Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2026 – 03:45 PM EDT

PDB ID	:	1R2C / pdb_00001r2c
Title	:	PHOTOSYNTHETIC REACTION CENTER BLASTOCHLORIS VIRIDIS (ATCC)
Authors	:	Baxter, R.H.; Ponomarenko, N.; Pahl, R.; Srajer, V.; Moffat, K.; Norris, J.R.
Deposited on	:	2003-09-26
Resolution	:	2.86 Å(reported)

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

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

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

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

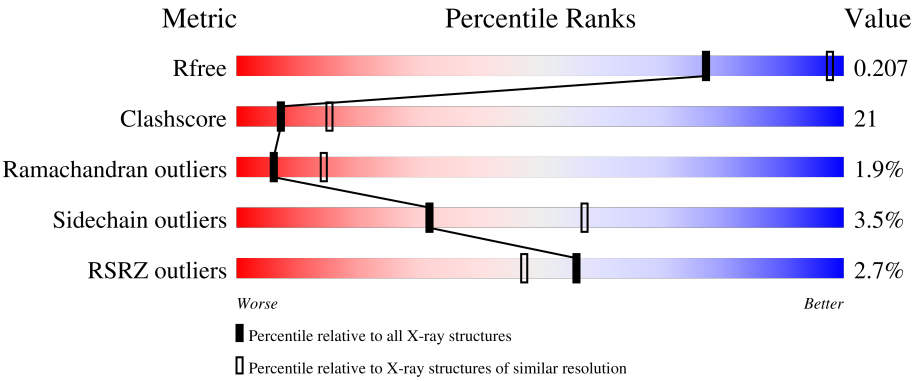
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.86 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	% 65% 32% ••
2	L	273	65% 32% •
3	M	323	% 64% 33% •
4	H	258	9% 52% 41% 6% •

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
5	HEC	C	1201	X	-	-	-
5	HEC	C	1202	X	-	-	-
5	HEC	C	1203	X	-	-	-
5	HEC	C	1204	X	-	-	-
6	BCB	L	302	X	-	-	-
6	BCB	L	304	X	-	-	-
6	BCB	M	1301	X	-	-	-
6	BCB	M	1303	X	-	-	-
7	BPB	M	401	X	-	X	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 10140 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 precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	332	Total	C	N	O	S	41	0	0
			2602	1640	466	478	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	273	Total	C	N	O	S	10	0	0
			2171	1459	350	355	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	323	Total	C	N	O	S	15	0	0
			2555	1702	419	423	11			

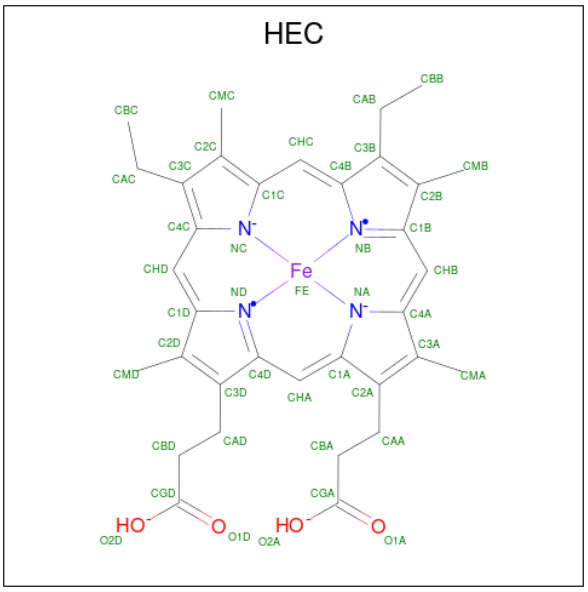
- Molecule 4 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	258	Total	C	N	O	S	98	0	0
			2018	1292	344	380	2			

There is a discrepancy between the modelled and reference sequences:

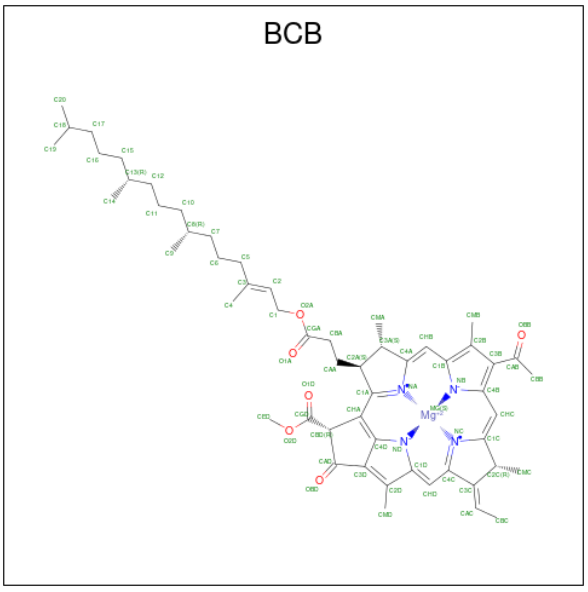
Chain	Residue	Modelled	Actual	Comment	Reference
H	1	FME	MET	modified residue	UNP P06008

- Molecule 5 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



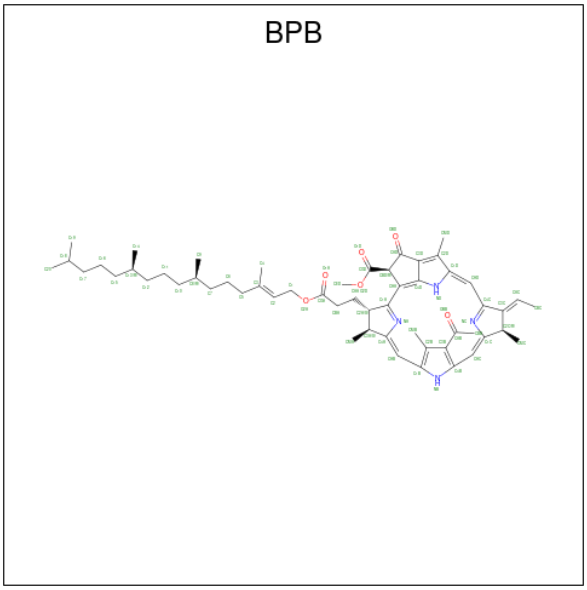
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is BACTERIOCHLOROPHYLL B (CCD ID: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).



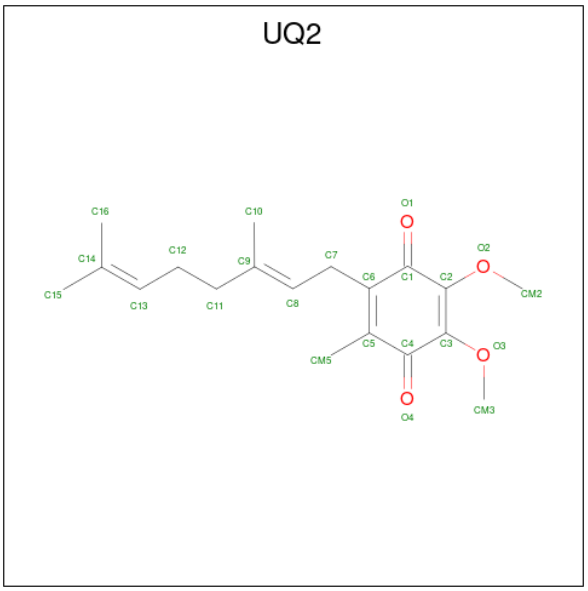
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	15	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 7 is BACTERIOPHEOPHYTIN B (CCD ID: BPB) (formula: $C_{55}H_{74}N_4O_6$).



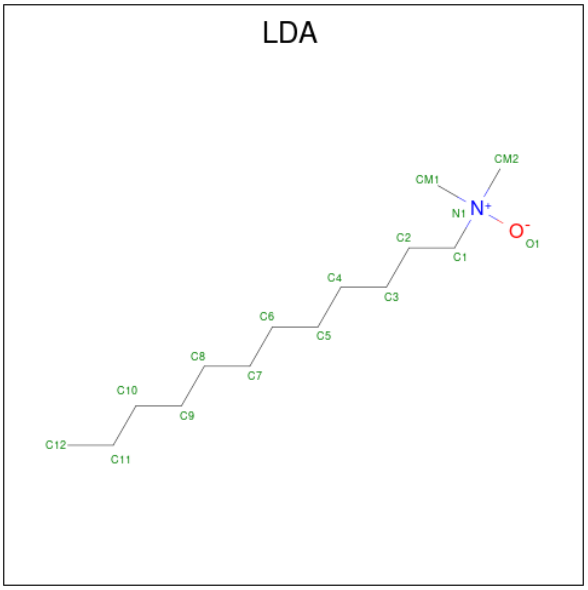
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 8 is UBIQUINONE-2 (CCD ID: UQ2) (formula: $C_{19}H_{26}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			23	19	4		

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	L	1	Total	C	N	O	3	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		

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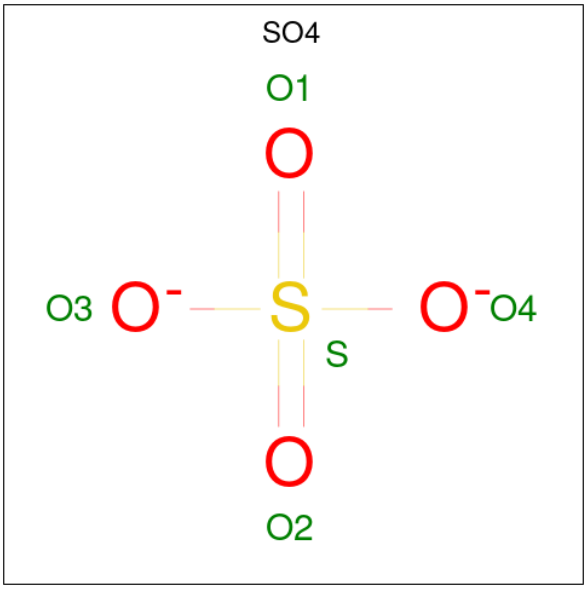
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total C N O 16 14 1 1	3	0
9	M	1	Total C N O 16 14 1 1	0	0
9	H	1	Total C N O 16 14 1 1	0	0

- Molecule 10 is FE (II) ION (CCD ID: FE2) (formula: Fe).

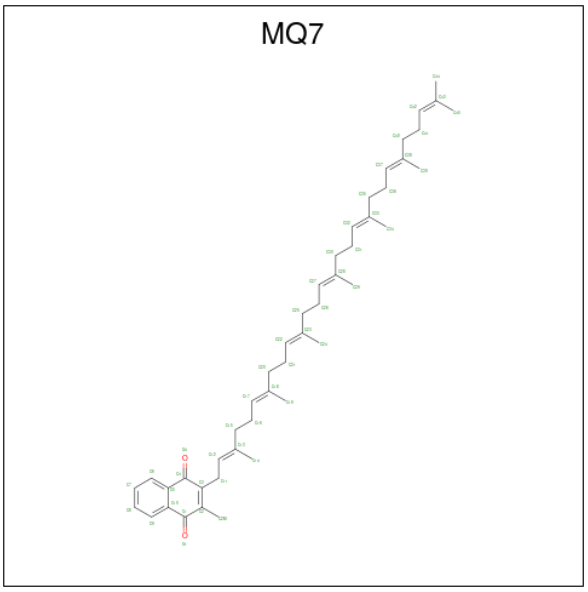
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	M	1	Total Fe 1 1	0	0

- Molecule 11 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



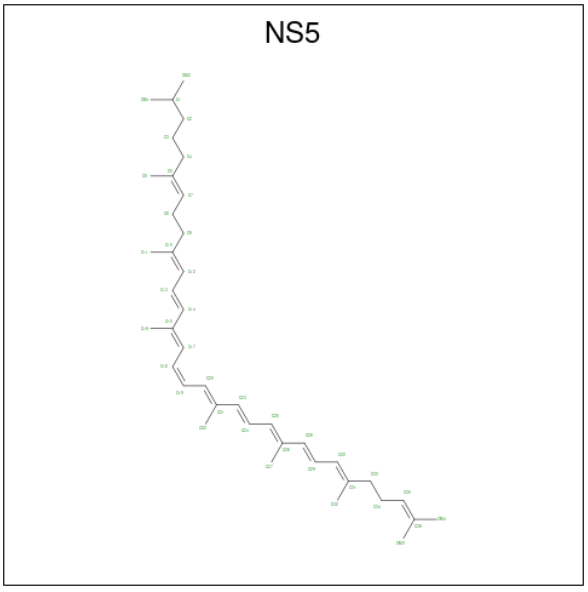
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total O S 5 4 1	0	0
11	M	1	Total O S 5 4 1	0	0
11	M	1	Total O S 5 4 1	0	0
11	H	1	Total O S 5 4 1	0	0

- Molecule 12 is MENAQUINONE-7 (CCD ID: MQ7) (formula: $C_{46}H_{64}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	M	1	Total C O 48 46 2	0	0

- Molecule 13 is 15-cis-1,2-dihydroneurosporene (CCD ID: NS5) (formula: $C_{40}H_{60}$).



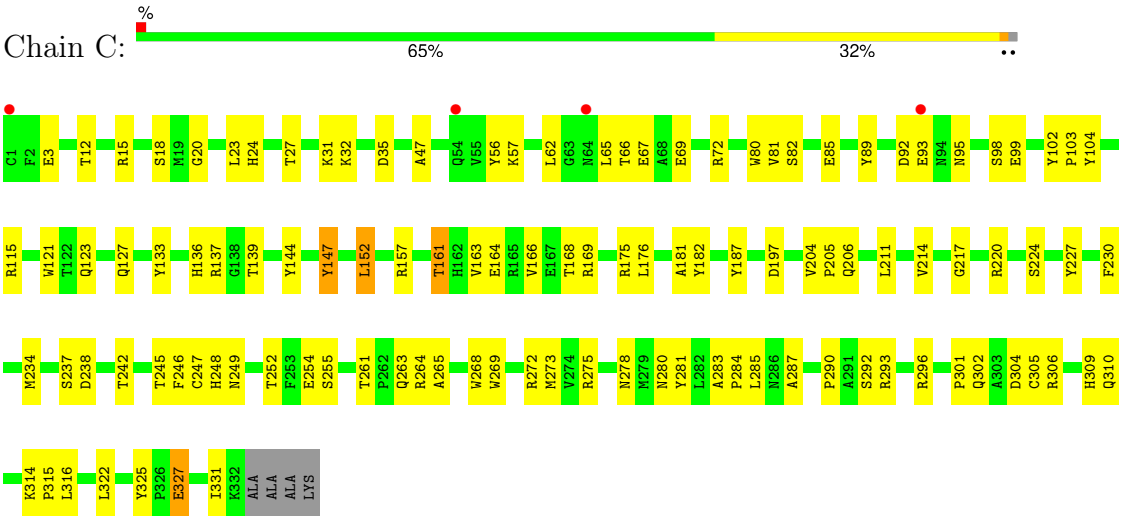
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	M	1	Total C 40 40	11	0

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.

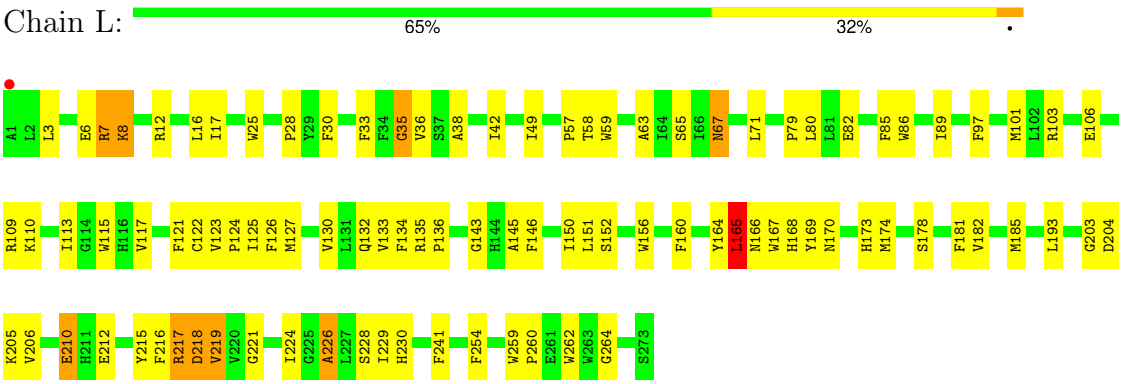
• Molecule 1: Photosynthetic reaction center cytochrome C subunit precursor

Chain C:



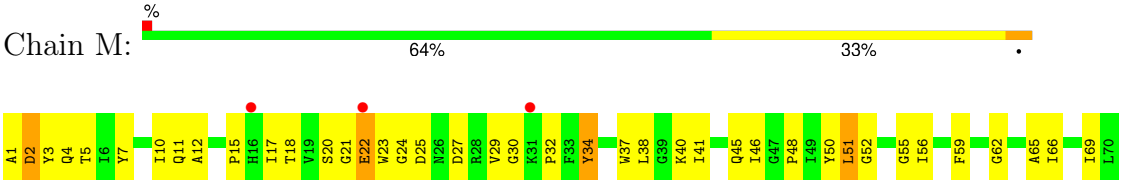
• Molecule 2: Reaction center protein L chain

Chain L:



• Molecule 3: Reaction center protein M chain

Chain M:

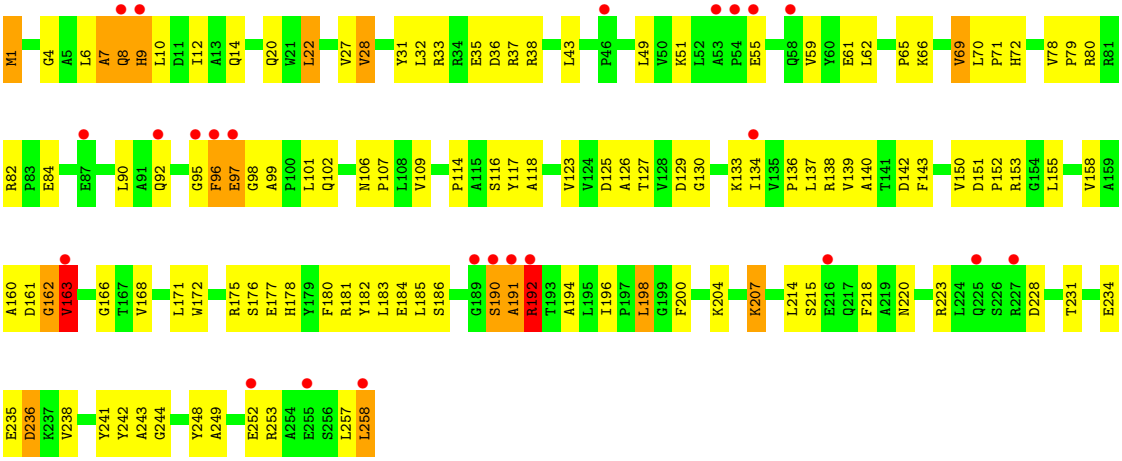




• Molecule 4: Reaction center protein H chain

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	223.50Å 223.50Å 112.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.83 – 2.86 48.83 – 2.86	Depositor EDS
% Data completeness (in resolution range)	97.3 (48.83-2.86) 97.4 (48.83-2.86)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.90 (at 2.86Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202 , 0.228 0.187 , 0.207	Depositor DCC
R_{free} test set	6311 reflections (9.82%)	wwPDB-VP
Wilson B-factor (Å^2)	59.3	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10140	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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: BPB, FME, MQ7, HEC, NS5, LDA, FE2, UQ2, BCB, SO4

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	0.46	0/2669	0.95	6/3637 (0.2%)
2	L	0.47	0/2259	0.99	11/3084 (0.4%)
3	M	0.47	0/2659	0.94	8/3637 (0.2%)
4	H	0.41	0/2055	0.91	3/2807 (0.1%)
All	All	0.45	0/9642	0.95	28/13165 (0.2%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	308	TYR	N-CA-C	-8.87	99.98	112.13
3	M	309	LEU	N-CA-C	-7.25	100.64	110.36
1	C	249	ASN	N-CA-C	-7.20	93.44	107.62
2	L	35	GLY	N-CA-C	-7.12	103.65	112.77
2	L	133	VAL	N-CA-C	7.00	118.06	111.48
3	M	200	HIS	N-CA-C	-6.84	103.76	111.07
3	M	95	PRO	N-CA-C	-6.45	102.83	110.70
1	C	280	ASN	N-CA-C	5.88	120.61	113.38
3	M	307	ALA	N-CA-C	-5.72	102.82	110.55
1	C	161	THR	N-CA-C	-5.69	102.50	110.35
2	L	217	ARG	N-CA-C	-5.65	105.04	111.14
2	L	259	TRP	CA-C-N	-5.57	113.16	119.28
2	L	259	TRP	C-N-CA	-5.57	113.16	119.28
2	L	67	ASN	N-CA-C	5.56	118.36	110.40
4	H	70	LEU	CA-C-N	5.46	125.28	119.28
4	H	70	LEU	C-N-CA	5.46	125.28	119.28
3	M	94	TYR	N-CA-C	5.45	117.81	110.29
4	H	28	VAL	N-CA-C	5.44	115.64	110.42
1	C	57	LYS	N-CA-C	5.40	117.99	111.40
2	L	134	PHE	N-CA-C	5.38	116.84	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	45	GLN	N-CA-C	5.28	117.35	109.59
2	L	219	VAL	N-CA-C	5.23	115.50	110.74
3	M	235	GLN	N-CA-C	-5.19	105.69	112.23
1	C	147	TYR	N-CA-C	-5.11	102.59	109.95
2	L	8	LYS	N-CA-C	5.05	118.55	112.38
2	L	133	VAL	CB-CA-C	-5.04	107.43	111.71
1	C	81	VAL	N-CA-C	5.03	116.44	111.67
2	L	30	PHE	N-CA-C	-5.02	102.27	110.20

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	2602	0	2579	77	0
2	L	2171	0	2098	93	0
3	M	2555	0	2452	114	0
4	H	2018	0	2020	121	0
5	C	172	0	120	8	0
6	L	132	0	144	18	0
6	M	132	0	143	26	0
7	L	65	0	74	12	0
7	M	65	0	74	21	0
8	L	23	0	26	4	0
9	H	16	0	31	4	0
9	L	16	0	31	2	0
9	M	64	0	124	11	0
10	M	1	0	0	0	0
11	H	5	0	0	0	0
11	M	15	0	0	0	0
12	M	48	0	64	0	0
13	M	40	0	60	5	0
All	All	10140	0	10040	405	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 21.

All (405) 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)
4:H:152:PRO:HA	4:H:155:LEU:HD12	1.31	1.05
7:M:401:BPB:H14	7:M:401:BPB:H17	1.39	1.03
3:M:32:PRO:HG3	3:M:48:PRO:HD3	1.39	1.02
6:L:302:BCB:HBD	6:L:302:BCB:HBA1	1.46	0.94
7:L:402:BPB:HBBA	3:M:208:TYR:HB3	1.47	0.94
2:L:182:VAL:HG22	6:M:1301:BCB:H12	1.49	0.94
1:C:152:LEU:HD22	1:C:175:ARG:HA	1.53	0.90
2:L:226:ALA:HA	8:L:502:UQ2:H3M2	1.57	0.86
7:L:402:BPB:HHC	7:L:402:BPB:HBBB	1.57	0.86
2:L:42:ILE:HD13	7:L:402:BPB:H4A	1.58	0.85
9:M:701:LDA:HM22	4:H:33:ARG:HE	1.45	0.81
9:M:702:LDA:H11	4:H:14:GLN:NE2	1.95	0.81
7:L:402:BPB:HBB	3:M:208:TYR:CD2	2.16	0.81
4:H:6:LEU:HB2	4:H:10:LEU:HD12	1.62	0.81
6:L:302:BCB:HBD	6:L:302:BCB:CBA	2.12	0.79
4:H:152:PRO:HG2	4:H:171:LEU:HD11	1.65	0.79
2:L:127:MET:HE3	2:L:130:VAL:HB	1.65	0.78
1:C:47:ALA:O	1:C:66:THR:HG21	1.84	0.78
3:M:79:PHE:O	3:M:81:PRO:HD3	1.84	0.78
4:H:258:LEU:HD23	4:H:258:LEU:H	1.48	0.77
1:C:62:LEU:HB3	1:C:65:LEU:HD12	1.67	0.77
7:M:401:BPB:H9A	7:M:401:BPB:H5	1.65	0.77
2:L:212:GLU:OE1	8:L:502:UQ2:H3M3	1.86	0.76
6:L:302:BCB:HBA1	6:L:302:BCB:CBD	2.16	0.76
4:H:231:THR:OG1	4:H:234:GLU:HG3	1.87	0.75
2:L:182:VAL:HG22	6:M:1301:BCB:C1	2.17	0.74
2:L:8:LYS:HD2	4:H:116:SER:HB3	1.67	0.74
7:L:402:BPB:CBB	3:M:208:TYR:HB3	2.17	0.74
4:H:33:ARG:HH11	4:H:33:ARG:HA	1.51	0.74
4:H:138:ARG:HD2	4:H:228:ASP:OD1	1.86	0.73
3:M:231:ARG:HH22	4:H:235:GLU:CD	1.96	0.73
2:L:230:HIS:CD2	3:M:221:ILE:HG13	2.24	0.72
4:H:80:ARG:NH2	4:H:82:ARG:HD2	2.05	0.72
4:H:106:ASN:ND2	4:H:109:VAL:HG23	2.04	0.71
2:L:181:PHE:CD2	7:M:401:BPB:HBB	2.25	0.71
1:C:278:ASN:HB3	1:C:302:GLN:HE21	1.55	0.71
4:H:114:PRO:HB2	4:H:244:GLY:HA2	1.74	0.70
3:M:200:HIS:CE1	3:M:204:ILE:HD11	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:GLU:N	1:C:254:GLU:OE1	2.24	0.69
1:C:152:LEU:CD2	1:C:175:ARG:HA	2.23	0.69
2:L:178:SER:O	2:L:182:VAL:HG23	1.93	0.69
4:H:160:ALA:HB3	4:H:214:LEU:HD23	1.75	0.69
2:L:182:VAL:CG2	6:M:1301:BCB:H12	2.24	0.68
3:M:29:VAL:CG1	3:M:51:LEU:HD13	2.22	0.68
4:H:138:ARG:HH22	4:H:184:GLU:CD	2.01	0.68
3:M:132:TYR:CE1	3:M:142:THR:HG21	2.29	0.68
3:M:241:THR:O	3:M:245:ARG:HG3	1.95	0.67
2:L:7:ARG:HD3	4:H:101:LEU:HD11	1.76	0.67
2:L:12:ARG:HD3	4:H:102:GLN:HE21	1.60	0.67
3:M:29:VAL:HG12	3:M:51:LEU:HD13	1.75	0.67
2:L:7:ARG:CD	4:H:101:LEU:HD11	2.25	0.66
1:C:95:ASN:ND2	1:C:98:SER:HB2	2.10	0.66
7:M:401:BPB:HHC	7:M:401:BPB:HBBB	1.78	0.66
2:L:226:ALA:O	2:L:229:ILE:HG22	1.96	0.65
2:L:80:LEU:HD12	2:L:80:LEU:H	1.62	0.65
3:M:159:GLY:HA3	13:M:600:NS5:H272	1.79	0.65
2:L:224:ILE:HG12	2:L:228:SER:HB3	1.79	0.64
3:M:299:HIS:HB3	9:M:702:LDA:H22	1.79	0.64
3:M:147:ASN:C	3:M:147:ASN:HD22	2.07	0.63
1:C:247:CYS:HA	1:C:261:THR:OG1	1.98	0.63
4:H:163:VAL:HG13	4:H:215:SER:HB3	1.81	0.63
1:C:82:SER:HB2	1:C:85:GLU:HB2	1.82	0.62
3:M:235:GLN:NE2	3:M:242:ALA:HB3	2.14	0.62
2:L:132:GLN:O	2:L:136:PRO:HG2	2.00	0.62
3:M:12:ALA:HB2	4:H:180:PHE:CE2	2.35	0.62
3:M:160:CYS:C	3:M:163:PRO:HD2	2.26	0.61
4:H:152:PRO:CG	4:H:171:LEU:HD11	2.30	0.61
1:C:169:ARG:HD2	3:M:78:HIS:CD2	2.35	0.60
3:M:162:HIS:HB3	3:M:163:PRO:HD3	1.83	0.60
2:L:35:GLY:CA	2:L:103:ARG:HD2	2.31	0.60
2:L:181:PHE:HB3	7:M:401:BPB:CBB	2.31	0.60
3:M:22:GLU:HB3	3:M:23:TRP:CE3	2.35	0.60
1:C:99:GLU:HG2	1:C:104:TYR:CE1	2.37	0.60
3:M:22:GLU:HB3	3:M:23:TRP:HE3	1.66	0.60
6:M:1303:BCB:HBA2	6:M:1303:BCB:HMA2	1.83	0.60
1:C:95:ASN:HD22	1:C:98:SER:HB2	1.67	0.60
2:L:182:VAL:HG13	6:M:1301:BCB:H43	1.82	0.60
4:H:190:SER:O	4:H:192:ARG:HG3	2.02	0.60
4:H:234:GLU:O	4:H:238:VAL:HG23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:302:BCB:H2C	6:M:1303:BCB:H2C	1.83	0.60
1:C:217:GLY:O	1:C:220:ARG:HG2	2.01	0.60
3:M:226:ARG:HD3	4:H:200:PHE:CZ	2.37	0.60
3:M:258:ALA:HB1	3:M:262:SER:OG	2.02	0.60
4:H:185:LEU:HD23	4:H:194:ALA:O	2.02	0.60
3:M:243:VAL:HG11	3:M:260:ILE:HB	1.84	0.59
1:C:123:GLN:HG3	1:C:269:TRP:CD2	2.38	0.59
7:L:402:BPB:HBBB	7:L:402:BPB:CHC	2.32	0.59
3:M:95:PRO:HD3	3:M:174:PRO:HB3	1.84	0.59
2:L:173:HIS:HD2	6:L:302:BCB:HED2	1.66	0.59
9:M:701:LDA:CM2	4:H:33:ARG:HE	2.15	0.59
4:H:117:TYR:HB2	4:H:236:ASP:HB3	1.83	0.58
1:C:152:LEU:HD22	1:C:175:ARG:HG2	1.85	0.58
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.39	0.58
4:H:139:VAL:HG21	4:H:228:ASP:HB3	1.86	0.58
5:C:1204:HEC:HBD1	5:C:1204:HEC:HHA	1.83	0.58
3:M:155:VAL:HG21	6:M:1303:BCB:H8	1.84	0.58
7:M:401:BPB:H17	7:M:401:BPB:C14	2.25	0.58
1:C:281:TYR:O	1:C:285:LEU:HG	2.04	0.58
1:C:123:GLN:HG3	1:C:269:TRP:CE3	2.39	0.58
2:L:49:ILE:HG12	2:L:89:ILE:HD13	1.85	0.58
4:H:33:ARG:HH11	4:H:33:ARG:CA	2.16	0.58
1:C:224:SER:HA	1:C:227:TYR:HD1	1.68	0.58
2:L:173:HIS:CD2	6:L:302:BCB:HED2	2.39	0.57
3:M:231:ARG:NH2	4:H:235:GLU:OE1	2.37	0.57
4:H:62:LEU:O	9:H:703:LDA:H11	2.05	0.57
4:H:151:ASP:OD1	4:H:153:ARG:HB2	2.04	0.57
2:L:101:MET:HE2	2:L:122:CYS:SG	2.45	0.57
3:M:195:TYR:CE2	6:M:1303:BCB:HMC2	2.40	0.56
1:C:161:THR:OG1	1:C:164:GLU:HG3	2.05	0.56
3:M:107:LEU:HA	3:M:111:GLY:HA3	1.86	0.56
1:C:99:GLU:HG2	1:C:104:TYR:CD1	2.40	0.56
3:M:2:ASP:OD1	3:M:4:GLN:HB2	2.04	0.56
1:C:65:LEU:HD11	1:C:327:GLU:HG2	1.87	0.56
3:M:202:PHE:CE2	4:H:20:GLN:HG2	2.41	0.56
4:H:59:VAL:O	9:H:703:LDA:H21	2.05	0.56
4:H:161:ASP:HB3	4:H:214:LEU:HD22	1.87	0.56
1:C:314:LYS:HE2	5:C:1204:HEC:O1D	2.06	0.55
1:C:283:ALA:HB3	1:C:284:PRO:HD3	1.87	0.55
2:L:169:TYR:CG	2:L:260:PRO:HG3	2.41	0.55
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:66:ILE:HD12	7:M:401:BPB:H7	1.89	0.55
3:M:265:ARG:HH11	3:M:265:ARG:HG2	1.71	0.55
2:L:8:LYS:HE3	4:H:84:GLU:OE1	2.06	0.55
4:H:65:PRO:HG3	9:H:703:LDA:H92	1.89	0.54
2:L:80:LEU:H	2:L:80:LEU:CD1	2.20	0.54
3:M:127:TRP:O	3:M:131:VAL:HG23	2.07	0.54
2:L:42:ILE:CD1	7:L:402:BPB:H4A	2.34	0.54
2:L:166:ASN:OD1	2:L:168:HIS:HB2	2.07	0.54
4:H:192:ARG:O	4:H:192:ARG:HD3	2.07	0.54
3:M:34:TYR:CD1	3:M:34:TYR:N	2.75	0.54
2:L:185:MET:HE1	6:M:1301:BCB:H42	1.90	0.54
2:L:241:PHE:CE2	7:L:402:BPB:H43	2.42	0.54
3:M:69:ILE:HG21	13:M:600:NS5:H111	1.89	0.54
3:M:206:PHE:CD2	3:M:273:MET:HB3	2.43	0.54
2:L:38:ALA:O	2:L:42:ILE:HG13	2.08	0.53
2:L:167:TRP:HE1	2:L:173:HIS:CD2	2.27	0.53
2:L:35:GLY:HA2	2:L:103:ARG:HD2	1.91	0.53
3:M:66:ILE:CD1	7:M:401:BPB:H7	2.38	0.53
4:H:8:GLN:O	4:H:10:LEU:N	2.42	0.53
1:C:325:TYR:HA	1:C:327:GLU:OE2	2.09	0.53
2:L:185:MET:CE	6:M:1301:BCB:H42	2.39	0.53
3:M:37:TRP:HA	3:M:40:LYS:HG3	1.91	0.53
2:L:79:PRO:HG2	2:L:82:GLU:HB2	1.91	0.53
4:H:166:GLY:HA3	4:H:186:SER:O	2.09	0.53
1:C:56:TYR:HB3	5:C:1201:HEC:O2A	2.08	0.53
2:L:7:ARG:NE	4:H:101:LEU:HD11	2.24	0.53
4:H:192:ARG:HD3	4:H:192:ARG:C	2.34	0.52
6:M:1301:BCB:HHC	6:M:1301:BCB:HBB2	1.91	0.52
3:M:21:GLY:C	3:M:23:TRP:N	2.66	0.52
4:H:106:ASN:HD22	4:H:109:VAL:HG23	1.73	0.52
1:C:230:PHE:CE2	3:M:185:THR:HG21	2.44	0.52
2:L:165:LEU:N	2:L:165:LEU:HD23	2.24	0.52
4:H:134:ILE:HD12	4:H:134:ILE:N	2.24	0.52
4:H:204:LYS:HB2	4:H:207:LYS:O	2.10	0.52
2:L:164:TYR:O	2:L:166:ASN:N	2.34	0.52
1:C:211:LEU:HD12	4:H:1:FME:O	2.09	0.52
3:M:212:LEU:C	3:M:212:LEU:HD23	2.35	0.52
3:M:235:GLN:HA	3:M:235:GLN:OE1	2.09	0.52
6:M:1301:BCB:HBB3	6:M:1303:BCB:H62	1.92	0.52
4:H:28:VAL:O	4:H:33:ARG:HG2	2.09	0.52
1:C:3:GLU:O	2:L:254:PHE:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:VAL:HG22	1:C:296:ARG:NH1	2.25	0.51
7:L:402:BPB:HBB	3:M:208:TYR:CG	2.43	0.51
3:M:206:PHE:CE2	3:M:273:MET:HB3	2.45	0.51
3:M:160:CYS:SG	13:M:600:NS5:H322	2.50	0.51
3:M:178:TRP:HA	3:M:178:TRP:CE3	2.46	0.51
3:M:243:VAL:CG1	3:M:260:ILE:HB	2.40	0.51
9:M:702:LDA:H11	4:H:14:GLN:HE21	1.75	0.51
1:C:272:ARG:HD2	1:C:272:ARG:N	2.25	0.51
3:M:17:ILE:HG22	3:M:18:THR:N	2.25	0.51
3:M:124:LEU:HD21	6:M:1303:BCB:H142	1.92	0.51
2:L:121:PHE:O	2:L:124:PRO:HG2	2.10	0.51
9:M:702:LDA:H11	4:H:14:GLN:HE22	1.74	0.51
3:M:73:MET:O	3:M:76:GLU:HB2	2.11	0.51
3:M:282:ILE:HD11	6:M:1303:BCB:OBD	2.11	0.51
7:M:401:BPB:C14	7:M:401:BPB:H10	2.41	0.51
4:H:192:ARG:NH2	4:H:223:ARG:HG2	2.26	0.51
4:H:258:LEU:H	4:H:258:LEU:CD2	2.21	0.51
4:H:249:ALA:HB3	4:H:253:ARG:NH1	2.26	0.50
4:H:183:LEU:HG	4:H:198:LEU:HD13	1.93	0.50
1:C:197:ASP:HB3	1:C:275:ARG:HD3	1.93	0.50
3:M:15:PRO:HD3	4:H:142:ASP:HB2	1.94	0.50
4:H:90:LEU:HD13	4:H:101:LEU:HD13	1.93	0.50
2:L:151:LEU:HD21	9:M:702:LDA:H123	1.93	0.50
2:L:210:GLU:OE1	4:H:176:SER:HB3	2.12	0.50
1:C:56:TYR:OH	1:C:67:GLU:HG3	2.12	0.50
3:M:21:GLY:C	3:M:23:TRP:H	2.18	0.50
3:M:198:PRO:HG3	9:M:702:LDA:H112	1.92	0.50
4:H:248:TYR:O	4:H:249:ALA:C	2.54	0.50
4:H:38:ARG:HA	4:H:79:PRO:HB3	1.94	0.50
4:H:220:ASN:HB2	4:H:241:TYR:OH	2.11	0.50
4:H:138:ARG:NH2	4:H:184:GLU:OE1	2.42	0.49
1:C:27:THR:HG22	1:C:31:LYS:HE2	1.93	0.49
3:M:241:THR:HG22	4:H:236:ASP:OD2	2.12	0.49
1:C:309:HIS:CE1	1:C:315:PRO:HD3	2.47	0.49
3:M:87:GLN:O	3:M:91:LEU:HG	2.13	0.49
3:M:173:VAL:HG22	3:M:183:TRP:CE2	2.48	0.49
3:M:17:ILE:HD11	4:H:175:ARG:O	2.12	0.49
2:L:28:PRO:O	3:M:252:TRP:HA	2.13	0.49
3:M:24:GLY:HA3	3:M:50:TYR:HE1	1.78	0.49
3:M:178:TRP:HA	3:M:178:TRP:HE3	1.77	0.49
1:C:65:LEU:HD21	1:C:327:GLU:CG	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:224:ILE:HG12	2:L:228:SER:CB	2.42	0.49
6:M:1303:BCB:HBB3	6:M:1303:BCB:HMB1	1.94	0.49
4:H:158:VAL:HG21	4:H:207:LYS:HD3	1.95	0.48
1:C:144:TYR:CD2	1:C:310:GLN:HG2	2.48	0.48
6:L:302:BCB:HBB3	6:L:302:BCB:HMB1	1.95	0.48
4:H:181:ARG:HH11	4:H:181:ARG:HG2	1.78	0.48
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.48	0.48
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.95	0.48
4:H:8:GLN:O	4:H:9:HIS:C	2.55	0.48
6:L:304:BCB:HMB3	6:L:304:BCB:CBB	2.43	0.48
6:M:1303:BCB:H143	7:M:401:BPB:CBA	2.44	0.48
6:L:302:BCB:HBA1	6:L:302:BCB:CHA	2.44	0.48
3:M:146:TRP:HA	3:M:146:TRP:CE3	2.47	0.48
1:C:206:GLN:HA	1:C:206:GLN:OE1	2.14	0.48
3:M:157:CYS:HA	3:M:161:ILE:HB	1.96	0.48
4:H:134:ILE:HG22	4:H:172:TRP:HE3	1.79	0.48
7:M:401:BPB:H10	7:M:401:BPB:H14B	1.96	0.47
4:H:27:VAL:O	4:H:31:TYR:HB3	2.14	0.47
2:L:3:LEU:HB2	2:L:6:GLU:HB2	1.95	0.47
3:M:59:PHE:HA	7:M:401:BPB:H4A	1.96	0.47
6:M:1303:BCB:OBB	6:M:1303:BCB:HHC	2.14	0.47
4:H:137:LEU:HA	4:H:140:ALA:HB3	1.97	0.47
1:C:65:LEU:HD21	1:C:327:GLU:HG2	1.96	0.47
4:H:10:LEU:HD12	4:H:10:LEU:O	2.14	0.47
1:C:12:THR:HG23	1:C:20:GLY:HA2	1.95	0.47
4:H:35:GLU:C	4:H:37:ARG:N	2.73	0.47
3:M:62:GLY:O	3:M:65:ALA:HB3	2.15	0.47
2:L:97:PHE:CE1	6:L:302:BCB:H101	2.50	0.47
2:L:217:ARG:O	2:L:221:GLY:HA2	2.15	0.47
3:M:69:ILE:O	3:M:73:MET:HG3	2.14	0.47
4:H:78:VAL:HA	4:H:79:PRO:C	2.39	0.47
4:H:127:THR:C	4:H:129:ASP:N	2.71	0.47
4:H:127:THR:O	4:H:129:ASP:N	2.47	0.47
1:C:18:SER:HB2	2:L:156:TRP:CD1	2.50	0.47
1:C:66:THR:OG1	1:C:69:GLU:HG3	2.15	0.47
2:L:109:ARG:HD3	2:L:115:TRP:CZ2	2.50	0.47
4:H:6:LEU:O	4:H:7:ALA:O	2.33	0.47
2:L:71:LEU:HD23	2:L:143:GLY:HA3	1.97	0.46
6:L:302:BCB:OBB	6:L:302:BCB:HHC	2.14	0.46
1:C:181:ALA:O	1:C:182:TYR:HB2	2.14	0.46
2:L:193:LEU:HD13	2:L:216:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:401:BPB:H6A	7:M:401:BPB:H4	1.55	0.46
2:L:210:GLU:OE1	2:L:210:GLU:N	2.49	0.46
4:H:196:ILE:HA	4:H:242:TYR:CE2	2.51	0.46
1:C:252:THR:HG23	1:C:255:SER:HB2	1.97	0.46
2:L:80:LEU:HD12	2:L:80:LEU:N	2.29	0.46
2:L:85:PHE:O	2:L:89:ILE:HG13	2.16	0.46
3:M:231:ARG:NH2	4:H:235:GLU:CD	2.68	0.46
2:L:123:VAL:N	2:L:124:PRO:HD2	2.30	0.46
6:M:1303:BCB:HAA2	6:M:1303:BCB:HBD	1.97	0.46
2:L:205:LYS:HA	4:H:69:VAL:HG13	1.96	0.46
13:M:600:NS5:H29	13:M:600:NS5:H271	1.83	0.46
9:L:705:LDA:HM22	9:L:705:LDA:H31	1.98	0.45
3:M:241:THR:N	4:H:118:ALA:HB2	2.31	0.45
4:H:107:PRO:HB2	4:H:248:TYR:CD2	2.51	0.45
2:L:117:VAL:HG11	3:M:249:PHE:CE2	2.52	0.45
2:L:65:SER:OG	2:L:67:ASN:OD1	2.28	0.45
3:M:29:VAL:HG11	3:M:51:LEU:HD13	1.98	0.45
3:M:41:ILE:C	3:M:41:ILE:HD12	2.41	0.45
2:L:165:LEU:HD23	2:L:165:LEU:H	1.82	0.45
6:L:304:BCB:OBB	6:L:304:BCB:HHC	2.16	0.45
3:M:195:TYR:CZ	6:M:1303:BCB:HMC2	2.52	0.45
4:H:66:LYS:HG2	4:H:78:VAL:HG23	1.97	0.45
7:L:402:BPB:HEDB	3:M:250:TRP:CZ3	2.52	0.45
1:C:304:ASP:C	1:C:304:ASP:OD1	2.60	0.45
5:C:1202:HEC:HMC1	5:C:1202:HEC:HBC3	1.98	0.45
2:L:168:HIS:HE2	6:L:302:BCB:HHC	1.82	0.45
3:M:258:ALA:HB1	3:M:262:SER:HG	1.81	0.45
2:L:212:GLU:HB3	8:L:502:UQ2:H2M3	1.98	0.44
3:M:227:PHE:CE1	4:H:243:ALA:HB2	2.52	0.44
4:H:33:ARG:O	4:H:37:ARG:HG3	2.17	0.44
2:L:215:TYR:O	2:L:219:VAL:HG23	2.17	0.44
3:M:1:ALA:O	3:M:2:ASP:C	2.60	0.44
4:H:215:SER:O	4:H:218:PHE:HB2	2.17	0.44
1:C:92:ASP:O	1:C:93:GLU:C	2.60	0.44
1:C:293:ARG:NE	5:C:1202:HEC:O2A	2.49	0.44
3:M:52:GLY:O	3:M:56:ILE:HG13	2.17	0.44
3:M:69:ILE:HG21	13:M:600:NS5:C11	2.47	0.44
2:L:146:PHE:HB3	2:L:156:TRP:CD2	2.53	0.44
2:L:206:VAL:O	4:H:71:PRO:HB3	2.17	0.44
2:L:185:MET:HE2	7:M:401:BPB:NB	2.32	0.44
1:C:127:GLN:O	1:C:322:LEU:HD22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:VAL:HA	1:C:205:PRO:HD3	1.86	0.44
7:L:402:BPB:CBB	3:M:208:TYR:CD2	2.95	0.44
1:C:176:LEU:HD11	1:C:187:TYR:O	2.18	0.44
1:C:237:SER:HB3	1:C:242:THR:O	2.17	0.44
4:H:137:LEU:C	4:H:139:VAL:N	2.75	0.44
1:C:147:TYR:CE1	1:C:301:PRO:HG3	2.53	0.43
1:C:245:THR:HA	1:C:248:HIS:O	2.18	0.43
4:H:143:PHE:CE1	4:H:175:ARG:HG2	2.53	0.43
3:M:7:TYR:HB2	3:M:40:LYS:O	2.18	0.43
3:M:132:TYR:O	3:M:135:ALA:HB3	2.19	0.43
3:M:181:ILE:HD12	6:M:1301:BCB:CED	2.47	0.43
3:M:184:LEU:HD21	6:M:1301:BCB:CAC	2.48	0.43
4:H:142:ASP:N	4:H:142:ASP:OD2	2.46	0.43
3:M:2:ASP:OD1	3:M:5:THR:HG23	2.17	0.43
4:H:160:ALA:C	4:H:162:GLY:H	2.26	0.43
1:C:139:THR:HG23	1:C:157:ARG:NH2	2.33	0.43
3:M:2:ASP:CG	3:M:5:THR:HG23	2.44	0.43
7:M:401:BPB:H19A	7:M:401:BPB:H15A	1.99	0.43
4:H:10:LEU:HD12	4:H:10:LEU:C	2.43	0.43
4:H:35:GLU:C	4:H:37:ARG:H	2.26	0.43
4:H:22:LEU:HD22	4:H:22:LEU:HA	1.89	0.43
2:L:86:TRP:CZ2	2:L:145:ALA:CB	3.01	0.43
2:L:218:ASP:O	3:M:50:TYR:HB3	2.18	0.43
7:M:401:BPB:HBBB	7:M:401:BPB:CHC	2.48	0.43
2:L:262:TRP:C	2:L:264:GLY:H	2.27	0.43
9:L:705:LDA:H32	9:M:701:LDA:HM11	1.99	0.43
3:M:55:GLY:O	3:M:59:PHE:HD1	2.01	0.43
3:M:176:GLY:C	3:M:179:PRO:HD2	2.44	0.43
1:C:247:CYS:HB3	1:C:264:ARG:HB2	1.99	0.43
3:M:1:ALA:O	3:M:3:TYR:N	2.52	0.43
3:M:77:VAL:HG21	3:M:84:PHE:HB2	2.00	0.43
2:L:135:ARG:CZ	2:L:160:PHE:CZ	3.01	0.43
3:M:11:GLN:O	4:H:180:PHE:HE2	2.01	0.43
3:M:265:ARG:HG2	3:M:265:ARG:NH1	2.32	0.43
1:C:305:CYS:SG	5:C:1204:HEC:HMB1	2.59	0.42
2:L:113:ILE:HB	3:M:223:ALA:O	2.19	0.42
3:M:62:GLY:HA3	7:M:401:BPB:H6	2.01	0.42
2:L:181:PHE:HD2	7:M:401:BPB:HBB	1.77	0.42
4:H:37:ARG:HD2	4:H:61:GLU:HB2	2.01	0.42
1:C:136:HIS:O	1:C:137:ARG:C	2.61	0.42
4:H:136:PRO:HA	4:H:172:TRP:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:180:PHE:O	4:H:198:LEU:HD23	2.19	0.42
4:H:182:TYR:OH	4:H:235:GLU:HB3	2.19	0.42
1:C:35:ASP:OD2	1:C:316:LEU:HA	2.19	0.42
2:L:58:THR:OG1	2:L:59:TRP:N	2.52	0.42
3:M:226:ARG:HD3	4:H:200:PHE:CE1	2.55	0.42
4:H:152:PRO:O	4:H:168:VAL:HB	2.19	0.42
1:C:115:ARG:NH1	1:C:331:ILE:HG13	2.35	0.42
3:M:283:LEU:HD23	3:M:283:LEU:HA	1.88	0.42
4:H:97:GLU:C	4:H:99:ALA:H	2.28	0.42
4:H:127:THR:C	4:H:129:ASP:H	2.28	0.42
2:L:25:TRP:O	4:H:98:GLY:HA3	2.20	0.42
2:L:150:ILE:O	6:L:304:BCB:HED1	2.19	0.42
6:L:304:BCB:H51	6:L:304:BCB:H8	1.92	0.42
6:M:1303:BCB:H143	7:M:401:BPB:HBA	2.02	0.42
4:H:4:GLY:O	4:H:12:ILE:HG12	2.20	0.42
2:L:167:TRP:NE1	2:L:173:HIS:CD2	2.88	0.42
3:M:38:LEU:HD22	3:M:46:ILE:HD11	2.01	0.42
6:M:1301:BCB:HBB3	6:M:1303:BCB:C6	2.49	0.42
4:H:72:HIS:CD2	4:H:126:ALA:HB3	2.55	0.42
1:C:246:PHE:CZ	1:C:263:GLN:HG2	2.55	0.42
1:C:234:MET:SD	2:L:165:LEU:HB3	2.60	0.42
3:M:125:GLY:O	3:M:129:ILE:HG12	2.20	0.42
4:H:106:ASN:HA	4:H:107:PRO:HD2	1.85	0.42
2:L:126:PHE:O	2:L:130:VAL:HG23	2.20	0.41
1:C:238:ASP:OD2	1:C:306:ARG:NH2	2.53	0.41
2:L:168:HIS:CE1	6:L:302:BCB:HMC2	2.55	0.41
4:H:125:ASP:CG	4:H:133:LYS:HD2	2.45	0.41
1:C:3:GLU:HB3	1:C:24:HIS:CE1	2.55	0.41
1:C:252:THR:HG23	1:C:252:THR:O	2.20	0.41
5:C:1202:HEC:CGD	5:C:1202:HEC:HHA	2.50	0.41
4:H:106:ASN:HD22	4:H:109:VAL:CG2	2.32	0.41
1:C:163:VAL:HA	1:C:168:THR:HG21	2.03	0.41
1:C:285:LEU:C	1:C:287:ALA:H	2.28	0.41
1:C:285:LEU:C	1:C:287:ALA:N	2.76	0.41
2:L:33:PHE:O	2:L:36:VAL:HB	2.20	0.41
3:M:20:SER:HA	3:M:25:ASP:OD2	2.20	0.41
3:M:29:VAL:HG22	3:M:30:GLY:N	2.34	0.41
7:M:401:BPB:HBA	7:M:401:BPB:H44	1.56	0.41
4:H:6:LEU:HD11	4:H:12:ILE:HD13	2.02	0.41
1:C:72:ARG:HG2	1:C:72:ARG:HH11	1.86	0.41
2:L:215:TYR:OH	3:M:131:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:302:BCB:C1	6:L:304:BCB:H2C	2.50	0.41
4:H:177:GLU:O	4:H:178:HIS:HB2	2.20	0.41
1:C:290:PRO:C	1:C:292:SER:N	2.79	0.41
3:M:258:ALA:HA	4:H:36:ASP:HB3	2.03	0.41
3:M:299:HIS:HB3	9:M:702:LDA:C2	2.46	0.41
1:C:265:ALA:O	1:C:268:TRP:HB3	2.21	0.41
2:L:12:ARG:HG3	2:L:12:ARG:HH11	1.86	0.41
2:L:58:THR:HG21	2:L:63:ALA:HB3	2.03	0.41
3:M:2:ASP:OD1	3:M:2:ASP:C	2.64	0.41
3:M:155:VAL:HG22	6:M:1301:BCB:HBB1	2.01	0.41
4:H:6:LEU:HB2	4:H:10:LEU:CD1	2.41	0.41
2:L:16:LEU:HD13	2:L:106:GLU:HG2	2.03	0.41
2:L:110:LYS:O	4:H:114:PRO:HG3	2.20	0.41
2:L:181:PHE:HB3	7:M:401:BPB:HBBB	2.03	0.41
3:M:10:ILE:HD13	4:H:152:PRO:HD3	2.03	0.41
3:M:124:LEU:CD2	6:M:1303:BCB:H142	2.50	0.41
3:M:183:TRP:CZ3	3:M:184:LEU:HD23	2.55	0.41
3:M:266:TRP:CE3	4:H:32:LEU:HD13	2.56	0.41
4:H:65:PRO:CG	9:H:703:LDA:H92	2.50	0.41
1:C:65:LEU:HD22	1:C:69:GLU:HB3	2.03	0.41
1:C:121:TRP:CE3	1:C:273:MET:HB2	2.56	0.40
1:C:137:ARG:CG	1:C:310:GLN:HE22	2.34	0.40
2:L:203:GLY:O	4:H:69:VAL:HG11	2.21	0.40
6:L:302:BCB:H62	6:L:302:BCB:H41	1.90	0.40
2:L:121:PHE:CE2	2:L:125:ILE:HD11	2.56	0.40
3:M:71:PHE:CD2	9:M:706:LDA:H71	2.57	0.40
4:H:181:ARG:HG2	4:H:181:ARG:NH1	2.36	0.40
1:C:56:TYR:HB3	5:C:1201:HEC:CGA	2.51	0.40
2:L:115:TRP:N	2:L:115:TRP:CD1	2.89	0.40
7:L:402:BPB:HHC	7:L:402:BPB:CBB	2.35	0.40
3:M:178:TRP:N	3:M:179:PRO:CD	2.85	0.40
4:H:97:GLU:C	4:H:99:ALA:N	2.78	0.40
4:H:150:VAL:CG1	4:H:151:ASP:N	2.84	0.40
1:C:85:GLU:HG2	1:C:89:TYR:CD1	2.56	0.40
2:L:224:ILE:HB	8:L:502:UQ2:H112	2.03	0.40
3:M:204:ILE:HG12	6:M:1303:BCB:CHB	2.51	0.40
2:L:170:ASN:O	2:L:174:MET:HG3	2.22	0.40
4:H:191:ALA:O	4:H:192:ARG:HB3	2.21	0.40
4:H:231:THR:O	4:H:234:GLU:N	2.55	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%)	299 (91%)	30 (9%)	1 (0%)	36 54
2	L	271/273 (99%)	251 (93%)	17 (6%)	3 (1%)	11 24
3	M	321/323 (99%)	299 (93%)	19 (6%)	3 (1%)	14 28
4	H	256/258 (99%)	216 (84%)	25 (10%)	15 (6%)	1 2
All	All	1178/1190 (99%)	1065 (90%)	91 (8%)	22 (2%)	6 14

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	57	PRO
4	H	7	ALA
4	H	8	GLN
4	H	9	HIS
4	H	96	PHE
4	H	257	LEU
2	L	165	LEU
3	M	2	ASP
3	M	177	ILE
4	H	49	LEU
4	H	130	GLY
4	H	162	GLY
4	H	163	VAL
2	L	226	ALA
4	H	55	GLU
4	H	191	ALA
4	H	95	GLY
4	H	192	ARG
4	H	51	LYS
3	M	193	ASN
4	H	43	LEU
1	C	214	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	281/282 (100%)	276 (98%)	5 (2%)	51 73
2	L	218/218 (100%)	211 (97%)	7 (3%)	34 59
3	M	249/249 (100%)	241 (97%)	8 (3%)	34 59
4	H	212/212 (100%)	198 (93%)	14 (7%)	15 32
All	All	960/961 (100%)	926 (96%)	34 (4%)	32 57

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	15	ARG
1	C	23	LEU
1	C	32	LYS
1	C	152	LEU
1	C	327	GLU
2	L	7	ARG
2	L	17	ILE
2	L	152	SER
2	L	165	LEU
2	L	204	ASP
2	L	210	GLU
2	L	218	ASP
3	M	22	GLU
3	M	27	ASP
3	M	34	TYR
3	M	51	LEU
3	M	147	ASN
3	M	181	ILE
3	M	194	PHE
3	M	214	PHE
4	H	22	LEU
4	H	69	VAL
4	H	92	GLN
4	H	96	PHE

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Mol	Chain	Res	Type
4	H	97	GLU
4	H	123	VAL
4	H	163	VAL
4	H	190	SER
4	H	192	ARG
4	H	198	LEU
4	H	207	LYS
4	H	236	ASP
4	H	252	GLU
4	H	258	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	24	HIS
1	C	58	ASN
1	C	94	ASN
1	C	95	ASN
1	C	286	ASN
1	C	302	GLN
1	C	310	GLN
2	L	158	ASN
2	L	183	ASN
2	L	213	ASN
2	L	239	ASN
3	M	16	HIS
3	M	147	ASN
4	H	8	GLN
4	H	58	GLN
4	H	102	GLN
4	H	106	ASN
4	H	220	ASN
4	H	229	GLN

5.3.3 RNA

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	$\#\|Z\| > 2$
4	FME	H	1	4	8,9,10	0.67	0	8,9,11	3.14	3 (37%)

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	1	FME	CA-N-CN	-7.21	111.74	122.82
4	H	1	FME	O1-CN-N	-4.09	114.75	125.32
4	H	1	FME	CE-SD-CG	-2.17	89.07	100.32

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 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	HEC	C	1202	1	50,50,50	0.92	3 (6%)	68,82,82	1.33	9 (13%)
6	BCB	L	302	2	68,74,74	1.36	8 (11%)	77,115,115	2.22	19 (24%)
11	SO4	M	802	-	4,4,4	0.45	0	6,6,6	0.54	0
7	BPB	L	402	-	57,70,70	1.64	9 (15%)	55,101,101	3.29	19 (34%)
5	HEC	C	1203	1	50,50,50	0.93	2 (4%)	68,82,82	0.94	4 (5%)
9	LDA	H	703	-	13,15,15	2.73	2 (15%)	14,17,17	0.49	0
7	BPB	M	401	-	57,70,70	1.72	12 (21%)	55,101,101	2.86	18 (32%)
9	LDA	M	702	-	13,15,15	2.18	2 (15%)	14,17,17	0.51	0
11	SO4	H	801	-	4,4,4	0.31	0	6,6,6	0.37	0
11	SO4	M	804	-	4,4,4	0.45	0	6,6,6	0.41	0
12	MQ7	M	501	-	49,49,49	1.67	17 (34%)	61,63,63	1.50	8 (13%)
9	LDA	M	704	-	13,15,15	2.61	2 (15%)	14,17,17	0.54	0
6	BCB	M	1303	3	68,74,74	1.26	7 (10%)	77,115,115	1.86	11 (14%)
5	HEC	C	1204	1	50,50,50	0.94	2 (4%)	68,82,82	1.35	8 (11%)
6	BCB	L	304	2	68,74,74	1.34	8 (11%)	77,115,115	2.12	11 (14%)
9	LDA	M	701	-	13,15,15	2.37	2 (15%)	14,17,17	0.64	0
8	UQ2	L	502	-	23,23,23	1.78	5 (21%)	30,31,31	1.29	3 (10%)
13	NS5	M	600	-	39,39,39	0.70	0	46,46,46	1.06	4 (8%)
9	LDA	M	706	-	13,15,15	2.54	2 (15%)	14,17,17	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	SO4	M	803	-	4,4,4	0.42	0	6,6,6	0.07	0
6	BCB	M	1301	3	68,74,74	1.31	8 (11%)	77,115,115	1.92	9 (11%)
5	HEC	C	1201	1	50,50,50	0.99	3 (6%)	68,82,82	1.29	7 (10%)
9	LDA	L	705	-	13,15,15	2.44	2 (15%)	14,17,17	0.57	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
5	HEC	C	1202	1	1/1/3/7	8/14/54/54	-
6	BCB	L	302	2	2/2/21/26	9/41/137/137	-
7	BPB	L	402	-	-	5/37/105/105	0/5/6/6
5	HEC	C	1203	1	1/1/3/7	8/14/54/54	-
9	LDA	H	703	-	-	1/13/13/13	-
7	BPB	M	401	-	1/1/18/23	12/37/105/105	0/5/6/6
9	LDA	M	702	-	-	0/13/13/13	-
12	MQ7	M	501	-	-	2/41/61/61	0/2/2/2
9	LDA	M	704	-	-	3/13/13/13	-
6	BCB	M	1303	3	4/4/21/26	7/41/137/137	-
5	HEC	C	1204	1	1/1/3/7	7/14/54/54	-
6	BCB	L	304	2	4/4/21/26	12/41/137/137	-
9	LDA	M	701	-	-	0/13/13/13	-
8	UQ2	L	502	-	-	3/15/39/39	0/1/1/1
13	NS5	M	600	-	-	8/43/43/43	-
9	LDA	M	706	-	-	0/13/13/13	-
6	BCB	M	1301	3	3/3/21/26	9/41/137/137	-
5	HEC	C	1201	1	1/1/3/7	6/14/54/54	-
9	LDA	L	705	-	-	0/13/13/13	-

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	H	703	LDA	O1-N1	-8.24	1.22	1.42
9	M	704	LDA	O1-N1	-8.12	1.22	1.42
9	M	701	LDA	O1-N1	-7.98	1.22	1.42
9	M	706	LDA	O1-N1	-7.88	1.22	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	702	LDA	O1-N1	-7.41	1.24	1.42
9	L	705	LDA	O1-N1	-7.11	1.24	1.42
9	H	703	LDA	C1-N1	-5.34	1.46	1.51
6	M	1301	BCB	MG-NA	5.28	2.18	2.06
7	L	402	BPB	C1D-C2D	5.28	1.45	1.39
7	M	401	BPB	C1D-C2D	5.27	1.45	1.39
8	L	502	UQ2	C7-C8	-5.22	1.42	1.50
9	L	705	LDA	C1-N1	-5.16	1.46	1.51
7	M	401	BPB	C3A-C2A	-4.92	1.50	1.54
7	L	402	BPB	C3A-C2A	-4.84	1.50	1.54
7	L	402	BPB	C1B-C2B	4.79	1.44	1.39
6	L	304	BCB	O2A-CGA	4.78	1.47	1.33
9	M	704	LDA	C1-N1	-4.66	1.46	1.51
9	M	706	LDA	C1-N1	-4.66	1.46	1.51
7	M	401	BPB	C1B-C2B	4.57	1.44	1.39
6	L	302	BCB	O2D-CGD	4.54	1.44	1.33
6	L	304	BCB	MG-NA	4.19	2.16	2.06
6	L	302	BCB	MG-NA	4.04	2.15	2.06
6	M	1301	BCB	O2A-CGA	3.68	1.44	1.33
6	L	304	BCB	O2D-CGD	3.62	1.42	1.33
7	L	402	BPB	O2D-CED	-3.59	1.37	1.45
6	L	302	BCB	MG-ND	-3.54	1.98	2.05
7	M	401	BPB	O2D-CED	-3.49	1.37	1.45
6	L	304	BCB	O2D-CED	-3.45	1.37	1.45
6	M	1303	BCB	MG-ND	-3.42	1.99	2.05
6	M	1303	BCB	O2D-CGD	3.41	1.41	1.33
6	M	1303	BCB	MG-NA	3.40	2.14	2.06
7	M	401	BPB	O2A-CGA	3.36	1.43	1.33
7	L	402	BPB	O2D-CGD	3.32	1.41	1.33
6	M	1301	BCB	O2D-CED	-3.30	1.37	1.45
7	M	401	BPB	O2D-CGD	3.29	1.41	1.33
5	C	1201	HEC	FE-NB	3.24	2.04	1.94
6	M	1303	BCB	O2D-CED	-3.24	1.38	1.45
6	L	302	BCB	O2D-CED	-3.05	1.38	1.45
7	L	402	BPB	C1-C2	-3.04	1.40	1.49
12	M	501	MQ7	C26-C27	-3.03	1.41	1.50
12	M	501	MQ7	C11-C12	-2.99	1.45	1.50
6	M	1303	BCB	O2A-CGA	2.97	1.42	1.33
9	M	701	LDA	C1-N1	-2.96	1.48	1.51
5	C	1204	HEC	FE-NB	2.94	2.03	1.94
12	M	501	MQ7	C12-C13	2.91	1.39	1.33
12	M	501	MQ7	C37-C38	2.90	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1301	BCB	C2-C3	2.90	1.39	1.33
7	M	401	BPB	C3B-C4B	2.85	1.46	1.41
7	M	401	BPB	C2-C3	2.84	1.39	1.33
6	L	302	BCB	C3B-C4B	2.82	1.46	1.41
8	L	502	UQ2	O3-CM3	-2.81	1.39	1.45
6	M	1303	BCB	C3B-C4B	2.80	1.46	1.41
7	L	402	BPB	C2-C3	2.77	1.39	1.33
8	L	502	UQ2	C8-C9	2.73	1.39	1.33
6	L	304	BCB	MG-ND	-2.73	2.00	2.05
7	M	401	BPB	C1-C2	-2.73	1.41	1.49
6	L	304	BCB	C3B-C4B	2.72	1.46	1.41
12	M	501	MQ7	C22-C23	2.70	1.39	1.33
5	C	1202	HEC	FE-NB	2.69	2.03	1.94
8	L	502	UQ2	O2-CM2	-2.69	1.39	1.45
6	L	302	BCB	C2-C3	2.68	1.39	1.33
6	L	304	BCB	C2-C3	2.68	1.39	1.33
12	M	501	MQ7	C42-C43	2.67	1.40	1.32
6	M	1301	BCB	MG-NC	2.65	2.12	2.06
12	M	501	MQ7	C27-C28	2.65	1.39	1.33
6	L	304	BCB	MG-NC	2.62	2.12	2.06
5	C	1204	HEC	FE-NC	2.60	2.03	1.95
6	M	1301	BCB	C3B-C4B	2.59	1.46	1.41
6	M	1303	BCB	C2-C3	2.55	1.38	1.33
5	C	1203	HEC	FE-ND	2.52	2.02	1.94
12	M	501	MQ7	C32-C33	2.51	1.38	1.33
7	L	402	BPB	C3B-C4B	2.43	1.45	1.41
7	L	402	BPB	C3B-C2B	-2.41	1.35	1.39
12	M	501	MQ7	C17-C18	2.36	1.38	1.33
9	M	702	LDA	C1-N1	-2.36	1.49	1.51
8	L	502	UQ2	C13-C14	2.36	1.39	1.32
5	C	1203	HEC	FE-NB	2.35	2.02	1.94
6	M	1301	BCB	CAC-C3C	2.23	1.39	1.33
5	C	1202	HEC	FE-NA	2.22	2.02	1.95
12	M	501	MQ7	C24-C23	2.18	1.56	1.50
12	M	501	MQ7	C10-C5	-2.17	1.37	1.40
12	M	501	MQ7	C3-C2	2.14	1.39	1.35
5	C	1201	HEC	FE-ND	2.14	2.01	1.94
5	C	1201	HEC	FE-NC	2.14	2.02	1.95
7	M	401	BPB	C3D-C4D	2.11	1.44	1.41
12	M	501	MQ7	C45-C43	2.09	1.56	1.50
6	L	302	BCB	C4-C3	2.09	1.55	1.50
5	C	1202	HEC	FE-ND	2.08	2.01	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	501	MQ7	C44-C43	2.08	1.56	1.50
7	M	401	BPB	CBC-CAC	2.06	1.57	1.49
12	M	501	MQ7	C40-C38	2.05	1.55	1.51
12	M	501	MQ7	C15-C13	2.04	1.55	1.51
6	L	302	BCB	C1-C2	-2.04	1.43	1.49
12	M	501	MQ7	C31-C32	-2.03	1.44	1.50
6	M	1301	BCB	MG-ND	-2.02	2.01	2.05
7	M	401	BPB	CHA-CBD	2.02	1.54	1.51

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	L	402	BPB	O2D-CGD-CBD	11.78	123.89	110.95
7	L	402	BPB	C1-C2-C3	11.36	144.81	126.20
7	M	401	BPB	O2D-CGD-CBD	11.17	123.22	110.95
7	M	401	BPB	C1-C2-C3	10.36	143.17	126.20
6	M	1301	BCB	C4A-NA-C1A	8.56	110.58	106.68
6	L	304	BCB	C4A-NA-C1A	8.32	110.48	106.68
6	M	1303	BCB	C4A-NA-C1A	7.95	110.30	106.68
6	L	302	BCB	C4A-NA-C1A	7.91	110.29	106.68
6	L	304	BCB	C1-C2-C3	7.19	137.98	126.20
7	L	402	BPB	C5-C3-C2	7.19	137.31	121.17
12	M	501	MQ7	C11-C12-C13	7.05	138.98	126.83
6	L	304	BCB	O2D-CGD-CBD	6.93	123.34	111.23
7	L	402	BPB	O1D-CGD-CBD	-6.92	114.23	124.72
7	L	402	BPB	O2A-CGA-CBA	6.74	132.39	111.83
6	M	1301	BCB	O2D-CGD-CBD	6.70	122.94	111.23
6	L	302	BCB	C1-C2-C3	-6.69	115.23	126.20
6	M	1301	BCB	C1-C2-C3	6.68	137.15	126.20
7	M	401	BPB	O1D-CGD-CBD	-6.65	114.63	124.72
6	L	302	BCB	O2D-CGD-CBD	6.52	122.63	111.23
7	L	402	BPB	O2A-CGA-O1A	-6.51	107.33	123.63
6	L	302	BCB	O2A-CGA-CBA	6.06	130.31	111.83
6	M	1303	BCB	O2D-CGD-CBD	5.67	121.13	111.23
7	M	401	BPB	C4D-CHA-CBD	-5.60	105.77	108.45
7	M	401	BPB	C5-C3-C2	5.49	133.48	121.17
7	L	402	BPB	C4D-CHA-CBD	-5.28	105.92	108.45
5	C	1202	HEC	CAC-C3C-C4C	-5.19	117.77	124.91
5	C	1202	HEC	CAC-C3C-C2C	5.15	135.03	126.89
6	M	1303	BCB	C1C-NC-C4C	5.02	108.97	106.68
6	L	302	BCB	O2A-CGA-O1A	-4.99	111.16	123.63
6	L	304	BCB	O1D-CGD-CBD	-4.92	114.81	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	304	BCB	C1C-NC-C4C	4.82	108.88	106.68
6	L	302	BCB	O1D-CGD-CBD	-4.70	115.25	124.52
6	M	1301	BCB	O1D-CGD-CBD	-4.59	115.46	124.52
6	M	1301	BCB	C1C-NC-C4C	4.35	108.66	106.68
6	L	304	BCB	OBB-CAB-C3B	4.14	127.75	120.43
7	L	402	BPB	C4-C3-C2	-4.13	113.01	123.63
5	C	1204	HEC	CAD-C3D-C4D	4.13	131.89	124.70
6	M	1303	BCB	C15-C13-C12	4.09	132.81	112.07
6	M	1303	BCB	O1D-CGD-CBD	-4.07	116.48	124.52
5	C	1201	HEC	CAC-C3C-C2C	4.04	133.28	126.89
6	L	304	BCB	C6-C5-C3	4.04	123.30	113.47
5	C	1204	HEC	CAB-C3B-C4B	-4.01	119.56	124.79
6	M	1303	BCB	O2A-CGA-CBA	3.94	123.85	111.83
5	C	1201	HEC	CAC-C3C-C4C	-3.88	119.58	124.91
5	C	1201	HEC	CAB-C3B-C4B	-3.80	119.84	124.79
5	C	1204	HEC	CAD-C3D-C2D	-3.71	120.91	127.87
7	L	402	BPB	OBD-CAD-CBD	-3.64	120.48	125.82
5	C	1201	HEC	CAD-C3D-C4D	3.63	131.02	124.70
5	C	1204	HEC	CAC-C3C-C2C	3.54	132.49	126.89
12	M	501	MQ7	C40-C38-C37	3.49	129.00	121.17
13	M	600	NS5	C19-C18-C17	3.48	130.65	123.52
8	L	502	UQ2	CM3-O3-C3	3.47	128.67	116.47
7	M	401	BPB	OBD-CAD-CBD	-3.35	120.91	125.82
6	L	302	BCB	CED-O2D-CGD	-3.30	108.42	115.92
5	C	1204	HEC	CAB-C3B-C2B	3.24	133.50	127.56
5	C	1204	HEC	CAC-C3C-C4C	-3.21	120.50	124.91
7	L	402	BPB	C4-C3-C5	-3.20	109.67	115.23
12	M	501	MQ7	C41-C42-C43	3.11	138.01	127.64
5	C	1202	HEC	CAD-C3D-C4D	3.11	130.11	124.70
5	C	1201	HEC	CAB-C3B-C2B	3.09	133.24	127.56
5	C	1201	HEC	CAD-C3D-C2D	-3.09	122.08	127.87
6	L	302	BCB	OBB-CAB-C3B	3.08	125.87	120.43
6	M	1301	BCB	CED-O2D-CGD	-3.07	108.96	115.92
5	C	1203	HEC	CAC-C3C-C2C	3.06	131.74	126.89
7	M	401	BPB	C4-C3-C2	-3.06	115.77	123.63
6	L	302	BCB	CAA-C2A-C3A	-3.03	104.81	113.00
6	L	302	BCB	C1C-NC-C4C	2.99	108.04	106.68
6	M	1303	BCB	C1-C2-C3	-2.95	121.37	126.20
7	M	401	BPB	C4D-ND-C1D	-2.92	105.38	108.87
6	L	304	BCB	CBC-CAC-C3C	-2.89	118.85	126.70
6	L	304	BCB	CBB-CAB-C3B	-2.88	114.33	120.40
7	L	402	BPB	C4D-ND-C1D	-2.87	105.43	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	M	501	MQ7	C39-C38-C40	-2.85	110.28	115.23
5	C	1204	HEC	CAA-C2A-C3A	-2.85	122.53	127.87
12	M	501	MQ7	C16-C17-C18	2.77	133.97	127.62
5	C	1204	HEC	CAA-C2A-C1A	2.75	130.45	124.85
6	M	1303	BCB	C6-C5-C3	2.75	120.16	113.47
12	M	501	MQ7	C26-C25-C23	-2.73	104.14	113.19
6	M	1303	BCB	O2A-CGA-O1A	-2.72	116.83	123.63
7	L	402	BPB	CMD-C2D-C3D	2.71	130.09	124.68
5	C	1202	HEC	CAB-C3B-C4B	-2.70	121.28	124.79
13	M	600	NS5	C16-C15-C14	-2.67	114.01	118.09
5	C	1203	HEC	CAC-C3C-C4C	-2.67	121.24	124.91
13	M	600	NS5	C18-C19-C20	2.65	128.95	123.52
5	C	1202	HEC	CAD-C3D-C2D	-2.62	122.96	127.87
7	M	401	BPB	CMD-C2D-C3D	2.60	129.88	124.68
7	M	401	BPB	C4-C3-C5	-2.58	110.74	115.23
7	M	401	BPB	O2A-CGA-CBA	2.58	119.71	111.83
6	M	1303	BCB	OBB-CAB-C3B	2.56	124.97	120.43
6	L	304	BCB	CAB-C3B-C2B	2.51	132.96	127.74
7	M	401	BPB	C2D-C1D-ND	2.49	111.23	109.43
5	C	1202	HEC	CMC-C2C-C1C	2.49	129.21	125.42
7	M	401	BPB	C6-C5-C3	-2.48	107.43	113.47
6	L	302	BCB	CAB-C3B-C2B	2.48	132.89	127.74
7	M	401	BPB	OBB-CAB-C3B	2.47	124.12	119.99
6	L	302	BCB	CBB-CAB-C3B	-2.47	115.19	120.40
6	M	1303	BCB	CAB-C3B-C2B	2.45	132.82	127.74
6	L	302	BCB	C2A-C1A-CHA	2.42	128.06	123.87
8	L	502	UQ2	C7-C6-C5	-2.37	120.82	124.89
12	M	501	MQ7	C41-C40-C38	2.35	120.98	113.19
6	M	1301	BCB	CAB-C3B-C2B	2.34	132.61	127.74
7	L	402	BPB	OBB-CAB-C3B	2.33	123.89	119.99
7	M	401	BPB	C3D-C4D-ND	2.30	110.65	107.71
7	L	402	BPB	OBD-CAD-C3D	2.28	131.44	127.89
13	M	600	NS5	C14-C15-C17	2.26	122.56	119.01
5	C	1202	HEC	CAB-C3B-C2B	2.25	131.70	127.56
6	L	302	BCB	CAA-C2A-C1A	2.22	119.26	111.97
7	L	402	BPB	C3D-C4D-ND	2.21	110.53	107.71
6	L	304	BCB	CMB-C2B-C1B	-2.20	122.06	125.42
5	C	1203	HEC	CAB-C3B-C4B	-2.20	121.92	124.79
6	L	302	BCB	C15-C13-C12	-2.20	100.91	112.07
12	M	501	MQ7	C11-C3-C2	-2.20	121.13	124.89
7	M	401	BPB	CED-O2D-CGD	2.19	120.89	115.92
6	L	302	BCB	CBC-CAC-C3C	-2.18	120.78	126.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	302	BCB	C3C-C4C-NC	2.18	113.15	110.45
7	L	402	BPB	CMA-C3A-C4A	-2.17	109.92	114.61
5	C	1201	HEC	CMA-C3A-C4A	2.17	128.56	124.73
6	L	302	BCB	C4D-CHA-C1A	2.12	123.77	121.24
7	L	402	BPB	C2D-C1D-ND	2.12	110.96	109.43
7	M	401	BPB	OBD-CAD-C3D	2.12	131.19	127.89
5	C	1203	HEC	CAB-C3B-C2B	2.11	131.44	127.56
7	M	401	BPB	C4A-C3A-C2A	2.10	104.83	102.84
7	L	402	BPB	C4A-C3A-C2A	2.10	104.83	102.84
7	L	402	BPB	C4B-NB-C1B	-2.07	105.81	108.82
6	L	302	BCB	C2A-C3A-C4A	2.06	105.20	101.87
5	C	1202	HEC	CAA-C2A-C3A	-2.06	124.01	127.87
6	M	1301	BCB	C4D-CHA-C1A	2.06	123.70	121.24
5	C	1202	HEC	CAA-C2A-C1A	2.04	129.00	124.85
6	M	1301	BCB	O2A-CGA-CBA	2.03	118.02	111.83
8	L	502	UQ2	C7-C8-C9	2.02	130.31	126.83

All (18) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	1201	HEC	NA
5	C	1202	HEC	NA
5	C	1203	HEC	NA
5	C	1204	HEC	NA
6	L	302	BCB	NA
6	L	302	BCB	ND
6	L	304	BCB	NA
6	L	304	BCB	C8
6	L	304	BCB	NC
6	L	304	BCB	ND
6	M	1301	BCB	NA
6	M	1301	BCB	NC
6	M	1301	BCB	ND
6	M	1303	BCB	NA
6	M	1303	BCB	C13
6	M	1303	BCB	NC
6	M	1303	BCB	ND
7	M	401	BPB	C13

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	302	BCB	CAD-CBD-CGD-O1D
6	L	302	BCB	CAD-CBD-CGD-O2D
6	M	1301	BCB	C2B-C3B-CAB-CBB
6	M	1301	BCB	C4B-C3B-CAB-OBB
6	M	1301	BCB	C4B-C3B-CAB-CBB
6	M	1301	BCB	C4C-C3C-CAC-CBC
6	M	1303	BCB	CAD-CBD-CGD-O1D
6	M	1303	BCB	CAD-CBD-CGD-O2D
7	M	401	BPB	C3A-C2A-CAA-CBA
13	M	600	NS5	C11-C10-C12-C13
13	M	600	NS5	C10-C12-C13-C14
13	M	600	NS5	C12-C13-C14-C15
6	L	302	BCB	CBD-CGD-O2D-CED
5	C	1201	HEC	C4B-C3B-CAB-CBB
5	C	1201	HEC	C2B-C3B-CAB-CBB
6	L	302	BCB	C4-C3-C5-C6
6	L	304	BCB	C4-C3-C5-C6
6	L	302	BCB	C2-C3-C5-C6
6	L	304	BCB	C2-C3-C5-C6
6	L	302	BCB	O1D-CGD-O2D-CED
5	C	1202	HEC	C2B-C3B-CAB-CBB
5	C	1203	HEC	C2B-C3B-CAB-CBB
5	C	1203	HEC	C2C-C3C-CAC-CBC
13	M	600	NS5	C13-C14-C15-C16
6	M	1303	BCB	C2A-CAA-CBA-CGA
5	C	1202	HEC	C4B-C3B-CAB-CBB
5	C	1204	HEC	C2B-C3B-CAB-CBB
5	C	1204	HEC	C4D-C3D-CAD-CBD
5	C	1203	HEC	C4C-C3C-CAC-CBC
5	C	1204	HEC	C2D-C3D-CAD-CBD
6	M	1301	BCB	CBD-CGD-O2D-CED
13	M	600	NS5	C13-C14-C15-C17
6	L	304	BCB	O2A-C1-C2-C3
6	M	1301	BCB	C2B-C3B-CAB-OBB
5	C	1203	HEC	C4B-C3B-CAB-CBB
7	M	401	BPB	CBA-CGA-O2A-C1
5	C	1201	HEC	C2C-C3C-CAC-CBC
7	M	401	BPB	C8-C10-C11-C12
7	M	401	BPB	O1A-CGA-O2A-C1
5	C	1201	HEC	C4C-C3C-CAC-CBC
9	H	703	LDA	C2-C3-C4-C5
6	L	304	BCB	CBD-CGD-O2D-CED
6	M	1303	BCB	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
5	C	1204	HEC	C2C-C3C-CAC-CBC
5	C	1204	HEC	C4B-C3B-CAB-CBB
6	M	1303	BCB	C12-C13-C15-C16
6	M	1301	BCB	O1D-CGD-O2D-CED
6	L	304	BCB	O1D-CGD-O2D-CED
7	L	402	BPB	CAA-CBA-CGA-O2A
5	C	1202	HEC	C2C-C3C-CAC-CBC
7	M	401	BPB	C15-C16-C17-C18
7	L	402	BPB	C4C-C3C-CAC-CBC
13	M	600	NS5	C32-C31-C33-C34
5	C	1202	HEC	C4C-C3C-CAC-CBC
7	M	401	BPB	CBD-CGD-O2D-CED
6	L	304	BCB	C12-C13-C15-C16
7	M	401	BPB	C6-C7-C8-C10
6	L	304	BCB	C4C-C3C-CAC-CBC
6	M	1303	BCB	C4-C3-C5-C6
5	C	1204	HEC	C4C-C3C-CAC-CBC
7	M	401	BPB	O1D-CGD-O2D-CED
8	L	502	UQ2	C12-C11-C9-C10
6	M	1301	BCB	CBA-CGA-O2A-C1
8	L	502	UQ2	C12-C11-C9-C8
6	M	1301	BCB	O1A-CGA-O2A-C1
6	L	302	BCB	CBA-CGA-O2A-C1
5	C	1202	HEC	CAA-CBA-CGA-O2A
6	L	302	BCB	C3A-C2A-CAA-CBA
5	C	1202	HEC	CAA-CBA-CGA-O1A
5	C	1204	HEC	C3D-CAD-CBD-CGD
6	L	302	BCB	O1A-CGA-O2A-C1
6	L	304	BCB	C6-C7-C8-C9
5	C	1201	HEC	CAA-CBA-CGA-O2A
12	M	501	MQ7	C39-C38-C40-C41
9	M	704	LDA	C3-C4-C5-C6
7	M	401	BPB	C10-C11-C12-C13
6	L	304	BCB	C11-C12-C13-C15
5	C	1201	HEC	CAA-CBA-CGA-O1A
8	L	502	UQ2	C4-C3-O3-CM3
12	M	501	MQ7	C37-C38-C40-C41
5	C	1202	HEC	CAD-CBD-CGD-O2D
5	C	1203	HEC	CAA-CBA-CGA-O2A
5	C	1203	HEC	CAD-CBD-CGD-O2D
7	L	402	BPB	C8-C10-C11-C12
7	L	402	BPB	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
13	M	600	NS5	C23-C24-C25-C26
5	C	1203	HEC	CAA-CBA-CGA-O1A
5	C	1202	HEC	CAD-CBD-CGD-O1D
5	C	1203	HEC	CAD-CBD-CGD-O1D
6	L	304	BCB	C10-C11-C12-C13
9	M	704	LDA	C7-C8-C9-C10
7	M	401	BPB	CAA-CBA-CGA-O2A
13	M	600	NS5	C7-C8-C9-C10
6	L	304	BCB	C6-C7-C8-C10
9	M	704	LDA	C4-C5-C6-C7
7	M	401	BPB	CAA-CBA-CGA-O1A
7	M	401	BPB	C4-C3-C5-C6
6	L	304	BCB	C8-C10-C11-C12
7	L	402	BPB	C2-C1-O2A-CGA
6	M	1303	BCB	CAA-CBA-CGA-O2A

There are no ring outliers.

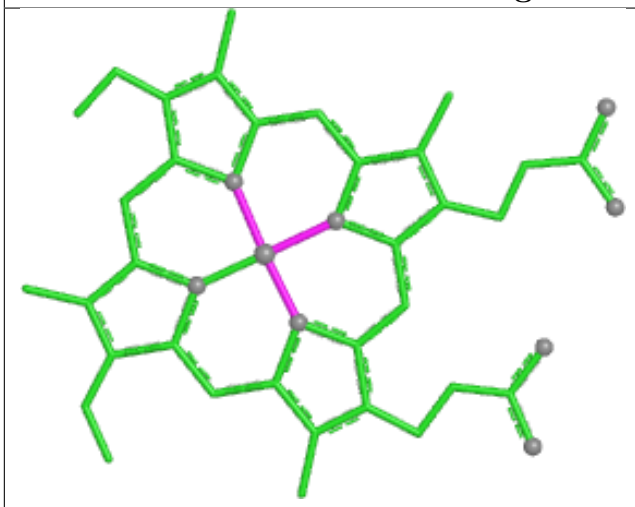
16 monomers are involved in 107 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1202	HEC	3	0
6	L	302	BCB	14	0
7	L	402	BPB	12	0
9	H	703	LDA	4	0
7	M	401	BPB	21	0
9	M	702	LDA	7	0
6	M	1303	BCB	16	0
5	C	1204	HEC	3	0
6	L	304	BCB	5	0
9	M	701	LDA	3	0
8	L	502	UQ2	4	0
13	M	600	NS5	5	0
9	M	706	LDA	1	0
6	M	1301	BCB	12	0
5	C	1201	HEC	2	0
9	L	705	LDA	2	0

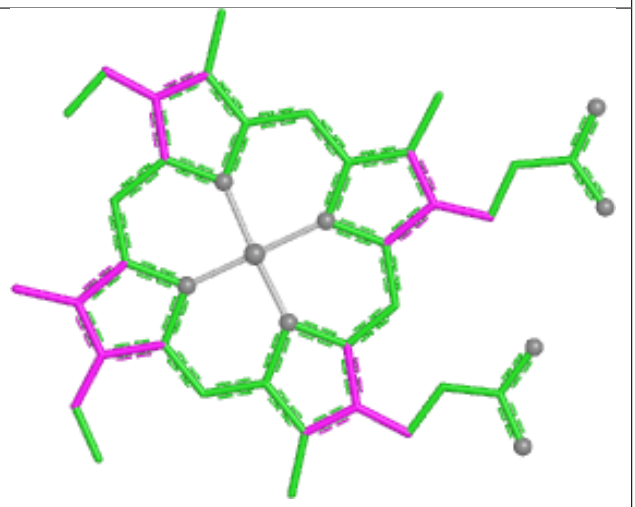
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

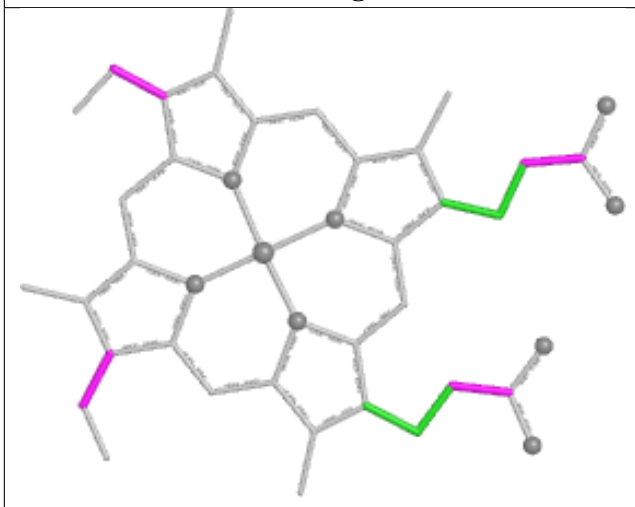
Ligand HEC C 1202



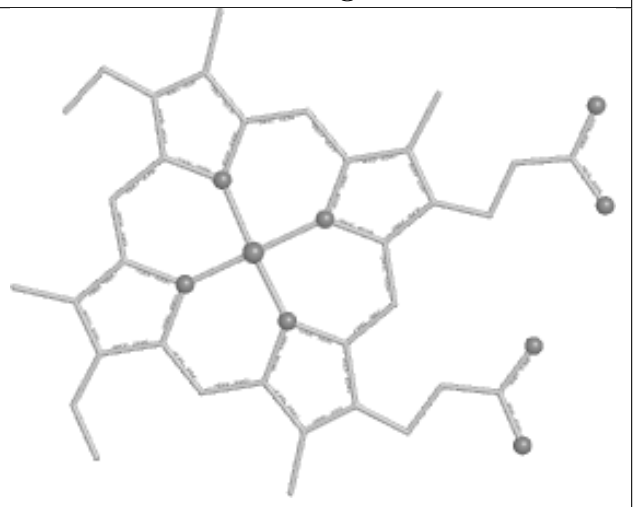
Bond lengths



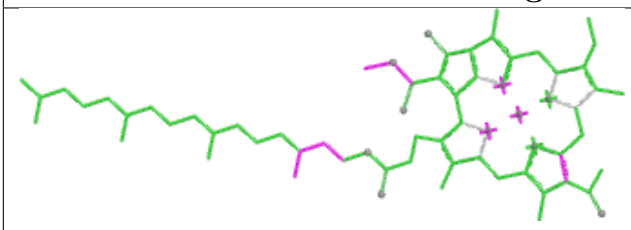
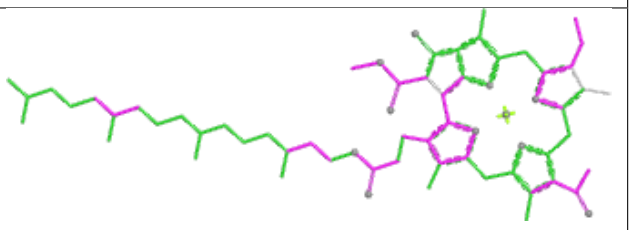
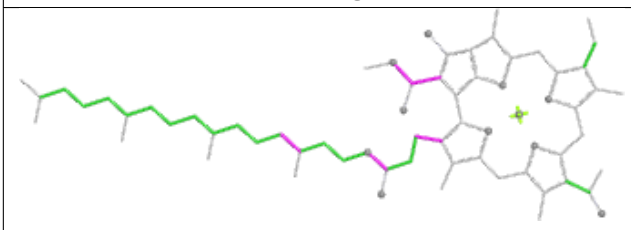
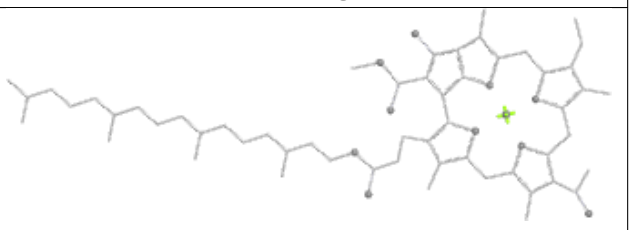
Bond angles

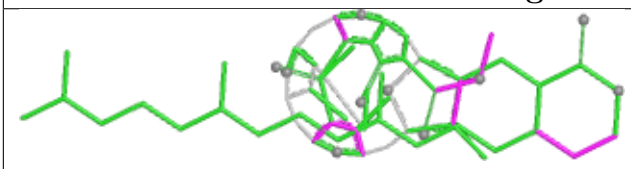
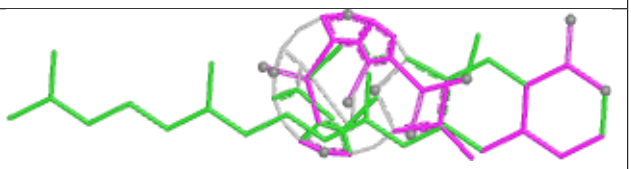
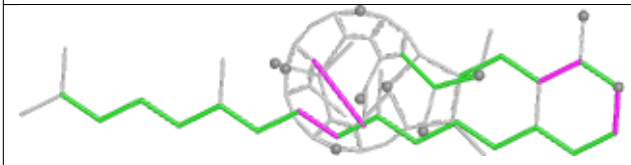
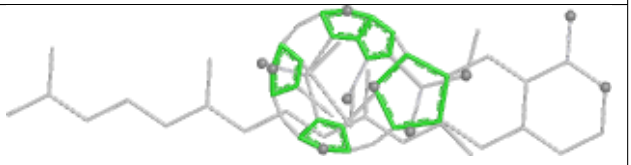


Torsions

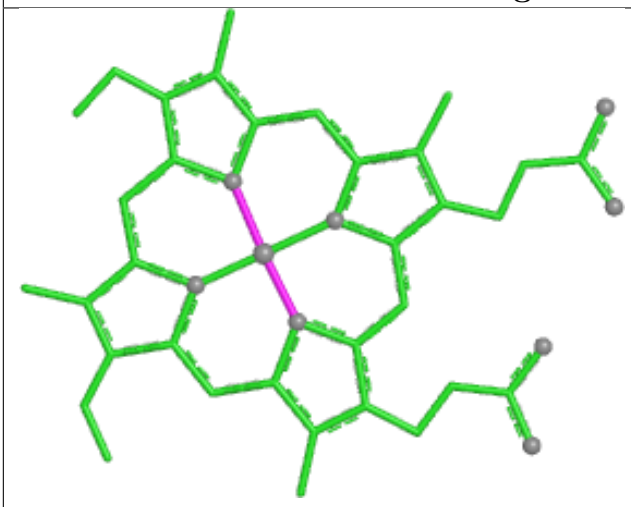


Rings

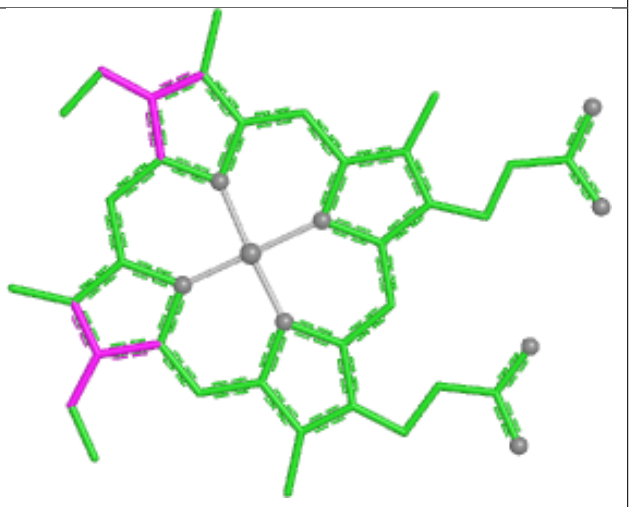
Ligand BCB L 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BPB L 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

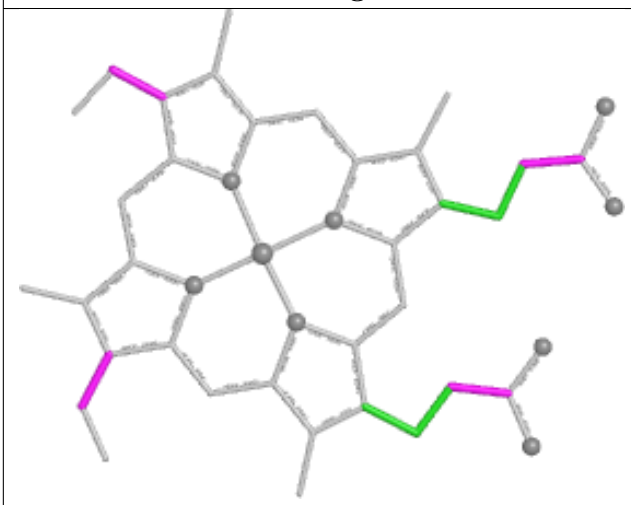
Ligand HEC C 1203



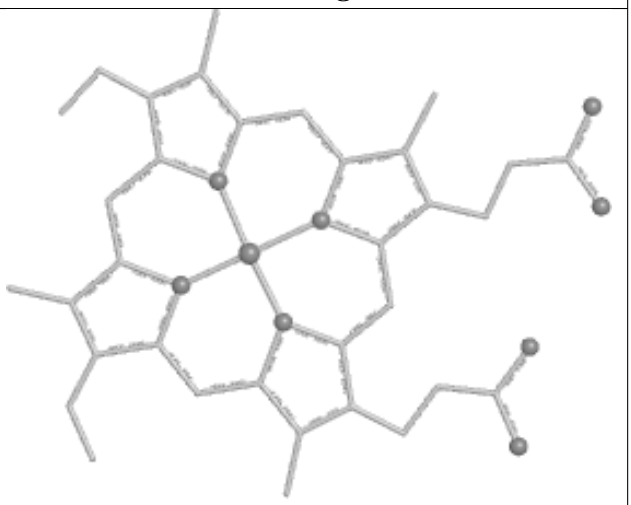
Bond lengths



Bond angles

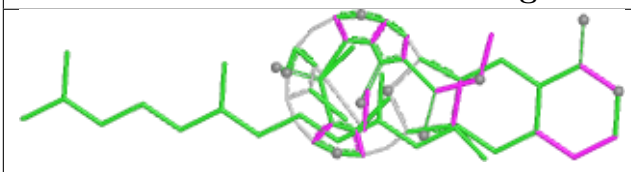


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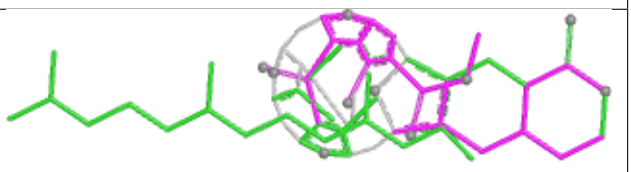


Rings

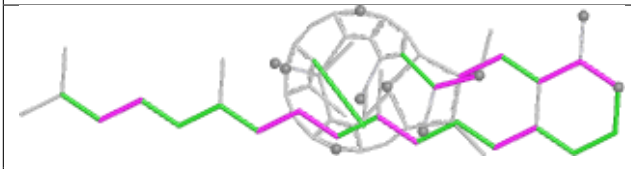
Ligand BPB M 401



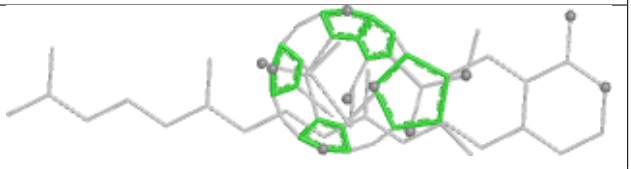
Bond lengths



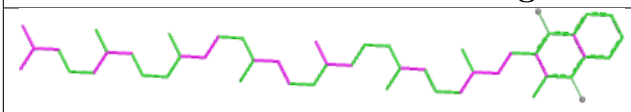
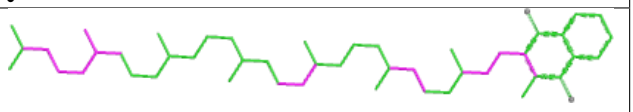
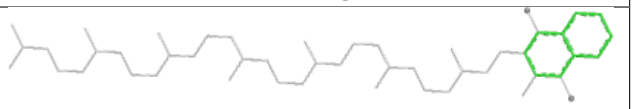
Bond angles

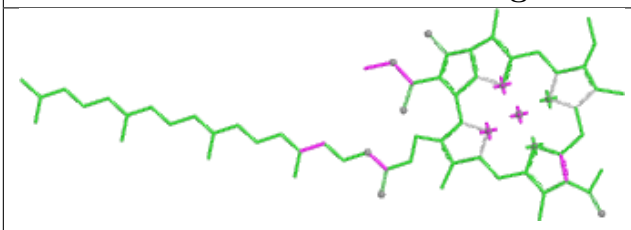
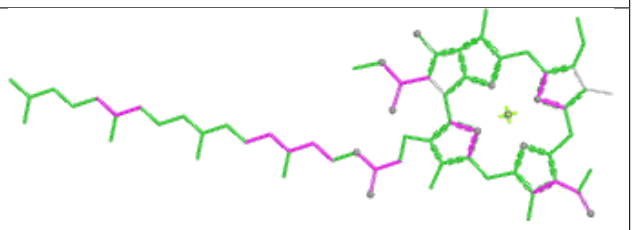
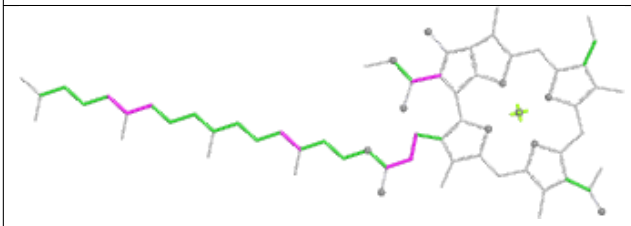
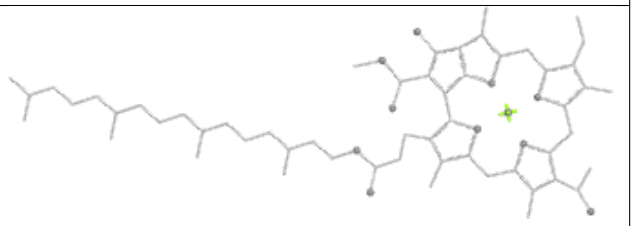


Torsions

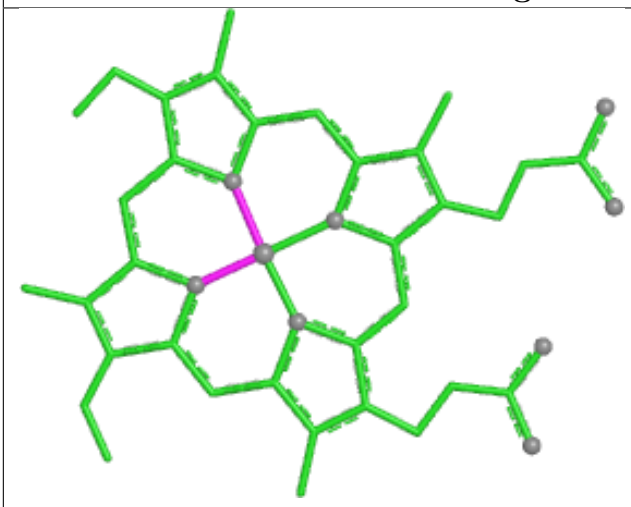


Rings

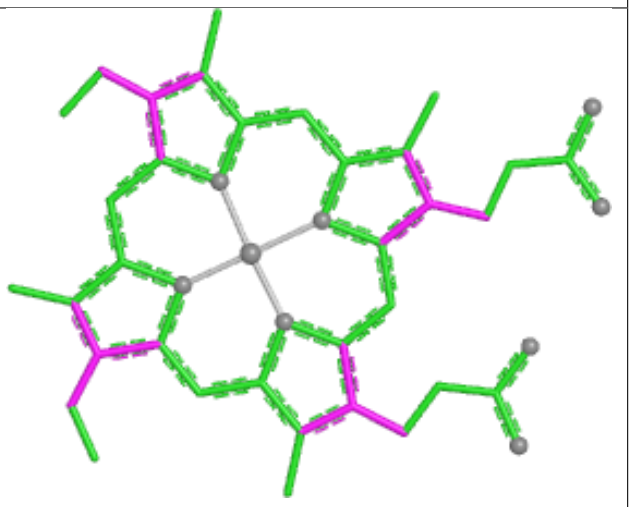
Ligand MQ7 M 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCB M 1303	
 Bond lengths	 Bond angles
 Torsions	 Rings

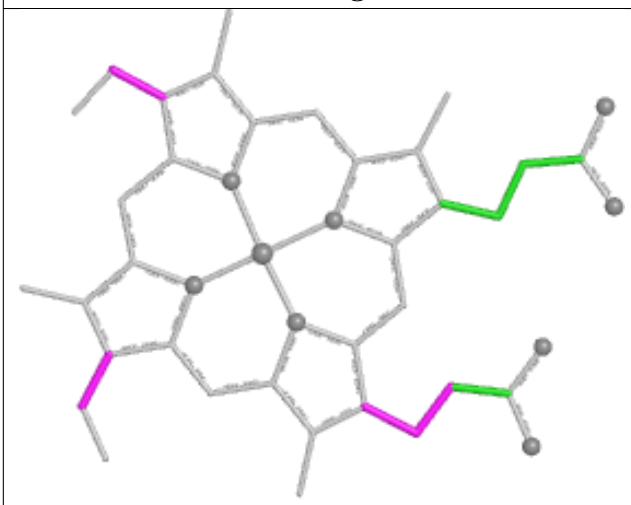
Ligand HEC C 1204



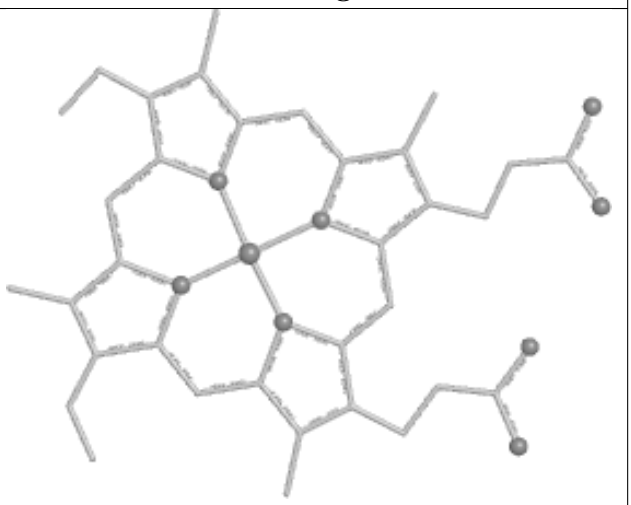
Bond lengths



Bond angles

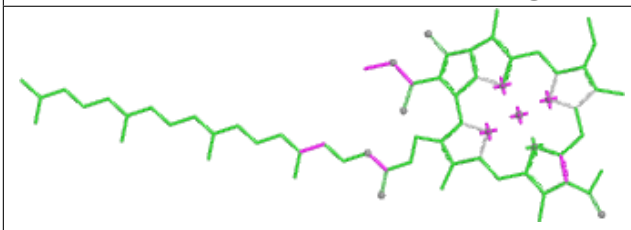


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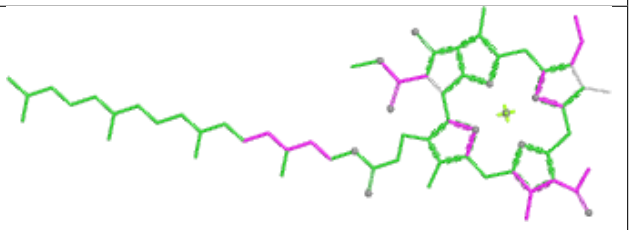


Rings

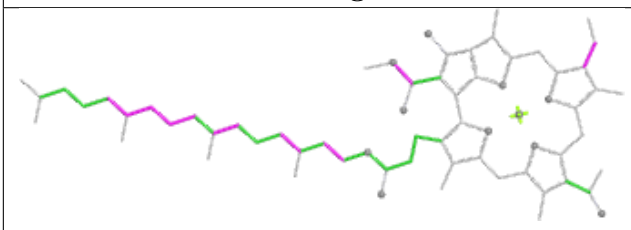
Ligand BCB L 304



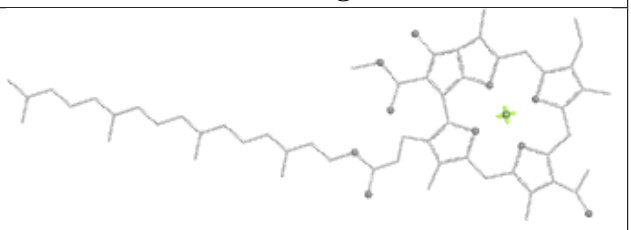
Bond lengths



Bond angles

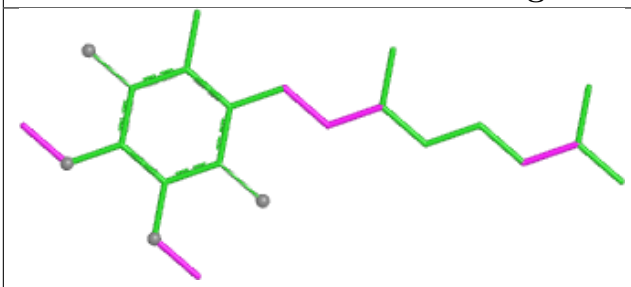


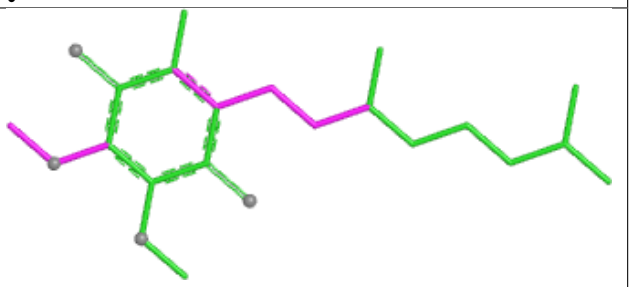
Torsions

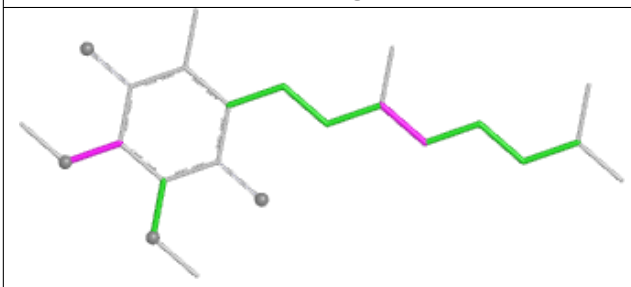


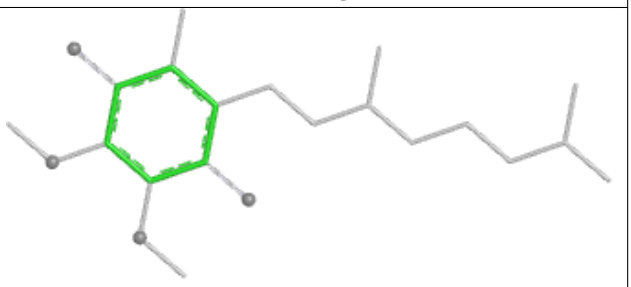
Rings

Ligand UQ2 L 502

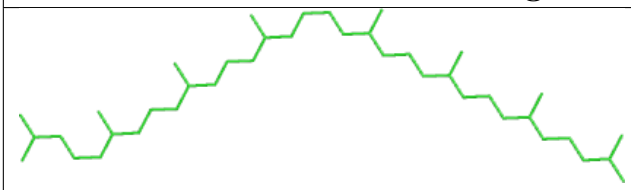

Bond lengths

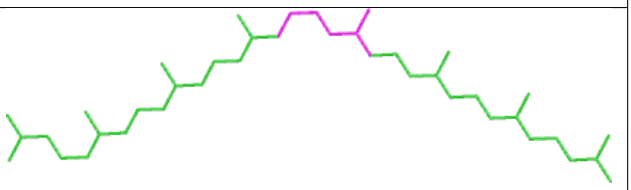

Bond angles

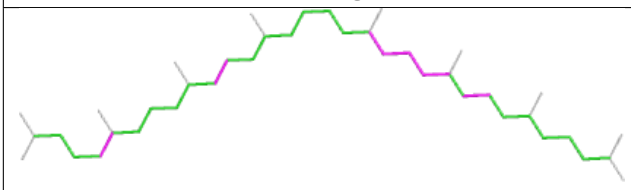

Torsions

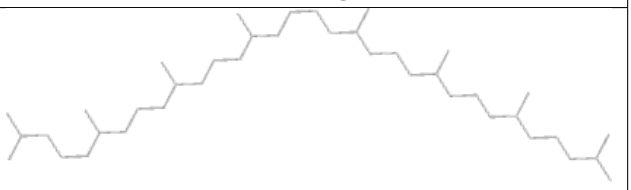

Rings

Ligand NS5 M 600

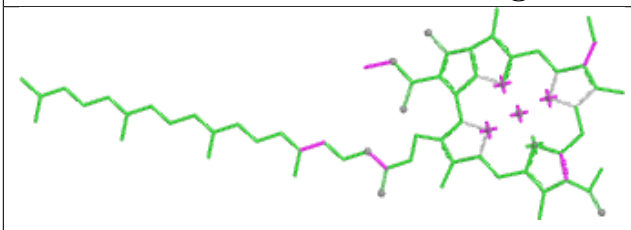

Bond lengths

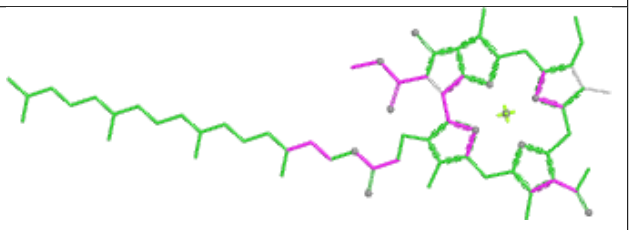

Bond angles

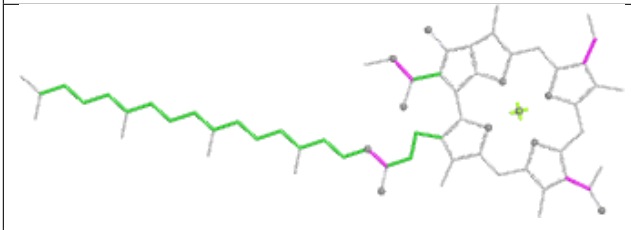

Torsions

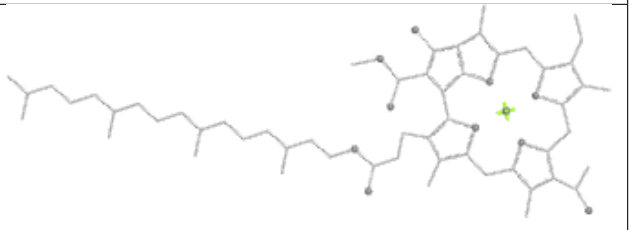

Rings

Ligand BCB M 1301

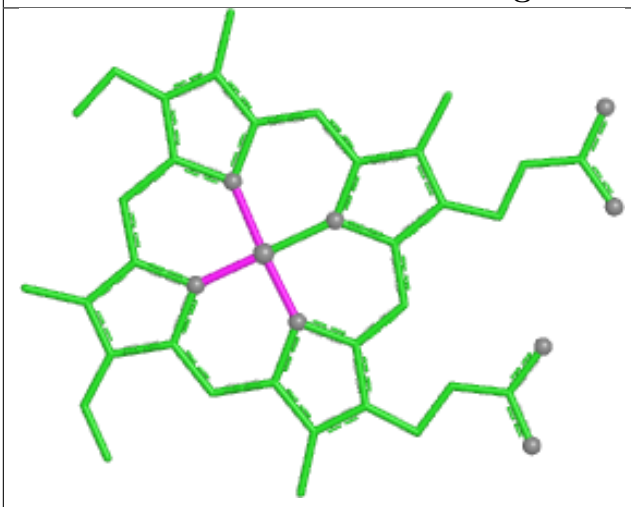

Bond lengths


Bond angles

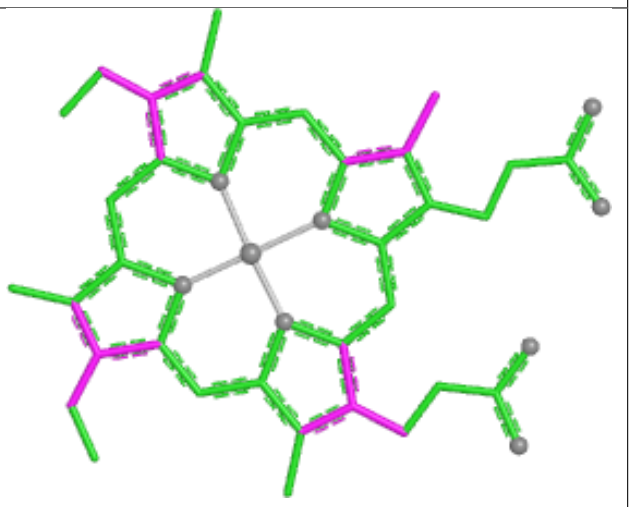

Torsions


Rings

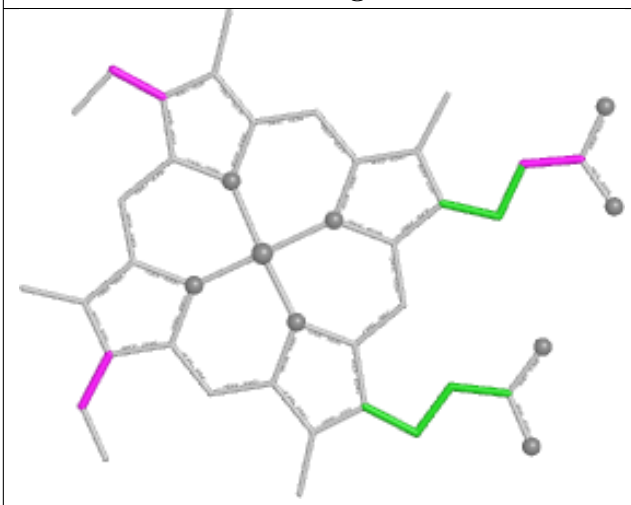
Ligand HEC C 1201



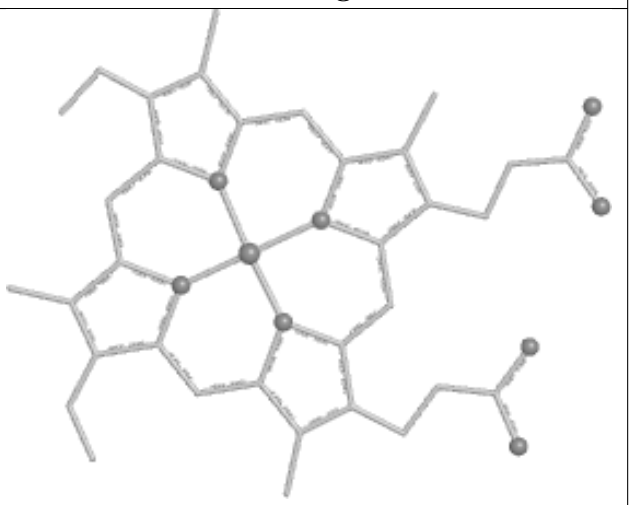
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.15	4 (1%)	76	71	23, 44, 65, 78	15 (4%)
2	L	273/273 (100%)	-0.27	1 (0%)	88	87	25, 42, 65, 76	6 (2%)
3	M	323/323 (100%)	-0.17	3 (0%)	81	76	25, 42, 66, 76	8 (2%)
4	H	251/258 (97%)	0.56	24 (9%)	13	11	27, 54, 83, 93	19 (7%)
All	All	1179/1190 (99%)	-0.03	32 (2%)	56	47	23, 46, 70, 93	48 (4%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	46	PRO	5.7
4	H	92	GLN	5.3
4	H	55	GLU	4.8
4	H	54	PRO	4.4
1	C	93	GLU	4.3
4	H	9	HIS	4.2
4	H	258	LEU	4.0
4	H	97	GLU	3.8
4	H	53	ALA	3.3
4	H	191	ALA	3.2
4	H	8	GLN	3.0
2	L	1	ALA	3.0
4	H	189	GLY	2.9
3	M	16	HIS	2.8
1	C	54	GLN	2.8
1	C	1	CYS	2.7
4	H	190	SER	2.7
3	M	22	GLU	2.6
1	C	64	ASN	2.6
4	H	96	PHE	2.5
4	H	225	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
4	H	252	GLU	2.4
4	H	255	GLU	2.3
4	H	163	VAL	2.3
4	H	87	GLU	2.3
4	H	216	GLU	2.2
4	H	192	ARG	2.2
4	H	95	GLY	2.2
4	H	134	ILE	2.2
3	M	31	LYS	2.1
4	H	58	GLN	2.0
4	H	227	ARG	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, 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
4	FME	H	1	10/11	0.93	0.13	53,55,63,65	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, 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
9	LDA	L	705	16/16	0.83	0.30	71,78,94,95	3
9	LDA	M	702	16/16	0.83	0.32	73,87,100,101	0
9	LDA	M	706	16/16	0.85	0.33	99,105,114,114	0
11	SO4	M	804	5/5	0.86	0.17	81,82,82,83	0
9	LDA	H	703	16/16	0.88	0.26	74,79,85,85	0
9	LDA	M	704	16/16	0.88	0.27	79,82,83,84	3

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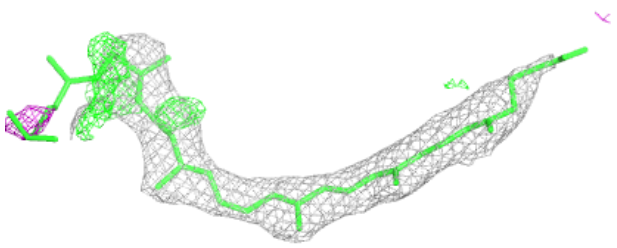
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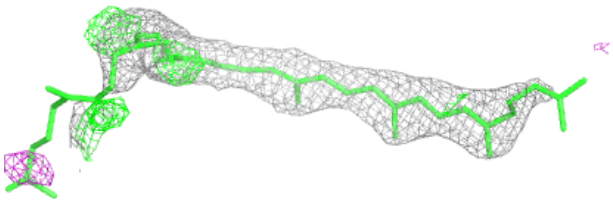
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	NS5	M	600	40/40	0.92	0.15	39,58,67,68	11
7	BPB	M	401	65/65	0.93	0.14	37,45,94,95	0
11	SO4	M	803	5/5	0.93	0.12	102,102,103,103	0
11	SO4	H	801	5/5	0.94	0.08	73,76,76,77	0
8	UQ2	L	502	23/23	0.95	0.20	48,49,50,50	23
9	LDA	M	701	16/16	0.95	0.13	48,50,52,52	0
6	BCB	M	1301	66/66	0.96	0.09	33,43,59,63	15
12	MQ7	M	501	48/48	0.96	0.11	36,45,67,70	0
7	BPB	L	402	65/65	0.96	0.10	31,41,45,47	0
6	BCB	L	302	66/66	0.97	0.08	10,20,42,43	0
6	BCB	M	1303	66/66	0.97	0.08	17,25,46,48	0
11	SO4	M	802	5/5	0.97	0.08	57,59,61,61	0
6	BCB	L	304	66/66	0.97	0.09	23,29,54,57	0
5	HEC	C	1201	43/43	0.98	0.08	47,51,61,65	0
5	HEC	C	1203	43/43	0.99	0.06	26,33,41,44	0
5	HEC	C	1204	43/43	0.99	0.07	32,36,48,53	0
5	HEC	C	1202	43/43	0.99	0.06	39,43,55,58	0
10	FE2	M	500	1/1	1.00	0.05	33,33,33,33	0

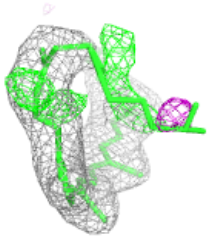
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

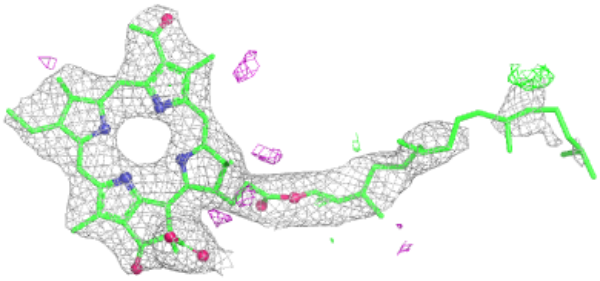


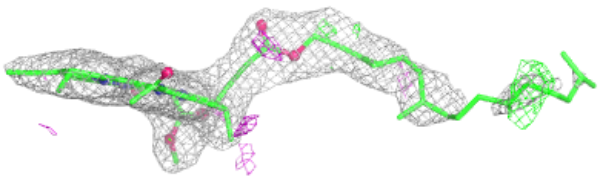


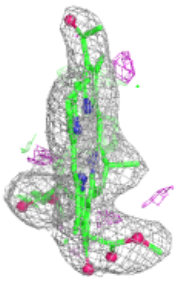


Electron density around BPB M 401:

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

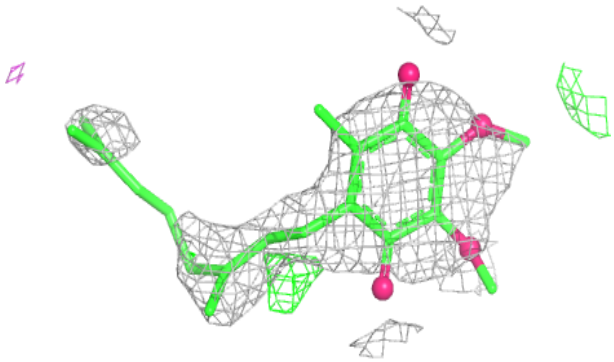


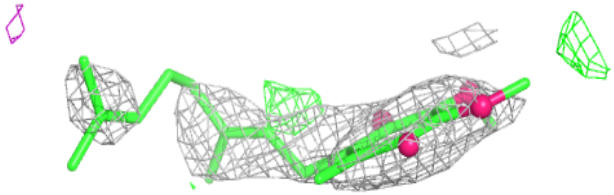


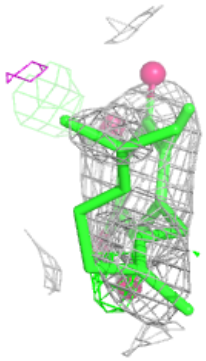


Electron density around UQ2 L 502:

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

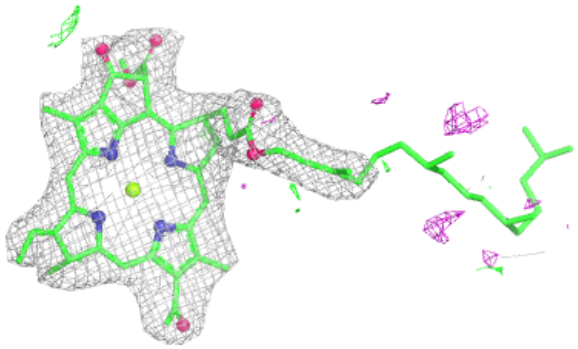


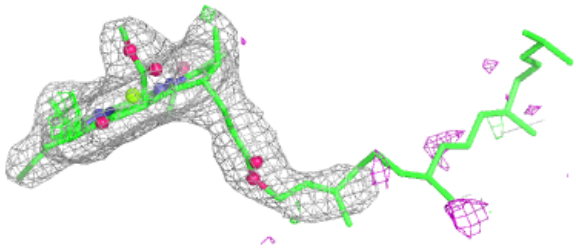


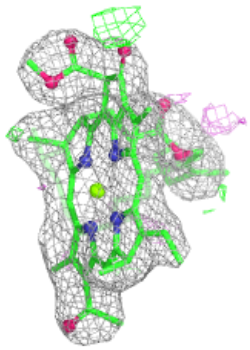


Electron density around BCB M 1301:

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

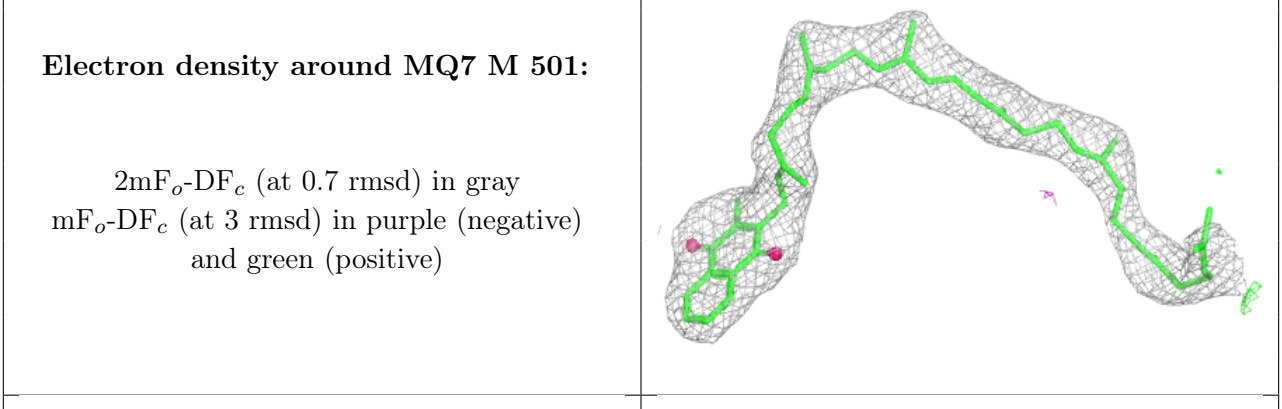






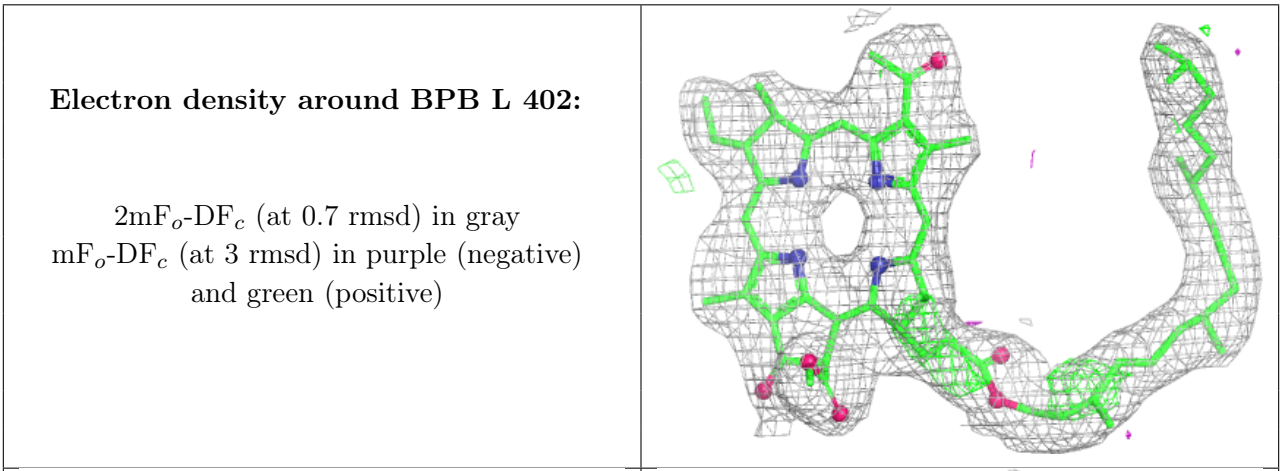
Electron density around MQ7 M 501:

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



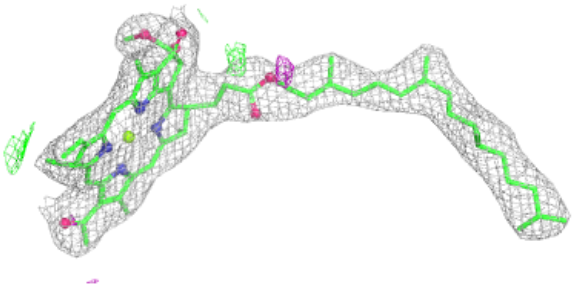
Electron density around BPB L 402:

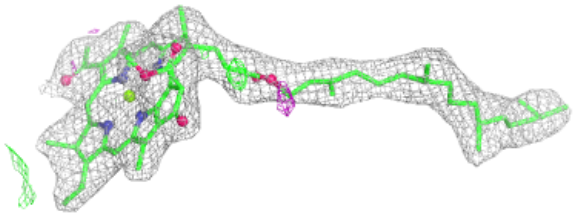
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

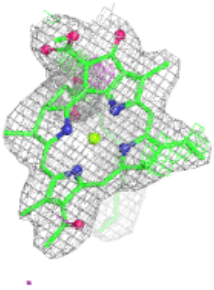


Electron density around BCB L 302:

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

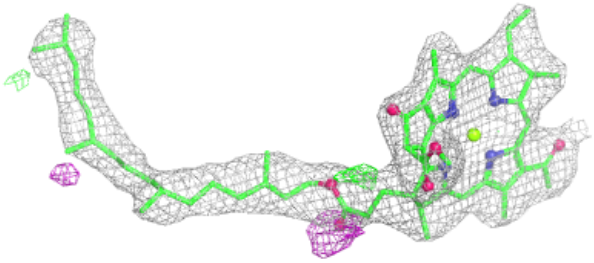


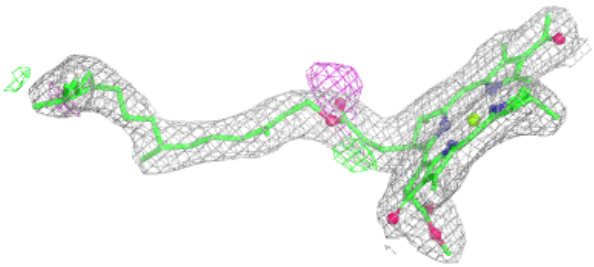


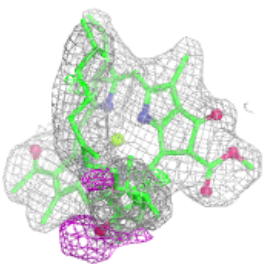


Electron density around BCB M 1303:

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

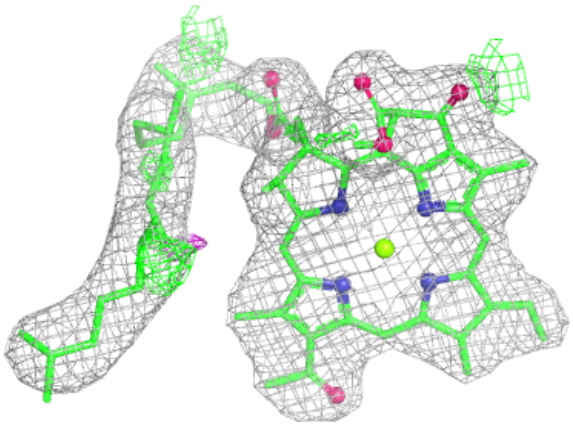


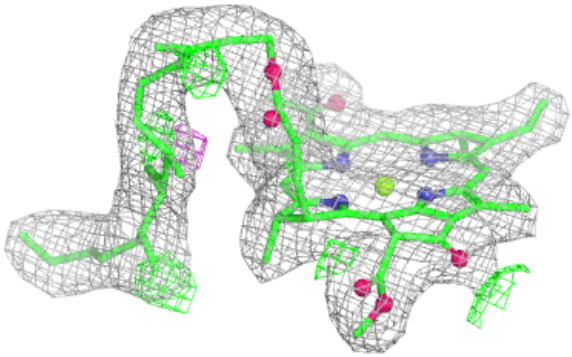


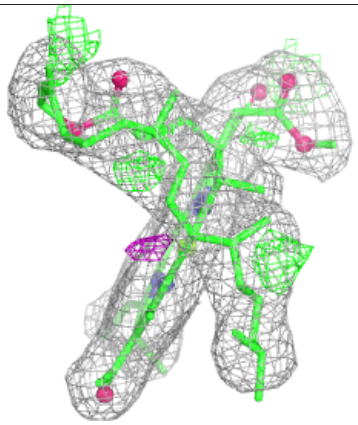


Electron density around BCB L 304:

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

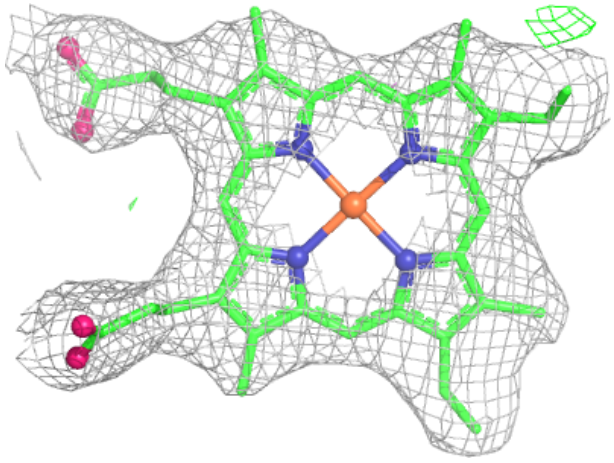


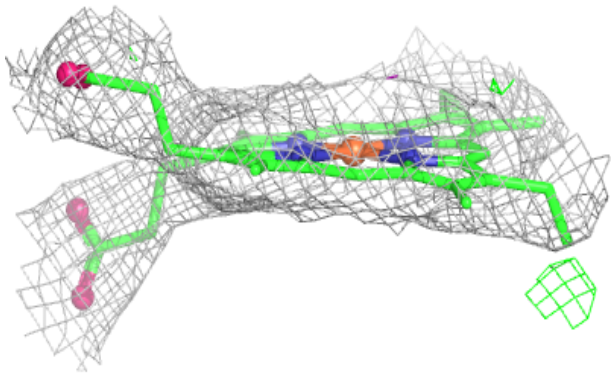




Electron density around HEC C 1201:

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

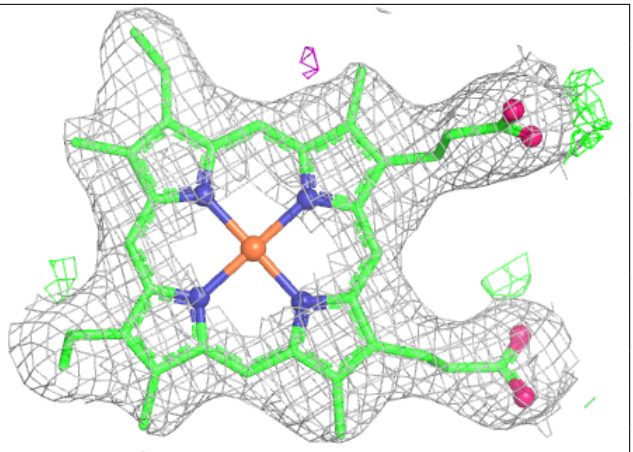


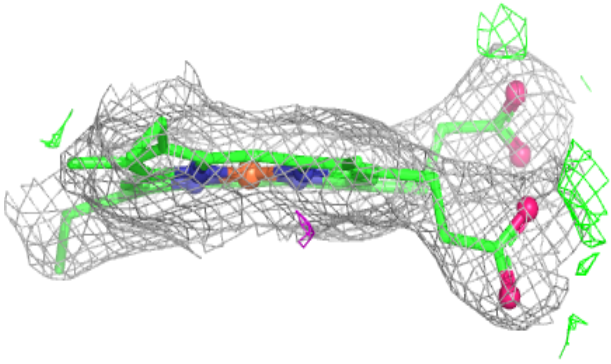




Electron density around HEC C 1203:

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

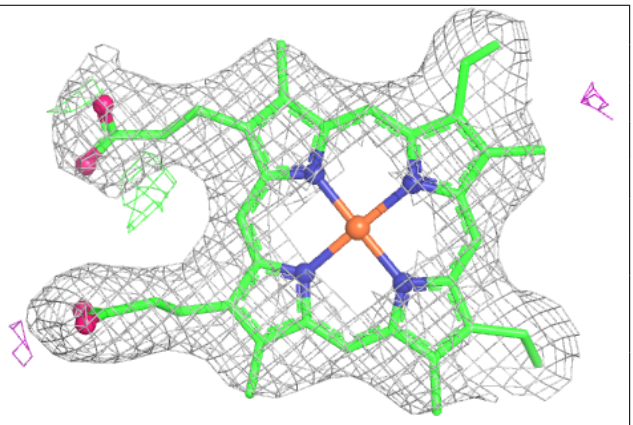


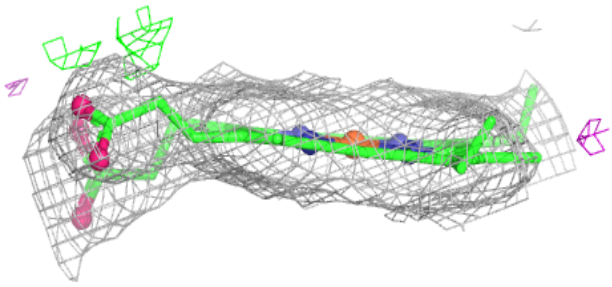




Electron density around HEC C 1204:

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

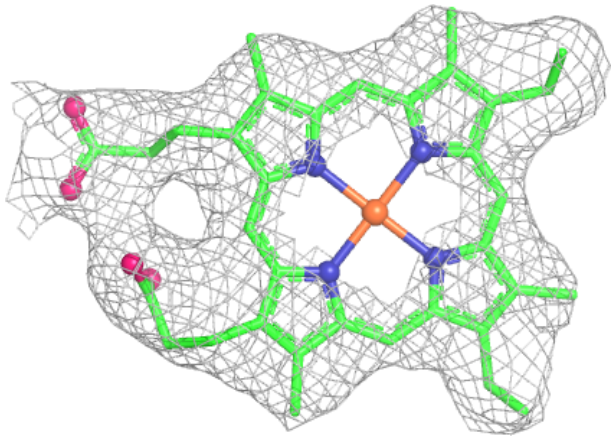


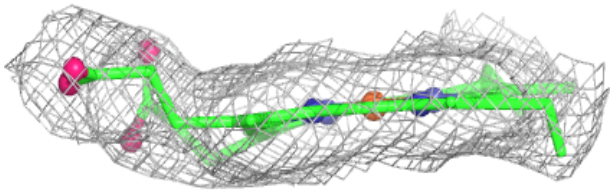


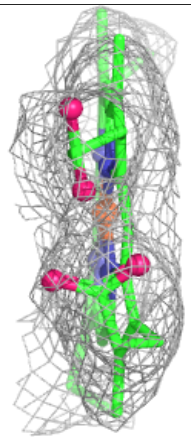


Electron density around HEC C 1202:

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







6.5 Other polymers

There are no such residues in this entry.