Full wwPDB X-ray Structure Validation Report (i)

Aug 25, 2026 – 10:42 am BST

PDB ID	:	2X5V / pdb_00002x5v
Title	:	80 microsecond laue diffraction snapshot from crystals of a photosynthetic reaction centre 3 millisecond following photoactivation.
Authors	:	Wohri, A.B.; Katona, G.; Johansson, L.C.; Fritz, E.; Malmerberg, E.; Andersson, M.; Vincent, J.; Eklund, M.; Cammarata, M.; Wulff, M.; Davidsson, J.; Groenhof, G.; Neutze, R.
Deposited on	:	2010-02-10
Resolution	:	3.00 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 (1)) were used in the production of this report:

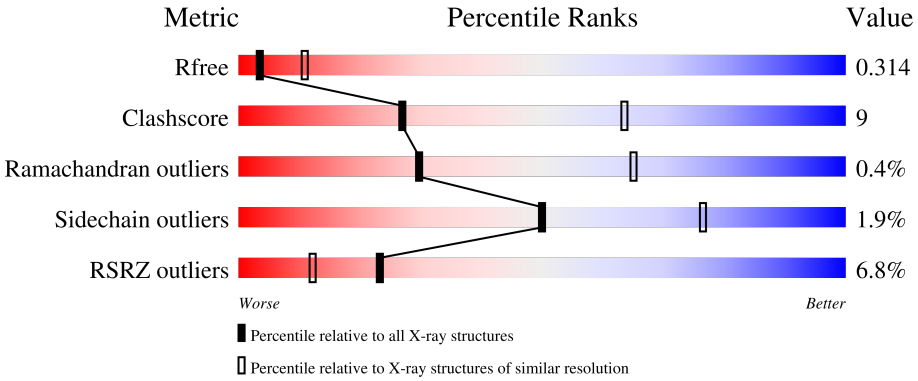
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	7% 84% 14%
2	H	258	12% 78% 14% 6%
3	L	274	6% 75% 23%
4	M	324	2% 80% 19%

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	1333	X	-	-	-
5	HEC	C	1334	X	-	-	-
5	HEC	C	1335	X	-	-	-
5	HEC	C	1336	X	-	-	-
6	BCB	L	1274	X	-	-	-
6	BCB	L	1275	X	-	-	-
6	BCB	M	1324	X	-	-	-
6	BCB	M	1325	X	-	-	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 9871 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	2602	1640	466	478	18	4	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	243	1906	1218	327	359	2	26	0	0

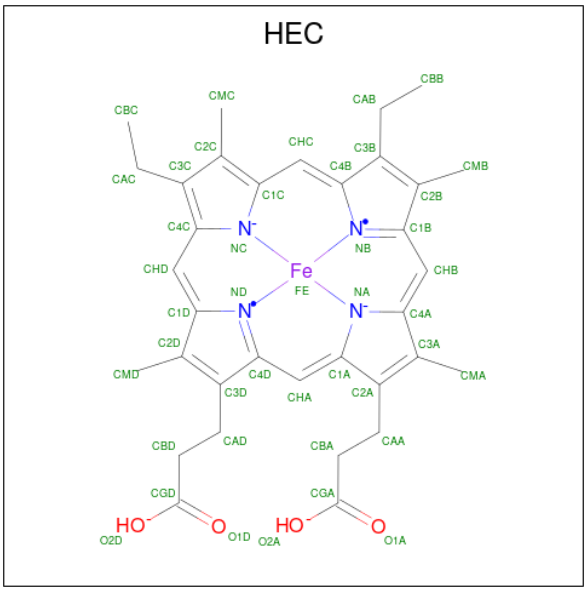
- Molecule 3 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	273	2196	1476	352	361	7	10	4	0

- Molecule 4 is a protein called REACTION CENTER PROTEIN M CHAIN.

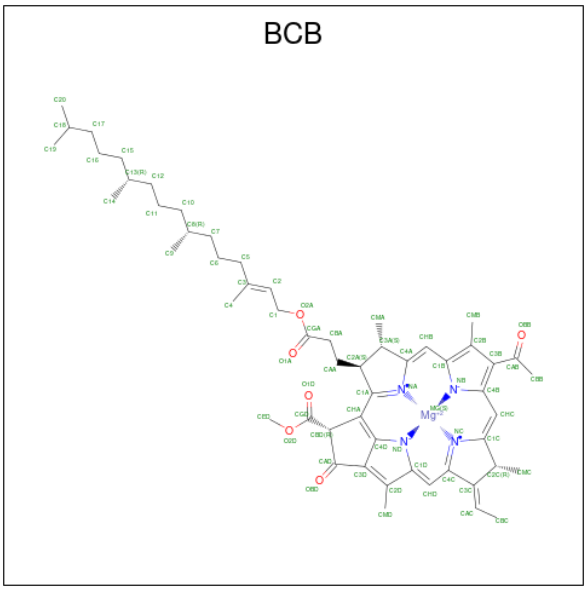
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	M	323	2555	1702	419	423	11	7	0	0

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



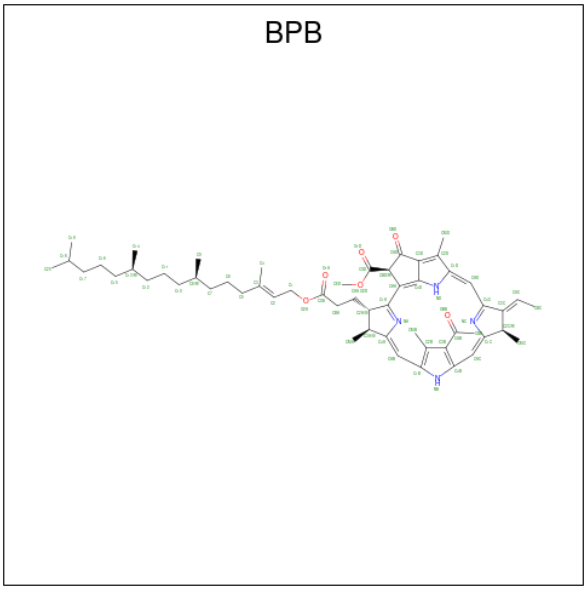
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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	0	0
			65	54	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: $C_{55}H_{74}N_4O_6$).

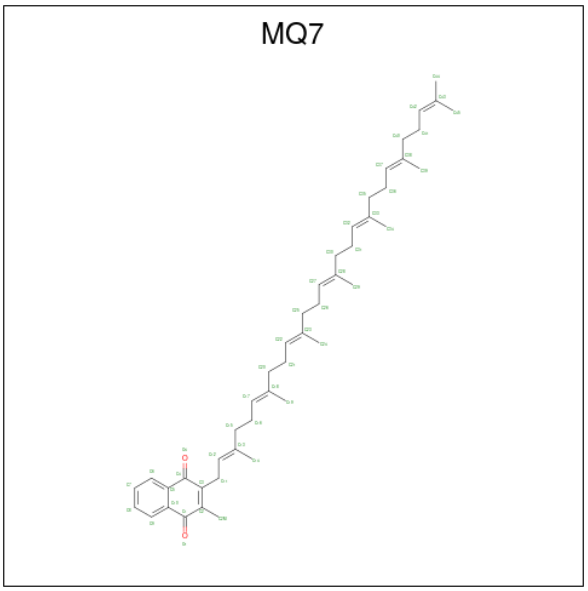


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			61	51	4	6		

- Molecule 8 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 9 is MENAQUINONE-7 (CCD ID: MQ7) (formula: $C_{46}H_{64}O_2$).



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

- Molecule 10 is water.

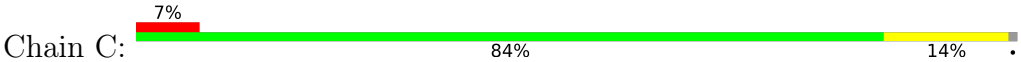
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	1	Total O 1 1	0	0
10	M	1	Total O 1 1	0	0

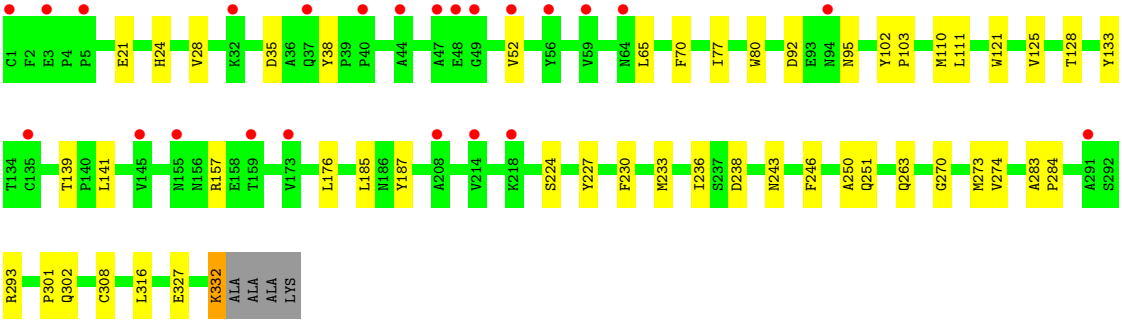
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT

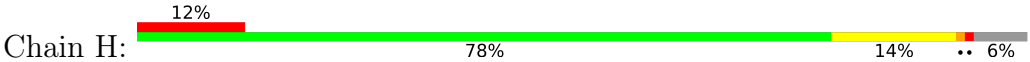
Chain C:

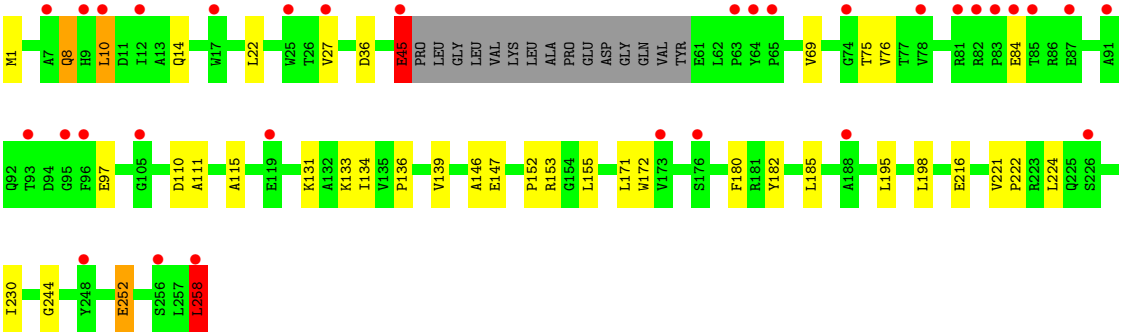




• Molecule 2: REACTION CENTER PROTEIN H CHAIN

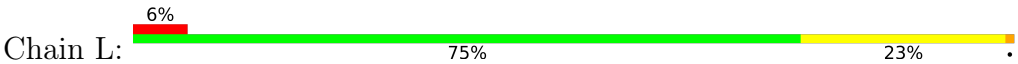
Chain H:

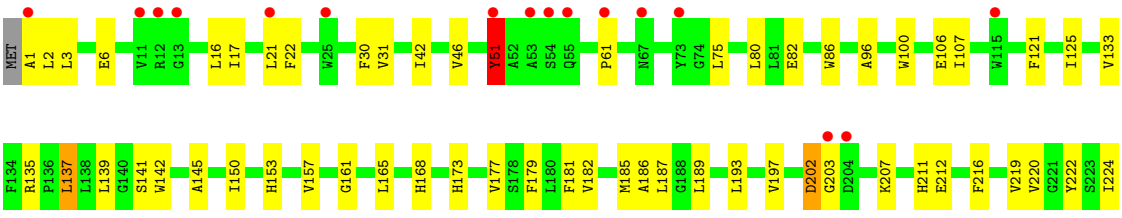




• Molecule 3: REACTION CENTER PROTEIN L CHAIN

Chain L:



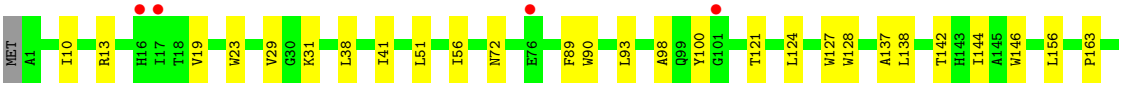


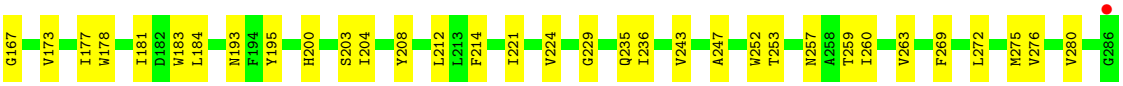


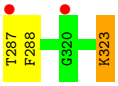
• Molecule 4: REACTION CENTER PROTEIN M CHAIN

Chain M:









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	85.69Å 143.47Å 178.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.18 – 3.00 46.18 – 3.00	Depositor EDS
% Data completeness (in resolution range)	90.6 (46.18-3.00) 90.5 (46.18-3.00)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.79 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.277 , 0.319 0.277 , 0.314	Depositor DCC
R_{free} test set	2049 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	45.4	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 31.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.76	EDS
Total number of atoms	9871	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FME, HEC, BCB, FE2, MQ7, BPB

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	0.78	1/2669 (0.0%)	0.78	2/3637 (0.1%)
2	H	1.11	6/1939 (0.3%)	1.15	9/2646 (0.3%)
3	L	0.96	2/2291 (0.1%)	0.88	4/3127 (0.1%)
4	M	0.79	2/2659 (0.1%)	0.83	3/3637 (0.1%)
All	All	0.90	11/9558 (0.1%)	0.90	18/13047 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	2
3	L	0	1
All	All	0	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	51	TYR	CB-CG	28.77	2.15	1.51
1	C	332	LYS	CB-CG	28.09	2.36	1.52
2	H	216	GLU	CB-CG	25.49	2.29	1.52
3	L	202	ASP	CB-CG	24.78	2.13	1.52
4	M	31	LYS	CG-CD	22.99	2.21	1.52
2	H	258	LEU	CB-CG	22.90	1.99	1.53
4	M	323	LYS	CB-CG	20.77	2.14	1.52
2	H	131	LYS	CD-CE	19.46	2.10	1.52
2	H	147	GLU	CG-CD	-13.69	1.17	1.52
2	H	45	GLU	CG-CD	8.20	1.72	1.52
2	H	84	GLU	CB-CG	6.58	1.72	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	97	GLU	CA-CB-CG	-25.99	62.13	114.10
2	H	97	GLU	CB-CG-CD	-20.56	77.64	112.60
2	H	84	GLU	CB-CG-CD	-15.49	86.27	112.60
4	M	31	LYS	CB-CG-CD	-14.49	77.97	111.30
3	L	51	TYR	CB-CG-CD2	-14.31	99.33	120.80
2	H	45	GLU	CG-CD-OE1	-14.17	85.80	118.40
2	H	216	GLU	CA-CB-CG	-12.65	88.81	114.10
3	L	51	TYR	CB-CG-CD1	11.70	138.35	120.80
2	H	45	GLU	CB-CG-CD	11.41	132.00	112.60
2	H	252	GLU	CB-CG-CD	10.10	129.78	112.60
2	H	216	GLU	CB-CG-CD	8.97	127.85	112.60
4	M	31	LYS	CG-CD-CE	-8.97	90.67	111.30
4	M	323	LYS	CA-CB-CG	-7.89	98.32	114.10
2	H	147	GLU	CB-CG-CD	-6.44	101.64	112.60
1	C	332	LYS	CB-CG-CD	6.01	125.12	111.30
3	L	202	ASP	CA-CB-CG	5.84	118.44	112.60
3	L	202	ASP	CB-CG-OD2	5.11	130.15	118.40
1	C	332	LYS	CA-CB-CG	-5.07	103.97	114.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	252	GLU	Sidechain
2	H	45	GLU	Sidechain
3	L	51	TYR	Sidechain

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	33	0
2	H	1906	0	1903	27	0
3	L	2196	0	2120	58	0
4	M	2555	0	2452	52	0
5	C	172	0	120	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	132	0	144	19	0
6	M	131	0	140	9	0
7	L	65	0	74	5	0
7	M	61	0	63	6	0
8	M	1	0	0	0	0
9	M	48	0	64	3	0
10	L	1	0	0	0	0
10	M	1	0	0	0	0
All	All	9871	0	9659	178	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 9.

All (178) 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)
3:L:168:HIS:CE1	6:L:1274:BCB:HMC2	2.13	0.84
3:L:121:PHE:CE2	3:L:125:ILE:HD11	2.17	0.80
3:L:168:HIS:NE2	6:L:1274:BCB:HMC2	1.99	0.78
7:L:1276:BPB:HHC	7:L:1276:BPB:HBBB	1.68	0.75
1:C:77:ILE:HD11	1:C:111:LEU:HD21	1.70	0.71
6:L:1275:BCB:HMD2	4:M:204:ILE:HD13	1.72	0.70
6:L:1274:BCB:HMB1	6:L:1274:BCB:HBB3	1.73	0.69
3:L:161[A]:GLY:HA3	6:L:1274:BCB:HBC3	1.76	0.66
7:M:1326:BPB:HHC	7:M:1326:BPB:HBBB	1.77	0.66
2:H:180:PHE:O	2:H:198:LEU:HD12	1.96	0.65
4:M:173:VAL:HG22	4:M:183:TRP:CD2	2.32	0.65
6:M:1325:BCB:HBB2	6:M:1325:BCB:HMB3	1.78	0.65
4:M:263:VAL:HG21	9:M:1328:MQ7:C1	2.27	0.64
4:M:275:MET:HA	4:M:275:MET:HE2	1.80	0.64
7:L:1276:BPB:HHC	7:L:1276:BPB:CBB	2.27	0.64
5:C:1335:HEC:HBB3	5:C:1335:HEC:HMB3	1.79	0.64
3:L:161[B]:GLY:HA3	6:L:1274:BCB:HBC3	1.80	0.63
3:L:179:PHE:HA	3:L:182:VAL:HG12	1.81	0.62
3:L:193:LEU:HD22	3:L:216:PHE:CE2	2.34	0.62
6:L:1275:BCB:CMD	4:M:204:ILE:HD13	2.29	0.61
3:L:182:VAL:HG13	3:L:236:LEU:HD22	1.82	0.61
2:H:10:LEU:CD1	2:H:14:GLN:HE22	2.13	0.61
1:C:270:GLY:O	1:C:274:VAL:HG23	2.01	0.61
3:L:16:LEU:HD13	3:L:106:GLU:HG2	1.83	0.61
3:L:181:PHE:CD2	7:M:1326:BPB:HBB	2.36	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:226:ALA:O	3:L:229:ILE:HG22	2.01	0.61
4:M:287:THR:HG22	4:M:288:PHE:CE1	2.36	0.60
1:C:283:ALA:HB2	1:C:302:GLN:NE2	2.17	0.60
5:C:1334:HEC:HMC3	5:C:1334:HEC:HBC3	1.83	0.60
6:L:1274:BCB:HMB1	6:L:1274:BCB:CBB	2.32	0.58
4:M:142:THR:HG1	4:M:146:TRP:CD1	2.23	0.57
2:H:10:LEU:HD11	2:H:14:GLN:HE22	1.68	0.56
2:H:69:VAL:HG22	2:H:75:THR:HG22	1.87	0.56
4:M:98:ALA:HB3	4:M:100:TYR:CZ	2.40	0.56
3:L:82[A]:GLU:OE1	3:L:82[A]:GLU:HA	2.05	0.56
6:L:1275:BCB:HBB2	6:L:1275:BCB:HMB3	1.87	0.56
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.41	0.56
1:C:65:LEU:HD11	1:C:327:GLU:CB	2.36	0.56
3:L:21:LEU:HD23	3:L:22:PHE:CE2	2.40	0.56
1:C:21:GLU:HA	1:C:243:ASN:HD21	1.71	0.55
4:M:19:VAL:HG12	4:M:138:LEU:HD22	1.89	0.55
2:H:133:LYS:HG2	2:H:134:ILE:HD13	1.89	0.55
1:C:176:LEU:HD11	1:C:187:TYR:O	2.07	0.54
1:C:52:VAL:HG11	1:C:70:PHE:CB	2.37	0.54
6:M:1324:BCB:HBB2	6:M:1324:BCB:HHC	1.89	0.54
3:L:207:LYS:HB3	3:L:211:HIS:CG	2.43	0.54
3:L:267:LEU:HD13	4:M:90:TRP:CH2	2.42	0.54
3:L:173:HIS:O	3:L:177:VAL:HG23	2.07	0.54
1:C:35:ASP:HB3	1:C:316:LEU:HD23	1.90	0.54
6:L:1274:BCB:HAC1	4:M:195:TYR:OH	2.08	0.53
2:H:172:TRP:HB2	2:H:182:TYR:HB2	1.91	0.53
3:L:3:LEU:HB2	3:L:6:GLU:HB2	1.90	0.53
1:C:246:PHE:CZ	1:C:263:GLN:HG2	2.44	0.53
1:C:52:VAL:HG11	1:C:70:PHE:HB2	1.91	0.53
1:C:65:LEU:HD11	1:C:327:GLU:HB2	1.91	0.53
2:H:136:PRO:HG2	2:H:139:VAL:HG23	1.89	0.53
1:C:24:HIS:O	1:C:28:VAL:HG23	2.09	0.53
3:L:181:PHE:HB3	7:M:1326:BPB:HBBA	1.91	0.52
4:M:124:LEU:HD21	6:M:1325:BCB:H112	1.91	0.52
3:L:135:ARG:NH2	3:L:139:LEU:HD11	2.24	0.52
1:C:273:MET:HE1	5:C:1336:HEC:C2C	2.40	0.52
3:L:107:ILE:HD12	4:M:253:THR:OG1	2.09	0.52
4:M:195:TYR:CE1	6:M:1325:BCB:HMC2	2.45	0.52
2:H:27:VAL:HG11	4:M:269:PHE:CE1	2.45	0.51
4:M:173:VAL:HG22	4:M:183:TRP:CE2	2.46	0.51
3:L:230:HIS:CD2	4:M:221:ILE:HG13	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:152:PRO:HG2	2:H:171:LEU:HD11	1.92	0.51
3:L:182:VAL:CG1	3:L:236:LEU:HD22	2.40	0.51
2:H:258:LEU:C	3:L:17:ILE:HG22	2.35	0.51
7:L:1276:BPB:HBB	4:M:208:TYR:CD2	2.46	0.51
1:C:141:LEU:HD22	1:C:293:ARG:NH1	2.26	0.51
4:M:41:ILE:HD12	4:M:41:ILE:C	2.35	0.51
3:L:150:ILE:O	6:L:1275:BCB:HED1	2.11	0.50
3:L:224:ILE:CD1	3:L:232:LEU:HD22	2.41	0.50
2:H:224:LEU:HD21	2:H:230:ILE:HD12	1.94	0.50
4:M:247:ALA:HB1	4:M:257:ASN:ND2	2.27	0.50
3:L:197:VAL:HG21	3:L:212:GLU:HG2	1.94	0.50
4:M:243:VAL:HG11	4:M:260:ILE:HB	1.94	0.50
6:L:1275:BCB:H43	6:L:1275:BCB:O1A	2.12	0.49
4:M:200:HIS:CE1	4:M:204:ILE:HD11	2.47	0.49
3:L:96:ALA:O	3:L:100:TRP:N	2.41	0.49
3:L:177:VAL:HG13	6:L:1274:BCB:CMB	2.42	0.49
3:L:186:ALA:HA	3:L:189:LEU:HD12	1.95	0.49
1:C:35:ASP:CB	1:C:316:LEU:HD23	2.43	0.49
2:H:69:VAL:HA	2:H:75:THR:HG22	1.94	0.49
6:L:1274:BCB:HMB2	6:M:1325:BCB:CHB	2.43	0.49
7:L:1276:BPB:HEDA	7:L:1276:BPB:HMAB	1.95	0.49
4:M:121:THR:HG23	4:M:156:LEU:HD21	1.95	0.49
4:M:72:ASN:CB	4:M:93:LEU:HD13	2.43	0.48
2:H:180:PHE:CD2	4:M:10:ILE:HG22	2.49	0.48
6:L:1274:BCB:CBB	6:L:1274:BCB:CMB	2.91	0.48
1:C:121:TRP:O	1:C:125:VAL:HG22	2.13	0.48
4:M:272:LEU:O	4:M:276:VAL:HG23	2.12	0.48
3:L:153:HIS:O	3:L:157:VAL:HG23	2.13	0.48
4:M:235:GLN:OE1	4:M:243:VAL:HG22	2.14	0.48
1:C:38:TYR:CE2	1:C:316:LEU:HD13	2.49	0.48
2:H:258:LEU:OXT	3:L:17:ILE:HG22	2.14	0.47
3:L:75:LEU:HA	3:L:142:TRP:CD1	2.48	0.47
1:C:233:MET:HA	1:C:236:ILE:HD12	1.96	0.47
5:C:1334:HEC:HBB3	5:C:1334:HEC:HMB1	1.96	0.47
3:L:100:TRP:CZ2	4:M:253:THR:HG22	2.49	0.47
2:H:110:ASP:O	2:H:111:ALA:HB3	2.15	0.47
3:L:187:LEU:HD13	4:M:214:PHE:CG	2.49	0.47
4:M:224:VAL:HG23	4:M:229:GLY:HA3	1.96	0.47
5:C:1335:HEC:HMC3	5:C:1335:HEC:HBC3	1.96	0.47
2:H:76:VAL:O	2:H:76:VAL:HG13	2.14	0.47
4:M:89:PHE:HB3	4:M:178:TRP:CD1	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:1325:BCB:HMB3	6:M:1325:BCB:CBB	2.44	0.47
4:M:173:VAL:HG22	4:M:183:TRP:CE3	2.50	0.47
3:L:193:LEU:HD11	3:L:212:GLU:HA	1.97	0.46
4:M:51:LEU:HD22	4:M:56:ILE:CG1	2.45	0.46
1:C:250:ALA:O	1:C:251:GLN:C	2.58	0.46
4:M:236:ILE:HG12	4:M:260:ILE:HG23	1.97	0.46
2:H:69:VAL:HG22	2:H:75:THR:CG2	2.45	0.46
3:L:82[A]:GLU:OE1	3:L:82[A]:GLU:CA	2.61	0.46
1:C:224:SER:O	1:C:227:TYR:HB2	2.15	0.46
4:M:287:THR:HG22	4:M:288:PHE:CD1	2.50	0.46
4:M:181:ILE:HG13	6:M:1324:BCB:HED3	1.97	0.46
1:C:52:VAL:HG13	1:C:65:LEU:O	2.16	0.46
2:H:180:PHE:HB3	2:H:198:LEU:HD11	1.98	0.46
4:M:195:TYR:CZ	6:M:1325:BCB:HMC2	2.51	0.45
1:C:185:LEU:HD11	1:C:230:PHE:CD2	2.52	0.45
2:H:8:GLN:HE21	2:H:8:GLN:HA	1.81	0.45
2:H:10:LEU:CD1	2:H:14:GLN:NE2	2.77	0.45
2:H:36:ASP:HA	4:M:259:THR:HG23	1.99	0.45
1:C:102:TYR:N	1:C:103:PRO:CD	2.79	0.45
3:L:177:VAL:HG13	6:L:1274:BCB:HMB3	1.97	0.45
3:L:100:TRP:CZ2	9:M:1328:MQ7:H291	2.51	0.45
3:L:187:LEU:HD13	4:M:214:PHE:CD2	2.52	0.45
5:C:1333:HEC:HBB3	5:C:1333:HEC:HMB1	1.99	0.45
1:C:139:THR:OG1	1:C:157:ARG:NH2	2.50	0.44
4:M:23:TRP:CH2	4:M:137:ALA:HB2	2.53	0.44
1:C:301:PRO:HG2	5:C:1334:HEC:HBD1	1.99	0.44
5:C:1334:HEC:CGD	5:C:1334:HEC:HHA	2.47	0.44
3:L:139:LEU:HD21	3:L:253:PRO:HD3	2.00	0.44
3:L:222:TYR:CZ	4:M:38:LEU:HD21	2.52	0.44
3:L:185:MET:HE1	7:M:1326:BPB:CED	2.47	0.44
3:L:86:TRP:CZ2	3:L:145:ALA:CB	3.01	0.44
3:L:216:PHE:O	3:L:220:VAL:HG22	2.18	0.44
4:M:29:VAL:HG21	4:M:51:LEU:HD12	1.99	0.44
6:L:1275:BCB:C3D	4:M:204:ILE:HG21	2.48	0.44
3:L:86:TRP:CZ2	3:L:145:ALA:HB3	2.52	0.44
3:L:1:ALA:C	3:L:2:LEU:HD12	2.43	0.43
3:L:224:ILE:HD12	3:L:232:LEU:HD22	2.00	0.43
3:L:121:PHE:CD2	3:L:125:ILE:HD11	2.54	0.43
4:M:184:LEU:HD11	6:M:1324:BCB:HHD	2.01	0.43
6:L:1274:BCB:H41	6:L:1274:BCB:H62	1.77	0.43
2:H:10:LEU:HD11	2:H:14:GLN:NE2	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:1334:HEC:HBB3	5:C:1334:HEC:CMB	2.49	0.43
7:L:1276:BPB:HBBA	4:M:208:TYR:HB3	1.99	0.43
1:C:38:TYR:CD2	1:C:316:LEU:HD13	2.54	0.43
2:H:115:ALA:HB2	2:H:244:GLY:HA3	2.01	0.43
3:L:165:LEU:HD12	3:L:258:GLY:HA3	2.01	0.42
3:L:61:PRO:O	3:L:150:ILE:HD12	2.20	0.42
1:C:308:CYS:SG	5:C:1336:HEC:HMC1	2.60	0.42
3:L:193:LEU:O	3:L:193:LEU:HD12	2.19	0.42
4:M:51:LEU:HD22	4:M:56:ILE:HG13	2.02	0.42
2:H:195:LEU:HD12	2:H:230:ILE:HD12	2.01	0.42
3:L:75:LEU:CD1	3:L:137:LEU:HD23	2.49	0.42
1:C:111:LEU:HA	5:C:1334:HEC:HBB2	2.01	0.42
1:C:141:LEU:HD22	1:C:293:ARG:HH11	1.85	0.42
2:H:221:VAL:HG13	2:H:222:PRO:HD2	2.02	0.42
4:M:163:PRO:O	4:M:167:GLY:N	2.52	0.42
3:L:42:ILE:O	3:L:46:VAL:HG23	2.21	0.41
3:L:202:ASP:HB3	3:L:203:GLY:H	1.74	0.41
1:C:283:ALA:N	1:C:284:PRO:CD	2.83	0.41
3:L:181:PHE:HB3	7:M:1326:BPB:CBB	2.50	0.41
6:L:1275:BCB:HMB3	6:L:1275:BCB:CBB	2.50	0.41
1:C:92:ASP:HB3	1:C:95:ASN:O	2.21	0.41
4:M:276:VAL:O	4:M:280:VAL:HG23	2.21	0.41
4:M:127:TRP:O	4:M:128:TRP:C	2.64	0.41
2:H:152:PRO:HA	2:H:155:LEU:HD12	2.03	0.41
4:M:260:ILE:HD13	9:M:1328:MQ7:H8	2.03	0.41
3:L:219:VAL:HG12	3:L:220:VAL:HG13	2.03	0.40
2:H:146:ALA:HB2	4:M:13:ARG:CG	2.52	0.40
1:C:110:MET:HE1	5:C:1334:HEC:C1D	2.51	0.40
3:L:30:PHE:HB2	4:M:252:TRP:HB3	2.04	0.40
3:L:185:MET:HE3	7:M:1326:BPB:NA	2.36	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%)	304 (92%)	26 (8%)	0	100	100
2	H	239/258 (93%)	221 (92%)	17 (7%)	1 (0%)	30	65
3	L	275/274 (100%)	255 (93%)	18 (6%)	2 (1%)	18	53
4	M	321/324 (99%)	303 (94%)	16 (5%)	2 (1%)	21	56
All	All	1165/1192 (98%)	1083 (93%)	77 (7%)	5 (0%)	30	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	M	177	ILE
2	H	153	ARG
4	M	193	ASN
3	L	31	VAL
3	L	133	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%)	278 (99%)	3 (1%)	65	83
2	H	200/212 (94%)	194 (97%)	6 (3%)	36	69
3	L	221/219 (101%)	215 (97%)	6 (3%)	39	71
4	M	249/250 (100%)	245 (98%)	4 (2%)	55	79
All	All	951/963 (99%)	932 (98%)	19 (2%)	50	76

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	128	THR
1	C	238	ASP
1	C	332	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	8	GLN
2	H	10	LEU
2	H	22	LEU
2	H	45	GLU
2	H	185	LEU
2	H	258	LEU
3	L	51	TYR
3	L	80	LEU
3	L	137	LEU
3	L	141[A]	SER
3	L	141[B]	SER
3	L	228	SER
4	M	144	ILE
4	M	203	SER
4	M	212	LEU
4	M	323	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	58	ASN
1	C	84	GLN
1	C	94	ASN
1	C	186	ASN
1	C	200	GLN
1	C	243	ASN
1	C	302	GLN
1	C	310	GLN
2	H	8	GLN
2	H	14	GLN
2	H	72	HIS
4	M	16	HIS
4	M	108	HIS
4	M	200	HIS
4	M	257	ASN

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	$\#\|Z\| > 2$
2	FME	H	1	2	8,9,10	0.79	0	7,9,11	3.18	3 (42%)

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	-	3/7/9/11	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1	FME	CA-N-CN	-7.14	111.84	122.82
2	H	1	FME	CE-SD-CG	3.21	111.43	100.40
2	H	1	FME	O1-CN-N	-2.32	119.16	125.27

There are no chirality outliers.

All (3) 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	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 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	BPB	L	1276	-	57,70,70	2.73	15 (26%)	56,101,101	2.38	17 (30%)
9	MQ7	M	1328	-	49,49,49	1.38	2 (4%)	60,63,63	1.31	7 (11%)
6	BCB	M	1325	4	68,74,74	2.12	17 (25%)	79,115,115	3.09	31 (39%)
6	BCB	M	1324	4	67,73,74	2.06	19 (28%)	77,113,115	3.04	25 (32%)
5	HEC	C	1336	1	50,50,50	2.00	7 (14%)	68,82,82	1.66	14 (20%)
6	BCB	L	1274	3	68,74,74	2.01	17 (25%)	79,115,115	2.82	24 (30%)
5	HEC	C	1333	1	50,50,50	1.98	7 (14%)	68,82,82	1.67	13 (19%)
6	BCB	L	1275	3	68,74,74	2.05	19 (27%)	79,115,115	2.94	22 (27%)
5	HEC	C	1334	1	50,50,50	2.08	8 (16%)	68,82,82	1.65	13 (19%)
7	BPB	M	1326	-	53,66,70	2.87	14 (26%)	51,96,101	2.45	17 (33%)
5	HEC	C	1335	1	50,50,50	2.05	8 (16%)	68,82,82	1.50	8 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BPB	L	1276	-	-	13/37/105/105	0/5/6/6
9	MQ7	M	1328	-	-	3/41/61/61	0/2/2/2
6	BCB	M	1325	4	3/3/21/26	18/41/137/137	-
6	BCB	M	1324	4	3/3/20/26	16/40/136/137	-
5	HEC	C	1336	1	1/1/3/7	7/14/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BCB	L	1274	3	3/3/21/26	9/41/137/137	-
5	HEC	C	1333	1	1/1/3/7	6/14/54/54	-
6	BCB	L	1275	3	3/3/21/26	10/41/137/137	-
5	HEC	C	1334	1	1/1/3/7	9/14/54/54	-
7	BPB	M	1326	-	-	14/33/101/105	0/5/6/6
5	HEC	C	1335	1	1/1/3/7	6/14/54/54	-

All (133) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1326	BPB	C1B-C2B	9.07	1.49	1.39
7	M	1326	BPB	C1D-C2D	8.56	1.49	1.39
7	L	1276	BPB	C1B-C2B	8.32	1.48	1.39
5	C	1335	HEC	C3D-C2D	8.17	1.54	1.36
7	L	1276	BPB	C1D-C2D	8.14	1.48	1.39
5	C	1333	HEC	C3D-C2D	7.95	1.53	1.36
5	C	1334	HEC	C3D-C2D	7.79	1.53	1.36
7	L	1276	BPB	CAC-C3C	7.77	1.53	1.33
7	M	1326	BPB	CAC-C3C	7.60	1.52	1.33
9	M	1328	MQ7	C3-C2	7.50	1.48	1.35
5	C	1336	HEC	C3D-C2D	7.50	1.52	1.36
5	C	1335	HEC	FE-ND	6.25	2.14	1.94
7	L	1276	BPB	C3D-C2D	6.11	1.50	1.39
5	C	1334	HEC	FE-ND	5.83	2.12	1.94
6	M	1325	BCB	O2D-CGD	5.74	1.47	1.33
6	L	1274	BCB	CAC-C3C	5.72	1.49	1.33
7	M	1326	BPB	O2D-CGD	5.66	1.47	1.33
7	M	1326	BPB	C3D-C2D	5.65	1.49	1.39
6	M	1324	BCB	O2D-CGD	5.58	1.46	1.33
6	L	1274	BCB	O2D-CGD	5.55	1.46	1.33
6	L	1275	BCB	CAC-C3C	5.39	1.48	1.33
6	M	1324	BCB	CAC-C3C	5.35	1.48	1.33
6	M	1325	BCB	CAC-C3C	5.32	1.48	1.33
6	L	1275	BCB	O2D-CGD	5.27	1.46	1.33
5	C	1333	HEC	FE-NB	5.22	2.11	1.94
6	M	1325	BCB	C3B-C4B	5.15	1.50	1.41
7	M	1326	BPB	C4D-CHA	5.13	1.47	1.39
7	L	1276	BPB	O2D-CGD	5.09	1.45	1.33
7	L	1276	BPB	C4D-CHA	5.01	1.47	1.39
5	C	1336	HEC	FE-ND	4.97	2.10	1.94
6	M	1325	BCB	CHC-C1C	4.89	1.48	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1274	BCB	CHC-C1C	4.86	1.48	1.37
9	M	1328	MQ7	C10-C5	4.81	1.48	1.40
7	L	1276	BPB	C3B-C2B	4.73	1.47	1.39
6	L	1275	BCB	O2A-CGA	4.72	1.47	1.33
5	C	1334	HEC	FE-NA	4.68	2.11	1.95
7	L	1276	BPB	OBD-CAD	4.66	1.28	1.22
6	L	1275	BCB	C3B-C4B	4.62	1.49	1.41
7	M	1326	BPB	O2A-CGA	4.61	1.46	1.33
6	M	1325	BCB	O2A-CGA	4.60	1.46	1.33
6	M	1324	BCB	CHC-C1C	4.58	1.48	1.37
6	M	1325	BCB	C2C-C3C	-4.55	1.45	1.51
7	L	1276	BPB	C3B-C4B	4.51	1.49	1.41
5	C	1333	HEC	FE-NC	4.46	2.10	1.95
5	C	1334	HEC	FE-NB	4.46	2.08	1.94
6	M	1324	BCB	O2A-CGA	4.44	1.46	1.33
6	L	1275	BCB	CHD-C1D	4.37	1.46	1.38
6	M	1325	BCB	CHC-C4B	4.31	1.49	1.39
7	M	1326	BPB	C3B-C2B	4.29	1.47	1.39
7	M	1326	BPB	OBD-CAD	4.27	1.28	1.22
6	L	1274	BCB	CHC-C4B	4.27	1.49	1.39
6	L	1275	BCB	CHC-C1C	4.26	1.47	1.37
6	L	1274	BCB	CHD-C1D	4.25	1.46	1.38
7	M	1326	BPB	C3B-C4B	4.24	1.48	1.41
6	L	1274	BCB	C3B-C4B	4.21	1.48	1.41
6	M	1324	BCB	CHD-C1D	4.19	1.46	1.38
6	M	1324	BCB	C2C-C3C	-4.19	1.46	1.51
6	L	1275	BCB	CHC-C4B	4.18	1.48	1.39
5	C	1335	HEC	FE-NA	4.18	2.09	1.95
6	L	1274	BCB	O2A-CGA	4.15	1.45	1.33
6	M	1325	BCB	OBD-CAD	4.12	1.29	1.22
6	L	1275	BCB	C2C-C3C	-4.10	1.46	1.51
6	M	1324	BCB	C3B-C4B	4.09	1.48	1.41
7	L	1276	BPB	O2A-CGA	4.07	1.45	1.33
5	C	1336	HEC	FE-NB	4.07	2.07	1.94
6	M	1325	BCB	C1D-ND	-4.02	1.32	1.37
6	M	1325	BCB	CHD-C1D	3.96	1.46	1.38
6	M	1324	BCB	C1D-ND	-3.94	1.32	1.37
5	C	1334	HEC	CBB-CAB	-3.93	1.33	1.51
5	C	1335	HEC	CBC-CAC	-3.93	1.34	1.51
5	C	1335	HEC	CBB-CAB	-3.92	1.34	1.51
5	C	1333	HEC	CBC-CAC	-3.89	1.34	1.51
5	C	1333	HEC	CBB-CAB	-3.87	1.34	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1334	HEC	CBC-CAC	-3.87	1.34	1.51
5	C	1336	HEC	FE-NC	3.83	2.08	1.95
5	C	1336	HEC	CBC-CAC	-3.80	1.34	1.51
5	C	1336	HEC	CBB-CAB	-3.79	1.34	1.51
6	M	1324	BCB	CHD-C4C	3.77	1.47	1.39
7	M	1326	BPB	CHA-CBD	-3.76	1.47	1.51
6	M	1324	BCB	CHC-C4B	3.76	1.47	1.39
7	L	1276	BPB	CHA-CBD	-3.67	1.47	1.51
6	L	1275	BCB	OBD-CAD	3.63	1.28	1.22
6	L	1274	BCB	C2C-C3C	-3.61	1.47	1.51
6	M	1324	BCB	OBD-CAD	3.54	1.28	1.22
6	L	1274	BCB	C3D-C2D	3.46	1.48	1.39
6	L	1275	BCB	CHD-C4C	3.46	1.47	1.39
6	M	1324	BCB	C3D-C2D	3.46	1.48	1.39
6	L	1274	BCB	CHD-C4C	3.42	1.47	1.39
5	C	1336	HEC	FE-NA	3.37	2.06	1.95
7	M	1326	BPB	C4C-NC	-3.37	1.27	1.37
5	C	1333	HEC	FE-ND	3.34	2.05	1.94
6	L	1274	BCB	OBD-CAD	3.32	1.28	1.22
7	L	1276	BPB	C4C-NC	-3.27	1.27	1.37
6	M	1325	BCB	C3D-C2D	3.26	1.48	1.39
6	L	1275	BCB	C1D-ND	-3.25	1.33	1.37
6	L	1275	BCB	C3D-C2D	3.25	1.48	1.39
6	L	1274	BCB	C1D-ND	-3.21	1.33	1.37
6	M	1325	BCB	CHD-C4C	3.20	1.46	1.39
6	L	1275	BCB	CHB-C1B	3.16	1.46	1.39
6	M	1324	BCB	CHB-C1B	3.11	1.46	1.39
6	L	1274	BCB	CHB-C1B	3.07	1.46	1.39
5	C	1334	HEC	FE-NC	3.07	2.05	1.95
6	M	1325	BCB	MG-NA	-2.99	1.99	2.06
6	M	1325	BCB	C1B-NB	-2.89	1.34	1.37
6	M	1325	BCB	CHB-C1B	2.87	1.45	1.39
5	C	1335	HEC	FE-NB	2.83	2.03	1.94
6	L	1275	BCB	C1B-NB	-2.77	1.34	1.37
6	L	1274	BCB	C1B-NB	-2.75	1.34	1.37
7	M	1326	BPB	C1D-ND	-2.67	1.33	1.38
7	L	1276	BPB	C1D-ND	-2.60	1.33	1.38
6	L	1275	BCB	C1B-C2B	2.54	1.49	1.43
6	M	1324	BCB	C4C-C3C	2.45	1.49	1.44
6	L	1275	BCB	MG-NA	-2.44	2.00	2.06
6	L	1274	BCB	C1B-C2B	2.44	1.49	1.43
6	M	1324	BCB	MG-NA	-2.42	2.00	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1324	BCB	C1B-C2B	2.33	1.48	1.43
7	L	1276	BPB	C3A-C2A	-2.31	1.52	1.54
7	M	1326	BPB	C3A-C2A	-2.28	1.52	1.54
6	M	1324	BCB	C4D-CHA	2.23	1.46	1.38
5	C	1333	HEC	FE-NA	2.22	2.02	1.95
6	L	1275	BCB	CHB-C4A	-2.16	1.32	1.37
5	C	1335	HEC	CMC-C2C	2.15	1.55	1.50
6	L	1274	BCB	C4D-CHA	2.13	1.46	1.38
6	M	1325	BCB	C1B-C2B	2.13	1.48	1.43
5	C	1335	HEC	CMD-C2D	2.11	1.55	1.50
6	L	1275	BCB	C3D-C4D	-2.09	1.39	1.44
6	M	1324	BCB	CHB-C4A	-2.09	1.32	1.37
6	M	1325	BCB	C4D-CHA	2.08	1.45	1.38
6	M	1324	BCB	C3D-C4D	-2.07	1.39	1.44
6	L	1274	BCB	CHB-C4A	-2.03	1.32	1.37
7	L	1276	BPB	CBD-CGD	-2.03	1.49	1.52
6	L	1275	BCB	C4D-CHA	2.01	1.45	1.38
5	C	1334	HEC	CMC-C2C	2.00	1.55	1.50

All (191) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	1324	BCB	C1C-NC-C4C	-15.57	99.71	106.71
6	M	1325	BCB	C1C-NC-C4C	-15.56	99.71	106.71
6	L	1275	BCB	C1C-NC-C4C	-15.24	99.85	106.71
6	L	1274	BCB	C1C-NC-C4C	-13.96	100.43	106.71
6	M	1325	BCB	C2B-C1B-NB	10.85	117.50	110.23
6	L	1275	BCB	C2B-C1B-NB	10.22	117.08	110.23
6	M	1324	BCB	C2B-C1B-NB	9.54	116.63	110.23
6	L	1274	BCB	C2B-C1B-NB	9.22	116.41	110.23
7	L	1276	BPB	O2D-CGD-CBD	7.46	120.45	111.00
7	L	1276	BPB	C3D-C4D-ND	7.18	117.51	107.72
6	L	1274	BCB	C4D-C3D-CAD	-7.09	99.74	108.10
7	M	1326	BPB	C3D-C4D-ND	6.95	117.20	107.72
5	C	1333	HEC	C1D-ND-C4D	6.77	112.07	105.07
5	C	1336	HEC	C1D-ND-C4D	6.75	112.04	105.07
5	C	1335	HEC	C1D-ND-C4D	6.60	111.89	105.07
6	M	1324	BCB	C4D-C3D-CAD	-6.60	100.32	108.10
6	M	1325	BCB	CMD-C2D-C1D	6.49	136.16	124.71
5	C	1334	HEC	C1D-ND-C4D	6.39	111.67	105.07
7	L	1276	BPB	CBC-CAC-C3C	-6.35	109.85	126.70
7	M	1326	BPB	O2D-CGD-CBD	6.30	118.98	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	L	1276	BPB	C2B-C1B-NB	6.20	113.81	109.53
6	L	1275	BCB	CMD-C2D-C1D	6.19	135.62	124.71
7	M	1326	BPB	CBC-CAC-C3C	-6.11	110.47	126.70
6	L	1275	BCB	C4D-C3D-CAD	-5.80	101.25	108.10
6	M	1324	BCB	C3D-C4D-ND	5.75	119.54	110.24
6	M	1324	BCB	O2D-CGD-CBD	5.74	121.47	111.27
7	M	1326	BPB	C2B-C1B-NB	5.70	113.46	109.53
6	M	1325	BCB	C3D-C4D-ND	5.58	119.27	110.24
6	M	1324	BCB	CMD-C2D-C1D	5.55	134.49	124.71
6	L	1275	BCB	C3D-C4D-ND	5.48	119.09	110.24
6	M	1325	BCB	O2D-CGD-CBD	5.47	120.99	111.27
6	M	1325	BCB	C4D-C3D-CAD	-5.44	101.68	108.10
6	L	1275	BCB	O2D-CGD-CBD	5.11	120.35	111.27
6	L	1274	BCB	C3D-C4D-ND	5.07	118.43	110.24
6	M	1325	BCB	C1D-ND-C4D	-4.66	103.03	106.33
6	L	1274	BCB	CMD-C2D-C1D	4.61	132.84	124.71
6	M	1324	BCB	C1D-ND-C4D	-4.33	103.26	106.33
7	M	1326	BPB	OBD-CAD-C3D	-4.33	120.79	127.98
6	M	1325	BCB	CMD-C2D-C3D	-4.28	117.77	127.61
6	L	1275	BCB	C2C-C1C-CHC	-4.27	113.58	123.64
6	M	1324	BCB	C2C-C1C-CHC	-4.27	113.58	123.64
6	L	1275	BCB	CMD-C2D-C3D	-4.25	117.85	127.61
6	M	1324	BCB	CAD-C3D-C2D	4.13	160.72	140.80
6	L	1274	BCB	CAD-C3D-C2D	4.09	160.56	140.80
6	M	1325	BCB	C4A-NA-C1A	4.09	108.54	106.71
6	L	1274	BCB	C4-C3-C5	4.04	122.08	115.27
7	M	1326	BPB	CMD-C2D-C3D	-4.00	117.20	124.68
5	C	1333	HEC	CBD-CAD-C3D	-4.00	101.53	112.63
6	L	1275	BCB	C1D-ND-C4D	-3.95	103.53	106.33
6	M	1324	BCB	CMD-C2D-C3D	-3.81	118.84	127.61
6	L	1275	BCB	CAD-C3D-C2D	3.79	159.08	140.80
6	L	1274	BCB	C2C-C1C-CHC	-3.78	114.74	123.64
5	C	1334	HEC	C4B-NB-C1B	3.75	108.95	105.07
6	M	1325	BCB	CAD-C3D-C2D	3.74	158.84	140.80
6	L	1274	BCB	C1D-ND-C4D	-3.74	103.68	106.33
7	L	1276	BPB	OBD-CAD-C3D	-3.62	121.97	127.98
6	M	1324	BCB	CHB-C4A-NA	3.61	129.51	124.51
6	M	1325	BCB	C2C-C1C-CHC	-3.58	115.22	123.64
6	M	1325	BCB	CHB-C4A-NA	3.38	129.19	124.51
5	C	1336	HEC	CBB-CAB-C3B	3.36	121.70	112.43
7	L	1276	BPB	CMD-C2D-C3D	-3.36	118.40	124.68
6	L	1275	BCB	CHB-C4A-NA	3.35	129.14	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1334	HEC	C4A-NA-C1A	3.34	108.62	105.35
6	L	1274	BCB	C1-C2-C3	-3.27	120.38	126.04
5	C	1336	HEC	C4B-NB-C1B	3.25	108.44	105.07
6	L	1275	BCB	OBD-CAD-C3D	-3.25	120.70	128.52
5	C	1334	HEC	CBC-CAC-C3C	3.21	121.29	112.43
5	C	1336	HEC	C4A-NA-C1A	3.21	108.49	105.35
5	C	1334	HEC	C4C-NC-C1C	3.20	108.48	105.35
6	M	1324	BCB	OBD-CAD-C3D	-3.20	120.83	128.52
6	L	1274	BCB	CHA-C4D-ND	-3.20	125.81	132.50
6	M	1324	BCB	CMB-C2B-C1B	3.19	130.23	125.37
6	L	1275	BCB	CHB-C1B-NB	-3.15	120.92	124.26
6	L	1274	BCB	O2D-CGD-CBD	3.12	116.82	111.27
6	M	1325	BCB	CBC-CAC-C3C	-3.11	117.63	126.72
7	M	1326	BPB	C1A-C2A-C3A	-3.10	99.89	102.84
6	M	1325	BCB	C4-C3-C5	3.10	120.48	115.27
6	L	1274	BCB	CED-O2D-CGD	3.06	122.86	115.94
7	M	1326	BPB	CED-O2D-CGD	3.05	122.84	115.94
6	L	1274	BCB	CMD-C2D-C3D	-3.05	120.60	127.61
6	M	1324	BCB	O2D-CGD-O1D	-3.04	117.89	123.84
6	M	1324	BCB	CHA-C4D-ND	-3.04	126.14	132.50
5	C	1336	HEC	CBC-CAC-C3C	3.02	120.74	112.43
5	C	1334	HEC	C2A-C1A-NA	-3.00	107.40	110.32
7	L	1276	BPB	C1A-C2A-C3A	-2.97	100.02	102.84
5	C	1336	HEC	CAD-C3D-C4D	2.92	129.76	124.66
5	C	1334	HEC	C3B-C4B-NB	-2.90	106.94	110.17
6	L	1274	BCB	OBD-CAD-C3D	-2.90	121.54	128.52
6	M	1325	BCB	CHD-C1D-ND	-2.89	121.80	124.45
6	L	1274	BCB	CHB-C4A-NA	2.88	128.50	124.51
6	L	1274	BCB	CBC-CAC-C3C	-2.86	118.35	126.72
6	M	1325	BCB	C1-C2-C3	-2.86	121.09	126.04
7	L	1276	BPB	CMB-C2B-C3B	2.85	130.01	124.68
9	M	1328	MQ7	C24-C23-C25	2.85	120.06	115.27
6	M	1325	BCB	CHA-C4D-ND	-2.83	126.57	132.50
7	M	1326	BPB	C4-C3-C5	2.82	120.02	115.27
5	C	1335	HEC	C4B-NB-C1B	2.82	107.99	105.07
7	M	1326	BPB	C3D-CAD-CBD	2.82	111.31	107.61
6	L	1275	BCB	C2A-C1A-CHA	-2.81	118.94	123.86
6	M	1325	BCB	C2D-C1D-ND	2.80	112.17	110.10
5	C	1336	HEC	C4C-NC-C1C	2.80	108.09	105.35
7	M	1326	BPB	C4D-ND-C1D	-2.79	105.99	108.83
7	M	1326	BPB	C4D-CHA-CBD	-2.79	107.25	108.52
5	C	1333	HEC	C4C-NC-C1C	2.79	108.08	105.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	L	1276	BPB	O1D-CGD-CBD	-2.78	120.11	124.74
5	C	1333	HEC	CBB-CAB-C3B	2.78	120.08	112.43
6	L	1275	BCB	CBC-CAC-C3C	-2.77	118.61	126.72
6	M	1325	BCB	CHB-C1B-NB	-2.75	121.34	124.26
6	M	1325	BCB	O2D-CGD-O1D	-2.73	118.50	123.84
6	L	1275	BCB	CHA-C4D-ND	-2.71	126.83	132.50
6	L	1275	BCB	CHC-C4B-C3B	-2.70	122.76	132.35
5	C	1333	HEC	CBC-CAC-C3C	2.68	119.83	112.43
9	M	1328	MQ7	C39-C38-C40	2.68	119.77	115.27
9	M	1328	MQ7	C2M-C2-C3	-2.67	120.04	124.40
5	C	1333	HEC	C4B-NB-C1B	2.67	107.83	105.07
5	C	1334	HEC	CBB-CAB-C3B	2.67	119.79	112.43
5	C	1333	HEC	C2A-C1A-NA	-2.66	107.73	110.32
5	C	1336	HEC	C2A-C1A-NA	-2.65	107.74	110.32
6	M	1324	BCB	CHC-C4B-C3B	-2.65	122.92	132.35
5	C	1335	HEC	CBC-CAC-C3C	2.65	119.73	112.43
7	L	1276	BPB	C4D-CHA-CBD	-2.64	107.33	108.52
6	L	1274	BCB	CHC-C4B-C3B	-2.63	123.00	132.35
6	L	1275	BCB	O2A-CGA-CBA	2.62	120.14	111.91
7	L	1276	BPB	C4D-ND-C1D	-2.61	106.17	108.83
5	C	1336	HEC	CHD-C1D-ND	2.59	127.57	124.37
6	M	1324	BCB	CBC-CAC-C3C	-2.55	119.26	126.72
7	M	1326	BPB	O1D-CGD-CBD	-2.55	120.49	124.74
6	L	1275	BCB	C1-O2A-CGA	2.55	123.13	116.44
6	M	1324	BCB	C2A-C1A-CHA	-2.54	119.41	123.86
5	C	1335	HEC	C4A-NA-C1A	2.53	107.83	105.35
7	L	1276	BPB	C3D-CAD-CBD	2.52	110.92	107.61
6	L	1274	BCB	CHB-C1B-NB	-2.52	121.59	124.26
5	C	1333	HEC	C4A-NA-C1A	2.49	107.79	105.35
5	C	1335	HEC	C4C-NC-C1C	2.49	107.78	105.35
6	L	1274	BCB	CBB-CAB-C3B	-2.48	115.12	120.43
6	L	1274	BCB	CAA-C2A-C1A	2.43	119.95	111.97
5	C	1335	HEC	CBB-CAB-C3B	2.42	119.11	112.43
9	M	1328	MQ7	C29-C28-C30	2.41	119.33	115.27
6	M	1325	BCB	O2A-CGA-CBA	2.41	119.48	111.91
5	C	1333	HEC	O2D-CGD-CBD	2.41	121.77	114.03
6	M	1325	BCB	OBD-CAD-C3D	-2.40	122.75	128.52
5	C	1333	HEC	C3B-C4B-NB	-2.37	107.53	110.17
6	L	1275	BCB	O2D-CGD-O1D	-2.37	119.21	123.84
6	M	1325	BCB	C1-O2A-CGA	2.36	122.64	116.44
5	C	1333	HEC	CAA-CBA-CGA	-2.35	108.54	113.60
5	C	1333	HEC	O1D-CGD-CBD	-2.35	115.53	123.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1336	HEC	C3D-C4D-ND	-2.34	108.09	110.36
9	M	1328	MQ7	C14-C13-C15	2.34	119.21	115.27
6	L	1274	BCB	CMB-C2B-C1B	2.33	128.92	125.37
9	M	1328	MQ7	C2M-C2-C1	2.33	120.13	116.27
6	L	1274	BCB	CHD-C4C-C3C	-2.31	123.00	125.89
6	L	1275	BCB	C4B-C3B-C2B	-2.31	104.64	108.36
6	M	1324	BCB	CHD-C1D-ND	-2.30	122.34	124.45
5	C	1333	HEC	CHD-C1D-ND	2.29	127.20	124.37
6	M	1324	BCB	CAB-C3B-C2B	-2.29	124.90	128.34
7	M	1326	BPB	C4A-C3A-C2A	-2.28	100.67	102.84
5	C	1334	HEC	C2B-C1B-NB	-2.27	107.17	109.88
7	L	1276	BPB	O2D-CGD-O1D	-2.26	119.41	123.84
6	M	1325	BCB	CAB-C3B-C2B	-2.26	124.96	128.34
6	M	1325	BCB	CAA-C2A-C1A	2.26	119.37	111.97
5	C	1335	HEC	C2A-C1A-NA	-2.26	108.13	110.32
7	M	1326	BPB	OBD-CAD-CBD	-2.25	122.52	125.82
6	M	1324	BCB	CED-O2D-CGD	2.25	121.02	115.94
6	M	1325	BCB	CED-O2D-CGD	2.25	121.02	115.94
5	C	1336	HEC	CAD-CBD-CGD	-2.23	108.80	113.60
7	L	1276	BPB	C6-C7-C8	-2.23	108.70	115.92
7	L	1276	BPB	O2A-CGA-O1A	-2.23	117.97	123.59
6	M	1324	BCB	C4A-NA-C1A	2.22	107.70	106.71
6	L	1275	BCB	CMB-C2B-C1B	2.21	128.74	125.37
6	M	1324	BCB	O2A-CGA-CBA	2.19	118.77	111.91
9	M	1328	MQ7	C21-C22-C23	-2.17	122.44	127.66
6	M	1325	BCB	CHB-C1B-C2B	-2.16	121.13	127.24
6	M	1325	BCB	CMB-C2B-C1B	2.13	128.62	125.37
5	C	1334	HEC	CHB-C1B-NB	2.13	126.74	124.42
6	M	1324	BCB	CHB-C1B-NB	-2.13	122.00	124.26
5	C	1334	HEC	CHA-C4D-ND	2.12	126.72	124.42
7	M	1326	BPB	C1-O2A-CGA	2.12	122.00	116.44
7	L	1276	BPB	O2A-CGA-CBA	2.11	118.54	111.91
5	C	1336	HEC	C3B-C4B-NB	-2.09	107.84	110.17
7	M	1326	BPB	C1-C2-C3	-2.08	122.45	126.04
6	M	1324	BCB	CHB-C1B-C2B	-2.08	121.37	127.24
7	L	1276	BPB	OBD-CAD-CBD	-2.07	122.78	125.82
6	L	1274	BCB	C2D-C1D-ND	2.07	111.63	110.10
6	M	1325	BCB	C4B-C3B-C2B	-2.05	105.06	108.36
5	C	1336	HEC	CHB-C4A-NA	2.04	126.65	124.44
5	C	1334	HEC	C3D-C4D-ND	-2.03	108.39	110.36
5	C	1335	HEC	C3B-C4B-NB	-2.03	107.90	110.17
6	M	1325	BCB	CHC-C4B-C3B	-2.02	125.15	132.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1334	HEC	CHA-C1A-NA	2.01	126.62	124.44
6	M	1325	BCB	C4D-CHA-C1A	2.01	123.69	121.25
5	C	1336	HEC	C2B-C1B-NB	-2.00	107.48	109.88

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	1333	HEC	NA
5	C	1334	HEC	NA
5	C	1335	HEC	NA
5	C	1336	HEC	NA
6	L	1274	BCB	ND
6	L	1274	BCB	NA
6	L	1274	BCB	NC
6	L	1275	BCB	ND
6	L	1275	BCB	NA
6	L	1275	BCB	NC
6	M	1324	BCB	ND
6	M	1324	BCB	NA
6	M	1324	BCB	NC
6	M	1325	BCB	ND
6	M	1325	BCB	NA
6	M	1325	BCB	NC

All (111) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1336	HEC	C3D-CAD-CBD-CGD
6	L	1274	BCB	C2C-C3C-CAC-CBC
6	L	1274	BCB	C4C-C3C-CAC-CBC
6	L	1274	BCB	C2-C3-C5-C6
6	L	1274	BCB	C4-C3-C5-C6
6	L	1275	BCB	C2C-C3C-CAC-CBC
6	L	1275	BCB	C4C-C3C-CAC-CBC
6	M	1324	BCB	C2B-C3B-CAB-OBB
6	M	1324	BCB	C2B-C3B-CAB-CBB
6	M	1324	BCB	C4B-C3B-CAB-OBB
6	M	1324	BCB	C4B-C3B-CAB-CBB
6	M	1324	BCB	C2C-C3C-CAC-CBC
6	M	1324	BCB	C4C-C3C-CAC-CBC
6	M	1325	BCB	C2A-CAA-CBA-CGA
6	M	1325	BCB	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	M	1325	BCB	C4C-C3C-CAC-CBC
6	M	1325	BCB	CAD-CBD-CGD-O1D
6	M	1325	BCB	CAD-CBD-CGD-O2D
7	L	1276	BPB	C2C-C3C-CAC-CBC
7	M	1326	BPB	C2C-C3C-CAC-CBC
7	M	1326	BPB	C4C-C3C-CAC-CBC
6	M	1324	BCB	CBD-CGD-O2D-CED
6	M	1325	BCB	CBD-CGD-O2D-CED
7	L	1276	BPB	CBD-CGD-O2D-CED
6	M	1324	BCB	O1D-CGD-O2D-CED
5	C	1333	HEC	C4B-C3B-CAB-CBB
7	M	1326	BPB	CBD-CGD-O2D-CED
5	C	1334	HEC	C4B-C3B-CAB-CBB
5	C	1333	HEC	C2B-C3B-CAB-CBB
5	C	1334	HEC	C2B-C3B-CAB-CBB
5	C	1336	HEC	C2B-C3B-CAB-CBB
7	L	1276	BPB	O1D-CGD-O2D-CED
5	C	1333	HEC	C2C-C3C-CAC-CBC
7	M	1326	BPB	O1D-CGD-O2D-CED
5	C	1334	HEC	C2C-C3C-CAC-CBC
5	C	1336	HEC	C4B-C3B-CAB-CBB
6	M	1325	BCB	O1D-CGD-O2D-CED
7	M	1326	BPB	C11-C10-C8-C9
5	C	1333	HEC	C4C-C3C-CAC-CBC
5	C	1334	HEC	C4C-C3C-CAC-CBC
7	L	1276	BPB	C8-C10-C11-C12
7	M	1326	BPB	C5-C6-C7-C8
5	C	1336	HEC	C2C-C3C-CAC-CBC
5	C	1335	HEC	C2B-C3B-CAB-CBB
7	M	1326	BPB	C8-C10-C11-C12
6	M	1324	BCB	C10-C11-C12-C13
7	L	1276	BPB	CBA-CGA-O2A-C1
5	C	1335	HEC	C2C-C3C-CAC-CBC
6	L	1275	BCB	C16-C17-C18-C19
5	C	1336	HEC	C4C-C3C-CAC-CBC
7	L	1276	BPB	C4-C3-C5-C6
7	L	1276	BPB	C2-C1-O2A-CGA
5	C	1335	HEC	C4C-C3C-CAC-CBC
7	L	1276	BPB	O1A-CGA-O2A-C1
6	L	1275	BCB	C11-C12-C13-C15
7	L	1276	BPB	C2-C3-C5-C6
6	L	1275	BCB	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	M	1325	BCB	C5-C6-C7-C8
6	M	1325	BCB	C13-C15-C16-C17
9	M	1328	MQ7	C38-C40-C41-C42
6	L	1275	BCB	C11-C12-C13-C14
5	C	1335	HEC	C4B-C3B-CAB-CBB
7	L	1276	BPB	C15-C16-C17-C18
6	M	1325	BCB	C10-C11-C12-C13
6	L	1274	BCB	C15-C16-C17-C18
6	M	1325	BCB	C11-C12-C13-C15
6	M	1325	BCB	C11-C12-C13-C14
7	M	1326	BPB	C11-C12-C13-C14
7	M	1326	BPB	C10-C11-C12-C13
5	C	1334	HEC	C3D-CAD-CBD-CGD
6	M	1325	BCB	O2A-C1-C2-C3
7	M	1326	BPB	C11-C12-C13-C15
6	L	1275	BCB	C2A-CAA-CBA-CGA
6	L	1274	BCB	CHA-CBD-CGD-O1D
6	L	1275	BCB	CHA-CBD-CGD-O1D
6	L	1275	BCB	CHA-CBD-CGD-O2D
6	M	1324	BCB	CHA-CBD-CGD-O1D
6	M	1324	BCB	CHA-CBD-CGD-O2D
6	M	1325	BCB	C3-C5-C6-C7
9	M	1328	MQ7	C18-C20-C21-C22
6	L	1274	BCB	CAD-CBD-CGD-O1D
6	M	1325	BCB	C11-C10-C8-C7
7	M	1326	BPB	C6-C7-C8-C10
6	M	1325	BCB	C11-C10-C8-C9
5	C	1334	HEC	CAA-CBA-CGA-O1A
5	C	1336	HEC	CAD-CBD-CGD-O1D
6	M	1324	BCB	C1A-C2A-CAA-CBA
5	C	1336	HEC	CAD-CBD-CGD-O2D
5	C	1334	HEC	CAD-CBD-CGD-O2D
5	C	1334	HEC	CAD-CBD-CGD-O1D
5	C	1334	HEC	CAA-CBA-CGA-O2A
5	C	1335	HEC	CAA-CBA-CGA-O2A
7	L	1276	BPB	C13-C15-C16-C17
6	M	1324	BCB	C4-C3-C5-C6
7	M	1326	BPB	C6-C7-C8-C9
7	L	1276	BPB	CAD-CBD-CGD-O2D
5	C	1333	HEC	CAA-CBA-CGA-O2A
7	M	1326	BPB	C4-C3-C5-C6
9	M	1328	MQ7	C34-C33-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	1335	HEC	CAA-CBA-CGA-O1A
6	M	1324	BCB	C2-C3-C5-C6
6	L	1274	BCB	CHA-CBD-CGD-O2D
6	M	1325	BCB	CHA-CBD-CGD-O1D
6	M	1325	BCB	CHA-CBD-CGD-O2D
7	M	1326	BPB	C11-C10-C8-C7
6	M	1324	BCB	C14-C13-C15-C16
5	C	1333	HEC	CAA-CBA-CGA-O1A
6	L	1275	BCB	C1A-C2A-CAA-CBA
7	L	1276	BPB	C3-C5-C6-C7
6	L	1274	BCB	C11-C10-C8-C7
6	M	1324	BCB	C12-C13-C15-C16

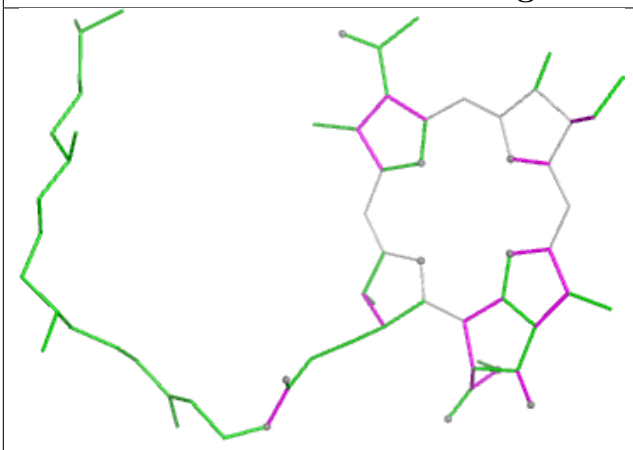
There are no ring outliers.

11 monomers are involved in 53 short contacts:

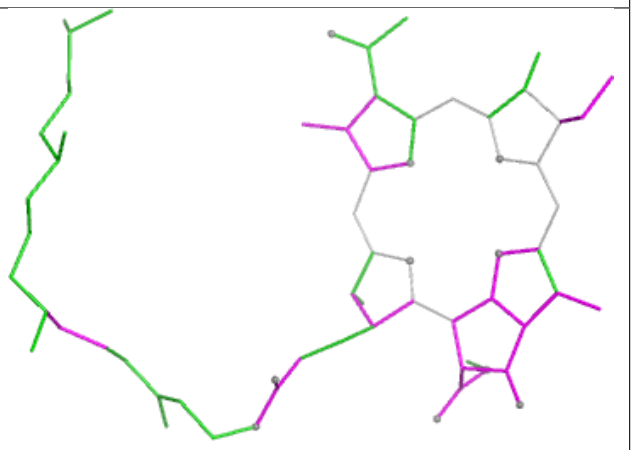
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	1276	BPB	5	0
9	M	1328	MQ7	3	0
6	M	1325	BCB	6	0
6	M	1324	BCB	3	0
5	C	1336	HEC	2	0
6	L	1274	BCB	12	0
5	C	1333	HEC	1	0
6	L	1275	BCB	7	0
5	C	1334	HEC	7	0
7	M	1326	BPB	6	0
5	C	1335	HEC	2	0

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.

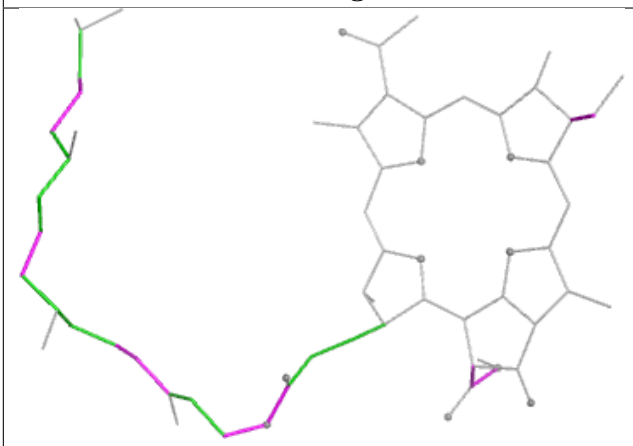
Ligand BPB L 1276



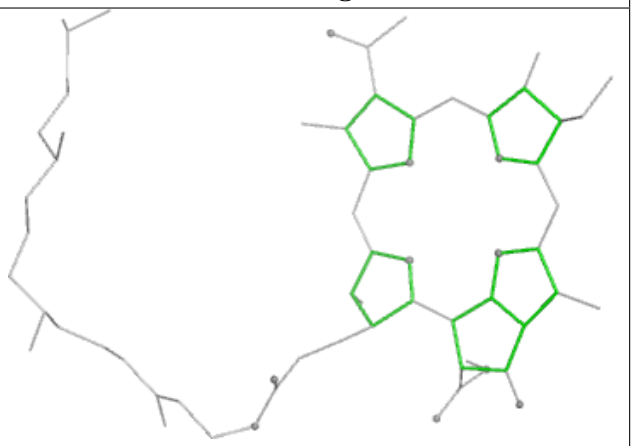
Bond lengths



Bond angles

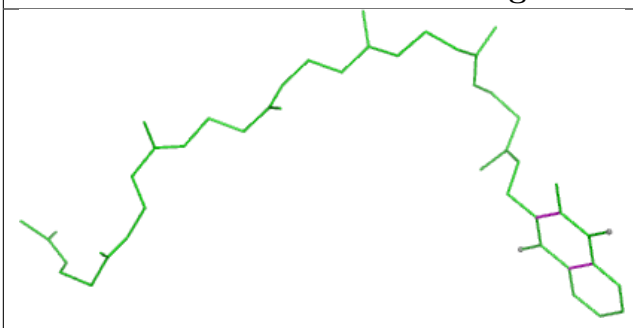


Torsions

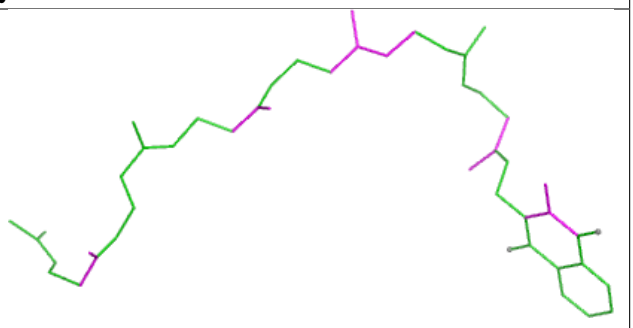


Rings

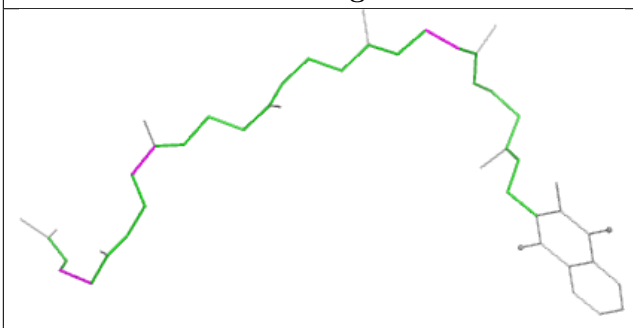
Ligand MQ7 M 1328



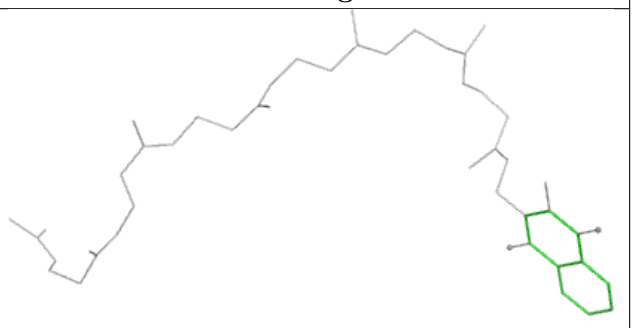
Bond lengths



Bond angles

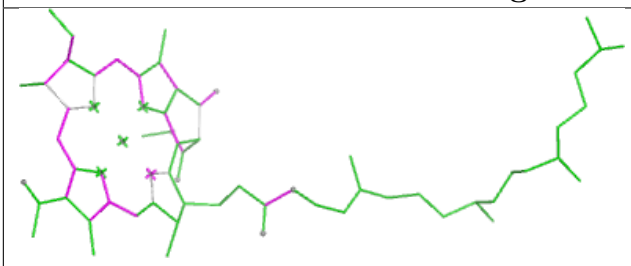


Torsions

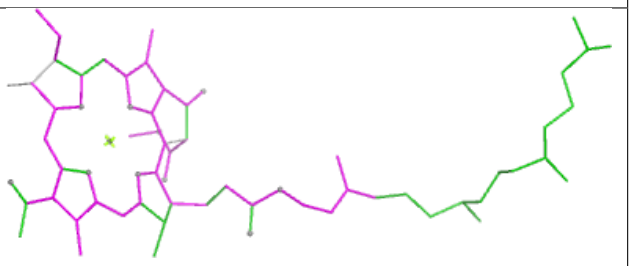


Rings

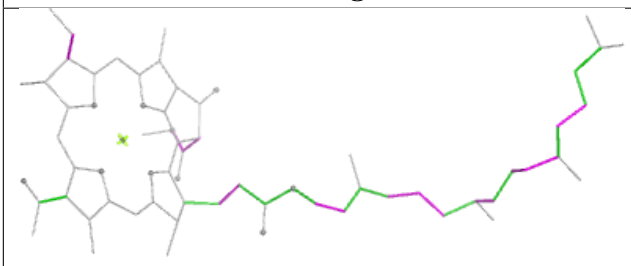
Ligand BCB M 1325



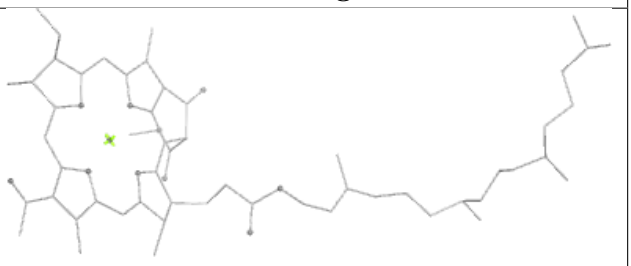
Bond lengths



Bond angles

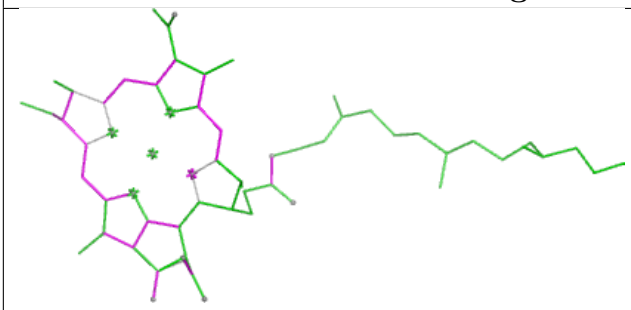


Torsions

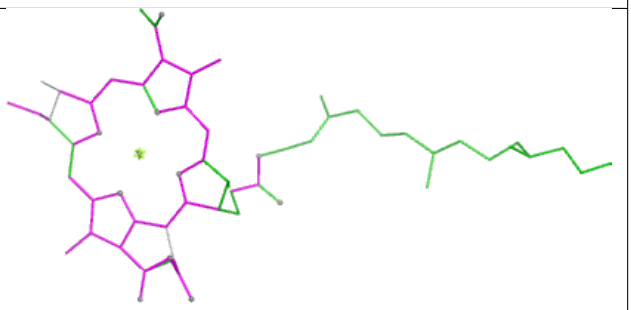


Rings

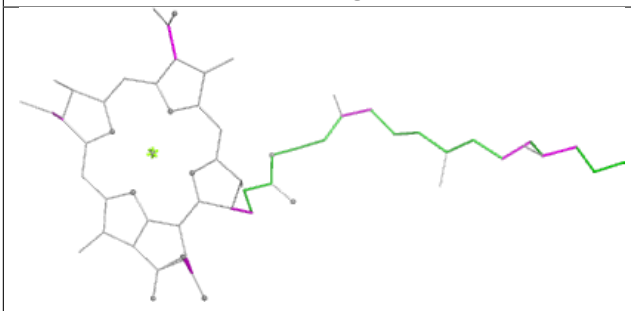
Ligand BCB M 1324



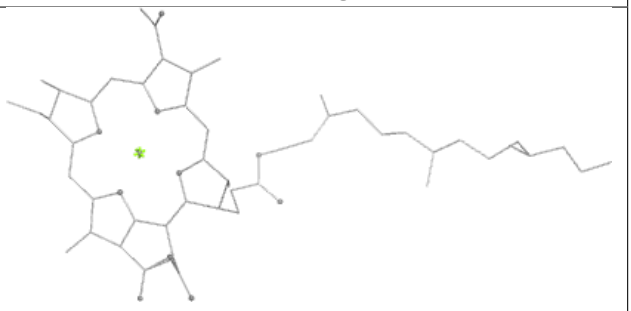
Bond lengths



Bond angles

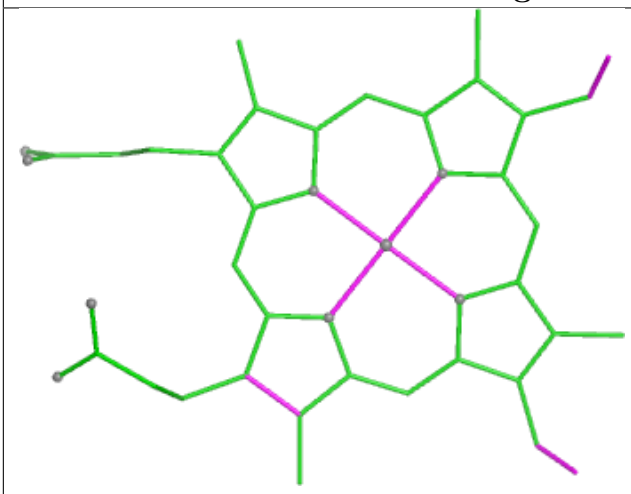


Torsions

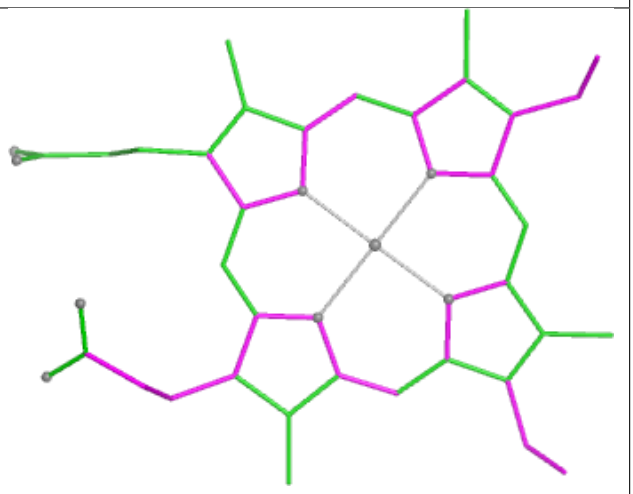


Rings

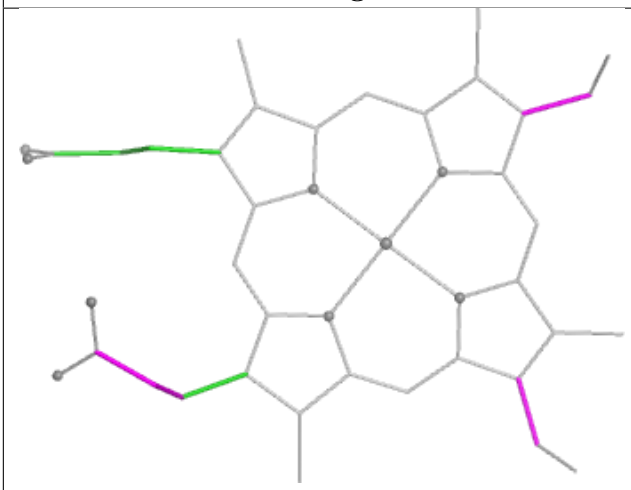
Ligand HEC C 1336



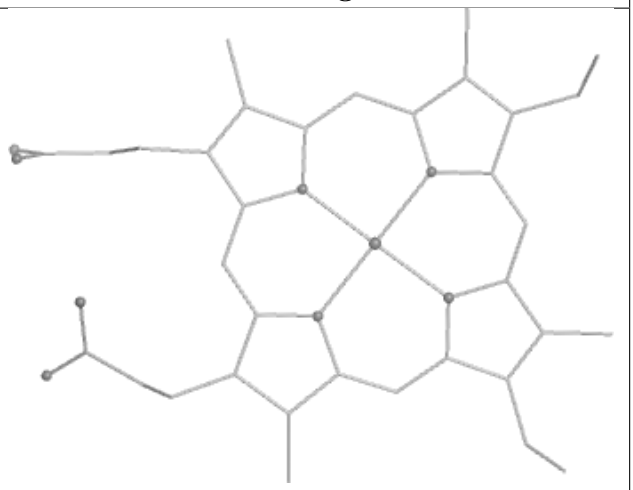
Bond lengths



Bond angles



Torsions

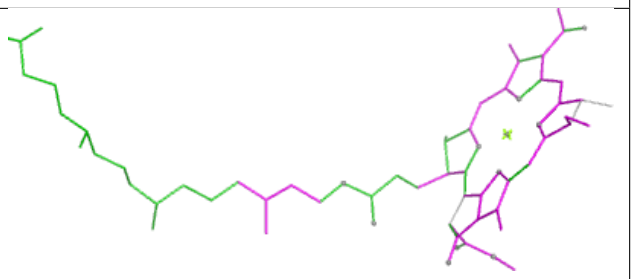


Rings

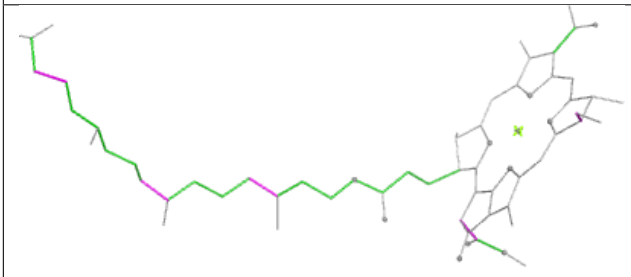
Ligand BCB L 1274



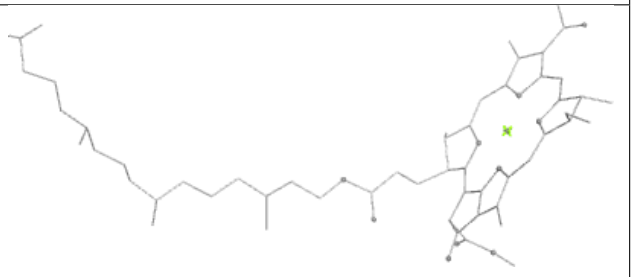
Bond lengths



Bond angles

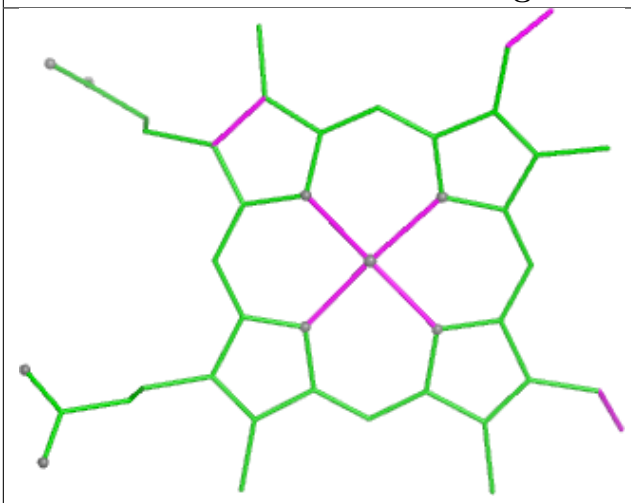


Torsions

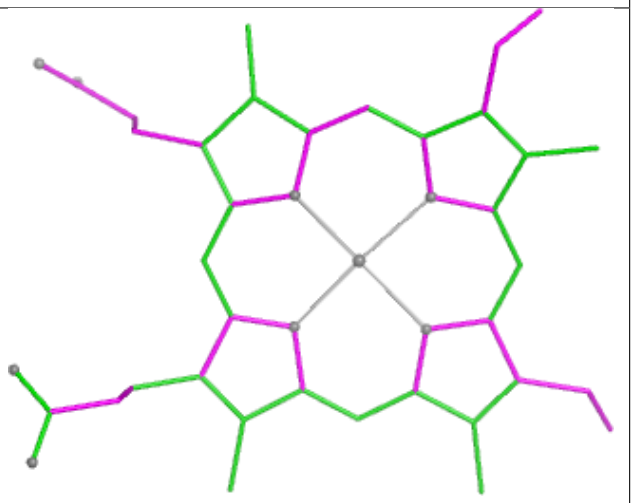


Rings

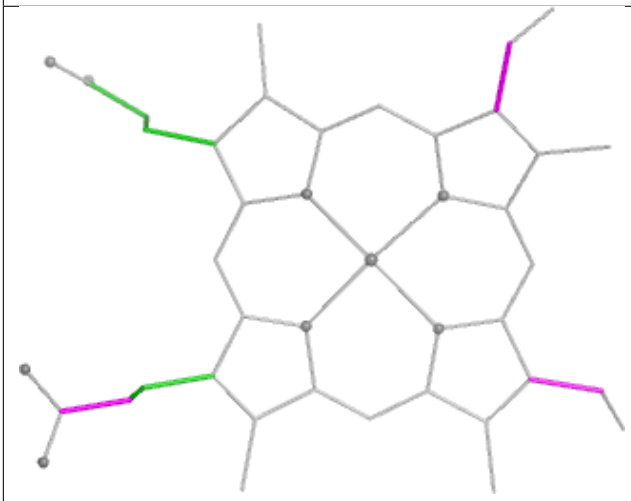
Ligand HEC C 1333



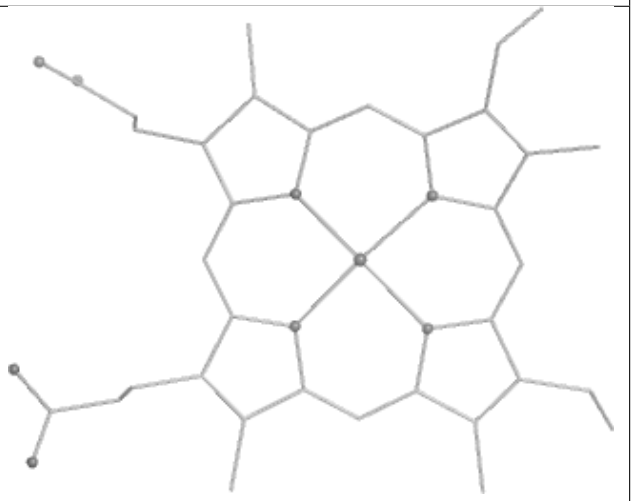
Bond lengths



Bond angles

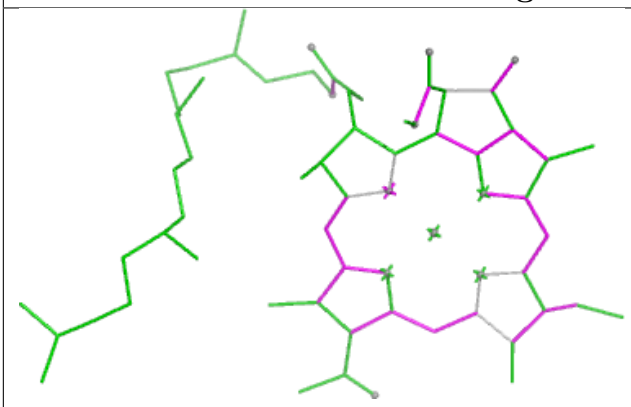


Torsions

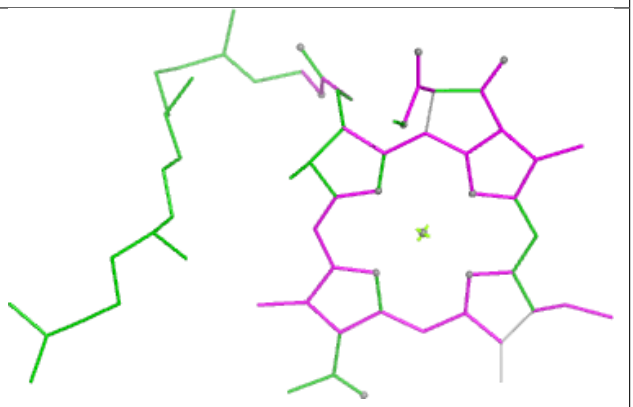


Rings

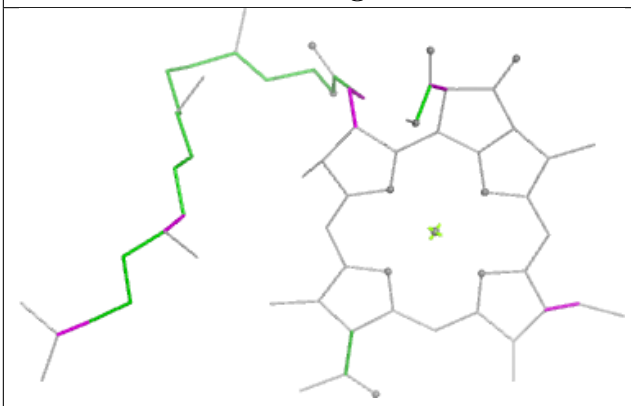
Ligand BCB L 1275



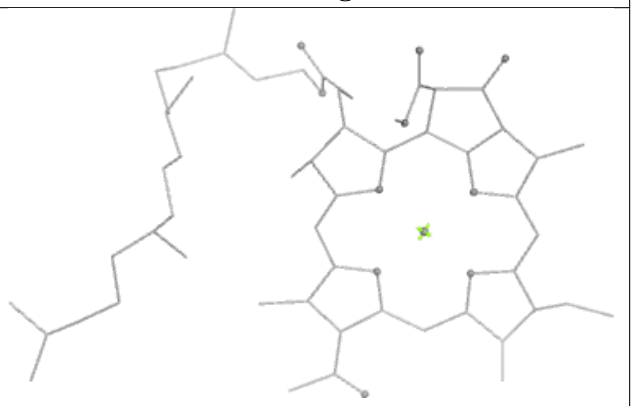
Bond lengths



Bond angles

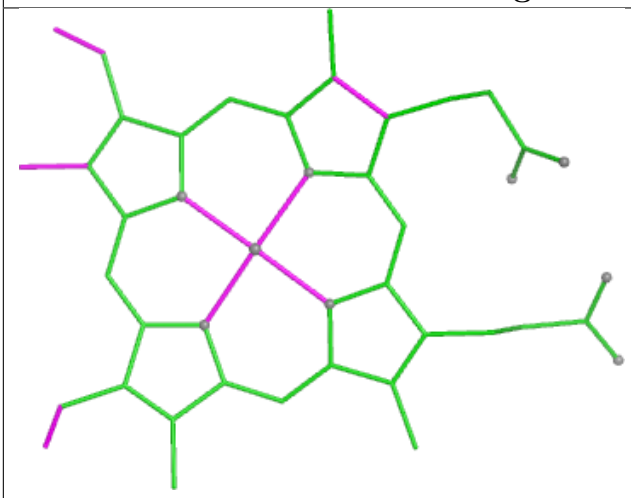


Torsions

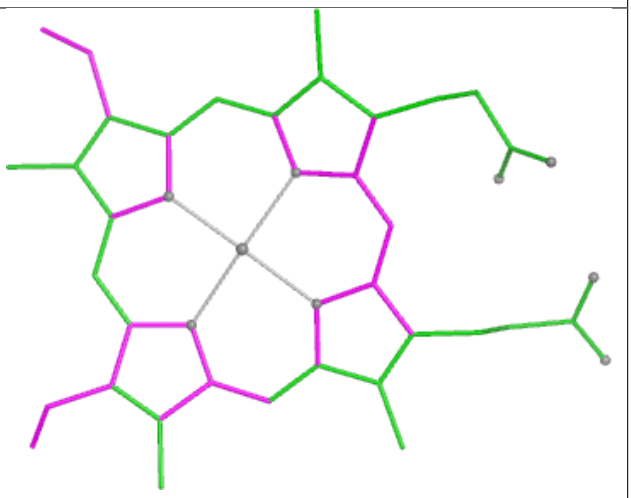


Rings

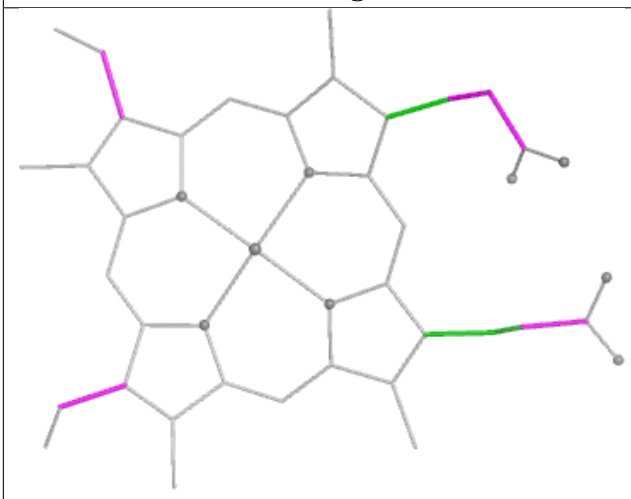
Ligand HEC C 1334



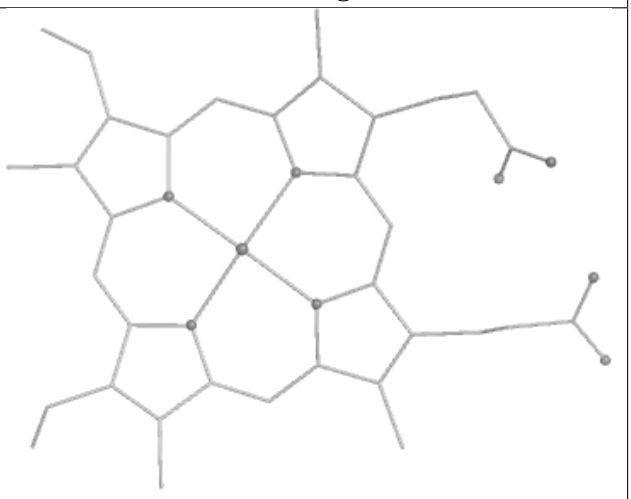
Bond lengths



Bond angles

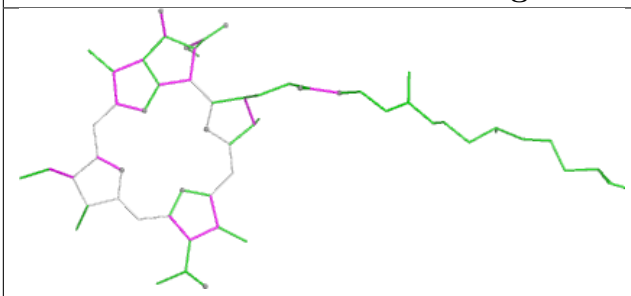


Torsions

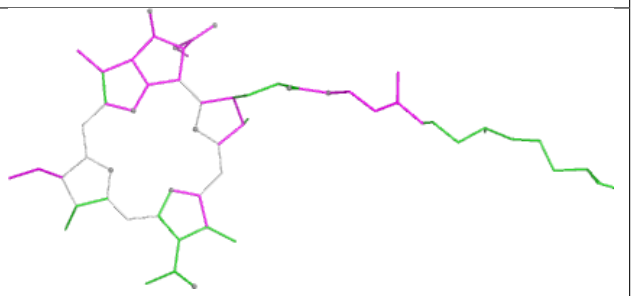


Rings

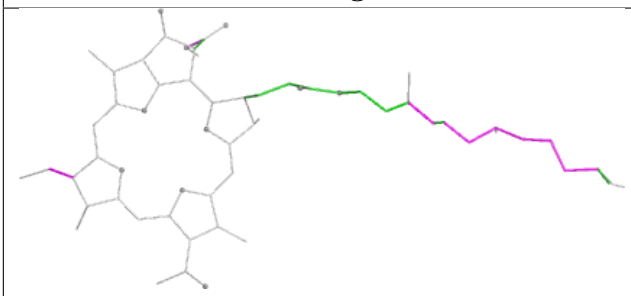
Ligand BPB M 1326



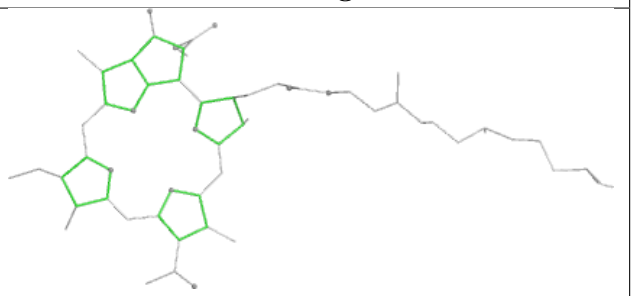
Bond lengths



Bond angles

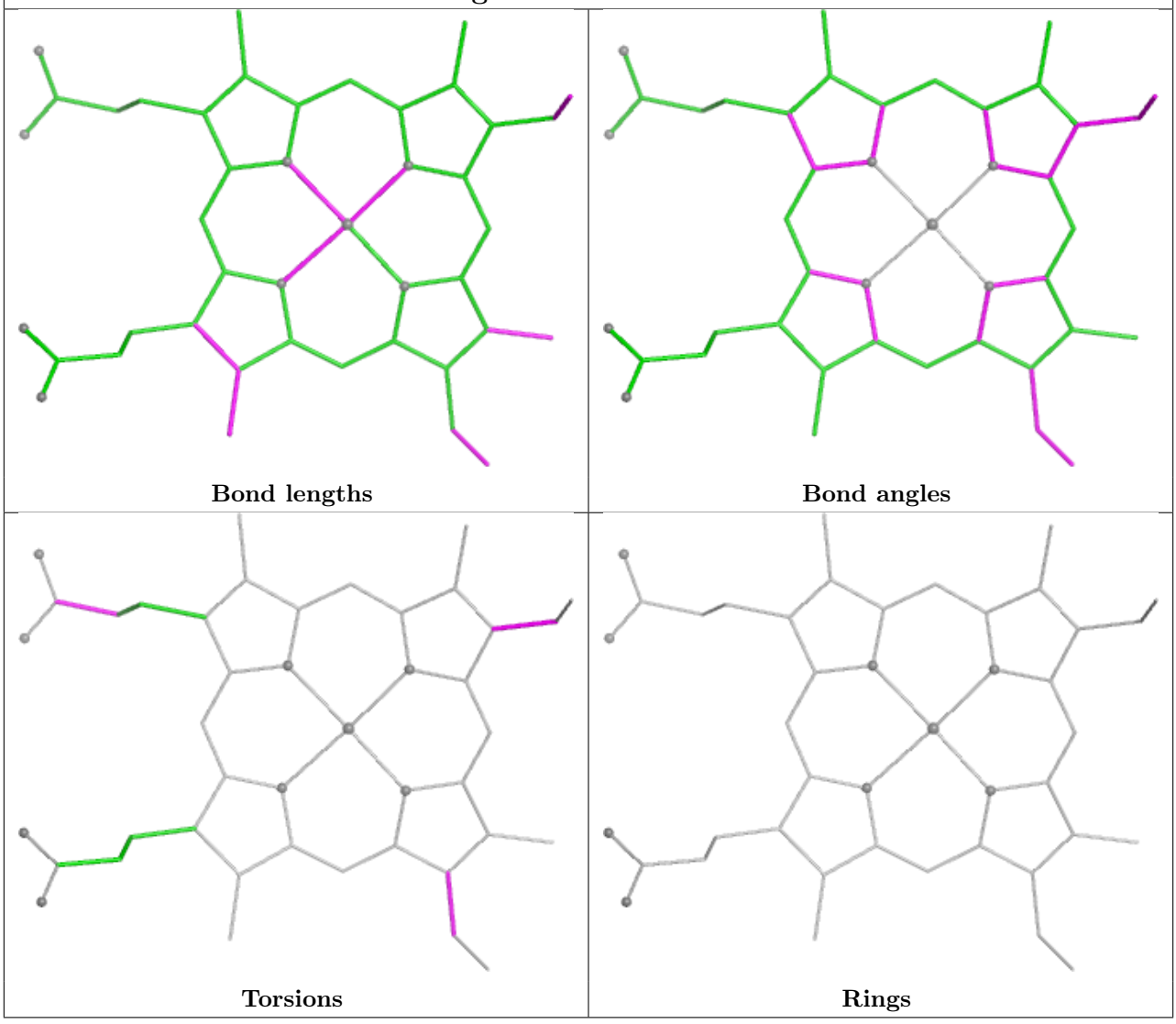


Torsions



Rings

Ligand HEC C 1335



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	C	332/336 (98%)	0.73	24 (7%) 21 11	18, 31, 45, 51	1 (0%)
2	H	242/258 (93%)	1.15	32 (13%) 7 4	22, 40, 64, 68	8 (3%)
3	L	273/274 (99%)	0.66	16 (5%) 28 14	9, 28, 48, 57	6 (2%)
4	M	323/324 (99%)	0.42	7 (2%) 62 39	16, 26, 41, 44	2 (0%)
All	All	1170/1192 (98%)	0.72	79 (6%) 23 12	9, 31, 49, 68	17 (1%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	94	ASN	5.0
2	H	85	THR	4.3
2	H	82	ARG	4.3
2	H	10	LEU	4.1
1	C	47	ALA	4.0
4	M	286	GLY	4.0
2	H	9	HIS	3.7
1	C	49	GLY	3.6
2	H	83	PRO	3.5
2	H	93	THR	3.4
2	H	45	GLU	3.3
2	H	81	ARG	3.3
1	C	218	LYS	3.2
4	M	320	GLY	3.1
3	L	13	GLY	3.1
1	C	135	CYS	3.1
1	C	208	ALA	3.0
3	L	51	TYR	3.0
4	M	16	HIS	3.0
2	H	258	LEU	2.9
3	L	54	SER	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	64	ASN	2.9
1	C	32	LYS	2.9
3	L	203	GLY	2.8
1	C	48	GLU	2.8
1	C	291	ALA	2.8
2	H	173	VAL	2.8
2	H	63	PRO	2.7
3	L	204	ASP	2.7
3	L	12	ARG	2.6
2	H	78	VAL	2.6
2	H	105	GLY	2.6
1	C	56	TYR	2.6
3	L	67	ASN	2.6
4	M	76	GLU	2.6
2	H	74	GLY	2.6
2	H	95	GLY	2.6
1	C	145	VAL	2.6
2	H	119	GLU	2.5
3	L	61	PRO	2.4
2	H	7	ALA	2.4
2	H	84	GLU	2.4
1	C	159	THR	2.4
4	M	101	GLY	2.4
4	M	287	THR	2.4
3	L	55	GLN	2.4
2	H	248	TYR	2.3
2	H	87	GLU	2.3
2	H	96	PHE	2.3
3	L	11	VAL	2.3
2	H	12	ILE	2.3
2	H	65	PRO	2.3
1	C	44	ALA	2.3
1	C	173	VAL	2.3
1	C	37	GLN	2.2
3	L	115	TRP	2.2
2	H	64	TYR	2.2
1	C	155	ASN	2.2
2	H	256	SER	2.2
1	C	3	GLU	2.2
3	L	21	LEU	2.2
1	C	214	VAL	2.2
2	H	226	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	17	TRP	2.2
1	C	52	VAL	2.1
3	L	73	TYR	2.1
4	M	17	ILE	2.1
2	H	91	ALA	2.1
3	L	1	ALA	2.1
1	C	40	PRO	2.1
2	H	27	VAL	2.1
1	C	59	VAL	2.1
1	C	1	CYS	2.1
3	L	53	ALA	2.1
2	H	176	SER	2.0
2	H	25	TRP	2.0
2	H	188	ALA	2.0
1	C	5	PRO	2.0
3	L	25	TRP	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
2	FME	H	1	10/11	0.66	0.21	67,67,68,68	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	MQ7	M	1328	48/48	0.84	0.19	39,41,47,48	0

Continued on next page...

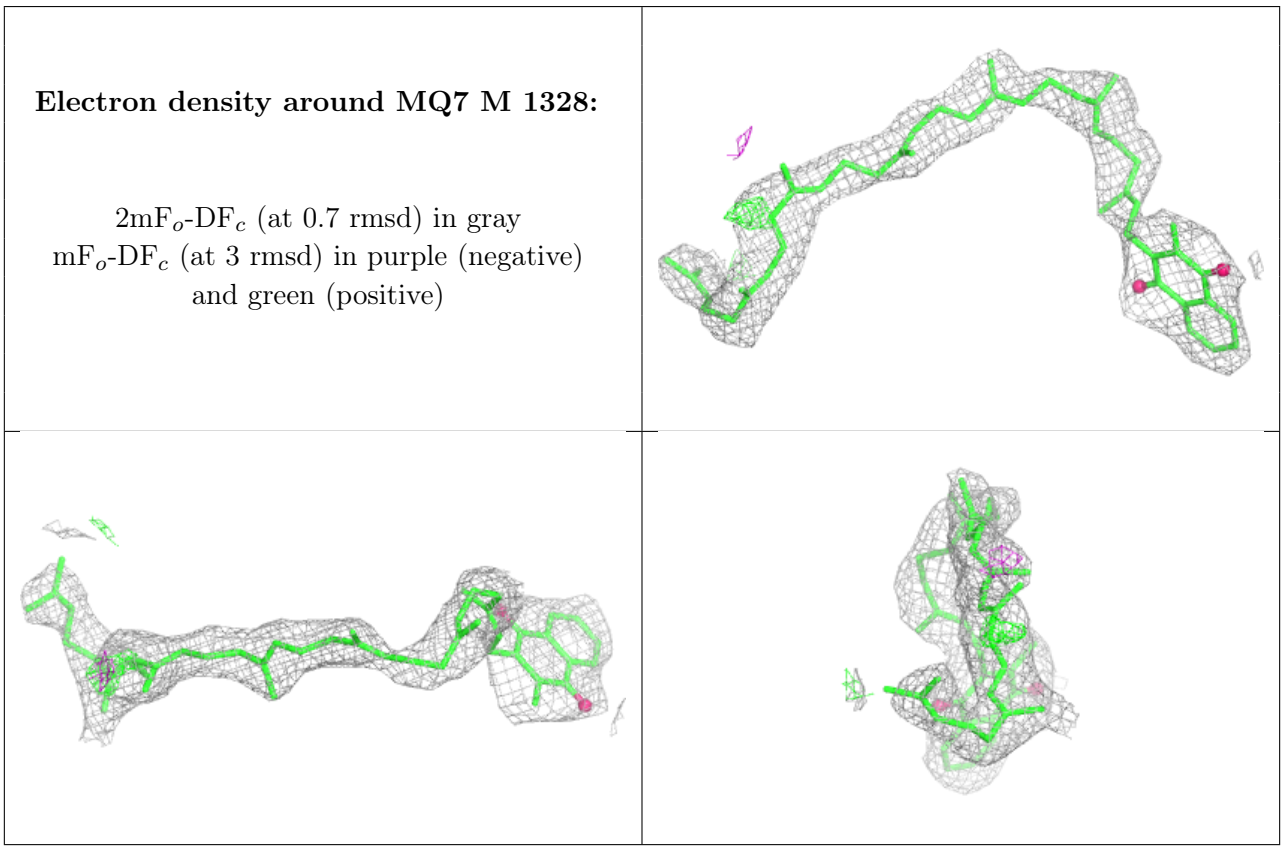
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	BCB	M	1324	65/66	0.89	0.15	18,20,48,49	0
7	BPB	M	1326	61/65	0.90	0.13	19,24,44,45	0
6	BCB	L	1275	66/66	0.91	0.13	18,21,28,28	0
7	BPB	L	1276	65/65	0.91	0.14	23,28,33,35	0
6	BCB	M	1325	66/66	0.92	0.13	15,18,26,27	0
5	HEC	C	1334	43/43	0.93	0.13	27,29,34,36	0
5	HEC	C	1333	43/43	0.94	0.12	25,32,33,34	0
6	BCB	L	1274	66/66	0.94	0.11	10,12,20,21	0
5	HEC	C	1336	43/43	0.95	0.13	25,28,33,34	0
5	HEC	C	1335	43/43	0.95	0.10	20,21,23,24	0
8	FE2	M	1327	1/1	0.98	0.02	24,24,24,24	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.

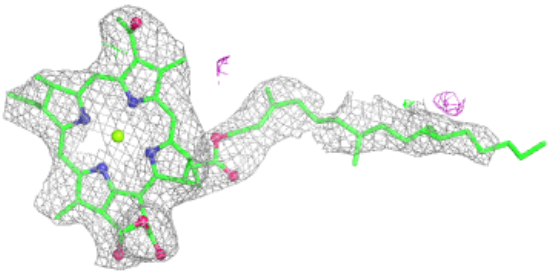
Electron density around MQ7 M 1328:

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

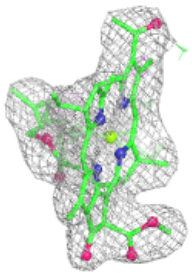


Electron density around BCB M 1324:

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

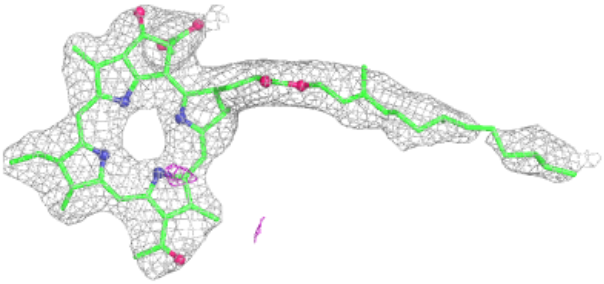


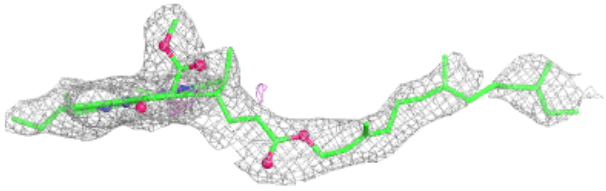


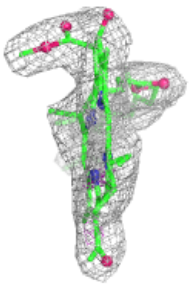


Electron density around BPB M 1326:

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

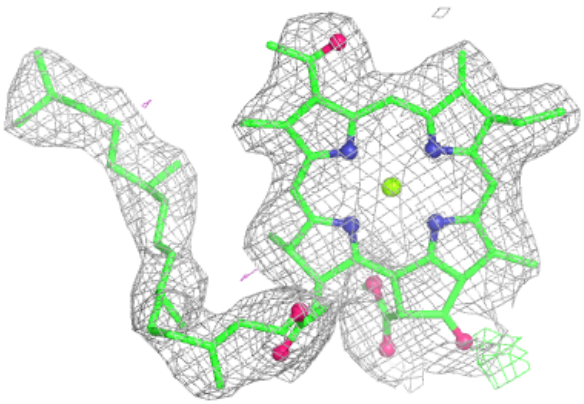


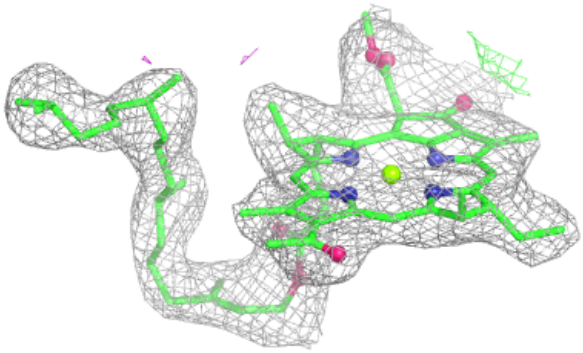


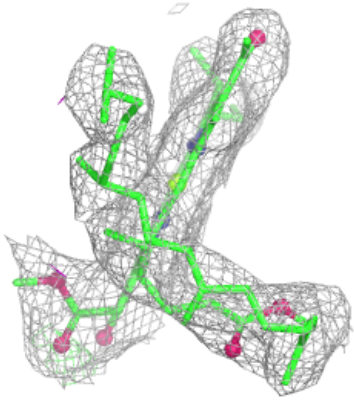


Electron density around BCB L 1275:

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

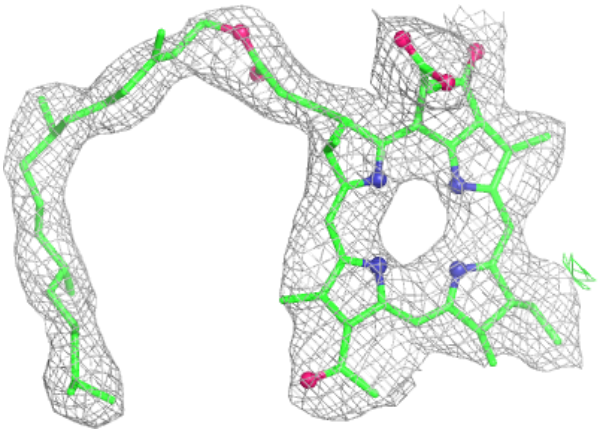


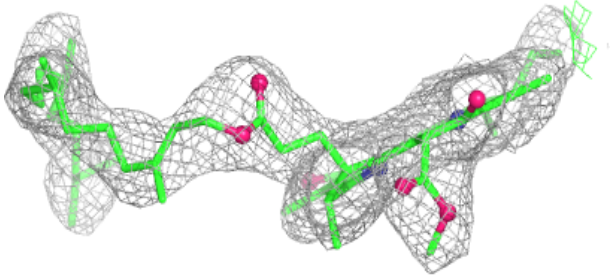


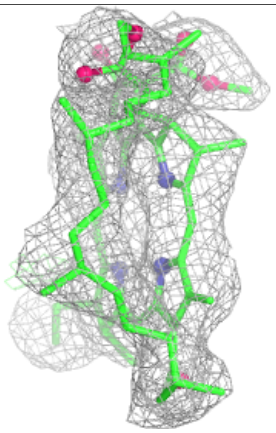


Electron density around BPB L 1276:

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

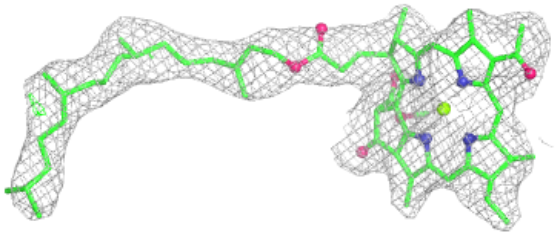


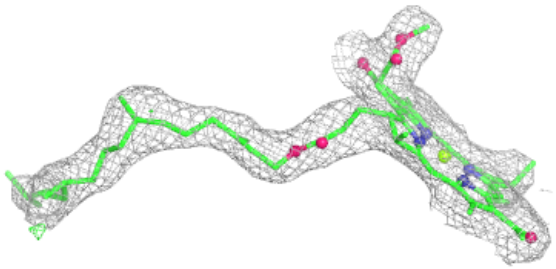


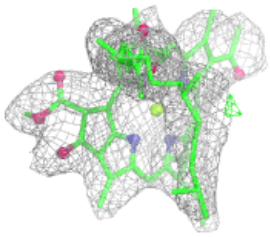


Electron density around BCB M 1325:

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

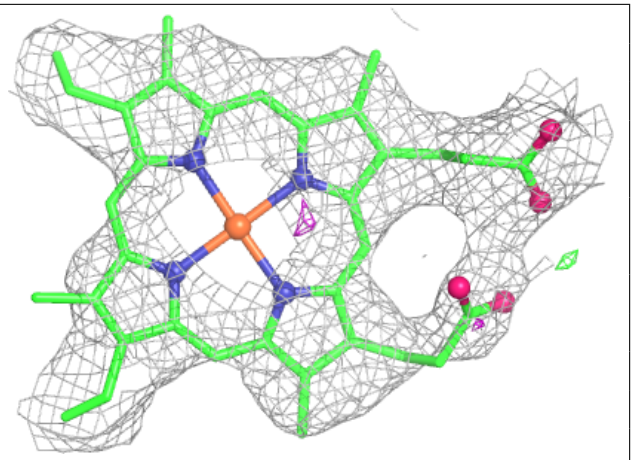


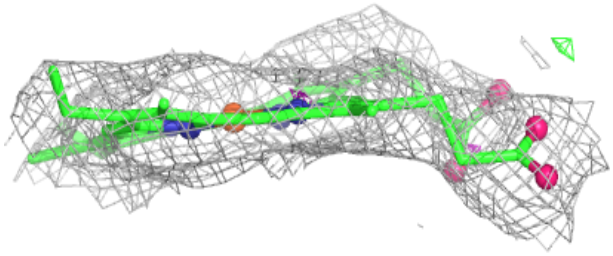


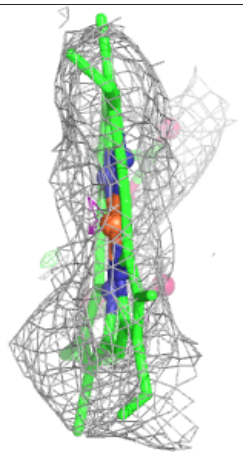


Electron density around HEC C 1334:

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

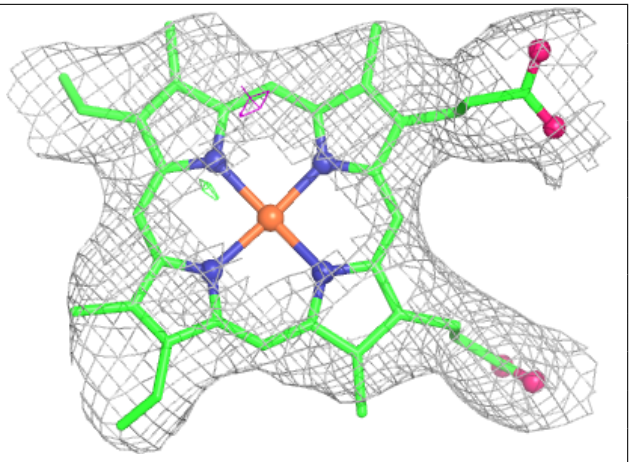


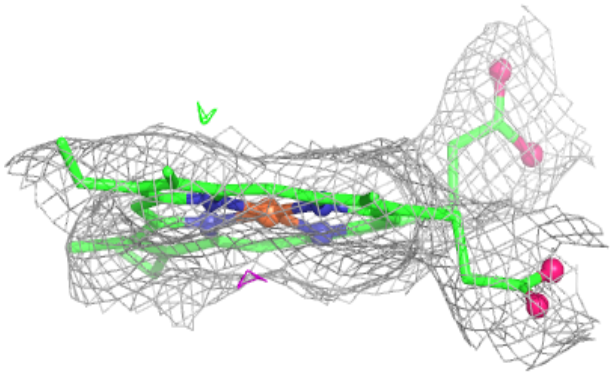


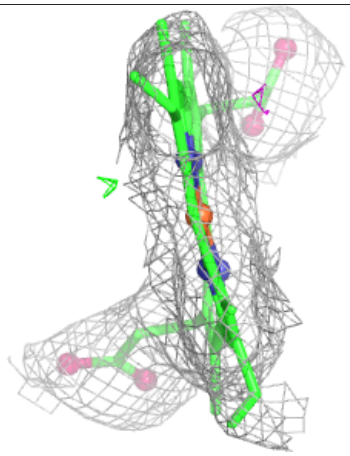


Electron density around HEC C 1333:

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

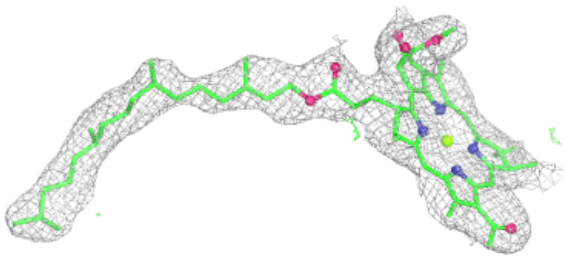


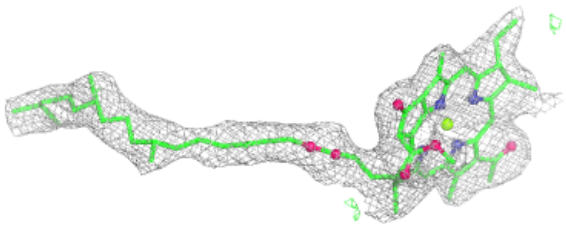


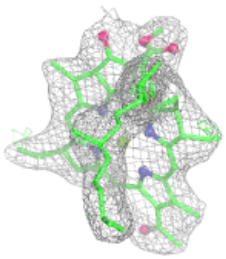


Electron density around BCB L 1274:

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

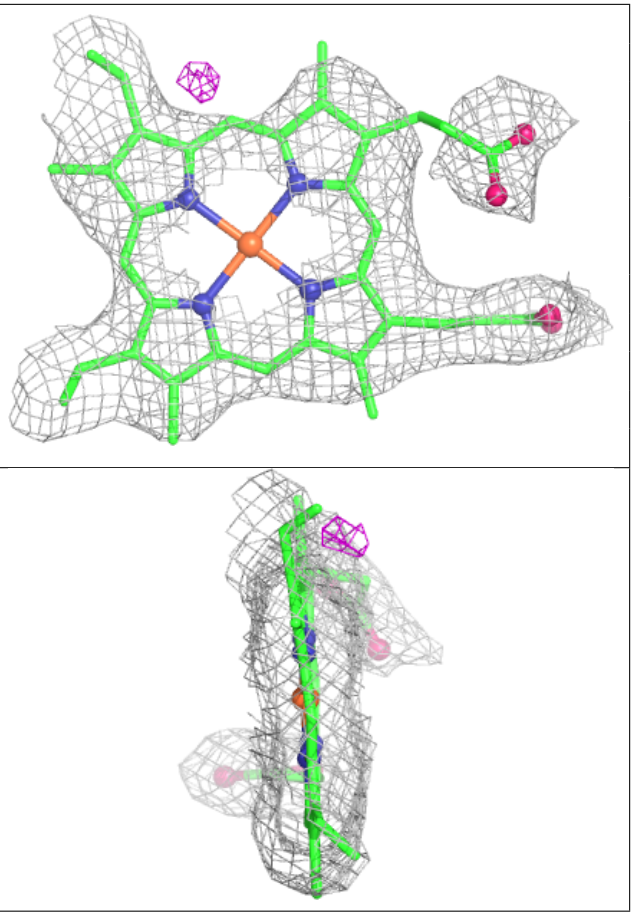






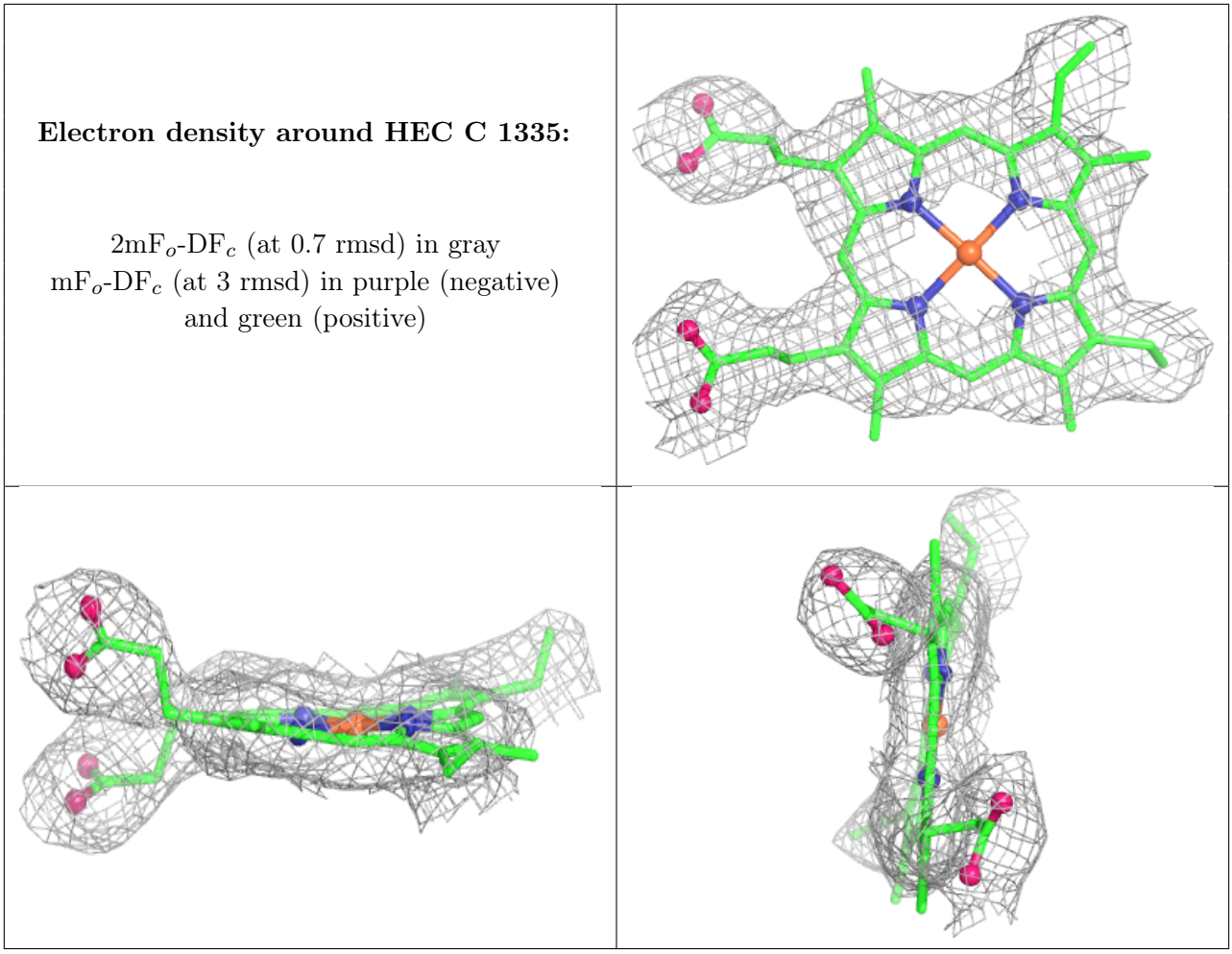
Electron density around HEC C 1336:

$2mF_o$-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 1335:

$2mF_o$-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.