Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2024 – 07:32 pm GMT

PDB ID	:	7Q7Q
Title	:	LIPIDIC CUBIC PHASE SERIAL FEMTOSECOND CRYSTALLOGRAPHY STRUCTURE OF A PHOTOSYNTHETIC REACTION CENTRE
Authors	:	Baath, P.; Banacore, A.; Neutze, R.
Deposited on	:	2021-11-09
Resolution	:	2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

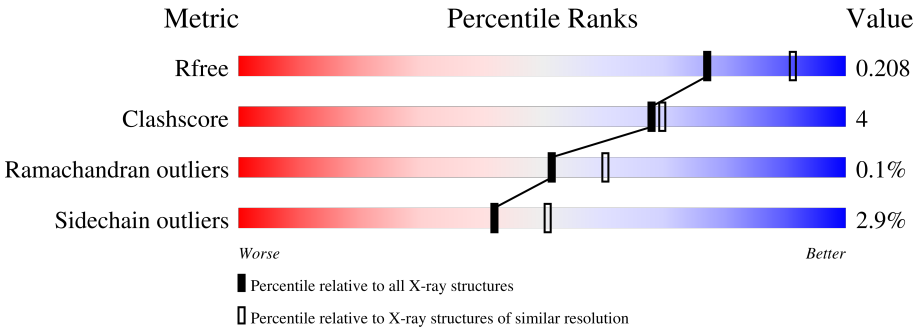
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)

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%

Mol	Chain	Length	Quality of chain
1	CCC	336	91% 7% ••
2	HHH	258	89% 6% 5%
3	LLL	273	93% 7%
4	MMM	323	92% 7% •

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	BPB	LLL	303	X	-	-	-
10	BPB	MMM	406	X	-	-	-
6	DGA	CCC	405	X	-	-	-
9	BCB	LLL	301	X	-	-	-
9	BCB	LLL	302	X	-	-	-
9	BCB	MMM	404	X	-	-	-
9	BCB	MMM	405	X	-	-	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 10609 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	CCC	332	Total	C	N	O	S	0	2	0
			2615	1648	470	479	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	HHH	246	Total	C	N	O	S	0	1	0
			1945	1243	335	365	2			

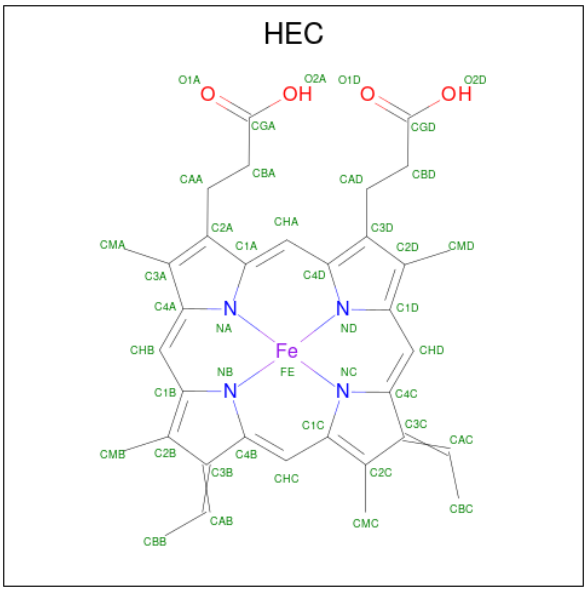
- Molecule 3 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	LLL	273	Total	C	N	O	S	0	1	0
			2172	1460	350	355	7			

- Molecule 4 is a protein called Reaction center protein M chain.

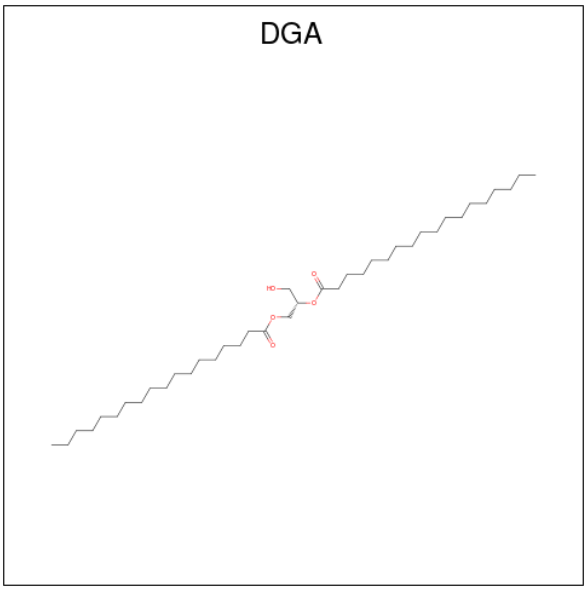
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	MMM	323	Total	C	N	O	S	0	1	0
			2565	1708	422	424	11			

- Molecule 5 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



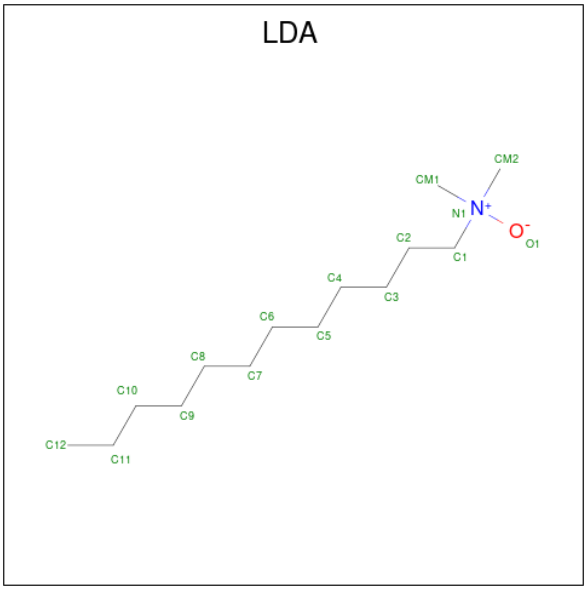
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	CCC	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	CCC	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	CCC	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	CCC	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$).



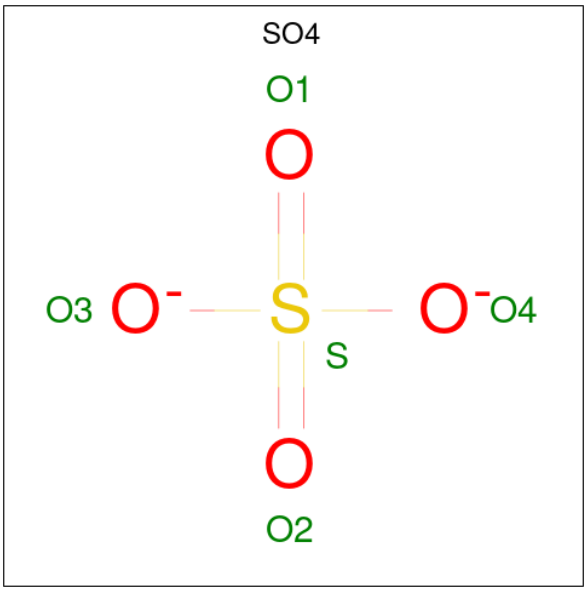
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	CCC	1	Total C O 44 39 5	21	0

- Molecule 7 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



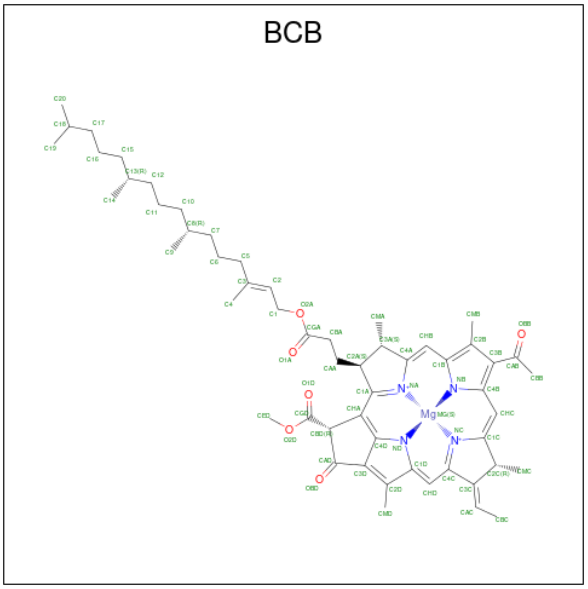
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	HHH	1	Total C N O 16 14 1 1	0	0
7	HHH	1	Total C N O 16 14 1 1	0	0
7	MMM	1	Total C N O 16 14 1 1	0	0
7	MMM	1	Total C N O 16 14 1 1	0	0
7	MMM	1	Total C N O 16 14 1 1	0	0
7	MMM	1	Total C N O 16 14 1 1	0	0
7	MMM	1	Total C N O 16 14 1 1	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



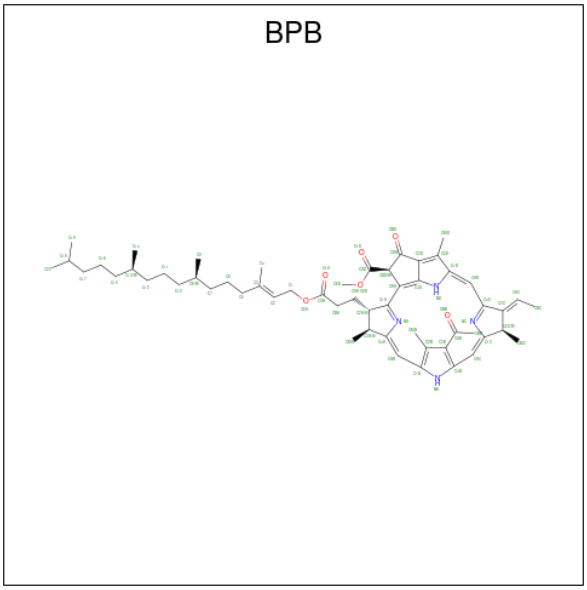
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	HHH	1	Total O S 5 4 1	0	0
8	MMM	1	Total O S 5 4 1	0	0
8	MMM	1	Total O S 5 4 1	0	0
8	MMM	1	Total O S 5 4 1	0	0
8	MMM	1	Total O S 5 4 1	0	0

- Molecule 9 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).



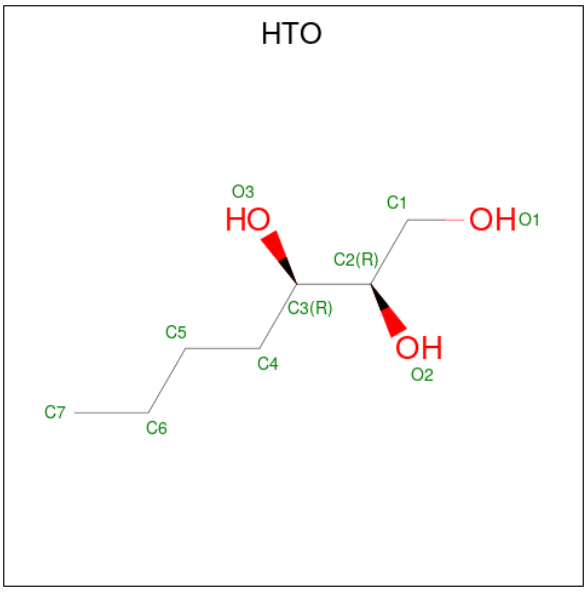
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	LLL	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	LLL	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	MMM	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	MMM	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 10 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: $C_{55}H_{74}N_4O_6$).



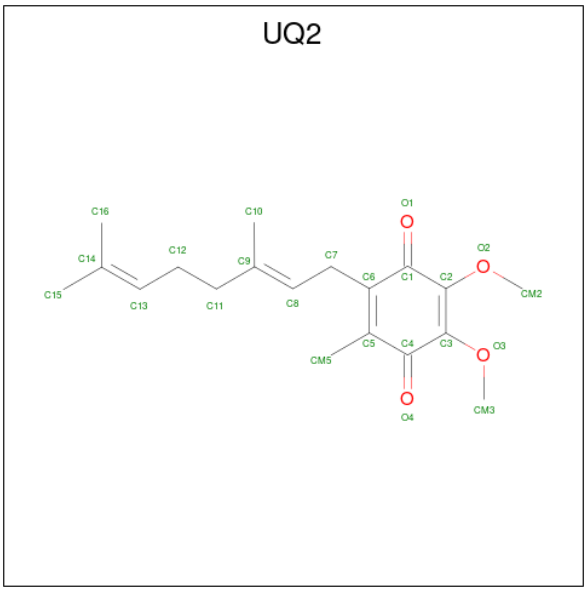
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	LLL	1	Total	C	N	O	0	0
			65	55	4	6		
10	MMM	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 11 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	LLL	1	Total C O 10 7 3	0	0
11	LLL	1	Total C O 10 7 3	0	0
11	LLL	1	Total C O 10 7 3	0	0
11	LLL	1	Total C O 10 7 3	0	0
11	LLL	1	Total C O 10 7 3	0	0
11	LLL	1	Total C O 10 7 3	0	0
11	MMM	1	Total C O 10 7 3	0	0
11	MMM	1	Total C O 10 7 3	0	0

- Molecule 12 is UBIQUINONE-2 (three-letter code: UQ2) (formula: $C_{19}H_{26}O_4$).

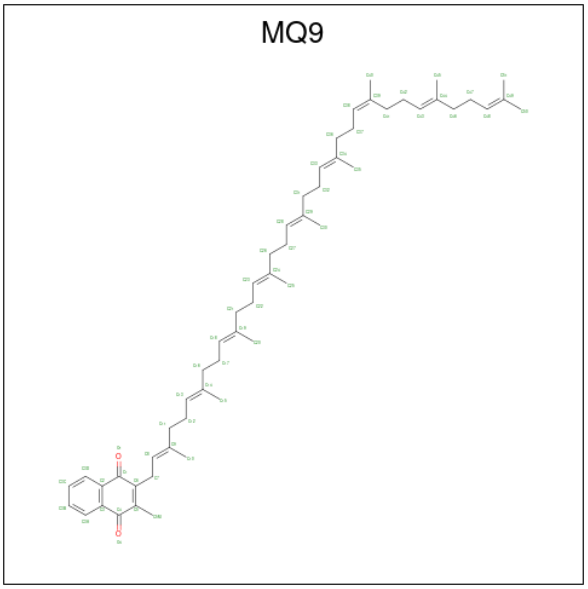


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	LLL	1	Total C O 23 19 4	0	0
12	MMM	1	Total C O 46 38 8	0	1

- Molecule 13 is FE (II) ION (three-letter code: FE2) (formula: Fe).

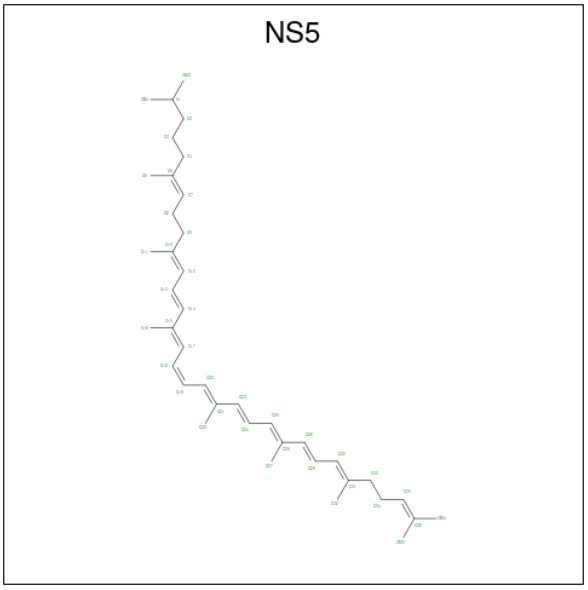
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	MMM	1	Total Fe 1 1	0	0

- Molecule 14 is MENAQUINONE-9 (three-letter code: MQ9) (formula: $C_{56}H_{80}O_2$).



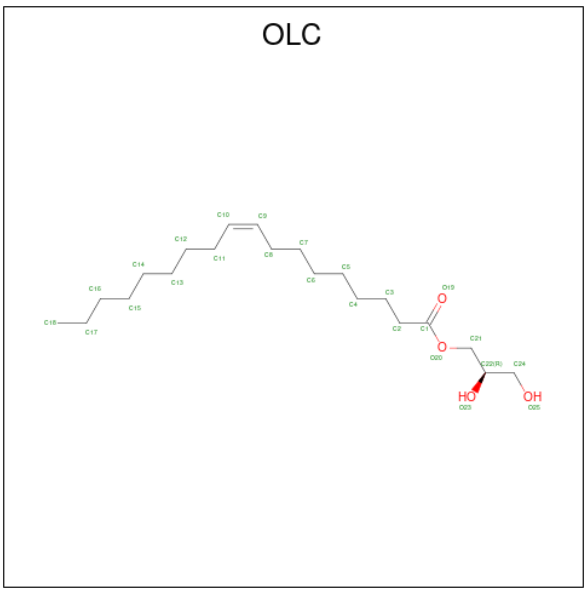
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	MMM	1	Total C O 58 56 2	0	0

- Molecule 15 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: $C_{40}H_{60}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	MMM	1	Total C 40 40	0	0

- Molecule 16 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	MMM	1	Total C O 25 21 4	0	0
16	MMM	1	Total C O 25 21 4	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	CCC	105	Total O 105 105	0	0
17	HHH	48	Total O 48 48	0	0
17	LLL	46	Total O 46 46	0	0
17	MMM	68	Total O 68 68	0	0

3 Residue-property plots (i)

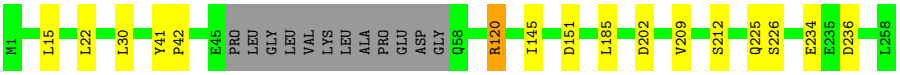
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

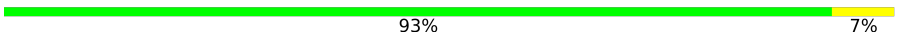
• Molecule 2: Reaction center protein H chain

Chain HHH:



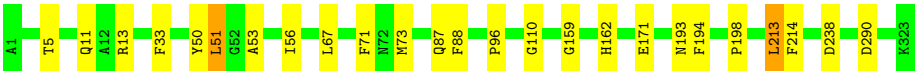
• Molecule 3: Reaction center protein L chain

Chain LLL:



• Molecule 4: Reaction center protein M chain

Chain MMM:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	84.66Å 125.13Å 182.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.70 – 2.25 23.69 – 1.27	Depositor EDS
% Data completeness (in resolution range)	99.9 (23.70-2.25) 96.3 (23.69-1.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.30 (at 1.27Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.168 , 0.203 0.177 , 0.208	Depositor DCC
R_{free} test set	24135 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	7.0	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 70.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10609	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCB, NS5, UQ2, DGA, HEC, FME, SO4, BPB, FE2, HTO, MQ9, OLC, LDA

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	CCC	0.66	0/2688	0.77	0/3662
2	HHH	0.64	0/1979	0.78	0/2700
3	LLL	0.64	0/2267	0.74	0/3095
4	MMM	0.62	0/2670	0.73	0/3652
All	All	0.64	0/9604	0.75	0/13109

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	CCC	2615	0	2597	16	0
2	HHH	1945	0	1941	6	0
3	LLL	2172	0	2097	20	0
4	MMM	2565	0	2458	16	0
5	CCC	172	0	120	5	0
6	CCC	44	0	72	1	0
7	HHH	32	0	62	1	0
7	MMM	80	0	155	6	0
8	HHH	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	MMM	20	0	0	1	0
9	LLL	132	0	144	6	0
9	MMM	132	0	144	4	0
10	LLL	65	0	74	1	0
10	MMM	65	0	74	5	0
11	LLL	60	0	96	0	0
11	MMM	20	0	32	1	0
12	LLL	23	0	26	4	0
12	MMM	46	0	52	7	0
13	MMM	1	0	0	0	0
14	MMM	58	0	80	0	0
15	MMM	40	0	60	5	0
16	MMM	50	0	80	0	0
17	CCC	105	0	0	0	0
17	HHH	48	0	0	2	0
17	LLL	46	0	0	0	0
17	MMM	68	0	0	2	0
All	All	10609	0	10364	78	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 4.

All (78) 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)
1:CCC:250:ALA:H	3:LLL:159:ASN:HD21	1.29	0.81
4:MMM:159:GLY:HA3	15:MMM:407:NS5:H272	1.64	0.80
10:MMM:406:BPB:HHC	10:MMM:406:BPB:HBBB	1.63	0.79
5:CCC:401:HEC:HBC3	5:CCC:401:HEC:HMC1	1.65	0.78
12:MMM:416[A]:UQ2:H101	12:MMM:416[A]:UQ2:H162	1.67	0.74
3:LLL:226:ALA:HA	12:LLL:309:UQ2:H3M2	1.70	0.73
3:LLL:181:PHE:HB3	10:MMM:406:BPB:HBBA	1.71	0.72
1:CCC:216:ARG:O	1:CCC:219:GLU:HG2	1.90	0.71
9:MMM:404:BCB:HBB2	9:MMM:404:BCB:HHC	1.73	0.69
10:LLL:303:BPB:HBBB	10:LLL:303:BPB:HMB	1.75	0.68
3:LLL:231:ARG:HD3	4:MMM:5:THR:O	1.95	0.67
12:MMM:416[A]:UQ2:H162	12:MMM:416[A]:UQ2:C10	2.29	0.62
4:MMM:162:HIS:HE1	4:MMM:171:GLU:OE1	1.83	0.61
3:LLL:181:PHE:CD2	10:MMM:406:BPB:HBB	2.35	0.61
4:MMM:71:PHE:HB3	11:MMM:415:HTO:O3	2.03	0.59
3:LLL:181:PHE:HB3	10:MMM:406:BPB:CBB	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:MMM:11:GLN:HE21	4:MMM:13:ARG:HH12	1.52	0.57
15:MMM:407:NS5:H31	15:MMM:407:NS5:H113	1.85	0.57
3:LLL:168:HIS:CE1	9:LLL:301:BCB:HMC2	2.40	0.57
15:MMM:407:NS5:H113	15:MMM:407:NS5:C3	2.35	0.57
4:MMM:73:MET:HE2	4:MMM:88:PHE:CE1	2.41	0.55
3:LLL:151:LEU:HD22	7:MMM:411:LDA:HM22	1.88	0.55
9:LLL:302:BCB:HMB1	9:LLL:302:BCB:HBB2	1.89	0.55
1:CCC:250:ALA:H	3:LLL:159:ASN:ND2	2.03	0.54
9:MMM:404:BCB:HHC	9:MMM:404:BCB:CBB	2.38	0.53
9:LLL:301:BCB:HBB3	9:LLL:301:BCB:HMB1	1.91	0.52
1:CCC:146[B]:ARG:HD2	1:CCC:179:TYR:CE1	2.45	0.52
2:HHH:234:GLU:OE2	17:HHH:1401:HOH:O	2.19	0.51
4:MMM:198:PRO:HG3	7:MMM:411:LDA:HM13	1.93	0.51
1:CCC:314:LYS:HG2	5:CCC:404:HEC:HBD2	1.92	0.51
2:HHH:120:ARG:NH1	4:MMM:238:ASP:O	2.42	0.51
3:LLL:212:GLU:HB3	12:LLL:309:UQ2:H2M3	1.92	0.51
3:LLL:168:HIS:HD2	17:MMM:514:HOH:O	1.94	0.50
6:CCC:405:DGA:HBV1	12:MMM:416[A]:UQ2:H102	1.94	0.49
2:HHH:145:ILE:HD13	2:HHH:151:ASP:HA	1.93	0.49
1:CCC:102:TYR:CD2	1:CCC:103:PRO:HD3	2.47	0.49
4:MMM:162:HIS:HD2	17:MMM:524:HOH:O	1.95	0.48
5:CCC:403:HEC:HMC1	5:CCC:403:HEC:HBC3	1.95	0.48
9:LLL:301:BCB:HMB1	9:LLL:301:BCB:CBB	2.43	0.48
5:CCC:401:HEC:HBC3	5:CCC:401:HEC:CMC	2.40	0.48
3:LLL:168:HIS:HE1	9:LLL:301:BCB:OBB	1.97	0.48
4:MMM:51:LEU:HD12	4:MMM:56:ILE:HG13	1.96	0.47
2:HHH:202:ASP:HB3	2:HHH:209:VAL:HB	1.96	0.47
3:LLL:190:HIS:HA	12:LLL:309:UQ2:O4	2.15	0.47
3:LLL:231:ARG:HG3	7:MMM:402:LDA:HM21	1.96	0.47
1:CCC:99:GLU:HG2	1:CCC:104:TYR:CE1	2.50	0.47
9:LLL:302:BCB:HMB1	9:LLL:302:BCB:CBB	2.46	0.46
9:MMM:405:BCB:CBB	9:MMM:405:BCB:HMB1	2.45	0.46
2:HHH:212:SER:HB2	17:HHH:1403:HOH:O	2.15	0.46
1:CCC:233:MET:HB3	5:CCC:403:HEC:C4B	2.46	0.46
1:CCC:146[A]:ARG:NH2	1:CCC:188:ASP:OD1	2.49	0.45
3:LLL:212:GLU:OE2	12:LLL:309:UQ2:H3M3	2.17	0.44
3:LLL:135:ARG:HB3	3:LLL:136:PRO:HD3	2.00	0.43
3:LLL:131:LEU:HD23	3:LLL:248:THR:HG21	2.01	0.43
1:CCC:252:THR:HG23	1:CCC:255:SER:HB2	2.00	0.43
1:CCC:102:TYR:N	1:CCC:103:PRO:CD	2.82	0.43
4:MMM:50:TYR:OH	8:MMM:418:SO4:O3	2.23	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HHH:41:TYR:HA	2:HHH:42:PRO:C	2.39	0.43
3:LLL:151:LEU:CD2	7:MMM:411:LDA:HM22	2.48	0.42
12:MMM:416[B]:UQ2:O1	12:MMM:416[B]:UQ2:H13	2.19	0.42
12:MMM:416[B]:UQ2:O1	12:MMM:416[B]:UQ2:H2M3	2.19	0.42
4:MMM:96:PRO:HD3	4:MMM:110:GLY:HA3	2.01	0.42
3:LLL:182:VAL:HG23	9:MMM:404:BCB:H43	2.02	0.42
15:MMM:407:NS5:H29	15:MMM:407:NS5:H271	1.83	0.42
12:MMM:416[A]:UQ2:H5M1	12:MMM:416[A]:UQ2:H72	1.71	0.42
12:MMM:416[B]:UQ2:H121	12:MMM:416[B]:UQ2:H101	1.61	0.42
4:MMM:53:ALA:HB3	7:MMM:409:LDA:H22	2.02	0.42
1:CCC:283:ALA:N	1:CCC:284:PRO:CD	2.83	0.42
7:HHH:1301:LDA:H123	7:MMM:411:LDA:H121	2.01	0.41
3:LLL:44:LEU:HD12	3:LLL:44:LEU:HA	1.87	0.41
4:MMM:51:LEU:HD13	4:MMM:51:LEU:HA	1.90	0.41
1:CCC:77:ILE:HD11	1:CCC:111:LEU:HD21	2.02	0.41
1:CCC:96:LEU:HD12	1:CCC:96:LEU:HA	1.83	0.41
1:CCC:173:VAL:HB	4:MMM:87:GLN:NE2	2.36	0.41
4:MMM:213:LEU:HD12	4:MMM:213:LEU:HA	1.88	0.41
1:CCC:69:GLU:O	1:CCC:72:ARG:HB3	2.21	0.40
10:MMM:406:BPB:H4	10:MMM:406:BPB:H6A	1.91	0.40
15:MMM:407:NS5:H111	15:MMM:407:NS5:H13	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CCC	332/336 (99%)	316 (95%)	16 (5%)	0	100	100
2	HHH	243/258 (94%)	237 (98%)	6 (2%)	0	100	100
3	LLL	272/273 (100%)	265 (97%)	7 (3%)	0	100	100
4	MMM	322/323 (100%)	314 (98%)	7 (2%)	1 (0%)	41	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1169/1190 (98%)	1132 (97%)	36 (3%)	1 (0%)	51 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	MMM	193	ASN

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	CCC	283/282 (100%)	275 (97%)	8 (3%)	43 52
2	HHH	204/212 (96%)	196 (96%)	8 (4%)	32 38
3	LLL	219/218 (100%)	213 (97%)	6 (3%)	44 54
4	MMM	250/249 (100%)	243 (97%)	7 (3%)	43 52
All	All	956/961 (100%)	927 (97%)	29 (3%)	42 50

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	1	CYS
1	CCC	38	TYR
1	CCC	48	GLU
1	CCC	71	LEU
1	CCC	96	LEU
1	CCC	146[A]	ARG
1	CCC	146[B]	ARG
1	CCC	332	LYS
2	HHH	15	LEU
2	HHH	22	LEU
2	HHH	30	LEU
2	HHH	120	ARG
2	HHH	185	LEU
2	HHH	225	GLN

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Mol	Chain	Res	Type
2	HHH	226	SER
2	HHH	236	ASP
3	LLL	12	ARG
3	LLL	82	GLU
3	LLL	94	LEU
3	LLL	249	ILE
3	LLL	271	PHE
3	LLL	272	TRP
4	MMM	33	PHE
4	MMM	51	LEU
4	MMM	67	LEU
4	MMM	194	PHE
4	MMM	213	LEU
4	MMM	214	PHE
4	MMM	290	ASP

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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FME	HHH	1	2	8,9,10	0.37	0	7,9,11	0.60	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	HHH	1	2	-	2/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	HHH	1	FME	O1-CN-N-CA
2	HHH	1	FME	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 39 ligands modelled in this entry, 1 is monoatomic - leaving 38 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	$\#\|Z\| > 2$
14	MQ9	MMM	403	-	59,59,59	0.38	0	72,75,75	0.44	0
12	UQ2	MMM	416[A]	-	23,23,23	1.94	2 (8%)	28,31,31	1.54	5 (17%)
11	HTO	LLL	306	-	9,9,9	0.48	0	10,10,10	0.52	0
7	LDA	MMM	413	-	12,15,15	0.17	0	14,17,17	0.24	0
11	HTO	MMM	408	-	9,9,9	0.56	0	10,10,10	0.65	0
11	HTO	MMM	415	-	9,9,9	0.77	0	10,10,10	0.55	0
5	HEC	CCC	402	1	32,50,50	1.66	4 (12%)	24,82,82	1.82	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	SO4	MMM	417	-	4,4,4	0.35	0	6,6,6	0.07	0
8	SO4	MMM	418	-	4,4,4	0.39	0	6,6,6	0.12	0
7	LDA	HHH	1301	-	12,15,15	0.16	0	14,17,17	0.18	0
9	BCB	MMM	404	-	63,74,74	1.70	14 (22%)	74,115,115	3.06	22 (29%)
5	HEC	CCC	404	1	32,50,50	1.63	5 (15%)	24,82,82	1.85	6 (25%)
11	HTO	LLL	307	-	9,9,9	0.80	0	10,10,10	1.29	1 (10%)
9	BCB	MMM	405	-	63,74,74	1.79	14 (22%)	74,115,115	2.87	26 (35%)
8	SO4	MMM	419	-	4,4,4	0.35	0	6,6,6	0.08	0
7	LDA	MMM	402	-	12,15,15	0.21	0	14,17,17	0.31	0
11	HTO	LLL	305	-	9,9,9	0.97	1 (11%)	10,10,10	1.05	0
7	LDA	MMM	412	-	12,15,15	0.24	0	14,17,17	0.24	0
7	LDA	MMM	409	-	12,15,15	0.11	0	14,17,17	0.28	0
11	HTO	LLL	308	-	9,9,9	0.55	0	10,10,10	0.69	0
9	BCB	LLL	301	-	63,74,74	1.73	13 (20%)	74,115,115	3.04	28 (37%)
8	SO4	HHH	1303	-	4,4,4	0.35	0	6,6,6	0.07	0
11	HTO	LLL	304	-	9,9,9	0.54	0	10,10,10	0.68	0
9	BCB	LLL	302	-	63,74,74	1.71	14 (22%)	74,115,115	2.88	20 (27%)
16	OLC	MMM	414	-	24,24,24	1.02	1 (4%)	25,25,25	1.08	2 (8%)
5	HEC	CCC	403	1	32,50,50	1.63	5 (15%)	24,82,82	1.76	5 (20%)
10	BPB	MMM	406	-	49,70,70	1.88	9 (18%)	47,101,101	1.95	8 (17%)
10	BPB	LLL	303	-	49,70,70	1.88	9 (18%)	47,101,101	1.61	8 (17%)
15	NS5	MMM	407	-	39,39,39	0.95	1 (2%)	44,46,46	1.64	8 (18%)
7	LDA	HHH	1302	-	12,15,15	0.11	0	14,17,17	0.25	0
16	OLC	MMM	410	-	24,24,24	0.96	1 (4%)	25,25,25	0.69	0
8	SO4	MMM	420	-	4,4,4	0.38	0	6,6,6	0.05	0
7	LDA	MMM	411	-	12,15,15	0.16	0	14,17,17	0.18	0
11	HTO	LLL	310	-	9,9,9	0.62	0	10,10,10	0.88	0
5	HEC	CCC	401	1	32,50,50	1.68	4 (12%)	24,82,82	2.19	5 (20%)
12	UQ2	LLL	309	-	23,23,23	1.92	2 (8%)	28,31,31	1.51	5 (17%)
6	DGA	CCC	405	-	43,43,43	2.88	3 (6%)	45,45,45	3.40	7 (15%)
12	UQ2	MMM	416[B]	-	23,23,23	1.95	2 (8%)	28,31,31	1.24	3 (10%)

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
14	MQ9	MMM	403	-	-	4/53/73/73	0/2/2/2
12	UQ2	MMM	416[A]	-	-	3/15/39/39	0/1/1/1
11	HTO	LLL	306	-	-	4/10/10/10	-
7	LDA	MMM	413	-	-	7/13/13/13	-
11	HTO	MMM	408	-	-	7/10/10/10	-
11	HTO	MMM	415	-	-	4/10/10/10	-
5	HEC	CCC	402	1	-	4/10/54/54	-
9	BCB	MMM	404	-	3/3/21/26	11/37/137/137	-
7	LDA	HHH	1301	-	-	7/13/13/13	-
5	HEC	CCC	404	1	-	0/10/54/54	-
11	HTO	LLL	307	-	-	2/10/10/10	-
9	BCB	MMM	405	-	3/3/21/26	9/37/137/137	-
7	LDA	MMM	402	-	-	5/13/13/13	-
11	HTO	LLL	305	-	-	6/10/10/10	-
7	LDA	MMM	412	-	-	8/13/13/13	-
7	LDA	MMM	409	-	-	9/13/13/13	-
11	HTO	LLL	308	-	-	3/10/10/10	-
9	BCB	LLL	301	-	3/3/21/26	5/37/137/137	-
11	HTO	LLL	304	-	-	2/10/10/10	-
9	BCB	LLL	302	-	3/3/21/26	5/37/137/137	-
16	OLC	MMM	414	-	-	11/24/24/24	-
5	HEC	CCC	403	1	-	0/10/54/54	-
10	BPB	MMM	406	-	1/1/18/23	16/37/105/105	0/5/6/6
10	BPB	LLL	303	-	1/1/18/23	5/37/105/105	0/5/6/6
15	NS5	MMM	407	-	-	5/43/43/43	-
7	LDA	HHH	1302	-	-	8/13/13/13	-
16	OLC	MMM	410	-	-	12/24/24/24	-
7	LDA	MMM	411	-	-	10/13/13/13	-
11	HTO	LLL	310	-	-	6/10/10/10	-
5	HEC	CCC	401	1	-	2/10/54/54	-
12	UQ2	LLL	309	-	-	3/15/39/39	0/1/1/1
6	DGA	CCC	405	-	1/1/3/3	19/45/45/45	-
12	UQ2	MMM	416[B]	-	-	6/15/39/39	0/1/1/1

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	CCC	405	DGA	CG1-CG2	-17.30	0.97	1.50
12	MMM	416[B]	UQ2	C6-C5	8.14	1.50	1.35
12	LLL	309	UQ2	C6-C5	7.95	1.49	1.35
12	MMM	416[A]	UQ2	C6-C5	7.82	1.49	1.35
10	LLL	303	BPB	CAC-C3C	7.30	1.52	1.33
10	MMM	406	BPB	CAC-C3C	6.44	1.49	1.33
5	CCC	403	HEC	C2B-C3B	-5.74	1.34	1.40
5	CCC	402	HEC	C2B-C3B	-5.70	1.34	1.40
9	MMM	405	BCB	C2C-C3C	-5.53	1.44	1.51
9	LLL	301	BCB	C2C-C3C	-5.31	1.44	1.51
9	LLL	302	BCB	CAC-C3C	5.29	1.48	1.33
5	CCC	401	HEC	C3C-C2C	-5.25	1.35	1.40
9	MMM	405	BCB	CAC-C3C	5.15	1.47	1.33
10	MMM	406	BPB	C3D-C2D	5.12	1.48	1.39
9	LLL	302	BCB	C3B-C2B	4.99	1.48	1.39
9	LLL	301	BCB	CAC-C3C	4.97	1.47	1.33
6	CCC	405	DGA	OG1-CA1	4.91	1.47	1.33
9	MMM	404	BCB	C2C-C3C	-4.90	1.45	1.51
9	MMM	404	BCB	CAC-C3C	4.88	1.46	1.33
6	CCC	405	DGA	OG2-CB1	4.82	1.47	1.34
9	LLL	302	BCB	C2C-C3C	-4.74	1.45	1.51
10	MMM	406	BPB	O2D-CGD	4.63	1.44	1.33
9	MMM	405	BCB	C3B-C2B	4.58	1.47	1.39
5	CCC	404	HEC	C3C-C2C	-4.58	1.36	1.40
16	MMM	414	OLC	O20-C1	4.58	1.46	1.33
9	MMM	405	BCB	C1D-ND	-4.52	1.32	1.37
9	MMM	404	BCB	C3B-C2B	4.48	1.47	1.39
10	LLL	303	BPB	OBD-CAD	4.41	1.28	1.22
16	MMM	410	OLC	O20-C1	4.33	1.46	1.33
10	MMM	406	BPB	C3B-C2B	4.26	1.47	1.39
9	LLL	301	BCB	CHD-C1D	4.23	1.46	1.38
10	LLL	303	BPB	O2D-CGD	4.19	1.43	1.33
9	MMM	404	BCB	O2A-CGA	4.11	1.45	1.33
9	LLL	301	BCB	O2D-CGD	4.07	1.43	1.33
5	CCC	404	HEC	C2B-C3B	-4.07	1.36	1.40
9	MMM	404	BCB	O2D-CGD	4.03	1.43	1.33
9	MMM	405	BCB	O2A-CGA	3.96	1.44	1.33
10	MMM	406	BPB	O2A-CGA	3.94	1.44	1.33
5	CCC	401	HEC	C2B-C3B	-3.86	1.36	1.40
9	LLL	301	BCB	C3B-C2B	3.86	1.46	1.39
9	LLL	302	BCB	O2D-CGD	3.75	1.42	1.33
10	LLL	303	BPB	C3B-C2B	3.63	1.45	1.39
9	MMM	405	BCB	OBD-CAD	3.61	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	LLL	302	BCB	O2A-CGA	3.54	1.43	1.33
10	MMM	406	BPB	OBD-CAD	3.54	1.27	1.22
9	LLL	301	BCB	OBD-CAD	3.45	1.28	1.22
10	LLL	303	BPB	O2A-CGA	3.44	1.43	1.33
12	MMM	416[A]	UQ2	C3-C2	3.42	1.50	1.36
12	MMM	416[B]	UQ2	C3-C2	3.39	1.50	1.36
9	MMM	404	BCB	C1D-ND	-3.38	1.33	1.37
9	MMM	405	BCB	O2D-CGD	3.37	1.41	1.33
5	CCC	402	HEC	C3C-C2C	-3.37	1.37	1.40
10	MMM	406	BPB	C4C-NC	-3.35	1.27	1.37
10	LLL	303	BPB	C3D-C2D	3.35	1.45	1.39
9	LLL	302	BCB	CHD-C1D	3.34	1.44	1.38
10	LLL	303	BPB	C3A-C2A	-3.32	1.51	1.54
10	LLL	303	BPB	CBD-CGD	-3.25	1.48	1.52
9	MMM	405	BCB	CHD-C1D	3.23	1.44	1.38
9	LLL	301	BCB	C1D-ND	-3.22	1.33	1.37
10	LLL	303	BPB	C4C-NC	-3.21	1.27	1.37
9	LLL	301	BCB	CHD-C4C	3.20	1.46	1.39
9	LLL	302	BCB	C3D-C2D	3.05	1.47	1.39
9	MMM	404	BCB	OBD-CAD	2.92	1.27	1.22
9	LLL	302	BCB	C4B-CHC	2.89	1.49	1.41
9	LLL	302	BCB	C1D-ND	-2.86	1.34	1.37
9	LLL	302	BCB	OBD-CAD	2.84	1.27	1.22
5	CCC	404	HEC	C3C-C4C	2.83	1.48	1.43
9	MMM	404	BCB	C3D-C2D	2.79	1.46	1.39
5	CCC	403	HEC	C3C-C2C	-2.77	1.37	1.40
9	LLL	301	BCB	O2A-CGA	2.77	1.41	1.33
12	LLL	309	UQ2	C3-C2	2.77	1.47	1.36
9	LLL	302	BCB	CHD-C4C	2.76	1.45	1.39
9	MMM	405	BCB	C4B-CHC	2.71	1.48	1.41
9	LLL	302	BCB	C1B-CHB	2.70	1.48	1.41
9	LLL	301	BCB	C1B-CHB	2.70	1.48	1.41
5	CCC	401	HEC	C4B-C3B	2.65	1.47	1.43
9	LLL	301	BCB	C4B-CHC	2.63	1.48	1.41
9	MMM	404	BCB	CHD-C1D	2.63	1.43	1.38
15	MMM	407	NS5	C30-C31	2.59	1.36	1.34
9	MMM	404	BCB	C4B-CHC	2.58	1.48	1.41
9	LLL	301	BCB	C3D-C2D	2.57	1.46	1.39
5	CCC	402	HEC	C3C-C4C	2.54	1.47	1.43
5	CCC	404	HEC	CBA-CGA	2.54	1.56	1.50
9	MMM	405	BCB	C3D-C2D	2.51	1.46	1.39
9	MMM	405	BCB	CHD-C4C	2.50	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	LLL	302	BCB	C3D-C4D	-2.48	1.38	1.44
9	LLL	301	BCB	C4D-CHA	2.43	1.47	1.38
5	CCC	402	HEC	CAD-C3D	2.43	1.55	1.52
9	MMM	404	BCB	C4D-CHA	2.43	1.47	1.38
9	MMM	404	BCB	CHD-C4C	2.35	1.44	1.39
9	MMM	405	BCB	C3D-C4D	-2.31	1.38	1.44
10	MMM	406	BPB	CBD-CGD	-2.25	1.49	1.52
5	CCC	401	HEC	C3C-C4C	2.24	1.47	1.43
9	MMM	405	BCB	C4D-CHA	2.22	1.46	1.38
9	MMM	404	BCB	MG-NA	-2.21	2.01	2.06
5	CCC	403	HEC	C3C-C4C	2.20	1.47	1.43
10	MMM	406	BPB	C3A-C2A	-2.18	1.52	1.54
5	CCC	403	HEC	C4B-C3B	2.17	1.47	1.43
9	MMM	405	BCB	C1B-CHB	2.10	1.46	1.41
9	LLL	302	BCB	C4D-CHA	2.07	1.45	1.38
9	MMM	404	BCB	C1B-CHB	2.06	1.46	1.41
11	LLL	305	HTO	C4-C3	2.05	1.56	1.52
5	CCC	403	HEC	CBA-CGA	2.03	1.55	1.50
5	CCC	404	HEC	O2A-CGA	-2.00	1.24	1.30

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	CCC	405	DGA	CG1-CG2-CG3	19.88	158.34	111.80
9	MMM	404	BCB	C1C-NC-C4C	-18.43	98.42	106.71
9	LLL	302	BCB	C1C-NC-C4C	-18.08	98.58	106.71
9	LLL	301	BCB	C1C-NC-C4C	-17.53	98.82	106.71
9	MMM	405	BCB	C1C-NC-C4C	-15.06	99.93	106.71
10	MMM	406	BPB	O2D-CGD-CBD	7.06	119.94	111.00
9	MMM	404	BCB	C4D-C3D-CAD	-6.51	100.42	108.10
9	LLL	301	BCB	C4A-NA-C1A	6.43	109.59	106.71
6	CCC	405	DGA	OG2-CG2-CG1	-6.42	85.16	108.40
5	CCC	401	HEC	CBA-CAA-C2A	-6.33	101.93	112.60
10	LLL	303	BPB	O2D-CGD-CBD	6.06	118.68	111.00
10	MMM	406	BPB	CBC-CAC-C3C	-5.98	110.83	126.70
9	LLL	301	BCB	C4D-C3D-CAD	-5.93	101.11	108.10
5	CCC	401	HEC	CBD-CAD-C3D	-5.88	102.58	112.62
5	CCC	402	HEC	CBA-CAA-C2A	-5.83	102.77	112.60
9	LLL	302	BCB	C4D-C3D-CAD	-5.68	101.41	108.10
9	MMM	405	BCB	O2D-CGD-CBD	5.62	121.26	111.27
6	CCC	405	DGA	OG1-CG1-CG2	5.61	124.77	108.43
9	MMM	405	BCB	CMD-C2D-C1D	5.60	134.59	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	MMM	405	BCB	O2D-CGD-O1D	-5.60	112.89	123.84
9	LLL	302	BCB	CMD-C2D-C1D	5.56	134.52	124.71
9	MMM	405	BCB	C4A-NA-C1A	5.50	109.18	106.71
10	MMM	406	BPB	C4-C3-C5	5.37	124.31	115.27
9	LLL	302	BCB	O2D-CGD-CBD	5.37	120.81	111.27
9	LLL	301	BCB	C1D-ND-C4D	-5.35	102.54	106.33
9	MMM	405	BCB	C4D-C3D-CAD	-5.34	101.80	108.10
9	MMM	404	BCB	CMD-C2D-C1D	5.25	133.97	124.71
15	MMM	407	NS5	C19-C20-C21	-5.23	119.85	127.31
9	LLL	301	BCB	CMD-C2D-C1D	5.07	133.65	124.71
9	LLL	302	BCB	OBD-CAD-C3D	-4.99	116.52	128.52
9	MMM	404	BCB	C1D-ND-C4D	-4.83	102.90	106.33
9	LLL	301	BCB	C3D-C4D-ND	4.77	117.96	110.24
9	MMM	404	BCB	O2D-CGD-CBD	4.68	119.58	111.27
5	CCC	403	HEC	CMC-C2C-C1C	-4.66	121.30	128.46
9	MMM	404	BCB	C3D-C4D-ND	4.60	117.68	110.24
9	LLL	301	BCB	OBD-CAD-C3D	-4.56	117.55	128.52
12	LLL	309	UQ2	CM3-O3-C3	4.52	132.49	116.47
6	CCC	405	DGA	OG2-CB1-CB2	4.50	121.21	111.50
9	MMM	405	BCB	C3D-C4D-ND	4.39	117.34	110.24
9	MMM	404	BCB	C4A-NA-C1A	4.32	108.65	106.71
9	MMM	405	BCB	CMB-C2B-C3B	4.30	132.72	124.68
9	MMM	404	BCB	C2D-C1D-ND	4.27	113.25	110.10
5	CCC	404	HEC	CMB-C2B-C1B	-4.22	121.98	128.46
9	MMM	404	BCB	OBD-CAD-C3D	-4.14	118.56	128.52
9	MMM	404	BCB	CHD-C4C-C3C	-4.10	120.76	125.89
9	LLL	301	BCB	C2D-C1D-ND	4.08	113.11	110.10
9	LLL	302	BCB	C2C-C1C-CHC	-4.03	114.15	123.64
9	LLL	301	BCB	C4-C3-C5	4.01	122.02	115.27
9	LLL	301	BCB	CHD-C4C-C3C	-3.97	120.92	125.89
10	LLL	303	BPB	CBC-CAC-C3C	-3.94	116.25	126.70
9	MMM	405	BCB	OBD-CAD-C3D	-3.92	119.08	128.52
12	MMM	416[A]	UQ2	CM5-C5-C6	-3.92	118.00	124.40
9	LLL	302	BCB	CMB-C2B-C3B	3.90	131.98	124.68
9	LLL	302	BCB	C3D-C4D-ND	3.88	116.52	110.24
5	CCC	404	HEC	CAD-CBD-CGD	-3.84	103.00	113.76
9	MMM	404	BCB	C2C-C1C-CHC	-3.79	114.71	123.64
16	MMM	414	OLC	O20-C1-C2	3.77	123.75	111.91
9	LLL	302	BCB	O2D-CGD-O1D	-3.71	116.58	123.84
15	MMM	407	NS5	C18-C19-C20	3.69	131.03	123.47
9	MMM	405	BCB	CHD-C4C-C3C	-3.68	121.28	125.89
9	MMM	405	BCB	CAA-C2A-C1A	3.67	124.00	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	MMM	405	BCB	C1D-ND-C4D	-3.64	103.75	106.33
9	MMM	404	BCB	CAD-C3D-C2D	3.61	158.23	140.80
9	LLL	301	BCB	CAD-C3D-C2D	3.58	158.07	140.80
9	MMM	405	BCB	CMD-C2D-C3D	-3.47	119.64	127.61
9	LLL	301	BCB	O2A-CGA-O1A	-3.44	114.91	123.59
9	MMM	404	BCB	CMB-C2B-C3B	3.40	131.03	124.68
5	CCC	402	HEC	CMB-C2B-C1B	-3.39	123.25	128.46
9	LLL	301	BCB	CMB-C2B-C3B	3.39	131.03	124.68
9	MMM	405	BCB	CAD-C3D-C2D	3.38	157.13	140.80
9	LLL	301	BCB	C1-C2-C3	-3.33	120.29	126.04
9	LLL	301	BCB	C2C-C1C-CHC	-3.31	115.84	123.64
5	CCC	403	HEC	CMC-C2C-C3C	3.29	129.69	125.82
9	LLL	302	BCB	CAD-C3D-C2D	3.25	156.47	140.80
12	MMM	416[A]	UQ2	C6-C5-C4	3.22	121.73	119.18
9	LLL	302	BCB	CMD-C2D-C3D	-3.20	120.25	127.61
5	CCC	404	HEC	CMB-C2B-C3B	3.20	129.59	125.82
6	CCC	405	DGA	OG1-CA1-CA2	3.20	121.94	111.91
9	MMM	405	BCB	CHB-C4A-NA	3.17	128.89	124.51
10	LLL	303	BPB	O1D-CGD-CBD	-3.12	119.54	124.74
15	MMM	407	NS5	C18-C17-C15	-3.09	122.91	127.31
10	LLL	303	BPB	C1A-C2A-C3A	-3.05	99.94	102.84
5	CCC	404	HEC	CBD-CAD-C3D	3.01	117.75	112.62
5	CCC	403	HEC	C1D-C2D-C3D	3.00	109.08	107.00
9	MMM	404	BCB	C1D-CHD-C4C	-3.00	119.59	126.06
9	LLL	301	BCB	CMD-C2D-C3D	-2.99	120.73	127.61
9	MMM	405	BCB	CED-O2D-CGD	2.95	122.62	115.94
6	CCC	405	DGA	OG1-CA1-OA1	-2.92	116.23	123.59
5	CCC	404	HEC	CMC-C2C-C1C	-2.90	124.01	128.46
10	MMM	406	BPB	C5-C3-C2	-2.89	115.28	121.12
9	MMM	404	BCB	CHB-C4A-NA	2.88	128.49	124.51
9	MMM	405	BCB	C2C-C1C-CHC	-2.87	116.88	123.64
5	CCC	403	HEC	CBA-CAA-C2A	-2.86	107.78	112.60
9	MMM	405	BCB	C1D-CHD-C4C	-2.86	119.89	126.06
11	LLL	307	HTO	C5-C4-C3	2.85	118.86	114.18
15	MMM	407	NS5	C6-C5-C7	-2.84	116.39	123.68
9	MMM	405	BCB	C2D-C1D-ND	2.84	112.19	110.10
12	LLL	309	UQ2	C10-C9-C11	2.83	120.03	115.27
9	LLL	302	BCB	O2A-CGA-O1A	-2.83	116.45	123.59
9	MMM	404	BCB	CHA-C4D-ND	-2.82	126.60	132.50
9	LLL	301	BCB	CHC-C1C-NC	-2.82	120.62	124.51
9	MMM	404	BCB	CMD-C2D-C3D	-2.78	121.21	127.61
16	MMM	414	OLC	O20-C1-O19	-2.77	116.59	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	MMM	404	BCB	CHC-C1C-NC	-2.77	120.68	124.51
9	LLL	302	BCB	C1D-ND-C4D	-2.76	104.38	106.33
15	MMM	407	NS5	C14-C15-C17	-2.72	114.77	118.94
10	MMM	406	BPB	C1A-C2A-C3A	-2.72	100.25	102.84
9	MMM	404	BCB	O2A-CGA-CBA	2.72	120.44	111.91
10	LLL	303	BPB	CMC-C2C-C1C	-2.69	109.84	114.36
9	LLL	301	BCB	CHA-C4D-ND	-2.67	126.90	132.50
5	CCC	401	HEC	CMB-C2B-C1B	-2.58	124.49	128.46
12	LLL	309	UQ2	C7-C8-C9	-2.58	122.49	126.79
9	LLL	301	BCB	O2A-CGA-CBA	2.57	119.97	111.91
12	MMM	416[A]	UQ2	C16-C14-C15	2.57	120.28	114.60
9	LLL	302	BCB	CHC-C1C-NC	-2.56	120.97	124.51
15	MMM	407	NS5	C16-C15-C17	2.56	126.50	122.92
5	CCC	402	HEC	CMC-C2C-C1C	-2.54	124.56	128.46
12	LLL	309	UQ2	O4-C4-C3	-2.54	115.54	120.93
12	MMM	416[B]	UQ2	C7-C8-C9	-2.51	122.61	126.79
9	MMM	404	BCB	C4D-CHA-C1A	2.50	124.29	121.25
15	MMM	407	NS5	C12-C13-C14	-2.48	115.47	123.22
9	LLL	301	BCB	CAA-C2A-C1A	2.46	120.02	111.97
12	MMM	416[B]	UQ2	C16-C14-C15	2.43	119.96	114.60
9	MMM	405	BCB	CHC-C1C-NC	-2.42	121.17	124.51
9	LLL	301	BCB	O2D-CGD-O1D	-2.41	119.13	123.84
5	CCC	403	HEC	CBD-CAD-C3D	-2.37	108.57	112.62
10	MMM	406	BPB	O2D-CGD-O1D	-2.37	119.21	123.84
10	MMM	406	BPB	O1D-CGD-CBD	-2.33	120.85	124.74
15	MMM	407	NS5	C6-C5-C4	2.31	119.16	115.27
9	LLL	302	BCB	C1D-CHD-C4C	-2.31	121.08	126.06
10	LLL	303	BPB	CMB-C2B-C3B	2.29	128.97	124.68
9	MMM	404	BCB	O2D-CGD-O1D	-2.29	119.35	123.84
5	CCC	401	HEC	CMB-C2B-C3B	2.28	128.50	125.82
9	MMM	405	BCB	C4D-CHA-C1A	2.28	124.02	121.25
10	MMM	406	BPB	CMC-C2C-C1C	-2.27	110.55	114.36
9	LLL	302	BCB	CHB-C4A-NA	2.24	127.61	124.51
9	LLL	301	BCB	C1D-CHD-C4C	-2.23	121.24	126.06
9	MMM	404	BCB	O2A-CGA-O1A	-2.22	117.99	123.59
9	LLL	302	BCB	C2D-C1D-ND	2.22	111.74	110.10
9	MMM	405	BCB	C4B-CHC-C1C	-2.20	125.75	130.12
6	CCC	405	DGA	OG2-CB1-OB1	-2.20	118.39	123.70
12	MMM	416[A]	UQ2	C7-C6-C1	2.19	121.11	118.48
9	MMM	405	BCB	CHA-C4D-ND	-2.19	127.92	132.50
9	LLL	302	BCB	C4B-CHC-C1C	-2.18	125.80	130.12
9	LLL	301	BCB	C3C-C4C-NC	2.16	112.94	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	LLL	301	BCB	C4B-CHC-C1C	-2.16	125.85	130.12
9	MMM	405	BCB	C1B-CHB-C4A	-2.15	125.85	130.12
10	LLL	303	BPB	C1-C2-C3	-2.15	122.33	126.04
9	LLL	301	BCB	O2D-CGD-CBD	2.14	115.07	111.27
5	CCC	401	HEC	CMC-C2C-C1C	-2.14	125.18	128.46
12	MMM	416[B]	UQ2	C10-C9-C11	2.13	118.86	115.27
5	CCC	404	HEC	CBA-CAA-C2A	-2.12	109.04	112.60
9	LLL	301	BCB	CED-O2D-CGD	2.11	120.72	115.94
12	MMM	416[A]	UQ2	C12-C13-C14	-2.10	120.58	127.75
5	CCC	402	HEC	CMD-C2D-C1D	-2.09	125.26	128.46
12	LLL	309	UQ2	C6-C5-C4	-2.08	117.54	119.18
9	MMM	405	BCB	CBC-CAC-C3C	-2.08	120.64	126.72
9	LLL	302	BCB	CHD-C4C-C3C	-2.07	123.30	125.89
10	LLL	303	BPB	CED-O2D-CGD	2.04	120.54	115.94
9	LLL	301	BCB	CHB-C4A-NA	2.01	127.29	124.51
9	LLL	301	BCB	C5-C3-C2	-2.00	117.07	121.12
9	MMM	405	BCB	CAA-C2A-C3A	-2.00	107.30	112.78
9	LLL	302	BCB	C2A-C1A-CHA	-2.00	120.36	123.86

All (15) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	CCC	405	DGA	CG2
9	LLL	301	BCB	NA
9	LLL	301	BCB	NC
9	LLL	301	BCB	ND
9	LLL	302	BCB	NA
9	LLL	302	BCB	NC
9	LLL	302	BCB	ND
9	MMM	404	BCB	NA
9	MMM	404	BCB	NC
9	MMM	404	BCB	ND
9	MMM	405	BCB	NA
9	MMM	405	BCB	NC
9	MMM	405	BCB	ND
10	LLL	303	BPB	C13
10	MMM	406	BPB	C13

All (208) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	CCC	405	DGA	CA2-CA1-OG1-CG1

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Mol	Chain	Res	Type	Atoms
6	CCC	405	DGA	OA1-CA1-OG1-CG1
7	HHH	1302	LDA	C2-C1-N1-O1
7	HHH	1302	LDA	C2-C1-N1-CM2
7	MMM	402	LDA	C2-C1-N1-CM1
7	MMM	402	LDA	C2-C1-N1-CM2
7	MMM	409	LDA	C2-C1-N1-CM2
7	MMM	411	LDA	C2-C1-N1-CM1
7	MMM	411	LDA	C2-C1-N1-CM2
7	MMM	411	LDA	N1-C1-C2-C3
7	MMM	412	LDA	C2-C1-N1-CM1
7	MMM	412	LDA	C2-C1-N1-CM2
9	LLL	301	BCB	C2C-C3C-CAC-CBC
9	MMM	404	BCB	C2C-C3C-CAC-CBC
9	MMM	404	BCB	C11-C10-C8-C9
9	MMM	405	BCB	C2A-CAA-CBA-CGA
9	MMM	405	BCB	C2C-C3C-CAC-CBC
9	MMM	405	BCB	CHA-CBD-CGD-O1D
9	MMM	405	BCB	CHA-CBD-CGD-O2D
9	MMM	405	BCB	CAD-CBD-CGD-O1D
9	MMM	405	BCB	CAD-CBD-CGD-O2D
10	LLL	303	BPB	C2C-C3C-CAC-CBC
10	MMM	406	BPB	C2C-C3C-CAC-CBC
11	LLL	305	HTO	C1-C2-C3-O3
11	LLL	305	HTO	O2-C2-C3-O3
11	LLL	305	HTO	O2-C2-C3-C4
11	LLL	305	HTO	O3-C3-C4-C5
11	LLL	308	HTO	O1-C1-C2-C3
11	LLL	310	HTO	C1-C2-C3-O3
11	LLL	310	HTO	O2-C2-C3-O3
11	LLL	310	HTO	O2-C2-C3-C4
11	MMM	408	HTO	C1-C2-C3-O3
11	MMM	408	HTO	O2-C2-C3-C4
11	MMM	415	HTO	C1-C2-C3-O3
11	MMM	415	HTO	C1-C2-C3-C4
11	MMM	415	HTO	O2-C2-C3-O3
11	MMM	415	HTO	O2-C2-C3-C4
12	LLL	309	UQ2	C9-C11-C12-C13
12	MMM	416[A]	UQ2	C9-C11-C12-C13
14	MMM	403	MQ9	C39-C41-C42-C43
16	MMM	410	OLC	C21-C22-C24-O25
16	MMM	410	OLC	O19-C1-O20-C21
16	MMM	410	OLC	C2-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
11	LLL	308	HTO	O1-C1-C2-O2
16	MMM	414	OLC	O19-C1-O20-C21
16	MMM	414	OLC	C2-C1-O20-C21
9	LLL	301	BCB	C4-C3-C5-C6
10	MMM	406	BPB	C4-C3-C5-C6
12	MMM	416[B]	UQ2	C12-C11-C9-C10
9	LLL	301	BCB	C2-C3-C5-C6
10	MMM	406	BPB	C2-C3-C5-C6
9	MMM	404	BCB	C14-C13-C15-C16
16	MMM	410	OLC	C1-C2-C3-C4
10	MMM	406	BPB	C3-C5-C6-C7
10	MMM	406	BPB	C13-C15-C16-C17
9	LLL	301	BCB	C15-C16-C17-C18
16	MMM	414	OLC	C1-C2-C3-C4
14	MMM	403	MQ9	C44-C46-C47-C48
11	LLL	307	HTO	O1-C1-C2-O2
10	MMM	406	BPB	C8-C10-C11-C12
6	CCC	405	DGA	CBB-CAB-CB9-CB8
6	CCC	405	DGA	CB2-CB3-CB4-CB5
6	CCC	405	DGA	OB1-CB1-OG2-CG2
16	MMM	410	OLC	C4-C5-C6-C7
10	LLL	303	BPB	C4-C3-C5-C6
9	MMM	405	BCB	C11-C12-C13-C14
6	CCC	405	DGA	CA1-CA2-CA3-CA4
6	CCC	405	DGA	CA3-CA4-CA5-CA6
6	CCC	405	DGA	CA4-CA5-CA6-CA7
11	LLL	304	HTO	C2-C3-C4-C5
6	CCC	405	DGA	CB2-CB1-OG2-CG2
7	MMM	412	LDA	C4-C5-C6-C7
16	MMM	414	OLC	C4-C5-C6-C7
6	CCC	405	DGA	CCA-CDA-CEA-CFA
16	MMM	414	OLC	C3-C4-C5-C6
9	MMM	404	BCB	C5-C6-C7-C8
16	MMM	414	OLC	C14-C15-C16-C17
11	MMM	408	HTO	O3-C3-C4-C5
6	CCC	405	DGA	CB5-CB6-CB7-CB8
16	MMM	414	OLC	C13-C14-C15-C16
10	LLL	303	BPB	O2A-C1-C2-C3
15	MMM	407	NS5	C32-C31-C33-C34
16	MMM	410	OLC	O23-C22-C24-O25
7	HHH	1301	LDA	C3-C4-C5-C6
7	HHH	1301	LDA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
7	HHH	1302	LDA	C6-C7-C8-C9
7	MMM	402	LDA	C5-C6-C7-C8
7	MMM	402	LDA	C4-C5-C6-C7
7	MMM	409	LDA	C4-C5-C6-C7
9	LLL	302	BCB	C12-C13-C15-C16
9	MMM	404	BCB	C12-C13-C15-C16
9	MMM	405	BCB	C11-C12-C13-C15
10	LLL	303	BPB	C2-C3-C5-C6
10	MMM	406	BPB	C11-C12-C13-C15
12	MMM	416[B]	UQ2	C12-C11-C9-C8
16	MMM	414	OLC	C10-C11-C12-C13
6	CCC	405	DGA	CB1-CB2-CB3-CB4
7	MMM	409	LDA	C11-C10-C9-C8
15	MMM	407	NS5	C7-C8-C9-C10
6	CCC	405	DGA	CAA-CBA-CCA-CDA
15	MMM	407	NS5	C30-C31-C33-C34
9	LLL	302	BCB	C14-C13-C15-C16
10	MMM	406	BPB	C11-C12-C13-C14
7	MMM	412	LDA	C5-C6-C7-C8
7	MMM	411	LDA	C6-C7-C8-C9
7	MMM	411	LDA	C7-C8-C9-C10
10	MMM	406	BPB	C5-C6-C7-C8
7	HHH	1301	LDA	C2-C3-C4-C5
16	MMM	410	OLC	C10-C11-C12-C13
7	MMM	413	LDA	C5-C6-C7-C8
11	LLL	304	HTO	O3-C3-C4-C5
7	MMM	413	LDA	C3-C4-C5-C6
6	CCC	405	DGA	CFA-CGA-CHA-CIA
7	HHH	1301	LDA	C9-C10-C11-C12
11	LLL	307	HTO	C4-C5-C6-C7
7	MMM	412	LDA	C2-C3-C4-C5
11	MMM	408	HTO	O2-C2-C3-O3
7	HHH	1302	LDA	C7-C8-C9-C10
11	LLL	306	HTO	C4-C5-C6-C7
14	MMM	403	MQ9	C40-C39-C41-C42
10	MMM	406	BPB	C11-C10-C8-C7
15	MMM	407	NS5	C2-C3-C4-C5
12	MMM	416[B]	UQ2	C3-C2-O2-CM2
11	MMM	408	HTO	C2-C3-C4-C5
6	CCC	405	DGA	CB4-CB5-CB6-CB7
14	MMM	403	MQ9	C38-C39-C41-C42
7	MMM	413	LDA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
11	LLL	308	HTO	C4-C5-C6-C7
6	CCC	405	DGA	CA2-CA3-CA4-CA5
6	CCC	405	DGA	CA7-CA8-CA9-CAA
16	MMM	410	OLC	O20-C21-C22-O23
7	HHH	1302	LDA	C3-C4-C5-C6
7	MMM	409	LDA	C2-C3-C4-C5
9	MMM	404	BCB	C3-C5-C6-C7
6	CCC	405	DGA	CG1-CG2-CG3-OXT
11	LLL	310	HTO	C1-C2-C3-C4
11	MMM	408	HTO	C1-C2-C3-C4
7	MMM	413	LDA	C9-C10-C11-C12
9	MMM	404	BCB	C8-C10-C11-C12
7	HHH	1302	LDA	C2-C3-C4-C5
9	MMM	404	BCB	C11-C10-C8-C7
10	MMM	406	BPB	C6-C7-C8-C10
9	MMM	404	BCB	CAD-CBD-CGD-O2D
10	LLL	303	BPB	CAD-CBD-CGD-O2D
7	MMM	409	LDA	C9-C10-C11-C12
7	MMM	409	LDA	C2-C1-N1-CM1
7	MMM	413	LDA	C2-C1-N1-CM2
9	LLL	302	BCB	C16-C17-C18-C19
11	LLL	305	HTO	C2-C3-C4-C5
7	MMM	402	LDA	C2-C3-C4-C5
7	MMM	411	LDA	C4-C5-C6-C7
7	MMM	412	LDA	C7-C8-C9-C10
7	MMM	409	LDA	C2-C1-N1-O1
7	MMM	411	LDA	C2-C1-N1-O1
7	MMM	412	LDA	C2-C1-N1-O1
9	LLL	301	BCB	CAD-CBD-CGD-O1D
10	MMM	406	BPB	C15-C16-C17-C18
16	MMM	414	OLC	C5-C6-C7-C8
7	MMM	412	LDA	C1-C2-C3-C4
16	MMM	414	OLC	C15-C16-C17-C18
10	MMM	406	BPB	C6-C7-C8-C9
7	MMM	411	LDA	C2-C3-C4-C5
9	LLL	302	BCB	C16-C17-C18-C20
16	MMM	410	OLC	O20-C21-C22-C24
9	MMM	404	BCB	C2-C1-O2A-CGA
7	HHH	1301	LDA	C6-C7-C8-C9
7	MMM	409	LDA	C5-C6-C7-C8
7	HHH	1301	LDA	C11-C10-C9-C8
7	HHH	1301	LDA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
16	MMM	410	OLC	C12-C13-C14-C15
11	LLL	306	HTO	C1-C2-C3-O3
10	MMM	406	BPB	O2A-C1-C2-C3
7	HHH	1302	LDA	C5-C6-C7-C8
5	CCC	402	HEC	CAA-CBA-CGA-O1A
12	MMM	416[A]	UQ2	C2-C3-O3-CM3
11	LLL	310	HTO	C3-C4-C5-C6
11	LLL	310	HTO	C4-C5-C6-C7
6	CCC	405	DGA	CCB-CDB-CEB-CFB
12	MMM	416[A]	UQ2	C1-C2-O2-CM2
11	MMM	408	HTO	C3-C4-C5-C6
7	MMM	409	LDA	C1-C2-C3-C4
5	CCC	402	HEC	CAA-CBA-CGA-O2A
12	MMM	416[B]	UQ2	C4-C3-O3-CM3
11	LLL	305	HTO	C3-C4-C5-C6
12	MMM	416[B]	UQ2	C9-C11-C12-C13
7	MMM	413	LDA	C11-C10-C9-C8
7	MMM	413	LDA	C1-C2-C3-C4
5	CCC	402	HEC	C3D-CAD-CBD-CGD
12	LLL	309	UQ2	C4-C3-O3-CM3
16	MMM	414	OLC	C9-C10-C11-C12
5	CCC	401	HEC	CAA-CBA-CGA-O1A
5	CCC	401	HEC	CAA-CBA-CGA-O2A
9	MMM	405	BCB	O2A-C1-C2-C3
11	LLL	306	HTO	O2-C2-C3-O3
11	LLL	306	HTO	C3-C4-C5-C6
16	MMM	410	OLC	C13-C14-C15-C16
9	LLL	302	BCB	CHA-CBD-CGD-O1D
15	MMM	407	NS5	C3-C4-C5-C6
10	MMM	406	BPB	C11-C10-C8-C9
12	MMM	416[B]	UQ2	C11-C12-C13-C14
10	MMM	406	BPB	C2-C1-O2A-CGA
7	HHH	1302	LDA	C9-C10-C11-C12
16	MMM	410	OLC	C2-C3-C4-C5
7	MMM	411	LDA	C9-C10-C11-C12
7	MMM	411	LDA	C1-C2-C3-C4
12	LLL	309	UQ2	C11-C12-C13-C14
9	MMM	404	BCB	C6-C7-C8-C10
5	CCC	402	HEC	CAD-CBD-CGD-O1D

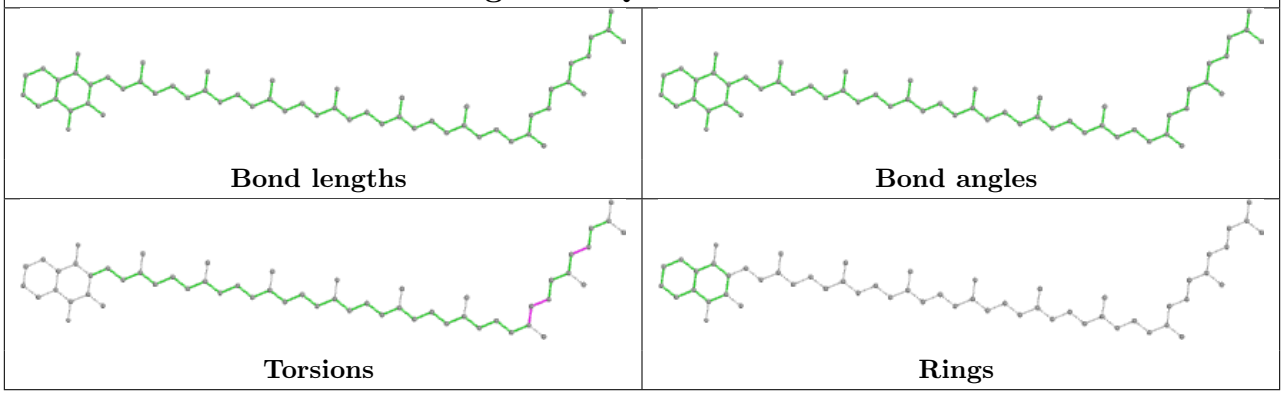
There are no ring outliers.

20 monomers are involved in 45 short contacts:

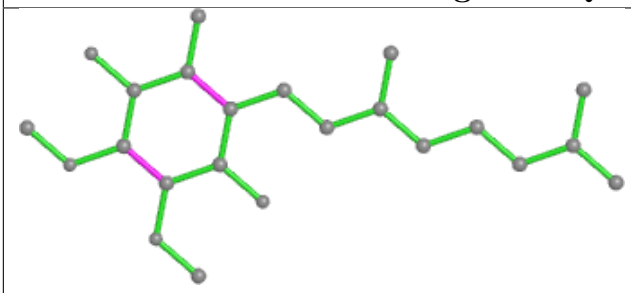
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	MMM	416[A]	UQ2	4	0
11	MMM	415	HTO	1	0
8	MMM	418	SO4	1	0
7	HHH	1301	LDA	1	0
9	MMM	404	BCB	3	0
5	CCC	404	HEC	1	0
9	MMM	405	BCB	1	0
7	MMM	402	LDA	1	0
7	MMM	409	LDA	1	0
9	LLL	301	BCB	4	0
9	LLL	302	BCB	2	0
5	CCC	403	HEC	2	0
10	MMM	406	BPB	5	0
10	LLL	303	BPB	1	0
15	MMM	407	NS5	5	0
7	MMM	411	LDA	4	0
5	CCC	401	HEC	2	0
12	LLL	309	UQ2	4	0
6	CCC	405	DGA	1	0
12	MMM	416[B]	UQ2	3	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.

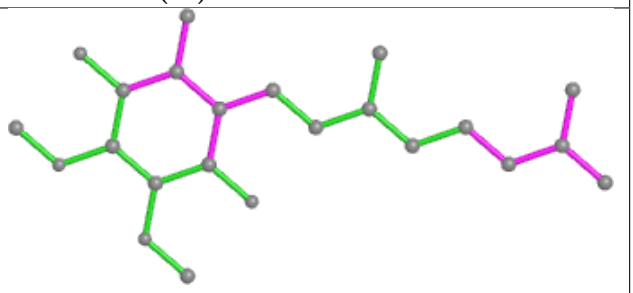
Ligand MQ9 MMM 403



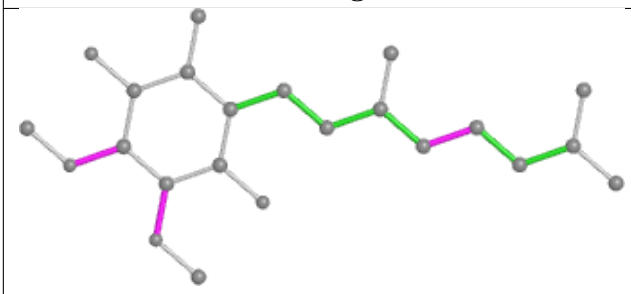
Ligand UQ2 MMM 416 (A)



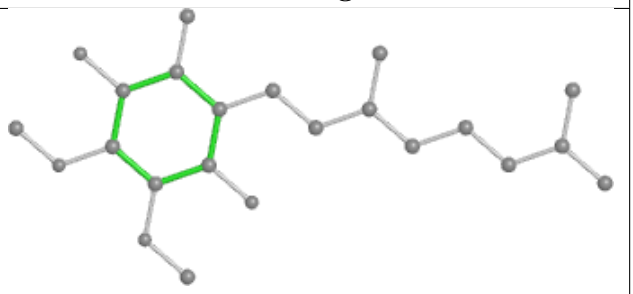
Bond lengths



Bond angles

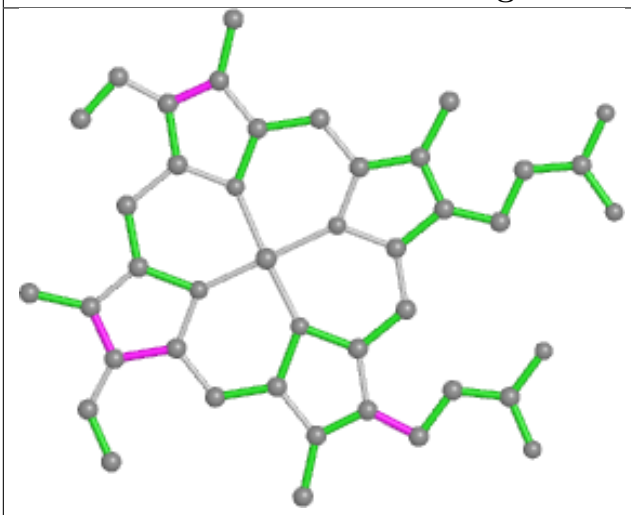


Torsions

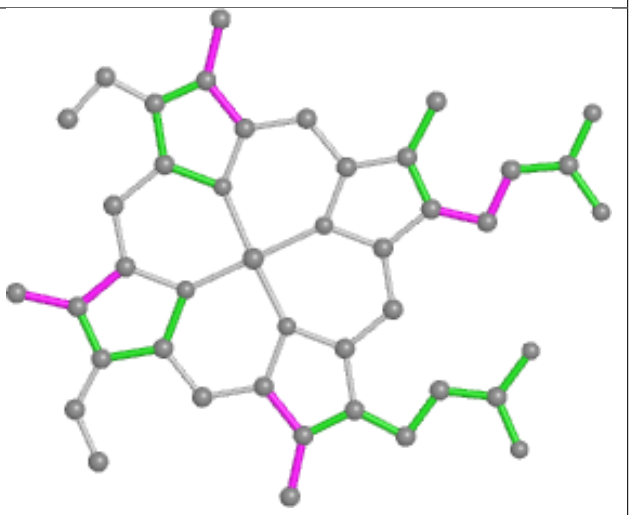


Rings

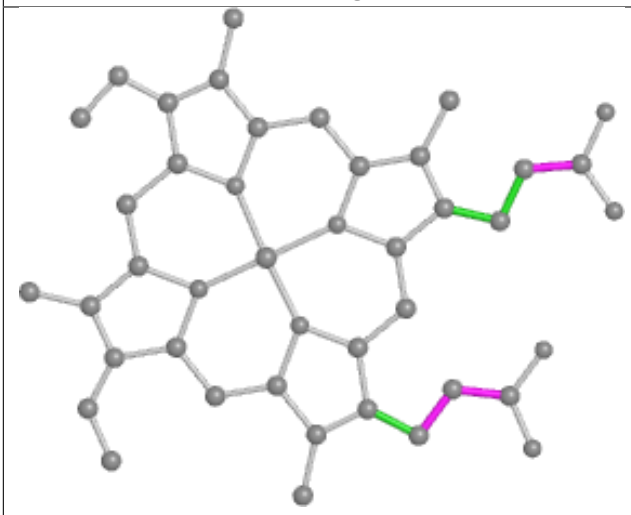
Ligand HEC CCC 402



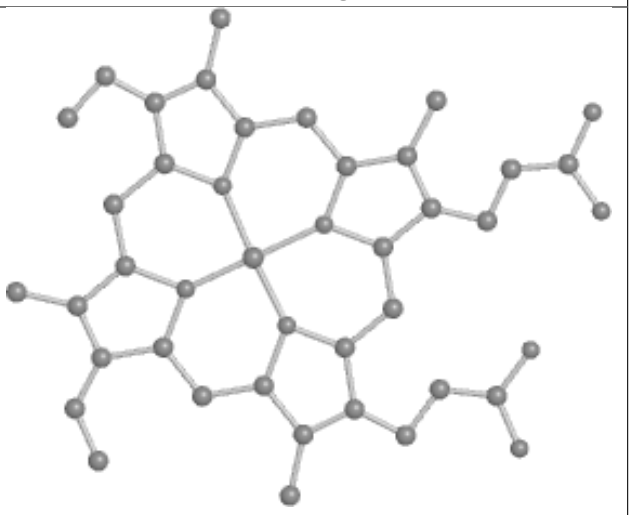
Bond lengths



Bond angles

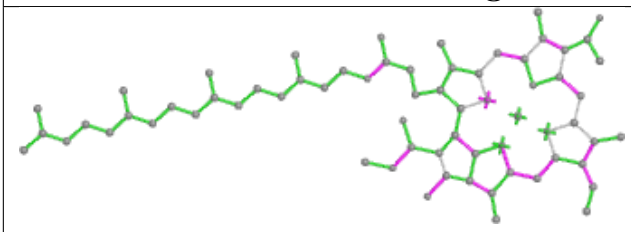


Torsions

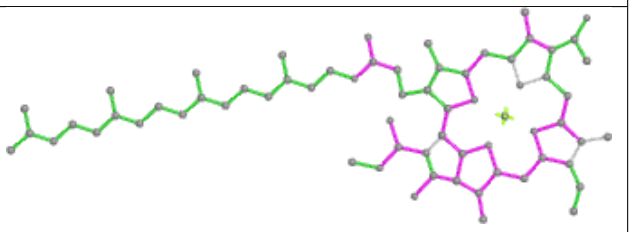


Rings

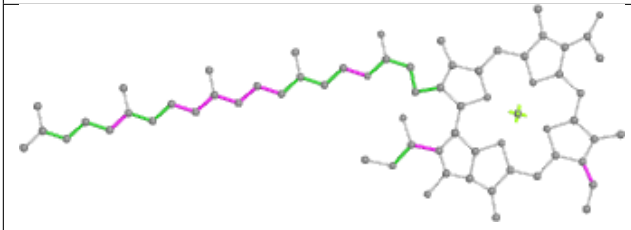
Ligand BCB MMM 404



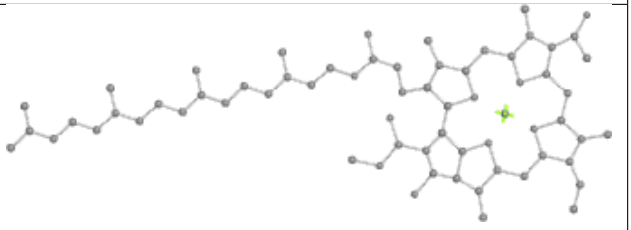
Bond lengths



Bond angles

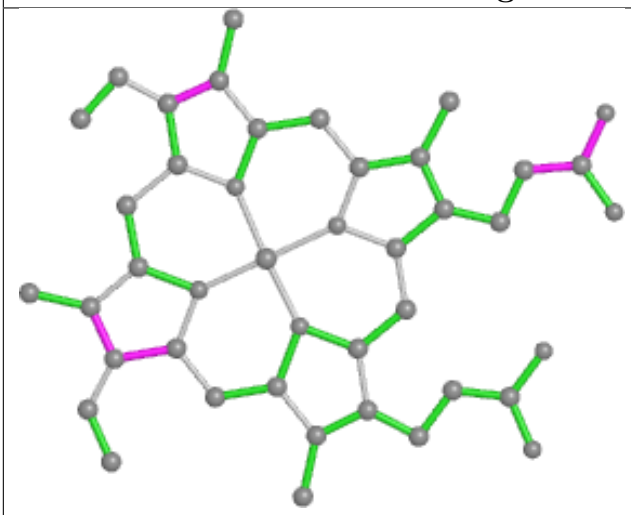


Torsions

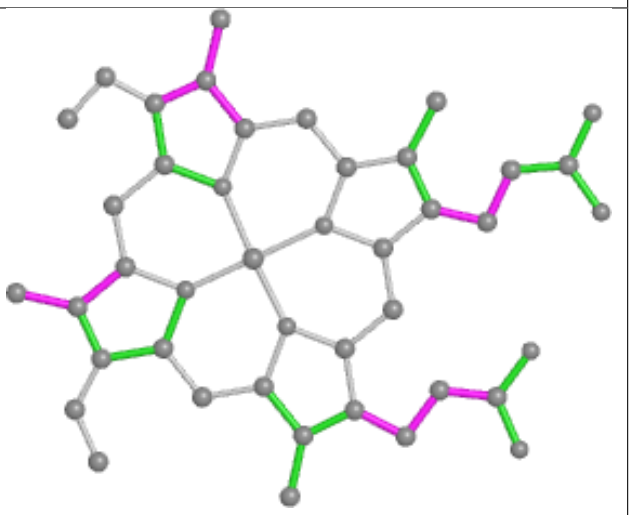


Rings

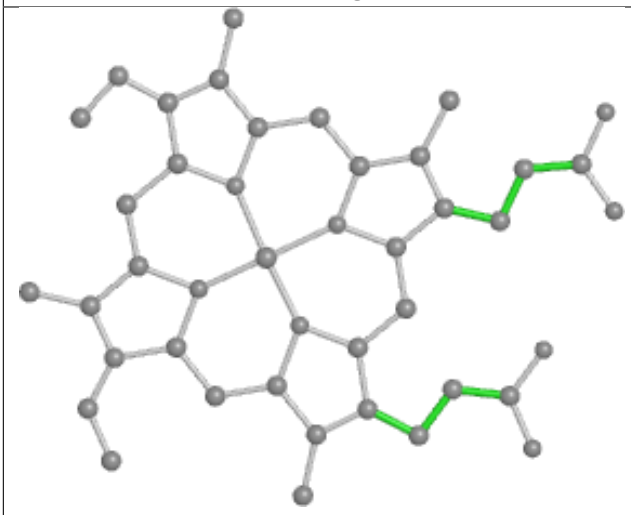
Ligand HEC CCC 404



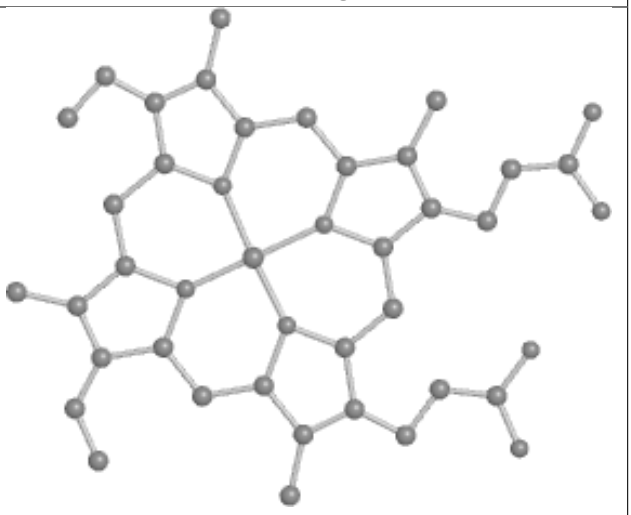
Bond lengths



Bond angles

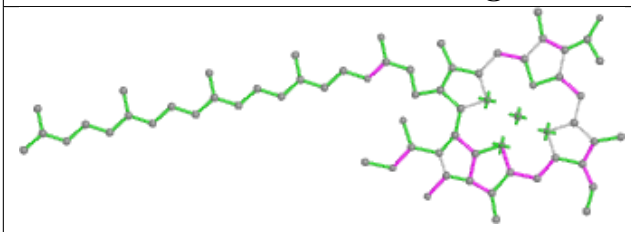


Torsions

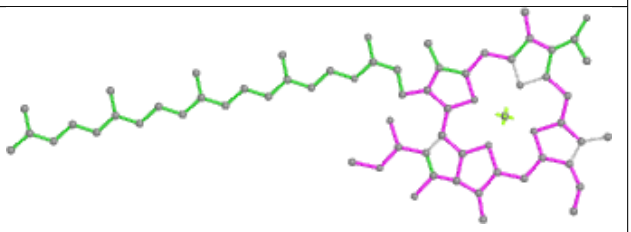


Rings

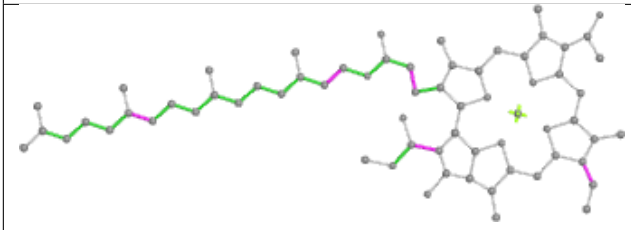
Ligand BCB MMM 405



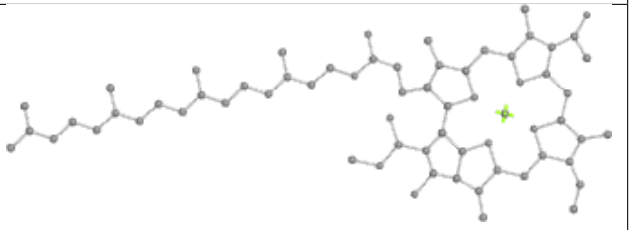
Bond lengths



Bond angles

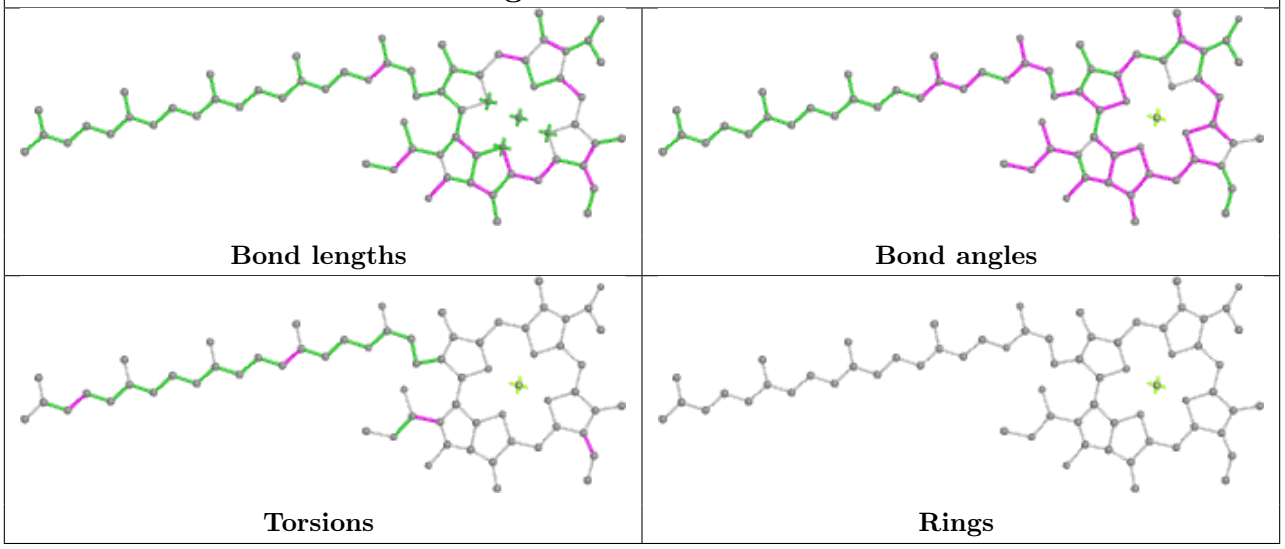


Torsions

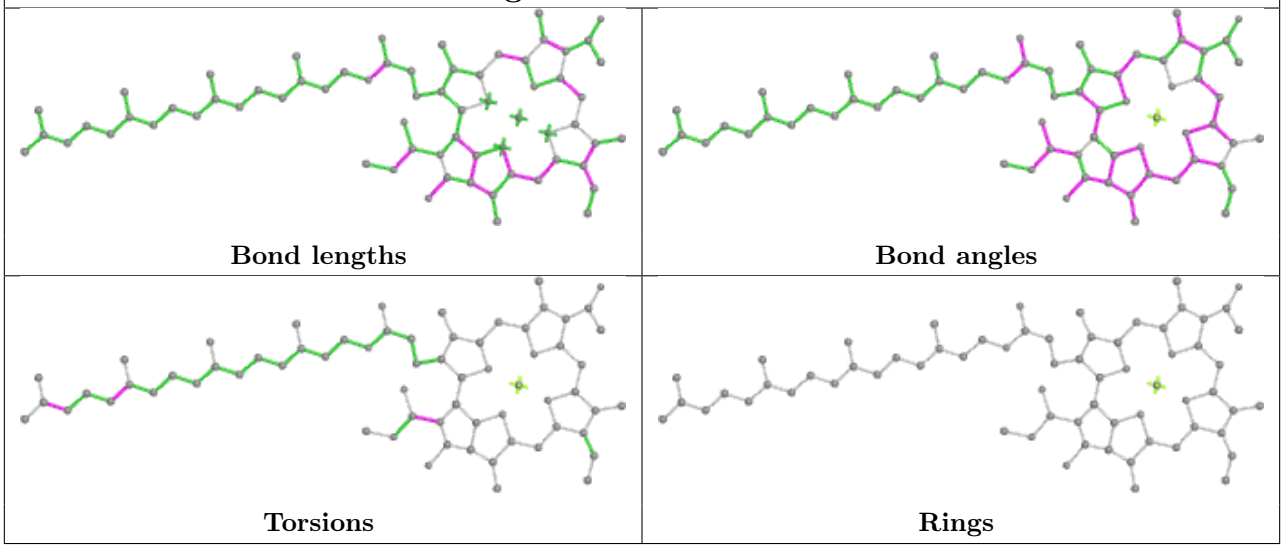


Rings

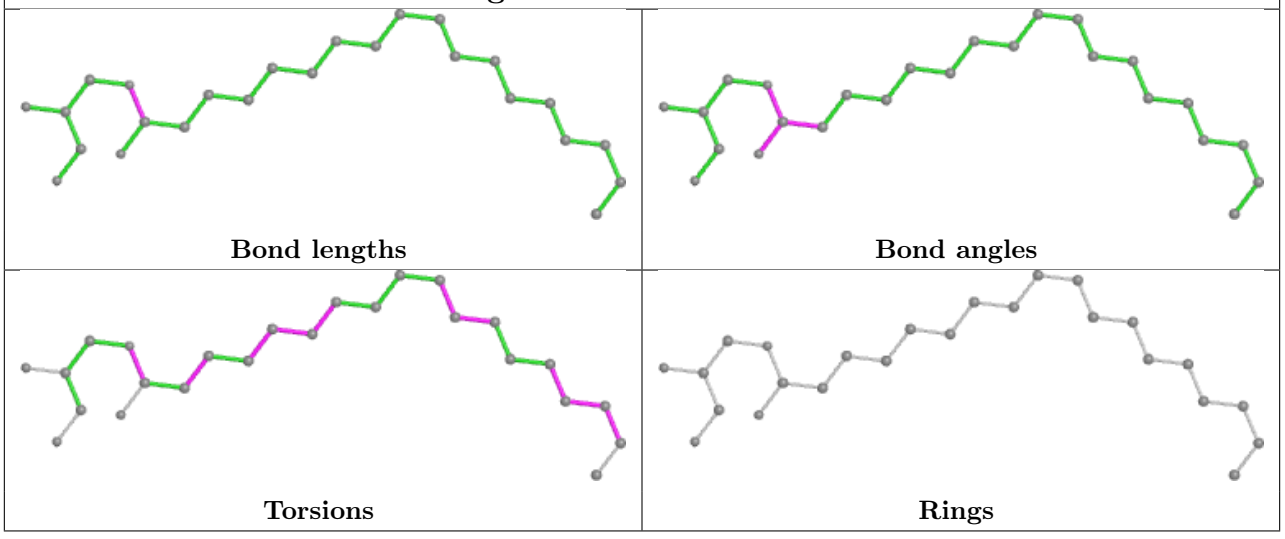
Ligand BCB LLL 301



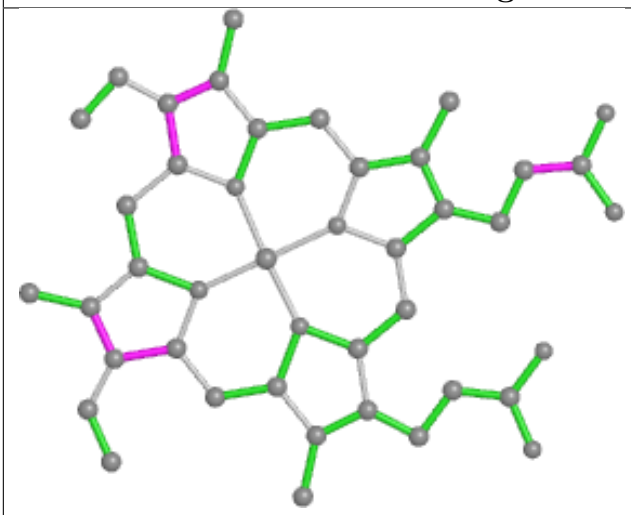
Ligand BCB LLL 302



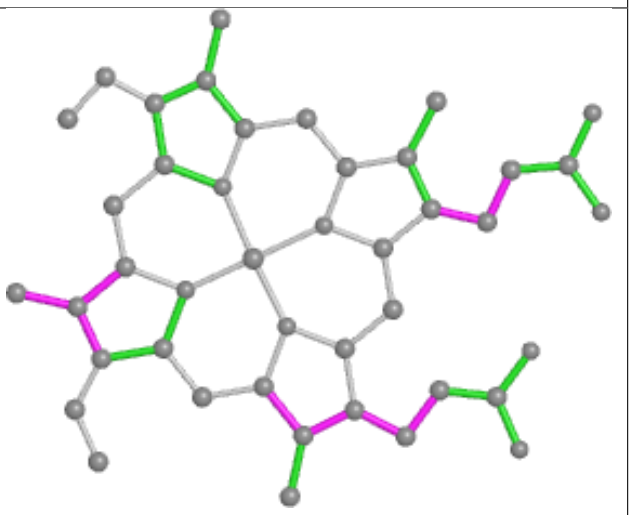
Ligand OLC MMM 414



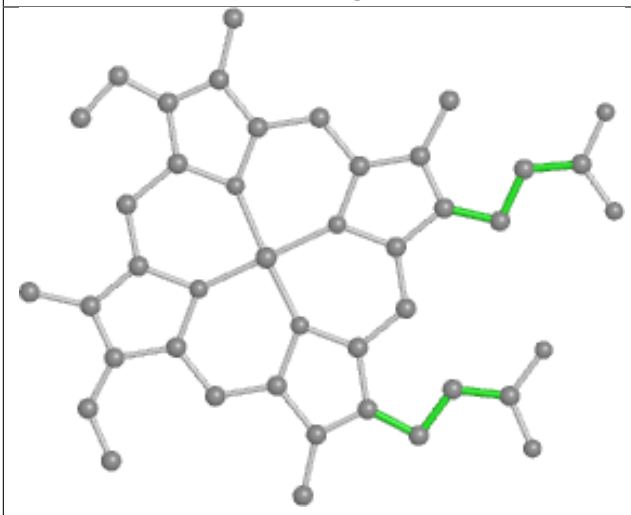
Ligand HEC CCC 403



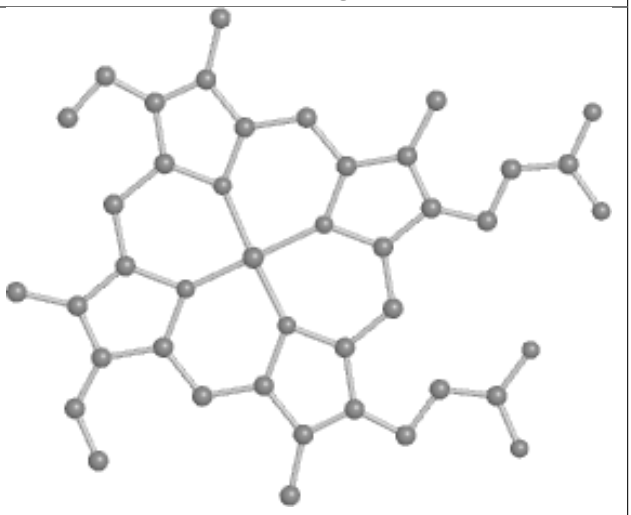
Bond lengths



Bond angles

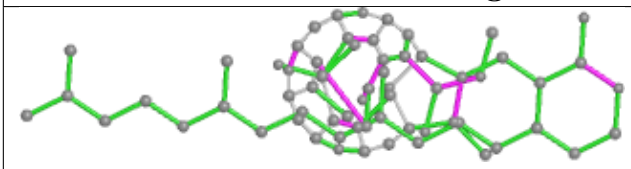


Torsions

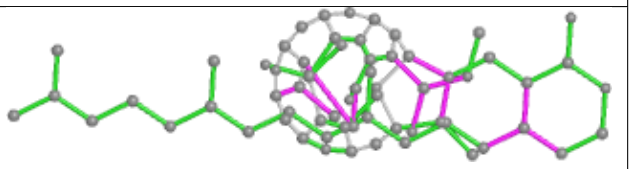


Rings

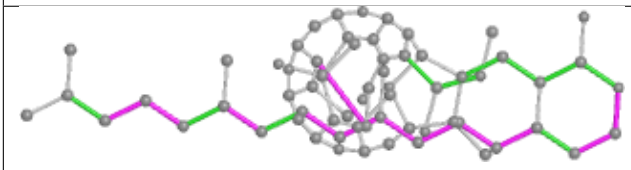
Ligand BPB MMM 406



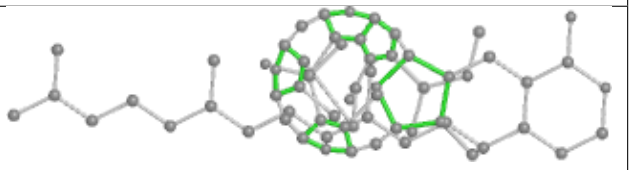
Bond lengths



Bond angles

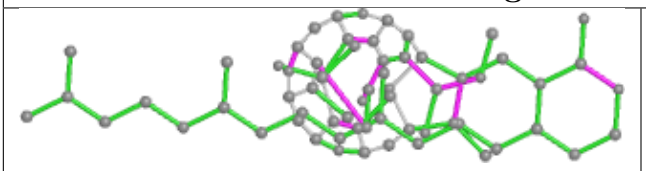


Torsions

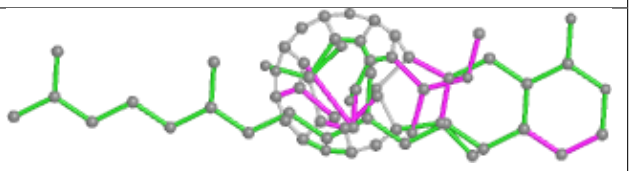


Rings

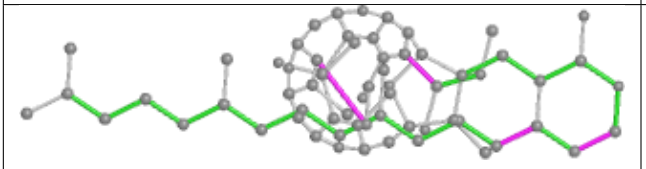
Ligand BPB LLL 303



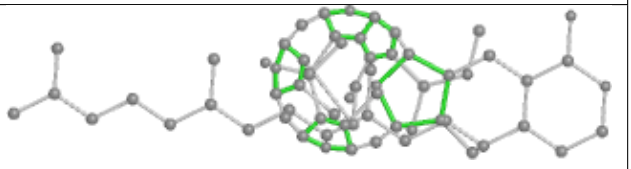
Bond lengths



Bond angles

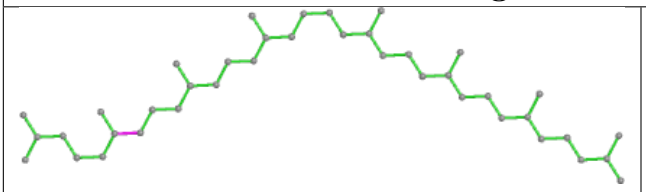


Torsions

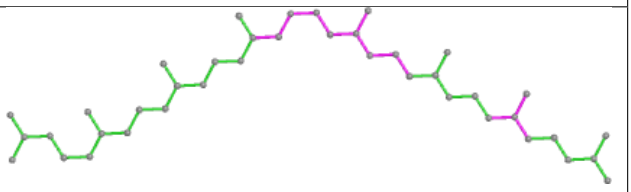


Rings

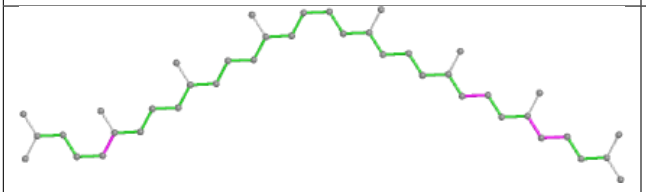
Ligand NS5 MMM 407



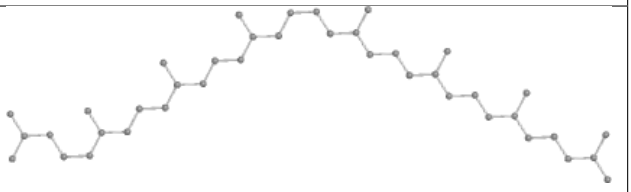
Bond lengths



Bond angles

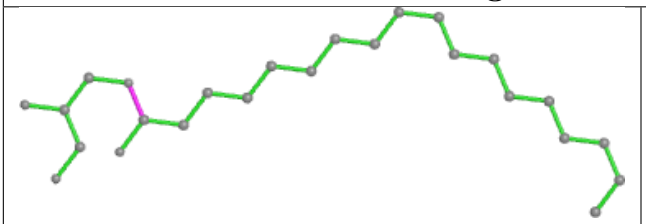


Torsions

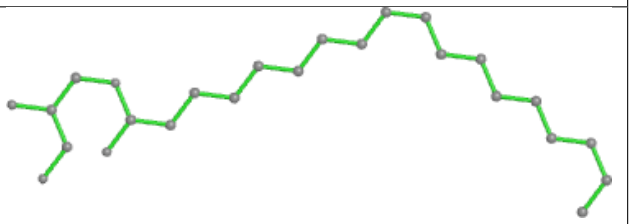


Rings

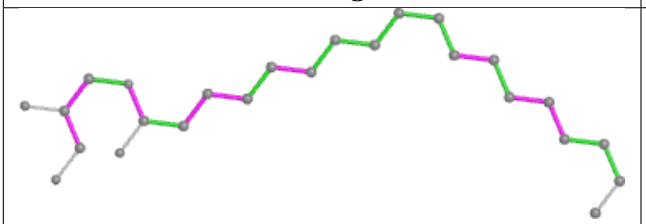
Ligand OLC MMM 410



Bond lengths



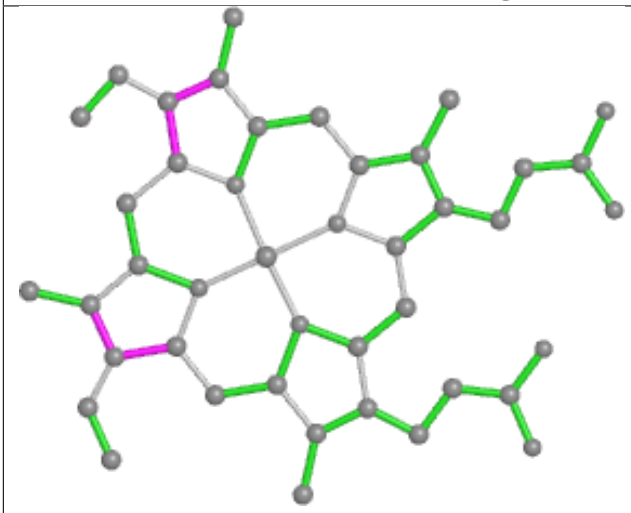
Bond angles



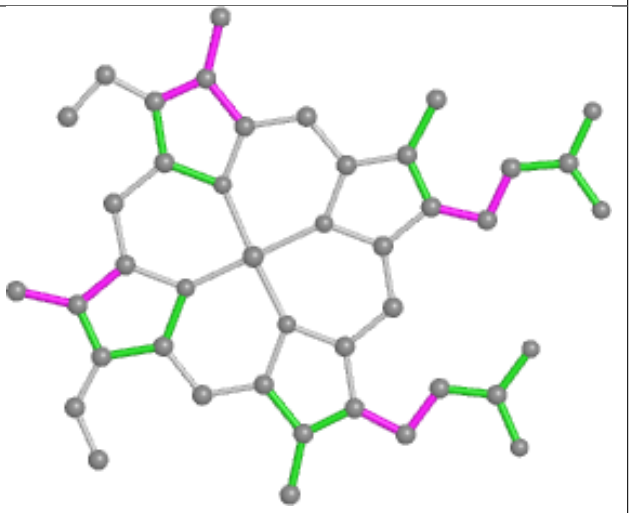
Torsions

Rings

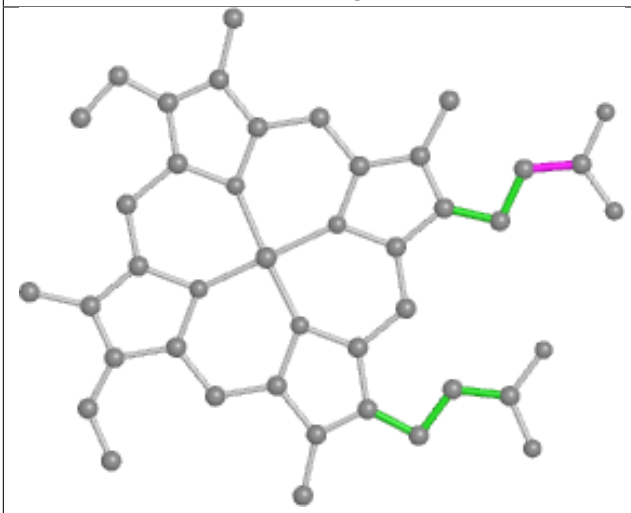
Ligand HEC CCC 401



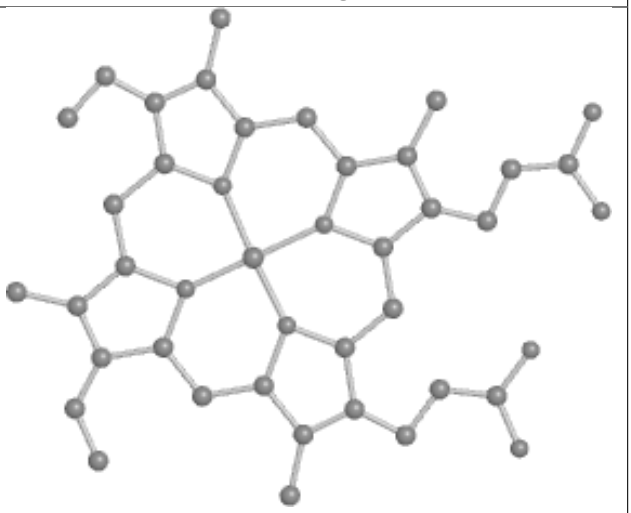
Bond lengths



Bond angles

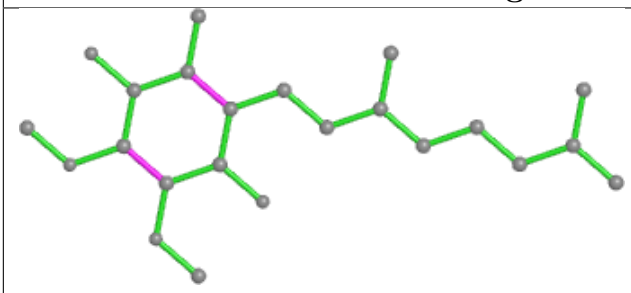


Torsions

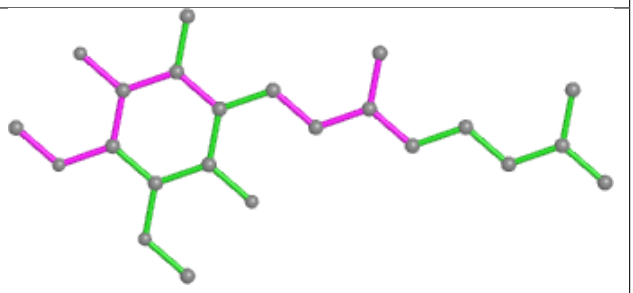


Rings

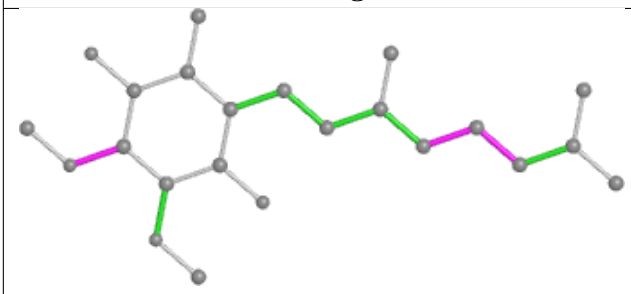
Ligand UQ2 LLL 309



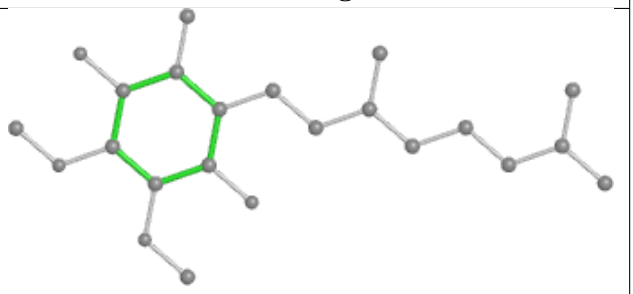
Bond lengths



Bond angles

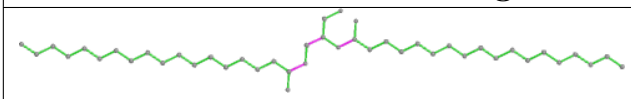


Torsions

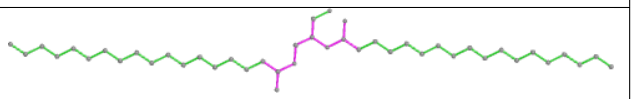


Rings

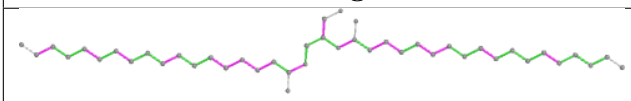
Ligand DGA CCC 405



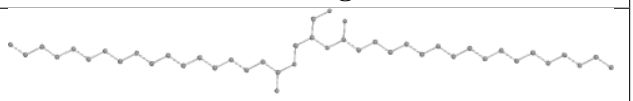
Bond lengths



Bond angles

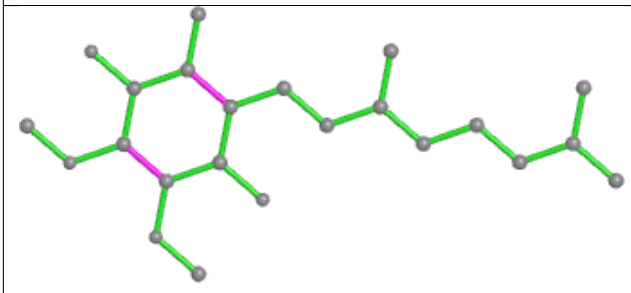


Torsions

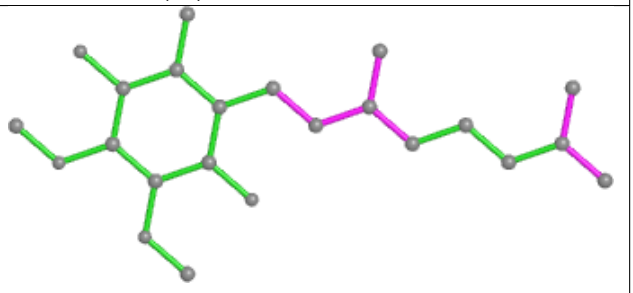


Rings

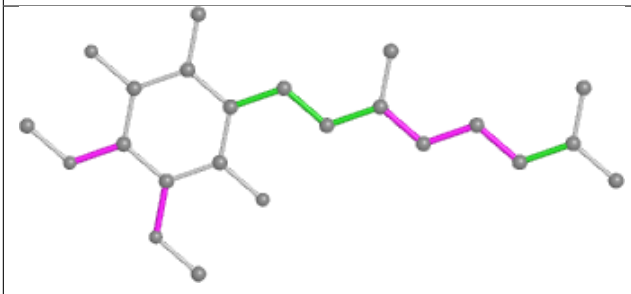
Ligand UQ2 MMM 416 (B)



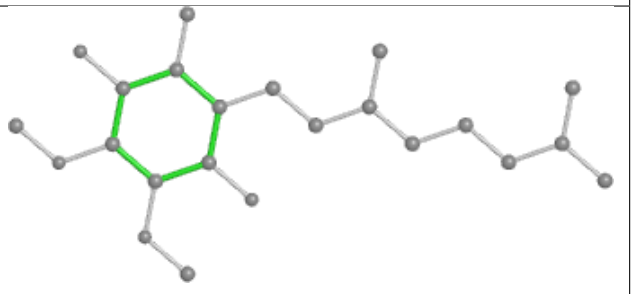
Bond lengths



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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

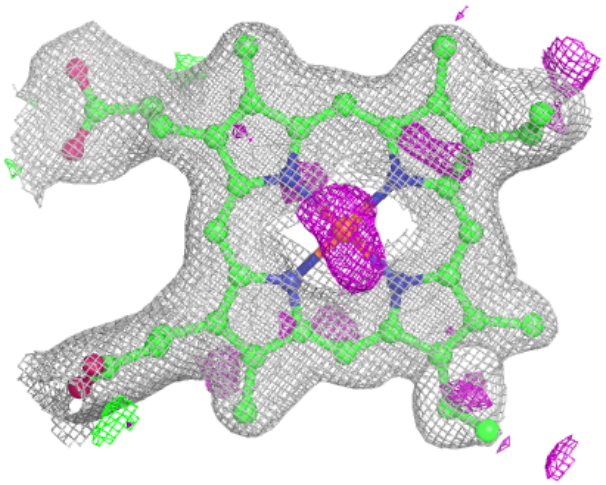
6.4 Ligands

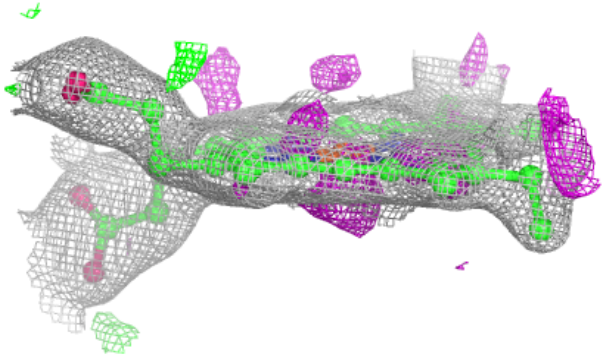
Unable to reproduce the depositors R factor - this section is therefore empty.

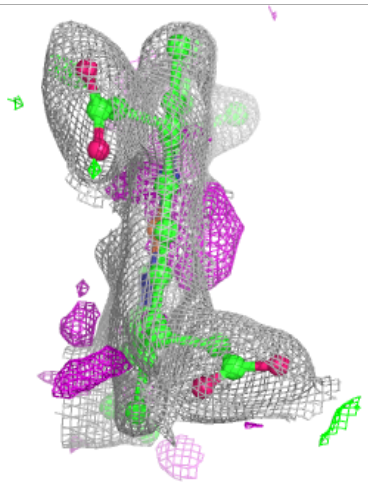
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEC CCC 401:

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

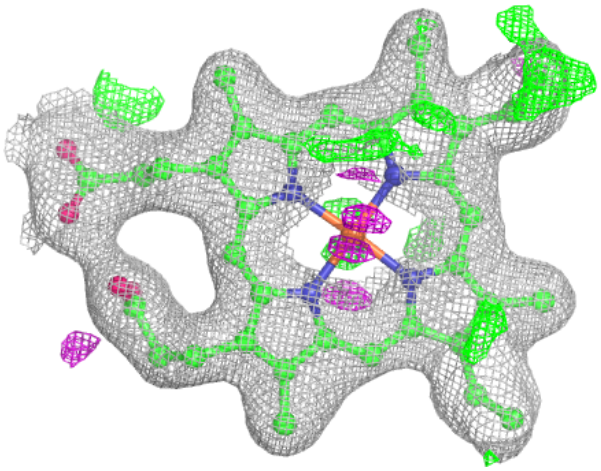


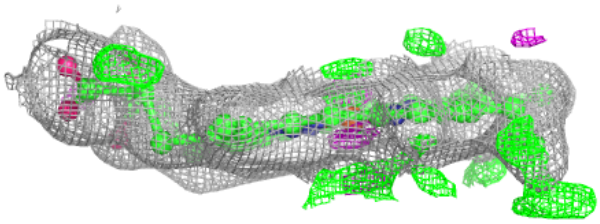


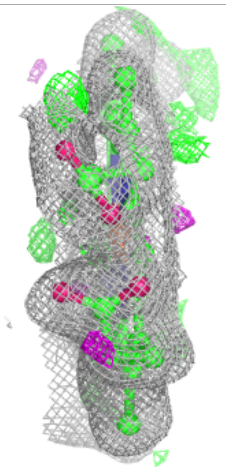


Electron density around HEC CCC 402:

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

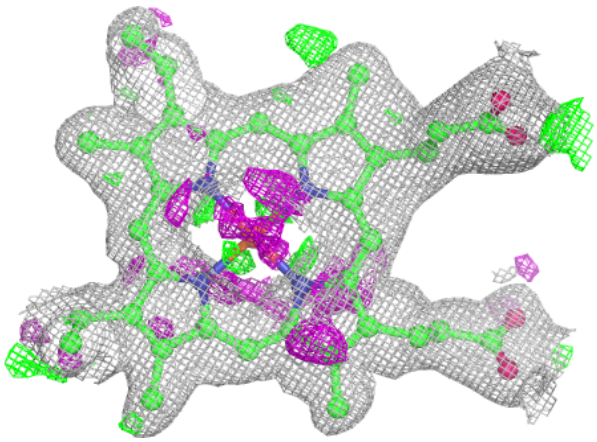


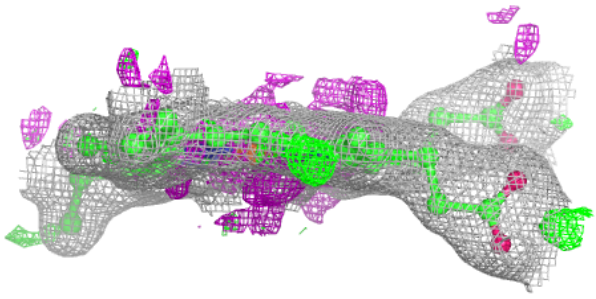


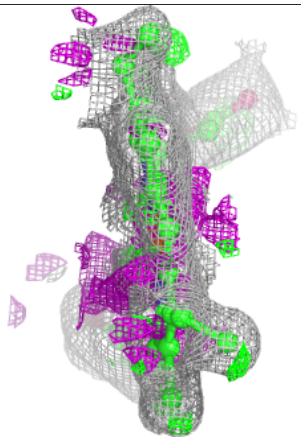


Electron density around HEC CCC 403:

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

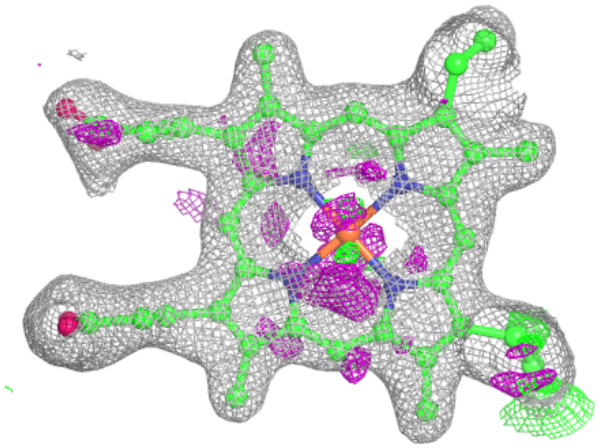


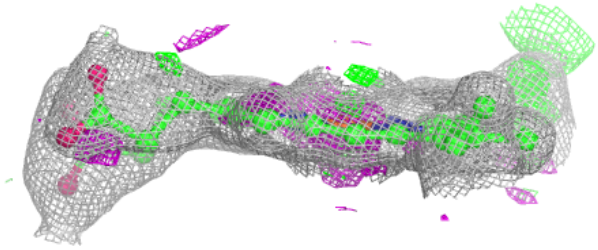


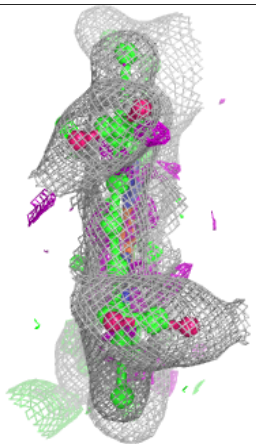


Electron density around HEC CCC 404:

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

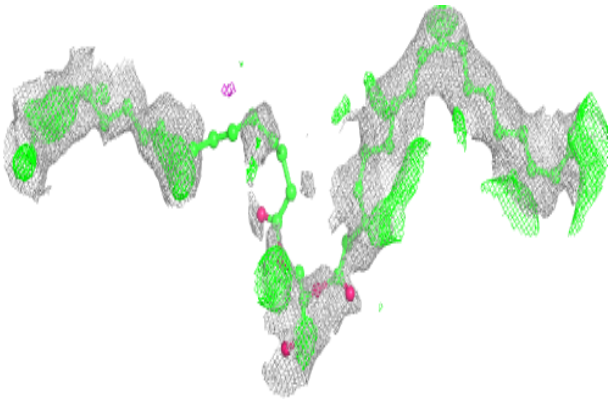


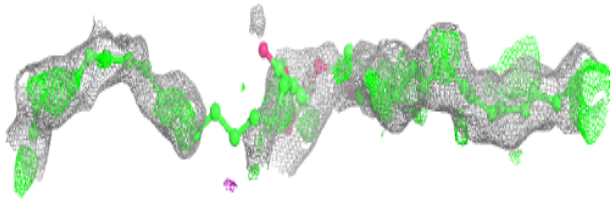


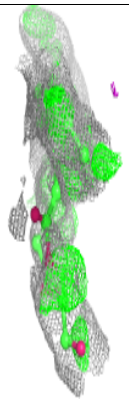


Electron density around DGA CCC 405:

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

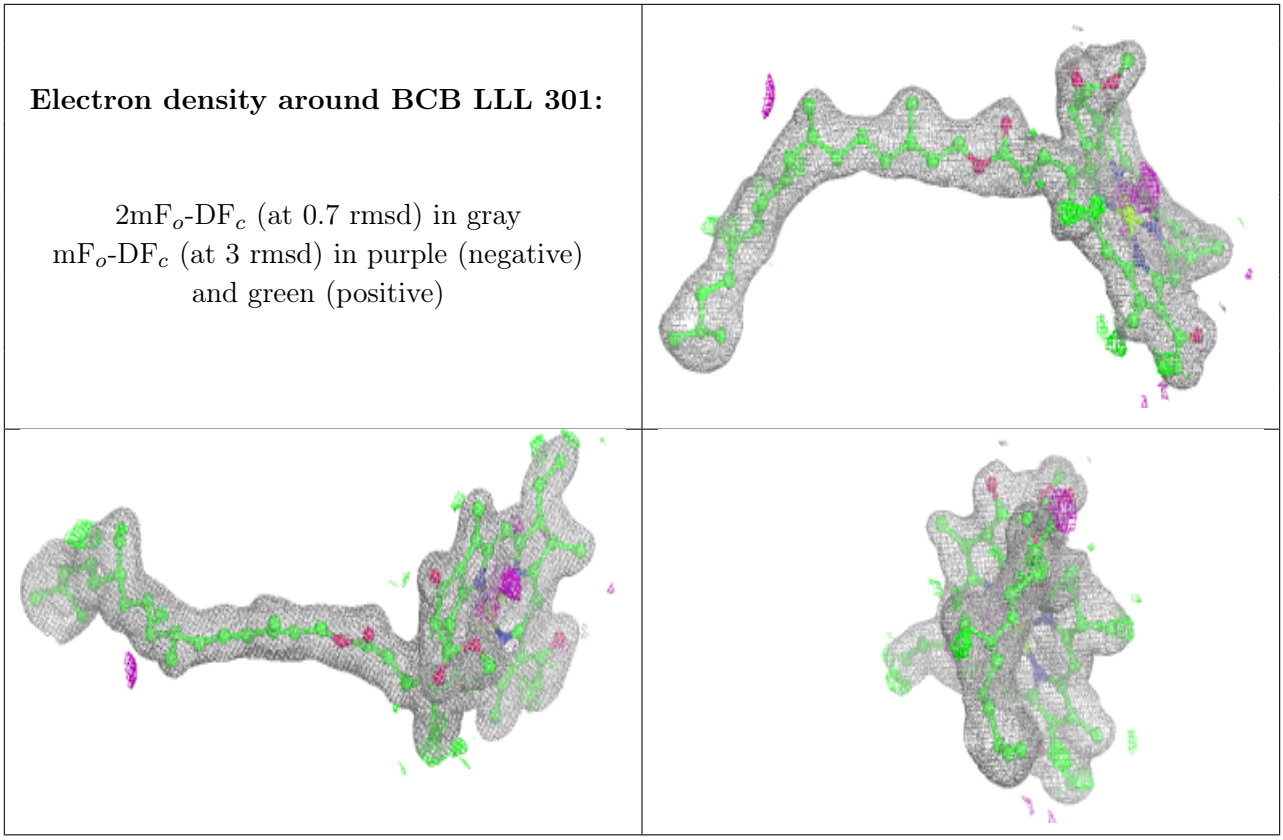






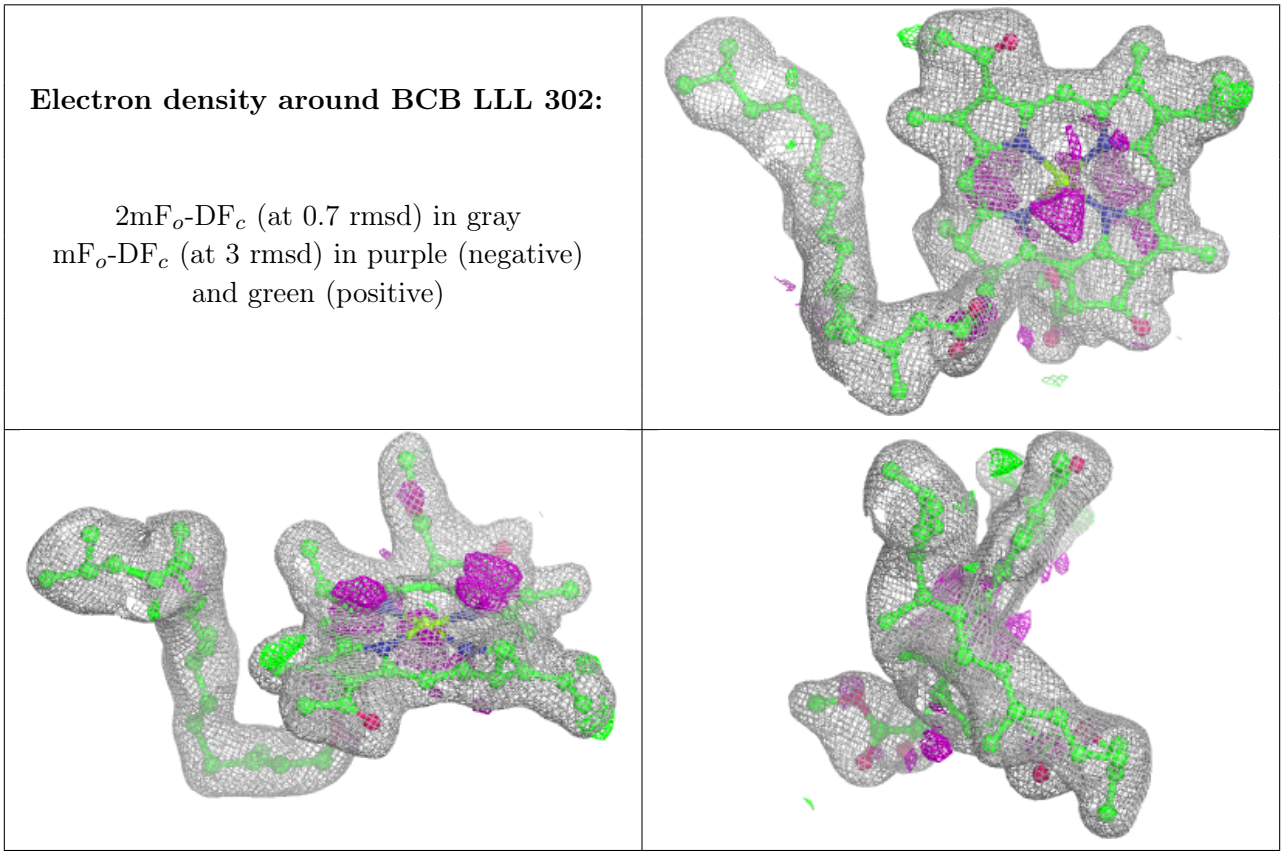
Electron density around BCB LLL 301:

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



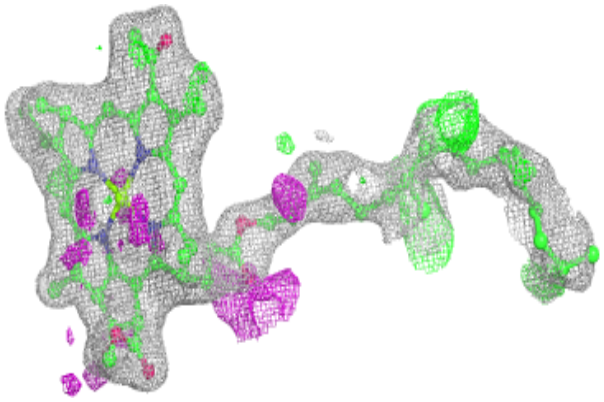
Electron density around BCB LLL 302:

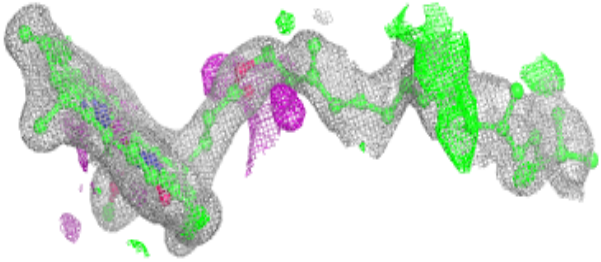
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

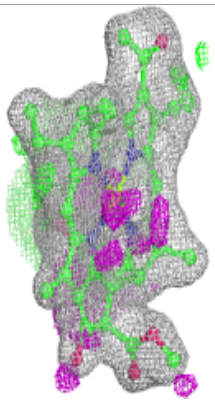


Electron density around BCB MMM 404:

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

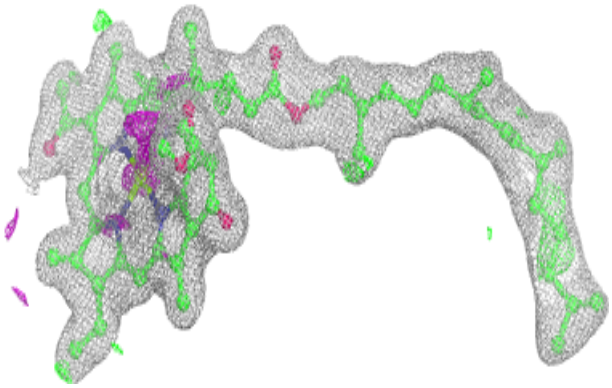


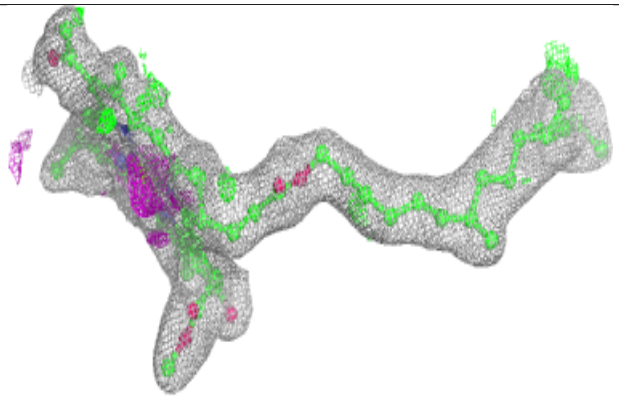




Electron density around BCB MMM 405:

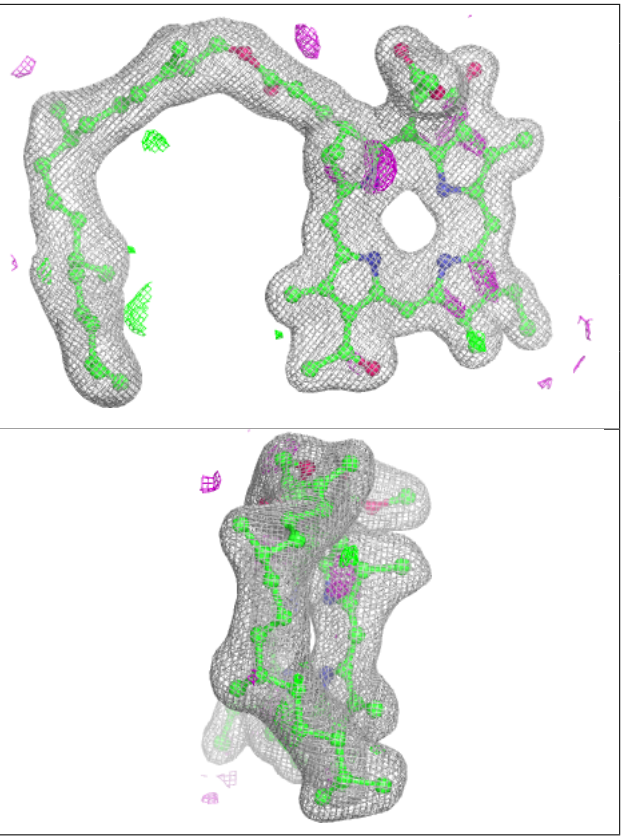
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





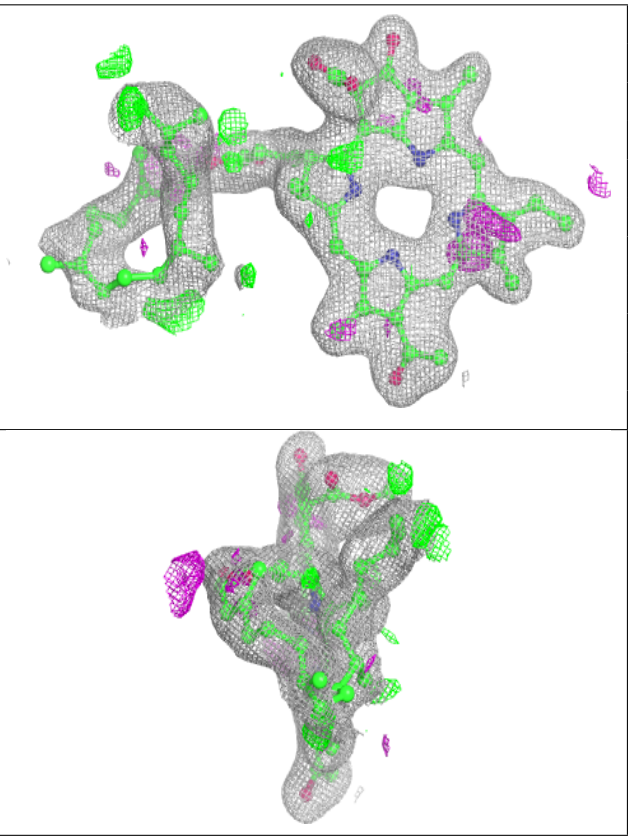
Electron density around BPB LLL 303:

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



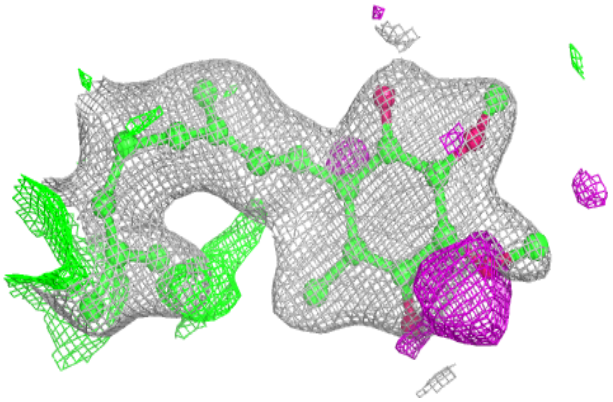
Electron density around BPB MMM 406:

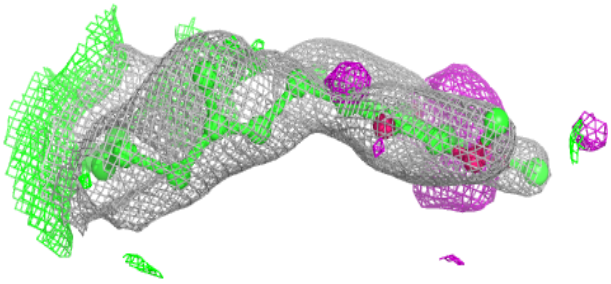
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

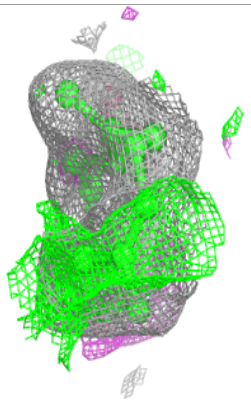


Electron density around UQ2 LLL 309:

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

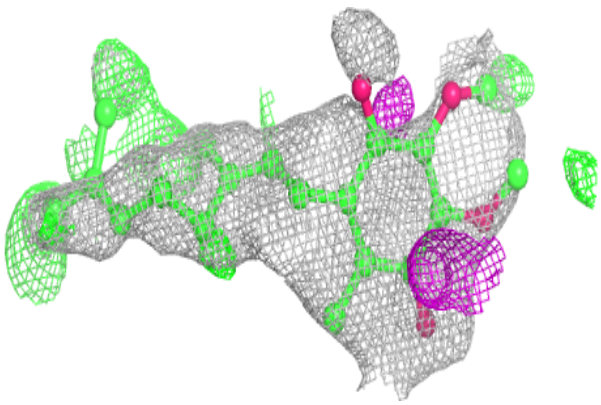


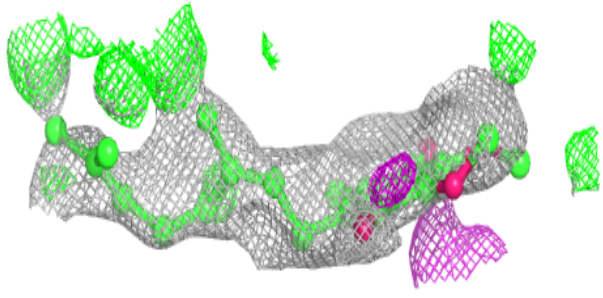


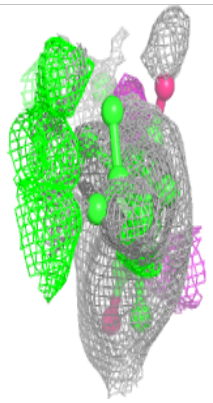


Electron density around UQ2 MMM 416 (A):

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

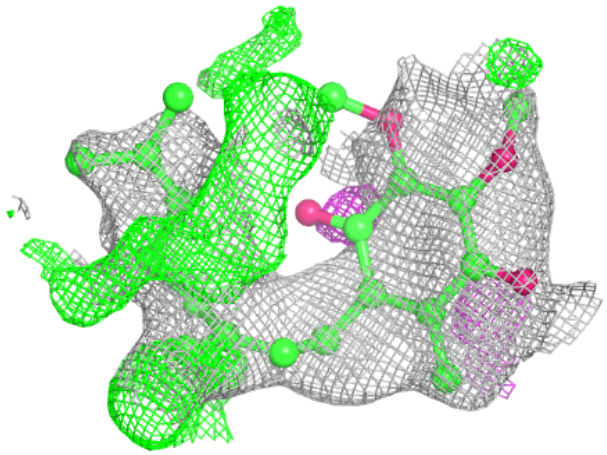


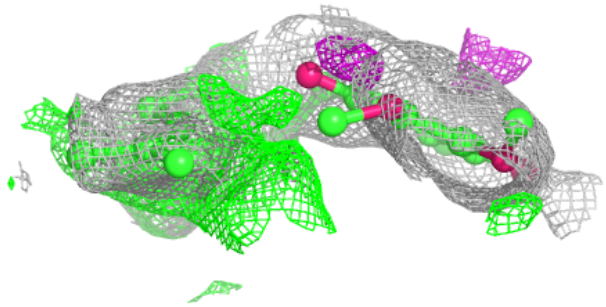


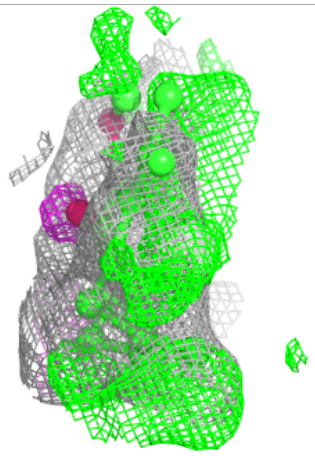


Electron density around UQ2 MMM 416 (B):

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

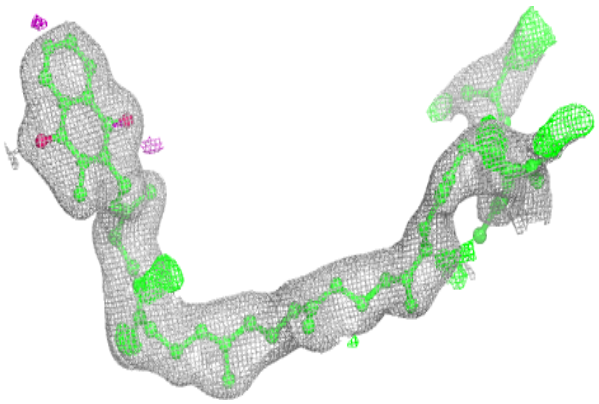


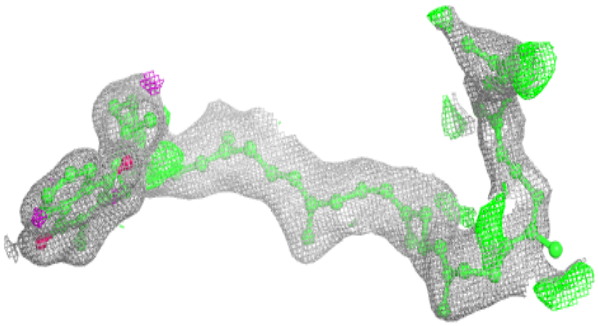


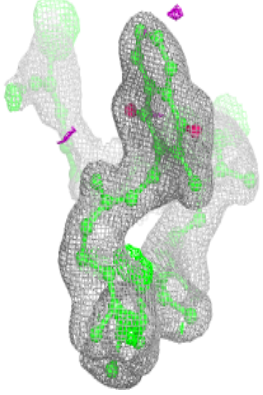


Electron density around MQ9 MMM 403:

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

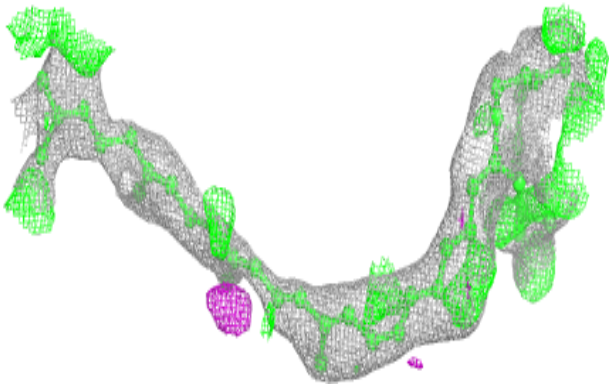


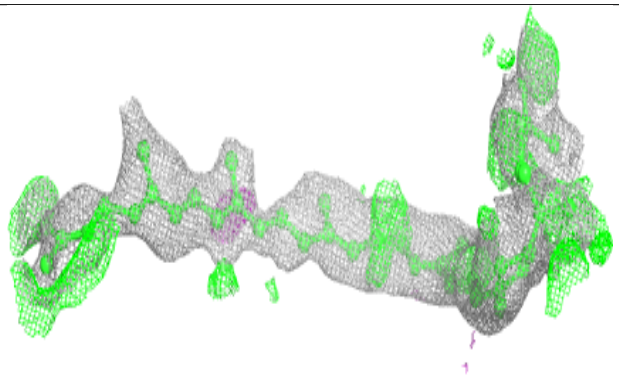


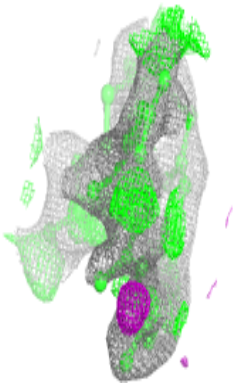


Electron density around NS5 MMM 407:

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

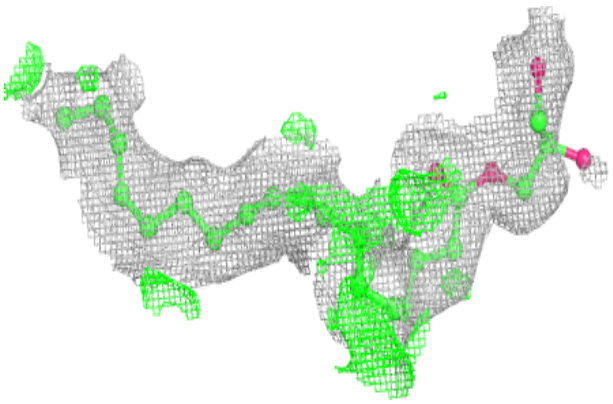


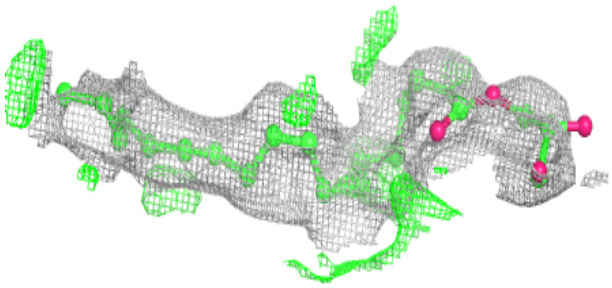


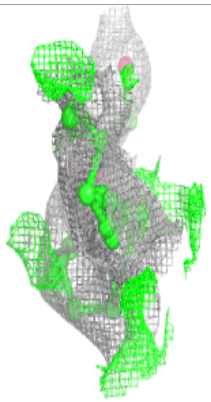


Electron density around OLC MMM 410:

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

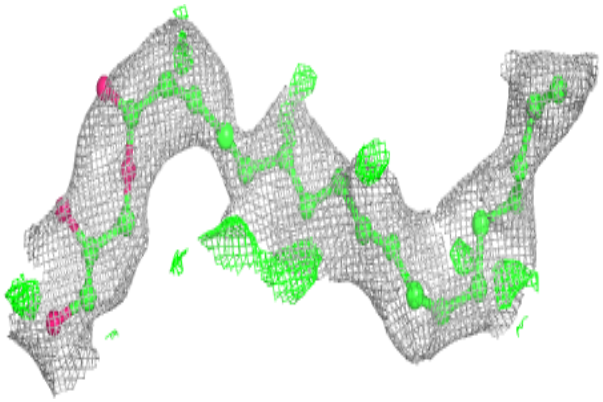


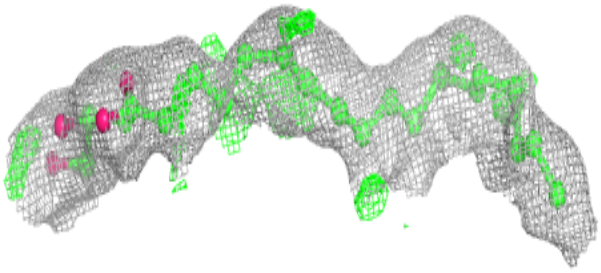


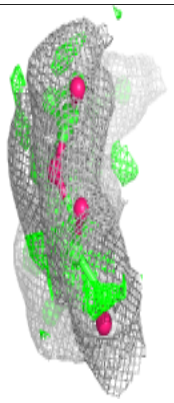


Electron density around OLC MMM 414:

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







6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.