Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 06:03 AM EDT

PDB ID	:	3D38 / pdb_00003d38
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 (i) symbol.

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

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

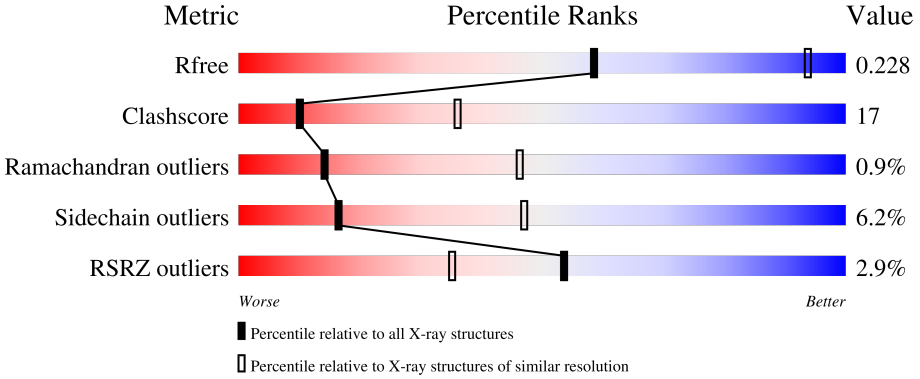
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	180053	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (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	4% 68% 29%
2	H	258	3% 66% 29%
3	L	273	2% 70% 26%
4	M	323	2% 70% 27%

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
6	HEC	C	401	X	-	-	-
6	HEC	C	402	X	-	-	-
6	HEC	C	403	X	-	-	-
6	HEC	C	404	X	-	-	-
7	HTO	C	706	-	-	-	X
7	HTO	C	707	-	-	-	X
7	HTO	H	705	-	-	-	X
9	BCB	L	400	X	-	-	-
9	BCB	L	401	X	-	-	-
9	BCB	M	400	X	-	-	-
9	BCB	M	401	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

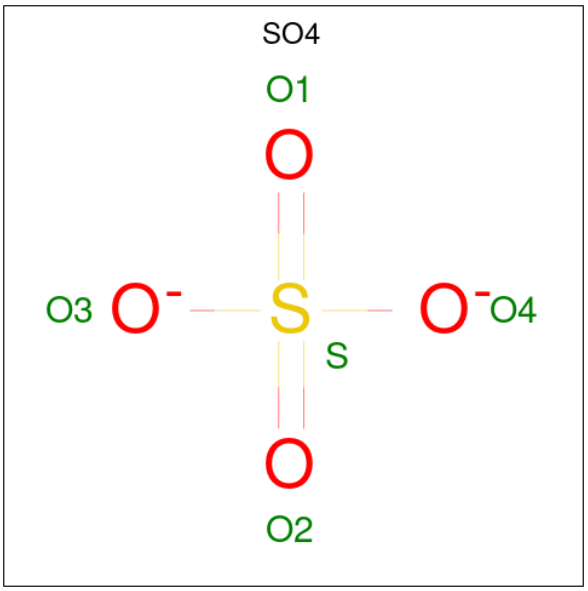
- Molecule 3 is a protein called Reaction center protein L chain.

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 (CCD ID: 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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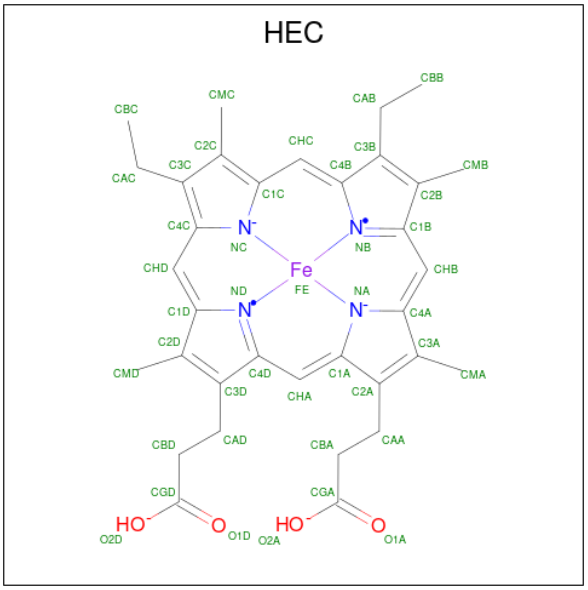
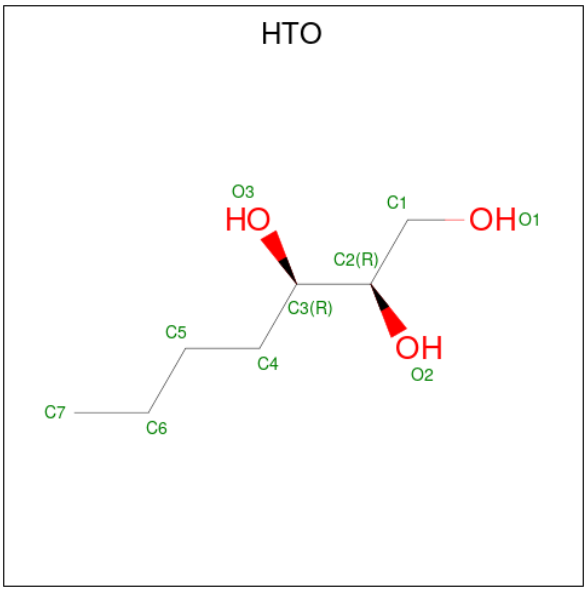
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	M	1	5	4	1	0	0

- Molecule 6 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



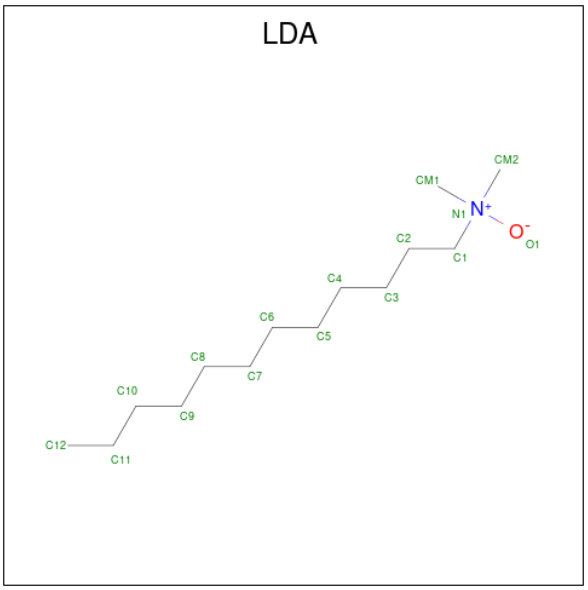
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
6	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
6	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
6	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
6	C	1	43	34	1	4	4	0	0

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



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

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



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

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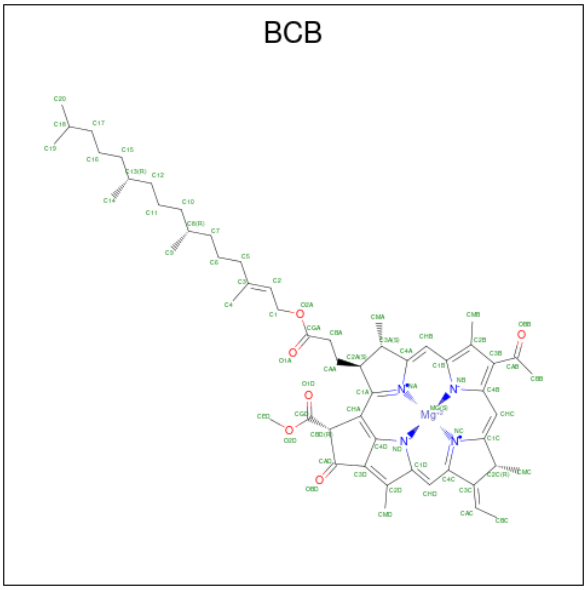
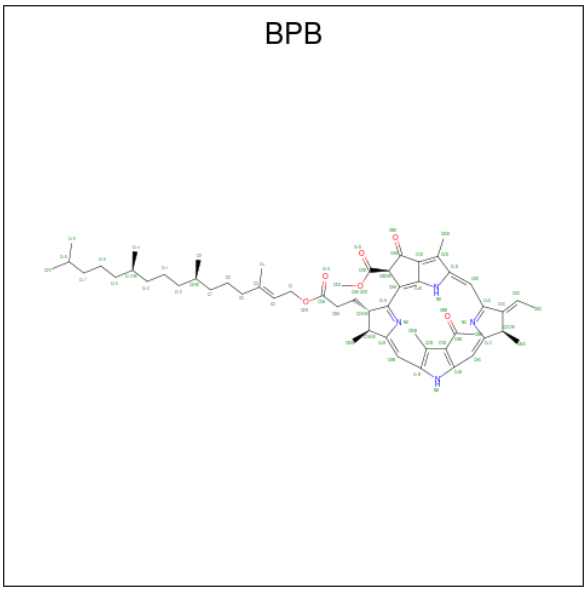
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	H	1	16	14	1	1	0	0
			Total	C	N	O		
8	L	1	16	14	1	1	0	0
			Total	C	N	O		
8	M	1	16	14	1	1	0	0

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



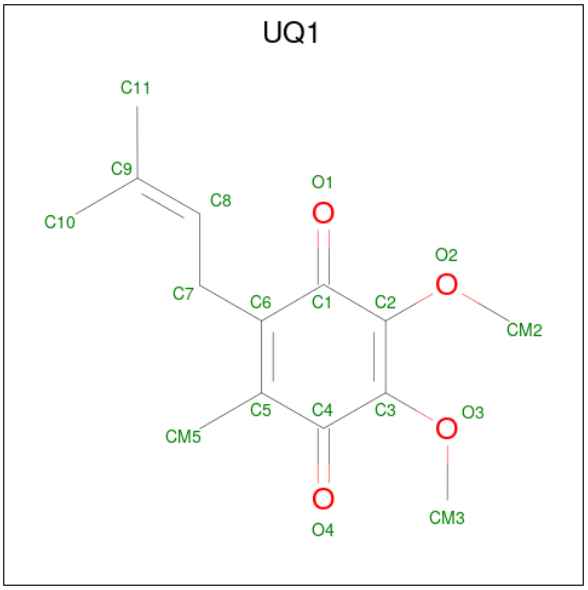
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
9	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	M	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	M	1	66	55	1	4	6	0	0

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



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

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

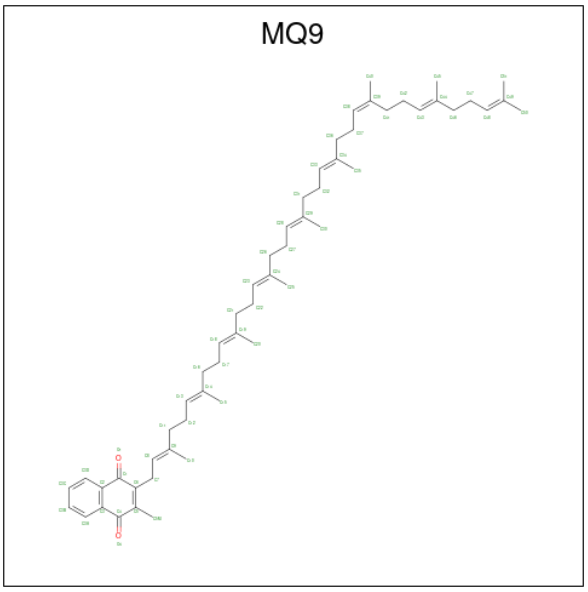


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
11	L	1	18	14	4	0	0
			Total	C	O		
11	L	1	18	14	4	0	0

- Molecule 12 is FE (II) ION (CCD ID: FE2) (formula: Fe).

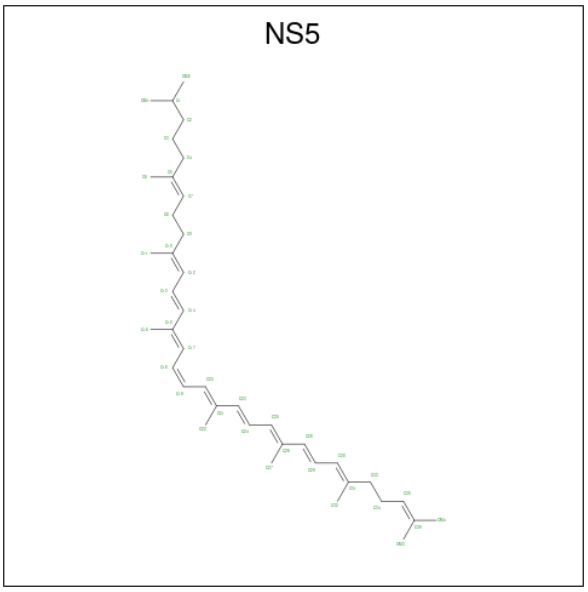
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
12	M	1	1	1	0	0

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



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

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



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

- Molecule 15 is water.

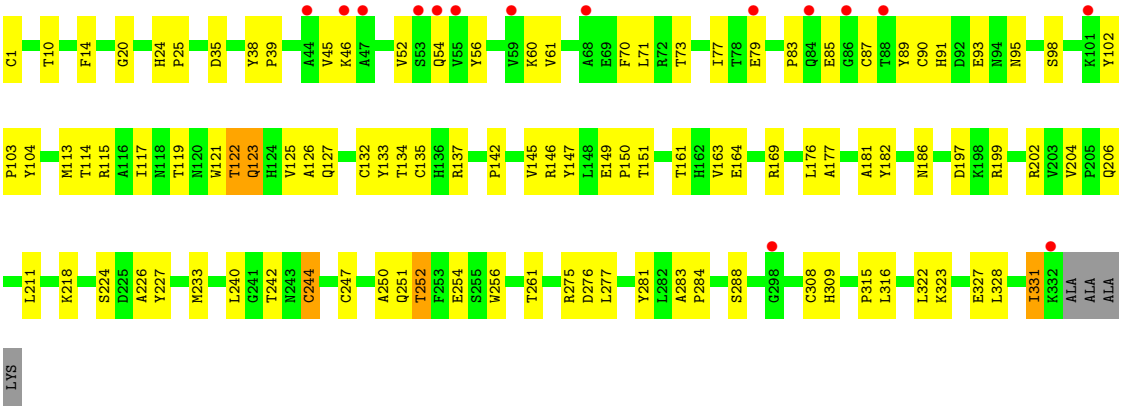
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
15	C	47	47	47	0	0
			Total	O		
15	H	28	28	28	0	0
			Total	O		
15	L	38	38	38	0	0
			Total	O		
15	M	46	46	46	0	0

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.

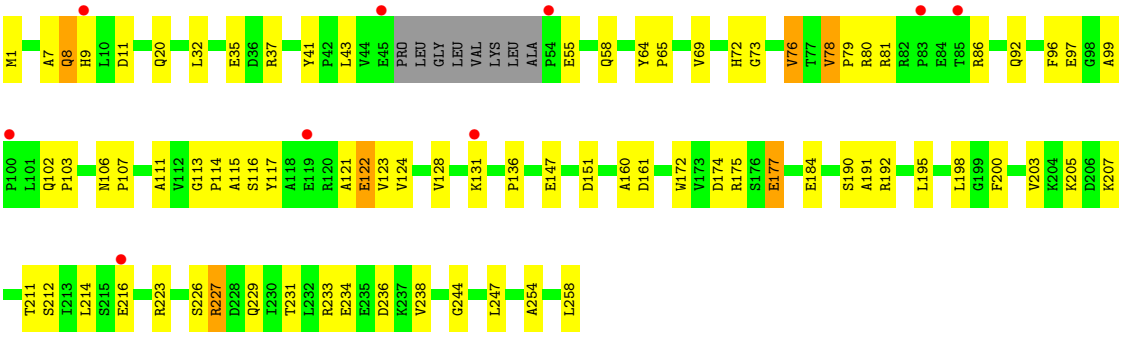
• Molecule 1: Photosynthetic reaction center cytochrome c subunit

Chain C: 4% 68% 29%



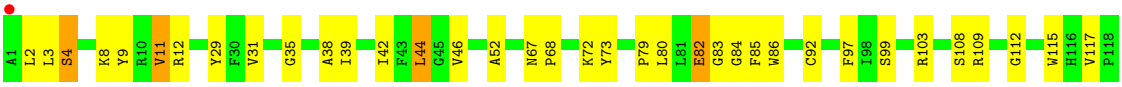
• Molecule 2: Reaction center protein H chain

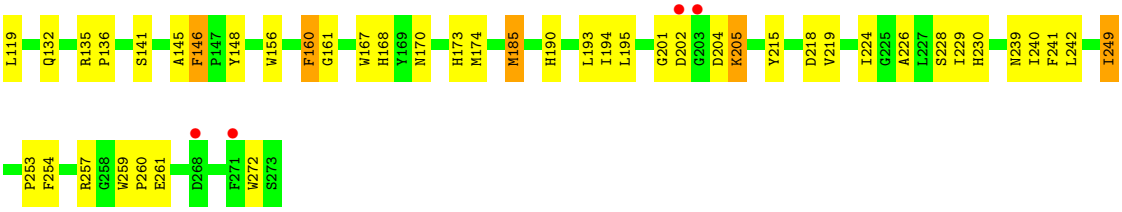
Chain H: 3% 66% 29%



• Molecule 3: Reaction center protein L chain

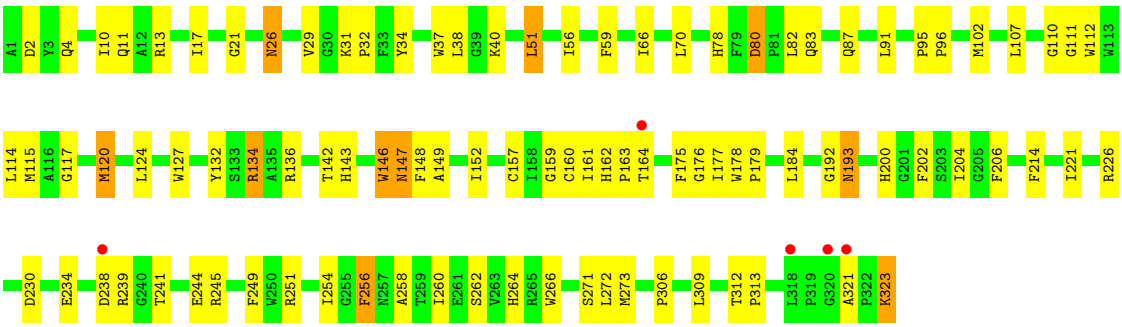
Chain L: 2% 70% 26%





• 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 50.00 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-3.21) 99.8 (50.00-3.21)	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 (5.05%)	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)	0.30 , 59.6	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FME, SO4, MQ9, HEC, BCB, NS5, BPB, FE2, HTO, LDA, 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	0.67	0/2665	0.96	5/3633 (0.1%)
2	H	0.72	0/1993	0.96	2/2720 (0.1%)
3	L	0.73	0/2259	0.94	2/3084 (0.1%)
4	M	0.68	0/2659	0.90	1/3637 (0.0%)
All	All	0.70	0/9576	0.94	10/13074 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	204	VAL	CA-C-N	6.58	126.61	119.90
1	C	204	VAL	C-N-CA	6.58	126.61	119.90
1	C	126	ALA	CB-CA-C	-5.71	109.46	117.23
2	H	177	GLU	N-CA-C	-5.41	102.51	110.52
4	M	309	LEU	N-CA-C	-5.40	102.43	110.20
1	C	61	VAL	N-CA-C	5.38	116.45	111.45
2	H	69	VAL	CB-CA-C	-5.15	106.34	111.80
1	C	142	PRO	O-C-N	5.14	123.57	121.15
3	L	146	PHE	CA-C-N	5.07	125.52	120.14
3	L	146	PHE	C-N-CA	5.07	125.52	120.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2598	0	2573	87	0
2	H	1958	0	1946	71	0
3	L	2171	0	2098	67	0
4	M	2555	0	2452	83	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	28	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	23	0
9	M	132	0	144	24	0
10	L	65	0	74	8	0
10	M	65	0	74	20	0
11	L	36	0	36	2	0
12	M	1	0	0	0	0
13	M	58	0	80	2	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	349	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 (349) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:C:123:GLN:HG2	15:C:854:HOH:O	1.69	0.93
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
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
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
10:L:402:BPB:HBBA	10:L:402:BPB:HMBB	1.66	0.77
10:L:402:BPB:HMBB	10:L:402:BPB:CBB	2.15	0.76
9:M:401:BCB:HMB3	9:M:401:BCB:CBB	2.15	0.76
4:M:258:ALA:HB1	4:M:262:SER:OG	1.84	0.76
9:M:401:BCB:HMB3	9:M:401:BCB:HBB2	1.67	0.76
2:H:227:ARG:HH11	2:H:227:ARG:CG	1.99	0.76
9:L:400:BCB:HMB3	9:L:400:BCB:CBB	2.17	0.75
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
4:M:120:MET:HE3	4:M:175:PHE:HE1	1.53	0.73
2:H:64:TYR:HE1	8:H:703:LDA:H31	1.50	0.73
3:L:79:PRO:HG2	3:L:82:GLU:HG3	1.69	0.73
9:L:401:BCB:HBB2	9:L:401:BCB:HMB3	1.69	0.73
1:C:52:VAL:HB	1:C:56:TYR:HD2	1.53	0.73
9:L:400:BCB:HMB3	9:L:400:BCB:HBB2	1.70	0.73
9:L:401:BCB:HMB3	9:L:401:BCB:CBB	2.18	0.73
2:H:76:VAL:HG13	2:H:80:ARG:HH12	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:400:BCB:HAA1	9:L:400:BCB:HBD	1.71	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
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: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
4:M:147:ASN:C	4:M:147:ASN:HD22	2.04	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
2:H:8:GLN:C	2:H:9:HIS:HD2	2.05	0.65
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.32	0.65
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
2:H:114:PRO:CG	2:H:247:LEU:HD23	2.29	0.61
4:M:117:GLY:HA3	14:M:600:NS5:H28	1.82	0.60
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
1:C:95:ASN:CG	1:C:98:SER:HB2	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:64:TYR:CE1	8:H:703:LDA:H12	2.38	0.59
9:M:401:BCB:CBB	9:M:401:BCB:CMB	2.80	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
3:L:185:MET:HE3	10:M:402:BPB:NA	2.19	0.57
9:L:401:BCB:CBB	9:L:401:BCB:CMB	2.82	0.57
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
9:L:400:BCB:CBB	9:L:400:BCB:CMB	2.83	0.56
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: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:121:ALA:C	2:H:123:VAL:H	2.14	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
10:L:402:BPB:CBB	10:L:402:BPB:CMB	2.80	0.56
1:C:177:ALA:HA	15:C:822:HOH:O	2.06	0.55
3:L:160:PHE:HD1	3:L:160:PHE:C	2.15	0.55
4:M:226:ARG:HG3	15:M:825:HOH:O	2.06	0.55
4:M:258:ALA:HB1	4:M:262:SER:HG	1.71	0.55
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
1:C:87:CYS:C	1:C:89:TYR:H	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:80:LEU:HD23	3:L:85:PHE:CE1	2.43	0.53
4:M:120:MET:CE	4:M:175:PHE:HE1	2.20	0.53
6:C:401:HEC:HBB3	6:C:401:HEC:CMB	2.38	0.53
3:L:259:TRP:O	3:L:260:PRO:C	2.52	0.53
3:L:160:PHE:C	3:L:160:PHE:CD1	2.84	0.53
1:C:197:ASP:HB3	1:C:275:ARG:HD3	1.91	0.53
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:113:GLY:C	2:H:115:ALA:H	2.16	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:8:GLN:C	2:H:9:HIS:CD2	2.87	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
1:C:133:TYR:O	1:C:134:THR:C	2.53	0.52
9:L:400:BCB:H2C	9:M:401:BCB:H2C	1.92	0.52
1:C:276:ASP:O	1:C:277:LEU:C	2.52	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
2:H:128:VAL:HG22	2:H:128:VAL:O	2.10	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
3:L:86:TRP:CZ2	3:L:145:ALA:CB	2.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:109:ARG:HD3	3:L:115:TRP:CZ2	2.46	0.49
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:231:THR:OG1	2:H:234:GLU:HG3	2.11	0.49
4:M:160:CYS:C	4:M:163:PRO:HD2	2.38	0.49
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
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
2:H:8:GLN:O	2:H:9:HIS:HD2	1.96	0.48
1:C:87:CYS:C	1:C:89:TYR:N	2.69	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
1:C:87:CYS:SG	6:C:401:HEC:C3B	3.00	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
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
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
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:147:TYR:C	1:C:149:GLU:H	2.22	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:80:ASP:OD1	4:M:80:ASP:C	2.58	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
6:C:403:HEC:CMC	6:C:403:HEC:HBC3	2.45	0.47
1:C:24:HIS:O	1:C:25:PRO:C	2.58	0.46
1:C:119:THR:HG21	1:C:331:ILE:HG22	1.98	0.46
4:M:120:MET:HE3	4:M:175:PHE:CE1	2.42	0.46
3:L:146:PHE:HB3	3:L:156:TRP:CD2	2.51	0.46
4:M:148:PHE:HB2	10:M:402:BPB:HMDB	1.98	0.46
1:C:10:THR:O	1:C:20:GLY:HA3	2.15	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
10:M:402:BPB:OBB	10:M:402:BPB:HMB	2.17	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
4:M:102:MET:HE2	4:M:164:THR:HG23	1.99	0.45
1:C:250:ALA:O	1:C:251:GLN:C	2.60	0.45
2:H:78:VAL:HA	2:H:79:PRO:C	2.41	0.45
4:M:238:ASP:O	4:M:239:ARG:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
4:M:147:ASN:C	4:M:147:ASN:ND2	2.73	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:176:GLY:C	4:M:179:PRO:HD2	2.44	0.43
4:M:254:ILE:HD12	4:M:256:PHE:CE1	2.54	0.43
1:C:281:TYR:C	1:C:284:PRO:HD2	2.44	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
1:C:226:ALA:O	1:C:227:TYR:C	2.62	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
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
2:H:174:ASP:C	2:H:174:ASP:OD1	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:247:CYS:HA	1:C:261:THR:OG1	2.20	0.42
3:L:239:ASN:O	3:L:240:ILE:C	2.63	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:102:TYR:C	1:C:104:TYR:N	2.77	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
3:L:3:LEU:O	3:L:4:SER:C	2.63	0.41
10:M:402:BPB:HMC	10:M:402:BPB:CBC	2.50	0.41
2:H:113:GLY:C	2:H:115:ALA:N	2.78	0.41
4:M:37:TRP:HD1	5:M:805:SO4:O1	2.02	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
2:H:151:ASP:OD1	2:H:151:ASP:C	2.64	0.41
4:M:271:SER:O	4:M:272:LEU:C	2.63	0.41
1:C:85:GLU:HG3	1:C:85:GLU:O	2.20	0.41
6:C:401:HEC:HBB3	6:C:401:HEC:HMB1	2.01	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:132:GLN:C	3:L:136:PRO:HG2	2.45	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:70:PHE:CD2	1:C:70:PHE:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:TYR:CD1	1:C:137:ARG:HA	2.55	0.41
2:H:121:ALA:C	2:H:123:VAL:N	2.78	0.41
4:M:87:GLN:O	4:M:91:LEU:HG	2.20	0.41
1:C:113:MET:O	1:C:114:THR:C	2.62	0.41
2:H:64:TYR:O	2:H:65:PRO:C	2.64	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
2:H:190:SER:O	2:H:191:ALA:C	2.63	0.40
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
3:L:170:ASN:OD1	3:L:170:ASN:C	2.64	0.40
4:M:160:CYS:SG	14:M:600:NS5:H29	2.60	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%)	36 67
2	H	246/258 (95%)	220 (89%)	22 (9%)	4 (2%)	7 35
3	L	271/273 (99%)	246 (91%)	24 (9%)	1 (0%)	30 61
4	M	321/323 (99%)	290 (90%)	26 (8%)	5 (2%)	7 35
All	All	1168/1190 (98%)	1050 (90%)	107 (9%)	11 (1%)	14 46

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%)	264 (94%)	16 (6%)	18	49
2	H	205/212 (97%)	192 (94%)	13 (6%)	16	46
3	L	218/218 (100%)	203 (93%)	15 (7%)	14	44
4	M	249/249 (100%)	234 (94%)	15 (6%)	17	48
All	All	952/961 (99%)	893 (94%)	59 (6%)	16	47

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

Mol	Chain	Res	Type
1	C	45	VAL
1	C	46	LYS
1	C	54	GLN
1	C	60	LYS
1	C	122	THR
1	C	123	GLN
1	C	127	GLN
1	C	151	THR
1	C	199	ARG
1	C	211	LEU
1	C	218	LYS

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Mol	Chain	Res	Type
1	C	244	CYS
1	C	252	THR
1	C	288	SER
1	C	323	LYS
1	C	331	ILE
2	H	8	GLN
2	H	11	ASP
2	H	76	VAL
2	H	78	VAL
2	H	81	ARG
2	H	97	GLU
2	H	205	LYS
2	H	207	LYS
2	H	211	THR
2	H	212	SER
2	H	223	ARG
2	H	227	ARG
2	H	258	LEU
3	L	2	LEU
3	L	4	SER
3	L	11	VAL
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	257	ARG
4	M	17	ILE
4	M	26	ASN
4	M	31	LYS
4	M	40	LYS
4	M	70	LEU
4	M	80	ASP
4	M	120	MET
4	M	134	ARG
4	M	136	ARG

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Mol	Chain	Res	Type
4	M	146	TRP
4	M	147	ASN
4	M	214	PHE
4	M	230	ASP
4	M	256	PHE
4	M	323	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	37	GLN
1	C	54	GLN
1	C	123	GLN
1	C	162	HIS
1	C	206	GLN
1	C	263	GLN
1	C	297	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
3	L	183	ASN
3	L	214	GLN
3	L	239	ASN
4	M	4	GLN
4	M	9	GLN
4	M	78	HIS
4	M	147	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	8,9,11	3.48	1 (12%)

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 (1) 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

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 oligosaccharides 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	$\#\|Z\| > 2$
5	SO4	C	814	-	4,4,4	0.24	0	6,6,6	0.35	0
6	HEC	C	402	1	50,50,50	1.23	4 (8%)	68,82,82	1.22	9 (13%)
5	SO4	H	806	-	4,4,4	0.27	0	6,6,6	0.22	0
5	SO4	C	815	-	4,4,4	0.27	0	6,6,6	0.15	0
5	SO4	M	802	-	4,4,4	0.29	0	6,6,6	0.24	0
7	HTO	H	705	-	9,9,9	0.73	0	10,10,10	0.86	0
8	LDA	L	702	-	13,15,15	2.26	2 (15%)	14,17,17	0.62	0
9	BCB	L	401	3	68,74,74	1.49	7 (10%)	77,115,115	1.99	15 (19%)
14	NS5	M	600	-	39,39,39	1.52	3 (7%)	46,46,46	1.99	14 (30%)
5	SO4	C	813	-	4,4,4	0.19	0	6,6,6	0.26	0
5	SO4	M	805	-	4,4,4	0.27	0	6,6,6	0.40	0
5	SO4	C	809	-	4,4,4	0.25	0	6,6,6	0.11	0
11	UQ1	L	503	-	18,18,18	2.31	2 (11%)	24,25,25	1.37	4 (16%)
5	SO4	H	812	-	4,4,4	0.27	0	6,6,6	0.19	0
9	BCB	L	400	3	68,74,74	1.53	10 (14%)	77,115,115	2.10	18 (23%)
11	UQ1	L	502	-	18,18,18	2.26	2 (11%)	24,25,25	1.53	5 (20%)
5	SO4	C	810	-	4,4,4	0.26	0	6,6,6	0.08	0
5	SO4	M	801	-	4,4,4	0.31	0	6,6,6	0.56	0
6	HEC	C	403	1	50,50,50	1.27	3 (6%)	68,82,82	1.12	5 (7%)
10	BPB	M	402	-	57,70,70	1.86	10 (17%)	55,101,101	2.15	11 (20%)
7	HTO	C	706	-	9,9,9	0.28	0	10,10,10	0.77	0
9	BCB	M	400	4	68,74,74	1.61	9 (13%)	77,115,115	1.90	18 (23%)
8	LDA	M	704	-	13,15,15	2.39	2 (15%)	14,17,17	0.44	0
13	MQ9	M	501	-	59,59,59	1.80	18 (30%)	73,75,75	1.57	21 (28%)
5	SO4	C	811	-	4,4,4	0.28	0	6,6,6	0.24	0
8	LDA	H	701	-	13,15,15	2.22	2 (15%)	14,17,17	0.47	0
5	SO4	C	808	-	4,4,4	0.22	0	6,6,6	0.20	0
5	SO4	M	804	-	4,4,4	0.26	0	6,6,6	0.29	0
9	BCB	M	401	4	68,74,74	1.60	10 (14%)	77,115,115	1.91	19 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	HEC	C	404	1	50,50,50	1.15	4 (8%)	68,82,82	1.30	6 (8%)
5	SO4	H	803	-	4,4,4	0.27	0	6,6,6	0.26	0
6	HEC	C	401	1	50,50,50	1.35	4 (8%)	68,82,82	1.15	5 (7%)
7	HTO	C	707	-	9,9,9	0.69	0	10,10,10	0.58	0
10	BPB	L	402	-	57,70,70	2.06	11 (19%)	55,101,101	2.10	15 (27%)
5	SO4	H	807	-	4,4,4	0.23	0	6,6,6	0.32	0
8	LDA	H	703	-	13,15,15	2.49	2 (15%)	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
6	HEC	C	402	1	1/1/3/7	6/14/54/54	-
7	HTO	H	705	-	-	8/10/10/10	-
8	LDA	L	702	-	-	11/13/13/13	-
9	BCB	L	401	3	2/2/21/26	9/41/137/137	-
14	NS5	M	600	-	-	14/43/43/43	-
11	UQ1	L	503	-	-	0/9/33/33	0/1/1/1
9	BCB	L	400	3	3/3/21/26	14/41/137/137	-
11	UQ1	L	502	-	-	3/9/33/33	0/1/1/1
6	HEC	C	403	1	1/1/3/7	7/14/54/54	-
10	BPB	M	402	-	-	15/37/105/105	0/5/6/6
7	HTO	C	706	-	-	5/10/10/10	-
9	BCB	M	400	4	2/2/21/26	12/41/137/137	-
8	LDA	M	704	-	-	9/13/13/13	-
13	MQ9	M	501	-	-	16/53/73/73	0/2/2/2
8	LDA	H	701	-	-	8/13/13/13	-
9	BCB	M	401	4	2/2/21/26	16/41/137/137	-
6	HEC	C	404	1	1/1/3/7	6/14/54/54	-
6	HEC	C	401	1	1/1/3/7	4/14/54/54	-
7	HTO	C	707	-	-	8/10/10/10	-
10	BPB	L	402	-	-	14/37/105/105	0/5/6/6
8	LDA	H	703	-	-	6/13/13/13	-

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	402	BPB	C1D-C2D	9.16	1.49	1.39
11	L	502	UQ1	C6-C5	8.27	1.50	1.35
11	L	503	UQ1	C6-C5	8.23	1.50	1.35
9	M	401	BCB	CAC-C3C	7.83	1.53	1.33
9	L	400	BCB	CAC-C3C	7.73	1.53	1.33
10	M	402	BPB	C1D-C2D	7.28	1.47	1.39
14	M	600	NS5	C35-C36	7.14	1.53	1.32
9	L	401	BCB	CAC-C3C	7.10	1.51	1.33
9	M	400	BCB	CAC-C3C	7.08	1.51	1.33
8	M	704	LDA	O1-N1	-7.05	1.24	1.42
8	L	702	LDA	O1-N1	-6.87	1.25	1.42
8	H	701	LDA	O1-N1	-6.60	1.26	1.42
8	H	703	LDA	C1-N1	-6.33	1.44	1.51
8	H	703	LDA	O1-N1	-6.28	1.26	1.42
10	L	402	BPB	C3A-C2A	-5.39	1.50	1.54
6	C	401	HEC	FE-NB	5.21	2.10	1.94
10	L	402	BPB	O2D-CGD	4.82	1.45	1.33
8	M	704	LDA	C1-N1	-4.77	1.46	1.51
10	M	402	BPB	O2A-CGA	4.61	1.46	1.33
9	M	400	BCB	O2A-CGA	4.54	1.46	1.33
9	M	400	BCB	C2C-C3C	-4.49	1.45	1.51
9	M	401	BCB	O2D-CGD	4.49	1.44	1.33
9	L	401	BCB	O2D-CGD	4.48	1.44	1.33
13	M	501	MQ9	C3-C4	-4.41	1.39	1.48
9	M	401	BCB	O2A-CGA	4.41	1.46	1.33
10	M	402	BPB	C3D-C2D	-4.35	1.32	1.39
8	H	701	LDA	C1-N1	-4.34	1.47	1.51
8	L	702	LDA	C1-N1	-4.26	1.47	1.51
9	L	400	BCB	O2A-CGA	4.14	1.45	1.33
10	L	402	BPB	O2A-CGA	4.12	1.45	1.33
11	L	503	UQ1	C3-C2	4.07	1.51	1.36
9	L	401	BCB	O2A-CGA	4.07	1.45	1.33
9	M	400	BCB	O2D-CGD	4.03	1.43	1.33
13	M	501	MQ9	C7-C8	-4.00	1.44	1.50
10	M	402	BPB	C1B-C2B	3.97	1.43	1.39
10	L	402	BPB	C3D-C4D	-3.96	1.35	1.41
10	M	402	BPB	C3D-C4D	-3.96	1.35	1.41
10	M	402	BPB	O2D-CGD	3.92	1.42	1.33
6	C	402	HEC	FE-NA	3.91	2.08	1.95
6	C	404	HEC	FE-NC	3.90	2.08	1.95
11	L	502	UQ1	C3-C2	3.86	1.50	1.36
6	C	402	HEC	FE-ND	3.80	2.06	1.94
9	L	400	BCB	O2D-CGD	3.80	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	403	HEC	FE-NB	3.79	2.06	1.94
10	L	402	BPB	C1B-C2B	3.75	1.43	1.39
9	M	400	BCB	MG-NA	3.67	2.15	2.06
10	M	402	BPB	C3A-C2A	-3.60	1.51	1.54
13	M	501	MQ9	C2-C1	-3.60	1.41	1.48
6	C	403	HEC	FE-ND	3.52	2.05	1.94
13	M	501	MQ9	C43-C44	3.46	1.41	1.33
10	L	402	BPB	C3D-C2D	-3.46	1.33	1.39
6	C	401	HEC	FE-ND	3.45	2.05	1.94
6	C	404	HEC	FE-ND	3.40	2.05	1.94
13	M	501	MQ9	C6-C1	-3.36	1.38	1.47
6	C	403	HEC	FE-NC	3.34	2.06	1.95
9	M	401	BCB	MG-NA	3.22	2.13	2.06
6	C	402	HEC	FE-NC	3.19	2.05	1.95
13	M	501	MQ9	C5-C4	-3.13	1.40	1.47
13	M	501	MQ9	C18-C19	3.03	1.40	1.33
9	M	400	BCB	MG-NC	3.01	2.13	2.06
14	M	600	NS5	C4-C5	2.99	1.57	1.51
6	C	401	HEC	FE-NC	2.95	2.04	1.95
9	L	401	BCB	MG-NC	2.91	2.13	2.06
10	L	402	BPB	C1D-ND	2.90	1.43	1.38
13	M	501	MQ9	C38-C39	2.90	1.39	1.33
13	M	501	MQ9	C13-C14	2.89	1.39	1.33
10	M	402	BPB	C1D-ND	2.87	1.43	1.38
10	L	402	BPB	C2-C3	2.84	1.39	1.33
13	M	501	MQ9	C28-C29	2.76	1.39	1.33
13	M	501	MQ9	C23-C24	2.73	1.39	1.33
6	C	404	HEC	FE-NB	2.71	2.03	1.94
6	C	401	HEC	FE-NA	2.65	2.03	1.95
9	L	400	BCB	MG-NC	2.63	2.12	2.06
9	L	401	BCB	C2C-C3C	-2.61	1.48	1.51
9	L	400	BCB	MG-NA	2.57	2.12	2.06
14	M	600	NS5	C7-C5	2.55	1.38	1.33
13	M	501	MQ9	C48-C49	2.54	1.40	1.32
13	M	501	MQ9	C8-C9	2.54	1.38	1.33
13	M	501	MQ9	C32-C33	-2.52	1.42	1.50
10	M	402	BPB	C2-C3	2.51	1.38	1.33
9	M	401	BCB	C3A-C2A	-2.48	1.47	1.54
13	M	501	MQ9	C27-C28	-2.45	1.43	1.50
9	L	400	BCB	C2-C3	2.39	1.38	1.33
9	L	401	BCB	C1-C2	-2.39	1.42	1.49
13	M	501	MQ9	C22-C23	-2.33	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	401	BCB	C1-C2	-2.32	1.42	1.49
10	M	402	BPB	C3B-C2B	-2.31	1.35	1.39
9	M	401	BCB	C4C-C3C	2.29	1.49	1.44
9	M	401	BCB	C2C-C3C	-2.28	1.48	1.51
13	M	501	MQ9	C17-C18	-2.27	1.43	1.50
9	L	401	BCB	MG-NA	2.26	2.11	2.06
6	C	402	HEC	FE-NB	2.25	2.01	1.94
13	M	501	MQ9	C6-C5	2.25	1.39	1.35
9	M	401	BCB	MG-ND	-2.24	2.01	2.05
9	M	400	BCB	C2-C3	2.20	1.38	1.33
9	M	400	BCB	C4C-C3C	2.19	1.49	1.44
9	L	400	BCB	C3A-C2A	-2.15	1.48	1.54
9	L	400	BCB	C2C-C3C	-2.15	1.49	1.51
9	M	400	BCB	C1-C2	-2.13	1.43	1.49
10	L	402	BPB	C3B-C2B	-2.12	1.36	1.39
9	L	400	BCB	C3B-C2B	-2.04	1.35	1.42
10	L	402	BPB	CHA-CBD	2.03	1.54	1.51
9	M	401	BCB	C3B-C2B	-2.03	1.35	1.42
6	C	404	HEC	FE-NA	2.03	2.01	1.95
9	L	400	BCB	C1-C2	-2.03	1.43	1.49

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	402	BPB	O2D-CGD-CBD	9.48	121.37	110.95
9	L	400	BCB	C1C-NC-C4C	9.07	110.82	106.68
10	L	402	BPB	O2D-CGD-CBD	7.98	119.71	110.95
9	L	400	BCB	C4A-NA-C1A	7.08	109.91	106.68
9	M	400	BCB	C4A-NA-C1A	6.97	109.86	106.68
10	M	402	BPB	C3D-C4D-ND	-6.90	98.86	107.71
9	L	401	BCB	C4A-NA-C1A	6.83	109.79	106.68
9	L	401	BCB	C1C-NC-C4C	6.55	109.67	106.68
10	L	402	BPB	C3D-C4D-ND	-6.47	99.41	107.71
9	M	401	BCB	C4A-NA-C1A	5.90	109.37	106.68
9	L	401	BCB	O2D-CGD-CBD	5.65	121.11	111.23
9	M	401	BCB	C1C-NC-C4C	5.62	109.24	106.68
9	M	400	BCB	O2D-CGD-CBD	5.45	120.76	111.23
14	M	600	NS5	C19-C20-C21	-5.37	119.75	127.28
9	L	400	BCB	C1D-ND-C4D	5.29	110.02	106.31
9	M	401	BCB	O2D-CGD-CBD	5.04	120.05	111.23
9	M	400	BCB	C1C-NC-C4C	4.87	108.90	106.68
10	M	402	BPB	CMD-C2D-C3D	4.61	133.89	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	L	400	BCB	O2D-CGD-CBD	4.32	118.78	111.23
9	M	400	BCB	C1D-ND-C4D	4.31	109.33	106.31
10	L	402	BPB	CMD-C2D-C3D	4.18	133.04	124.68
14	M	600	NS5	C34-C35-C36	-4.18	113.69	127.64
9	L	401	BCB	C1-C2-C3	-4.11	119.46	126.20
10	L	402	BPB	O1D-CGD-CBD	-3.93	118.76	124.72
14	M	600	NS5	CM4-C36-C35	-3.89	110.97	122.66
9	M	401	BCB	C1D-ND-C4D	3.85	109.01	106.31
14	M	600	NS5	CM3-C36-C35	-3.84	111.13	122.66
9	L	401	BCB	C1D-ND-C4D	3.81	108.99	106.31
10	M	402	BPB	O1D-CGD-CBD	-3.78	118.98	124.72
9	L	400	BCB	CHA-C4D-ND	3.73	140.25	132.55
13	M	501	MQ9	C32-C33-C34	-3.70	119.15	127.62
9	M	401	BCB	C1-C2-C3	-3.70	120.14	126.20
9	M	401	BCB	C2A-C1A-CHA	3.63	130.16	123.87
9	M	400	BCB	CHA-C4D-ND	3.59	139.95	132.55
9	L	401	BCB	CHA-C4D-ND	3.51	139.79	132.55
9	L	401	BCB	C4-C3-C5	3.51	121.31	115.23
11	L	502	UQ1	C7-C8-C9	-3.50	117.36	127.25
14	M	600	NS5	C29-C30-C31	-3.43	122.87	127.69
13	M	501	MQ9	C35-C34-C36	3.39	121.11	115.23
11	L	502	UQ1	C7-C6-C5	-3.36	119.14	124.89
9	M	401	BCB	CHA-C4D-ND	3.34	139.44	132.55
9	M	400	BCB	C4-C3-C5	3.29	120.94	115.23
14	M	600	NS5	C6-C5-C4	3.24	120.86	115.23
13	M	501	MQ9	C5M-C5-C6	-3.19	119.20	124.45
9	M	400	BCB	O2A-CGA-CBA	3.15	121.45	111.83
9	L	401	BCB	CBC-CAC-C3C	-3.14	118.17	126.70
10	L	402	BPB	O2A-CGA-CBA	3.14	121.41	111.83
9	M	400	BCB	C1-C2-C3	-3.13	121.08	126.20
9	M	400	BCB	CBC-CAC-C3C	-3.07	118.37	126.70
14	M	600	NS5	C18-C17-C15	-3.05	123.00	127.28
10	M	402	BPB	CMA-C3A-C4A	-3.03	108.07	114.61
11	L	503	UQ1	C7-C6-C5	-2.99	119.77	124.89
9	L	400	BCB	C2D-C1D-ND	-2.98	107.17	110.13
6	C	404	HEC	C3D-C4D-ND	-2.97	107.48	110.35
14	M	600	NS5	C13-C12-C10	-2.96	123.52	127.69
9	L	400	BCB	O2A-CGA-CBA	2.93	120.76	111.83
9	L	401	BCB	O1D-CGD-CBD	-2.92	118.76	124.52
9	L	401	BCB	O2A-CGA-CBA	2.92	120.73	111.83
10	M	402	BPB	O2A-CGA-CBA	2.91	120.69	111.83
9	M	401	BCB	CBC-CAC-C3C	-2.90	118.84	126.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	M	401	BCB	C4-C3-C5	2.88	120.23	115.23
9	M	400	BCB	O2D-CGD-O1D	-2.87	118.25	123.85
13	M	501	MQ9	C12-C13-C14	-2.87	121.06	127.62
6	C	404	HEC	C2A-C1A-NA	-2.86	107.56	110.32
11	L	502	UQ1	CM5-C5-C6	-2.86	119.75	124.45
14	M	600	NS5	C12-C13-C14	-2.83	115.00	123.20
10	M	402	BPB	C2B-C1B-NB	-2.81	107.40	109.43
6	C	402	HEC	C4B-NB-C1B	2.78	108.50	105.21
9	L	400	BCB	CAA-CBA-CGA	-2.77	105.35	113.21
9	M	401	BCB	O2A-CGA-CBA	2.76	120.25	111.83
14	M	600	NS5	C32-C31-C33	2.75	120.00	115.23
10	L	402	BPB	C2B-C1B-NB	-2.74	107.45	109.43
11	L	503	UQ1	CM5-C5-C6	-2.73	119.95	124.45
13	M	501	MQ9	C7-C6-C5	-2.72	120.23	124.89
6	C	401	HEC	C2A-C1A-NA	-2.71	107.70	110.32
13	M	501	MQ9	C17-C18-C19	-2.70	121.43	127.62
6	C	401	HEC	C1D-ND-C4D	2.69	108.40	105.21
6	C	404	HEC	CAD-CBD-CGD	-2.69	106.53	113.67
9	L	400	BCB	CBC-CAC-C3C	-2.67	119.45	126.70
6	C	402	HEC	C1D-ND-C4D	2.66	108.36	105.21
14	M	600	NS5	C11-C10-C9	2.66	119.84	115.23
13	M	501	MQ9	C27-C28-C29	-2.64	121.57	127.62
9	M	401	BCB	C6-C5-C3	-2.63	107.07	113.47
9	L	400	BCB	C6-C5-C3	-2.60	107.14	113.47
13	M	501	MQ9	C20-C19-C21	2.60	119.73	115.23
10	L	402	BPB	C6-C7-C8	-2.58	107.38	115.97
9	M	401	BCB	O2D-CGD-O1D	-2.56	118.86	123.85
6	C	404	HEC	C4B-NB-C1B	2.54	108.21	105.21
13	M	501	MQ9	C15-C14-C16	2.53	119.62	115.23
13	M	501	MQ9	C22-C23-C24	-2.53	121.83	127.62
6	C	403	HEC	C2A-C1A-NA	-2.52	107.89	110.32
13	M	501	MQ9	C37-C38-C39	-2.52	121.86	127.62
13	M	501	MQ9	C7-C8-C9	-2.51	122.51	126.83
9	L	400	BCB	C2A-C1A-CHA	2.51	128.22	123.87
13	M	501	MQ9	C10-C9-C11	2.50	119.57	115.23
9	L	400	BCB	C6-C7-C8	-2.48	107.71	115.97
6	C	404	HEC	C1D-ND-C4D	2.48	108.15	105.21
9	L	400	BCB	C2B-C1B-NB	-2.48	107.76	110.33
11	L	503	UQ1	C11-C9-C10	2.46	120.26	114.59
14	M	600	NS5	C30-C29-C28	-2.46	116.08	123.20
6	C	403	HEC	C4B-NB-C1B	2.45	108.11	105.21
9	L	400	BCB	C4-C3-C5	2.45	119.48	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	403	HEC	C1D-ND-C4D	2.45	108.10	105.21
9	M	401	BCB	C2D-C1D-ND	-2.43	107.72	110.13
9	M	401	BCB	CGD-CBD-CAD	-2.42	103.00	110.85
9	L	400	BCB	CGD-CBD-CAD	-2.38	103.13	110.85
9	L	400	BCB	C1-C2-C3	-2.38	122.30	126.20
14	M	600	NS5	C24-C25-C26	-2.38	123.94	127.28
10	L	402	BPB	C1-C2-C3	-2.37	122.31	126.20
9	L	400	BCB	O2D-CGD-O1D	-2.37	119.23	123.85
10	L	402	BPB	CED-O2D-CGD	2.35	121.24	115.92
9	M	400	BCB	C2D-C1D-ND	-2.35	107.81	110.13
14	M	600	NS5	C6-C5-C7	-2.34	117.61	123.63
10	M	402	BPB	CAA-CBA-CGA	-2.34	106.57	113.21
6	C	402	HEC	C3B-C4B-NB	-2.33	107.62	110.17
10	L	402	BPB	C4-C3-C5	2.30	119.22	115.23
9	M	401	BCB	C6-C7-C8	-2.30	108.33	115.97
10	L	402	BPB	CMA-C3A-C4A	-2.28	109.69	114.61
9	M	400	BCB	C2B-C1B-NB	-2.28	107.97	110.33
11	L	502	UQ1	C7-C6-C1	2.28	121.16	118.52
6	C	404	HEC	CAD-C3D-C2D	-2.27	123.61	127.87
13	M	501	MQ9	C30-C29-C31	2.27	119.17	115.23
9	L	400	BCB	C3A-C2A-C1A	2.26	104.73	101.34
10	L	402	BPB	CAA-CBA-CGA	-2.25	106.81	113.21
9	L	401	BCB	C2D-C1D-ND	-2.25	107.90	110.13
9	L	401	BCB	O2A-CGA-O1A	-2.25	118.01	123.63
13	M	501	MQ9	C40-C39-C41	2.23	119.10	115.23
6	C	402	HEC	C2A-C1A-NA	-2.23	108.17	110.32
6	C	402	HEC	C3D-C4D-ND	-2.22	108.21	110.35
9	M	401	BCB	C2B-C1B-NB	-2.20	108.05	110.33
6	C	402	HEC	CHB-C1B-NB	2.19	126.78	124.42
9	M	400	BCB	CGD-CBD-CAD	-2.19	103.75	110.85
9	M	400	BCB	C3C-C4C-NC	-2.18	107.75	110.45
6	C	402	HEC	C2B-C1B-NB	-2.18	107.39	109.90
6	C	401	HEC	C3C-C4C-NC	-2.17	107.75	110.15
9	M	401	BCB	C11-C10-C8	-2.17	108.77	115.97
6	C	403	HEC	C3D-C4D-ND	-2.16	108.26	110.35
10	M	402	BPB	O2D-CGD-O1D	-2.16	119.64	123.85
6	C	402	HEC	C2D-C1D-ND	-2.15	107.37	109.84
13	M	501	MQ9	C25-C24-C26	2.14	118.95	115.23
6	C	401	HEC	C3D-C4D-ND	-2.14	108.28	110.35
9	M	401	BCB	C3A-C2A-C1A	2.13	104.53	101.34
13	M	501	MQ9	C42-C43-C44	-2.13	122.74	127.62
9	L	401	BCB	CHC-C4B-NB	2.12	127.23	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	M	400	BCB	CHC-C4B-NB	2.12	127.23	124.05
13	M	501	MQ9	C8-C7-C6	-2.12	106.86	112.08
11	L	503	UQ1	C7-C8-C9	-2.12	121.26	127.25
6	C	403	HEC	C3B-C4B-NB	-2.12	107.85	110.17
13	M	501	MQ9	C51-C49-C50	2.12	119.46	114.59
10	L	402	BPB	C11-C10-C8	-2.11	108.95	115.97
11	L	502	UQ1	C11-C9-C10	2.10	119.42	114.59
9	M	400	BCB	C2A-C1A-CHA	2.10	127.50	123.87
9	M	400	BCB	C2A-C3A-C4A	2.09	105.24	101.87
10	M	402	BPB	C4-C3-C5	2.08	118.84	115.23
9	M	401	BCB	C11-C12-C13	-2.08	109.06	115.97
9	M	400	BCB	C6-C7-C8	-2.07	109.10	115.97
6	C	401	HEC	C4B-NB-C1B	2.07	107.65	105.21
10	M	402	BPB	C1-C2-C3	-2.06	122.81	126.20
13	M	501	MQ9	C47-C48-C49	-2.06	120.77	127.64
10	L	402	BPB	C16-C15-C13	-2.05	109.16	115.97
9	L	401	BCB	C6-C5-C3	-2.05	108.48	113.47
10	L	402	BPB	C11-C12-C13	-2.02	109.24	115.97
6	C	402	HEC	C3C-C4C-NC	-2.02	107.92	110.15
9	L	401	BCB	C16-C15-C13	-2.01	109.27	115.97
13	M	501	MQ9	C35-C34-C33	-2.01	118.47	123.63

All (13) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	401	HEC	NA
6	C	402	HEC	NA
6	C	403	HEC	NA
6	C	404	HEC	NA
9	L	400	BCB	NC
9	L	400	BCB	NA
9	L	400	BCB	ND
9	L	401	BCB	NC
9	L	401	BCB	NA
9	M	400	BCB	NC
9	M	400	BCB	NA
9	M	401	BCB	NC
9	M	401	BCB	NA

All (191) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
8	M	704	LDA	C2-C1-N1-CM1
8	M	704	LDA	C2-C1-N1-CM2
9	L	400	BCB	C1A-C2A-CAA-CBA
9	L	401	BCB	CHA-CBD-CGD-O1D
9	L	401	BCB	CHA-CBD-CGD-O2D
9	M	400	BCB	C2C-C3C-CAC-CBC
9	M	401	BCB	C2C-C3C-CAC-CBC
9	M	401	BCB	CAD-CBD-CGD-O1D
9	M	401	BCB	CAD-CBD-CGD-O2D
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-CM4
13	M	501	MQ9	C47-C48-C49-C50
14	M	600	NS5	C34-C35-C36-CM3
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
6	C	401	HEC	C2B-C3B-CAB-CBB
13	M	501	MQ9	C14-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
14	M	600	NS5	C31-C33-C34-C35
6	C	403	HEC	C2C-C3C-CAC-CBC
9	L	400	BCB	C4-C3-C5-C6
9	L	400	BCB	C2-C3-C5-C6
9	M	401	BCB	C2A-CAA-CBA-CGA
6	C	403	HEC	C4C-C3C-CAC-CBC
7	H	705	HTO	O1-C1-C2-O2
13	M	501	MQ9	C29-C31-C32-C33
13	M	501	MQ9	C34-C36-C37-C38
13	M	501	MQ9	C39-C41-C42-C43
10	L	402	BPB	C8-C10-C11-C12
10	M	402	BPB	C8-C10-C11-C12
9	M	401	BCB	C13-C15-C16-C17
6	C	401	HEC	C4B-C3B-CAB-CBB
9	M	400	BCB	C13-C15-C16-C17
9	L	400	BCB	C15-C16-C17-C18
6	C	402	HEC	C2C-C3C-CAC-CBC
9	L	400	BCB	C8-C10-C11-C12
10	L	402	BPB	C16-C17-C18-C19
8	L	702	LDA	C5-C6-C7-C8
8	H	703	LDA	C2-C3-C4-C5
8	L	702	LDA	C11-C10-C9-C8
10	L	402	BPB	C16-C17-C18-C20
10	L	402	BPB	C3A-C2A-CAA-CBA
7	H	705	HTO	O1-C1-C2-C3
8	M	704	LDA	C5-C6-C7-C8
8	H	703	LDA	C6-C7-C8-C9
9	M	401	BCB	C3-C5-C6-C7
8	M	704	LDA	C1-C2-C3-C4
8	L	702	LDA	C6-C7-C8-C9
8	H	703	LDA	C1-C2-C3-C4
6	C	404	HEC	C4D-C3D-CAD-CBD
14	M	600	NS5	C13-C14-C15-C16
10	M	402	BPB	C16-C17-C18-C19
8	L	702	LDA	C3-C4-C5-C6
8	H	703	LDA	C11-C10-C9-C8
10	M	402	BPB	C3-C5-C6-C7
9	L	401	BCB	C15-C16-C17-C18
9	L	400	BCB	C3-C5-C6-C7
8	L	702	LDA	C4-C5-C6-C7
8	H	701	LDA	C6-C7-C8-C9
10	M	402	BPB	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
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
10	M	402	BPB	C16-C17-C18-C20
9	M	400	BCB	C8-C10-C11-C12
9	M	401	BCB	C5-C6-C7-C8
9	M	401	BCB	C8-C10-C11-C12
9	M	400	BCB	C11-C10-C8-C9
9	M	400	BCB	C14-C13-C15-C16
9	M	401	BCB	C11-C12-C13-C14
7	H	705	HTO	O3-C3-C4-C5
7	H	705	HTO	O2-C2-C3-O3
8	M	704	LDA	C7-C8-C9-C10
10	L	402	BPB	O2A-C1-C2-C3
8	H	701	LDA	C7-C8-C9-C10
6	C	404	HEC	C2D-C3D-CAD-CBD
8	H	703	LDA	C9-C10-C11-C12
7	H	705	HTO	C4-C5-C6-C7
10	L	402	BPB	C6-C7-C8-C9
10	M	402	BPB	C6-C7-C8-C9
6	C	402	HEC	C4C-C3C-CAC-CBC
9	L	400	BCB	C11-C12-C13-C15
9	L	401	BCB	C11-C10-C8-C7
9	M	400	BCB	C12-C13-C15-C16
9	L	400	BCB	C3A-C2A-CAA-CBA
8	H	701	LDA	C9-C10-C11-C12
10	L	402	BPB	C1A-C2A-CAA-CBA
11	L	502	UQ1	C2-C3-O3-CM3
8	M	704	LDA	C3-C4-C5-C6
9	M	401	BCB	C6-C7-C8-C9
8	M	704	LDA	C9-C10-C11-C12
14	M	600	NS5	C7-C8-C9-C10
9	L	401	BCB	C11-C10-C8-C9
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
13	M	501	MQ9	C45-C44-C46-C47
7	C	706	HTO	O3-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
9	M	400	BCB	C16-C17-C18-C19
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	C16-C17-C18-C20
8	H	701	LDA	C4-C5-C6-C7
14	M	600	NS5	C11-C10-C9-C8
9	L	400	BCB	C11-C12-C13-C14
8	H	701	LDA	C2-C1-N1-O1
10	M	402	BPB	CAD-CBD-CGD-O2D
10	M	402	BPB	CAD-CBD-CGD-O1D
9	M	400	BCB	C16-C17-C18-C20
9	L	400	BCB	C6-C7-C8-C9
9	L	401	BCB	C11-C12-C13-C14
9	L	401	BCB	C12-C13-C15-C16
8	H	701	LDA	C5-C6-C7-C8
8	M	704	LDA	N1-C1-C2-C3
6	C	403	HEC	C2B-C3B-CAB-CBB
11	L	502	UQ1	C5-C6-C7-C8
7	C	706	HTO	C2-C3-C4-C5
7	C	707	HTO	C2-C3-C4-C5
7	H	705	HTO	C2-C3-C4-C5
10	M	402	BPB	C11-C12-C13-C14
11	L	502	UQ1	C1-C2-O2-CM2
9	M	401	BCB	C16-C17-C18-C20
6	C	402	HEC	CAA-CBA-CGA-O1A
6	C	402	HEC	CAA-CBA-CGA-O2A
14	M	600	NS5	C12-C10-C9-C8
9	L	401	BCB	C14-C13-C15-C16
8	L	702	LDA	C7-C8-C9-C10
6	C	404	HEC	C2C-C3C-CAC-CBC
10	L	402	BPB	C11-C12-C13-C15
10	M	402	BPB	C12-C13-C15-C16
10	M	402	BPB	C4-C3-C5-C6
13	M	501	MQ9	C38-C39-C41-C42
9	M	401	BCB	C16-C17-C18-C19
6	C	402	HEC	CAD-CBD-CGD-O2D
6	C	403	HEC	CAA-CBA-CGA-O2A
6	C	404	HEC	CAD-CBD-CGD-O2D
9	M	400	BCB	C6-C7-C8-C9
10	L	402	BPB	C11-C12-C13-C14
10	M	402	BPB	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
6	C	401	HEC	CAA-CBA-CGA-O2A
6	C	402	HEC	CAD-CBD-CGD-O1D
6	C	401	HEC	CAA-CBA-CGA-O1A
6	C	403	HEC	CAA-CBA-CGA-O1A
13	M	501	MQ9	C9-C11-C12-C13
14	M	600	NS5	C23-C24-C25-C26
6	C	404	HEC	CAD-CBD-CGD-O1D
14	M	600	NS5	C13-C14-C15-C17
9	M	400	BCB	C6-C7-C8-C10
9	M	401	BCB	C11-C10-C8-C7
6	C	403	HEC	C4B-C3B-CAB-CBB
7	C	707	HTO	C4-C5-C6-C7
9	M	401	BCB	C11-C10-C8-C9
6	C	404	HEC	C2B-C3B-CAB-CBB
10	L	402	BPB	C2-C3-C5-C6
9	L	400	BCB	C16-C17-C18-C19
7	C	707	HTO	C3-C4-C5-C6
10	L	402	BPB	C4-C3-C5-C6
10	M	402	BPB	C14-C13-C15-C16
9	L	400	BCB	C5-C6-C7-C8
10	L	402	BPB	C13-C15-C16-C17
6	C	403	HEC	CAD-CBD-CGD-O2D

There are no ring outliers.

19 monomers are involved in 119 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	402	HEC	9	0
7	H	705	HTO	2	0
8	L	702	LDA	2	0
9	L	401	BCB	9	0
14	M	600	NS5	11	0
5	M	805	SO4	1	0
9	L	400	BCB	17	0
11	L	502	UQ1	2	0
6	C	403	HEC	5	0
10	M	402	BPB	20	0
7	C	706	HTO	1	0
9	M	400	BCB	10	0
13	M	501	MQ9	2	0
9	M	401	BCB	15	0
6	C	404	HEC	2	0

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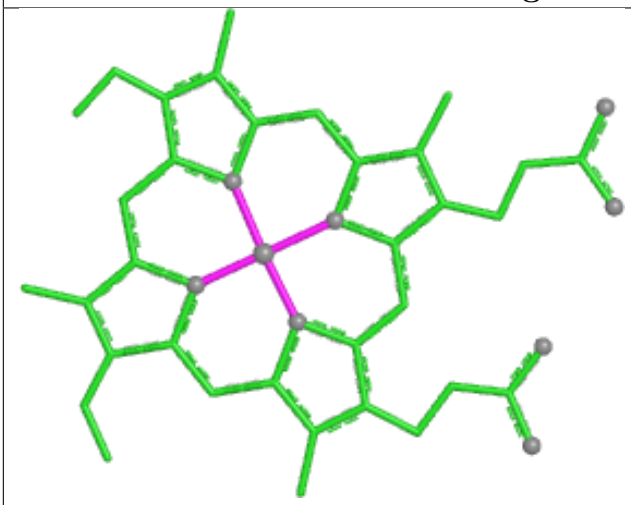
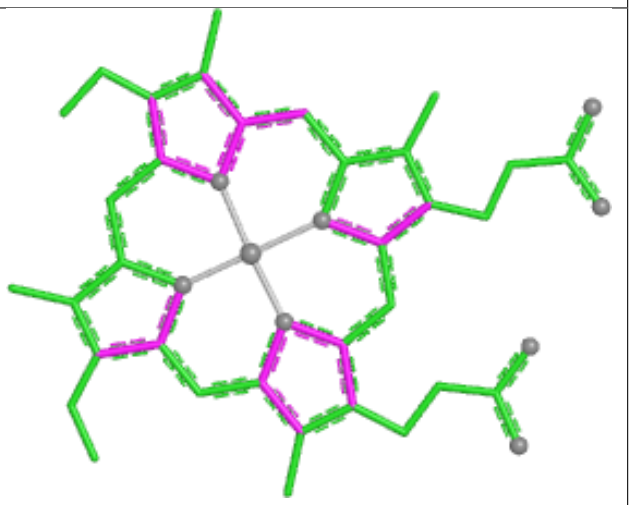
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	401	HEC	12	0
10	L	402	BPB	8	0
5	H	807	SO4	1	0
8	H	703	LDA	6	0

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.

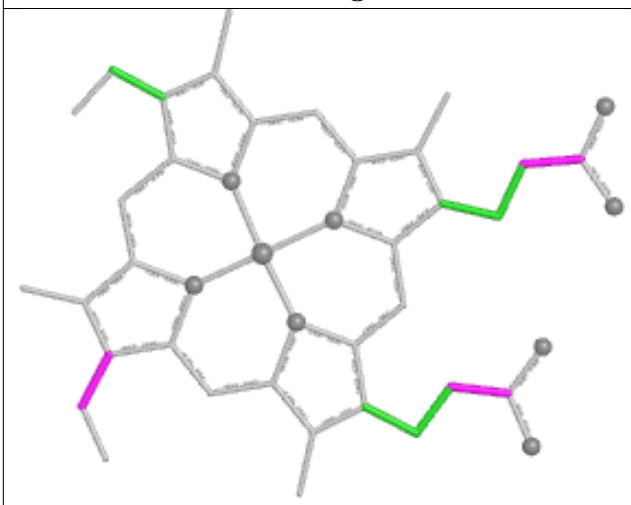
Ligand HEC C 402



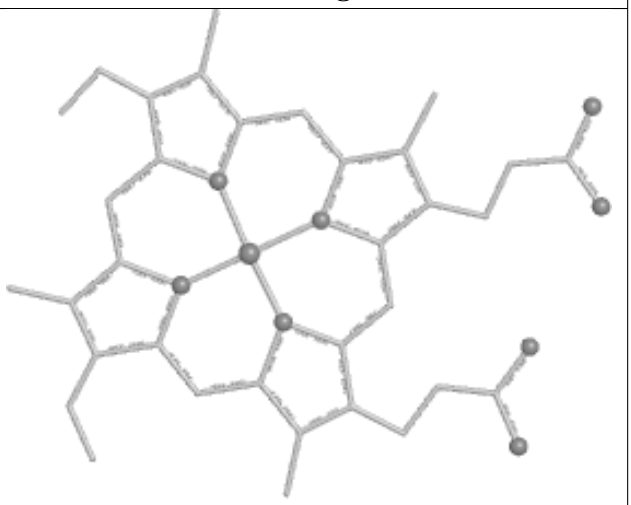
Bond lengths



Bond angles

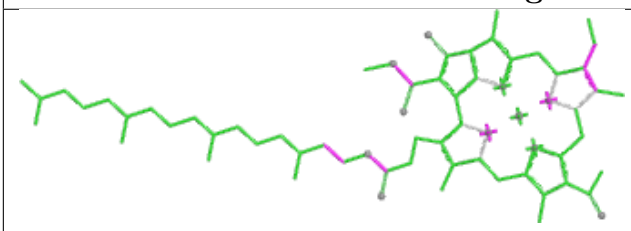


Torsions

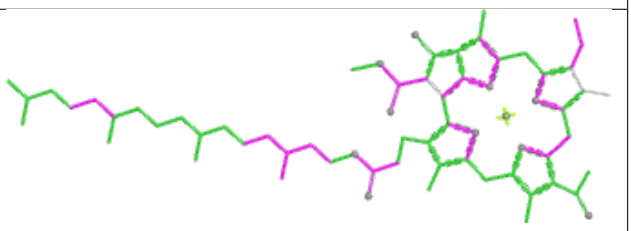


Rings

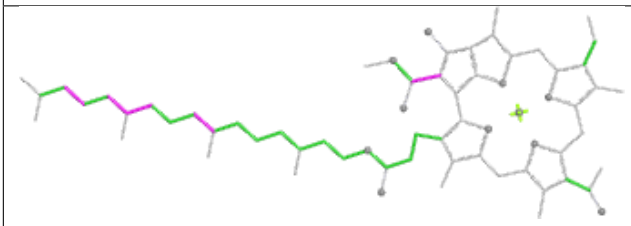
Ligand BCB L 401



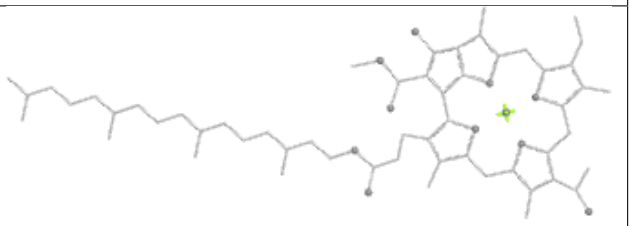
Bond lengths



Bond angles

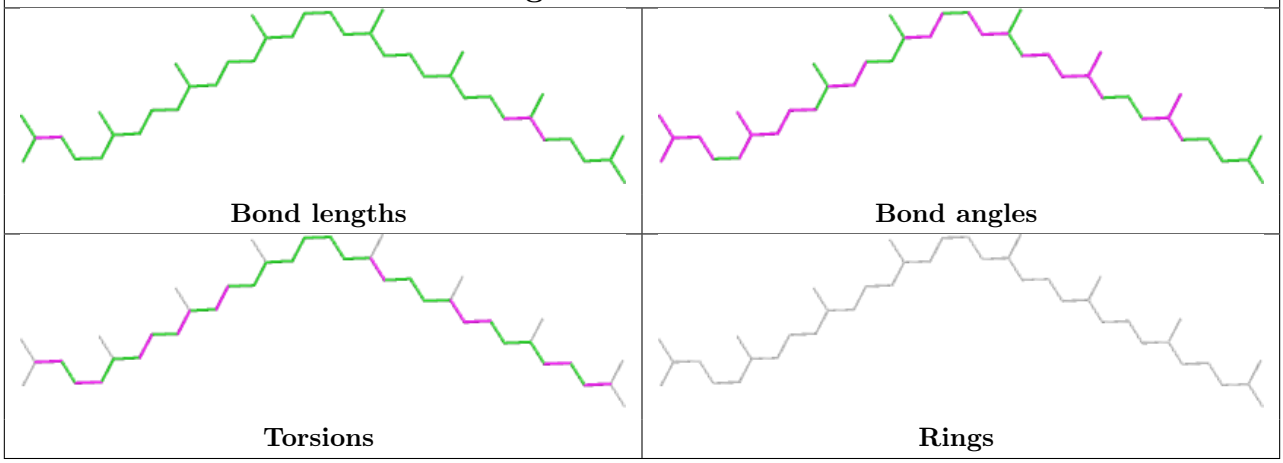


Torsions

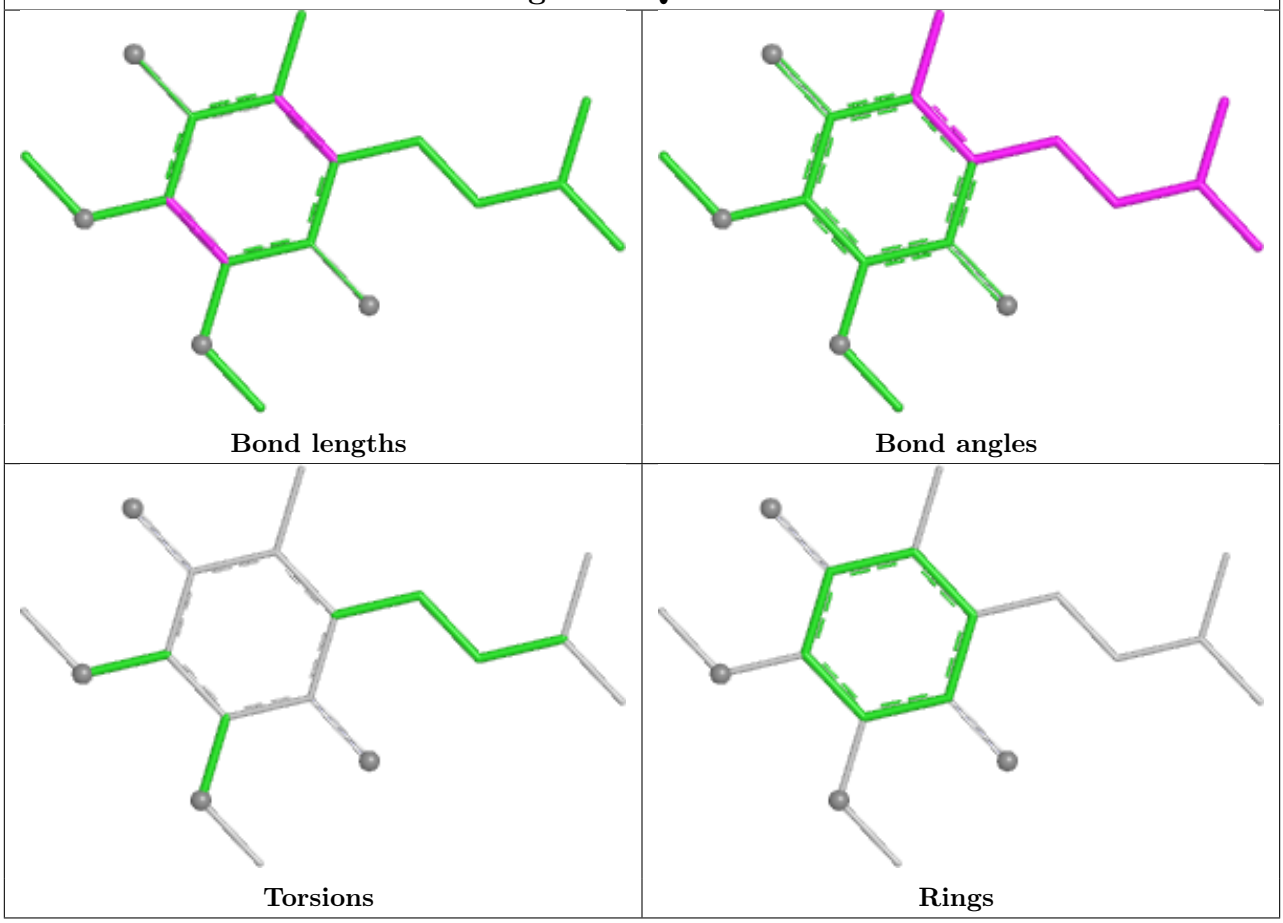


Rings

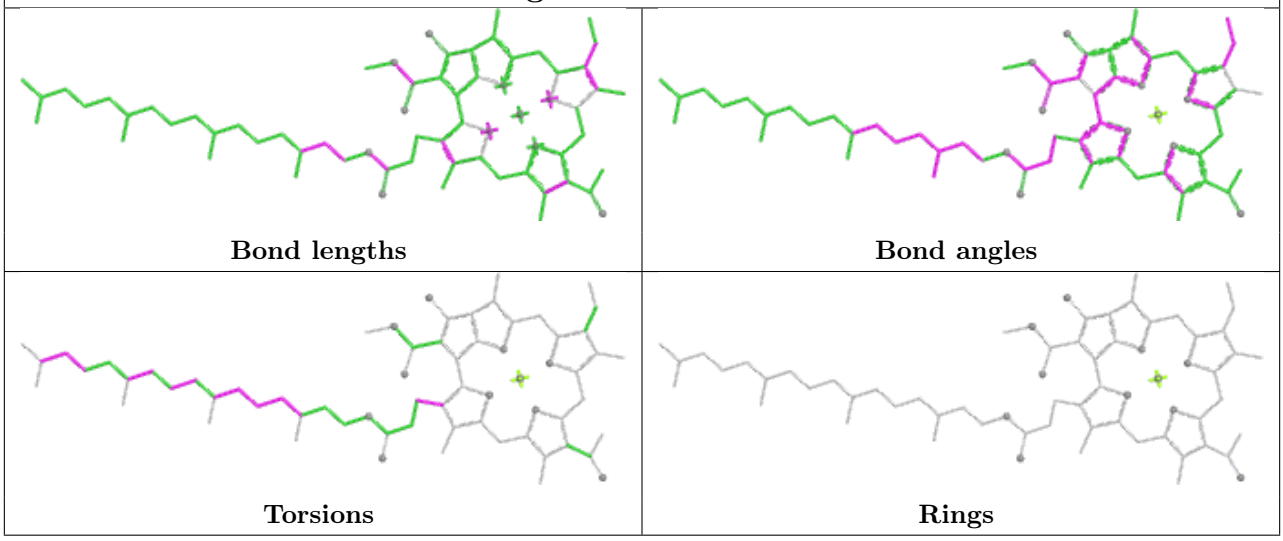
Ligand NS5 M 600



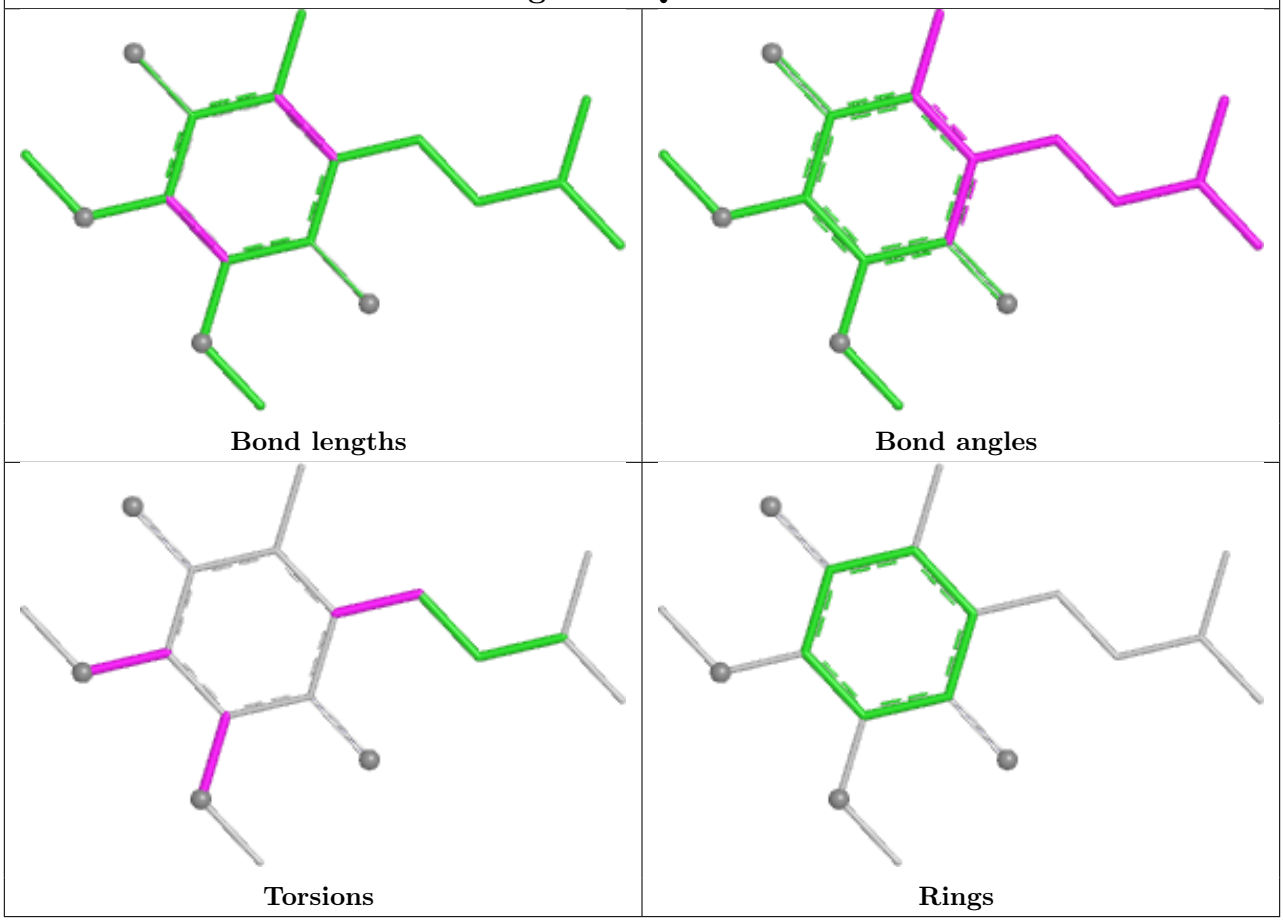
Ligand UQ1 L 503



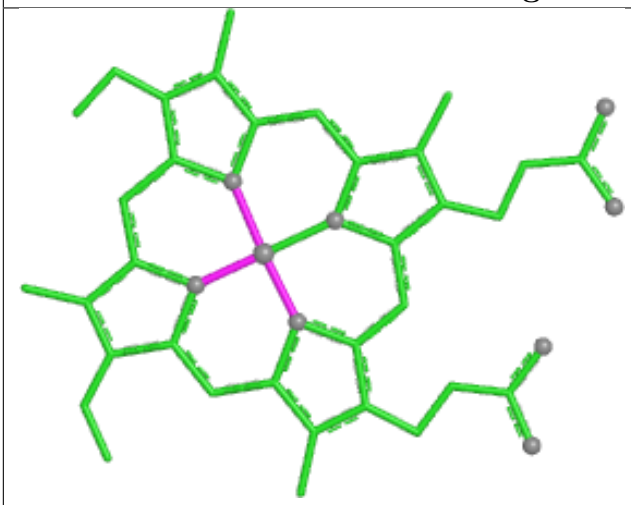
Ligand BCB L 400



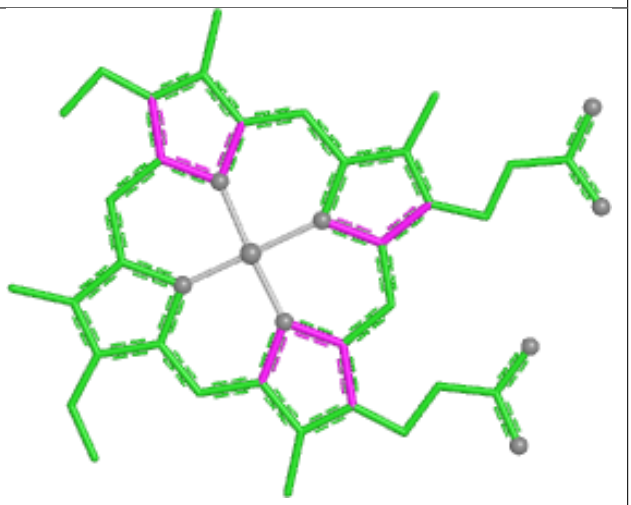
Ligand UQ1 L 502



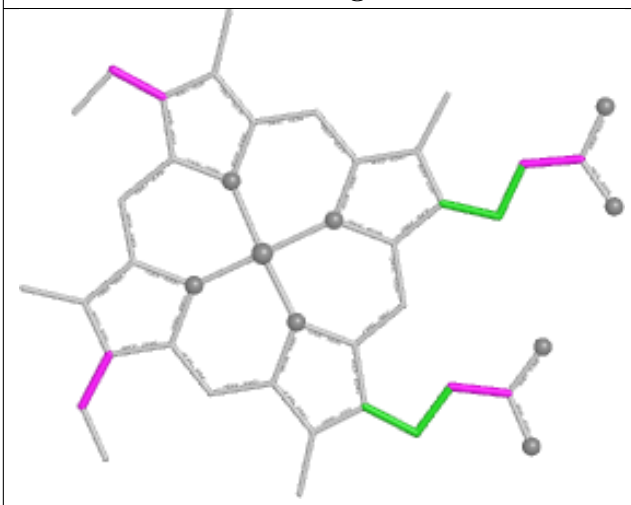
Ligand HEC C 403



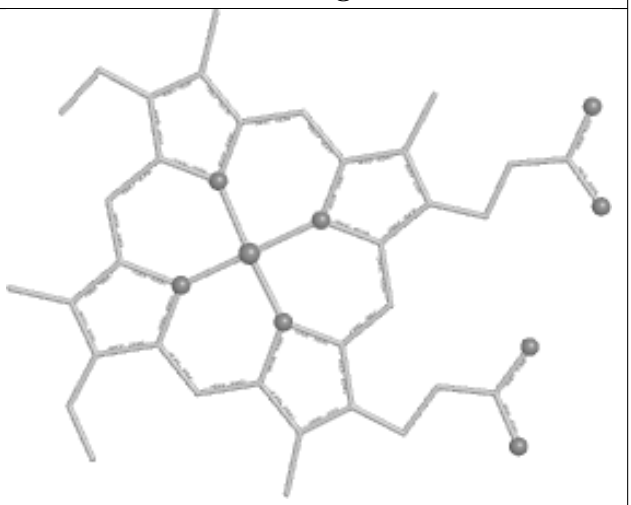
Bond lengths



Bond angles

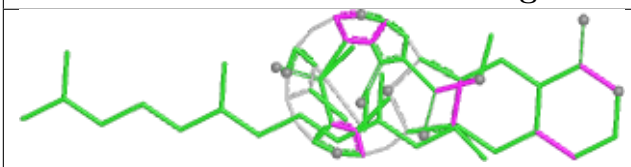


Torsions



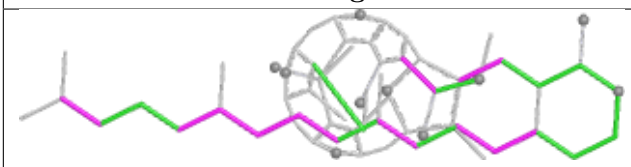
Rings

Ligand BPB M 402

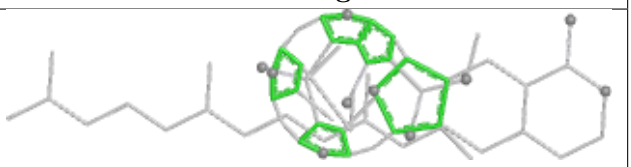


Bond lengths

Bond angles

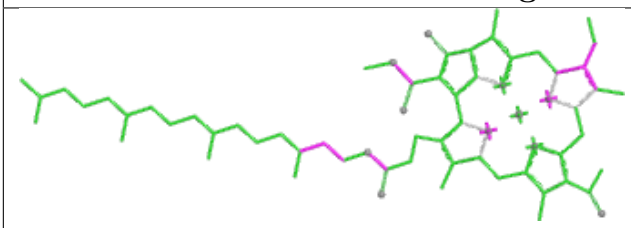


Torsions

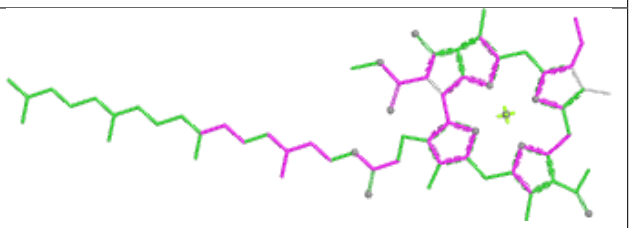


Rings

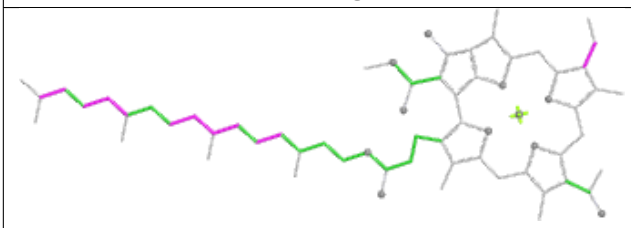
Ligand BCB M 400



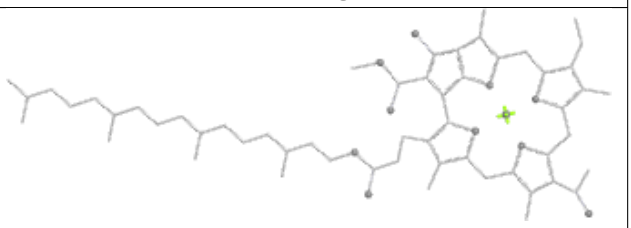
Bond lengths



Bond angles

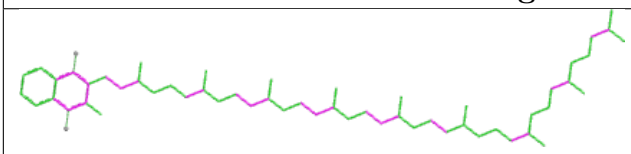


Torsions

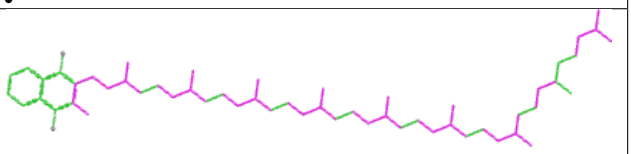


Rings

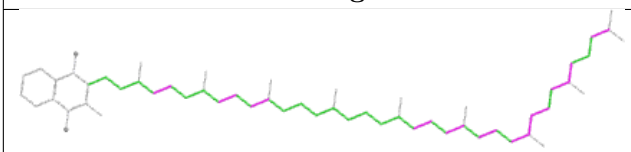
Ligand MQ9 M 501



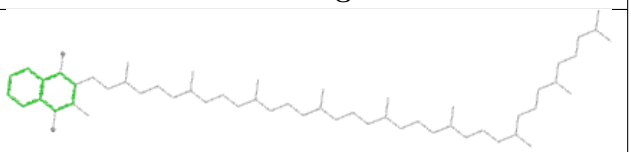
Bond lengths



Bond angles

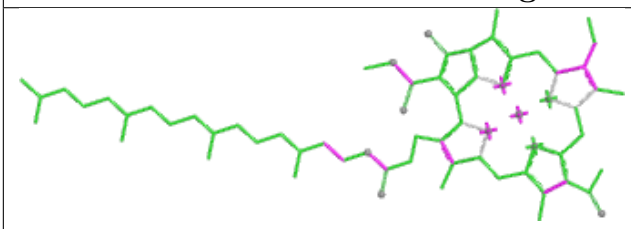


Torsions

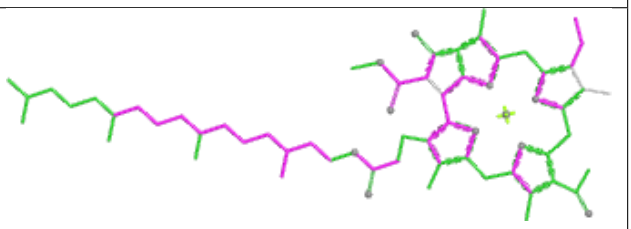


Rings

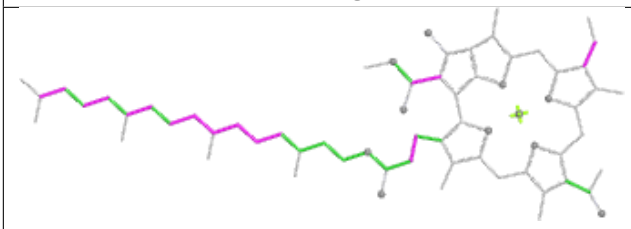
Ligand BCB M 401



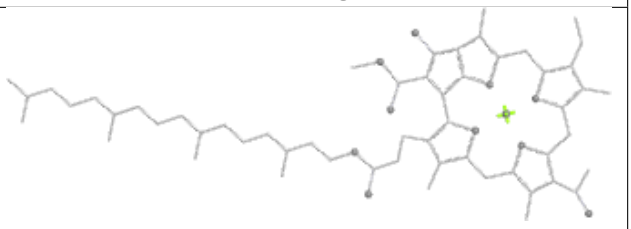
Bond lengths



Bond angles

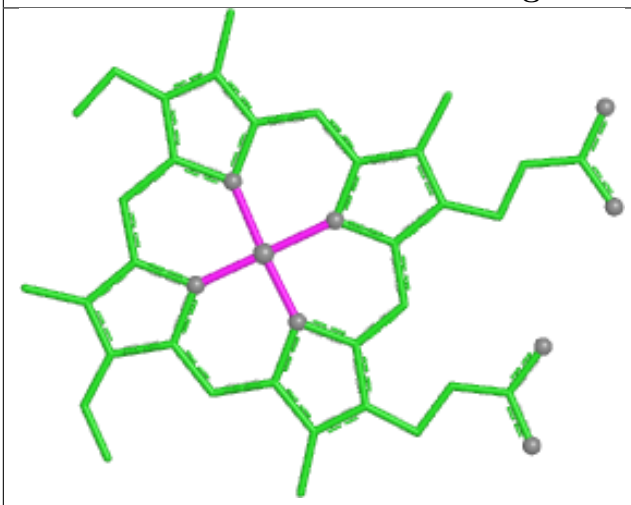


Torsions

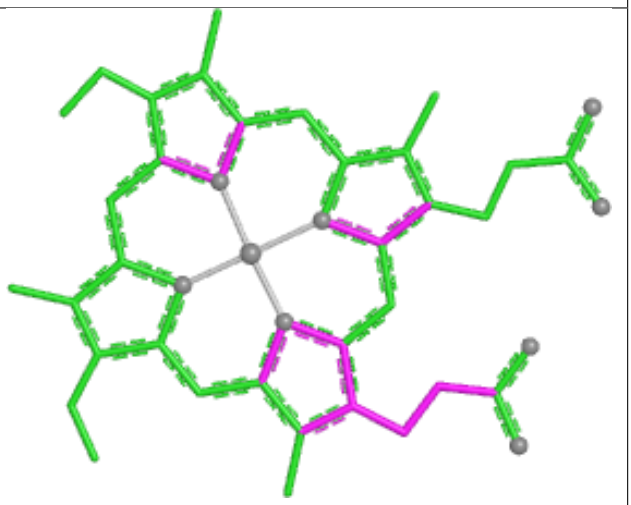


Rings

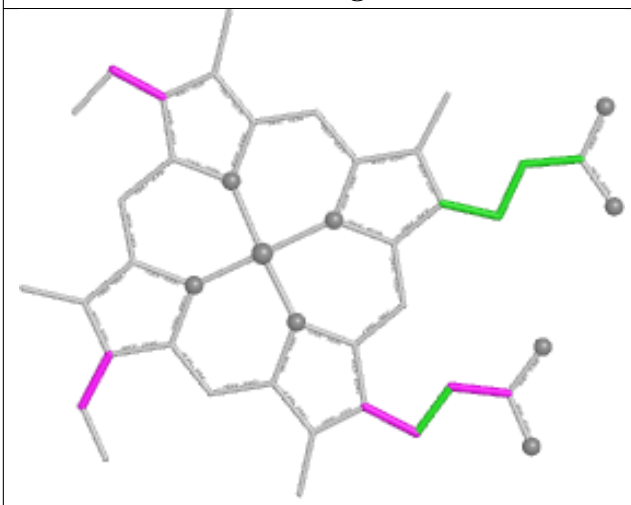
Ligand HEC C 404



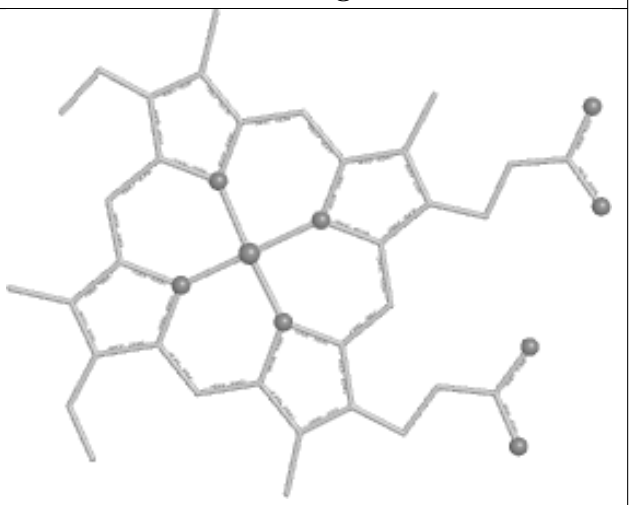
Bond lengths



Bond angles

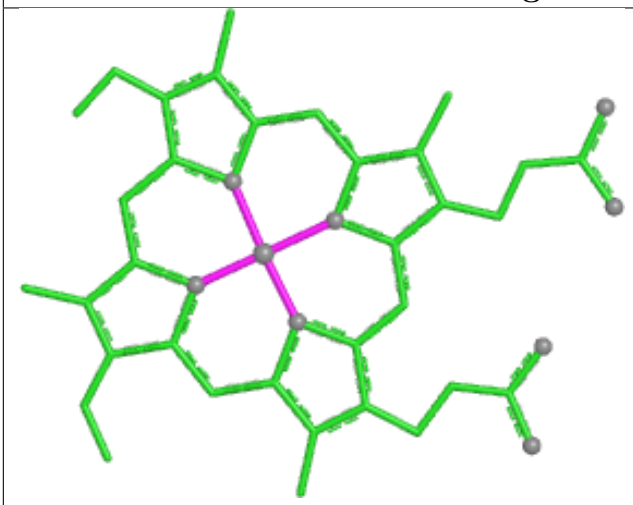


Torsions

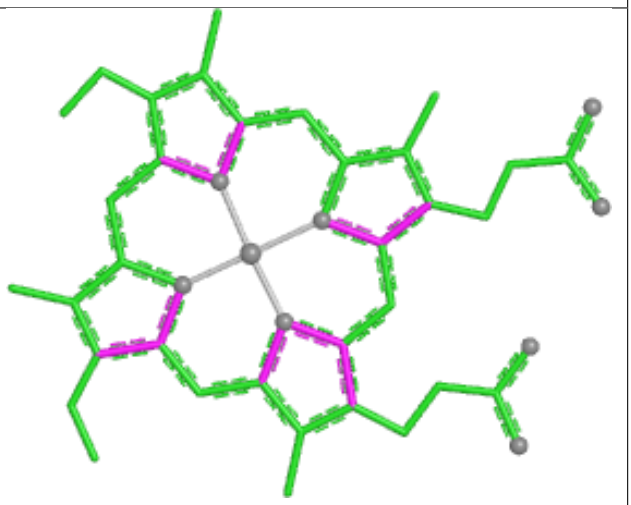


Rings

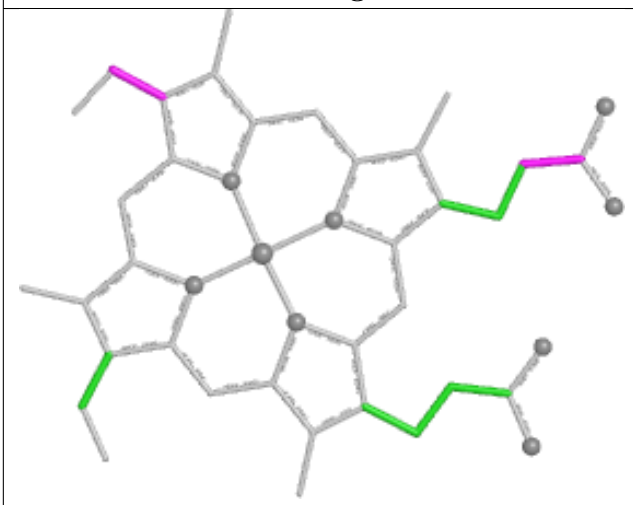
Ligand HEC C 401



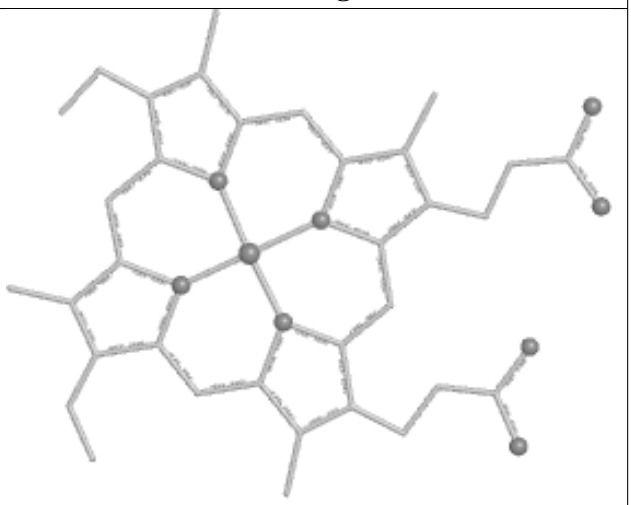
Bond lengths



Bond angles

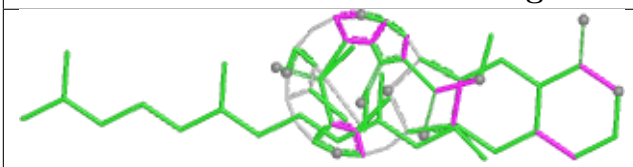


Torsions

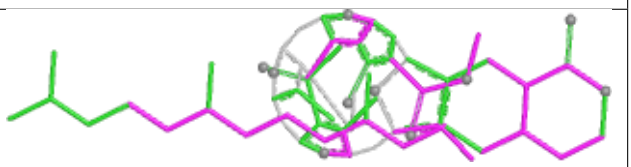


Rings

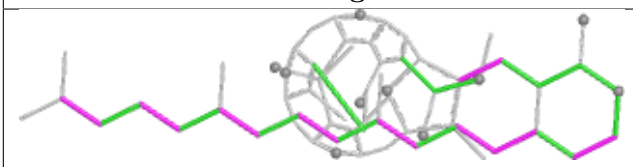
Ligand BPB L 402



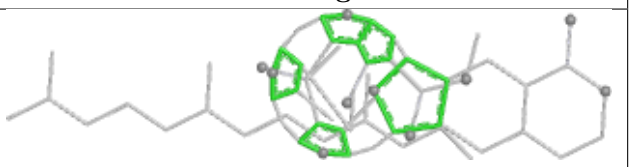
Bond lengths



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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	C	332/336 (98%)	0.05	15 (4%)	38	24	46, 74, 113, 124	0
2	H	249/258 (96%)	0.14	9 (3%)	46	29	50, 73, 99, 105	0
3	L	273/273 (100%)	-0.31	5 (1%)	67	48	37, 54, 74, 85	0
4	M	323/323 (100%)	-0.27	5 (1%)	72	52	42, 60, 89, 117	0
All	All	1177/1190 (98%)	-0.10	34 (2%)	53	35	37, 66, 102, 124	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	85	THR	4.3
2	H	54	PRO	4.2
3	L	1	ALA	4.0
2	H	45	GLU	3.8
4	M	321	ALA	3.4
1	C	84	GLN	3.4
4	M	318	LEU	3.2
2	H	83	PRO	3.1
1	C	332	LYS	3.1
1	C	54	GLN	3.0
4	M	320	GLY	2.9
2	H	9	HIS	2.8
3	L	203	GLY	2.7
1	C	55	VAL	2.7
1	C	59	VAL	2.7
3	L	271	PHE	2.6
1	C	44	ALA	2.5
1	C	53	SER	2.4
2	H	119	GLU	2.4
4	M	164	THR	2.4
1	C	88	THR	2.3

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Mol	Chain	Res	Type	RSRZ
3	L	202	ASP	2.3
1	C	298	GLY	2.2
2	H	131	LYS	2.2
2	H	100	PRO	2.2
1	C	79	GLU	2.2
1	C	46	LYS	2.1
1	C	47	ALA	2.1
1	C	68	ALA	2.1
1	C	101	LYS	2.1
4	M	238	ASP	2.1
3	L	268	ASP	2.0
2	H	216	GLU	2.0
1	C	86	GLY	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FME	H	1	10/11	0.75	0.22	104,105,115,117	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	C	808	5/5	0.48	0.31	104,104,104,104	5
7	HTO	H	705	10/10	0.60	1.17	56,59,61,61	10
7	HTO	C	706	10/10	0.66	1.28	56,57,58,58	10
7	HTO	C	707	10/10	0.75	0.76	44,48,49,49	10

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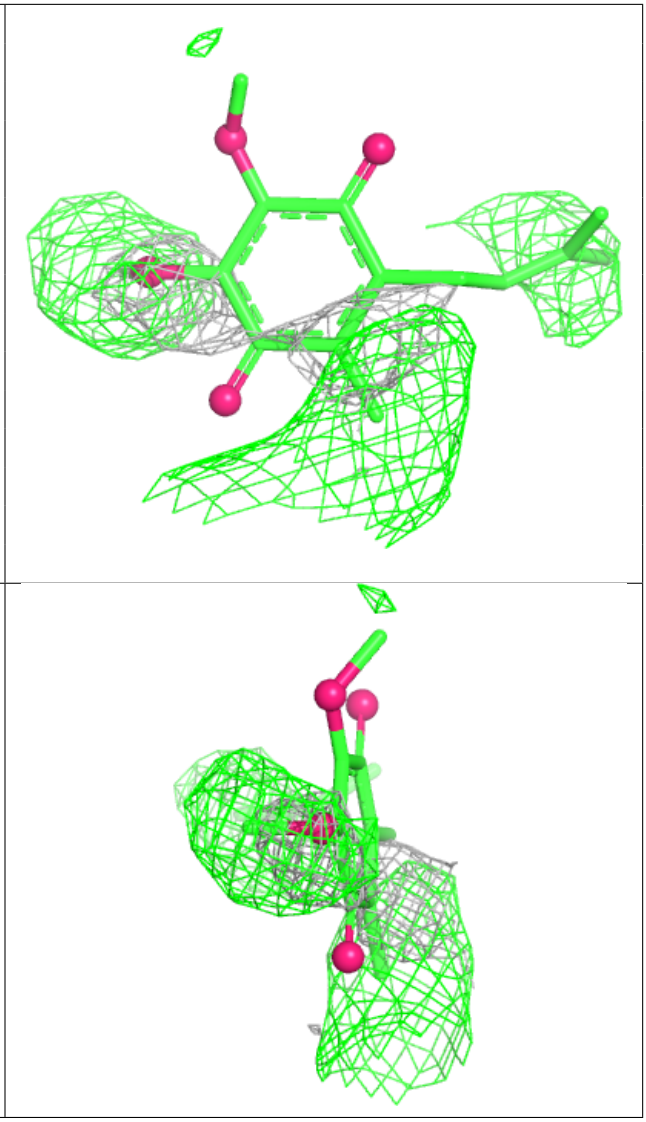
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	H	812	5/5	0.76	0.23	92,92,93,93	5
5	SO4	H	803	5/5	0.76	0.23	82,82,83,83	5
5	SO4	C	809	5/5	0.81	0.21	109,110,110,110	5
5	SO4	H	807	5/5	0.84	0.17	108,108,108,109	5
5	SO4	C	814	5/5	0.86	0.18	48,48,49,50	5
5	SO4	C	813	5/5	0.87	0.18	79,79,80,80	5
5	SO4	C	810	5/5	0.87	0.18	88,88,88,88	5
11	UQ1	L	503	18/18	0.87	0.42	73,76,78,78	18
5	SO4	M	805	5/5	0.91	0.14	64,65,65,67	5
14	NS5	M	600	40/40	0.91	0.22	65,71,100,101	4
5	SO4	H	806	5/5	0.92	0.10	72,72,73,73	5
8	LDA	M	704	16/16	0.92	0.25	68,70,73,73	16
5	SO4	C	811	5/5	0.93	0.19	76,76,76,77	5
10	BPB	M	402	65/65	0.93	0.17	61,67,123,124	0
5	SO4	M	802	5/5	0.93	0.14	89,89,90,90	0
8	LDA	H	703	16/16	0.93	0.19	54,58,60,61	16
11	UQ1	L	502	18/18	0.94	0.22	63,65,66,66	18
5	SO4	M	804	5/5	0.95	0.07	94,95,96,96	0
5	SO4	M	801	5/5	0.96	0.08	61,62,63,63	0
9	BCB	M	400	66/66	0.96	0.12	37,48,107,108	0
13	MQ9	M	501	58/58	0.96	0.12	40,64,102,103	0
6	HEC	C	401	43/43	0.96	0.13	99,110,118,120	0
5	SO4	C	815	5/5	0.97	0.10	40,40,41,41	5
8	LDA	L	702	16/16	0.97	0.12	67,73,79,80	0
8	LDA	H	701	16/16	0.97	0.11	54,57,68,68	0
9	BCB	L	400	66/66	0.98	0.08	37,40,45,49	0
9	BCB	M	401	66/66	0.98	0.09	36,41,63,68	0
10	BPB	L	402	65/65	0.98	0.08	38,51,60,60	0
9	BCB	L	401	66/66	0.98	0.08	41,44,59,64	0
6	HEC	C	404	43/43	0.99	0.06	52,55,68,73	0
6	HEC	C	402	43/43	0.99	0.08	73,76,80,81	0
6	HEC	C	403	43/43	0.99	0.07	46,48,52,54	0
12	FE2	M	500	1/1	1.00	0.01	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.

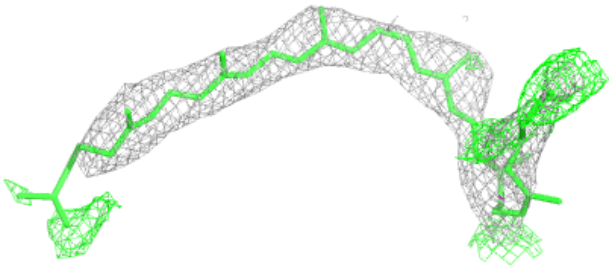
Electron density around UQ1 L 503:

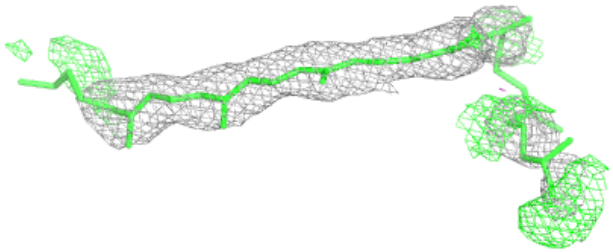
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

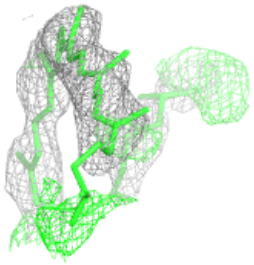


Electron density around NS5 M 600:

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

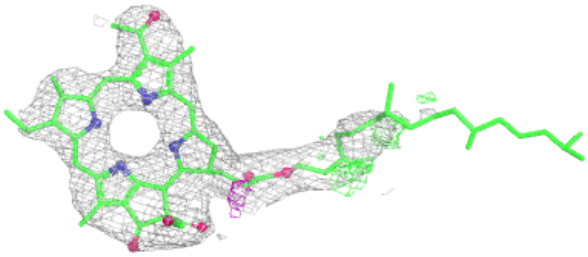


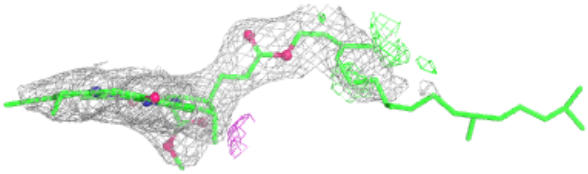


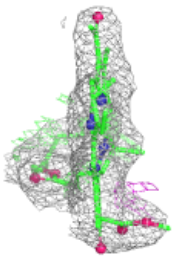


Electron density around BPB M 402:

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

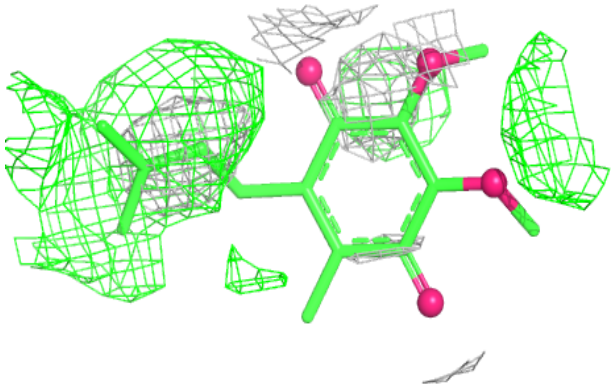


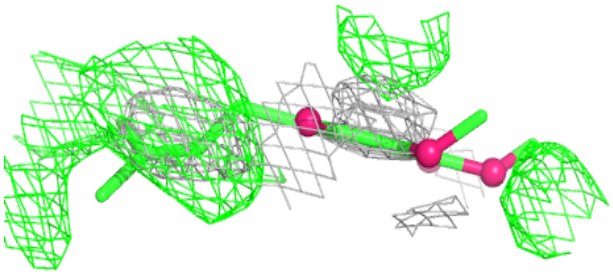


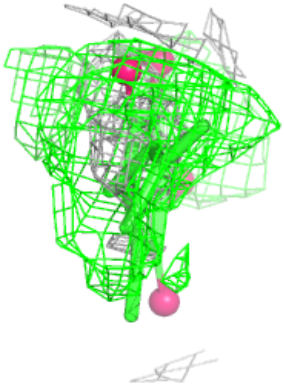


Electron density around UQ1 L 502:

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

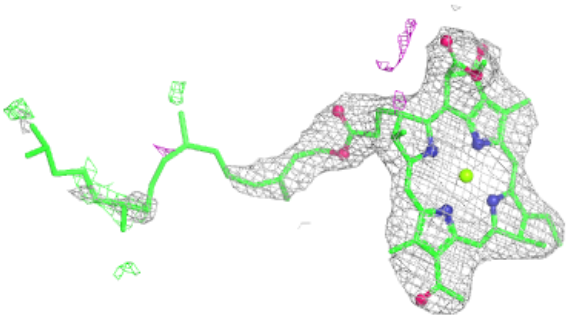


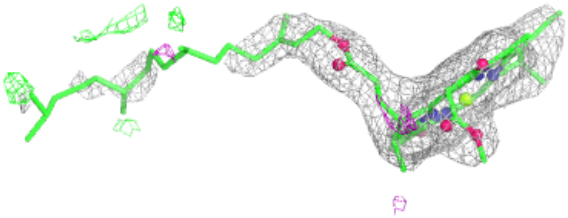


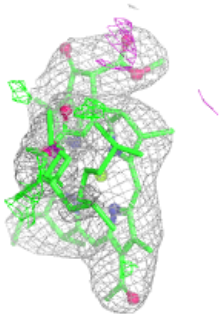


Electron density around BCB M 400:

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

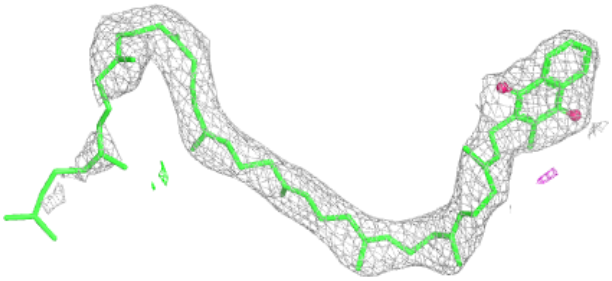


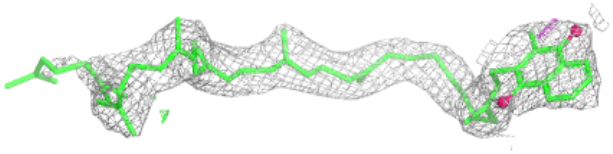




Electron density around MQ9 M 501:

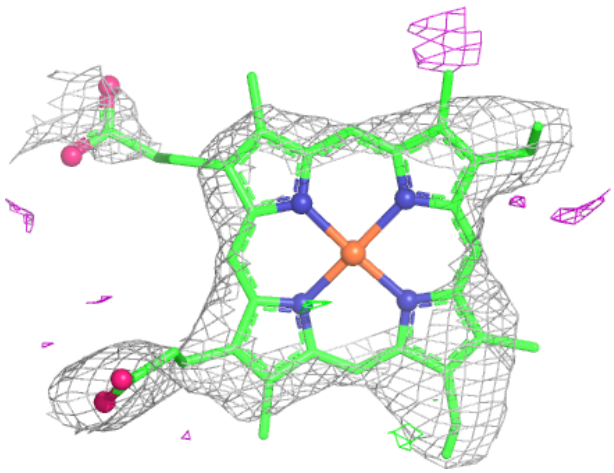
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

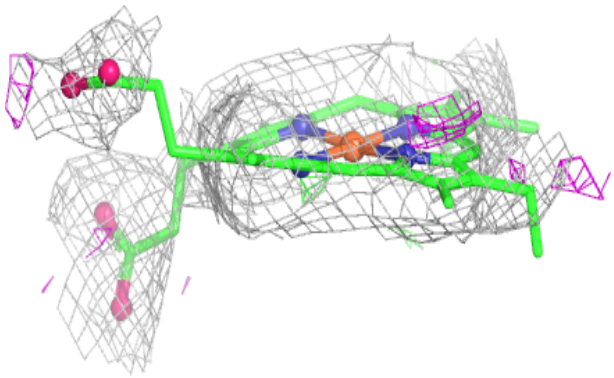


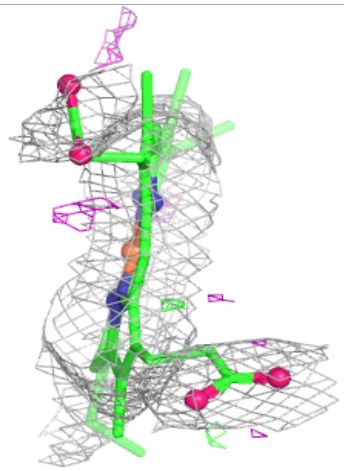


Electron density around HEC C 401:

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

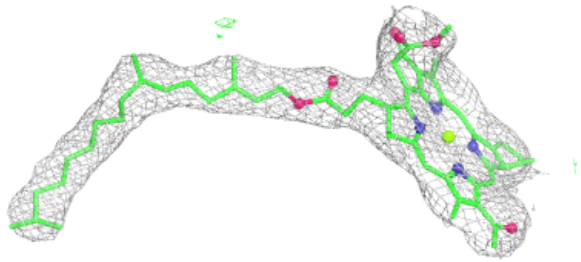


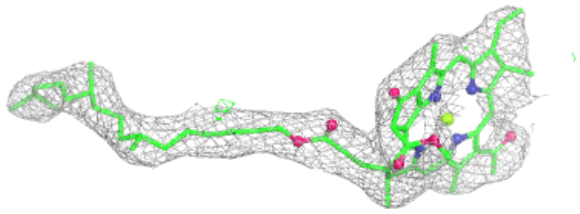


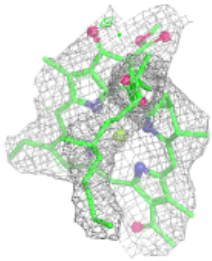


Electron density around BCB L 400:

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

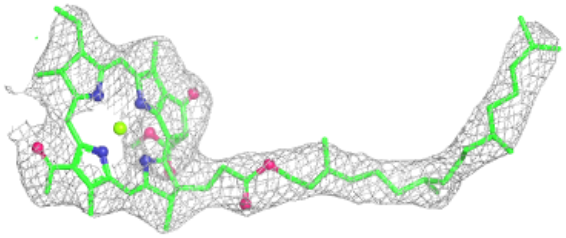


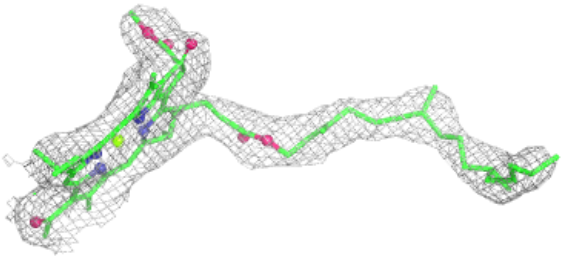


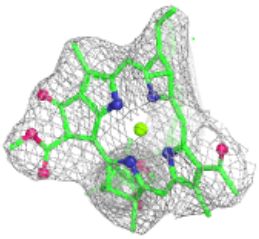


Electron density around BCB M 401:

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

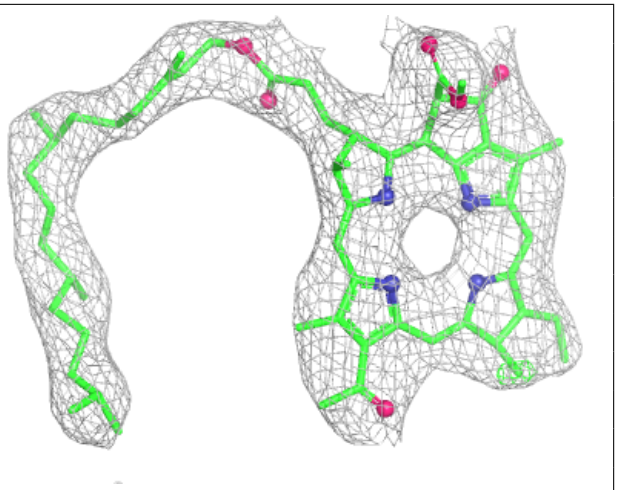


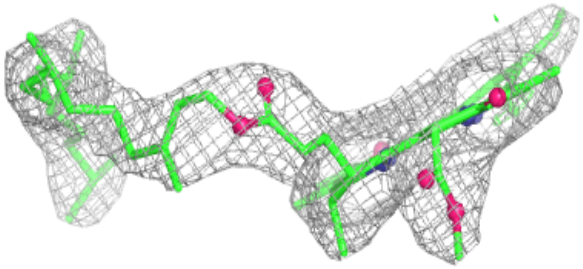


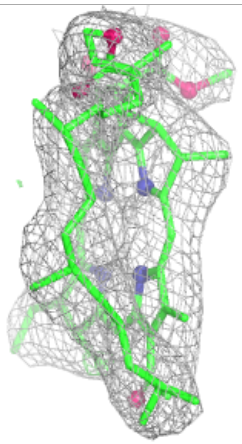


Electron density around BPB L 402:

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

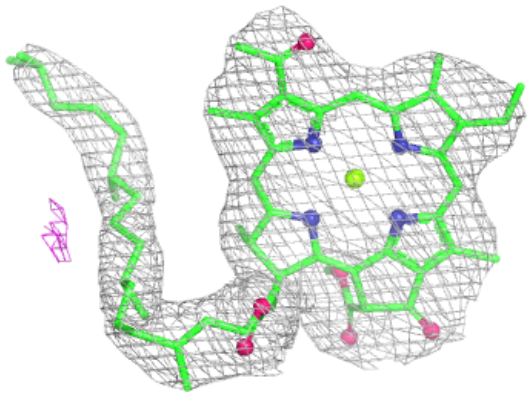


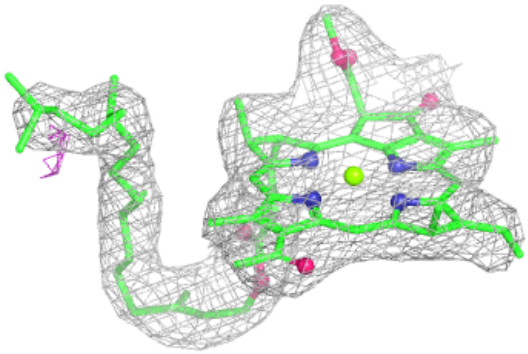


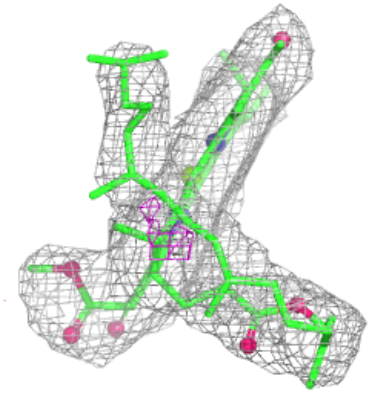


Electron density around BCB L 401:

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

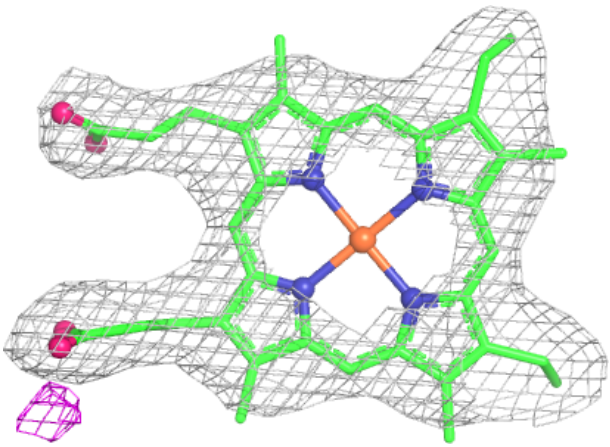


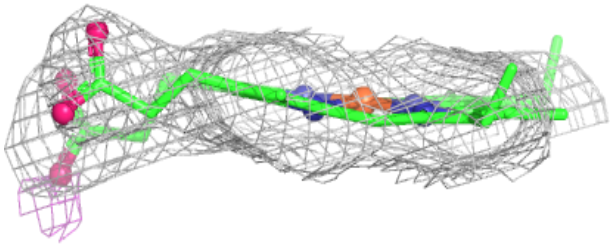


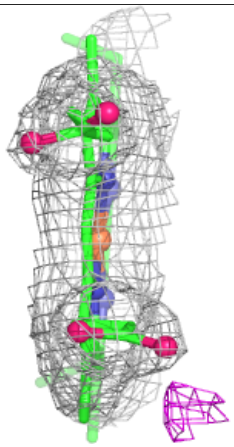


Electron density around HEC C 404:

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

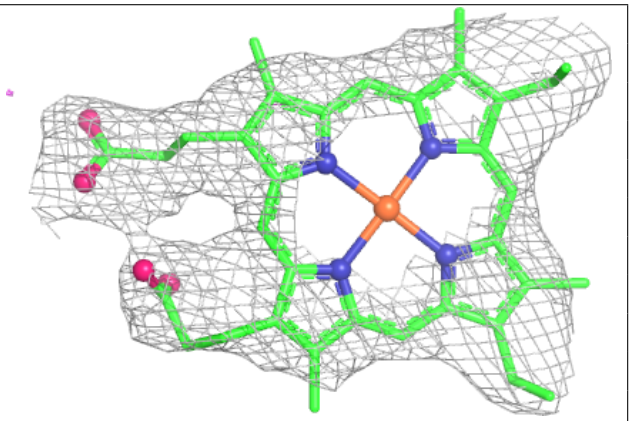


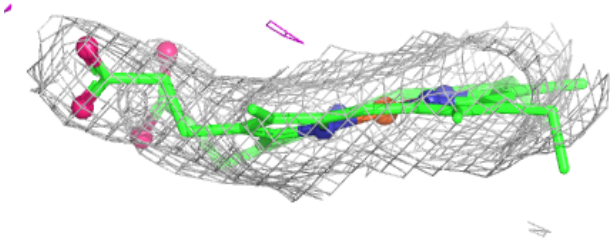


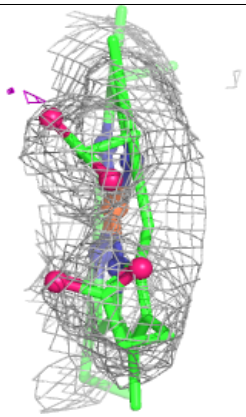


Electron density around HEC C 402:

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

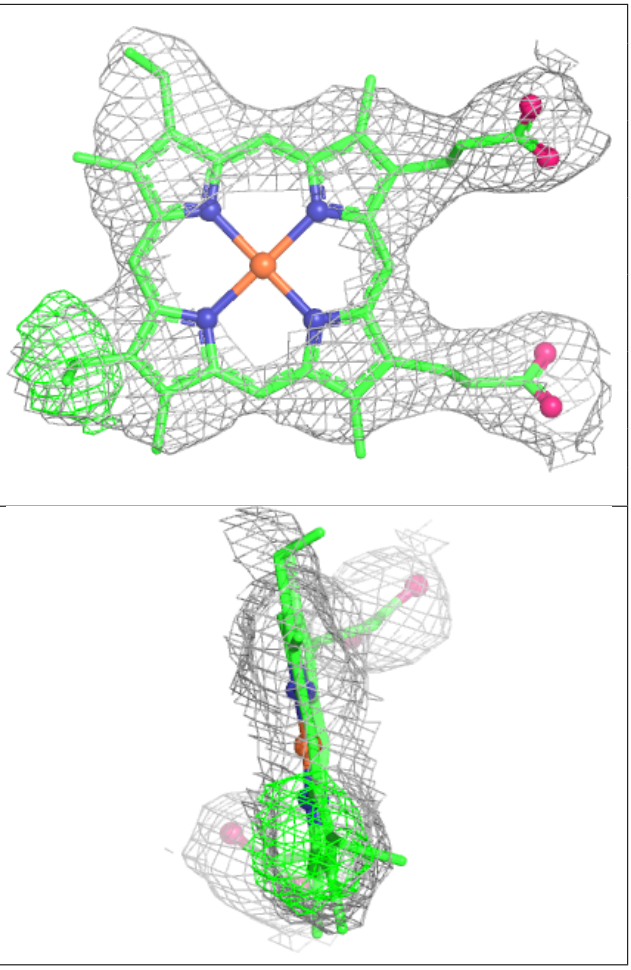






Electron density around HEC C 403:

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



6.5 Other polymers (i)

There are no such residues in this entry.