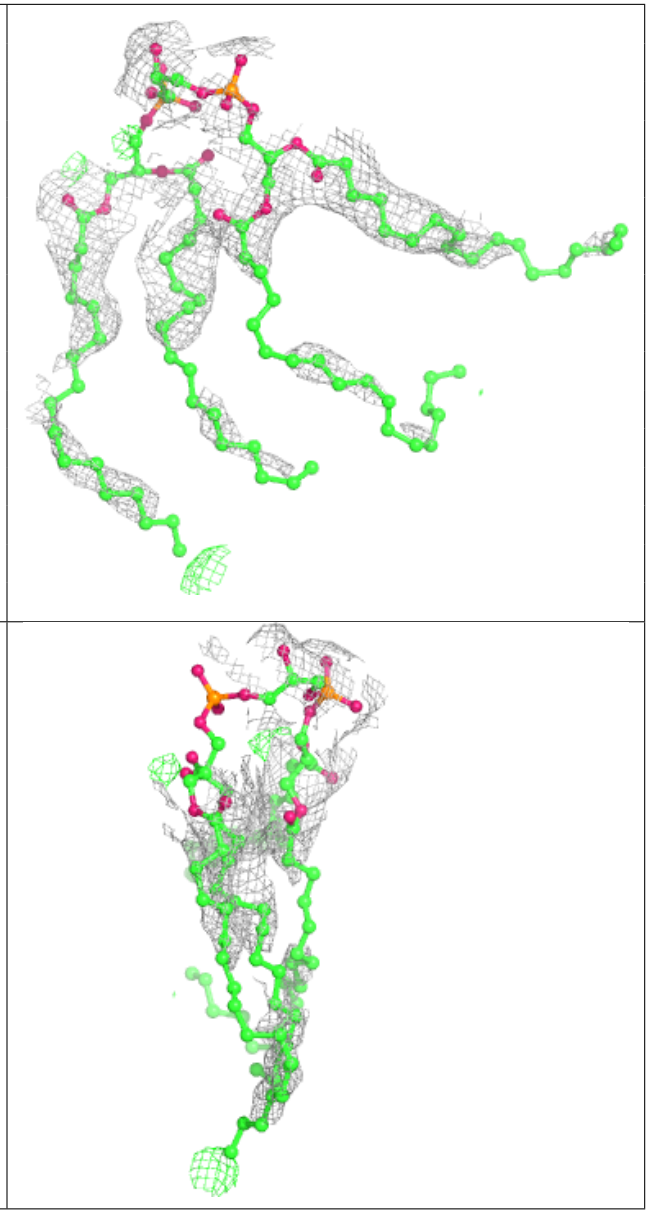
Electron density around BCL S 103:

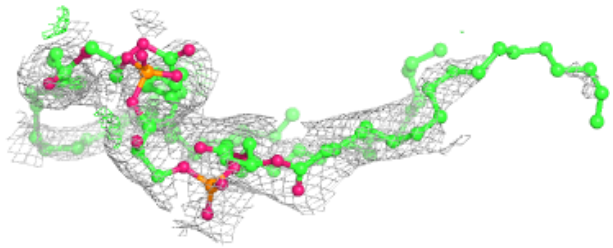
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CDL M 406:

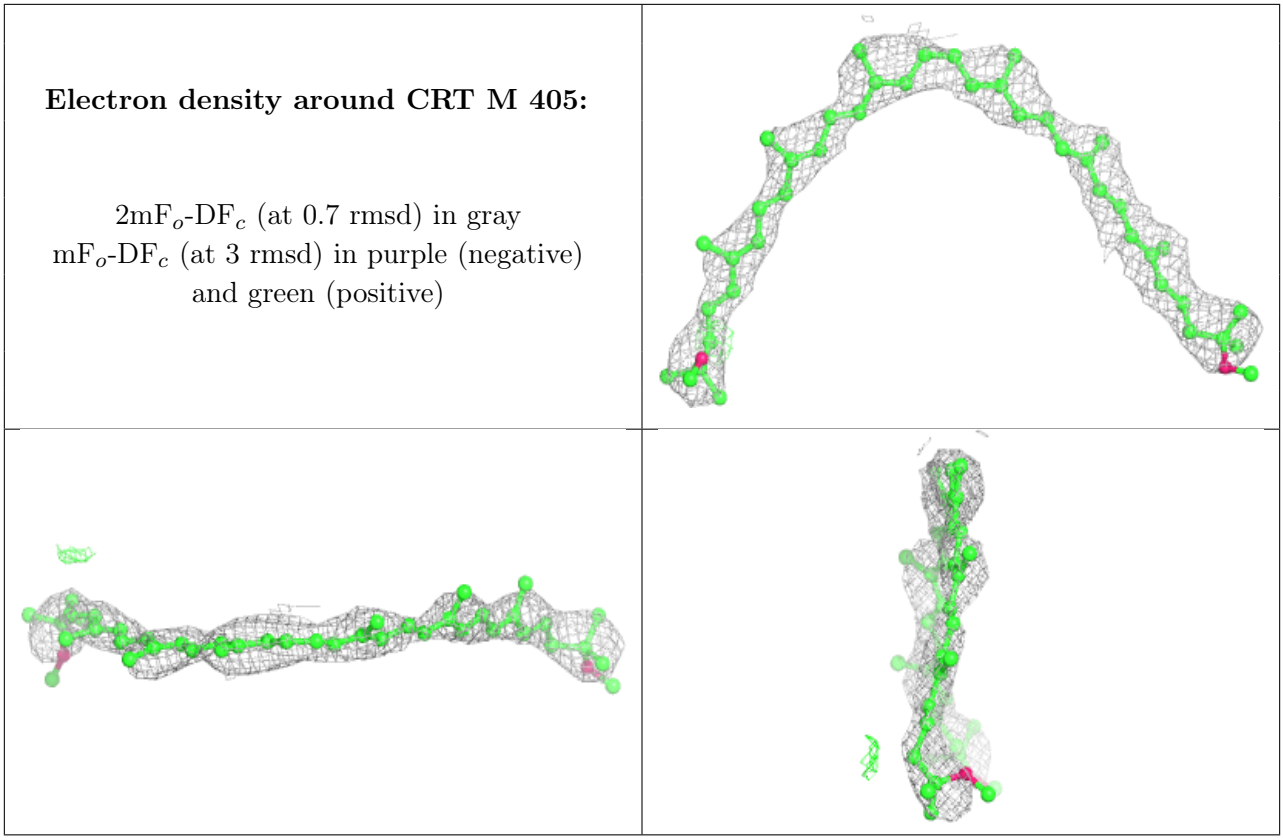
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





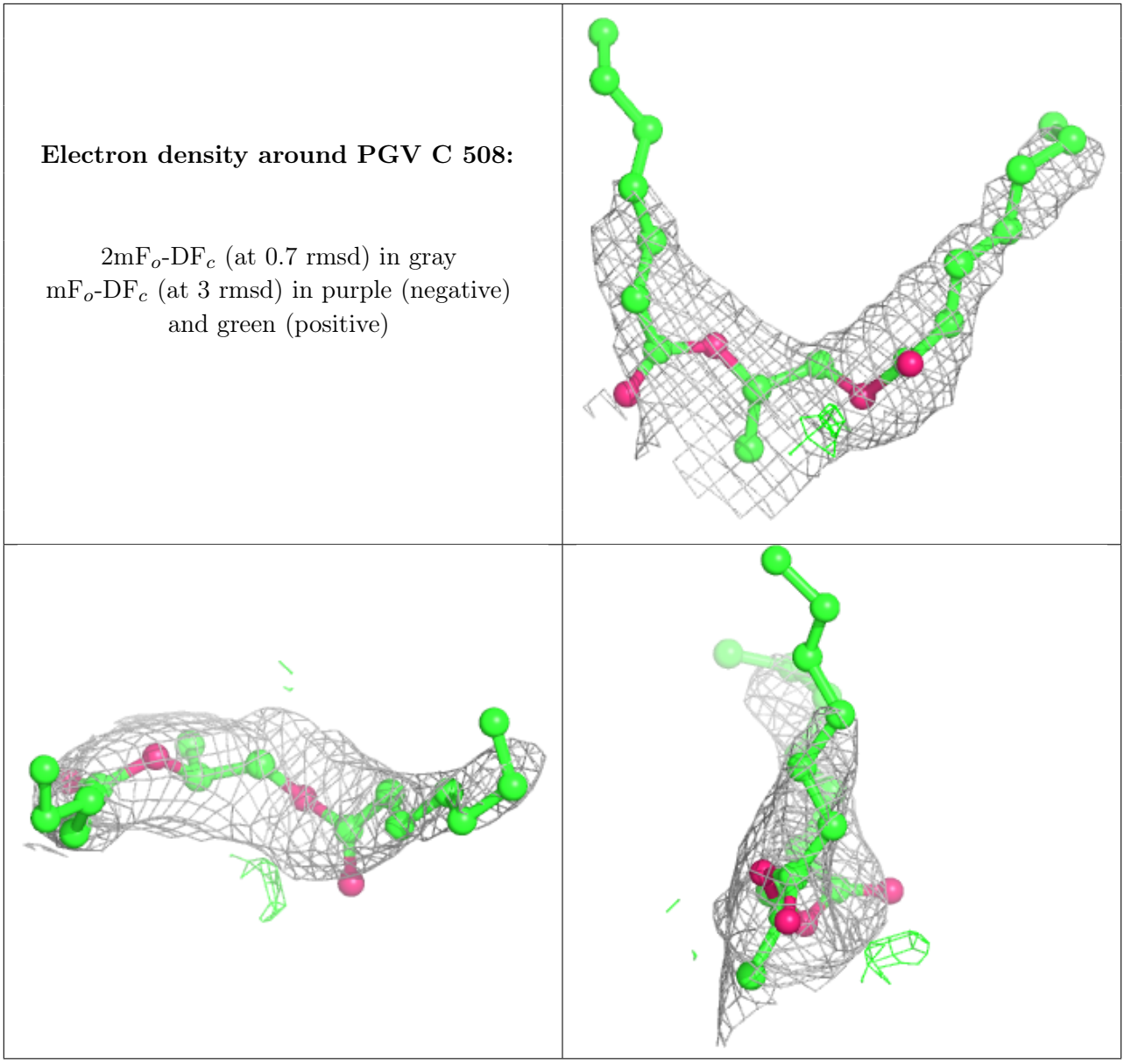
Electron density around CRT M 405:

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



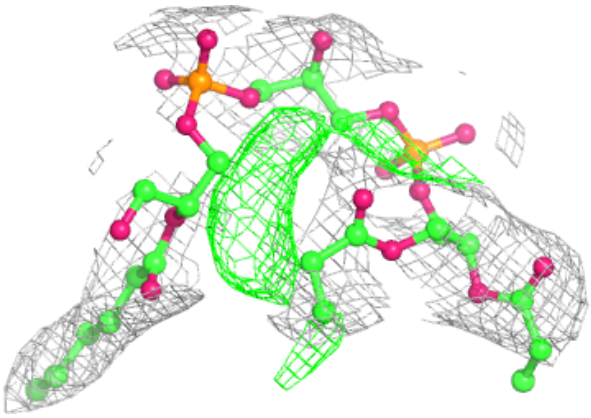
Electron density around PGV C 508:

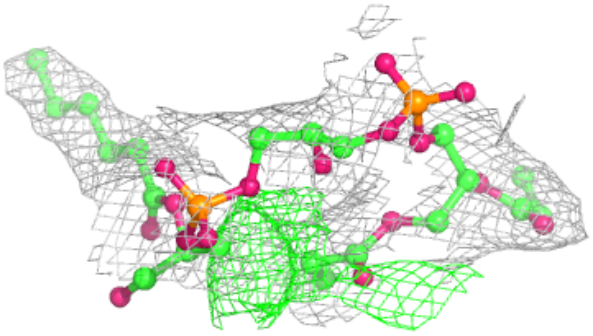
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

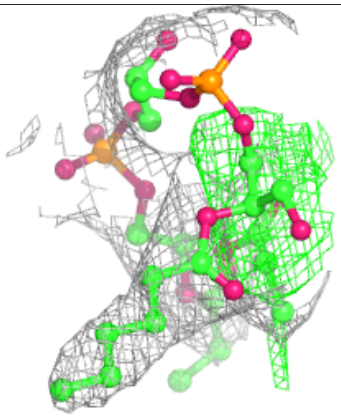


Electron density around CDL M 412:

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

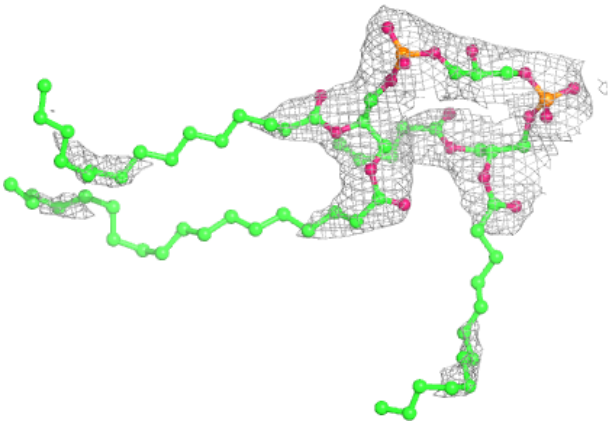


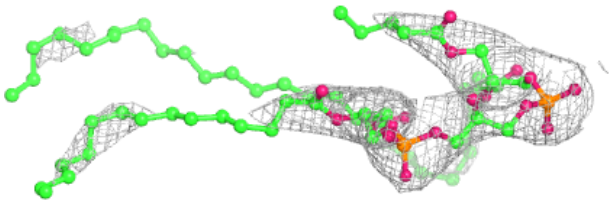


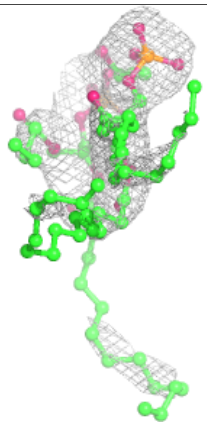


Electron density around CDL H 305:

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

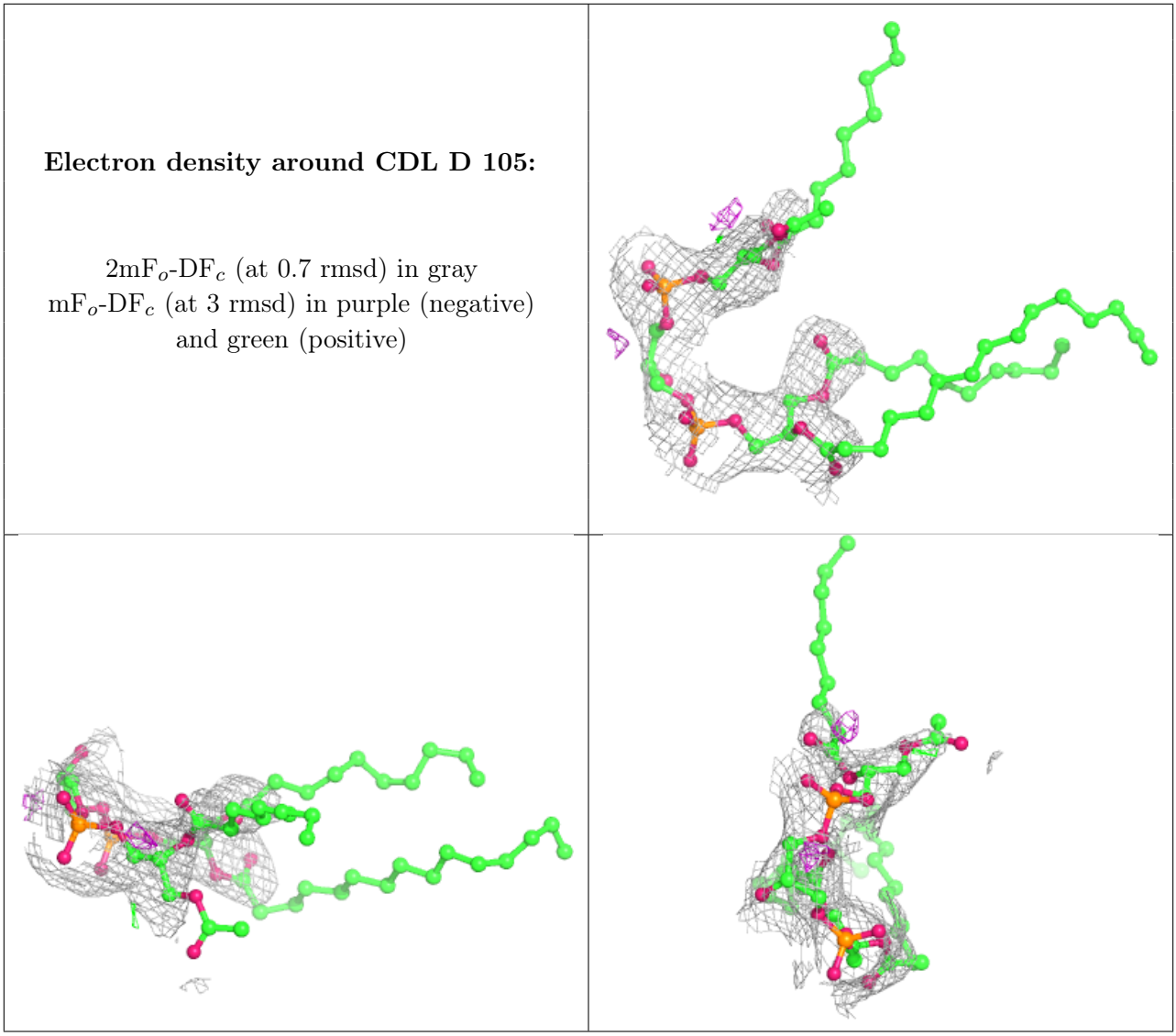






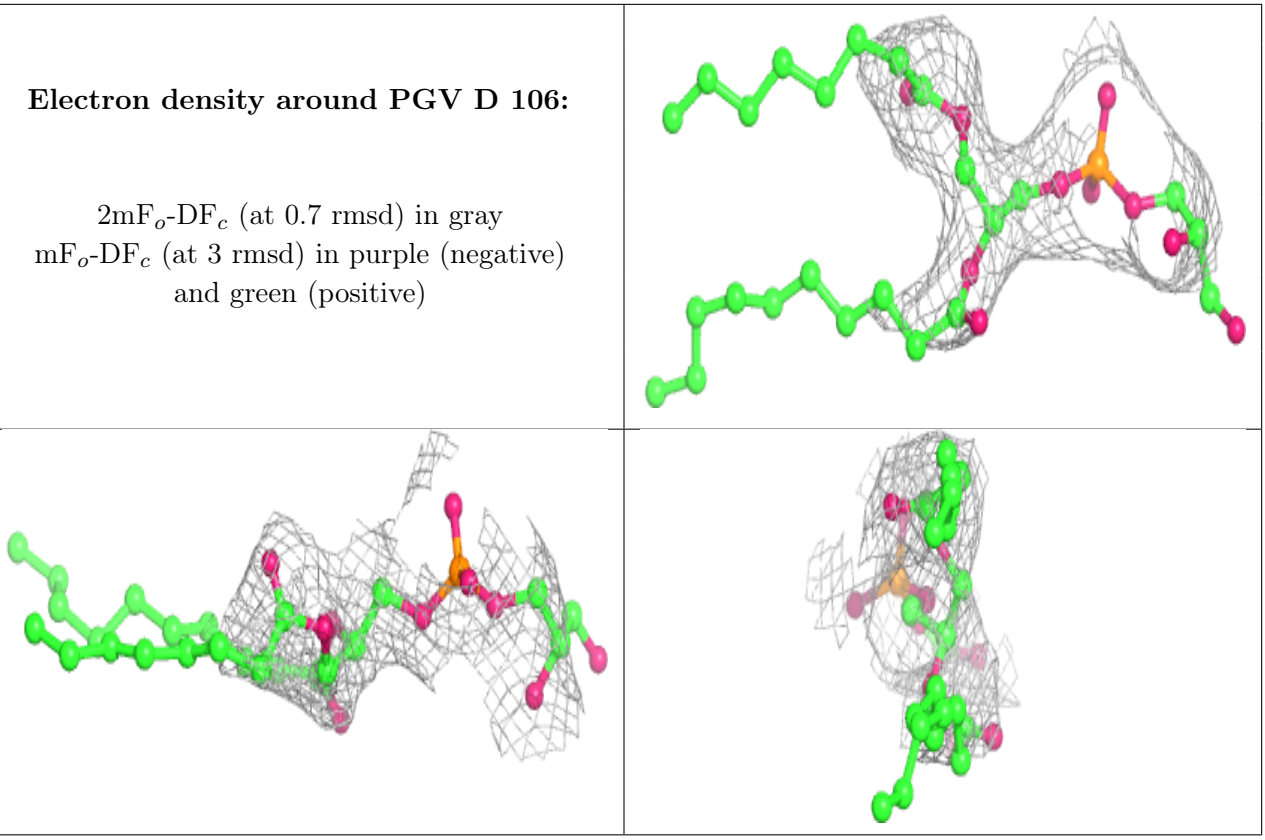
Electron density around CDL D 105:

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



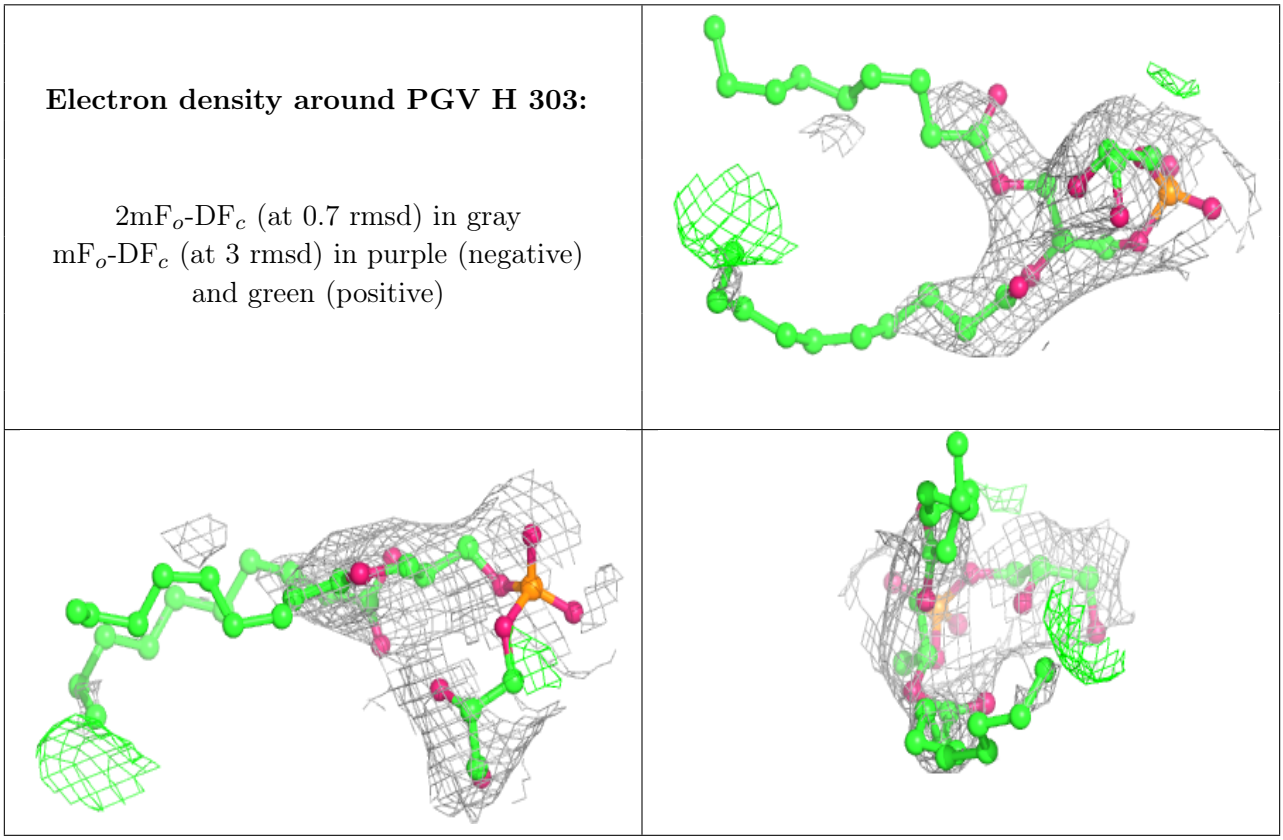
Electron density around PGV D 106:

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



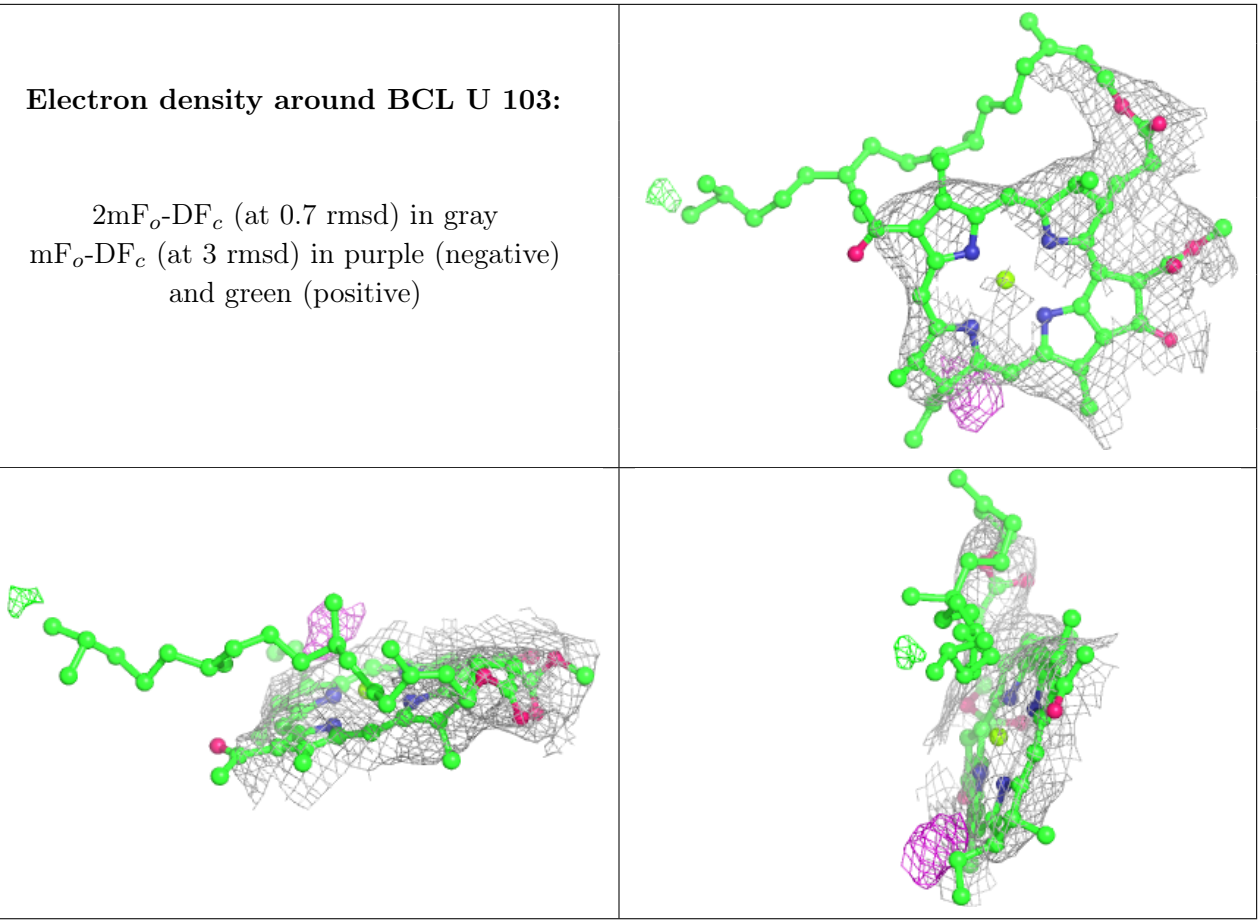
Electron density around PGV H 303:

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



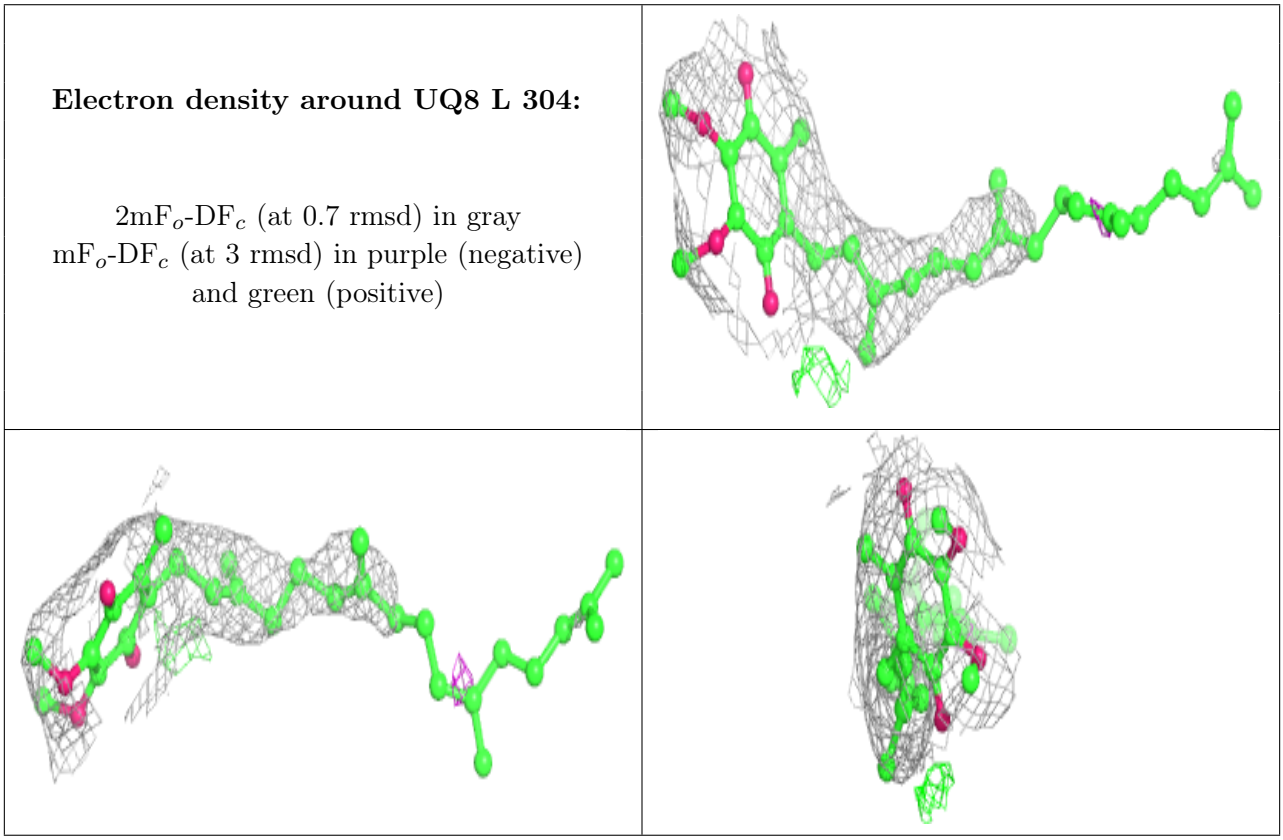
Electron density around BCL U 103:

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



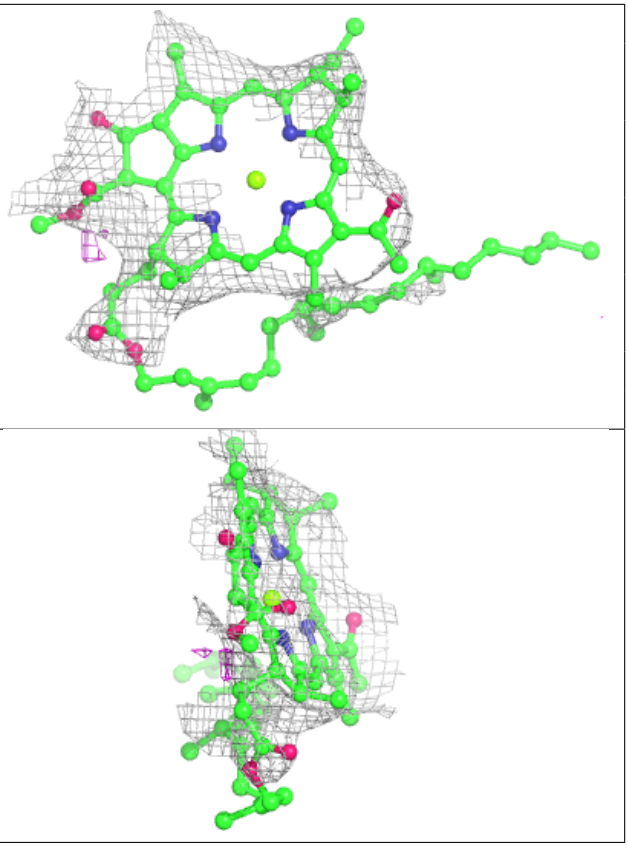
Electron density around UQ8 L 304:

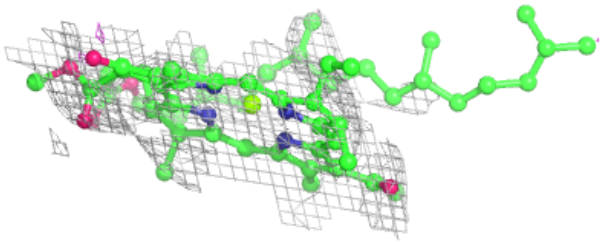
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around BCL 5 103:

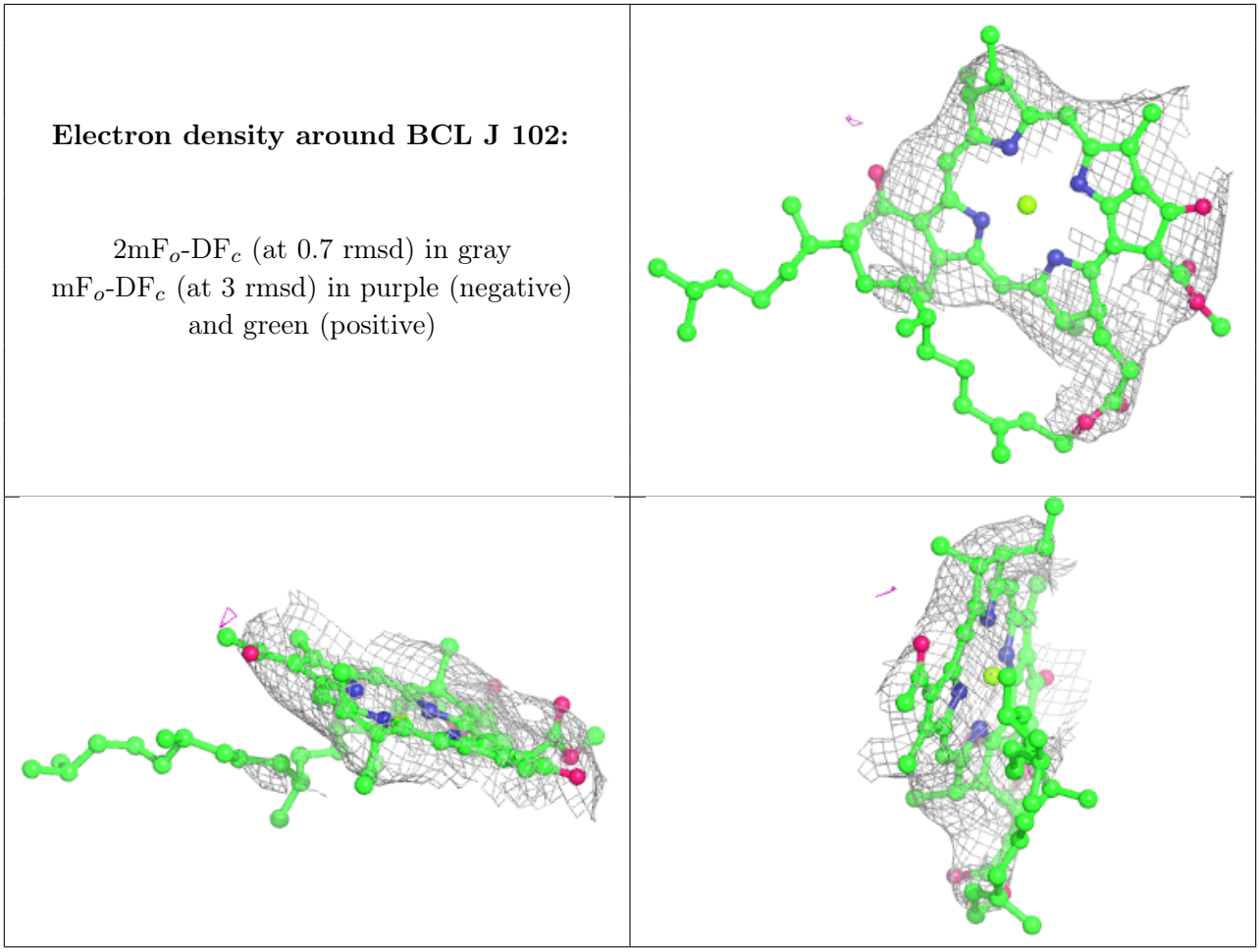
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





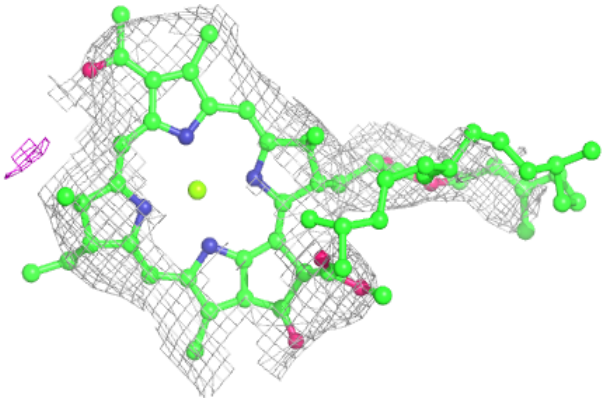
Electron density around BCL J 102:

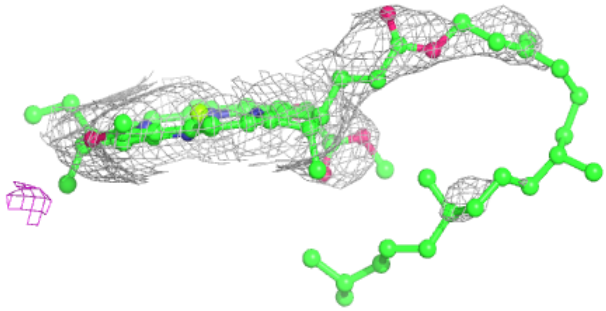
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

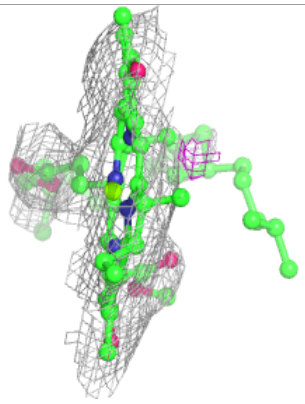


Electron density around BCL K 101:

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

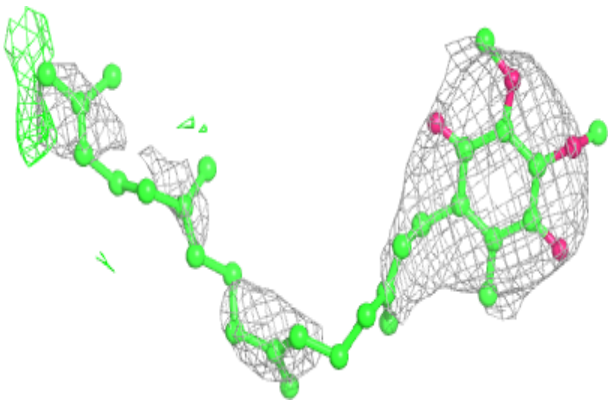


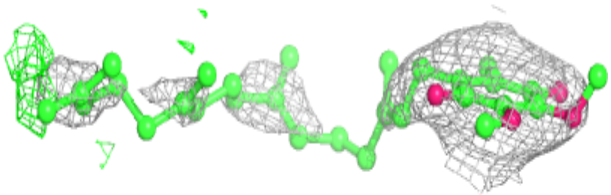


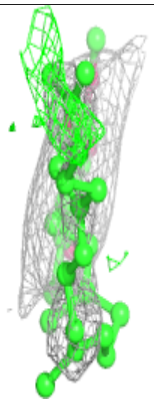


Electron density around UQ8 L 310:

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

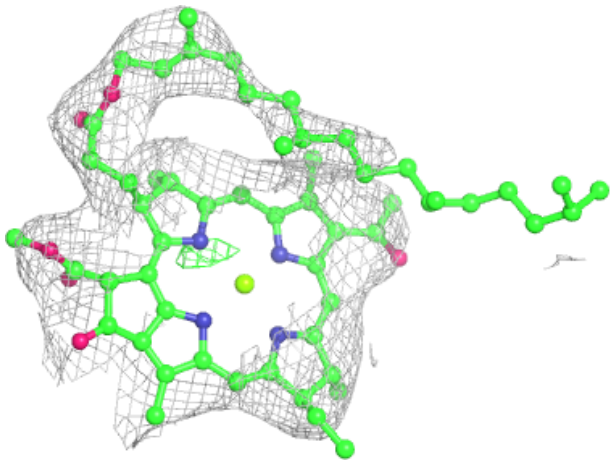


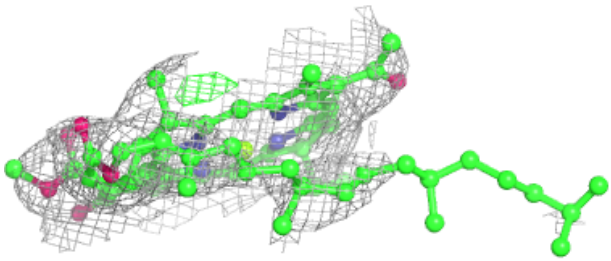


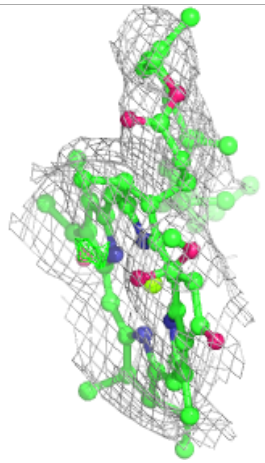


Electron density around BCL Q 103:

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

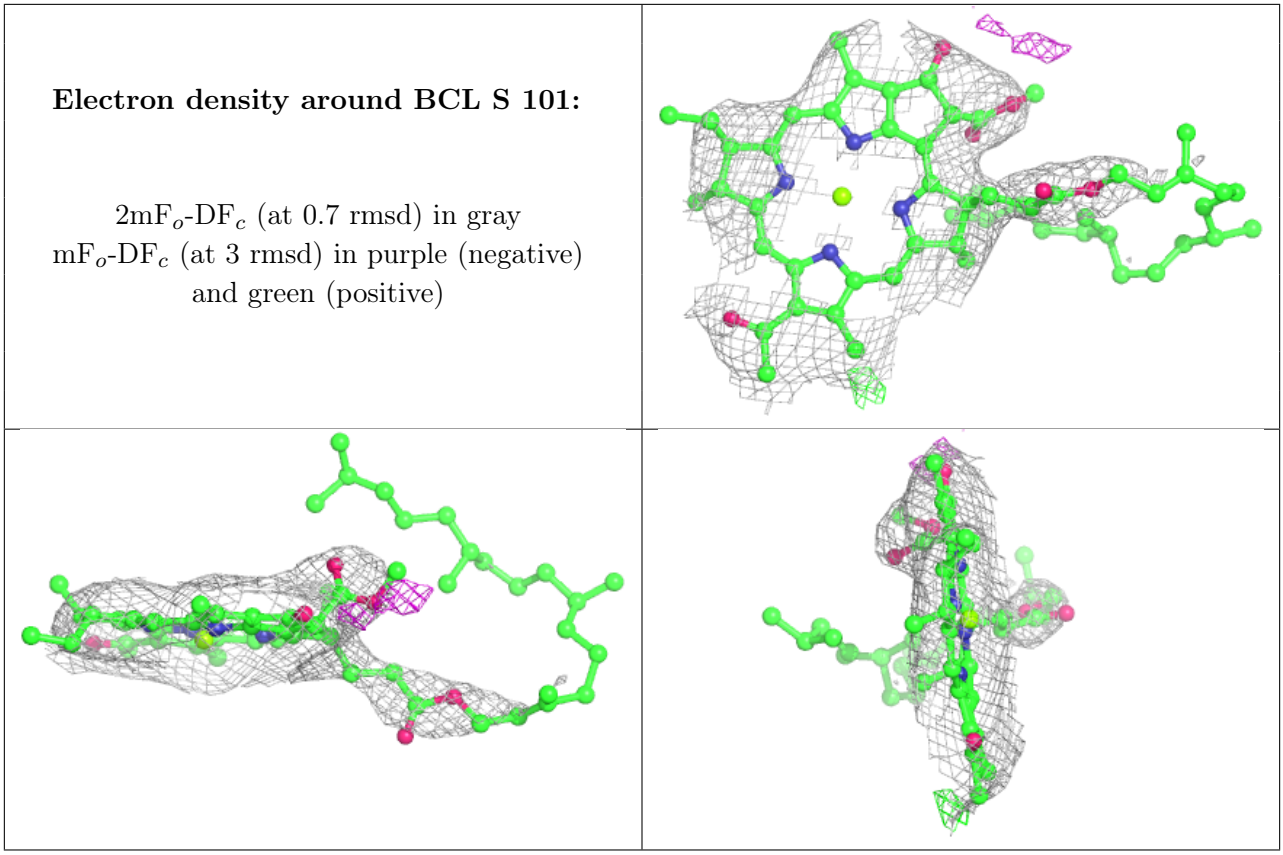






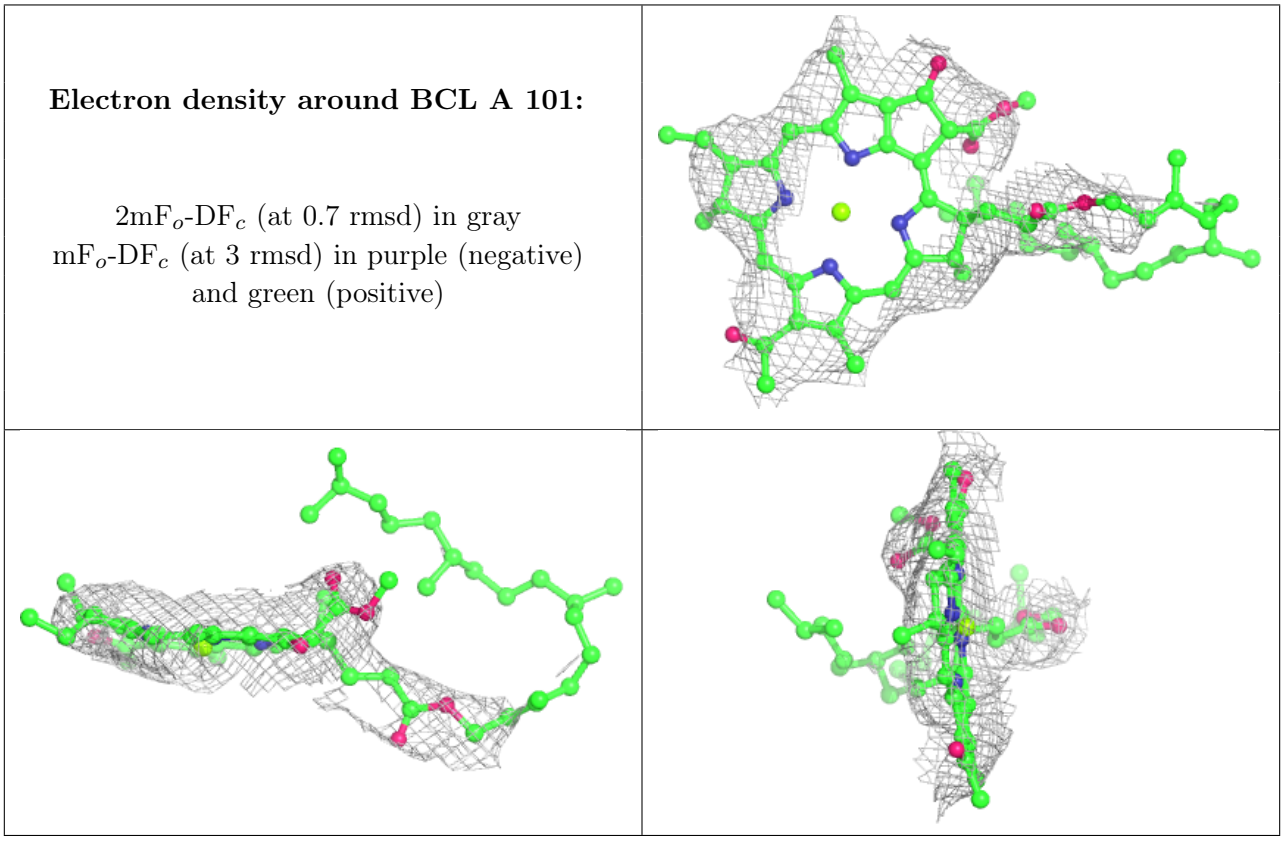
Electron density around BCL S 101:

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



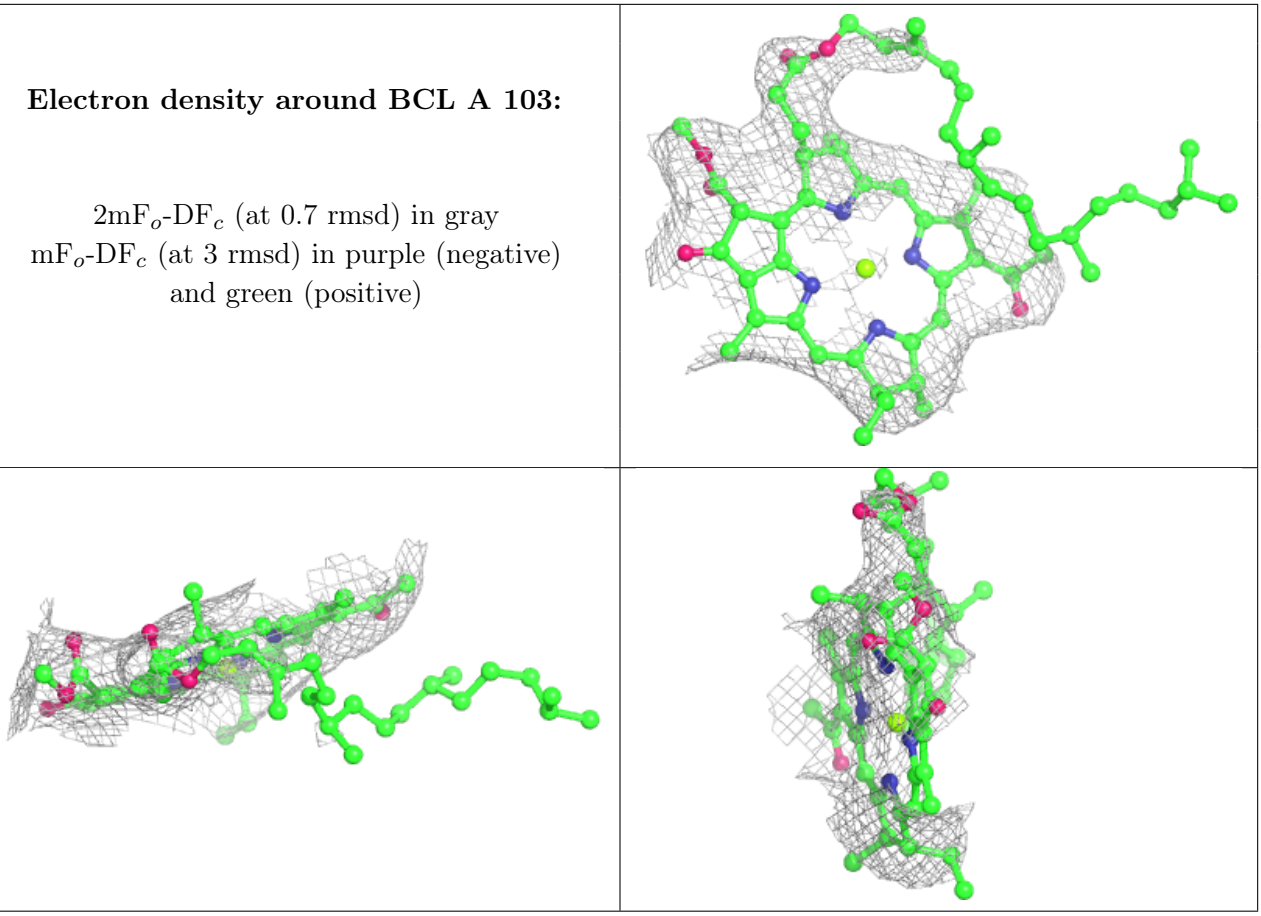
Electron density around BCL A 101:

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



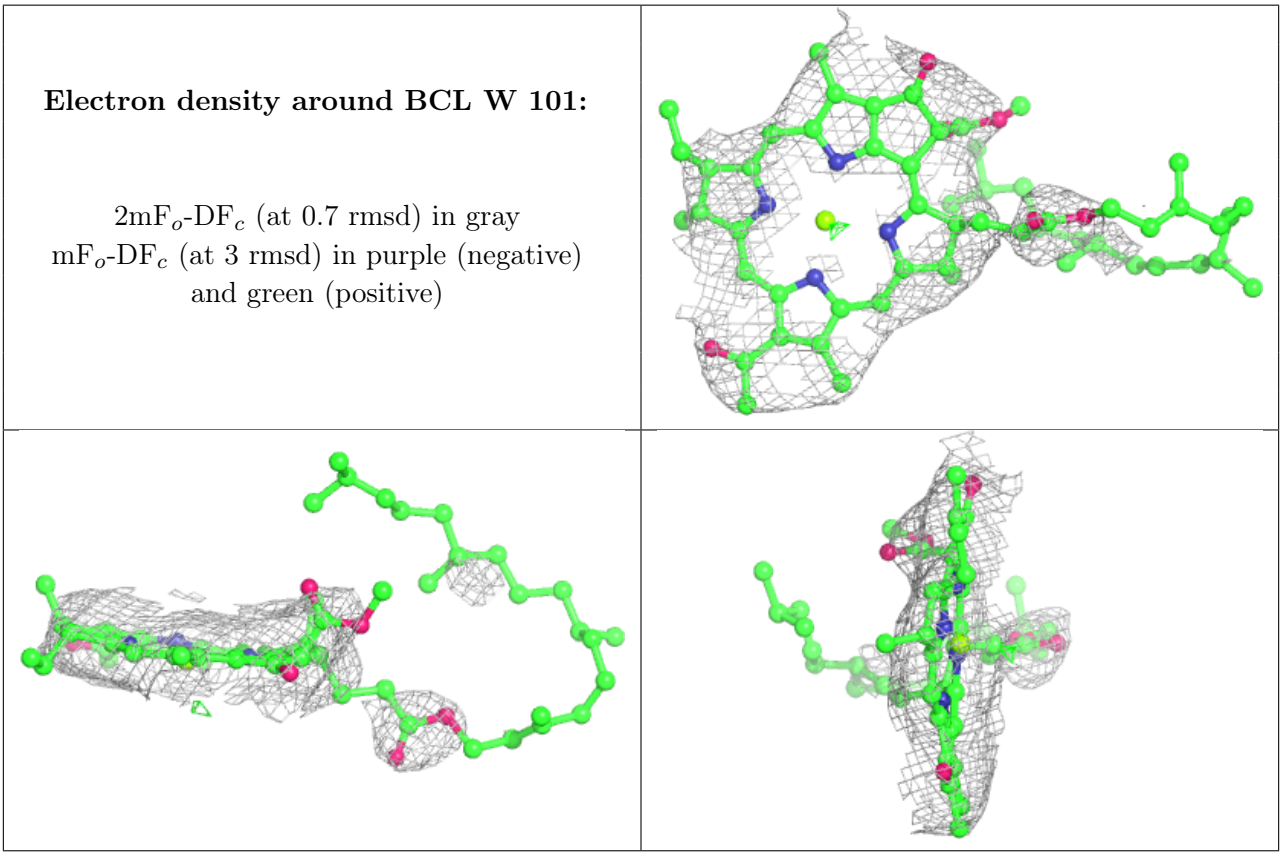
Electron density around BCL A 103:

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



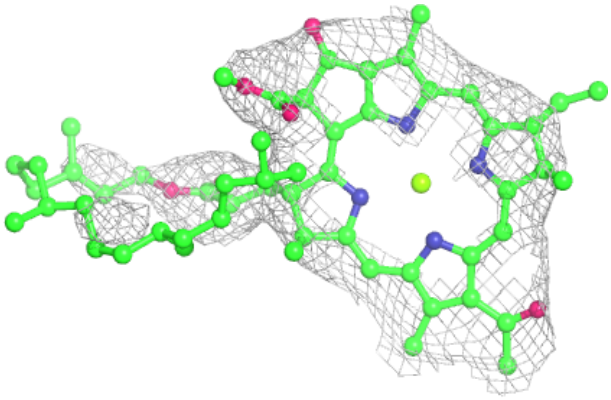
Electron density around BCL W 101:

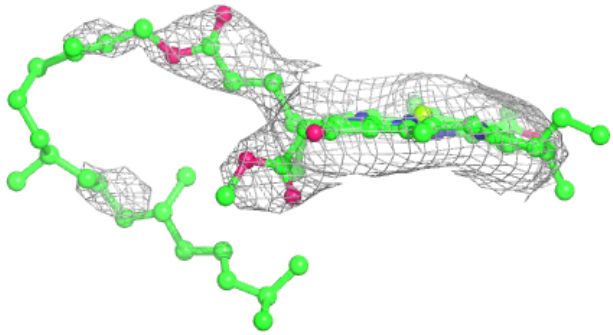
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

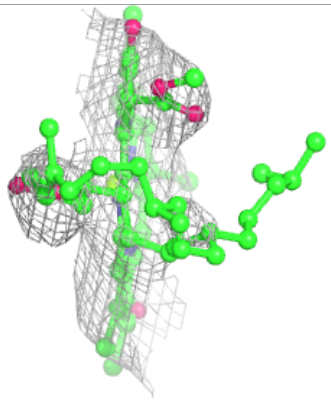


Electron density around BCL O 101:

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

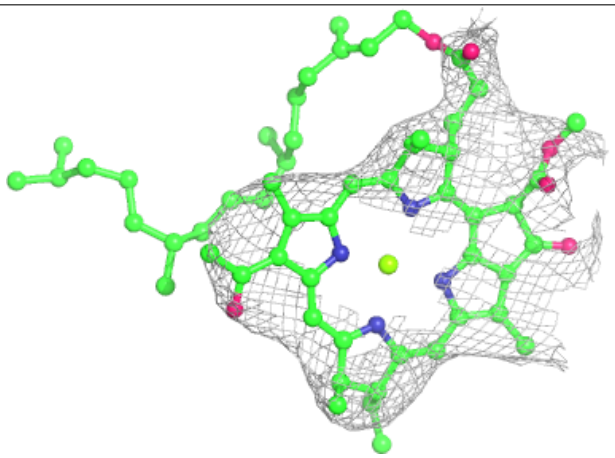


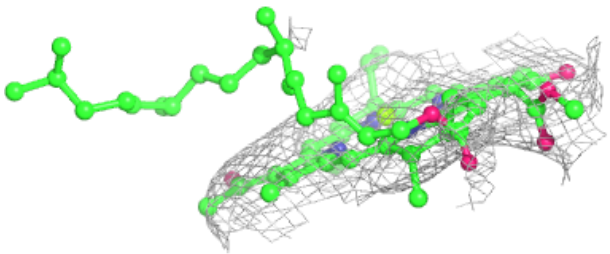


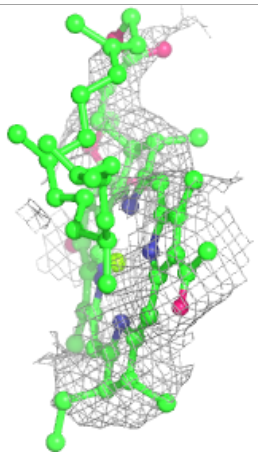


Electron density around BCL 9 103:

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

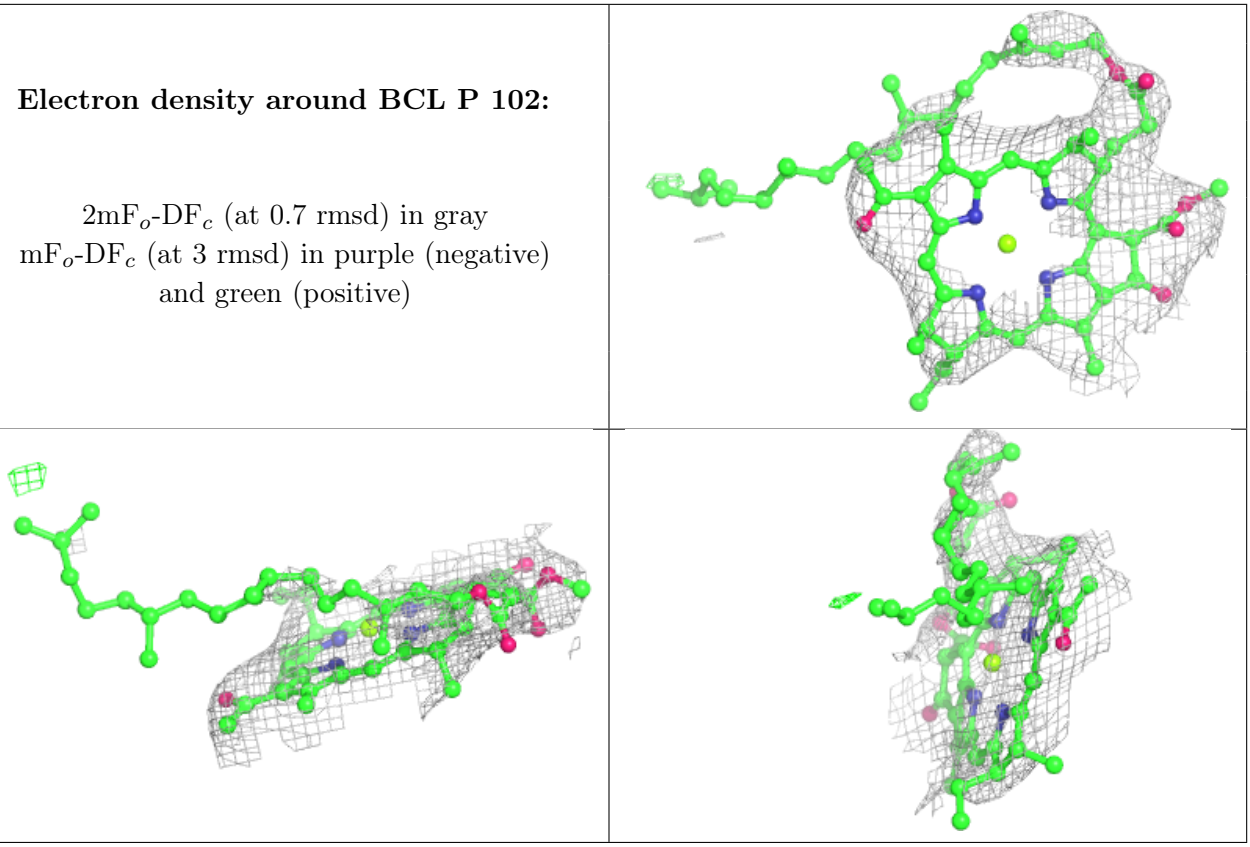






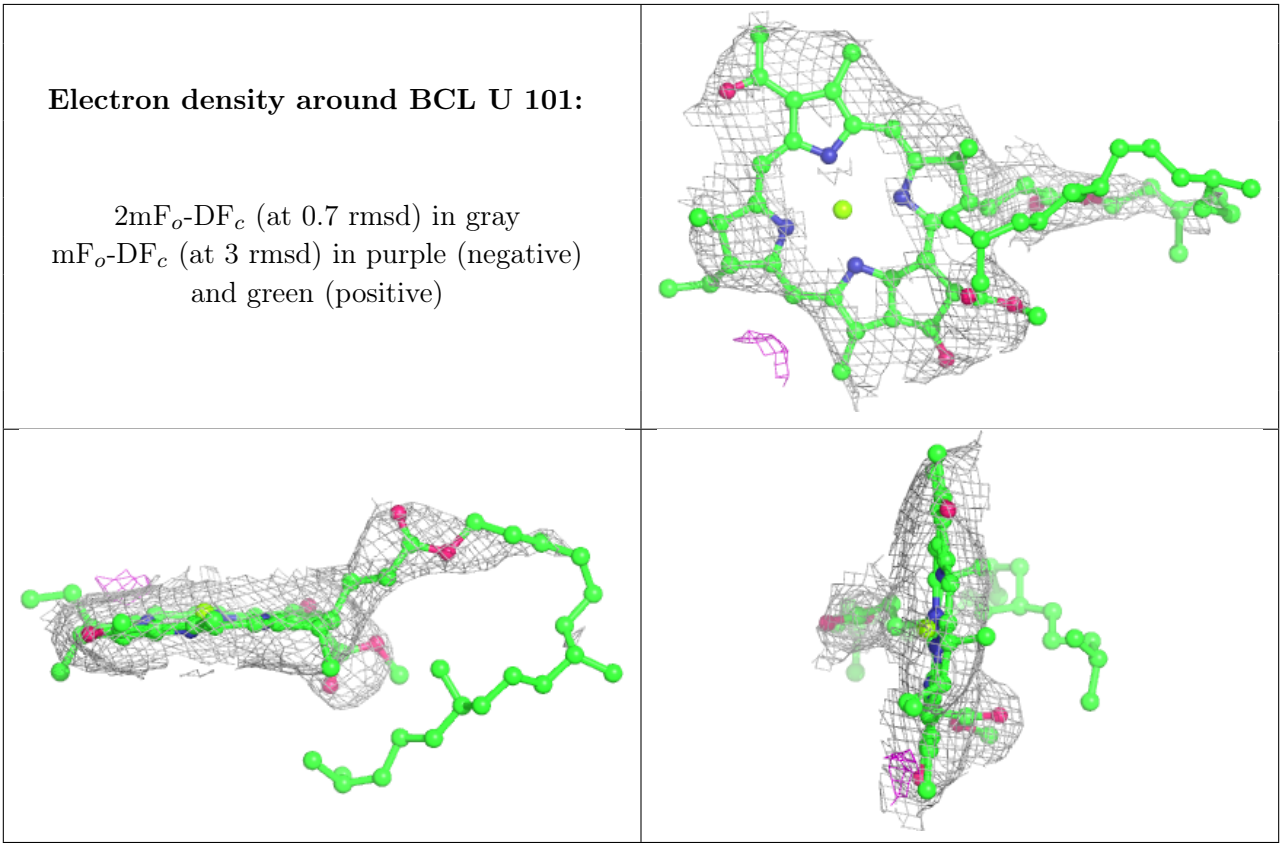
Electron density around BCL P 102:

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



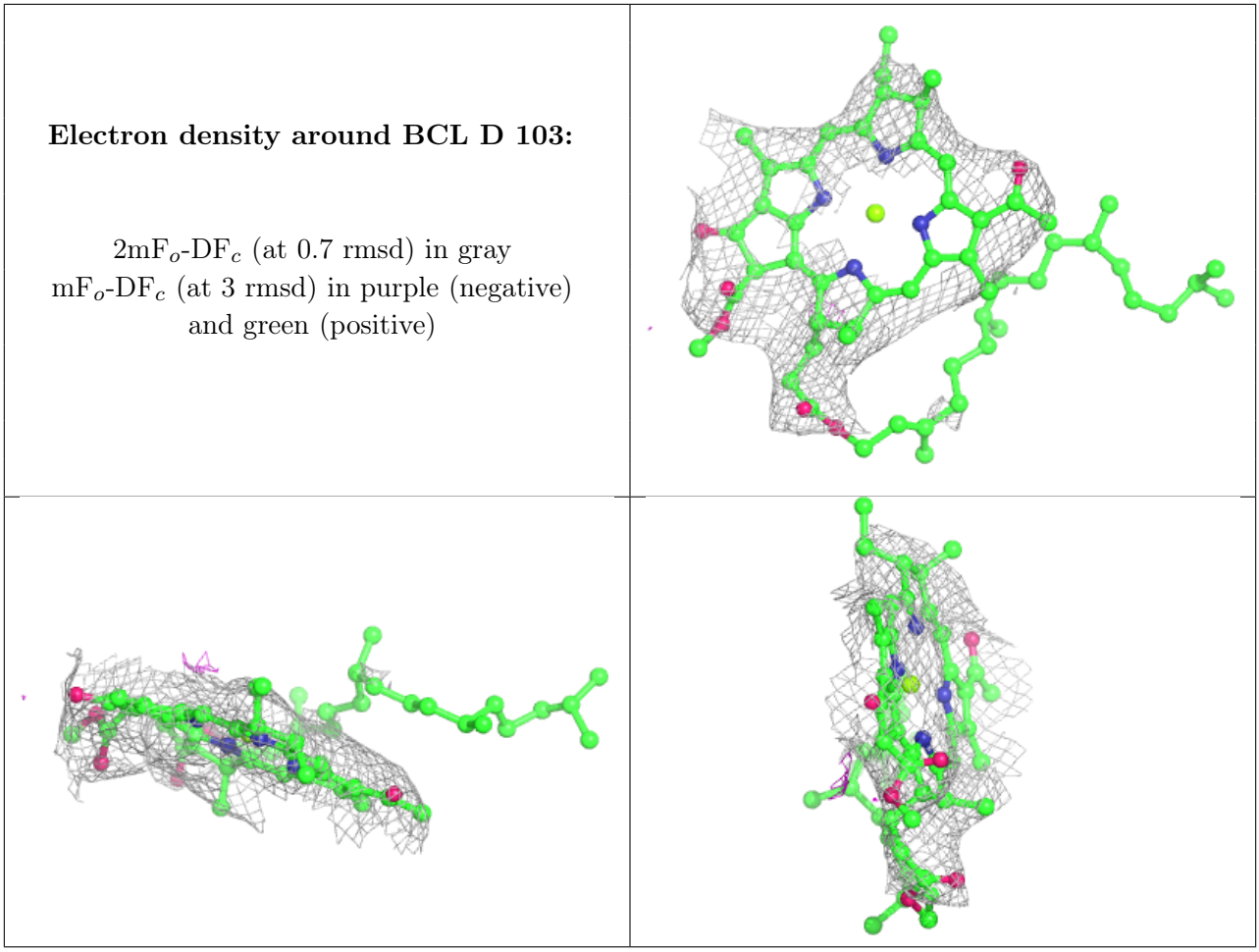
Electron density around BCL U 101:

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



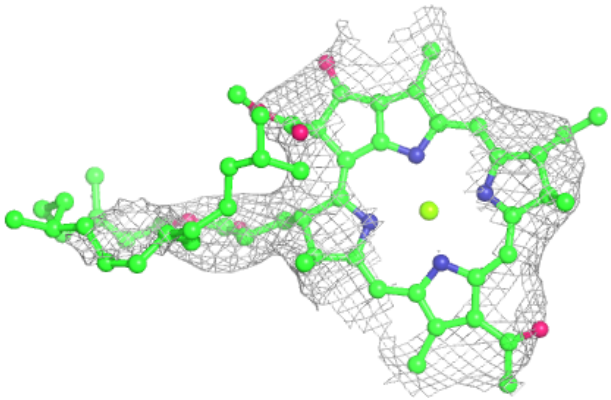
Electron density around BCL D 103:

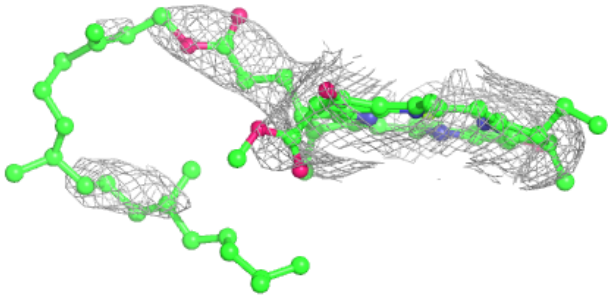
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

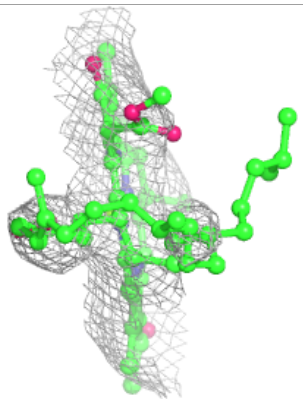


Electron density around BCL F 101:

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

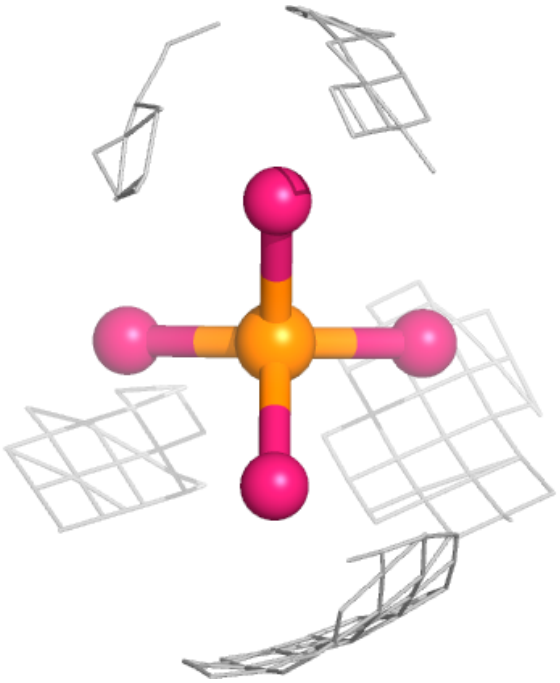


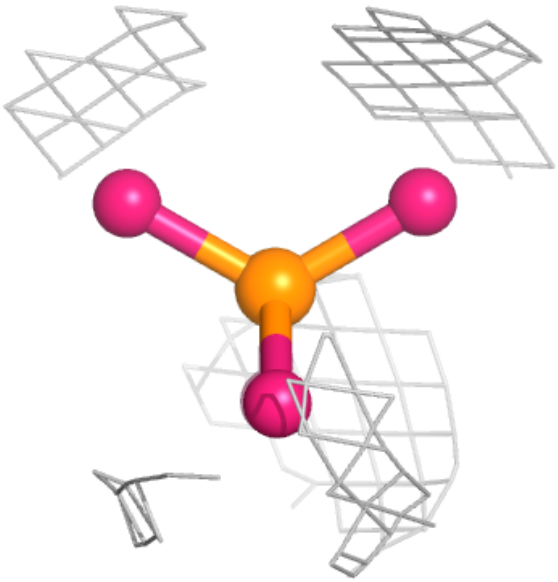


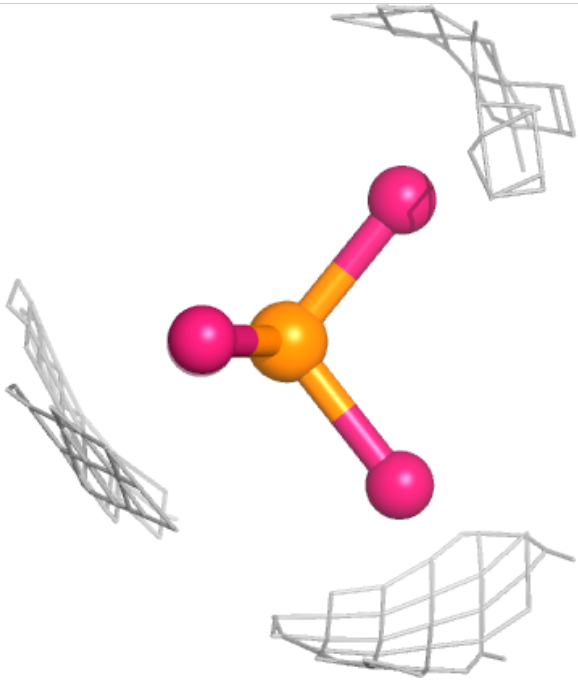


Electron density around PEF M 408:

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

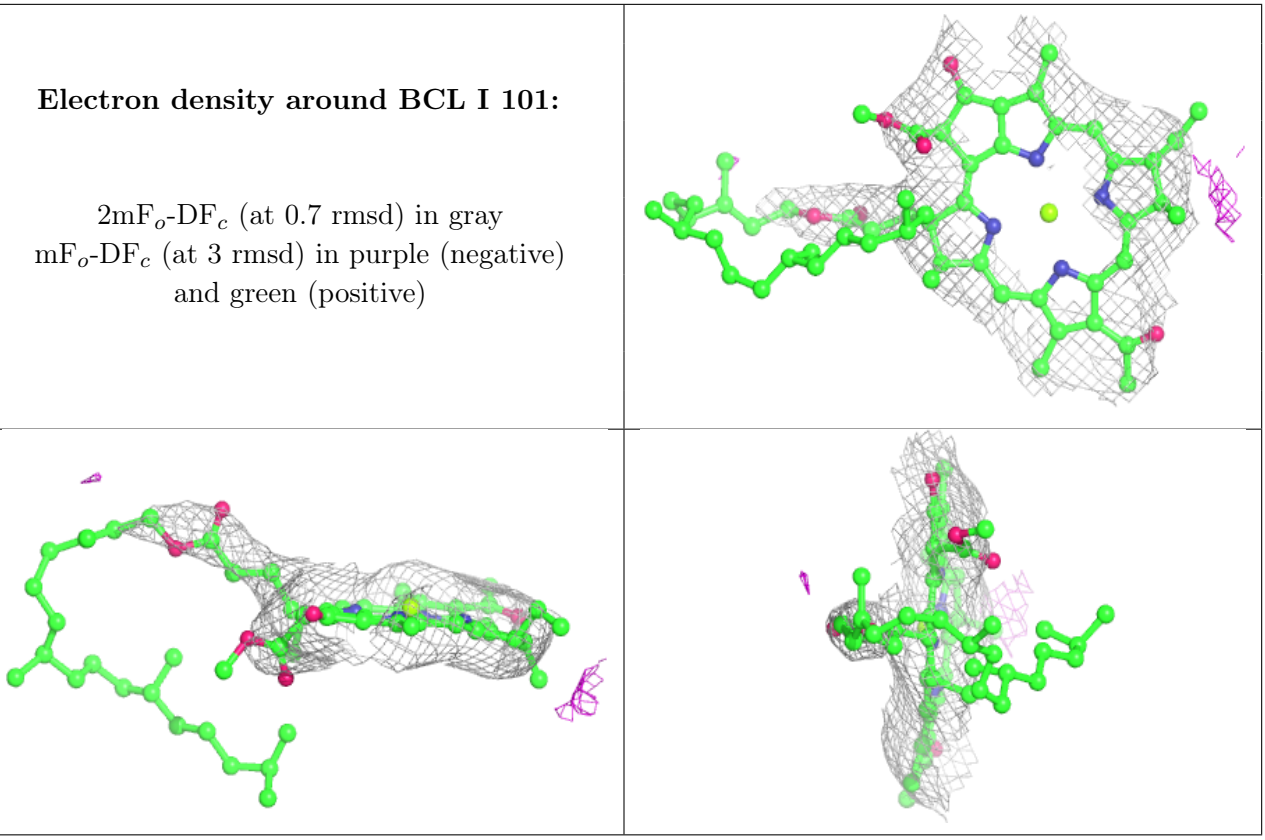






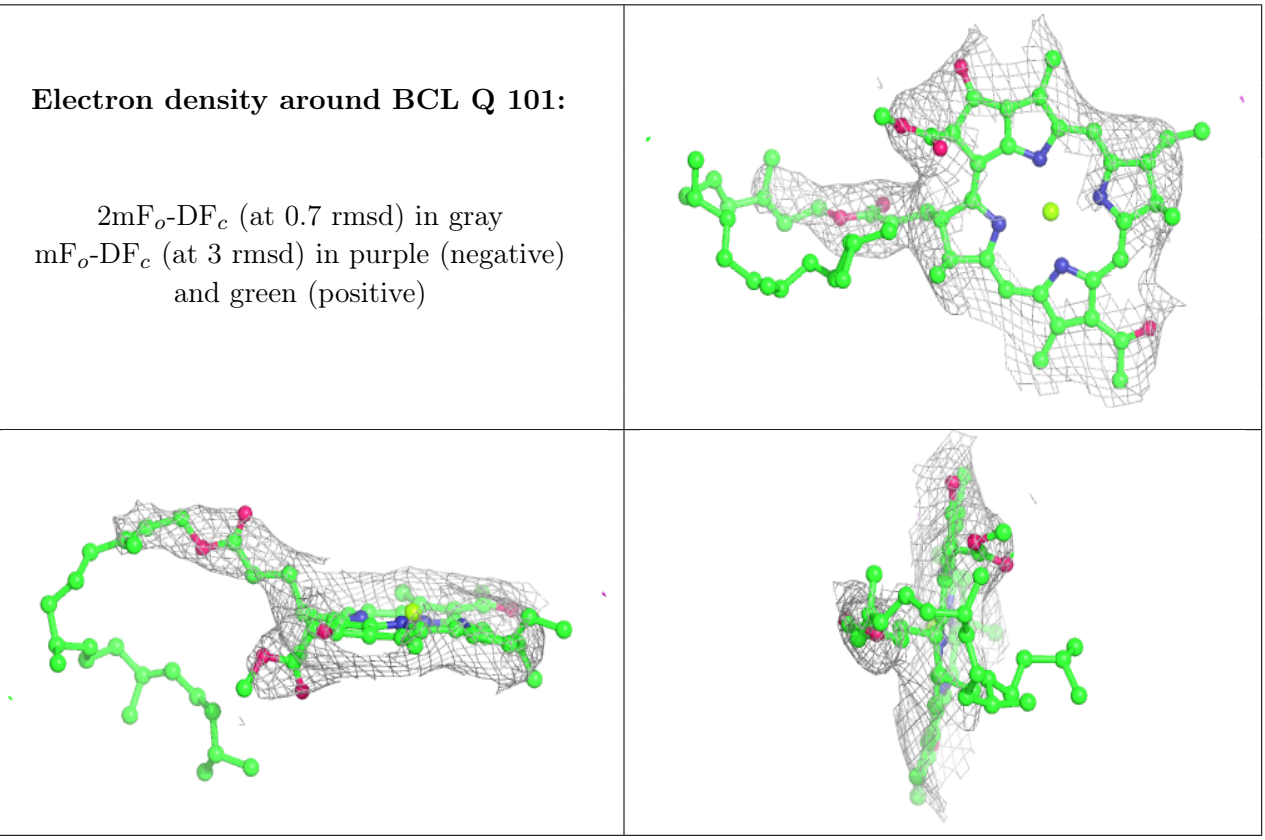
Electron density around BCL I 101:

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



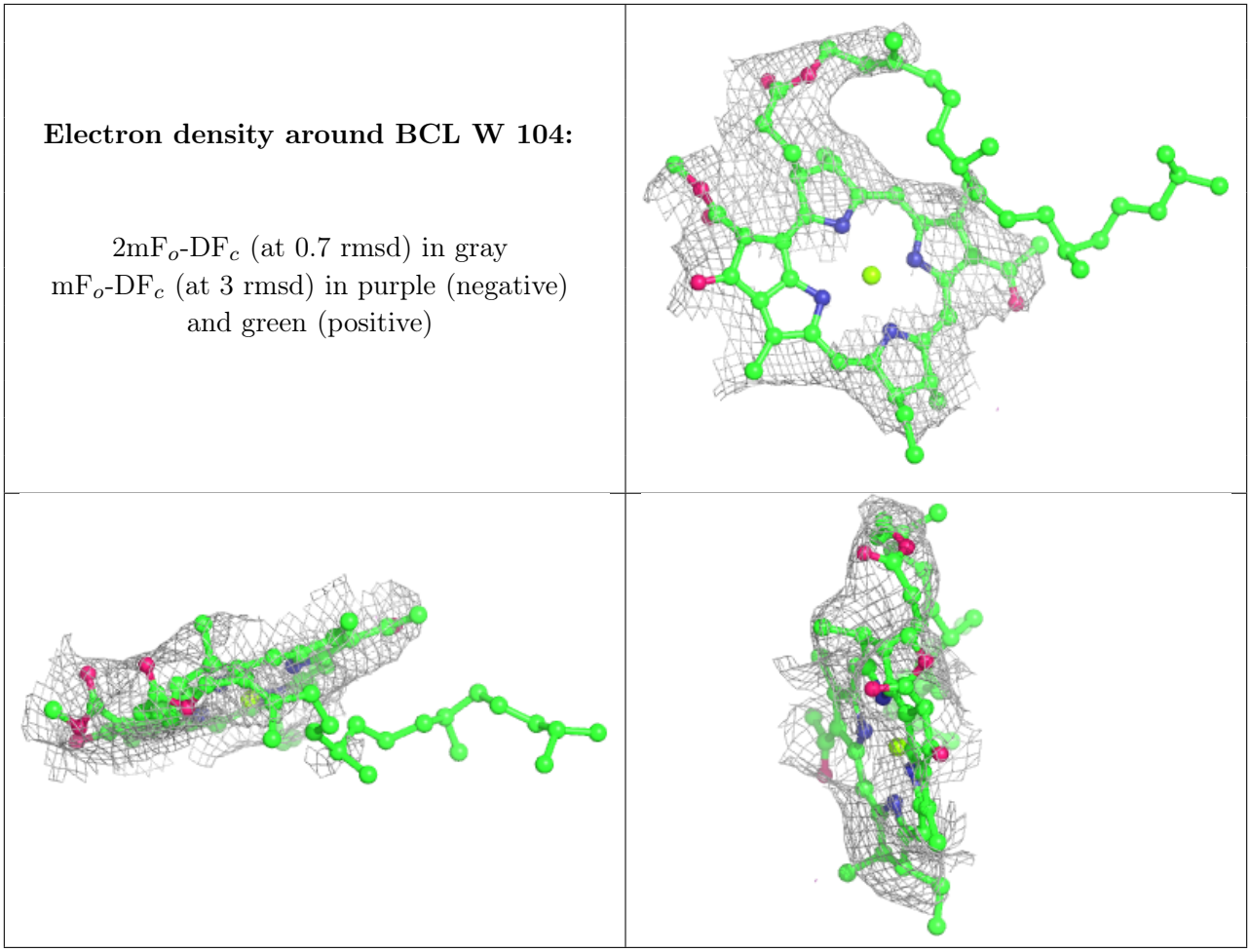
Electron density around BCL Q 101:

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



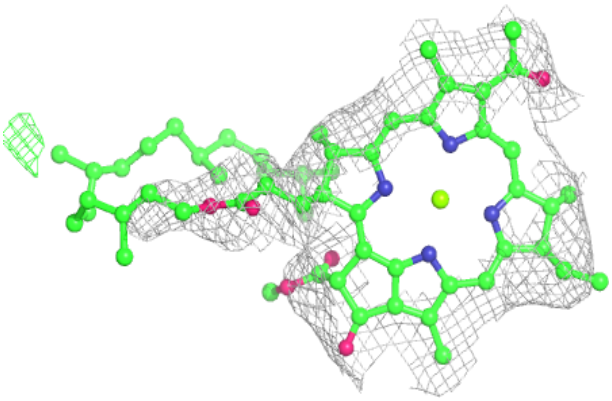
Electron density around BCL W 104:

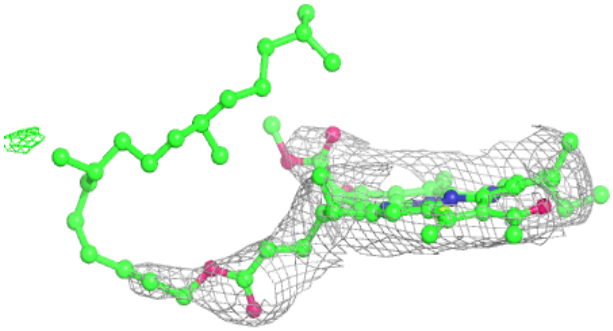
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

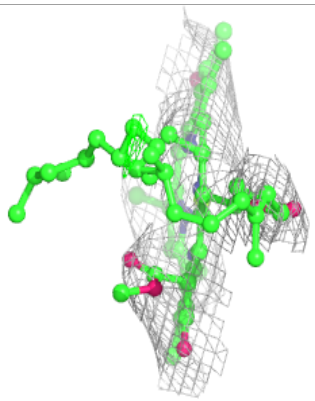


Electron density around BCL 5 101:

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

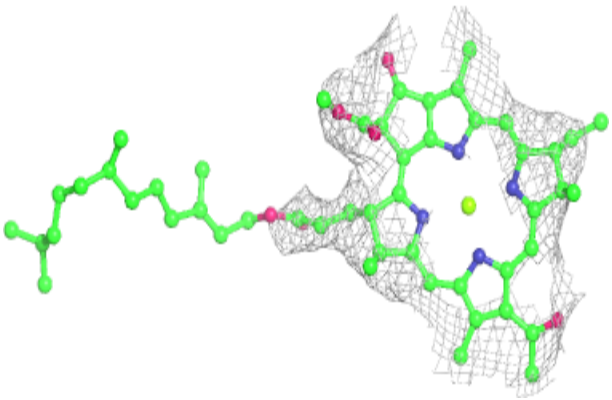


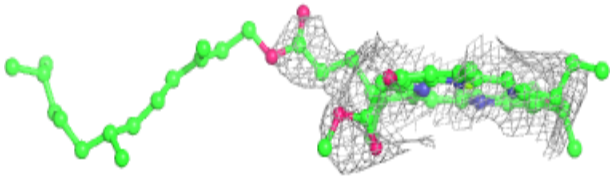


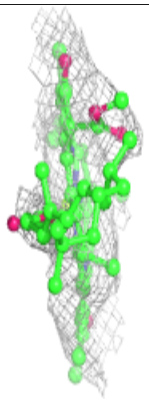


Electron density around BCL 7 101:

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

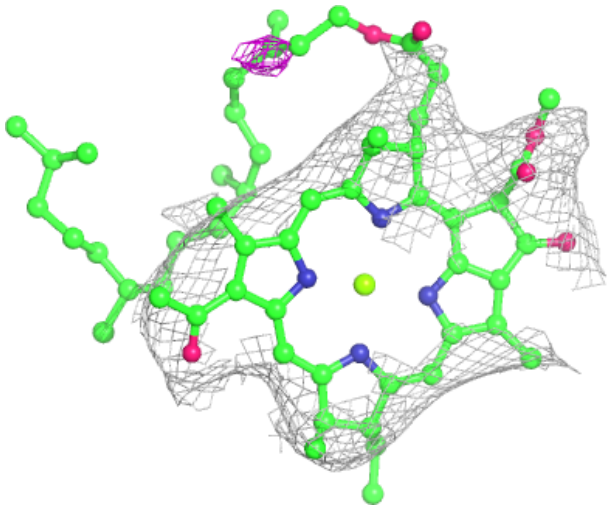


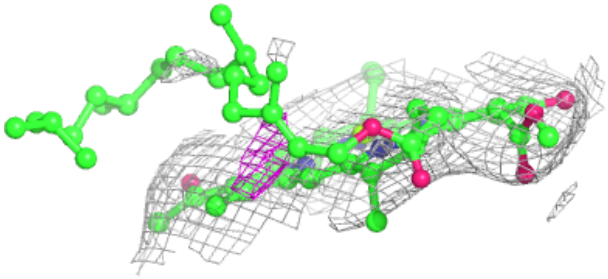


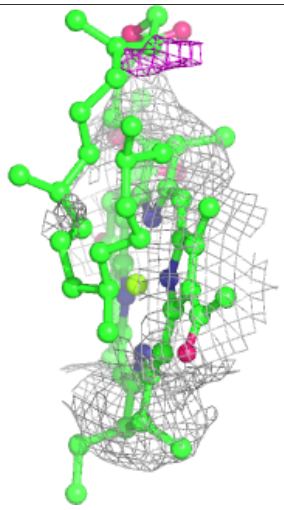


Electron density around BCL 7 103:

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

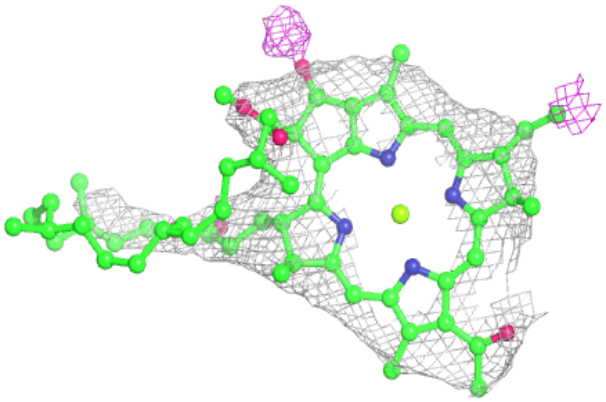


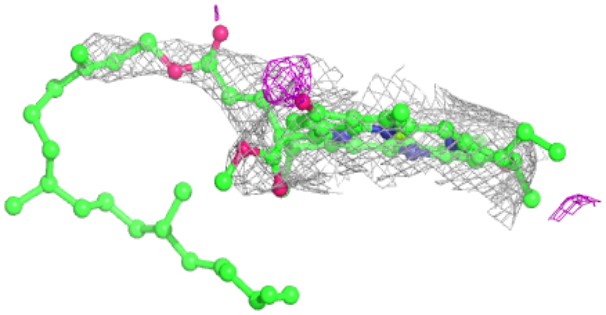


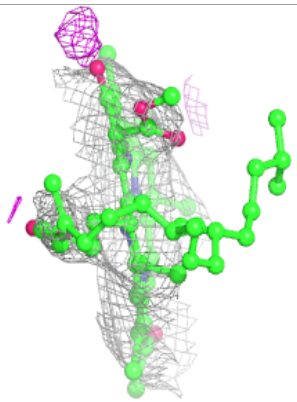


Electron density around BCL D 101:

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

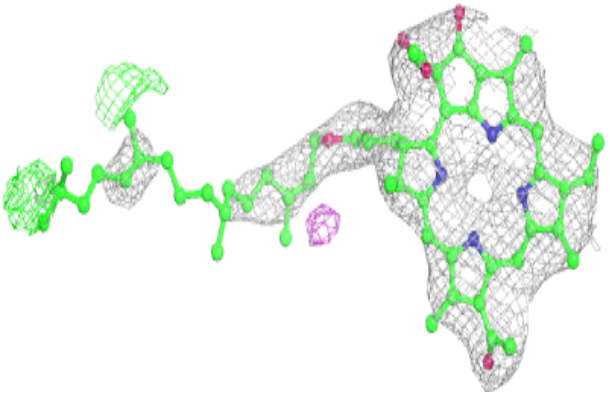


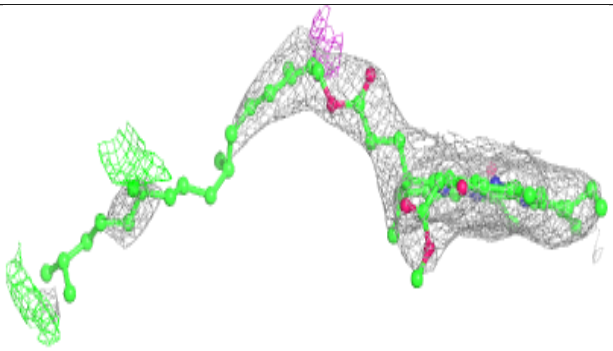


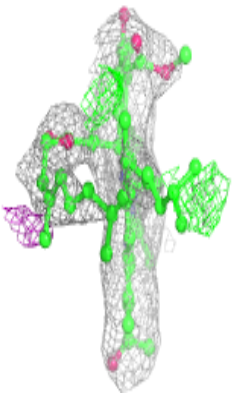


Electron density around BPH M 402:

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

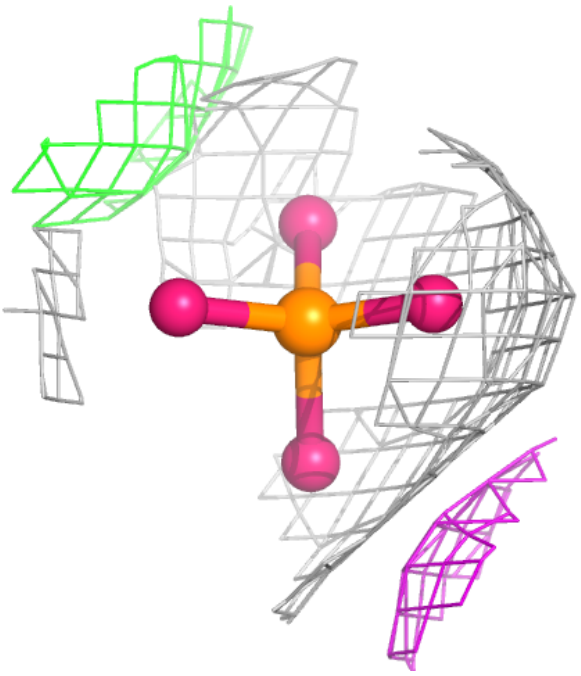


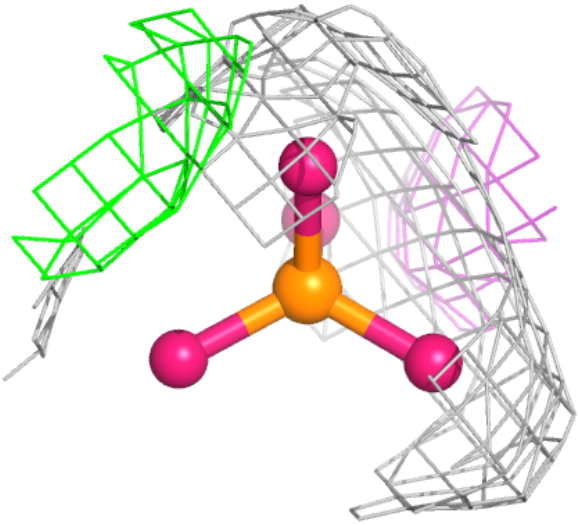


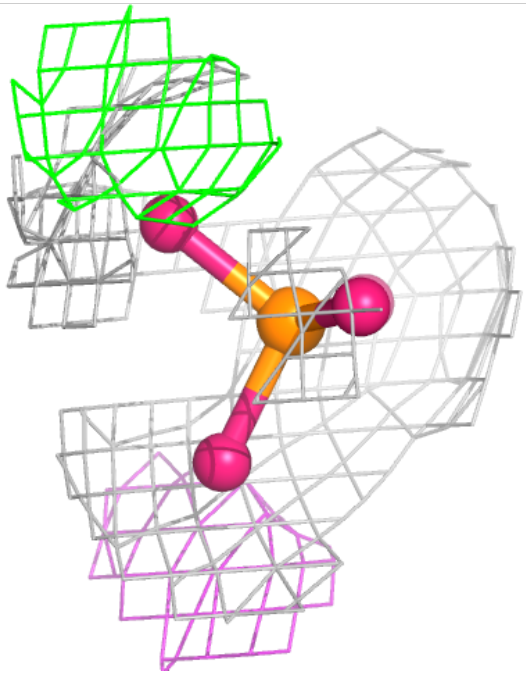


Electron density around PEF M 409:

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

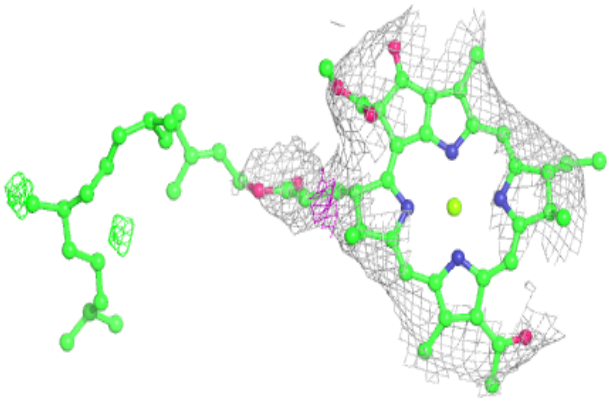


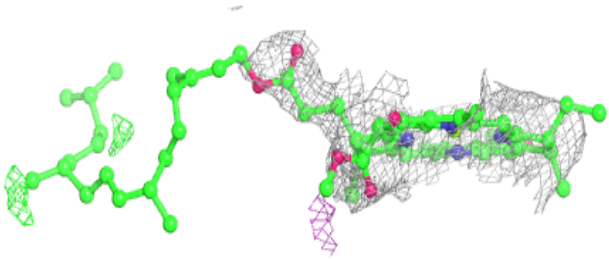


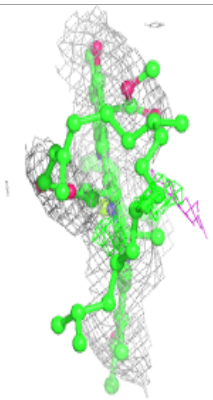


Electron density around BCL 9 101:

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

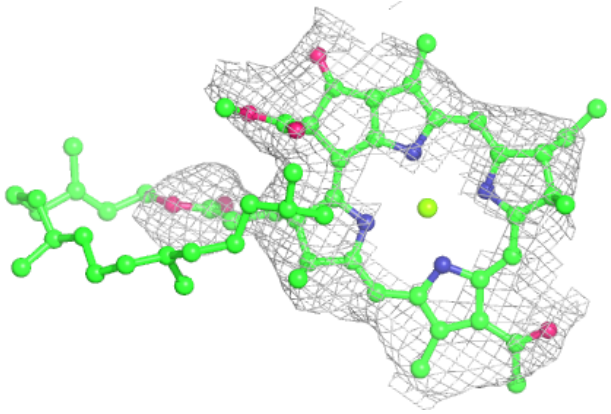


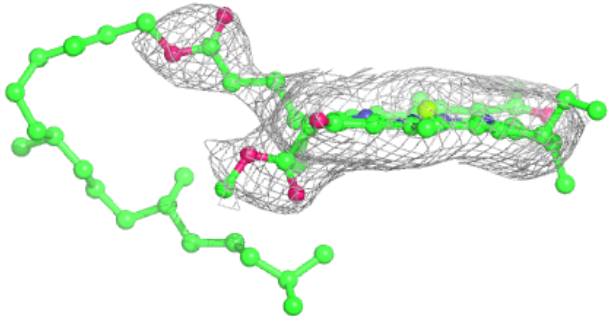


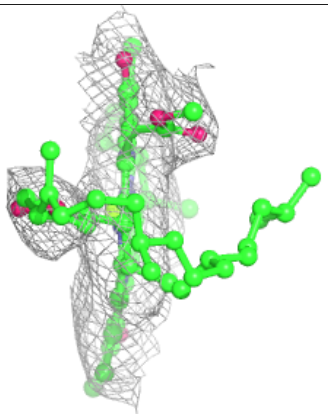


Electron density around BCL Y 101:

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

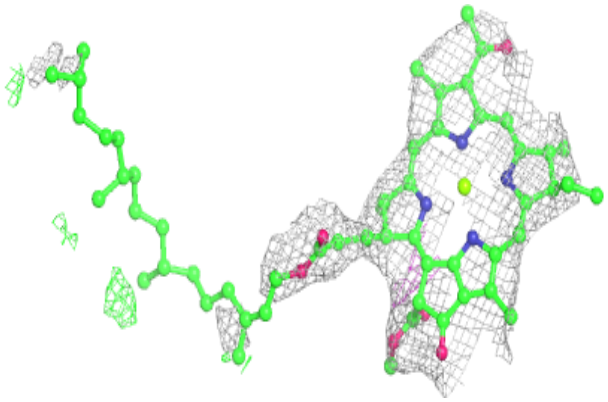


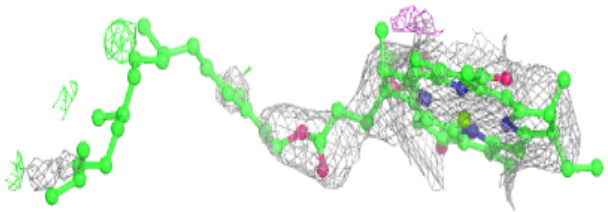


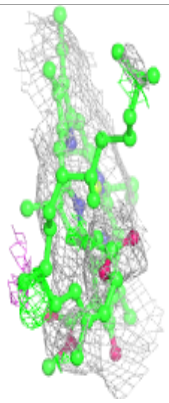


Electron density around BCL 1 101:

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

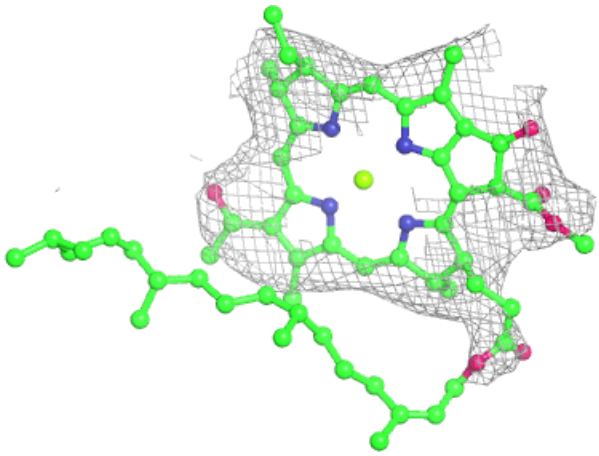


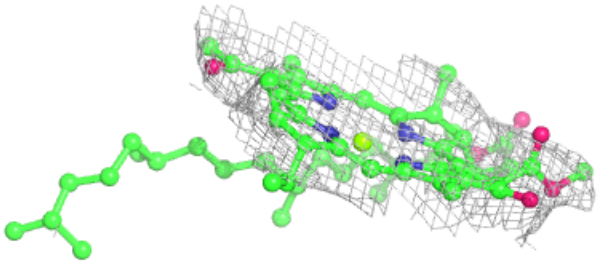


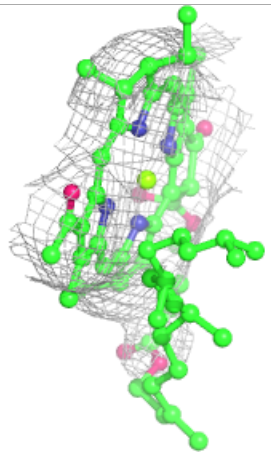


Electron density around BCL 2 102:

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

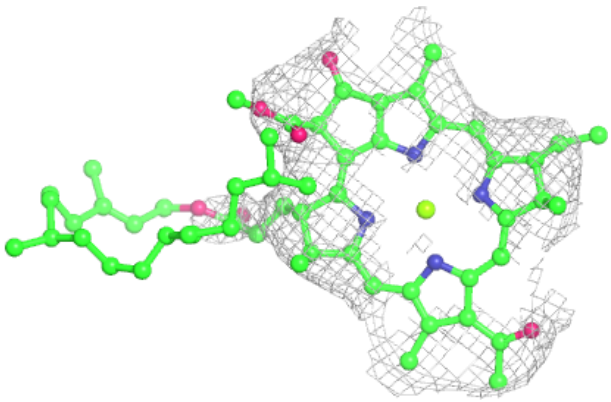


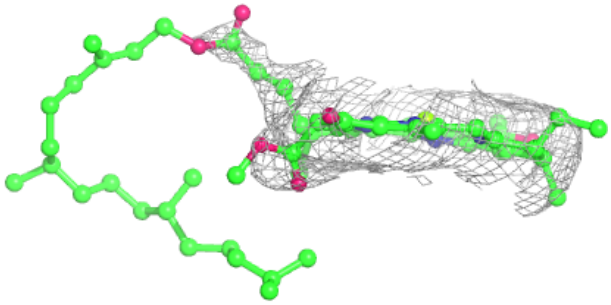


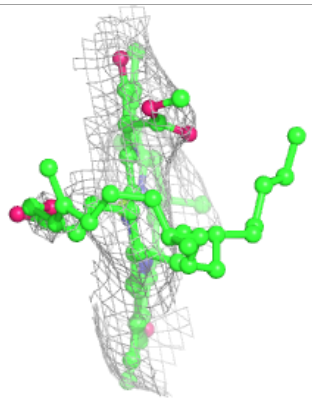


Electron density around BCL 3 101:

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

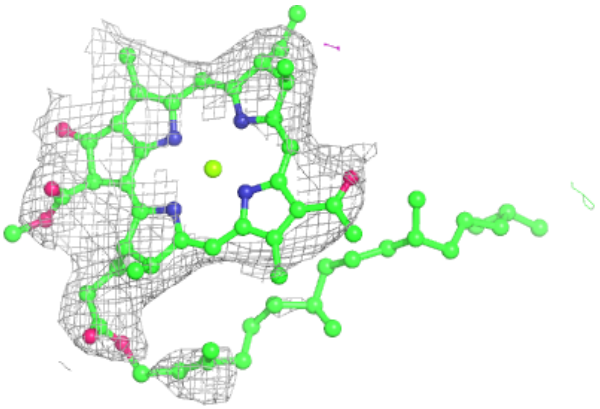


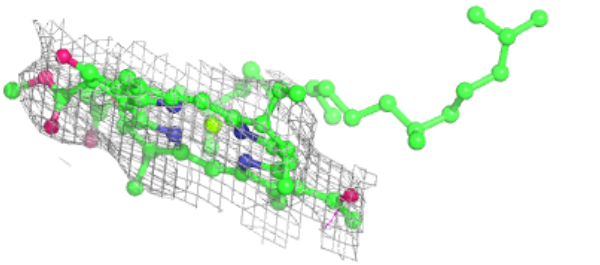


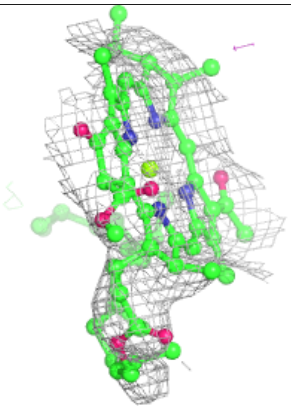


Electron density around BCL 4 102:

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

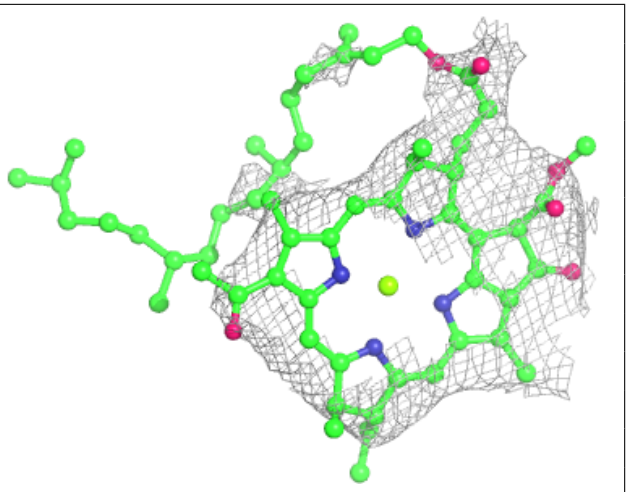


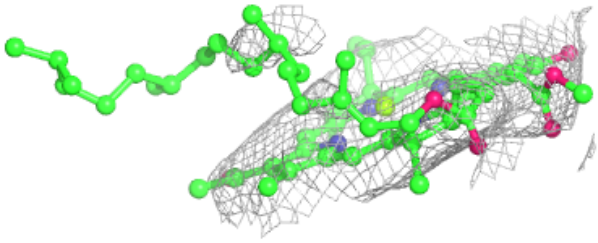


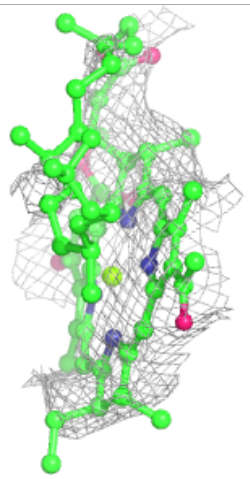


Electron density around BCL F 103:

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

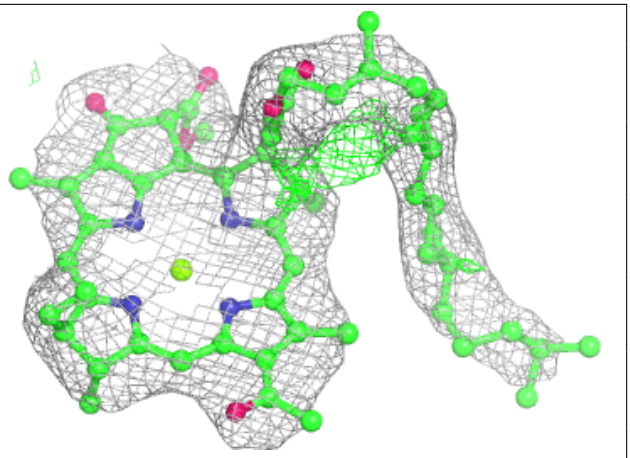


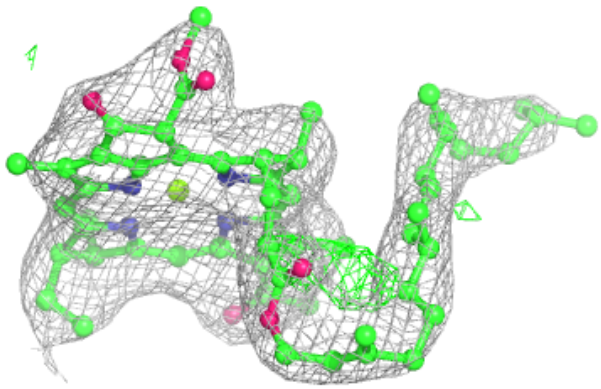


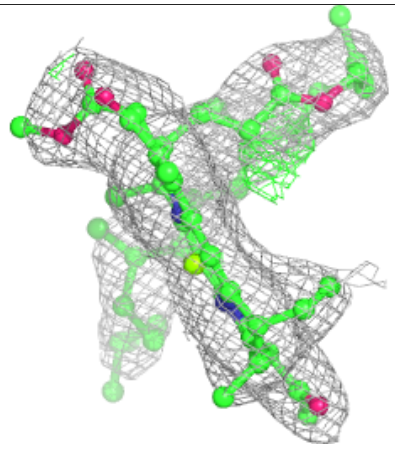


Electron density around BCL L 301:

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

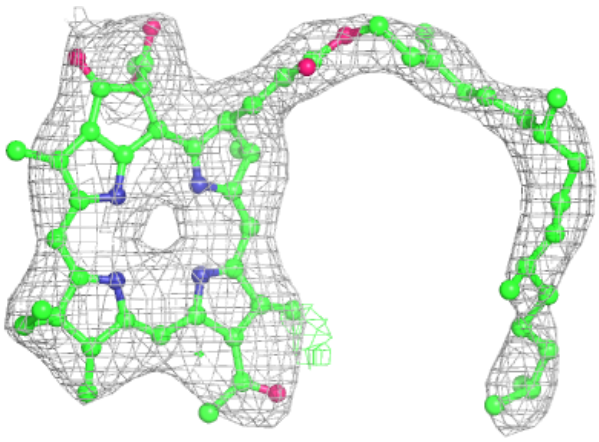


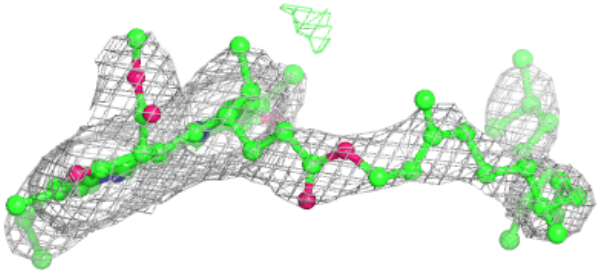


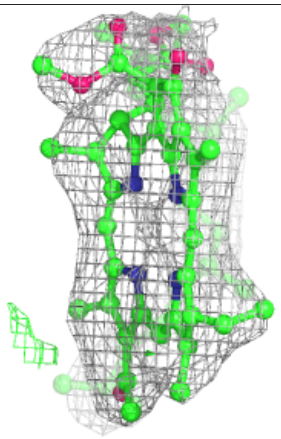


Electron density around BPH L 303:

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

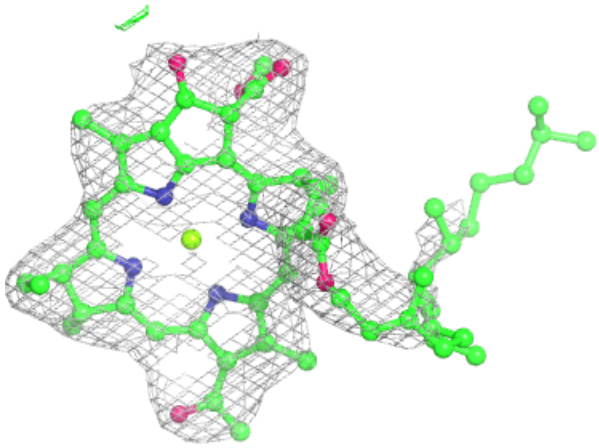


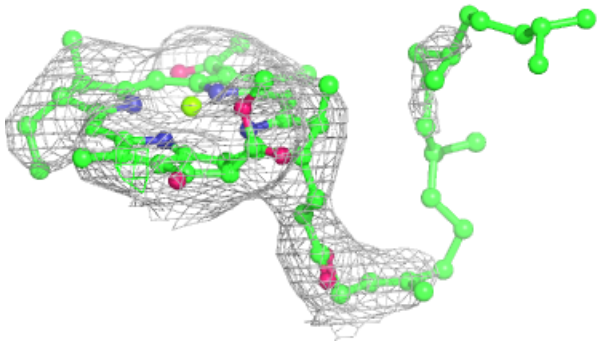


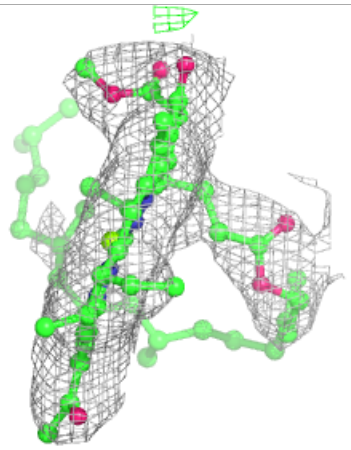


Electron density around BCL L 305:

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

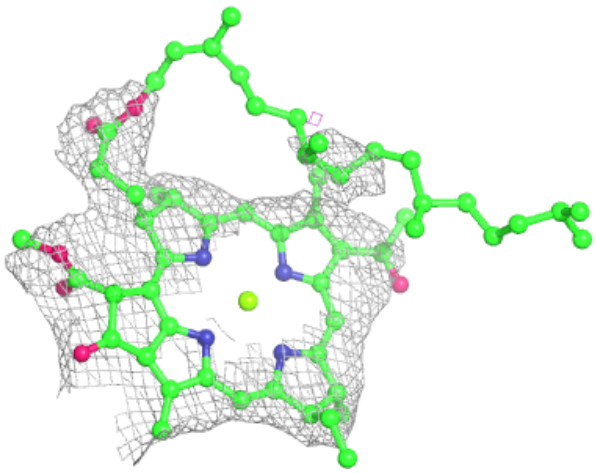


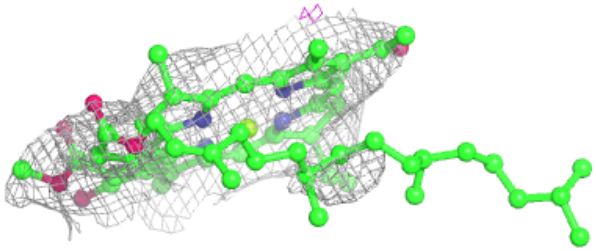


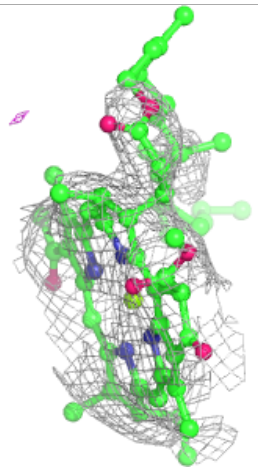


Electron density around BCL Y 103:

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

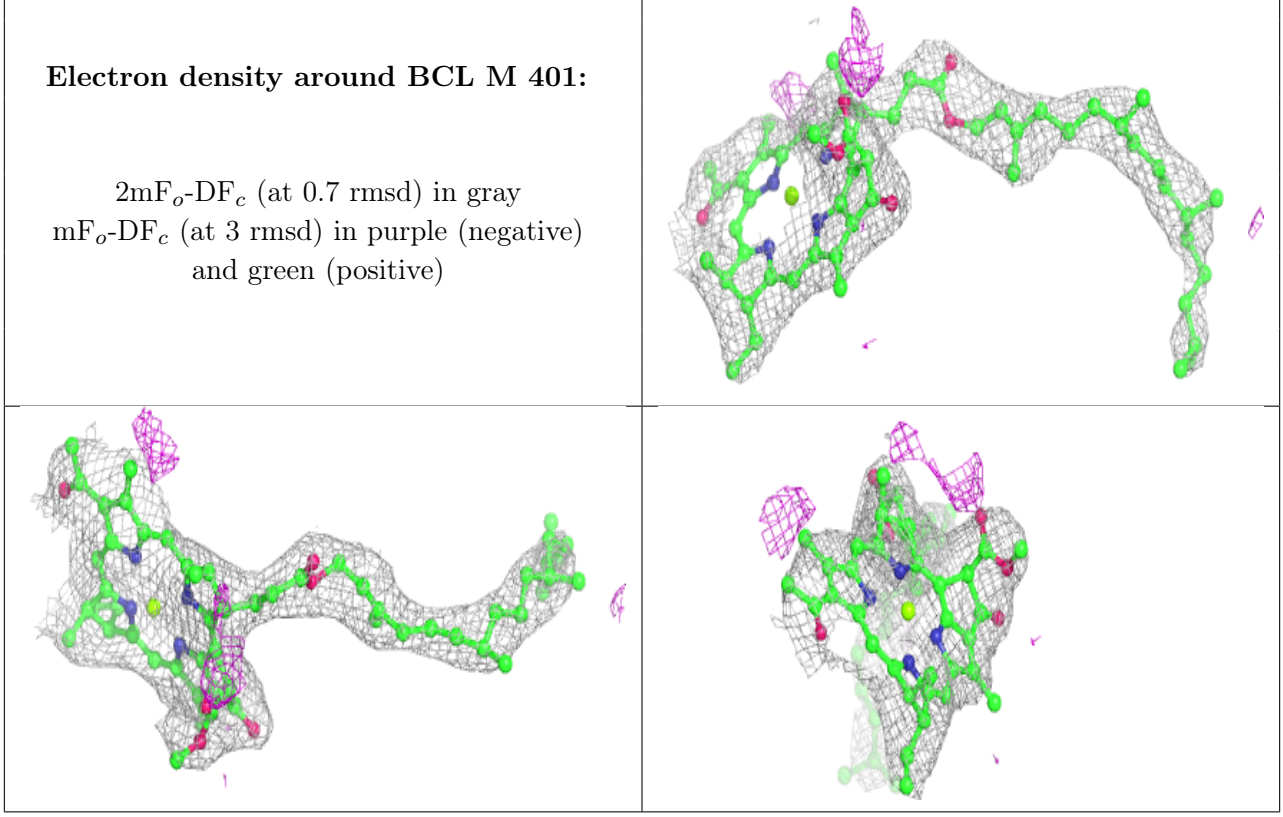






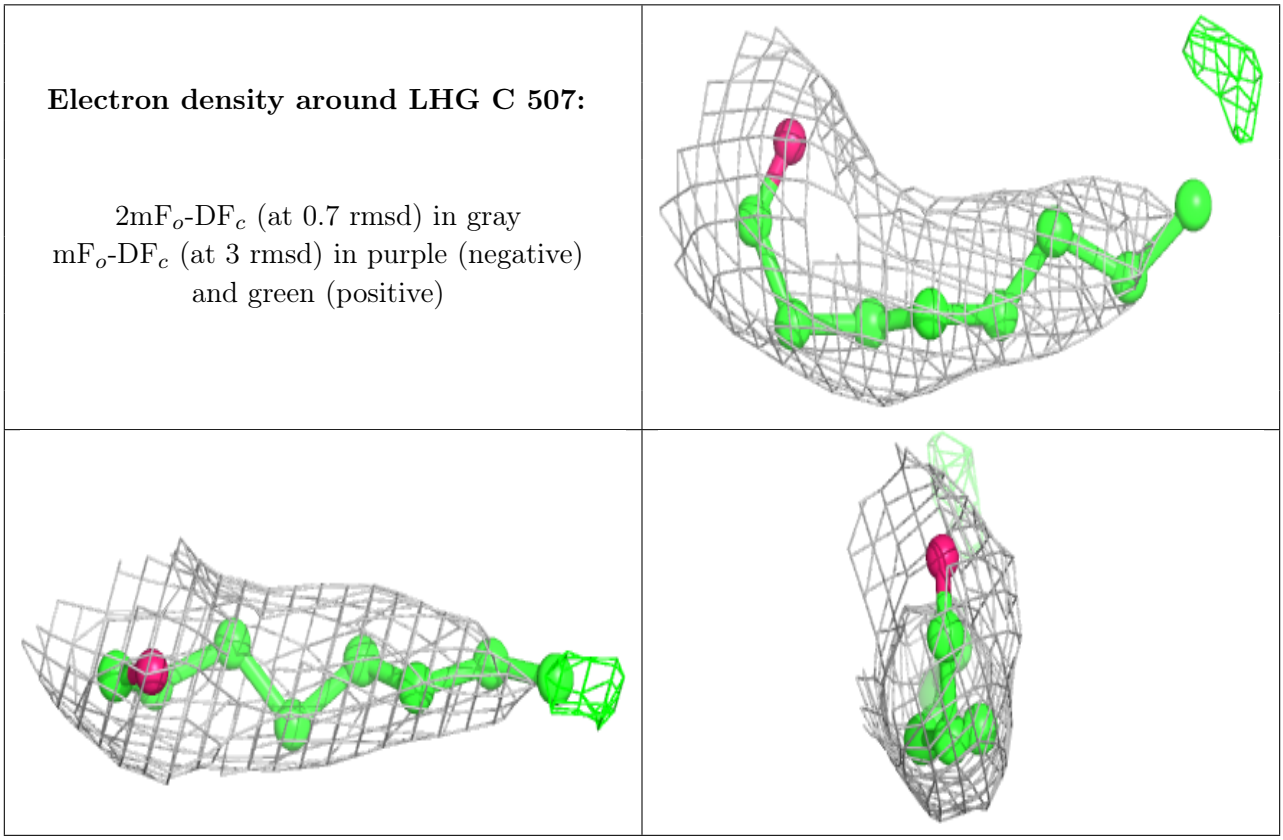
Electron density around BCL M 401:

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



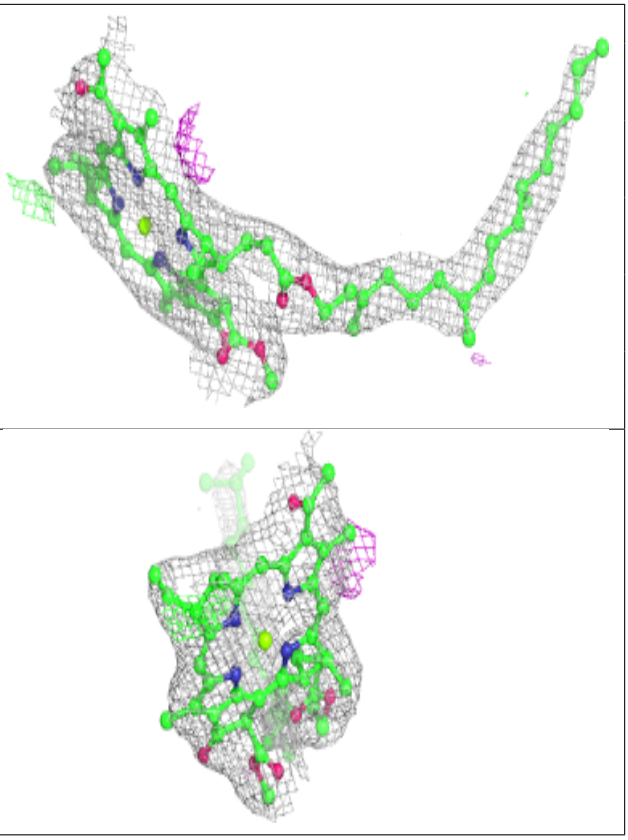
Electron density around LHG C 507:

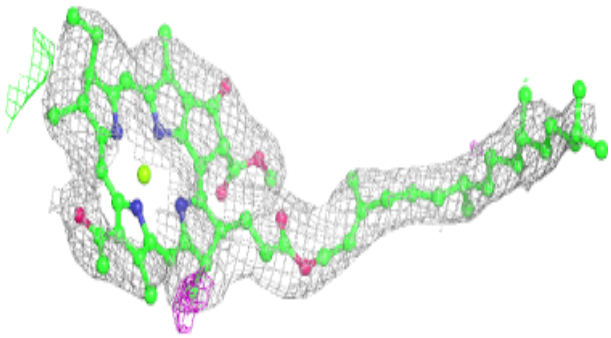
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around BCL L 302:

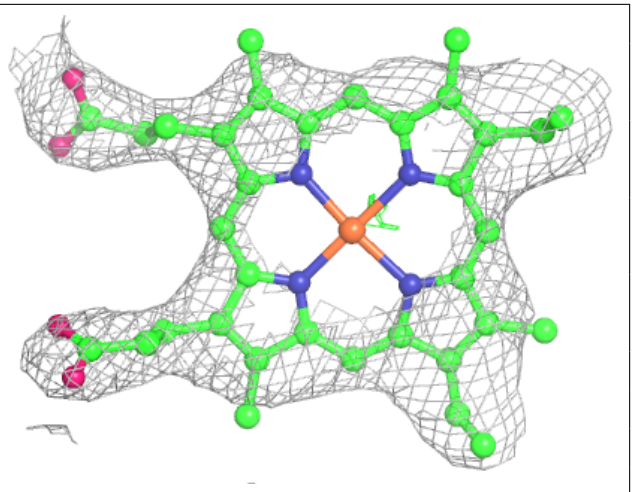
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

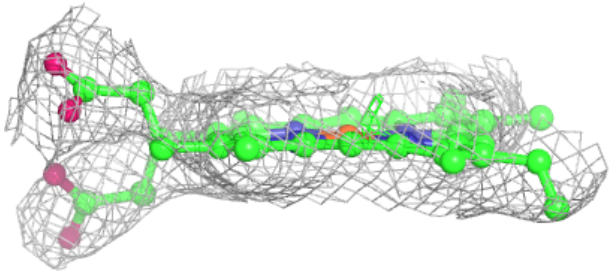


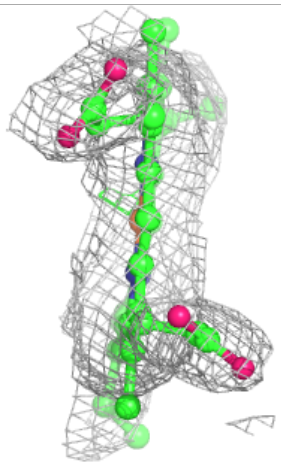


Electron density around HEM C 503:

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

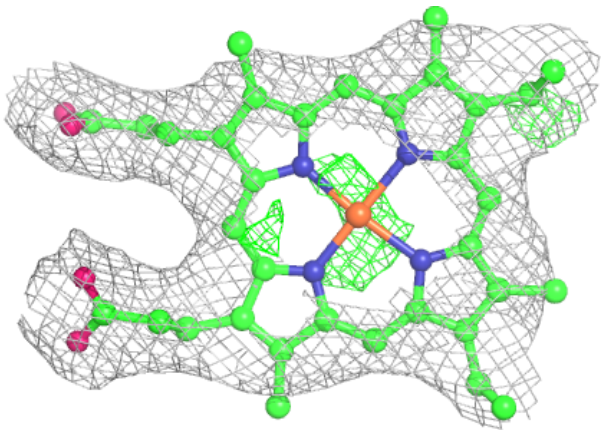


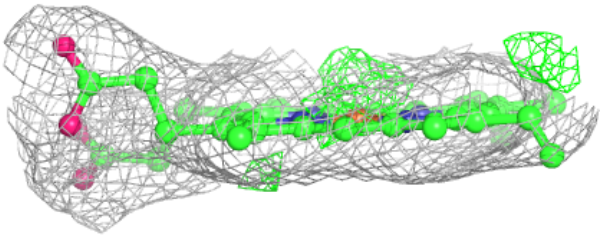


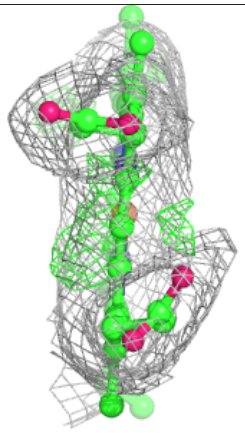


Electron density around HEM C 504:

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

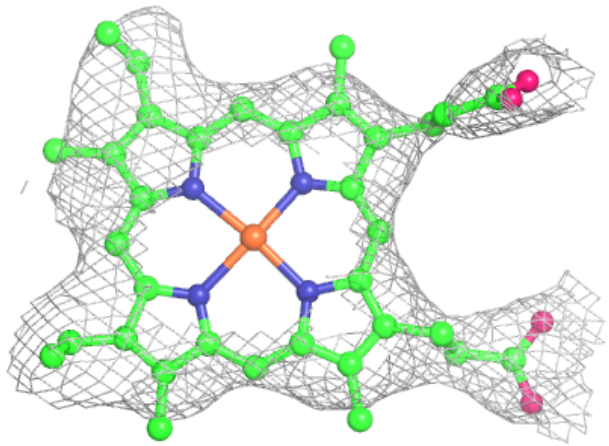


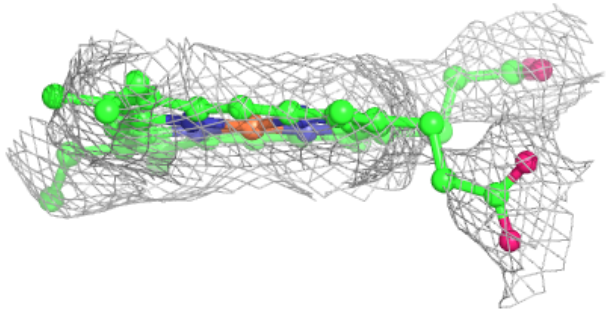


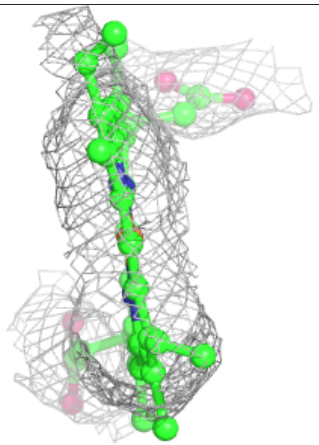


Electron density around HEM C 501:

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

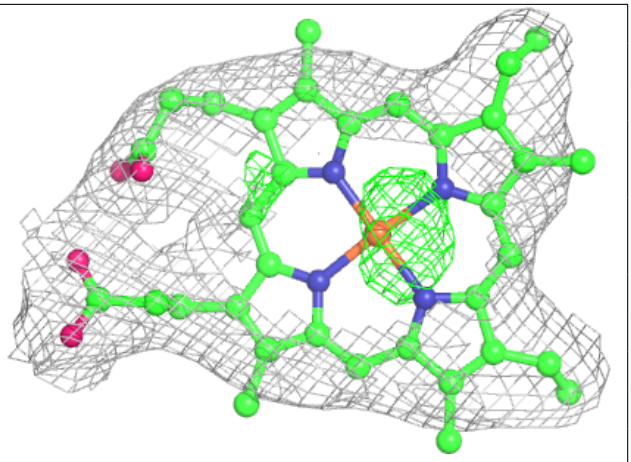


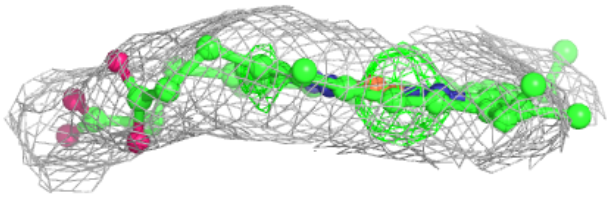


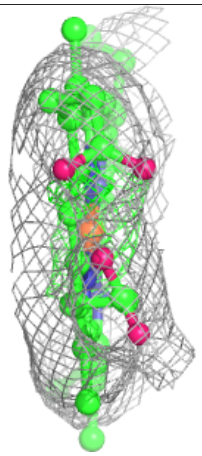


Electron density around HEM C 502:

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

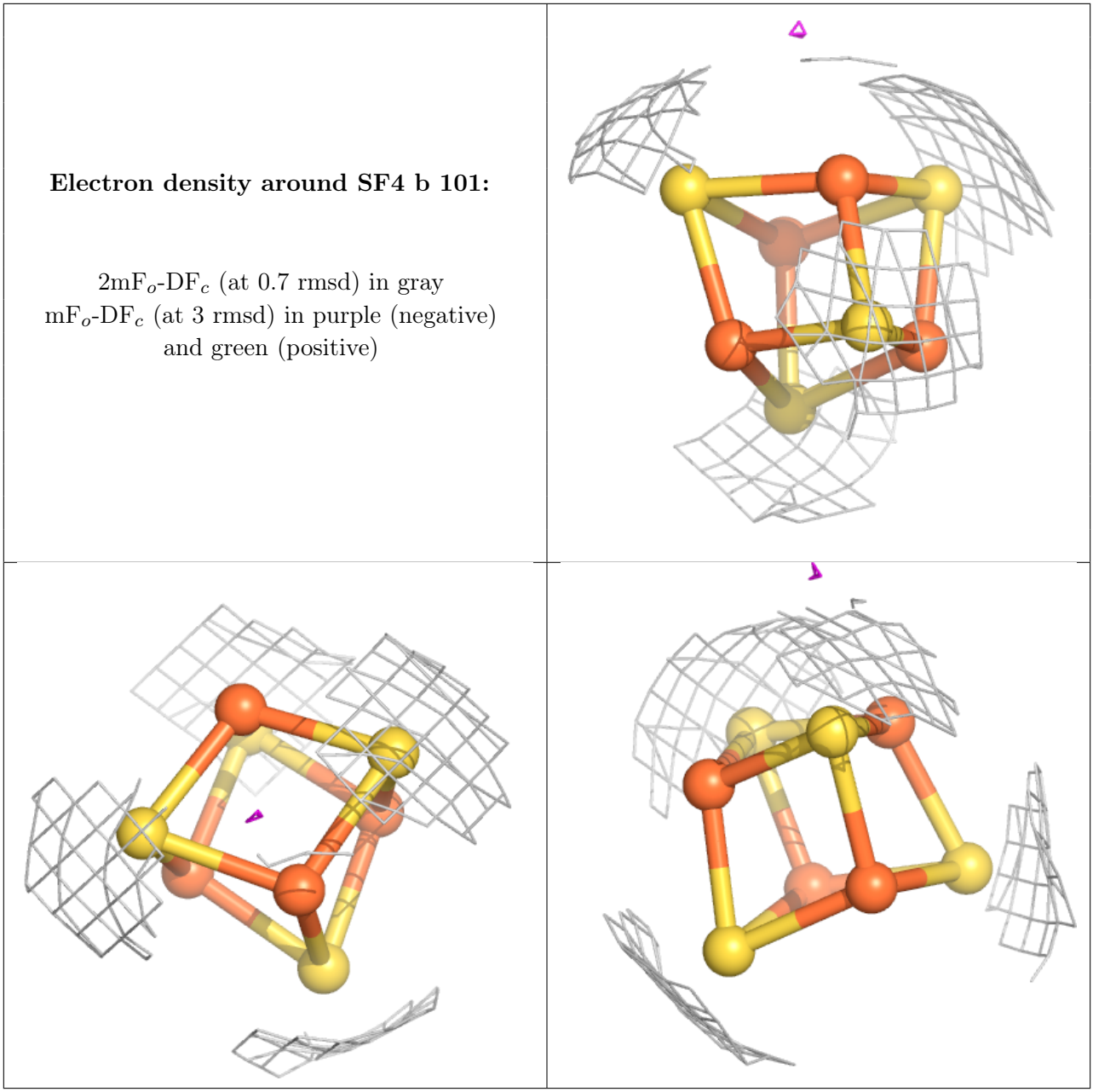






Electron density around SF4 b 101:

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



6.5 Other polymers

There are no such residues in this entry.