Full wwPDB X-ray Structure Validation Report

Aug 23, 2023 – 02:00 PM EDT

PDB ID	:	3D38
Title	:	Crystal structure of new trigonal form of photosynthetic reaction center from Blastochloris viridis. Crystals grown in microfluidics by detergent capture.
Authors	:	Li, L.; Nachtergaele, S.H.M.; Seddon, A.M.; Tereshko, V.; Ponomarenko, N.; Ismagilov, R.F.; Accelerated Technologies Center for Gene to 3D Structure (ATCG3D)
Deposited on	:	2008-05-09
Resolution	:	3.21 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 (1)) were used in the production of this report:

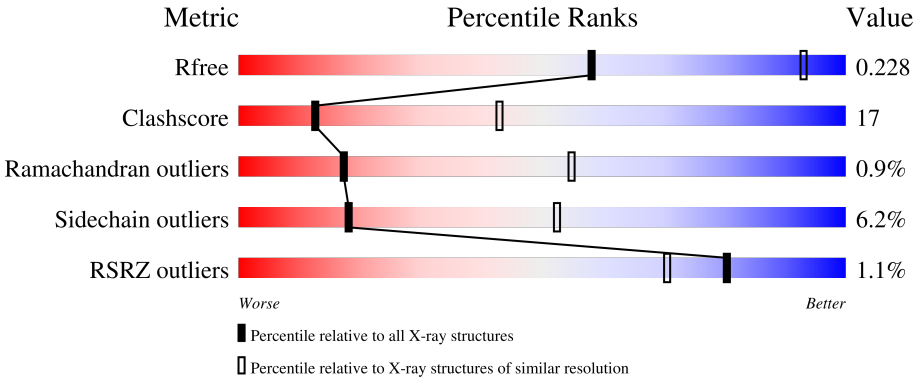
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.21 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	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

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	336	2% 73% 24%
2	H	258	% 67% 27%
3	L	273	% 72% 26%
4	M	323	72% 25%

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
11	UQ1	L	503	-	-	-	X
5	SO4	C	809	-	-	-	X
7	HTO	H	705	-	-	-	X

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 10311 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
			Total	C	N	O	S			
1	C	332	2598	1637	465	478	18	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	250	1958	1251	335	370	2	0	0	0

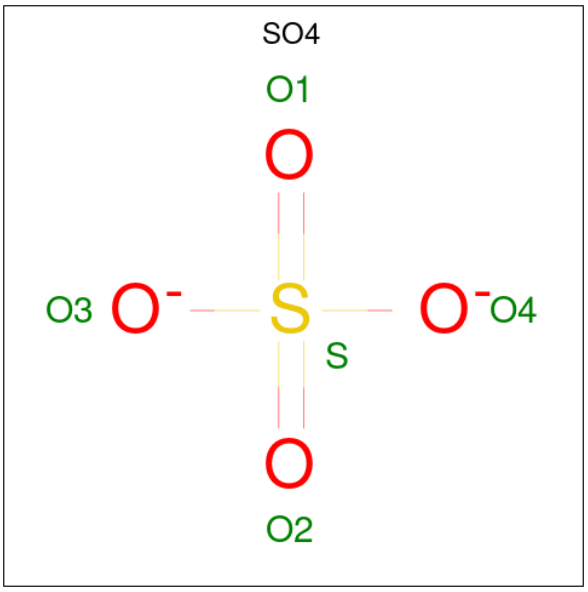
- Molecule 3 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	273	2171	1459	350	355	7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	M	323	2555	1702	419	423	11	0	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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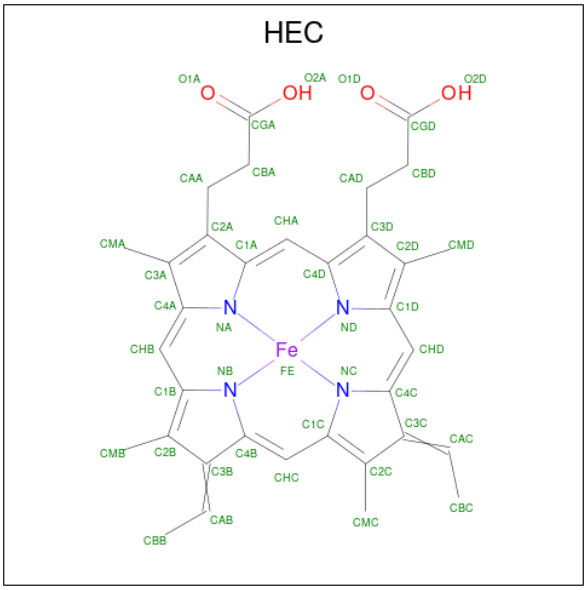
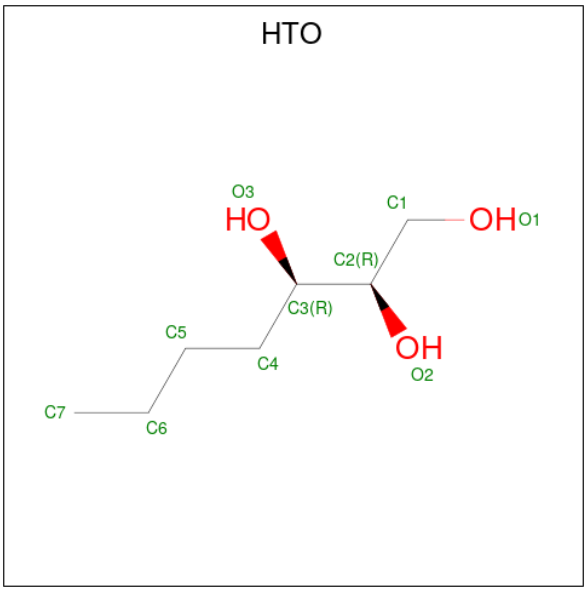
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	1	Total O S 5 4 1	0	0

- Molecule 6 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



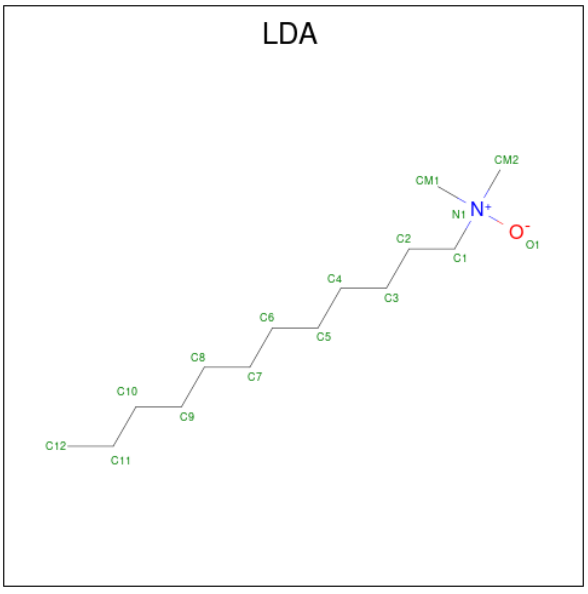
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C Fe N O 43 34 1 4 4	0	0
6	C	1	Total C Fe N O 43 34 1 4 4	0	0
6	C	1	Total C Fe N O 43 34 1 4 4	0	0
6	C	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 7 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



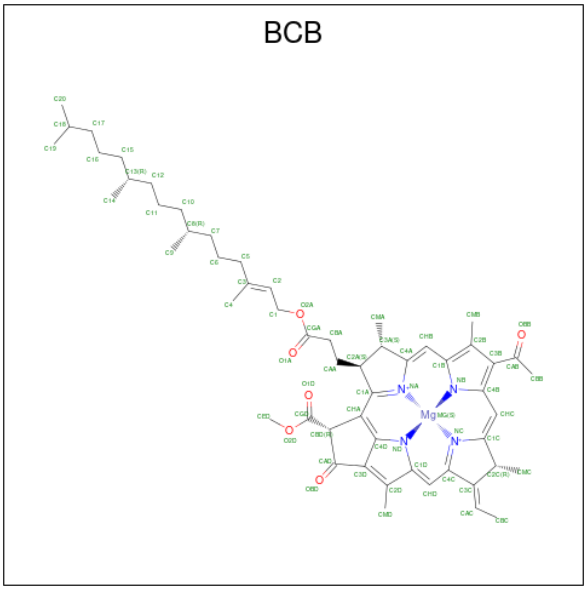
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 10 7 3	0	0
7	C	1	Total C O 10 7 3	0	0
7	H	1	Total C O 10 7 3	0	0

- Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



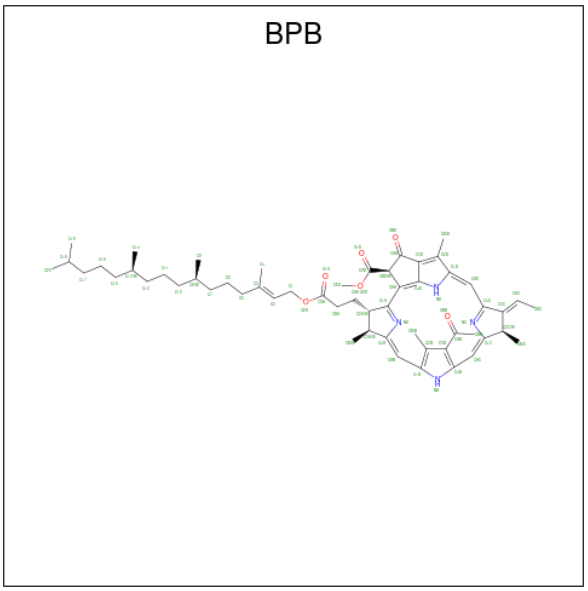
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	L	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		

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



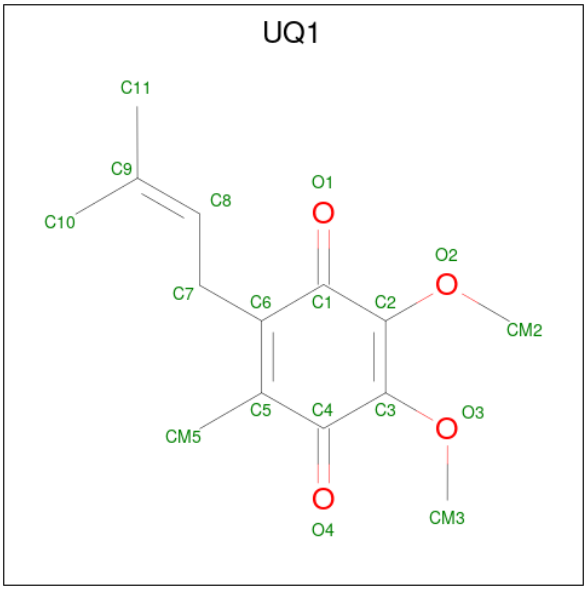
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



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

- Molecule 11 is UBIQUINONE-1 (three-letter code: UQ1) (formula: $C_{14}H_{18}O_4$).

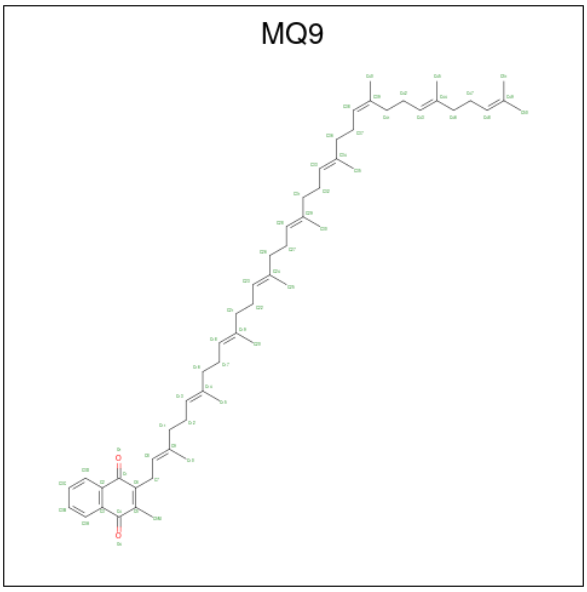


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	L	1	Total C O 18 14 4	0	0
11	L	1	Total C O 18 14 4	0	0

- Molecule 12 is FE (II) ION (three-letter code: FE2) (formula: Fe).

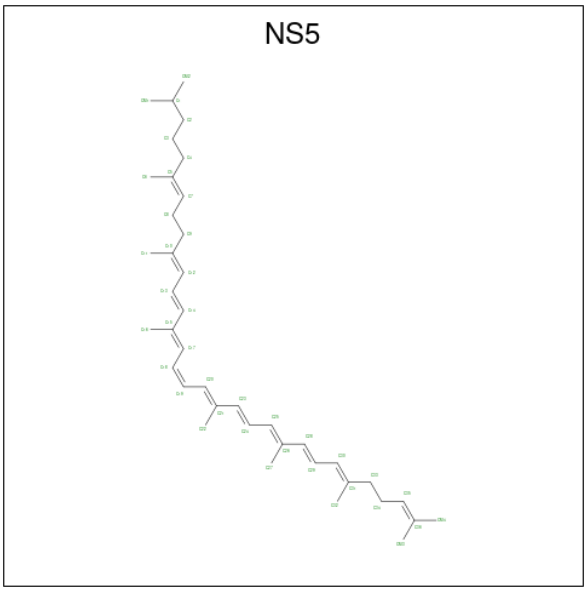
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	M	1	Total Fe 1 1	0	0

- Molecule 13 is MENAQUINONE-9 (three-letter code: MQ9) (formula: $C_{56}H_{80}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	M	1	Total C O 58 56 2	0	0

- Molecule 14 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: $C_{40}H_{60}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	M	1	Total C 40 40	0	0

- Molecule 15 is water.

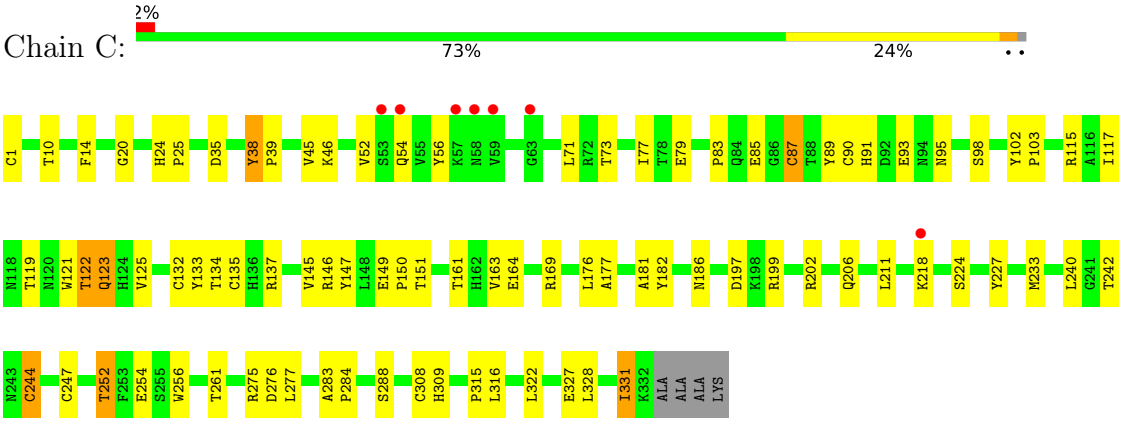
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	C	47	Total O 47 47	0	0
15	H	28	Total O 28 28	0	0
15	L	38	Total O 38 38	0	0
15	M	46	Total O 46 46	0	0

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 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.

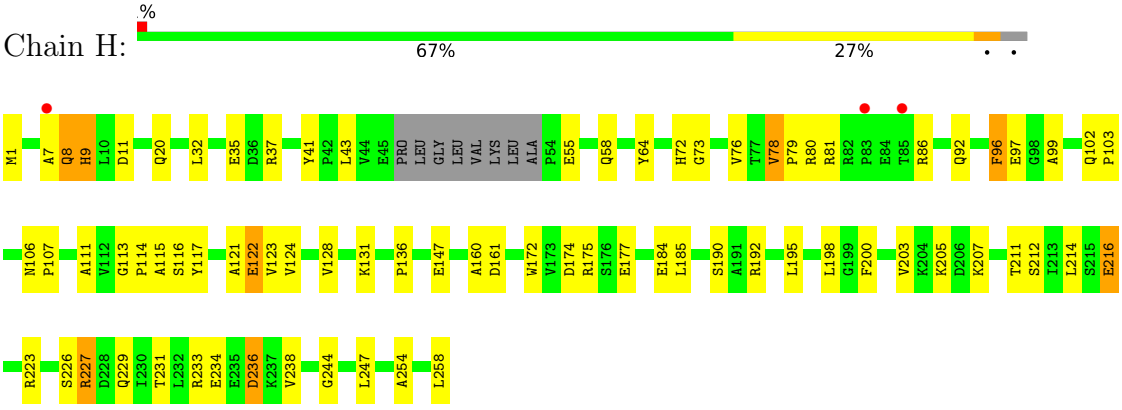
• Molecule 1: Photosynthetic reaction center cytochrome c subunit

Chain C:



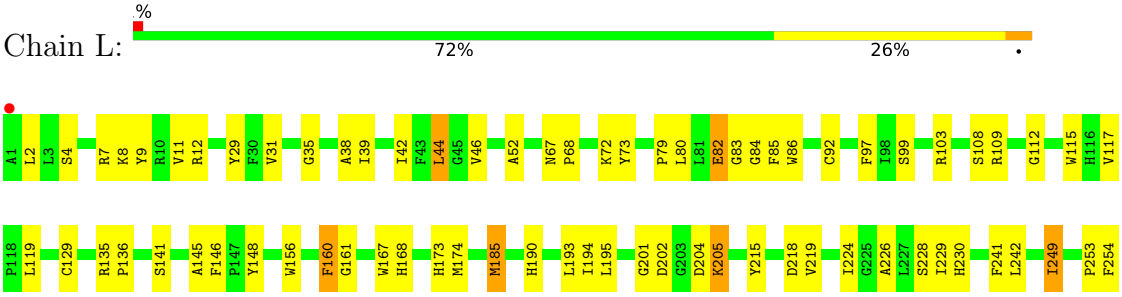
• Molecule 2: Reaction center protein H chain

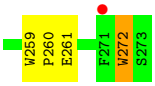
Chain H:



• Molecule 3: Reaction center protein L chain

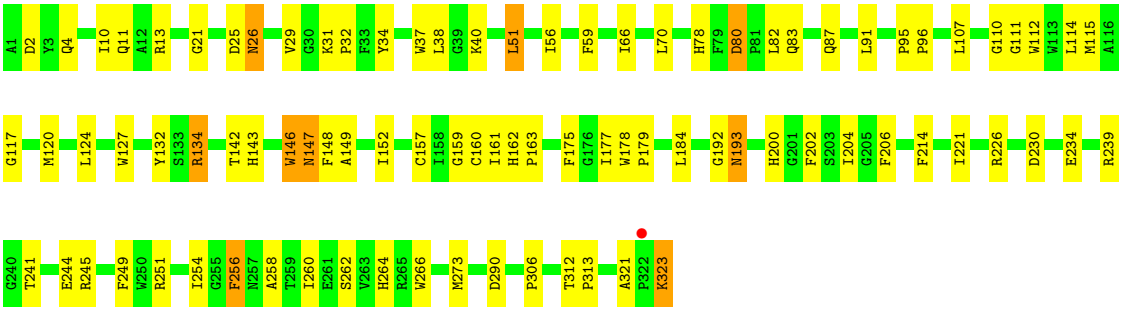
Chain L:





• Molecule 4: Reaction center protein M chain

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	241.17Å 241.17Å 113.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.21 47.92 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-3.21) 99.6 (47.92-3.21)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.4.0073	Depositor
R, R_{free}	0.192 , 0.224 0.196 , 0.228	Depositor DCC
R_{free} test set	3145 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	74.4	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 68.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10311	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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: SO4, HEC, MQ9, NS5, FE2, HTO, FME, BPB, LDA, BCB, UQ1

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	0.53	1/2665 (0.0%)	0.64	0/3633
2	H	0.59	0/1993	0.68	0/2720
3	L	0.60	1/2259 (0.0%)	0.66	0/3084
4	M	0.57	0/2659	0.65	1/3637 (0.0%)
All	All	0.57	2/9576 (0.0%)	0.66	1/13074 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	87	CYS	CB-SG	-5.84	1.72	1.81
3	L	129	CYS	CB-SG	-5.38	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	70	LEU	CA-CB-CG	7.57	132.71	115.30

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	2598	0	2573	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1958	0	1946	65	0
3	L	2171	0	2098	64	0
4	M	2555	0	2452	76	0
5	C	35	0	0	0	0
5	H	20	0	0	1	0
5	M	20	0	0	1	0
6	C	172	0	125	31	0
7	C	20	0	32	1	0
7	H	10	0	16	2	0
8	H	32	0	62	6	0
8	L	16	0	31	2	0
8	M	16	0	31	0	0
9	L	132	0	144	24	0
9	M	132	0	144	27	0
10	L	65	0	74	9	0
10	M	65	0	74	20	0
11	L	36	0	36	4	0
12	M	1	0	0	0	0
13	M	58	0	80	3	0
14	M	40	0	60	11	0
15	C	47	0	0	9	0
15	H	28	0	0	5	0
15	L	38	0	0	3	0
15	M	46	0	0	7	0
All	All	10311	0	9978	337	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 17.

All (337) 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:C:90:CYS:SG	6:C:401:HEC:HAC	1.31	1.69
1:C:132:CYS:SG	6:C:402:HEC:HAB	1.48	1.52
1:C:244:CYS:SG	6:C:403:HEC:HAB	1.54	1.47
1:C:132:CYS:SG	6:C:402:HEC:CAB	2.08	1.39
1:C:135:CYS:SG	6:C:402:HEC:CAC	2.12	1.37
1:C:90:CYS:SG	6:C:401:HEC:CAC	2.16	1.33
1:C:87:CYS:SG	6:C:401:HEC:HAB	1.77	1.24
1:C:135:CYS:SG	6:C:402:HEC:HAC	1.78	1.19
1:C:244:CYS:SG	6:C:403:HEC:CAB	2.37	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:CYS:SG	6:C:401:HEC:CAB	2.39	1.09
1:C:87:CYS:HG	6:C:401:HEC:HAB	1.05	1.00
3:L:193:LEU:HD23	11:L:502:UQ1:HM32	1.44	0.99
9:M:401:BCB:C2	10:M:402:BPB:HBBB	1.94	0.98
1:C:117:ILE:HD11	1:C:277:LEU:HD21	1.42	0.97
1:C:284:PRO:HA	15:C:857:HOH:O	1.65	0.96
3:L:205:LYS:H	3:L:205:LYS:HD3	1.28	0.96
1:C:132:CYS:HG	6:C:402:HEC:HAB	1.24	0.95
10:L:402:BPB:HMB	10:L:402:BPB:CBB	1.99	0.93
1:C:123:GLN:HG2	15:C:854:HOH:O	1.69	0.93
9:M:401:BCB:CBB	9:M:401:BCB:HMB1	1.99	0.93
9:L:401:BCB:CBB	9:L:401:BCB:HMB1	2.01	0.90
3:L:205:LYS:HD3	3:L:205:LYS:N	1.86	0.90
2:H:114:PRO:HG3	2:H:247:LEU:HD23	1.53	0.89
2:H:64:TYR:CE1	8:H:703:LDA:H31	2.07	0.88
9:L:400:BCB:CBB	9:L:400:BCB:HMB1	2.01	0.87
3:L:112:GLY:HA2	15:L:608:HOH:O	1.76	0.85
2:H:55:GLU:HB2	2:H:58:GLN:HE21	1.41	0.84
9:M:400:BCB:CBB	9:M:400:BCB:HHC	2.09	0.83
1:C:181:ALA:O	1:C:182:TYR:HB2	1.78	0.83
1:C:90:CYS:HG	6:C:401:HEC:HAC	1.39	0.83
6:C:401:HEC:HMB1	6:C:401:HEC:HBB3	1.62	0.82
2:H:92:GLN:HB2	15:H:901:HOH:O	1.81	0.81
4:M:260:ILE:HG22	15:M:816:HOH:O	1.81	0.81
4:M:159:GLY:HA3	14:M:600:NS5:H272	1.62	0.81
1:C:135:CYS:SG	6:C:402:HEC:C3C	2.68	0.81
3:L:83:GLY:HA2	15:L:638:HOH:O	1.82	0.80
4:M:258:ALA:HB1	4:M:262:SER:OG	1.84	0.76
2:H:227:ARG:HH11	2:H:227:ARG:CG	1.99	0.76
9:M:400:BCB:HHC	9:M:400:BCB:HBB2	1.69	0.74
9:L:400:BCB:O1A	9:L:401:BCB:HBC2	1.86	0.74
2:H:64:TYR:HE1	8:H:703:LDA:H31	1.50	0.73
10:L:402:BPB:HMB	10:L:402:BPB:HBBB	1.69	0.73
3:L:79:PRO:HG2	3:L:82:GLU:HG3	1.69	0.73
1:C:52:VAL:HB	1:C:56:TYR:HD2	1.53	0.73
9:M:401:BCB:HMB1	9:M:401:BCB:HBB3	1.70	0.73
2:H:76:VAL:HG13	2:H:80:ARG:HH12	1.55	0.72
9:L:400:BCB:HAA1	9:L:400:BCB:HBD	1.71	0.71
9:L:401:BCB:HMB1	9:L:401:BCB:HBB2	1.72	0.71
9:L:400:BCB:HMB1	9:L:400:BCB:HBB3	1.73	0.71
10:L:402:BPB:HMB	10:L:402:BPB:HBBA	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:401:BCB:HMB1	9:M:401:BCB:HBB2	1.71	0.71
6:C:403:HEC:HMC1	6:C:403:HEC:HBC3	1.72	0.71
1:C:322:LEU:HD12	15:C:834:HOH:O	1.89	0.70
10:M:402:BPB:CBB	10:M:402:BPB:HHC	2.22	0.70
2:H:203:VAL:HG11	4:M:10:ILE:HD11	1.74	0.70
9:M:400:BCB:CBB	14:M:600:NS5:H223	2.21	0.69
9:M:401:BCB:C1	10:M:402:BPB:CBB	2.71	0.69
2:H:227:ARG:HH11	2:H:227:ARG:HG3	1.56	0.69
4:M:26:ASN:OD1	15:M:840:HOH:O	2.10	0.69
1:C:133:TYR:CE1	1:C:137:ARG:HA	2.28	0.69
9:L:401:BCB:HMB1	9:L:401:BCB:HBB3	1.73	0.69
10:M:402:BPB:H7A	10:M:402:BPB:H4	1.75	0.69
2:H:123:VAL:HG11	7:H:705:HTO:H52	1.75	0.68
3:L:205:LYS:H	3:L:205:LYS:CD	2.04	0.68
9:L:400:BCB:HMB1	9:L:400:BCB:HBB2	1.74	0.68
9:M:401:BCB:H12	10:M:402:BPB:HBB	1.75	0.68
9:M:400:BCB:HBB2	14:M:600:NS5:H223	1.76	0.67
4:M:127:TRP:CD1	10:M:402:BPB:HBA	2.28	0.67
3:L:97:PHE:CE1	9:L:400:BCB:H121	2.30	0.66
4:M:107:LEU:HA	4:M:111:GLY:HA3	1.76	0.66
2:H:114:PRO:HG3	2:H:247:LEU:CD2	2.26	0.66
1:C:163:VAL:HG23	15:L:633:HOH:O	1.96	0.66
9:M:401:BCB:H12	10:M:402:BPB:CBB	2.26	0.65
1:C:77:ILE:CG2	6:C:401:HEC:HBC3	2.27	0.65
3:L:135:ARG:HB3	3:L:136:PRO:HD3	1.79	0.65
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.32	0.65
4:M:258:ALA:HB1	4:M:262:SER:HG	1.62	0.64
2:H:116:SER:HB3	3:L:8:LYS:HD2	1.80	0.64
2:H:227:ARG:HG3	2:H:227:ARG:NH1	2.11	0.64
3:L:224:ILE:HG12	3:L:228:SER:HB3	1.80	0.63
3:L:160:PHE:HD1	3:L:160:PHE:O	1.82	0.62
1:C:117:ILE:CD1	1:C:277:LEU:HD21	2.24	0.62
4:M:51:LEU:HD23	4:M:56:ILE:HD11	1.82	0.62
2:H:55:GLU:HB2	2:H:58:GLN:NE2	2.12	0.62
6:C:404:HEC:HBD2	6:C:404:HEC:HHA	1.82	0.62
9:M:401:BCB:C1	10:M:402:BPB:HBBB	2.29	0.61
4:M:147:ASN:C	4:M:147:ASN:HD22	2.04	0.61
2:H:114:PRO:CG	2:H:247:LEU:HD23	2.29	0.61
2:H:8:GLN:C	2:H:9:HIS:HD2	2.05	0.60
10:M:402:BPB:OBB	10:M:402:BPB:HMB	2.01	0.60
4:M:117:GLY:HA3	14:M:600:NS5:H28	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:123:VAL:HG12	2:H:124:VAL:N	2.17	0.59
1:C:132:CYS:SG	6:C:402:HEC:C3B	2.89	0.59
1:C:146:ARG:NH2	1:C:150:PRO:HA	2.18	0.59
1:C:242:THR:HA	15:C:843:HOH:O	2.02	0.59
2:H:64:TYR:CE1	8:H:703:LDA:H12	2.38	0.59
2:H:227:ARG:HB2	15:H:904:HOH:O	2.02	0.59
10:M:402:BPB:HBBB	10:M:402:BPB:HHC	1.83	0.58
1:C:161:THR:OG1	1:C:164:GLU:HG3	2.03	0.58
3:L:201:GLY:O	3:L:202:ASP:HB2	2.02	0.58
2:H:122:GLU:HA	2:H:122:GLU:OE1	2.04	0.58
8:H:703:LDA:HM12	15:H:574:HOH:O	2.04	0.58
1:C:117:ILE:HD11	1:C:277:LEU:CD2	2.26	0.57
9:L:400:BCB:HAA1	9:L:400:BCB:CBD	2.34	0.57
4:M:11:GLN:HB3	4:M:13:ARG:HH12	1.69	0.57
2:H:96:PHE:CE2	2:H:99:ALA:HB2	2.39	0.57
4:M:59:PHE:HA	10:M:402:BPB:H4A	1.86	0.57
1:C:283:ALA:N	1:C:284:PRO:CD	2.67	0.57
4:M:110:GLY:HA2	15:M:830:HOH:O	2.05	0.56
4:M:29:VAL:HG22	4:M:51:LEU:HD13	1.86	0.56
1:C:73:THR:O	1:C:77:ILE:HG13	2.05	0.56
1:C:91:HIS:HE1	6:C:401:HEC:ND	2.00	0.56
9:M:401:BCB:C2	10:M:402:BPB:CBB	2.76	0.56
3:L:167:TRP:HE1	3:L:173:HIS:CD2	2.23	0.56
4:M:132:TYR:CE1	4:M:142:THR:HG21	2.40	0.56
3:L:185:MET:HE3	10:M:402:BPB:NA	2.21	0.56
3:L:79:PRO:CG	3:L:82:GLU:HG3	2.36	0.56
4:M:114:LEU:HD11	14:M:600:NS5:H351	1.87	0.56
2:H:123:VAL:CG1	2:H:124:VAL:N	2.69	0.56
2:H:7:ALA:O	2:H:8:GLN:HG2	2.06	0.56
1:C:177:ALA:HA	15:C:822:HOH:O	2.06	0.55
4:M:120:MET:CE	4:M:175:PHE:HE1	2.20	0.55
4:M:226:ARG:HG3	15:M:825:HOH:O	2.06	0.55
1:C:95:ASN:CG	1:C:98:SER:HB2	2.28	0.54
4:M:117:GLY:CA	14:M:600:NS5:H28	2.36	0.54
3:L:8:LYS:HE2	3:L:9:TYR:CE2	2.42	0.54
4:M:59:PHE:HA	10:M:402:BPB:C4	2.38	0.54
9:L:400:BCB:H11	9:L:401:BCB:H2C	1.91	0.53
4:M:323:LYS:HD3	4:M:323:LYS:N	2.22	0.53
1:C:1:CYS:HA	15:C:861:HOH:O	2.07	0.53
3:L:80:LEU:HD23	3:L:85:PHE:CE1	2.43	0.53
1:C:197:ASP:HB3	1:C:275:ARG:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:162:HIS:HB3	4:M:163:PRO:HD3	1.91	0.53
1:C:115:ARG:HA	1:C:328:LEU:O	2.08	0.52
1:C:169:ARG:HE	4:M:78:HIS:CE1	2.27	0.52
2:H:37:ARG:HG2	2:H:41:TYR:CE1	2.45	0.52
4:M:2:ASP:OD1	4:M:4:GLN:HB2	2.09	0.52
4:M:206:PHE:CD2	4:M:273:MET:HB3	2.44	0.52
1:C:52:VAL:HB	1:C:56:TYR:CD2	2.41	0.52
9:M:401:BCB:C3	10:M:402:BPB:HBBB	2.37	0.52
2:H:136:PRO:HA	2:H:172:TRP:HA	1.91	0.52
2:H:128:VAL:HG22	2:H:128:VAL:O	2.10	0.52
3:L:195:LEU:HB3	4:M:143:HIS:CD2	2.45	0.52
1:C:182:TYR:CG	3:L:261:GLU:HA	2.45	0.52
1:C:224:SER:HA	1:C:227:TYR:HD1	1.73	0.52
2:H:117:TYR:HB2	2:H:236:ASP:HB3	1.91	0.52
1:C:182:TYR:CE1	3:L:261:GLU:HG3	2.45	0.52
9:L:400:BCB:H2C	9:M:401:BCB:H2C	1.92	0.52
2:H:121:ALA:C	2:H:123:VAL:H	2.14	0.51
4:M:95:PRO:HB2	4:M:96:PRO:HD2	1.92	0.51
9:M:400:BCB:HBB3	9:M:401:BCB:H41	1.91	0.51
1:C:206:GLN:HG2	7:C:706:HTO:H61	1.93	0.51
9:M:400:BCB:HBB1	14:M:600:NS5:H223	1.92	0.51
9:L:400:BCB:H152	10:L:402:BPB:H44	1.93	0.51
4:M:34:TYR:CD1	4:M:34:TYR:N	2.79	0.51
4:M:120:MET:HE3	4:M:175:PHE:HE1	1.75	0.51
3:L:86:TRP:CZ2	3:L:145:ALA:CB	2.93	0.51
3:L:160:PHE:HD1	3:L:160:PHE:C	2.15	0.51
2:H:161:ASP:HB3	2:H:214:LEU:HD22	1.93	0.51
2:H:72:HIS:HB2	7:H:705:HTO:H42	1.92	0.50
2:H:102:GLN:HB2	2:H:103:PRO:HD2	1.93	0.50
3:L:80:LEU:HA	3:L:84:GLY:HA3	1.94	0.50
4:M:110:GLY:CA	15:M:830:HOH:O	2.59	0.50
1:C:233:MET:HB3	6:C:403:HEC:C4B	2.41	0.50
4:M:192:GLY:O	4:M:193:ASN:HB3	2.12	0.50
3:L:39:ILE:HD12	13:M:501:MQ9:H43	1.93	0.50
1:C:102:TYR:N	1:C:103:PRO:CD	2.75	0.50
15:H:555:HOH:O	4:M:234:GLU:HB2	2.11	0.50
1:C:121:TRP:O	1:C:125:VAL:HG22	2.12	0.50
2:H:76:VAL:HG13	2:H:80:ARG:NH1	2.23	0.50
1:C:35:ASP:OD2	1:C:316:LEU:HA	2.13	0.49
3:L:160:PHE:C	3:L:160:PHE:CD1	2.84	0.49
3:L:109:ARG:HD3	3:L:115:TRP:CZ2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:CYS:CB	6:C:403:HEC:HAB	2.38	0.49
9:M:400:BCB:HHC	9:M:400:BCB:HBB3	1.90	0.49
4:M:200:HIS:CE1	4:M:204:ILE:HD11	2.47	0.49
1:C:252:THR:HA	15:C:817:HOH:O	2.12	0.49
2:H:8:GLN:O	2:H:9:HIS:HD2	1.96	0.49
2:H:231:THR:OG1	2:H:234:GLU:HG3	2.11	0.49
6:C:402:HEC:HBC3	6:C:402:HEC:HMC1	1.94	0.48
2:H:136:PRO:HD3	2:H:172:TRP:CZ3	2.48	0.48
3:L:52:ALA:HB2	3:L:85:PHE:CD2	2.47	0.48
3:L:167:TRP:NE1	3:L:173:HIS:CD2	2.81	0.48
9:L:401:BCB:OBB	9:L:401:BCB:HHC	2.13	0.48
6:C:401:HEC:HBB3	6:C:401:HEC:CMB	2.38	0.48
3:L:194:ILE:HG13	4:M:264:HIS:CD2	2.49	0.48
4:M:178:TRP:N	4:M:179:PRO:CD	2.76	0.48
3:L:259:TRP:O	3:L:260:PRO:C	2.52	0.48
9:M:400:BCB:HBA1	9:M:400:BCB:C4A	2.44	0.48
3:L:35:GLY:CA	3:L:103:ARG:HD2	2.44	0.48
4:M:83:GLN:HB3	4:M:87:GLN:HE21	1.78	0.48
4:M:256:PHE:CD1	4:M:256:PHE:N	2.82	0.48
2:H:8:GLN:C	2:H:9:HIS:CD2	2.87	0.48
1:C:87:CYS:C	1:C:89:TYR:H	2.16	0.47
1:C:87:CYS:SG	6:C:401:HEC:C3B	3.00	0.47
2:H:113:GLY:C	2:H:115:ALA:H	2.16	0.47
9:L:401:BCB:HBA1	9:L:401:BCB:C4A	2.44	0.47
4:M:204:ILE:HG12	9:M:401:BCB:CHB	2.44	0.47
9:M:400:BCB:OBB	9:M:400:BCB:HMB1	2.15	0.47
1:C:90:CYS:SG	6:C:401:HEC:C3C	2.97	0.47
2:H:96:PHE:H	2:H:96:PHE:HD2	1.62	0.47
11:L:502:UQ1:O4	11:L:502:UQ1:HM33	2.15	0.47
2:H:234:GLU:O	2:H:238:VAL:HG23	2.14	0.47
9:L:400:BCB:H203	9:L:400:BCB:H161	1.57	0.47
9:L:401:BCB:HMD2	9:M:401:BCB:HBB3	1.95	0.47
1:C:308:CYS:O	1:C:315:PRO:HB3	2.14	0.47
3:L:67:ASN:HB3	3:L:68:PRO:HD2	1.97	0.47
9:L:400:BCB:H112	9:L:401:BCB:HBB2	1.96	0.47
1:C:133:TYR:O	1:C:134:THR:C	2.53	0.47
2:H:131:LYS:HE3	2:H:175:ARG:HH12	1.79	0.47
2:H:190:SER:HB3	2:H:192:ARG:HG2	1.96	0.47
4:M:184:LEU:HD21	9:M:400:BCB:CAC	2.45	0.47
3:L:215:TYR:O	3:L:219:VAL:HG23	2.15	0.47
4:M:160:CYS:SG	14:M:600:NS5:H322	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:112:TRP:O	4:M:115:MET:HB2	2.15	0.47
1:C:276:ASP:O	1:C:277:LEU:C	2.52	0.47
1:C:119:THR:HG21	1:C:331:ILE:HG22	1.98	0.46
3:L:146:PHE:HB3	3:L:156:TRP:CD2	2.51	0.46
1:C:10:THR:O	1:C:20:GLY:HA3	2.15	0.46
1:C:87:CYS:C	1:C:89:TYR:N	2.69	0.46
1:C:123:GLN:CG	15:C:854:HOH:O	2.43	0.46
10:L:402:BPB:H6A	10:L:402:BPB:H2	1.60	0.46
1:C:115:ARG:NH1	1:C:327:GLU:O	2.47	0.46
3:L:35:GLY:HA2	3:L:103:ARG:HD2	1.98	0.46
3:L:242:LEU:HD23	3:L:242:LEU:HA	1.77	0.46
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.51	0.46
4:M:21:GLY:HA3	15:M:835:HOH:O	2.15	0.46
3:L:52:ALA:CB	3:L:85:PHE:CD2	2.99	0.46
3:L:249:ILE:HD13	3:L:249:ILE:HA	1.80	0.46
2:H:64:TYR:CD1	8:H:703:LDA:H31	2.50	0.45
3:L:230:HIS:CD2	4:M:221:ILE:HG13	2.51	0.45
2:H:20:GLN:HG2	4:M:202:PHE:CE2	2.51	0.45
8:L:702:LDA:H21	8:L:702:LDA:HM11	1.50	0.45
10:M:402:BPB:HMC	10:M:402:BPB:H55	1.98	0.45
1:C:79:GLU:HA	1:C:83:PRO:HB3	1.98	0.45
2:H:216:GLU:H	2:H:216:GLU:HG3	1.54	0.45
4:M:124:LEU:HD21	9:M:401:BCB:H112	1.98	0.45
4:M:239:ARG:HD3	4:M:244:GLU:HG2	1.99	0.45
3:L:190:HIS:HD1	11:L:502:UQ1:HM33	1.82	0.45
3:L:241:PHE:CE2	10:L:402:BPB:H43	2.52	0.45
3:L:253:PRO:HB2	3:L:254:PHE:CD2	2.51	0.45
2:H:254:ALA:HB2	15:H:562:HOH:O	2.17	0.45
3:L:168:HIS:CE1	9:L:400:BCB:HHC	2.52	0.44
2:H:172:TRP:HE1	2:H:184:GLU:HB2	1.82	0.44
3:L:272:TRP:HB3	4:M:82:LEU:HD21	1.97	0.44
4:M:157:CYS:HA	4:M:161:ILE:HB	1.98	0.44
4:M:323:LYS:CD	4:M:323:LYS:H	2.29	0.44
1:C:150:PRO:HG3	1:C:176:LEU:HD13	1.99	0.44
2:H:113:GLY:CA	3:L:11:VAL:HG11	2.47	0.44
2:H:172:TRP:CE2	2:H:195:LEU:HD21	2.52	0.44
2:H:41:TYR:CE2	2:H:43:LEU:HD21	2.53	0.44
4:M:160:CYS:C	4:M:163:PRO:HD2	2.38	0.44
2:H:174:ASP:O	2:H:177:GLU:O	2.35	0.44
3:L:42:ILE:O	3:L:46:VAL:HG23	2.18	0.44
10:L:402:BPB:OBB	10:L:402:BPB:HHC	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:198:LEU:HD23	2:H:198:LEU:HA	1.82	0.44
1:C:38:TYR:HD1	1:C:39:PRO:HD2	1.82	0.44
1:C:202:ARG:HH12	1:C:256:TRP:HE1	1.64	0.44
3:L:38:ALA:HB2	3:L:99:SER:HB3	2.00	0.43
1:C:240:LEU:HD22	1:C:309:HIS:CG	2.53	0.43
2:H:200:PHE:CZ	4:M:226:ARG:HD3	2.53	0.43
9:M:401:BCB:HHC	9:M:401:BCB:OBB	2.17	0.43
3:L:168:HIS:HE1	9:L:400:BCB:OBB	2.01	0.43
4:M:143:HIS:ND1	4:M:143:HIS:N	2.66	0.43
9:M:401:BCB:CBB	9:M:401:BCB:CMB	2.80	0.43
3:L:174:MET:HE3	9:M:400:BCB:HED3	2.01	0.43
9:L:400:BCB:H62	9:L:400:BCB:H41	1.41	0.43
4:M:254:ILE:HD12	4:M:256:PHE:CE1	2.54	0.43
3:L:29:TYR:CG	13:M:501:MQ9:H33	2.53	0.43
3:L:218:ASP:HB3	4:M:134:ARG:HD2	2.01	0.43
3:L:226:ALA:O	3:L:229:ILE:HG22	2.18	0.43
2:H:160:ALA:HB3	2:H:214:LEU:HD23	2.00	0.43
2:H:8:GLN:O	2:H:8:GLN:CG	2.66	0.42
3:L:44:LEU:HB3	3:L:92:CYS:SG	2.59	0.42
3:L:168:HIS:HD2	15:M:809:HOH:O	2.01	0.42
4:M:323:LYS:N	4:M:323:LYS:CD	2.82	0.42
10:L:402:BPB:HMC	10:L:402:BPB:H55	2.02	0.42
4:M:323:LYS:H	4:M:323:LYS:CE	2.32	0.42
3:L:72:LYS:HE3	3:L:73:TYR:CE2	2.54	0.42
6:C:403:HEC:HBC3	6:C:403:HEC:CMC	2.45	0.42
4:M:80:ASP:OD1	4:M:80:ASP:C	2.58	0.42
4:M:241:THR:O	4:M:245:ARG:HG3	2.19	0.42
3:L:52:ALA:HB2	3:L:85:PHE:CG	2.54	0.42
9:L:401:BCB:HBC3	9:L:401:BCB:HMC1	2.00	0.42
4:M:127:TRP:NE1	10:M:402:BPB:HBA	2.34	0.42
4:M:251:ARG:HA	4:M:256:PHE:O	2.19	0.42
1:C:93:GLU:H	1:C:93:GLU:HG2	1.66	0.42
3:L:185:MET:HE1	10:M:402:BPB:HMAB	2.02	0.42
3:L:86:TRP:CZ2	3:L:145:ALA:HB3	2.55	0.42
4:M:178:TRP:HA	4:M:178:TRP:CE3	2.55	0.42
10:M:402:BPB:CBB	10:M:402:BPB:CHC	2.94	0.42
2:H:8:GLN:O	2:H:9:HIS:CD2	2.72	0.42
2:H:115:ALA:HB2	2:H:244:GLY:HA3	2.02	0.42
8:L:702:LDA:H22	8:L:702:LDA:H52	1.80	0.42
1:C:24:HIS:O	1:C:25:PRO:C	2.58	0.42
1:C:247:CYS:HA	1:C:261:THR:OG1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:502:UQ1:HM51	11:L:502:UQ1:H71	1.72	0.42
4:M:146:TRP:O	4:M:149:ALA:HB3	2.20	0.42
14:M:600:NS5:H41	14:M:600:NS5:H81	1.86	0.42
1:C:102:TYR:N	1:C:103:PRO:HD2	2.35	0.41
1:C:147:TYR:C	1:C:149:GLU:H	2.22	0.41
6:C:404:HEC:HBD2	6:C:404:HEC:CHA	2.49	0.41
2:H:102:GLN:HB2	2:H:102:GLN:HE21	1.69	0.41
10:M:402:BPB:HMC	10:M:402:BPB:CBC	2.50	0.41
4:M:37:TRP:HD1	5:M:805:SO4:O1	2.02	0.41
13:M:501:MQ9:C8	13:M:501:MQ9:H5M3	2.50	0.41
1:C:132:CYS:CB	6:C:402:HEC:HAB	2.40	0.41
1:C:206:GLN:HE22	1:C:254:GLU:HB2	1.85	0.41
1:C:14:PHE:CD2	4:M:306:PRO:HD2	2.55	0.41
1:C:145:VAL:O	1:C:146:ARG:HD2	2.19	0.41
1:C:85:GLU:HG3	1:C:85:GLU:O	2.20	0.41
2:H:233:ARG:HD3	5:H:807:SO4:O4	2.20	0.41
4:M:38:LEU:HA	4:M:38:LEU:HD12	1.79	0.41
4:M:66:ILE:HG23	14:M:600:NS5:H82	2.01	0.41
1:C:132:CYS:CB	6:C:402:HEC:CAB	2.97	0.41
3:L:195:LEU:CB	4:M:143:HIS:CD2	3.04	0.41
1:C:71:LEU:HD23	1:C:71:LEU:HA	1.97	0.41
1:C:122:THR:HG22	15:C:847:HOH:O	2.21	0.41
2:H:32:LEU:HD13	4:M:266:TRP:CD2	2.55	0.41
2:H:64:TYR:OH	8:H:703:LDA:HM11	2.21	0.41
2:H:86:ARG:NH2	2:H:111:ALA:HB3	2.36	0.41
4:M:95:PRO:CB	4:M:96:PRO:HD2	2.50	0.41
2:H:106:ASN:HA	2:H:107:PRO:HD2	1.87	0.41
2:H:113:GLY:HA2	3:L:11:VAL:HG13	2.03	0.41
2:H:226:SER:HB2	2:H:229:GLN:HG2	2.03	0.41
3:L:148:TYR:CE1	10:L:402:BPB:H14B	2.56	0.41
1:C:133:TYR:CD1	1:C:137:ARG:HA	2.55	0.41
4:M:87:GLN:O	4:M:91:LEU:HG	2.20	0.41
4:M:148:PHE:CZ	4:M:152:ILE:HD11	2.56	0.41
4:M:312:THR:HA	4:M:313:PRO:HD3	1.88	0.41
3:L:161:GLY:HA3	9:L:400:BCB:HAC1	2.03	0.40
9:L:400:BCB:H141	9:L:400:BCB:H162	1.92	0.40
1:C:77:ILE:HG22	6:C:401:HEC:HBC3	2.00	0.40
3:L:117:VAL:HG11	4:M:249:PHE:CE2	2.57	0.40
4:M:239:ARG:HD3	4:M:244:GLU:CG	2.51	0.40
4:M:160:CYS:SG	14:M:600:NS5:H29	2.60	0.40
2:H:78:VAL:HA	2:H:79:PRO:C	2.41	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	330/336 (98%)	294 (89%)	35 (11%)	1 (0%)	41 74
2	H	246/258 (95%)	220 (89%)	22 (9%)	4 (2%)	9 42
3	L	271/273 (99%)	246 (91%)	24 (9%)	1 (0%)	34 69
4	M	321/323 (99%)	290 (90%)	26 (8%)	5 (2%)	9 42
All	All	1168/1190 (98%)	1050 (90%)	107 (9%)	11 (1%)	17 55

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	147	GLU
2	H	73	GLY
4	M	32	PRO
4	M	51	LEU
4	M	193	ASN
1	C	186	ASN
4	M	321	ALA
2	H	35	GLU
2	H	122	GLU
4	M	177	ILE
3	L	31	VAL

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	280/282 (99%)	266 (95%)	14 (5%)	24	59
2	H	205/212 (97%)	188 (92%)	17 (8%)	11	40
3	L	218/218 (100%)	203 (93%)	15 (7%)	15	48
4	M	249/249 (100%)	236 (95%)	13 (5%)	23	58
All	All	952/961 (99%)	893 (94%)	59 (6%)	18	52

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	38	TYR
1	C	45	VAL
1	C	46	LYS
1	C	54	GLN
1	C	122	THR
1	C	123	GLN
1	C	151	THR
1	C	199	ARG
1	C	211	LEU
1	C	218	LYS
1	C	244	CYS
1	C	252	THR
1	C	288	SER
1	C	331	ILE
2	H	8	GLN
2	H	9	HIS
2	H	11	ASP
2	H	78	VAL
2	H	81	ARG
2	H	96	PHE
2	H	97	GLU
2	H	185	LEU
2	H	205	LYS
2	H	207	LYS
2	H	211	THR
2	H	212	SER
2	H	216	GLU
2	H	223	ARG
2	H	227	ARG
2	H	236	ASP
2	H	258	LEU
3	L	2	LEU
3	L	4	SER

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Mol	Chain	Res	Type
3	L	7	ARG
3	L	12	ARG
3	L	44	LEU
3	L	82	GLU
3	L	108	SER
3	L	119	LEU
3	L	141	SER
3	L	160	PHE
3	L	185	MET
3	L	204	ASP
3	L	205	LYS
3	L	249	ILE
3	L	272	TRP
4	M	25	ASP
4	M	26	ASN
4	M	31	LYS
4	M	40	LYS
4	M	80	ASP
4	M	134	ARG
4	M	146	TRP
4	M	147	ASN
4	M	214	PHE
4	M	230	ASP
4	M	256	PHE
4	M	290	ASP
4	M	323	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	37	GLN
1	C	54	GLN
1	C	123	GLN
1	C	206	GLN
1	C	302	GLN
2	H	9	HIS
2	H	58	GLN
2	H	102	GLN
2	H	106	ASN
2	H	225	GLN
3	L	55	GLN
3	L	168	HIS

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Mol	Chain	Res	Type
3	L	183	ASN
3	L	239	ASN
4	M	4	GLN
4	M	9	GLN
4	M	78	HIS
4	M	147	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	H	1	2	8,9,10	0.83	0	7,9,11	3.72	2 (28%)

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	H	1	2	-	4/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1	FME	CA-N-CN	-9.15	108.76	122.82
2	H	1	FME	CE-SD-CG	2.39	108.62	100.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

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 37 ligands modelled in this entry, 1 is monoatomic - leaving 36 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	$\#\|Z\| > 2$
7	HTO	C	706	-	9,9,9	0.27	0	10,10,10	0.75	0
5	SO4	H	807	-	4,4,4	0.13	0	6,6,6	0.33	0
9	BCB	M	401	4	54,74,74	2.12	8 (14%)	52,115,115	2.02	15 (28%)
9	BCB	L	401	3	54,74,74	1.93	6 (11%)	52,115,115	2.11	11 (21%)
11	UQ1	L	502	-	18,18,18	2.19	2 (11%)	22,25,25	1.37	4 (18%)
9	BCB	L	400	3	54,74,74	2.02	7 (12%)	52,115,115	1.95	14 (26%)
7	HTO	C	707	-	9,9,9	0.66	0	10,10,10	0.55	0
5	SO4	M	804	-	4,4,4	0.16	0	6,6,6	0.29	0
7	HTO	H	705	-	9,9,9	0.69	0	10,10,10	0.83	0
5	SO4	C	809	-	4,4,4	0.14	0	6,6,6	0.10	0
13	MQ9	M	501	-	59,59,59	1.80	18 (30%)	72,75,75	1.56	20 (27%)
6	HEC	C	403	1	32,50,50	1.76	3 (9%)	24,82,82	1.28	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	BPB	L	402	-	49,70,70	1.84	6 (12%)	47,101,101	1.96	15 (31%)
8	LDA	L	702	-	12,15,15	2.10	1 (8%)	14,17,17	0.63	0
8	LDA	M	704	-	12,15,15	2.16	1 (8%)	14,17,17	0.44	0
9	BCB	M	400	4	54,74,74	1.78	6 (11%)	52,115,115	2.02	13 (25%)
5	SO4	H	806	-	4,4,4	0.17	0	6,6,6	0.26	0
5	SO4	H	812	-	4,4,4	0.16	0	6,6,6	0.19	0
6	HEC	C	401	1	32,50,50	1.95	3 (9%)	24,82,82	1.26	1 (4%)
5	SO4	C	814	-	4,4,4	0.12	0	6,6,6	0.36	0
6	HEC	C	402	1	32,50,50	1.79	2 (6%)	24,82,82	1.47	3 (12%)
5	SO4	C	815	-	4,4,4	0.15	0	6,6,6	0.23	0
5	SO4	C	811	-	4,4,4	0.17	0	6,6,6	0.23	0
8	LDA	H	701	-	12,15,15	2.03	1 (8%)	14,17,17	0.47	0
5	SO4	H	803	-	4,4,4	0.17	0	6,6,6	0.24	0
14	NS5	M	600	-	39,39,39	1.57	3 (7%)	44,46,46	1.93	13 (29%)
5	SO4	M	801	-	4,4,4	0.21	0	6,6,6	0.63	0
5	SO4	C	810	-	4,4,4	0.15	0	6,6,6	0.09	0
11	UQ1	L	503	-	18,18,18	2.23	2 (11%)	22,25,25	1.23	2 (9%)
10	BPB	M	402	-	49,70,70	1.77	7 (14%)	47,101,101	1.98	10 (21%)
6	HEC	C	404	1	32,50,50	1.73	2 (6%)	24,82,82	1.46	3 (12%)
5	SO4	M	802	-	4,4,4	0.18	0	6,6,6	0.19	0
5	SO4	C	808	-	4,4,4	0.11	0	6,6,6	0.19	0
5	SO4	M	805	-	4,4,4	0.18	0	6,6,6	0.42	0
5	SO4	C	813	-	4,4,4	0.09	0	6,6,6	0.27	0
8	LDA	H	703	-	12,15,15	1.92	1 (8%)	14,17,17	0.53	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
7	HTO	C	706	-	-	5/10/10/10	-
9	BCB	M	401	4	-	17/37/177/177	-
9	BCB	L	401	3	-	9/37/177/177	-
11	UQ1	L	502	-	-	4/9/33/33	0/1/1/1
9	BCB	L	400	3	-	16/37/177/177	-
7	HTO	C	707	-	-	8/10/10/10	-
7	HTO	H	705	-	-	8/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	MQ9	M	501	-	-	16/53/73/73	0/2/2/2
6	HEC	C	403	1	-	4/10/54/54	-
10	BPB	L	402	-	-	15/37/105/105	0/5/6/6
8	LDA	L	702	-	-	11/13/13/13	-
9	BCB	M	400	4	-	13/37/177/177	-
8	LDA	M	704	-	-	9/13/13/13	-
6	HEC	C	402	1	-	4/10/54/54	-
6	HEC	C	401	1	-	2/10/54/54	-
8	LDA	H	701	-	-	8/13/13/13	-
14	NS5	M	600	-	-	14/43/43/43	-
11	UQ1	L	503	-	-	0/9/33/33	0/1/1/1
10	BPB	M	402	-	-	14/37/105/105	0/5/6/6
6	HEC	C	404	1	-	4/10/54/54	-
8	LDA	H	703	-	-	6/13/13/13	-

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	502	UQ1	C6-C5	8.12	1.50	1.35
11	L	503	UQ1	C6-C5	8.07	1.50	1.35
9	M	401	BCB	CAC-C3C	7.87	1.53	1.33
10	L	402	BPB	CAC-C3C	7.79	1.53	1.33
9	L	400	BCB	CAC-C3C	7.77	1.53	1.33
10	M	402	BPB	CAC-C3C	7.76	1.53	1.33
9	M	401	BCB	C3A-C2A	-7.64	1.47	1.54
9	L	401	BCB	C4C-NC	7.63	1.42	1.35
14	M	600	NS5	C35-C36	7.45	1.53	1.32
8	M	704	LDA	O1-N1	-7.40	1.24	1.42
8	L	702	LDA	O1-N1	-7.20	1.25	1.42
9	L	401	BCB	CAC-C3C	7.14	1.51	1.33
9	M	400	BCB	CAC-C3C	7.12	1.51	1.33
9	L	400	BCB	C4C-NC	7.04	1.41	1.35
8	H	701	LDA	O1-N1	-6.92	1.26	1.42
6	C	401	HEC	C2B-C3B	-6.90	1.33	1.40
6	C	402	HEC	C2B-C3B	-6.72	1.33	1.40
9	L	400	BCB	C3A-C2A	-6.66	1.48	1.54
8	H	703	LDA	O1-N1	-6.59	1.26	1.42
9	M	401	BCB	C4C-NC	6.55	1.41	1.35
6	C	401	HEC	C3C-C2C	-6.12	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	403	HEC	C3C-C2C	-5.75	1.34	1.40
6	C	404	HEC	C3C-C2C	-5.74	1.34	1.40
6	C	404	HEC	C2B-C3B	-5.60	1.34	1.40
6	C	403	HEC	C2B-C3B	-5.43	1.35	1.40
9	M	400	BCB	C3A-C2A	-5.40	1.49	1.54
10	L	402	BPB	C3A-C2A	-5.11	1.50	1.54
10	L	402	BPB	O2D-CGD	4.87	1.45	1.33
6	C	402	HEC	C3C-C2C	-4.69	1.35	1.40
10	M	402	BPB	O2A-CGA	4.60	1.46	1.33
9	M	401	BCB	O2D-CGD	4.54	1.44	1.33
9	M	400	BCB	O2A-CGA	4.53	1.46	1.33
9	L	401	BCB	O2D-CGD	4.53	1.44	1.33
13	M	501	MQ9	C3-C4	-4.52	1.39	1.48
9	L	401	BCB	C3A-C2A	-4.44	1.50	1.54
13	M	501	MQ9	C7-C8	-4.41	1.44	1.50
9	M	401	BCB	O2A-CGA	4.40	1.46	1.33
9	L	400	BCB	O2A-CGA	4.13	1.45	1.33
10	L	402	BPB	O2A-CGA	4.11	1.45	1.33
9	M	400	BCB	O2D-CGD	4.08	1.43	1.33
9	L	401	BCB	O2A-CGA	4.06	1.45	1.33
10	M	402	BPB	C3D-C2D	-4.02	1.32	1.39
10	M	402	BPB	O2D-CGD	3.96	1.42	1.33
9	L	400	BCB	O2D-CGD	3.84	1.42	1.33
9	M	400	BCB	C4C-NC	3.82	1.38	1.35
13	M	501	MQ9	C2-C1	-3.69	1.41	1.48
11	L	503	UQ1	C3-C2	3.62	1.51	1.36
13	M	501	MQ9	C5-C4	-3.53	1.40	1.48
11	L	502	UQ1	C3-C2	3.43	1.50	1.36
10	M	402	BPB	C3A-C2A	-3.41	1.51	1.54
13	M	501	MQ9	C6-C1	-3.36	1.38	1.47
13	M	501	MQ9	C43-C44	3.35	1.41	1.33
10	L	402	BPB	C3D-C2D	-3.17	1.33	1.39
14	M	600	NS5	C4-C5	2.96	1.57	1.51
13	M	501	MQ9	C18-C19	2.95	1.40	1.33
13	M	501	MQ9	C38-C39	2.82	1.39	1.33
13	M	501	MQ9	C13-C14	2.81	1.39	1.33
10	L	402	BPB	C2-C3	2.76	1.39	1.33
13	M	501	MQ9	C28-C29	2.68	1.39	1.33
13	M	501	MQ9	C48-C49	2.68	1.40	1.32
13	M	501	MQ9	C23-C24	2.65	1.39	1.33
6	C	403	HEC	C4B-C3B	2.62	1.47	1.43
14	M	600	NS5	C7-C5	2.48	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	501	MQ9	C8-C9	2.47	1.38	1.33
10	M	402	BPB	C2-C3	2.44	1.38	1.33
9	L	400	BCB	C2-C3	2.33	1.38	1.33
13	M	501	MQ9	C32-C33	-2.32	1.42	1.50
9	M	401	BCB	CHD-C4C	2.27	1.41	1.37
13	M	501	MQ9	C27-C28	-2.26	1.43	1.50
9	L	401	BCB	C1-C2	-2.23	1.42	1.49
13	M	501	MQ9	C6-C5	2.21	1.39	1.35
9	M	401	BCB	C1-C2	-2.17	1.42	1.49
6	C	401	HEC	C4B-C3B	2.17	1.47	1.43
9	M	400	BCB	C2-C3	2.15	1.38	1.33
13	M	501	MQ9	C22-C23	-2.15	1.43	1.50
9	L	400	BCB	C3B-C2B	-2.13	1.35	1.39
9	M	401	BCB	C3B-C2B	-2.12	1.35	1.39
13	M	501	MQ9	C17-C18	-2.09	1.43	1.50
10	M	402	BPB	C3B-C2B	-2.08	1.35	1.39

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	402	BPB	O2D-CGD-CBD	8.19	121.37	111.00
9	L	401	BCB	O2D-CGD-CBD	7.99	121.11	111.00
9	M	400	BCB	O2D-CGD-CBD	7.71	120.76	111.00
9	M	401	BCB	O2D-CGD-CBD	7.14	120.05	111.00
10	L	402	BPB	O2D-CGD-CBD	6.88	119.71	111.00
9	L	400	BCB	O2D-CGD-CBD	6.15	118.78	111.00
9	L	400	BCB	C4D-C3D-CAD	-6.02	107.54	116.53
9	M	400	BCB	C4D-C3D-CAD	-5.77	107.91	116.53
9	M	401	BCB	C4D-C3D-CAD	-5.58	108.20	116.53
9	L	401	BCB	C4D-C3D-CAD	-5.44	108.41	116.53
14	M	600	NS5	C19-C20-C21	-5.30	119.75	127.31
10	M	402	BPB	CMD-C2D-C3D	4.92	133.89	124.68
10	L	402	BPB	CMD-C2D-C3D	4.47	133.04	124.68
14	M	600	NS5	C34-C35-C36	-4.11	113.69	127.75
14	M	600	NS5	CM4-C36-C35	-4.04	110.97	122.65
14	M	600	NS5	CM3-C36-C35	-3.99	111.13	122.65
9	L	401	BCB	C1-C2-C3	-3.80	119.46	126.04
9	L	400	BCB	CMC-C2C-C1C	-3.65	108.23	114.36
9	M	401	BCB	CMC-C2C-C1C	-3.61	108.30	114.36
9	L	401	BCB	C4-C3-C5	3.59	121.31	115.27
9	L	401	BCB	O1D-CGD-CBD	-3.59	118.76	124.74
10	L	402	BPB	O1D-CGD-CBD	-3.59	118.76	124.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	M	501	MQ9	C32-C33-C34	-3.53	119.15	127.66
13	M	501	MQ9	C35-C34-C36	3.47	121.11	115.27
10	M	402	BPB	O1D-CGD-CBD	-3.45	118.98	124.74
9	M	401	BCB	C1-C2-C3	-3.41	120.14	126.04
9	M	400	BCB	C4-C3-C5	3.37	120.94	115.27
14	M	600	NS5	C6-C5-C4	3.32	120.86	115.27
9	L	401	BCB	CBC-CAC-C3C	-3.22	118.17	126.70
9	L	401	BCB	CHA-C1A-C2A	-3.21	125.76	133.31
13	M	501	MQ9	C5M-C5-C6	-3.19	119.20	124.40
11	L	502	UQ1	C7-C8-C9	-3.16	117.36	127.26
9	M	400	BCB	CBC-CAC-C3C	-3.14	118.37	126.70
9	M	400	BCB	O2A-CGA-CBA	3.04	121.45	111.91
10	L	402	BPB	O2A-CGA-CBA	3.03	121.41	111.91
14	M	600	NS5	C18-C17-C15	-3.02	123.00	127.31
9	M	401	BCB	CBC-CAC-C3C	-2.96	118.84	126.70
9	M	401	BCB	C4-C3-C5	2.95	120.23	115.27
6	C	404	HEC	CBA-CAA-C2A	-2.93	107.67	112.60
10	M	402	BPB	CMA-C3A-C4A	-2.88	108.07	114.38
9	M	400	BCB	C1-C2-C3	-2.87	121.08	126.04
9	M	400	BCB	O2D-CGD-O1D	-2.86	118.25	123.84
11	L	502	UQ1	CM5-C5-C6	-2.85	119.75	124.40
9	L	400	BCB	O2A-CGA-CBA	2.82	120.76	111.91
14	M	600	NS5	C32-C31-C33	2.81	120.00	115.27
9	L	401	BCB	O2A-CGA-CBA	2.81	120.73	111.91
9	M	401	BCB	CMA-C3A-C4A	-2.80	108.24	114.38
10	M	402	BPB	O2A-CGA-CBA	2.80	120.69	111.91
6	C	402	HEC	CBA-CAA-C2A	-2.78	107.91	112.60
9	M	400	BCB	CMA-C3A-C4A	-2.77	108.31	114.38
13	M	501	MQ9	C12-C13-C14	-2.74	121.06	127.66
9	L	400	BCB	CBC-CAC-C3C	-2.73	119.45	126.70
11	L	503	UQ1	CM5-C5-C6	-2.72	119.95	124.40
14	M	600	NS5	C11-C10-C9	2.71	119.84	115.27
9	L	400	BCB	CAA-CBA-CGA	-2.70	105.35	113.25
9	M	401	BCB	O2A-CGA-CBA	2.66	120.25	111.91
13	M	501	MQ9	C20-C19-C21	2.65	119.73	115.27
10	L	402	BPB	C6-C7-C8	-2.64	107.38	115.92
14	M	600	NS5	C12-C13-C14	-2.63	115.00	123.22
6	C	403	HEC	CBA-CAA-C2A	-2.62	108.19	112.60
13	M	501	MQ9	C15-C14-C16	2.59	119.62	115.27
13	M	501	MQ9	C17-C18-C19	-2.59	121.43	127.66
6	C	404	HEC	CAD-CBD-CGD	-2.58	106.53	113.76
13	M	501	MQ9	C7-C8-C9	-2.57	122.51	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	L	503	UQ1	C11-C9-C10	2.56	120.26	114.60
13	M	501	MQ9	C10-C9-C11	2.56	119.57	115.27
9	M	401	BCB	O2D-CGD-O1D	-2.54	118.86	123.84
10	M	402	BPB	CBC-CAC-C3C	-2.54	119.95	126.70
9	L	400	BCB	C6-C7-C8	-2.54	107.71	115.92
13	M	501	MQ9	C27-C28-C29	-2.53	121.57	127.66
9	L	400	BCB	C4-C3-C5	2.51	119.48	115.27
10	L	402	BPB	CBC-CAC-C3C	-2.50	120.07	126.70
6	C	402	HEC	CMC-C2C-C1C	-2.49	124.63	128.46
9	M	400	BCB	C4C-CHD-C1D	2.48	125.37	118.67
9	L	400	BCB	CMA-C3A-C4A	-2.47	108.97	114.38
9	M	400	BCB	CHA-C1A-C2A	-2.47	127.50	133.31
6	C	404	HEC	CMC-C2C-C1C	-2.46	124.68	128.46
9	M	401	BCB	C6-C5-C3	-2.44	107.07	113.45
13	M	501	MQ9	C22-C23-C24	-2.42	121.83	127.66
10	M	402	BPB	CMC-C2C-C1C	-2.42	110.30	114.36
9	L	400	BCB	C6-C5-C3	-2.41	107.14	113.45
13	M	501	MQ9	C37-C38-C39	-2.41	121.86	127.66
9	M	401	BCB	CGD-CBD-CAD	-2.39	103.00	110.73
14	M	600	NS5	C6-C5-C7	-2.36	117.61	123.68
14	M	600	NS5	C24-C25-C26	-2.36	123.94	127.31
9	L	400	BCB	O2D-CGD-O1D	-2.36	119.23	123.84
13	M	501	MQ9	C5M-C5-C4	2.35	120.17	116.27
9	M	401	BCB	C6-C7-C8	-2.35	108.33	115.92
9	L	400	BCB	CGD-CBD-CAD	-2.35	103.13	110.73
10	L	402	BPB	C4-C3-C5	2.35	119.22	115.27
10	L	402	BPB	CED-O2D-CGD	2.34	121.24	115.94
6	C	402	HEC	CMB-C2B-C1B	-2.32	124.89	128.46
13	M	501	MQ9	C30-C29-C31	2.31	119.17	115.27
10	M	402	BPB	CAA-CBA-CGA	-2.29	106.57	113.25
14	M	600	NS5	C30-C29-C28	-2.29	116.08	123.22
13	M	501	MQ9	C40-C39-C41	2.27	119.10	115.27
10	L	402	BPB	CMC-C2C-C1C	-2.27	110.54	114.36
9	M	400	BCB	O1D-CGD-CBD	-2.27	120.95	124.74
11	L	502	UQ1	C7-C6-C1	2.23	121.16	118.48
6	C	401	HEC	CMC-C2C-C1C	-2.22	125.05	128.46
9	M	401	BCB	C11-C10-C8	-2.21	108.77	115.92
9	L	401	BCB	O2A-CGA-O1A	-2.21	118.01	123.59
10	L	402	BPB	CAA-CBA-CGA	-2.20	106.81	113.25
13	M	501	MQ9	C51-C49-C50	2.20	119.46	114.60
9	M	401	BCB	O1D-CGD-CBD	-2.20	121.08	124.74
13	M	501	MQ9	C25-C24-C26	2.19	118.95	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	L	502	UQ1	C11-C9-C10	2.18	119.42	114.60
9	L	400	BCB	CHA-C1A-C2A	-2.17	128.22	133.31
9	L	400	BCB	C1-C2-C3	-2.17	122.30	126.04
6	C	403	HEC	CMC-C2C-C1C	-2.16	125.14	128.46
10	L	402	BPB	C1-C2-C3	-2.16	122.31	126.04
9	M	400	BCB	CGD-CBD-CAD	-2.16	103.75	110.73
10	L	402	BPB	C11-C10-C8	-2.16	108.95	115.92
10	M	402	BPB	O2D-CGD-O1D	-2.14	119.64	123.84
10	L	402	BPB	CMA-C3A-C4A	-2.14	109.69	114.38
9	L	401	BCB	CMA-C3A-C4A	-2.13	109.72	114.38
9	M	401	BCB	C11-C12-C13	-2.12	109.06	115.92
10	M	402	BPB	C4-C3-C5	2.12	118.84	115.27
9	M	400	BCB	C6-C7-C8	-2.11	109.10	115.92
10	L	402	BPB	C16-C15-C13	-2.09	109.16	115.92
10	L	402	BPB	C11-C12-C13	-2.07	109.24	115.92
9	L	401	BCB	C16-C15-C13	-2.06	109.27	115.92
13	M	501	MQ9	C47-C48-C49	-2.04	120.77	127.75
13	M	501	MQ9	C42-C43-C44	-2.04	122.74	127.66
13	M	501	MQ9	C35-C34-C33	-2.03	118.47	123.68
14	M	600	NS5	C22-C21-C20	-2.01	120.11	122.92

There are no chirality outliers.

All (187) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	404	HEC	C2D-C3D-CAD-CBD
6	C	404	HEC	C4D-C3D-CAD-CBD
7	C	706	HTO	C1-C2-C3-O3
7	C	706	HTO	O2-C2-C3-O3
7	C	706	HTO	O2-C2-C3-C4
7	C	707	HTO	C1-C2-C3-O3
7	C	707	HTO	C1-C2-C3-C4
7	C	707	HTO	O2-C2-C3-O3
7	C	707	HTO	O2-C2-C3-C4
7	C	707	HTO	O3-C3-C4-C5
7	H	705	HTO	C1-C2-C3-O3
7	H	705	HTO	O2-C2-C3-C4
8	H	703	LDA	N1-C1-C2-C3
8	L	702	LDA	C2-C1-N1-O1
8	L	702	LDA	C2-C1-N1-CM1
8	L	702	LDA	N1-C1-C2-C3
8	M	704	LDA	C2-C1-N1-O1

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Mol	Chain	Res	Type	Atoms
8	M	704	LDA	C2-C1-N1-CM1
8	M	704	LDA	C2-C1-N1-CM2
9	M	400	BCB	C2C-C3C-CAC-CBC
9	M	401	BCB	C2A-CAA-CBA-CGA
9	M	401	BCB	C2C-C3C-CAC-CBC
9	M	401	BCB	CAD-CBD-CGD-O1D
9	M	401	BCB	CAD-CBD-CGD-O2D
10	L	402	BPB	O2A-C1-C2-C3
13	M	501	MQ9	C17-C18-C19-C20
13	M	501	MQ9	C17-C18-C19-C21
13	M	501	MQ9	C37-C38-C39-C40
13	M	501	MQ9	C37-C38-C39-C41
13	M	501	MQ9	C42-C43-C44-C45
13	M	501	MQ9	C47-C48-C49-C51
14	M	600	NS5	C25-C26-C28-C29
14	M	600	NS5	C27-C26-C28-C29
14	M	600	NS5	C28-C29-C30-C31
14	M	600	NS5	C34-C35-C36-CM3
14	M	600	NS5	C34-C35-C36-CM4
13	M	501	MQ9	C47-C48-C49-C50
9	M	400	BCB	C3-C5-C6-C7
10	L	402	BPB	C3-C5-C6-C7
14	M	600	NS5	C2-C3-C4-C5
13	M	501	MQ9	C32-C33-C34-C35
13	M	501	MQ9	C32-C33-C34-C36
9	L	400	BCB	C4-C3-C5-C6
9	L	400	BCB	C2-C3-C5-C6
13	M	501	MQ9	C14-C16-C17-C18
14	M	600	NS5	C31-C33-C34-C35
14	M	600	NS5	C13-C14-C15-C16
10	M	402	BPB	C8-C10-C11-C12
10	L	402	BPB	C8-C10-C11-C12
7	H	705	HTO	O1-C1-C2-O2
9	M	401	BCB	C13-C15-C16-C17
9	M	400	BCB	C13-C15-C16-C17
10	L	402	BPB	C11-C12-C13-C15
9	L	400	BCB	C15-C16-C17-C18
13	M	501	MQ9	C29-C31-C32-C33
13	M	501	MQ9	C34-C36-C37-C38
13	M	501	MQ9	C39-C41-C42-C43
9	L	400	BCB	C8-C10-C11-C12
7	H	705	HTO	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
8	L	702	LDA	C5-C6-C7-C8
10	L	402	BPB	C16-C17-C18-C19
8	H	703	LDA	C2-C3-C4-C5
8	L	702	LDA	C11-C10-C9-C8
9	M	400	BCB	C6-C7-C8-C9
8	M	704	LDA	C5-C6-C7-C8
10	L	402	BPB	C16-C17-C18-C20
8	L	702	LDA	C6-C7-C8-C9
8	H	703	LDA	C6-C7-C8-C9
8	L	702	LDA	C3-C4-C5-C6
10	L	402	BPB	C3A-C2A-CAA-CBA
8	M	704	LDA	C1-C2-C3-C4
9	M	401	BCB	C3-C5-C6-C7
8	H	703	LDA	C1-C2-C3-C4
8	L	702	LDA	C4-C5-C6-C7
8	H	701	LDA	C6-C7-C8-C9
8	H	703	LDA	C11-C10-C9-C8
9	L	401	BCB	C12-C13-C15-C16
9	M	400	BCB	C6-C7-C8-C10
11	L	502	UQ1	C2-C3-O3-CM3
9	L	401	BCB	C15-C16-C17-C18
9	L	400	BCB	C3-C5-C6-C7
10	M	402	BPB	C3-C5-C6-C7
9	L	401	BCB	C14-C13-C15-C16
9	M	400	BCB	C11-C10-C8-C9
9	M	401	BCB	C6-C7-C8-C9
10	L	402	BPB	C11-C12-C13-C14
8	M	704	LDA	C7-C8-C9-C10
10	M	402	BPB	C16-C17-C18-C19
9	M	400	BCB	C8-C10-C11-C12
9	M	401	BCB	C5-C6-C7-C8
10	M	402	BPB	C10-C11-C12-C13
9	M	401	BCB	C8-C10-C11-C12
8	H	701	LDA	C7-C8-C9-C10
7	C	706	HTO	O3-C3-C4-C5
7	H	705	HTO	O3-C3-C4-C5
10	M	402	BPB	C16-C17-C18-C20
11	L	502	UQ1	C5-C6-C7-C8
7	H	705	HTO	C4-C5-C6-C7
8	H	703	LDA	C9-C10-C11-C12
7	H	705	HTO	O2-C2-C3-O3
9	L	400	BCB	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
9	L	401	BCB	C11-C10-C8-C7
9	M	400	BCB	C11-C10-C8-C7
9	M	401	BCB	C6-C7-C8-C10
9	M	401	BCB	C11-C12-C13-C15
10	L	402	BPB	C6-C7-C8-C10
10	M	402	BPB	C6-C7-C8-C10
9	M	400	BCB	C14-C13-C15-C16
9	M	401	BCB	C11-C12-C13-C14
10	L	402	BPB	C6-C7-C8-C9
10	M	402	BPB	C6-C7-C8-C9
8	H	701	LDA	C9-C10-C11-C12
8	M	704	LDA	N1-C1-C2-C3
14	M	600	NS5	C7-C8-C9-C10
9	L	400	BCB	C3A-C2A-CAA-CBA
8	M	704	LDA	C3-C4-C5-C6
8	M	704	LDA	C9-C10-C11-C12
10	L	402	BPB	C1A-C2A-CAA-CBA
9	M	400	BCB	C12-C13-C15-C16
14	M	600	NS5	CM2-C1-C2-C3
8	L	702	LDA	C2-C3-C4-C5
8	H	701	LDA	C2-C1-N1-CM1
8	H	701	LDA	C2-C1-N1-CM2
8	L	702	LDA	C2-C1-N1-CM2
7	C	706	HTO	C2-C3-C4-C5
7	C	707	HTO	C2-C3-C4-C5
7	H	705	HTO	C2-C3-C4-C5
9	L	400	BCB	C16-C17-C18-C20
13	M	501	MQ9	C45-C44-C46-C47
8	H	701	LDA	C4-C5-C6-C7
9	M	400	BCB	C16-C17-C18-C19
8	H	701	LDA	C2-C1-N1-O1
10	M	402	BPB	CAD-CBD-CGD-O1D
9	L	400	BCB	C6-C7-C8-C10
9	L	401	BCB	C11-C12-C13-C15
10	M	402	BPB	C11-C12-C13-C15
9	L	400	BCB	C11-C12-C13-C14
9	L	401	BCB	C11-C10-C8-C9
8	H	701	LDA	C5-C6-C7-C8
14	M	600	NS5	C11-C10-C9-C8
9	L	401	BCB	CHA-CBD-CGD-O1D
9	L	401	BCB	CHA-CBD-CGD-O2D
9	L	400	BCB	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
9	L	401	BCB	C11-C12-C13-C14
10	M	402	BPB	C11-C12-C13-C14
9	M	400	BCB	C16-C17-C18-C20
11	L	502	UQ1	C1-C2-O2-CM2
6	C	402	HEC	CAA-CBA-CGA-O2A
6	C	402	HEC	CAA-CBA-CGA-O1A
8	L	702	LDA	C7-C8-C9-C10
10	L	402	BPB	C4-C3-C5-C6
10	L	402	BPB	C2-C3-C5-C6
9	M	401	BCB	C16-C17-C18-C20
10	M	402	BPB	C12-C13-C15-C16
9	L	400	BCB	C1A-C2A-CAA-CBA
9	M	401	BCB	C16-C17-C18-C19
6	C	402	HEC	CAD-CBD-CGD-O2D
14	M	600	NS5	C13-C14-C15-C17
14	M	600	NS5	C12-C10-C9-C8
6	C	403	HEC	CAA-CBA-CGA-O2A
10	M	402	BPB	C4-C3-C5-C6
13	M	501	MQ9	C38-C39-C41-C42
6	C	404	HEC	CAD-CBD-CGD-O2D
6	C	401	HEC	CAA-CBA-CGA-O2A
9	M	401	BCB	C11-C10-C8-C9
11	L	502	UQ1	C1-C6-C7-C8
10	M	402	BPB	C3A-C2A-CAA-CBA
9	M	400	BCB	CAD-CBD-CGD-O2D
10	L	402	BPB	CAD-CBD-CGD-O2D
6	C	401	HEC	CAA-CBA-CGA-O1A
6	C	402	HEC	CAD-CBD-CGD-O1D
9	M	401	BCB	O2A-C1-C2-C3
6	C	403	HEC	CAA-CBA-CGA-O1A
6	C	404	HEC	CAD-CBD-CGD-O1D
9	M	401	BCB	C11-C10-C8-C7
10	M	402	BPB	C14-C13-C15-C16
14	M	600	NS5	C23-C24-C25-C26
7	C	707	HTO	C4-C5-C6-C7
9	L	400	BCB	C16-C17-C18-C19
7	C	707	HTO	C3-C4-C5-C6
6	C	403	HEC	CAD-CBD-CGD-O2D
9	L	400	BCB	CAD-CBD-CGD-O1D
9	L	400	BCB	C11-C10-C8-C7
6	C	403	HEC	CAD-CBD-CGD-O1D
9	L	400	BCB	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
10	L	402	BPB	C13-C15-C16-C17
13	M	501	MQ9	C44-C46-C47-C48

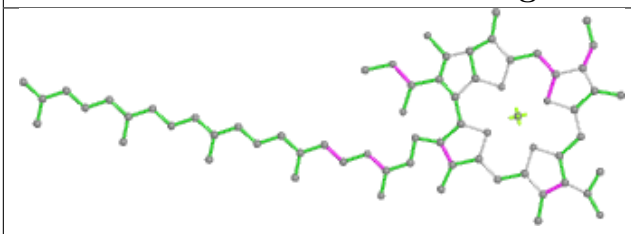
There are no ring outliers.

19 monomers are involved in 129 short contacts:

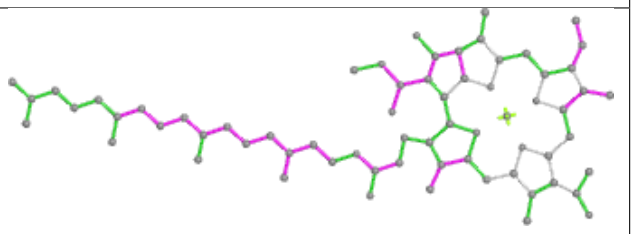
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	706	HTO	1	0
5	H	807	SO4	1	0
9	M	401	BCB	17	0
9	L	401	BCB	10	0
11	L	502	UQ1	4	0
9	L	400	BCB	17	0
7	H	705	HTO	2	0
13	M	501	MQ9	3	0
6	C	403	HEC	6	0
10	L	402	BPB	9	0
8	L	702	LDA	2	0
9	M	400	BCB	11	0
6	C	401	HEC	13	0
6	C	402	HEC	10	0
14	M	600	NS5	11	0
10	M	402	BPB	20	0
6	C	404	HEC	2	0
5	M	805	SO4	1	0
8	H	703	LDA	6	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.

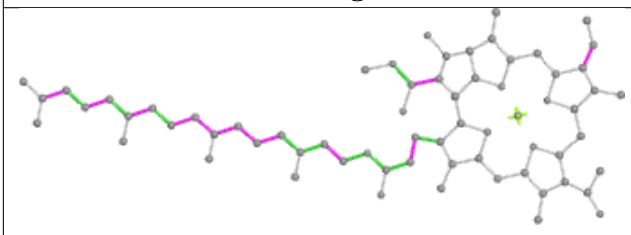
Ligand BCB M 401



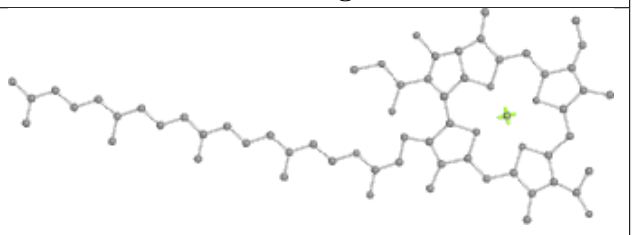
Bond lengths



Bond angles

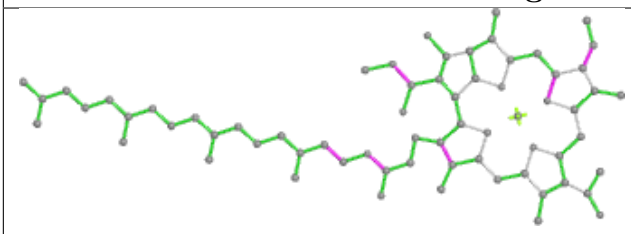


Torsions

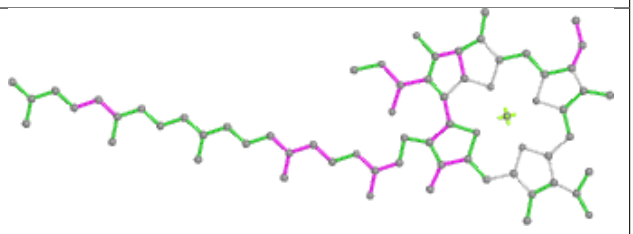


Rings

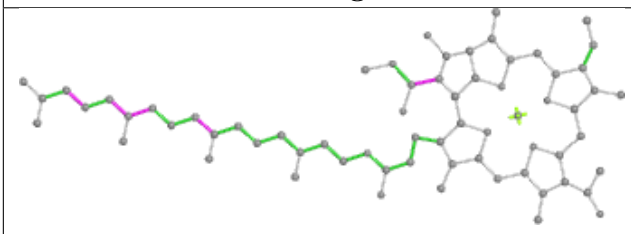
Ligand BCB L 401



Bond lengths



Bond angles



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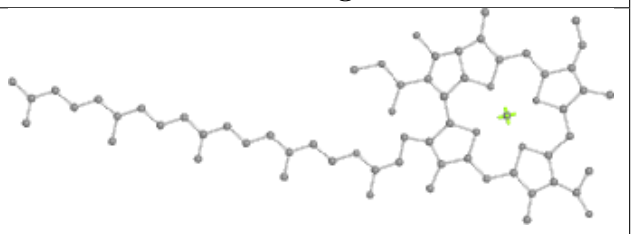
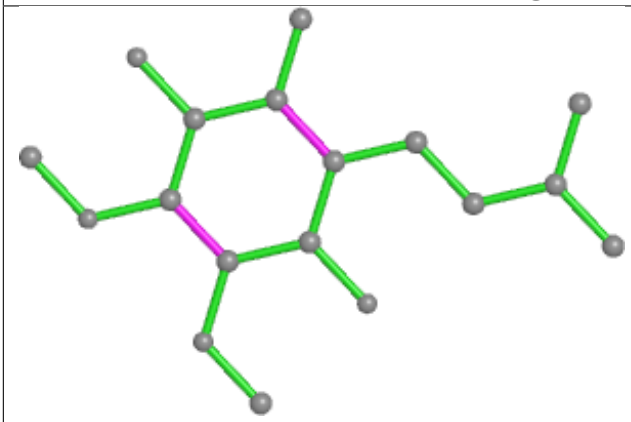


Rings

Ligand UQ1 L 502



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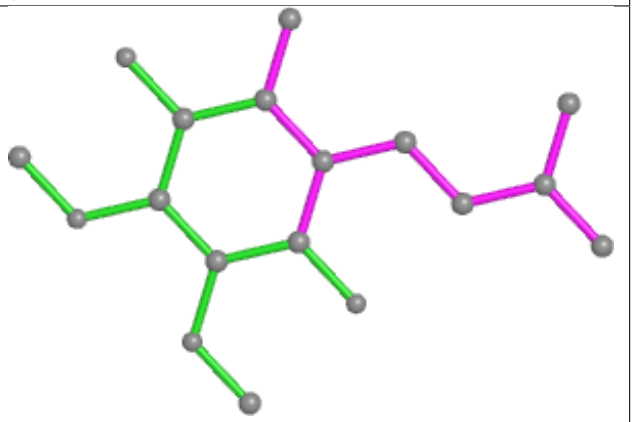
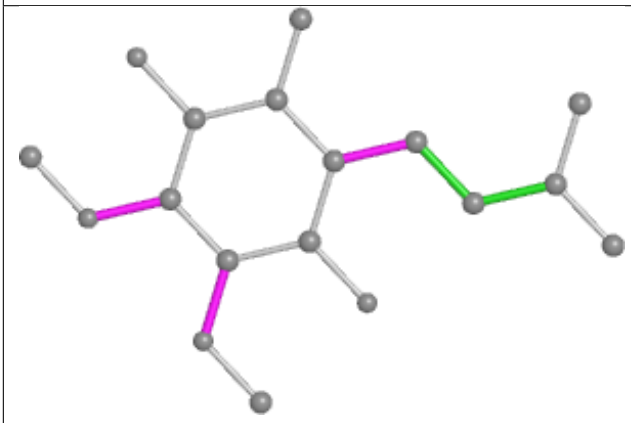


Bond angles



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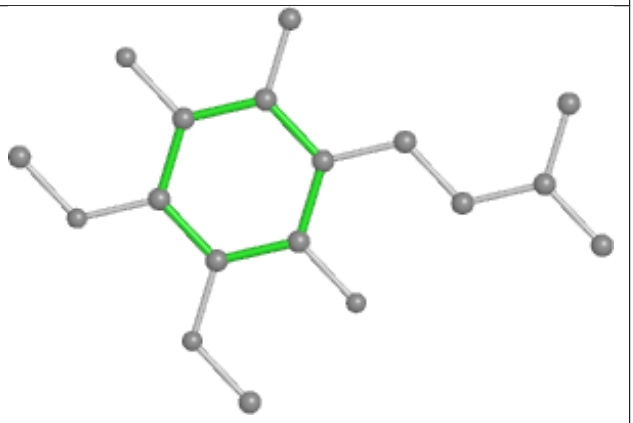
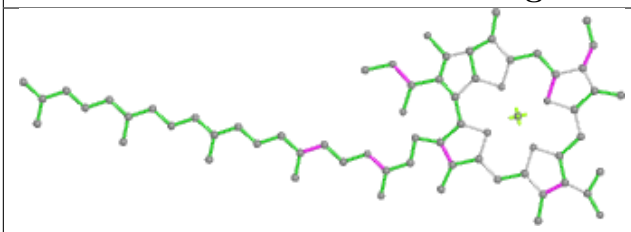


Rings

Ligand BCB L 400



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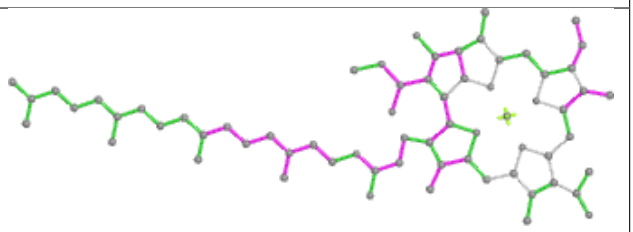
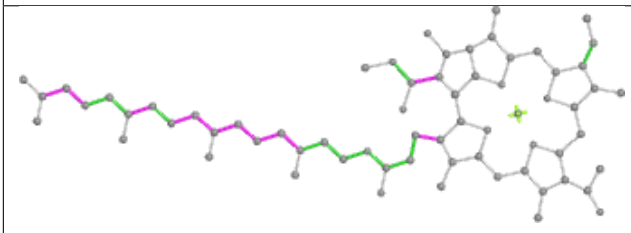
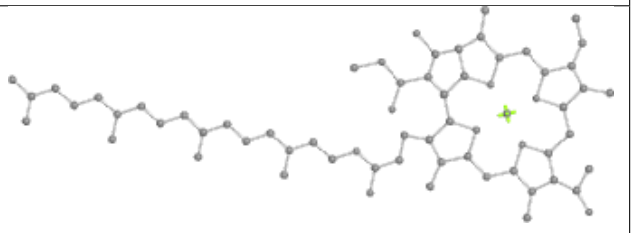


Bond angles

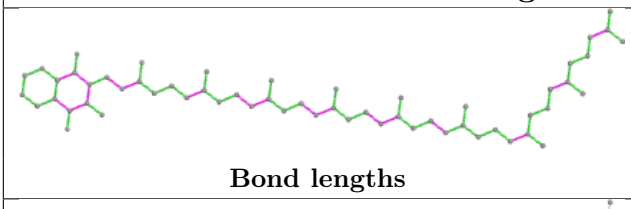


Torsions

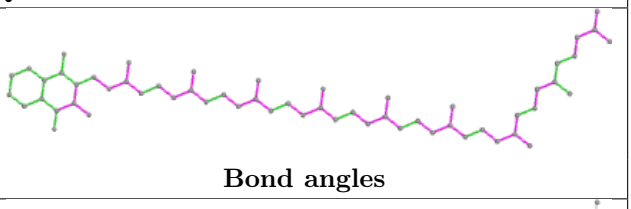


Rings

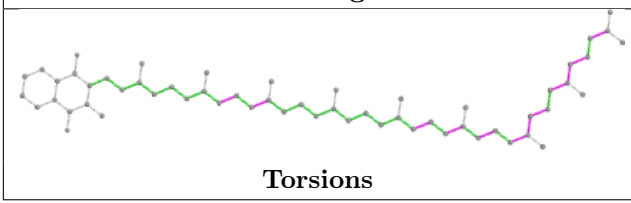
Ligand MQ9 M 501



Bond lengths



Bond angles



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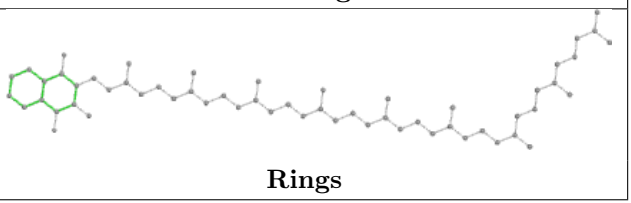
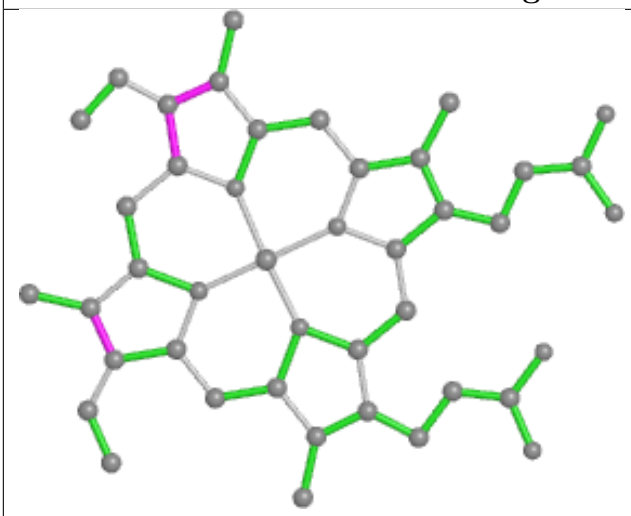


Rings

Ligand HEC C 403



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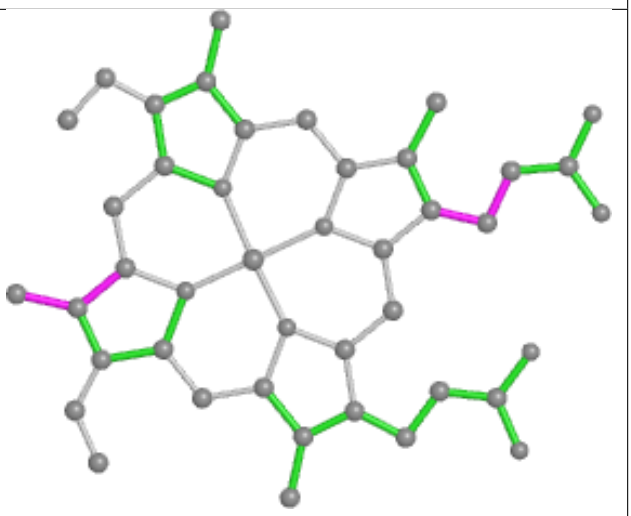

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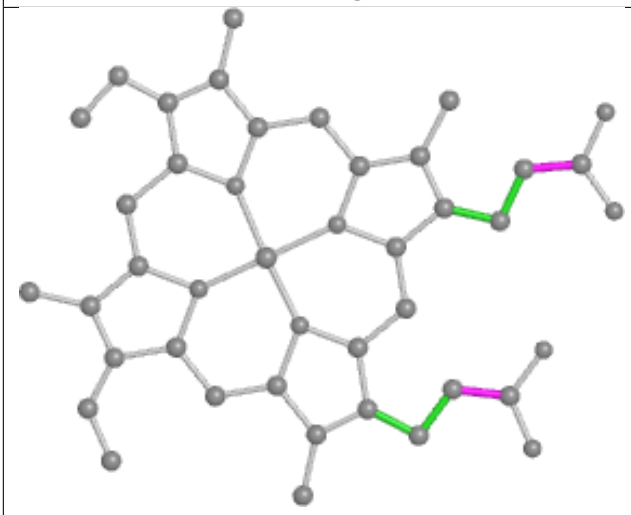

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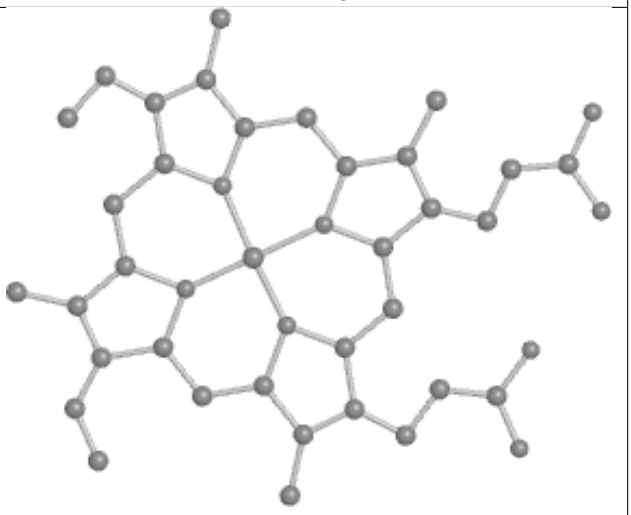
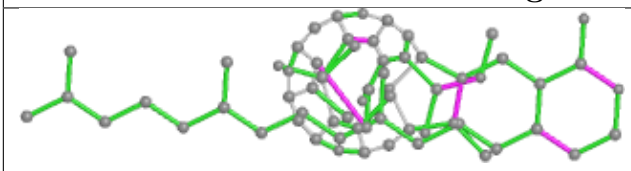


Rings

Ligand BPB L 402



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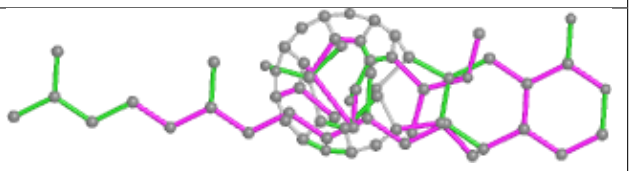

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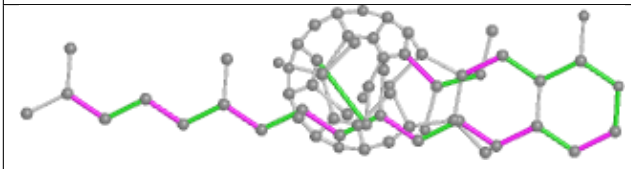

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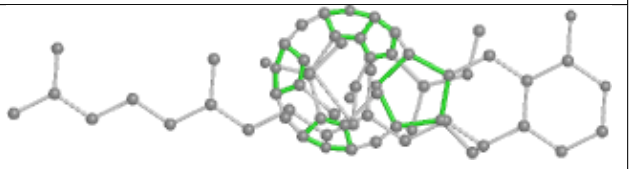
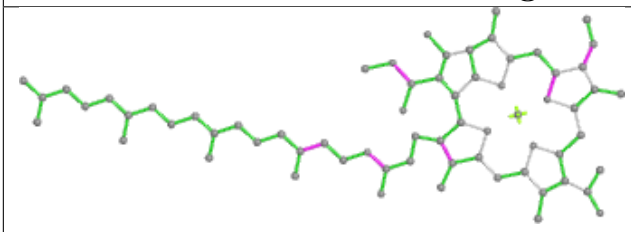


Rings

Ligand BCB M 400



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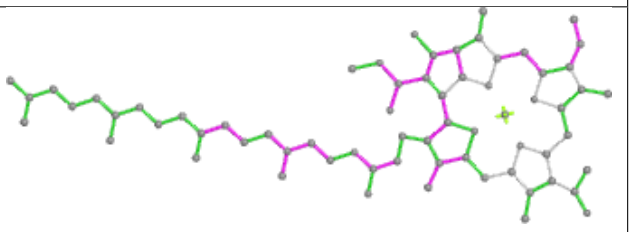

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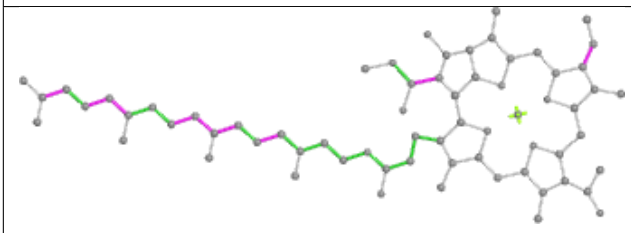

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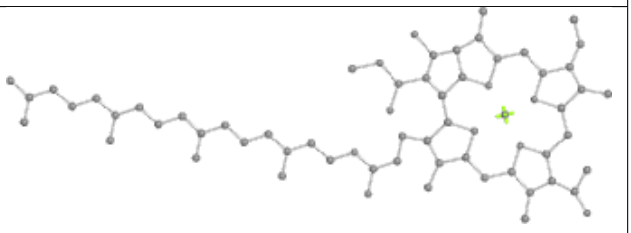
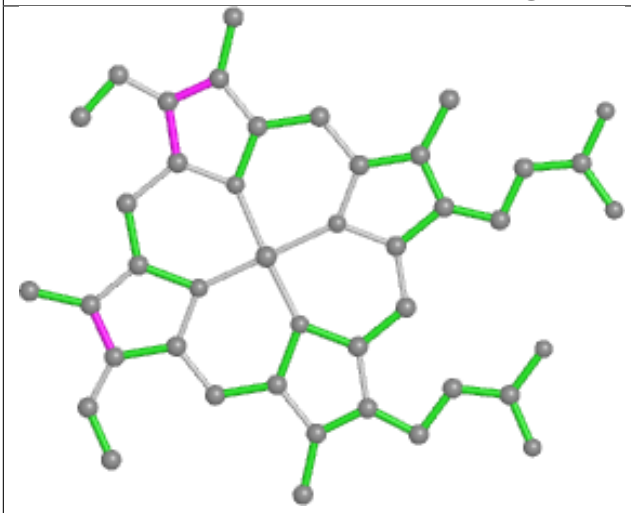
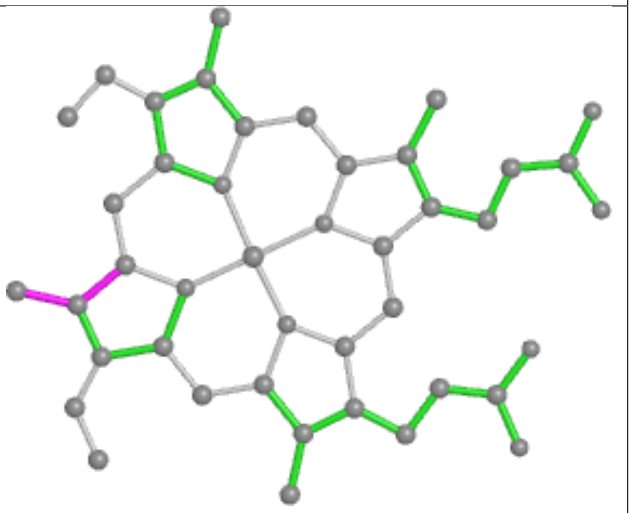


Rings

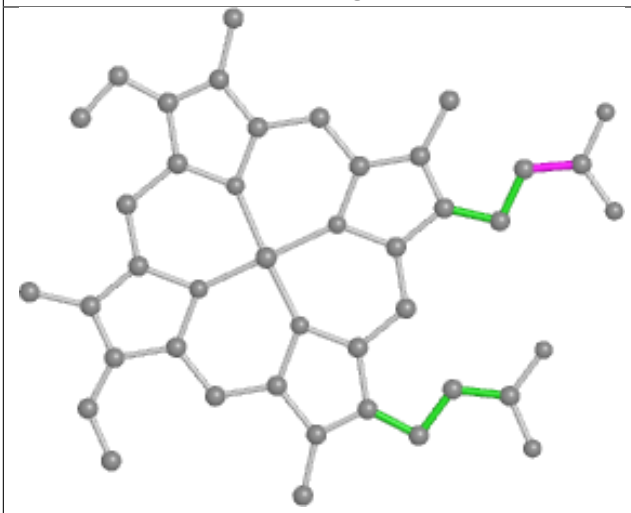
Ligand HEC C 401



Bond lengths



Bond angles



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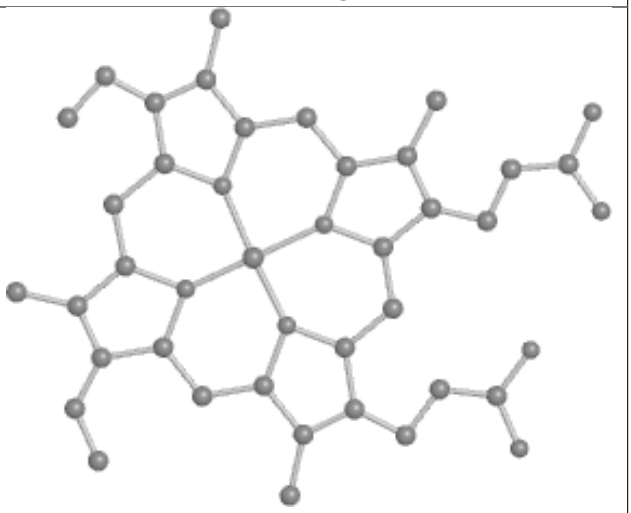
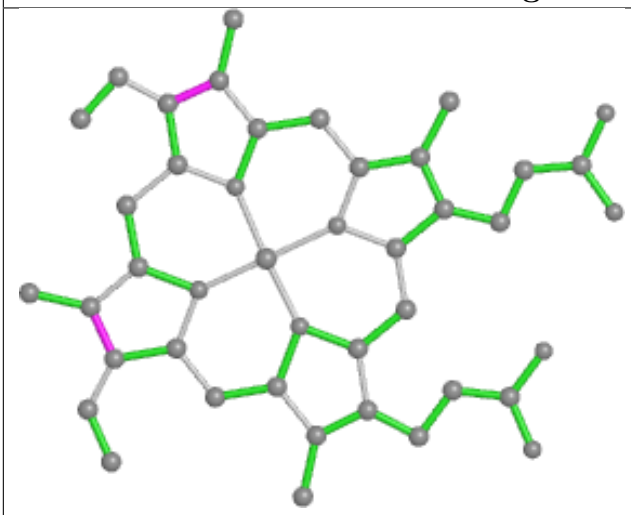


Rings

Ligand HEC C 402



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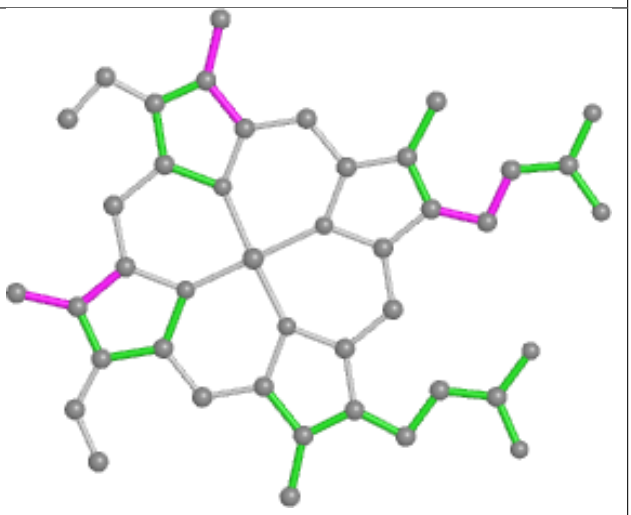
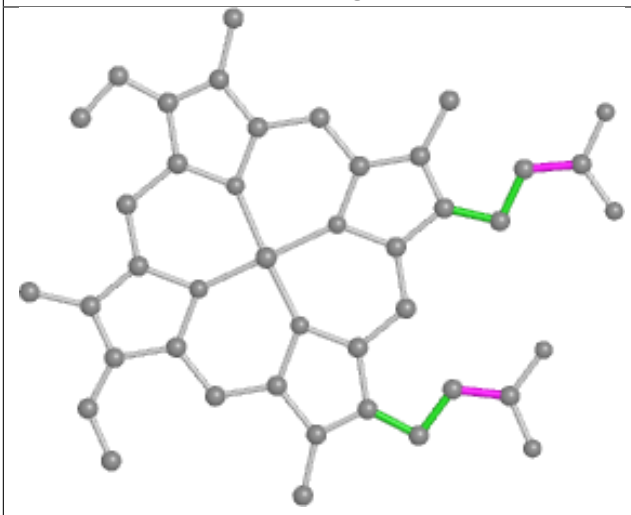


Bond angles



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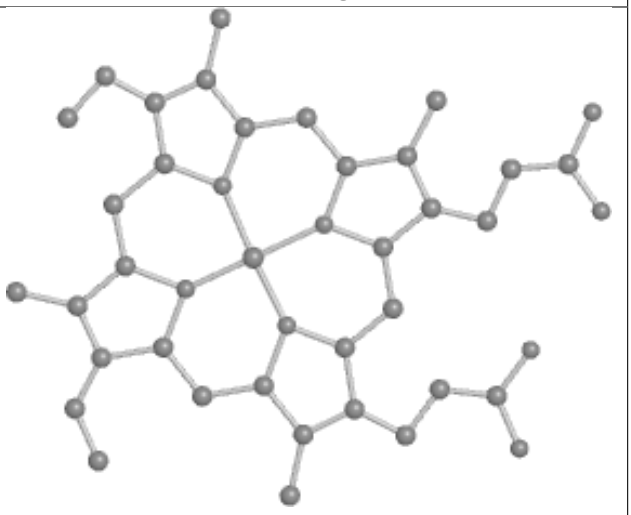
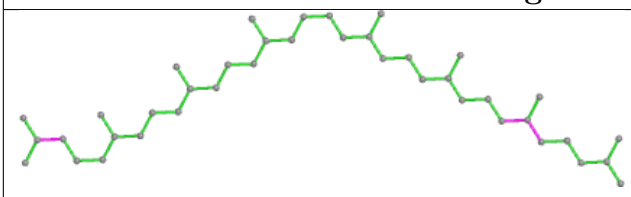
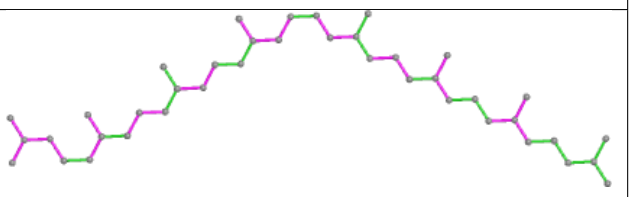


Rings

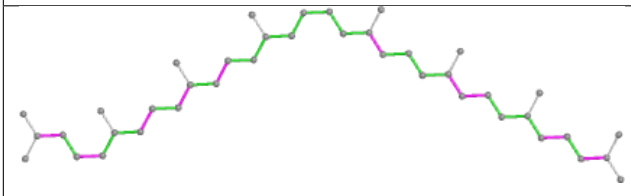
Ligand NS5 M 600



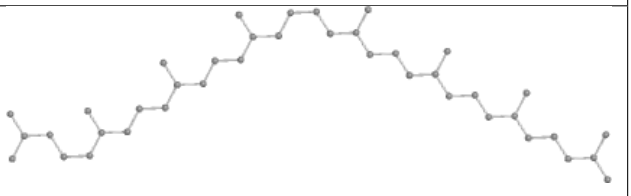
Bond lengths



Bond angles

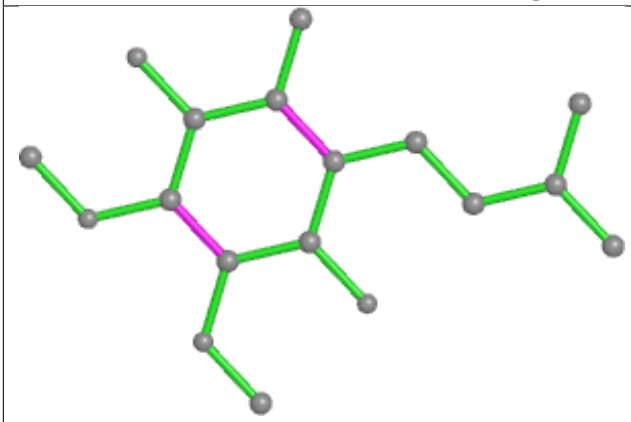


Torsions

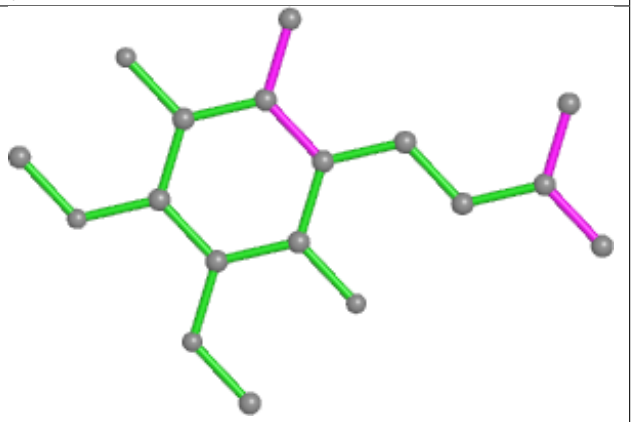


Rings

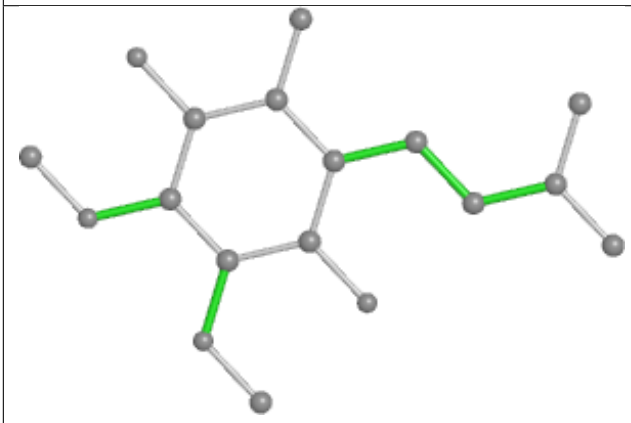
Ligand UQ1 L 503



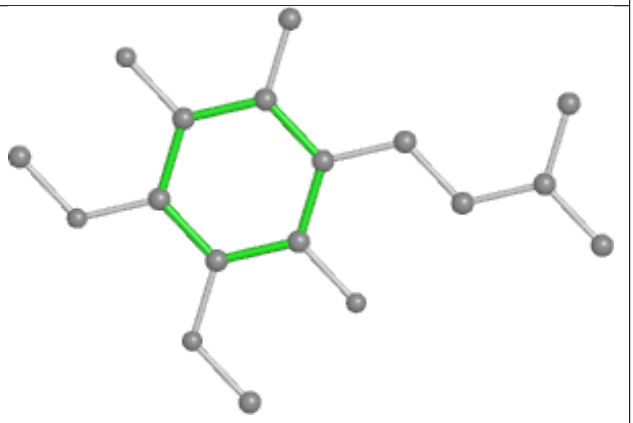
Bond lengths



Bond angles

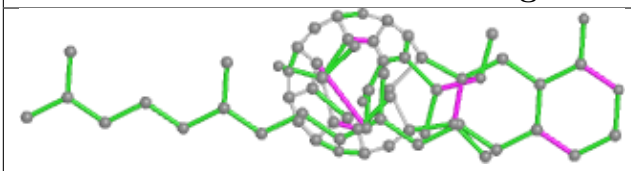


Torsions

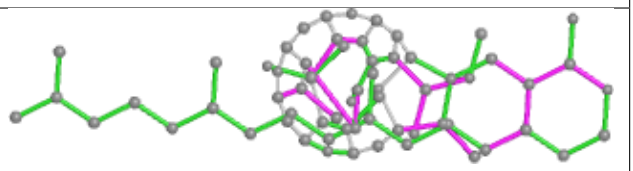


Rings

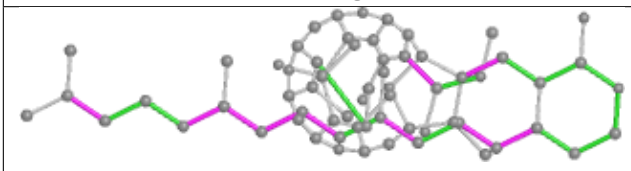
Ligand BPB M 402



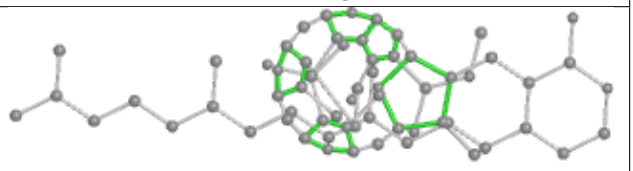
Bond lengths



Bond angles

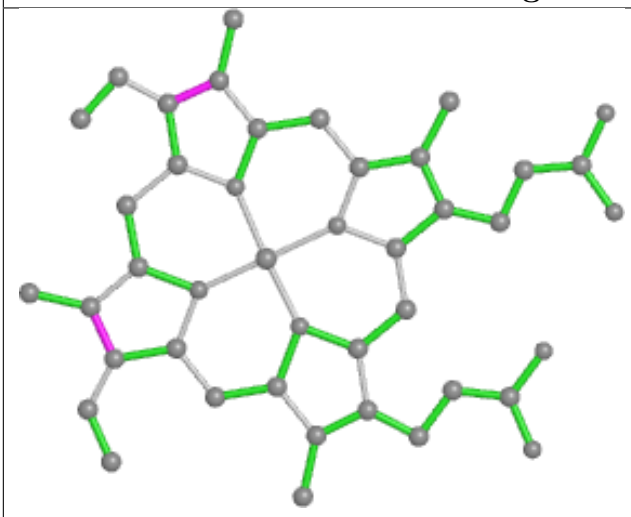


Torsions

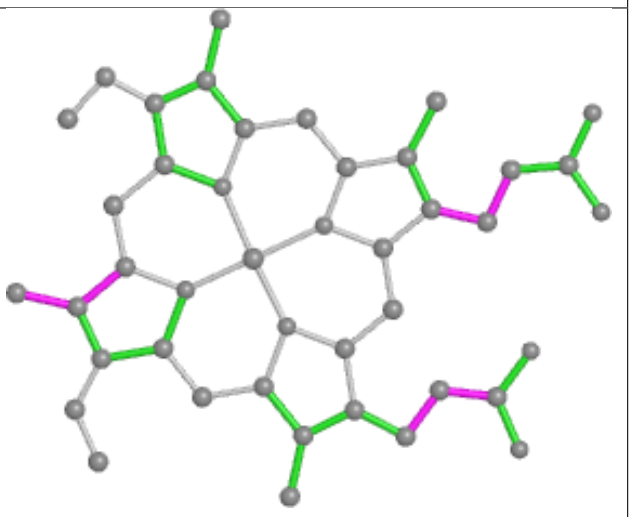


Rings

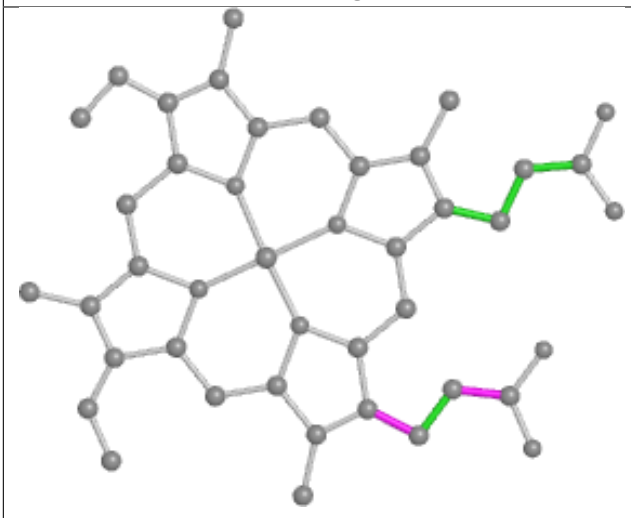
Ligand HEC C 404



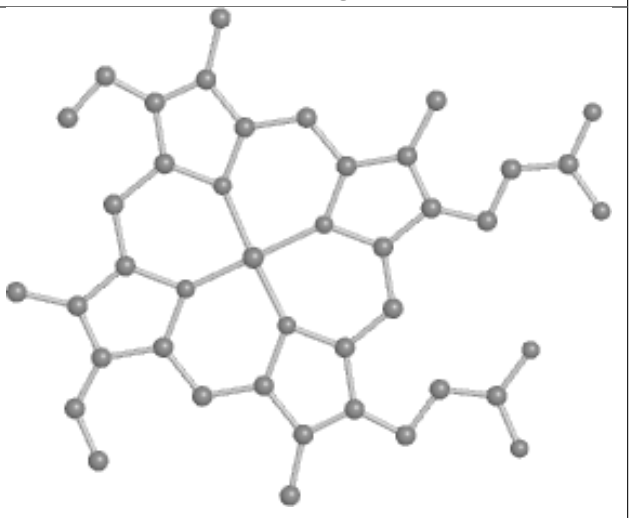
Bond lengths



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	332/336 (98%)	-0.24	7 (2%)	63	50	46, 74, 113, 124	0
2	H	249/258 (96%)	-0.19	3 (1%)	79	68	50, 73, 99, 105	0
3	L	273/273 (100%)	-0.58	2 (0%)	87	82	37, 54, 74, 85	0
4	M	323/323 (100%)	-0.51	1 (0%)	94	92	42, 60, 89, 117	0
All	All	1177/1190 (98%)	-0.38	13 (1%)	80	70	37, 66, 102, 124	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	85	THR	3.7
1	C	59	VAL	3.6
1	C	54	GLN	3.0
1	C	53	SER	2.8
2	H	83	PRO	2.7
3	L	271	PHE	2.5
1	C	218	LYS	2.4
1	C	58	ASN	2.4
4	M	322	PRO	2.3
1	C	63	GLY	2.2
2	H	7	ALA	2.1
3	L	1	ALA	2.1
1	C	57	LYS	2.0

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

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
2	FME	H	1	10/11	0.77	0.37	104,105,115,117	0

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
5	SO4	C	808	5/5	0.47	0.40	104,104,104,104	5
5	SO4	C	809	5/5	0.48	0.54	109,110,110,110	5
7	HTO	H	705	10/10	0.55	0.59	56,59,61,61	10
11	UQ1	L	503	18/18	0.62	0.59	73,76,78,78	18
5	SO4	H	812	5/5	0.76	0.33	92,92,93,93	5
5	SO4	H	803	5/5	0.77	0.34	82,82,83,83	5
7	HTO	C	707	10/10	0.77	0.39	44,48,49,49	10
5	SO4	C	810	5/5	0.80	0.42	88,88,88,88	5
5	SO4	H	807	5/5	0.81	0.42	108,108,108,109	5
5	SO4	C	813	5/5	0.82	0.43	79,79,80,80	5
5	SO4	C	811	5/5	0.85	0.60	76,76,76,77	5
14	NS5	M	600	40/40	0.87	0.28	65,71,100,101	4
7	HTO	C	706	10/10	0.88	0.71	56,57,58,58	10
10	BPB	M	402	65/65	0.89	0.28	61,67,123,124	0
11	UQ1	L	502	18/18	0.89	0.40	63,65,66,66	18
13	MQ9	M	501	58/58	0.91	0.25	40,64,102,103	0
8	LDA	M	704	16/16	0.91	0.41	68,70,73,73	16
5	SO4	C	814	5/5	0.92	0.37	48,48,49,50	5
5	SO4	C	815	5/5	0.92	0.25	40,40,41,41	5
8	LDA	H	703	16/16	0.94	0.39	54,58,60,61	16
5	SO4	H	806	5/5	0.95	0.14	72,72,73,73	5
5	SO4	M	804	5/5	0.95	0.18	94,95,96,96	0
8	LDA	L	702	16/16	0.95	0.36	67,73,79,80	0
8	LDA	H	701	16/16	0.96	0.17	54,57,68,68	0
5	SO4	M	801	5/5	0.96	0.11	61,62,63,63	0
5	SO4	M	805	5/5	0.96	0.09	64,65,65,67	5
6	HEC	C	401	43/43	0.96	0.27	99,110,118,120	0
10	BPB	L	402	65/65	0.96	0.19	38,51,60,60	0

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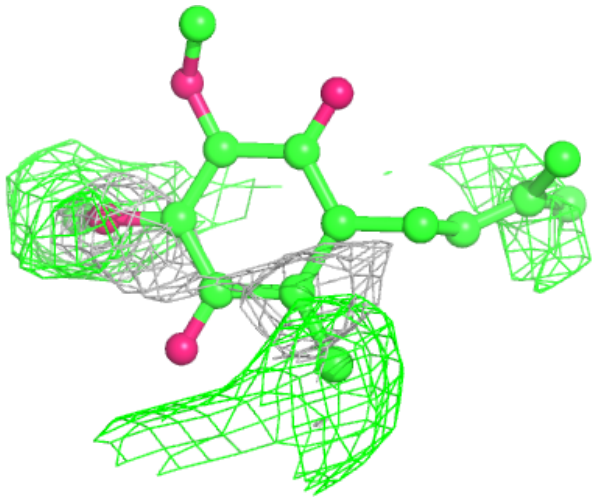
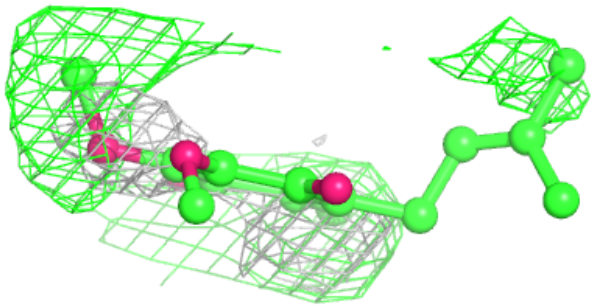
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	BCB	L	401	66/66	0.97	0.19	41,44,59,64	0
9	BCB	M	400	66/66	0.97	0.18	37,48,107,108	0
9	BCB	L	400	66/66	0.98	0.18	37,40,45,49	0
6	HEC	C	403	43/43	0.98	0.19	46,48,52,54	0
6	HEC	C	404	43/43	0.98	0.16	52,55,68,73	0
9	BCB	M	401	66/66	0.98	0.18	36,41,63,68	0
6	HEC	C	402	43/43	0.98	0.19	73,76,80,81	0
5	SO4	M	802	5/5	0.99	0.09	89,89,90,90	0
12	FE2	M	500	1/1	1.00	0.16	50,50,50,50	0

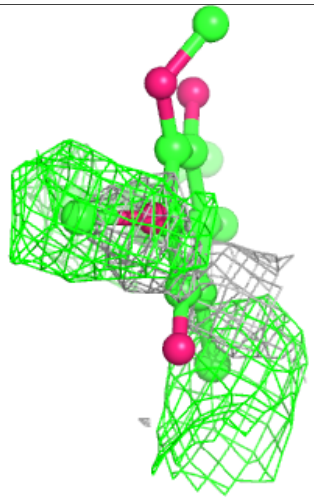
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UQ1 L 503:

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

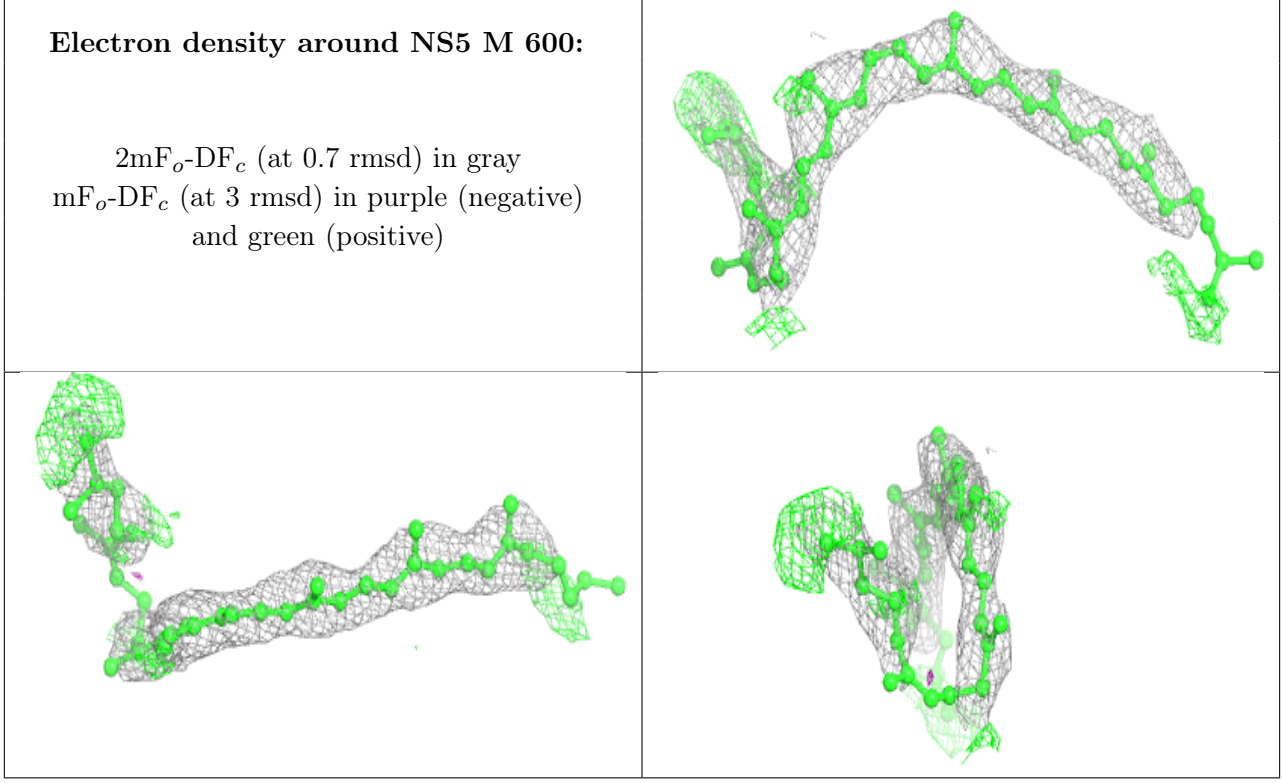






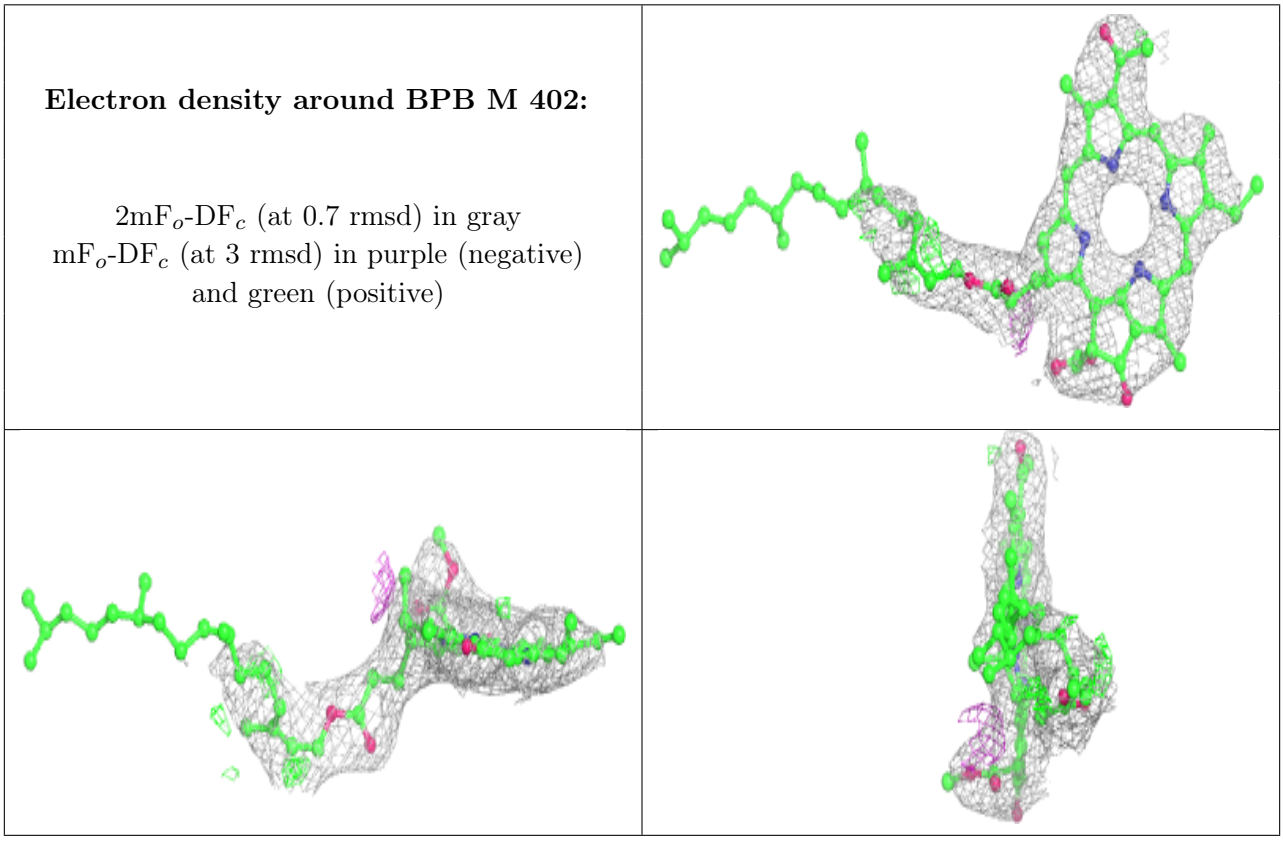
Electron density around NS5 M 600:

$2mF_o$-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 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 UQ1 L 502:

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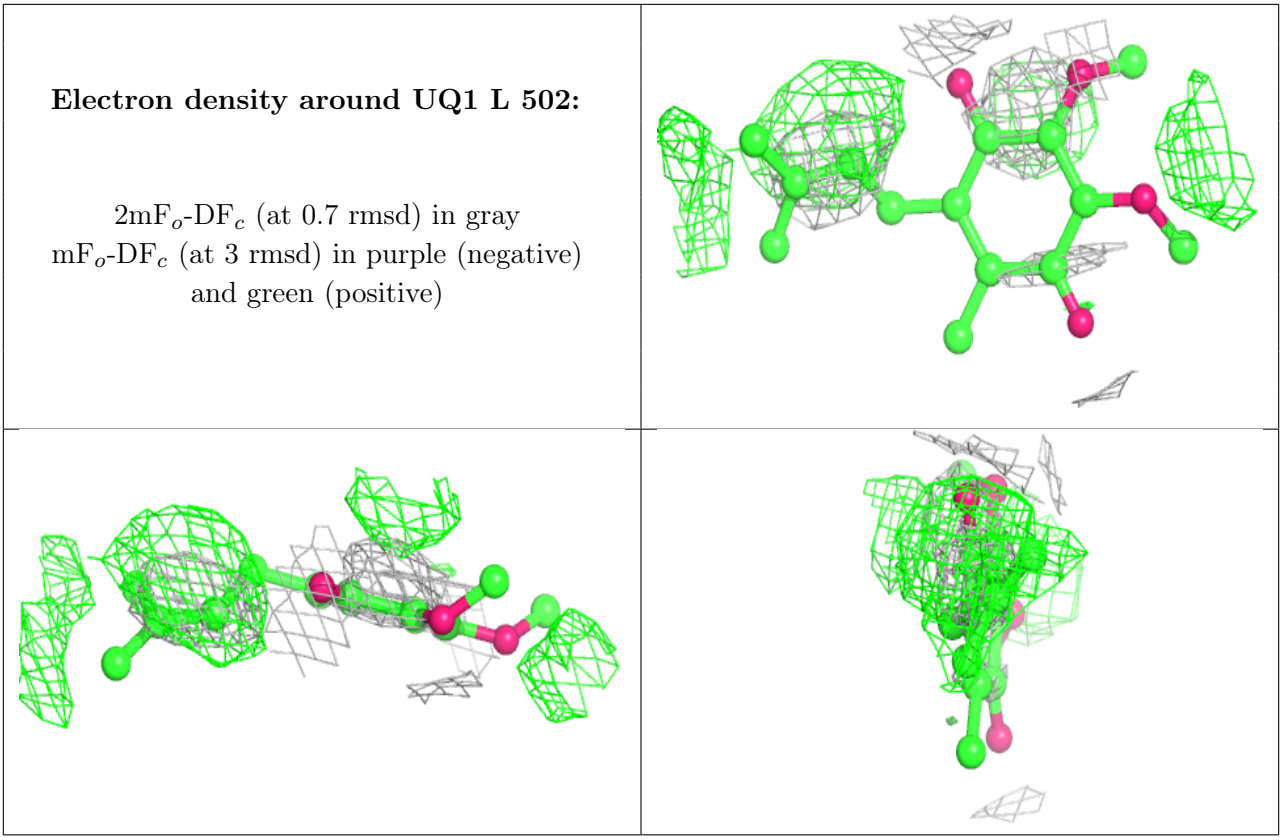
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around MQ9 M 501:

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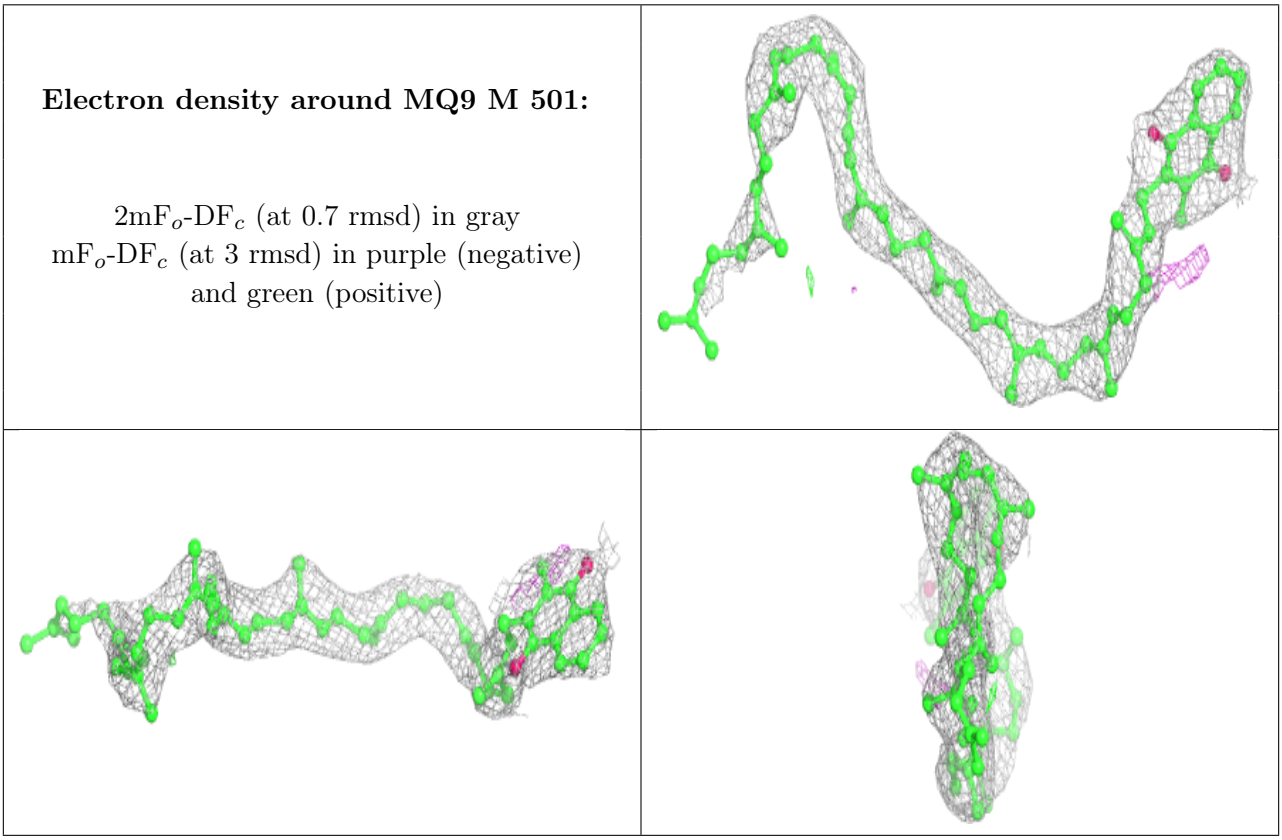
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HEC C 401:

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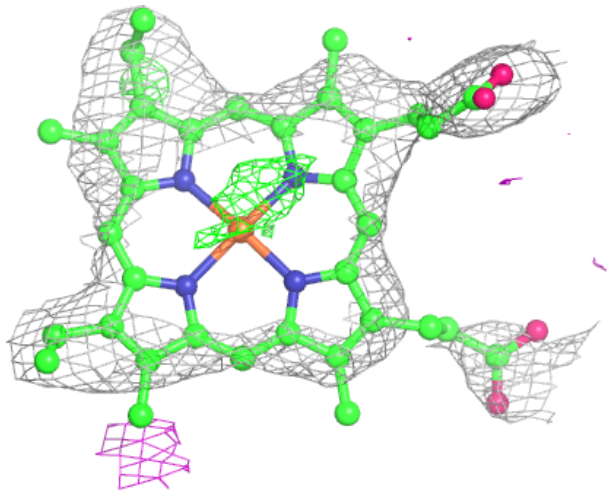
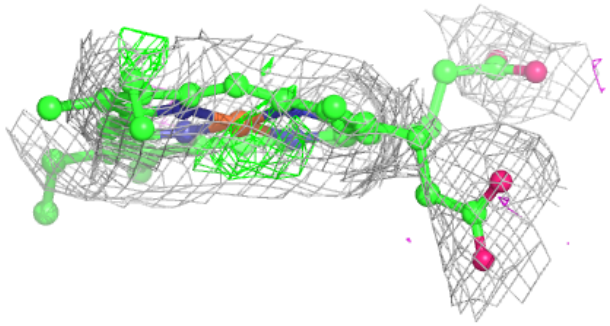
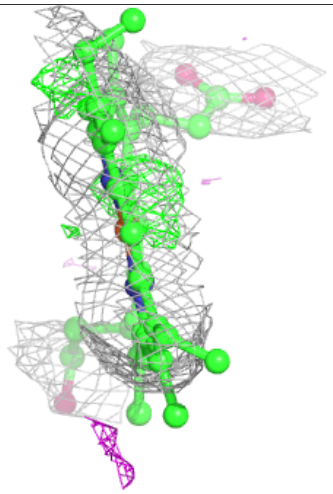
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

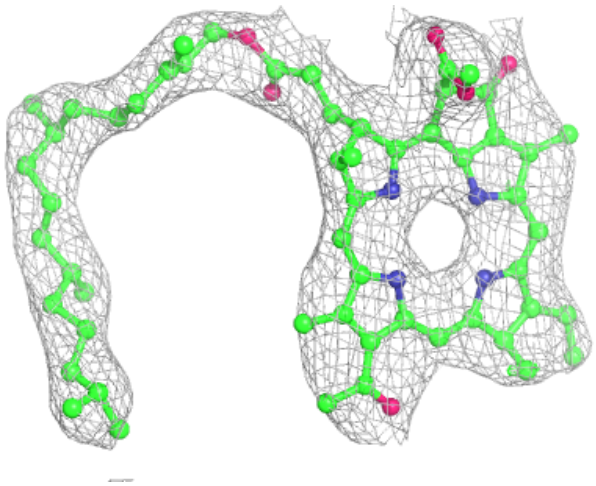


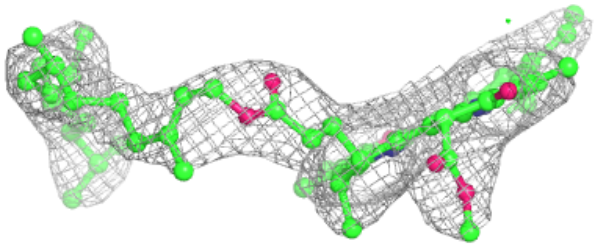


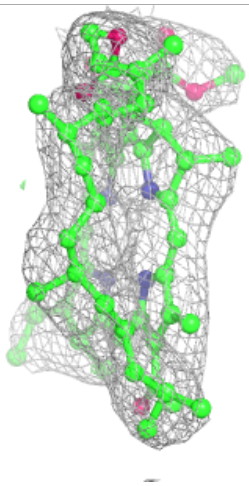


Electron density around BPB L 402:

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

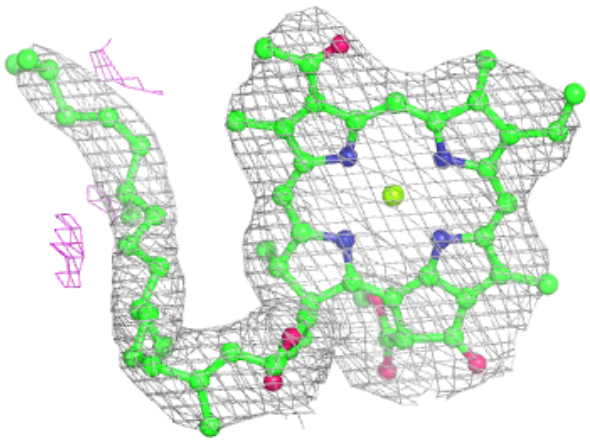


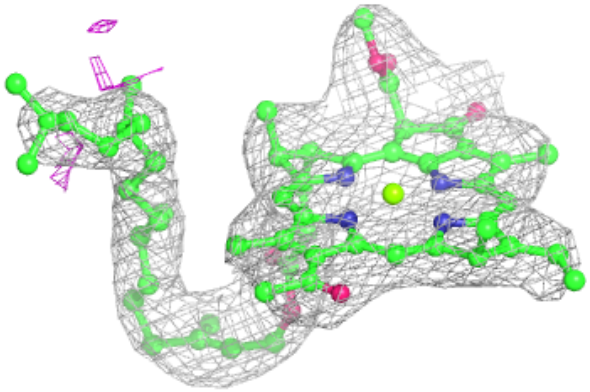


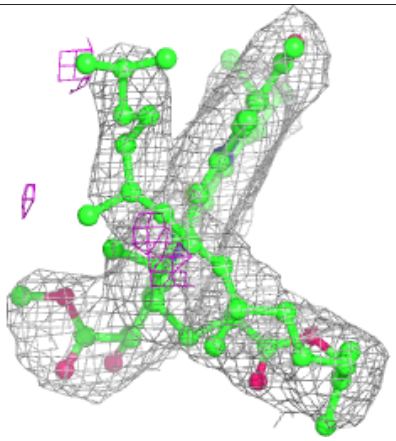


Electron density around BCB L 401:

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

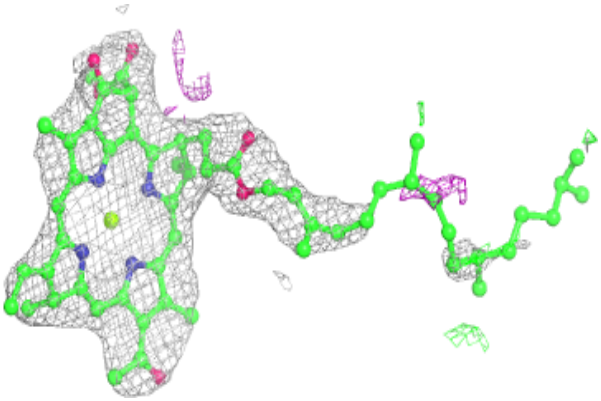


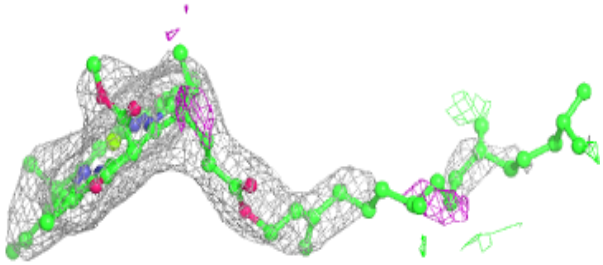


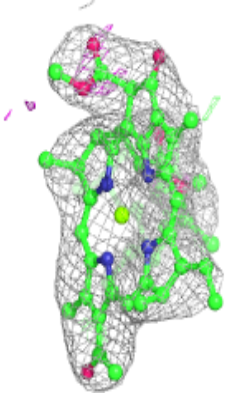


Electron density around BCB M 400:

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

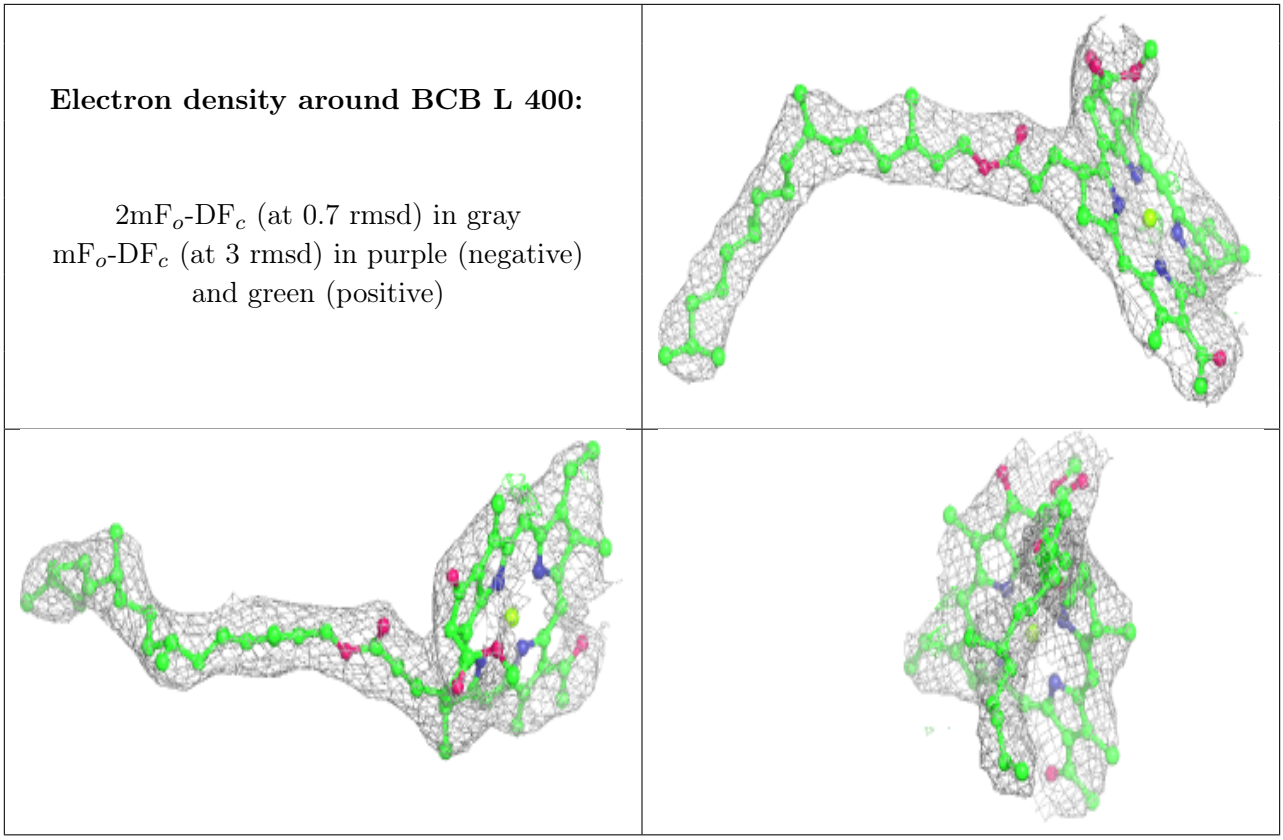






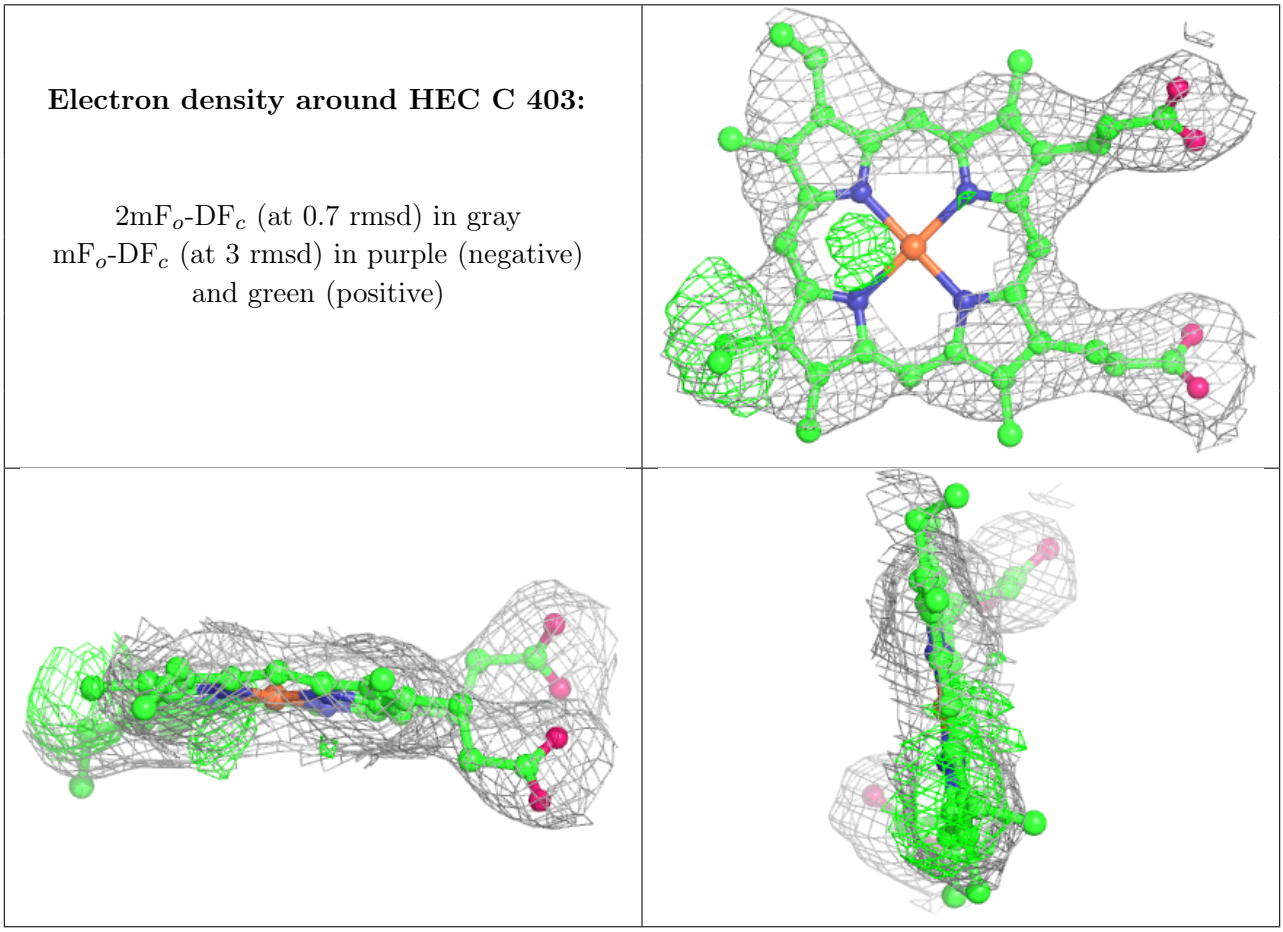
Electron density around BCB L 400:

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



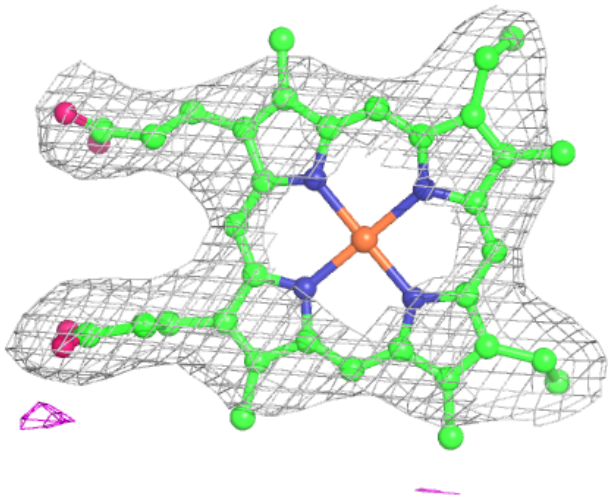
Electron density around HEC C 403:

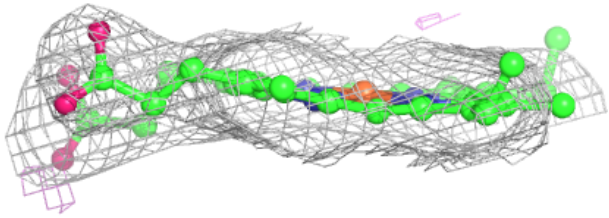
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

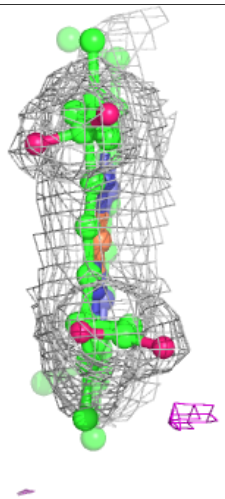


Electron density around HEC C 404:

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

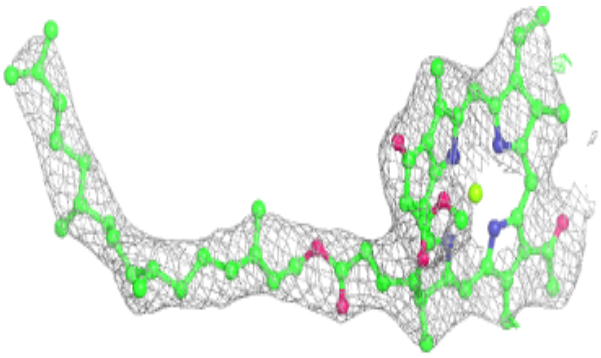


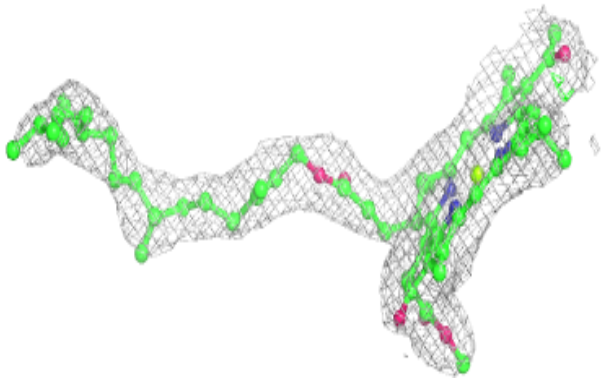


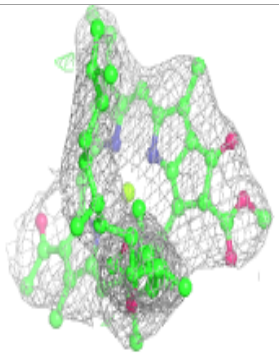


Electron density around BCB M 401:

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

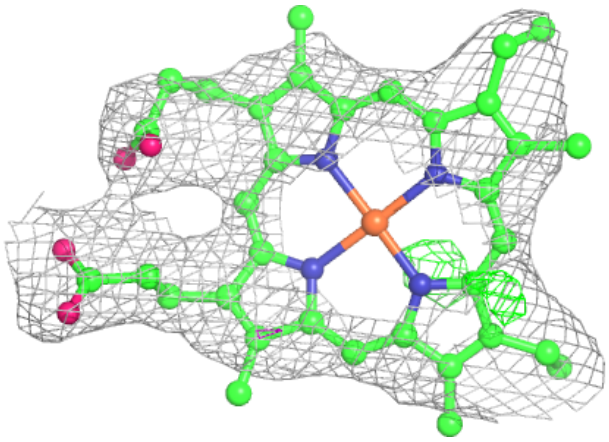


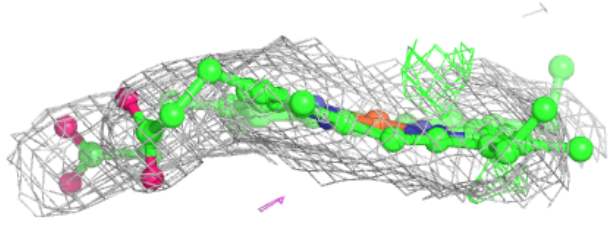


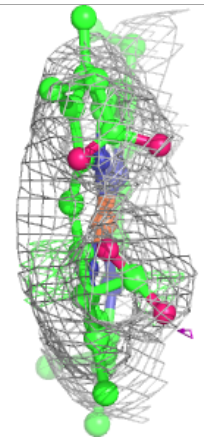


Electron density around HEC C 402:

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







6.5 Other polymers (i)

There are no such residues in this entry.