Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 07:39 PM EDT

PDB ID	:	2X5V
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 (i)) were used in the production of this report:

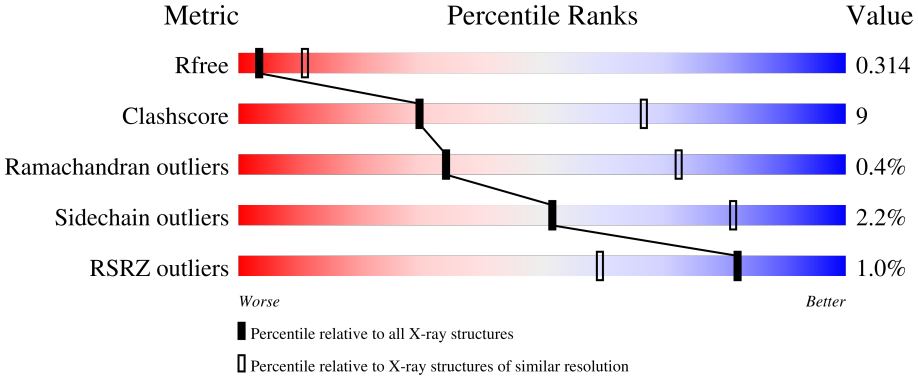
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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	84% 14% ••
2	H	258	3% 79% 14% •• 6%
3	L	274	75% 24%
4	M	324	81% 18% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	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

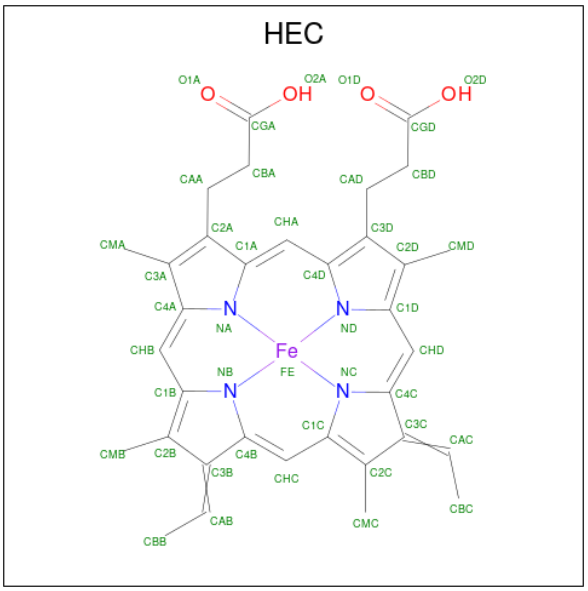
- Molecule 3 is a protein called REACTION CENTER PROTEIN L CHAIN.

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.

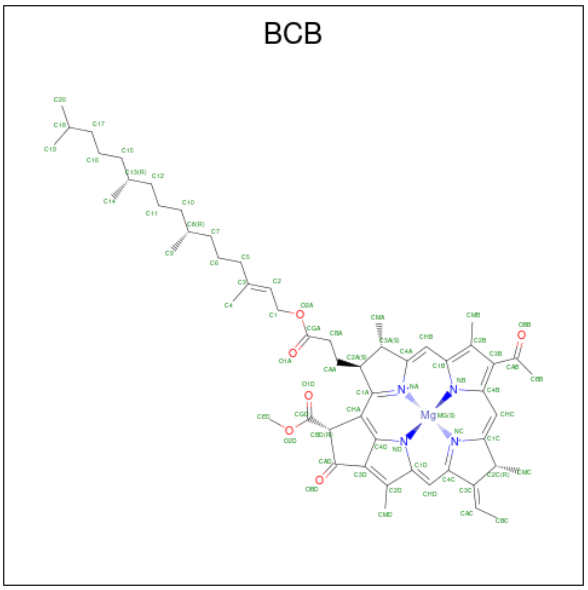
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	M	323	2555	1702	419	423	11	7	0	0

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



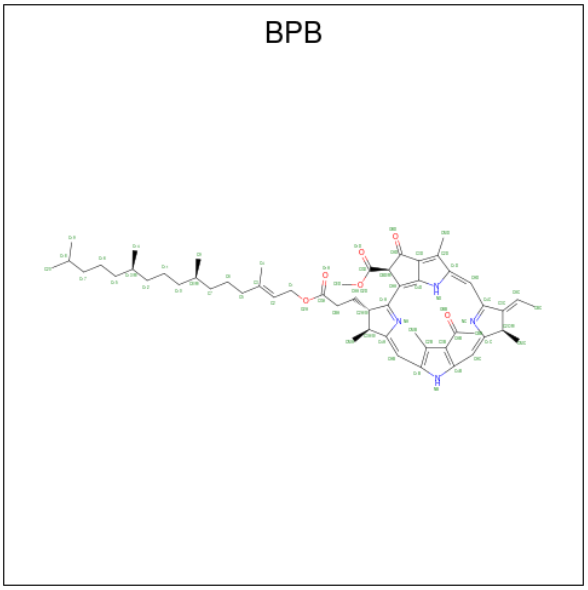
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	C	1	43	34	1	4	4	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
6	L	1	66	55	1	4	6	0	0
6	L	1	66	55	1	4	6	0	0
6	M	1	65	54	1	4	6	0	0
6	M	1	66	55	1	4	6	0	0

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

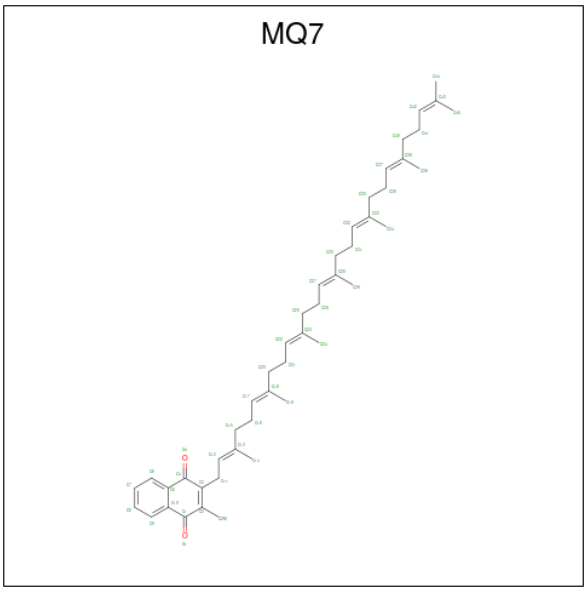


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	L	1	65	55	4	6	0	0
7	M	1	61	51	4	6	0	0

- Molecule 8 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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



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

- Molecule 10 is water.

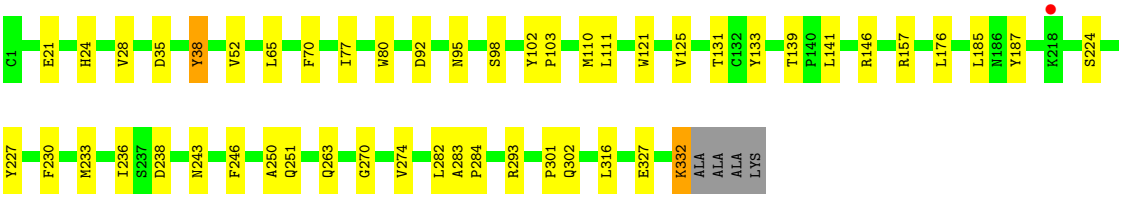
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	L	1	1	1	0	0
			Total	O		
10	M	1	1	1	0	0

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.

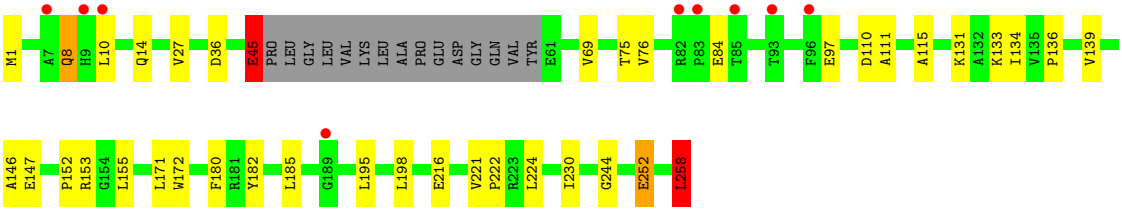
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT

Chain C:



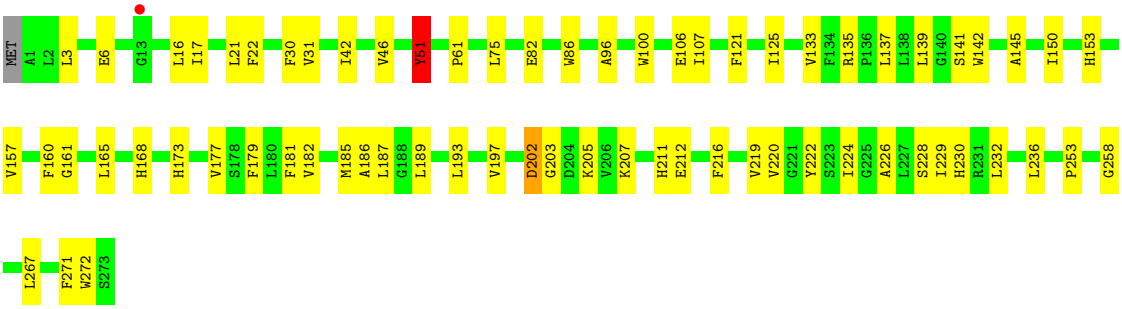
• Molecule 2: REACTION CENTER PROTEIN H CHAIN

Chain H:



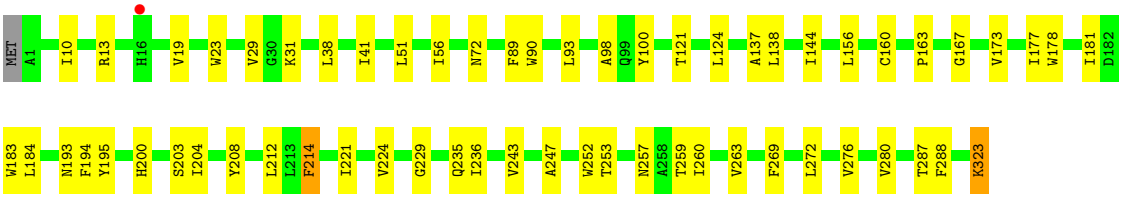
• Molecule 3: REACTION CENTER PROTEIN L CHAIN

Chain L:



• Molecule 4: REACTION CENTER PROTEIN M CHAIN

Chain M:


MET
A1
I10
R13
H16
V19
W23
V29
G30
K31
L38
I41
L51
I56
N72
F89
W90
L93
A98
Q99
Y100
T121
L124
A137
L138
I144
L156
C160
P163
G167
V173
I177
W178
I181
D182
W183
L184
N193
F194
Y195
H200
S203
I204
Y208
L212
L213
F214
I221
V224
G229
Q235
I236
V243
A247
W252
T253
N257
A258
T259
I260
V263
F269
L272
V276
V280
T287
F288
K323

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) 90.6 (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)	0.30 , 34.2	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	0.75	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 (i)

5.1 Standard geometry (i)

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

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	0.73	1/2669 (0.0%)	0.56	1/3637 (0.0%)
2	H	1.37	7/1939 (0.4%)	0.90	9/2646 (0.3%)
3	L	1.16	2/2291 (0.1%)	1.02	4/3127 (0.1%)
4	M	0.71	2/2659 (0.1%)	0.56	3/3637 (0.1%)
All	All	1.00	12/9558 (0.1%)	0.76	17/13047 (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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	51	TYR	CB-CG	42.20	2.15	1.51
2	H	216	GLU	CB-CG	40.41	2.29	1.52
1	C	332	LYS	CB-CG	31.18	2.36	1.52
3	L	202	ASP	CB-CG	29.64	2.13	1.51
2	H	131	LYS	CD-CE	23.83	2.10	1.51
4	M	323	LYS	CB-CG	23.05	2.14	1.52
2	H	147	GLU	CG-CD	-22.75	1.17	1.51
4	M	31	LYS	CG-CD	20.29	2.21	1.52
2	H	258	LEU	CB-CG	16.11	1.99	1.52
2	H	45	GLU	CG-CD	13.73	1.72	1.51
2	H	84	GLU	CB-CG	10.55	1.72	1.52
2	H	252	GLU	CG-CD	5.93	1.60	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	51	TYR	CB-CG-CD2	-36.12	99.33	121.00
3	L	51	TYR	CB-CG-CD1	28.92	138.35	121.00
2	H	97	GLU	CA-CB-CG	-23.31	62.13	113.40
2	H	45	GLU	CG-CD-OE1	-16.25	85.80	118.30
2	H	97	GLU	CB-CG-CD	-13.54	77.64	114.20
3	L	202	ASP	CB-CG-OD2	13.17	130.15	118.30
4	M	31	LYS	CB-CG-CD	-12.94	77.97	111.60
2	H	216	GLU	CA-CB-CG	-11.18	88.81	113.40
2	H	84	GLU	CB-CG-CD	-10.34	86.27	114.20
3	L	202	ASP	CB-CG-OD1	-10.18	109.14	118.30
4	M	31	LYS	CG-CD-CE	-7.08	90.67	111.90
4	M	323	LYS	CA-CB-CG	-6.86	98.32	113.40
2	H	45	GLU	CB-CG-CD	6.59	132.00	114.20
2	H	258	LEU	CB-CG-CD2	-5.94	100.90	111.00
2	H	252	GLU	CB-CG-CD	5.77	129.78	114.20
1	C	332	LYS	CB-CG-CD	5.20	125.12	111.60
2	H	216	GLU	CB-CG-CD	5.06	127.85	114.20

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	35	0
2	H	1906	0	1903	27	0
3	L	2196	0	2120	59	0
4	M	2555	0	2452	50	0
5	C	172	0	120	16	0
6	L	132	0	144	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	131	0	140	10	0
7	L	65	0	74	6	0
7	M	61	0	63	5	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	183	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 (183) 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:NE2	6:L:1274:BCB:HMC2	1.85	0.92
3:L:177:VAL:HG13	6:L:1274:BCB:HMB3	1.59	0.84
3:L:121:PHE:CE2	3:L:125:ILE:HD11	2.17	0.80
5:C:1334:HEC:HBB3	5:C:1334:HEC:HMB1	1.66	0.76
6:L:1274:BCB:CBB	6:L:1274:BCB:HMB1	2.15	0.75
7:L:1276:BPB:HHC	7:L:1276:BPB:HBBB	1.68	0.75
5:C:1333:HEC:HBB3	5:C:1333:HEC:HMB1	1.69	0.73
3:L:168:HIS:CE1	6:L:1274:BCB:HMC2	2.25	0.71
1:C:77:ILE:HD11	1:C:111:LEU:HD21	1.70	0.71
6:L:1274:BCB:HMB1	6:L:1274:BCB:HBB3	1.73	0.70
6:M:1325:BCB:HMB1	6:M:1325:BCB:HBB2	1.73	0.70
5:C:1333:HEC:HBC3	5:C:1333:HEC:HMC1	1.75	0.68
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
6:M:1325:BCB:HMB1	6:M:1325:BCB:CBB	2.25	0.66
2:H:180:PHE:O	2:H:198:LEU:HD12	1.96	0.65
6:L:1275:BCB:HMD1	4:M:204:ILE:HD13	1.78	0.65
4:M:173:VAL:HG22	4:M:183:TRP:CD2	2.32	0.65
4:M:263:VAL:HG21	9:M:1328:MQ7:C1	2.27	0.64
7:L:1276:BPB:HHC	7:L:1276:BPB:CBB	2.27	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
6:L:1275:BCB:CMD	4:M:204:ILE:HD13	2.29	0.62
3:L:193:LEU:HD22	3:L:216:PHE:CE2	2.34	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:L:226:ALA:O	3:L:229:ILE:HG22	2.01	0.61
6:L:1275:BCB:HMB1	6:L:1275:BCB:HBB2	1.83	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
6:L:1275:BCB:HMB1	6:L:1275:BCB:CBB	2.32	0.60
5:C:1336:HEC:HBB3	5:C:1336:HEC:HMB1	1.83	0.59
5:C:1334:HEC:HBC3	5:C:1334:HEC:HMC1	1.85	0.58
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
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
6:L:1275:BCB:HMD1	4:M:204:ILE:CD1	2.36	0.56
6:L:1275:BCB:HMD2	6:M:1325:BCB:HBB3	1.87	0.56
5:C:1335:HEC:HMB1	5:C:1335:HEC:HBB3	1.87	0.55
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:168:HIS:CD2	6:L:1274:BCB:HMC2	2.42	0.54
3:L:267:LEU:HD13	4:M:90:TRP:CH2	2.42	0.54
6:L:1274:BCB:HMB1	6:L:1274:BCB:HBB2	1.90	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
5:C:1336:HEC:HBC3	5:C:1336:HEC:HMC1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:C:131:THR:O	5:C:1334:HEC:HMC3	2.10	0.51
3:L:230:HIS:CD2	4:M:221:ILE:HG13	2.46	0.51
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
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
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: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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:M:41:ILE:HD12	4:M:41:ILE:C	2.35	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
2:H:258:LEU:C	3:L:17:ILE:HG22	2.35	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
6:L:1275:BCB:HMD2	6:M:1325:BCB:CBB	2.46	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: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
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: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
3:L:185:MET:HE3	7:M:1326:BPB:NA	2.33	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:160:PHE:CD2	6:L:1274:BCB:HMD1	2.54	0.43
5:C:1335:HEC:HBC3	5:C:1335:HEC:HMC1	2.01	0.43
1:C:110:MET:HE1	5:C:1334:HEC:C1D	2.49	0.42
3:L:165:LEU:HD12	3:L:258:GLY:HA3	2.01	0.42
3:L:205:LYS:O	3:L:207:LYS:NZ	2.42	0.42
3:L:61:PRO:O	3:L:150:ILE:HD12	2.20	0.42
1:C:282:LEU:HD22	5:C:1334:HEC:HMD2	2.01	0.42
3:L:168:HIS:CE1	6:L:1274:BCB:CMC	3.00	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
1:C:274:VAL:HG22	5:C:1336:HEC:HMC2	2.01	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
1:C:250:ALA:O	1:C:251:GLN:C	2.58	0.42
1:C:282:LEU:CD2	5:C:1334:HEC:HMD2	2.50	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
6:L:1275:BCB:HMB2	7:L:1276:BPB:HMBA	2.02	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
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
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
3:L:30:PHE:HB2	4:M:252:TRP:HB3	2.04	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%)	34	72
3	L	275/274 (100%)	255 (93%)	18 (6%)	2 (1%)	22	60
4	M	321/324 (99%)	303 (94%)	16 (5%)	2 (1%)	25	64
All	All	1165/1192 (98%)	1083 (93%)	77 (7%)	5 (0%)	34	72

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%)	276 (98%)	5 (2%)	59	85
2	H	200/212 (94%)	196 (98%)	4 (2%)	55	83
3	L	221/219 (101%)	215 (97%)	6 (3%)	44	77
4	M	249/250 (100%)	242 (97%)	7 (3%)	43	77
All	All	951/963 (99%)	929 (98%)	22 (2%)	52	80

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	38	TYR
1	C	98	SER
1	C	146	ARG
1	C	238	ASP
1	C	332	LYS
2	H	8	GLN
2	H	45	GLU
2	H	185	LEU
2	H	258	LEU
3	L	51	TYR
3	L	141[A]	SER
3	L	141[B]	SER
3	L	228	SER
3	L	271	PHE
3	L	272	TRP
4	M	144	ILE
4	M	160	CYS
4	M	194	PHE
4	M	203	SER
4	M	212	LEU
4	M	214	PHE
4	M	323	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	58	ASN
1	C	84	GLN
1	C	94	ASN
1	C	302	GLN
1	C	310	GLN
2	H	8	GLN
2	H	14	GLN
2	H	72	HIS
2	H	220	ASN
4	M	108	HIS
4	M	257	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FME	H	1	2	8,9,10	0.80	0	8,9,11	2.86	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
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	O1-CN-N	-2.38	119.16	125.32
2	H	1	FME	CE-SD-CG	2.15	111.43	100.32

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 monosaccharides 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	$\#\|Z\| > 2$
5	HEC	C	1333	1	32,50,50	2.34	5 (15%)	30,82,82	2.05	7 (23%)
5	HEC	C	1336	1	32,50,50	2.32	6 (18%)	30,82,82	1.32	3 (10%)
6	BCB	M	1325	4	63,74,74	2.88	14 (22%)	72,115,115	2.89	26 (36%)
7	BPB	M	1326	-	45,66,70	2.02	8 (17%)	43,96,101	1.94	12 (27%)
6	BCB	M	1324	-	62,73,74	2.81	16 (25%)	70,113,115	2.89	20 (28%)
9	MQ7	M	1328	-	49,49,49	1.41	2 (4%)	61,63,63	1.32	8 (13%)
5	HEC	C	1334	1	32,50,50	2.27	5 (15%)	30,82,82	1.58	6 (20%)
7	BPB	L	1276	-	49,70,70	1.97	9 (18%)	48,101,101	1.89	12 (25%)
6	BCB	L	1274	3	63,74,74	2.82	13 (20%)	72,115,115	2.67	21 (29%)
6	BCB	L	1275	3	63,74,74	2.71	15 (23%)	72,115,115	2.75	19 (26%)
5	HEC	C	1335	1	32,50,50	2.33	5 (15%)	30,82,82	1.62	5 (16%)

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	1333	1	-	2/10/54/54	-
5	HEC	C	1336	1	-	3/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BCB	M	1325	4	3/3/21/26	16/37/137/137	-
7	BPB	M	1326	-	-	14/33/101/105	0/5/6/6
6	BCB	M	1324	-	3/3/20/26	12/36/136/137	-
9	MQ7	M	1328	-	-	3/41/61/61	0/2/2/2
5	HEC	C	1334	1	-	5/10/54/54	-
7	BPB	L	1276	-	-	12/37/105/105	0/5/6/6
6	BCB	L	1274	3	3/3/21/26	7/37/137/137	-
6	BCB	L	1275	3	3/3/21/26	10/37/137/137	-
5	HEC	C	1335	1	-	2/10/54/54	-

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1325	BCB	CHC-C1C	16.73	1.48	1.33
6	L	1274	BCB	CHC-C1C	16.64	1.48	1.33
6	M	1324	BCB	CHC-C1C	15.95	1.48	1.33
6	L	1275	BCB	CHC-C1C	15.18	1.47	1.33
9	M	1328	MQ7	C3-C2	7.65	1.48	1.35
7	L	1276	BPB	C3D-C2D	6.29	1.50	1.39
5	C	1335	HEC	C2B-C3B	-6.28	1.33	1.40
6	L	1274	BCB	CAC-C3C	6.17	1.49	1.33
5	C	1333	HEC	C2B-C3B	-6.13	1.33	1.40
5	C	1333	HEC	C3C-C2C	-6.09	1.33	1.40
5	C	1336	HEC	C2B-C3B	-5.99	1.34	1.40
5	C	1336	HEC	C3C-C2C	-5.86	1.34	1.40
5	C	1334	HEC	C2B-C3B	-5.85	1.34	1.40
7	M	1326	BPB	C3D-C2D	5.82	1.49	1.39
6	L	1275	BCB	CAC-C3C	5.80	1.48	1.33
6	M	1324	BCB	CAC-C3C	5.77	1.48	1.33
6	M	1325	BCB	CAC-C3C	5.73	1.48	1.33
6	M	1325	BCB	O2D-CGD	5.68	1.47	1.33
7	M	1326	BPB	O2D-CGD	5.60	1.47	1.33
5	C	1335	HEC	C3D-C2D	5.55	1.54	1.37
5	C	1334	HEC	C3C-C2C	-5.53	1.34	1.40
6	M	1324	BCB	O2D-CGD	5.53	1.46	1.33
6	L	1274	BCB	O2D-CGD	5.50	1.46	1.33
5	C	1333	HEC	C3D-C2D	5.39	1.53	1.37
5	C	1334	HEC	C3D-C2D	5.27	1.53	1.37
6	L	1275	BCB	O2D-CGD	5.22	1.46	1.33
5	C	1335	HEC	C3C-C2C	-5.20	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1336	HEC	C3D-C2D	5.07	1.52	1.37
7	L	1276	BPB	O2D-CGD	5.04	1.45	1.33
7	L	1276	BPB	OBD-CAD	4.97	1.28	1.22
9	M	1328	MQ7	C10-C5	4.90	1.48	1.40
7	L	1276	BPB	C3B-C2B	4.85	1.47	1.39
7	M	1326	BPB	CHA-CBD	-4.76	1.47	1.52
6	L	1275	BCB	O2A-CGA	4.73	1.47	1.33
7	L	1276	BPB	CHA-CBD	-4.66	1.47	1.52
7	M	1326	BPB	O2A-CGA	4.62	1.46	1.33
6	M	1325	BCB	O2A-CGA	4.61	1.46	1.33
7	M	1326	BPB	OBD-CAD	4.56	1.28	1.22
6	M	1325	BCB	C2C-C3C	-4.55	1.45	1.51
6	L	1274	BCB	C3B-C2B	4.53	1.47	1.39
6	M	1324	BCB	O2A-CGA	4.45	1.46	1.33
7	M	1326	BPB	C3B-C2B	4.38	1.47	1.39
6	L	1275	BCB	CHD-C1D	4.33	1.46	1.38
6	L	1275	BCB	C3B-C2B	4.26	1.46	1.39
6	L	1274	BCB	CHD-C1D	4.21	1.46	1.38
5	C	1334	HEC	CBB-CAB	-4.19	1.33	1.49
5	C	1335	HEC	CBC-CAC	-4.19	1.34	1.49
6	M	1324	BCB	C2C-C3C	-4.19	1.46	1.51
5	C	1335	HEC	CBB-CAB	-4.18	1.34	1.49
6	L	1274	BCB	O2A-CGA	4.16	1.45	1.33
6	M	1324	BCB	CHD-C1D	4.15	1.46	1.38
5	C	1333	HEC	CBC-CAC	-4.14	1.34	1.49
6	M	1325	BCB	OBD-CAD	4.12	1.29	1.22
5	C	1333	HEC	CBB-CAB	-4.12	1.34	1.49
5	C	1334	HEC	CBC-CAC	-4.12	1.34	1.49
6	L	1275	BCB	C2C-C3C	-4.10	1.46	1.51
7	L	1276	BPB	O2A-CGA	4.08	1.45	1.33
6	M	1324	BCB	C3B-C2B	4.04	1.46	1.39
6	M	1325	BCB	C3B-C2B	4.04	1.46	1.39
5	C	1336	HEC	CBC-CAC	-4.03	1.34	1.49
5	C	1336	HEC	CBB-CAB	-4.02	1.34	1.49
6	M	1325	BCB	CHD-C1D	3.93	1.46	1.38
6	M	1325	BCB	C1D-ND	-3.82	1.32	1.37
6	M	1324	BCB	CHD-C4C	3.79	1.47	1.39
6	M	1324	BCB	C1D-ND	-3.75	1.32	1.37
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	3.51	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1324	BCB	C3D-C2D	3.51	1.48	1.39
6	L	1275	BCB	CHD-C4C	3.48	1.47	1.39
6	L	1274	BCB	CHD-C4C	3.45	1.47	1.39
7	M	1326	BPB	C4C-NC	-3.37	1.27	1.37
6	L	1274	BCB	OBD-CAD	3.32	1.28	1.22
6	M	1325	BCB	C3D-C2D	3.31	1.48	1.39
6	L	1275	BCB	C3D-C2D	3.30	1.48	1.39
7	L	1276	BPB	C4C-NC	-3.27	1.27	1.37
6	M	1325	BCB	CHD-C4C	3.22	1.46	1.39
6	L	1275	BCB	C1D-ND	-3.10	1.33	1.37
6	L	1274	BCB	C1D-ND	-3.06	1.33	1.37
6	M	1325	BCB	MG-NA	-2.99	1.99	2.06
6	M	1325	BCB	C4B-CHC	2.91	1.49	1.41
6	L	1274	BCB	C4B-CHC	2.88	1.49	1.41
6	L	1275	BCB	C4B-CHC	2.81	1.48	1.41
6	M	1324	BCB	C4B-CHC	2.46	1.47	1.41
7	L	1276	BPB	C3A-C2A	-2.46	1.52	1.54
6	L	1275	BCB	MG-NA	-2.44	2.00	2.06
6	M	1324	BCB	MG-NA	-2.42	2.00	2.06
7	M	1326	BPB	C3A-C2A	-2.42	1.52	1.54
6	M	1324	BCB	C4C-C3C	2.36	1.49	1.44
6	M	1324	BCB	C4D-CHA	2.31	1.46	1.38
6	L	1274	BCB	C4D-CHA	2.21	1.46	1.38
7	L	1276	BPB	CBD-CGD	-2.20	1.49	1.52
5	C	1336	HEC	CAA-C2A	2.19	1.56	1.52
6	M	1325	BCB	C4D-CHA	2.16	1.45	1.38
6	L	1275	BCB	C3D-C4D	-2.10	1.39	1.44
6	M	1324	BCB	C3D-C4D	-2.08	1.39	1.44
6	L	1275	BCB	C4D-CHA	2.08	1.45	1.38

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	1324	BCB	C1C-NC-C4C	-15.28	99.71	106.68
6	M	1325	BCB	C1C-NC-C4C	-15.28	99.71	106.68
6	L	1275	BCB	C1C-NC-C4C	-14.96	99.85	106.68
6	L	1274	BCB	C1C-NC-C4C	-13.70	100.43	106.68
7	L	1276	BPB	O2D-CGD-CBD	8.65	120.45	110.95
6	L	1274	BCB	C4D-C3D-CAD	-7.70	99.74	108.11
7	M	1326	BPB	O2D-CGD-CBD	7.31	118.98	110.95
6	M	1324	BCB	C4D-C3D-CAD	-7.17	100.32	108.11
5	C	1333	HEC	CBD-CAD-C3D	-6.55	101.53	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	1325	BCB	CMD-C2D-C1D	6.49	136.16	124.73
6	L	1275	BCB	C4D-C3D-CAD	-6.31	101.25	108.11
6	L	1275	BCB	CMD-C2D-C1D	6.18	135.62	124.73
6	M	1325	BCB	C4D-C3D-CAD	-5.92	101.68	108.11
6	M	1324	BCB	C3D-C4D-ND	5.88	119.54	109.99
6	M	1324	BCB	O2D-CGD-CBD	5.86	121.47	111.23
6	M	1325	BCB	C3D-C4D-ND	5.71	119.27	109.99
6	L	1275	BCB	C3D-C4D-ND	5.60	119.09	109.99
6	M	1325	BCB	O2D-CGD-CBD	5.58	120.99	111.23
6	M	1324	BCB	CMD-C2D-C1D	5.54	134.49	124.73
6	L	1275	BCB	O2D-CGD-CBD	5.22	120.35	111.23
6	L	1274	BCB	C3D-C4D-ND	5.20	118.43	109.99
6	M	1325	BCB	C1D-ND-C4D	-4.68	103.03	106.31
6	L	1274	BCB	CMD-C2D-C1D	4.61	132.84	124.73
6	M	1324	BCB	C1D-ND-C4D	-4.35	103.26	106.31
6	M	1325	BCB	CMD-C2D-C3D	-4.32	117.77	127.69
6	L	1275	BCB	C2C-C1C-CHC	-4.32	113.58	123.70
6	M	1324	BCB	C2C-C1C-CHC	-4.31	113.58	123.70
6	L	1275	BCB	CMD-C2D-C3D	-4.29	117.85	127.69
6	M	1325	BCB	C4A-NA-C1A	4.09	108.54	106.68
6	L	1275	BCB	C1D-ND-C4D	-3.96	103.53	106.31
6	L	1274	BCB	C4-C3-C5	3.94	122.08	115.23
6	M	1324	BCB	CMD-C2D-C3D	-3.86	118.84	127.69
6	L	1274	BCB	C2C-C1C-CHC	-3.82	114.74	123.70
6	L	1274	BCB	C1D-ND-C4D	-3.75	103.68	106.31
7	M	1326	BPB	CMD-C2D-C3D	-3.75	117.20	124.68
6	M	1325	BCB	C2C-C1C-CHC	-3.62	115.22	123.70
5	C	1335	HEC	CBB-CAB-C3B	-3.58	119.11	127.49
6	L	1274	BCB	C1-C2-C3	-3.55	120.38	126.20
6	M	1324	BCB	CHB-C4A-NA	3.54	129.51	124.40
6	M	1325	BCB	CBC-CAC-C3C	-3.34	117.63	126.70
6	M	1325	BCB	CHB-C4A-NA	3.32	129.19	124.40
5	C	1335	HEC	CBC-CAC-C3C	-3.32	119.73	127.49
6	L	1275	BCB	OBD-CAD-C3D	-3.30	120.70	128.42
5	C	1334	HEC	CBB-CAB-C3B	-3.29	119.79	127.49
6	L	1275	BCB	CHB-C4A-NA	3.28	129.14	124.40
5	C	1333	HEC	CBC-CAC-C3C	-3.27	119.83	127.49
6	L	1274	BCB	CHA-C4D-ND	-3.27	125.81	132.55
6	M	1324	BCB	OBD-CAD-C3D	-3.25	120.83	128.42
6	L	1274	BCB	O2D-CGD-CBD	3.20	116.82	111.23
5	C	1333	HEC	CBB-CAB-C3B	-3.17	120.08	127.49
7	L	1276	BPB	CMD-C2D-C3D	-3.15	118.40	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	1325	BCB	C1-C2-C3	-3.12	121.09	126.20
6	M	1324	BCB	CHA-C4D-ND	-3.11	126.14	132.55
7	M	1326	BPB	C1A-C2A-C3A	-3.10	99.89	102.84
6	L	1274	BCB	CMD-C2D-C3D	-3.09	120.60	127.69
6	L	1274	BCB	CBC-CAC-C3C	-3.08	118.35	126.70
6	L	1274	BCB	CED-O2D-CGD	3.06	122.86	115.92
6	M	1324	BCB	O2D-CGD-O1D	-3.06	117.89	123.85
7	M	1326	BPB	CED-O2D-CGD	3.05	122.84	115.92
6	M	1325	BCB	CMB-C2B-C3B	3.04	130.76	124.68
7	L	1276	BPB	O1D-CGD-CBD	-3.04	120.11	124.72
6	M	1325	BCB	C4-C3-C5	3.03	120.48	115.23
6	L	1275	BCB	CBC-CAC-C3C	-2.98	118.61	126.70
7	L	1276	BPB	C1A-C2A-C3A	-2.97	100.02	102.84
6	M	1324	BCB	C1B-CHB-C4A	-2.96	124.39	130.04
6	L	1274	BCB	OBD-CAD-C3D	-2.94	121.54	128.42
6	L	1275	BCB	CMB-C2B-C3B	2.92	130.51	124.68
6	M	1325	BCB	CHA-C4D-ND	-2.90	126.57	132.55
5	C	1336	HEC	CBC-CAC-C3C	-2.88	120.74	127.49
6	L	1274	BCB	CHB-C4A-NA	2.84	128.50	124.40
6	L	1275	BCB	C2A-C1A-CHA	-2.84	118.94	123.87
5	C	1335	HEC	CMC-C2C-C1C	-2.82	124.33	128.46
7	M	1326	BPB	C3D-CAD-CBD	2.82	111.31	107.61
7	M	1326	BPB	O1D-CGD-CBD	-2.79	120.49	124.72
9	M	1328	MQ7	C24-C23-C25	2.78	120.06	115.23
6	L	1275	BCB	CHA-C4D-ND	-2.77	126.83	132.55
6	L	1274	BCB	CMB-C2B-C3B	2.76	130.20	124.68
7	M	1326	BPB	C4-C3-C5	2.76	120.02	115.23
6	M	1325	BCB	O2D-CGD-O1D	-2.75	118.50	123.85
6	M	1324	BCB	CBC-CAC-C3C	-2.74	119.26	126.70
6	L	1275	BCB	O2A-CGA-CBA	2.72	120.14	111.83
9	M	1328	MQ7	C11-C3-C2	-2.70	120.26	124.89
9	M	1328	MQ7	C2M-C2-C3	-2.68	120.04	124.45
6	L	1275	BCB	C1-O2A-CGA	2.68	123.13	116.65
7	L	1276	BPB	CMB-C2B-C3B	2.67	130.01	124.68
5	C	1334	HEC	CBC-CAC-C3C	-2.65	121.29	127.49
5	C	1333	HEC	CBA-CAA-C2A	-2.65	108.19	112.55
9	M	1328	MQ7	C39-C38-C40	2.62	119.77	115.23
6	M	1324	BCB	C2A-C1A-CHA	-2.57	119.41	123.87
7	L	1276	BPB	C3D-CAD-CBD	2.52	110.92	107.61
6	M	1325	BCB	O2A-CGA-CBA	2.51	119.48	111.83
5	C	1336	HEC	CBB-CAB-C3B	-2.48	121.70	127.49
6	M	1325	BCB	C1-O2A-CGA	2.47	122.64	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1333	HEC	CMB-C2B-C1B	-2.47	124.84	128.46
5	C	1333	HEC	O2D-CGD-CBD	2.46	121.77	114.00
6	L	1274	BCB	CAA-C2A-C1A	2.43	119.95	111.97
6	M	1325	BCB	OBD-CAD-C3D	-2.42	122.75	128.42
6	L	1274	BCB	C4B-CHC-C1C	-2.42	125.43	130.04
5	C	1334	HEC	CMB-C2B-C1B	-2.39	124.96	128.46
5	C	1334	HEC	C1D-C2D-C3D	-2.39	105.34	107.00
5	C	1333	HEC	O1D-CGD-CBD	-2.38	115.53	123.09
6	L	1275	BCB	O2D-CGD-O1D	-2.38	119.21	123.85
9	M	1328	MQ7	C29-C28-C30	2.36	119.33	115.23
5	C	1335	HEC	CBA-CAA-C2A	-2.36	108.66	112.55
5	C	1334	HEC	CBD-CAD-C3D	-2.35	108.58	112.54
6	M	1324	BCB	CMB-C2B-C3B	2.34	129.37	124.68
5	C	1335	HEC	C1D-C2D-C3D	-2.33	105.38	107.00
6	L	1274	BCB	CHD-C4C-C3C	-2.32	123.00	125.91
9	M	1328	MQ7	C14-C13-C15	2.29	119.21	115.23
7	M	1326	BPB	C1-C2-C3	-2.29	122.45	126.20
7	L	1276	BPB	O2D-CGD-O1D	-2.28	119.41	123.85
7	M	1326	BPB	C4A-C3A-C2A	-2.28	100.67	102.84
6	M	1324	BCB	O2A-CGA-CBA	2.27	118.77	111.83
6	L	1274	BCB	C1B-CHB-C4A	-2.27	125.72	130.04
9	M	1328	MQ7	C21-C22-C23	-2.27	122.44	127.62
7	L	1276	BPB	O2A-CGA-O1A	-2.26	117.97	123.63
6	M	1325	BCB	CAA-C2A-C1A	2.26	119.37	111.97
7	M	1326	BPB	OBD-CAD-CBD	-2.25	122.52	125.82
6	M	1324	BCB	CED-O2D-CGD	2.25	121.02	115.92
6	M	1325	BCB	CED-O2D-CGD	2.25	121.02	115.92
6	M	1324	BCB	C4A-NA-C1A	2.24	107.70	106.68
7	M	1326	BPB	C1-O2A-CGA	2.21	122.00	116.65
7	L	1276	BPB	O2A-CGA-CBA	2.20	118.54	111.83
7	L	1276	BPB	C6-C7-C8	-2.18	108.70	115.97
6	L	1275	BCB	C1B-CHB-C4A	-2.14	125.96	130.04
6	M	1325	BCB	CHD-C1D-ND	-2.13	121.80	124.80
5	C	1334	HEC	C3B-C4B-NB	-2.12	106.94	110.94
5	C	1336	HEC	CMB-C2B-C1B	-2.09	125.40	128.46
6	L	1275	BCB	O1D-CGD-CBD	-2.08	120.42	124.52
7	L	1276	BPB	OBD-CAD-CBD	-2.07	122.78	125.82
6	M	1325	BCB	C2D-C1D-ND	2.06	112.17	110.13
7	M	1326	BPB	O2A-CGA-CBA	2.06	118.12	111.83
6	M	1325	BCB	C4D-CHA-C1A	2.05	123.69	121.24
6	M	1325	BCB	O1D-CGD-CBD	-2.05	120.48	124.52
6	M	1324	BCB	C1-O2A-CGA	2.03	121.58	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	1274	BCB	CGD-CBD-CAD	-2.02	104.30	110.85
6	M	1325	BCB	CHD-C4C-C3C	-2.01	123.39	125.91
9	M	1328	MQ7	C31-C32-C33	-2.01	123.03	127.62
7	L	1276	BPB	CMA-C3A-C4A	-2.01	110.28	114.61

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	L	1274	BCB	NC
6	L	1274	BCB	NA
6	L	1274	BCB	ND
6	L	1275	BCB	NC
6	L	1275	BCB	NA
6	L	1275	BCB	ND
6	M	1324	BCB	NC
6	M	1324	BCB	NA
6	M	1324	BCB	ND
6	M	1325	BCB	NC
6	M	1325	BCB	NA
6	M	1325	BCB	ND

All (86) 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	1275	BCB	C2C-C3C-CAC-CBC
6	L	1275	BCB	C4C-C3C-CAC-CBC
6	L	1275	BCB	CHA-CBD-CGD-O1D
6	L	1275	BCB	CHA-CBD-CGD-O2D
6	M	1324	BCB	C2C-C3C-CAC-CBC
6	M	1324	BCB	C4C-C3C-CAC-CBC
6	M	1324	BCB	CHA-CBD-CGD-O1D
6	M	1324	BCB	CHA-CBD-CGD-O2D
6	M	1325	BCB	C2C-C3C-CAC-CBC
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

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Mol	Chain	Res	Type	Atoms
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
7	M	1326	BPB	CBD-CGD-O2D-CED
6	L	1274	BCB	C4-C3-C5-C6
6	L	1274	BCB	C2-C3-C5-C6
6	M	1325	BCB	C2A-CAA-CBA-CGA
7	L	1276	BPB	O1D-CGD-O2D-CED
7	M	1326	BPB	O1D-CGD-O2D-CED
6	M	1325	BCB	O1D-CGD-O2D-CED
7	M	1326	BPB	C11-C10-C8-C9
5	C	1334	HEC	C3D-CAD-CBD-CGD
7	L	1276	BPB	C8-C10-C11-C12
7	M	1326	BPB	C5-C6-C7-C8
7	M	1326	BPB	C8-C10-C11-C12
7	L	1276	BPB	CBA-CGA-O2A-C1
6	M	1324	BCB	C10-C11-C12-C13
7	L	1276	BPB	C2-C1-O2A-CGA
6	L	1275	BCB	C16-C17-C18-C19
7	L	1276	BPB	O1A-CGA-O2A-C1
6	L	1275	BCB	C16-C17-C18-C20
6	M	1325	BCB	C5-C6-C7-C8
6	M	1325	BCB	C13-C15-C16-C17
6	M	1325	BCB	C11-C12-C13-C15
7	M	1326	BPB	C11-C12-C13-C14
9	M	1328	MQ7	C38-C40-C41-C42
7	L	1276	BPB	C4-C3-C5-C6
7	L	1276	BPB	C2-C3-C5-C6
7	L	1276	BPB	C15-C16-C17-C18
6	M	1325	BCB	C10-C11-C12-C13
6	M	1325	BCB	C11-C12-C13-C14
6	L	1274	BCB	C15-C16-C17-C18
7	M	1326	BPB	C11-C12-C13-C15
7	M	1326	BPB	C10-C11-C12-C13
6	L	1275	BCB	C2A-CAA-CBA-CGA
6	M	1325	BCB	O2A-C1-C2-C3
6	M	1325	BCB	C3-C5-C6-C7
6	M	1325	BCB	C11-C10-C8-C7
7	M	1326	BPB	C6-C7-C8-C10
6	L	1274	BCB	CAD-CBD-CGD-O2D
6	L	1274	BCB	CAD-CBD-CGD-O1D

Continued on next page...

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

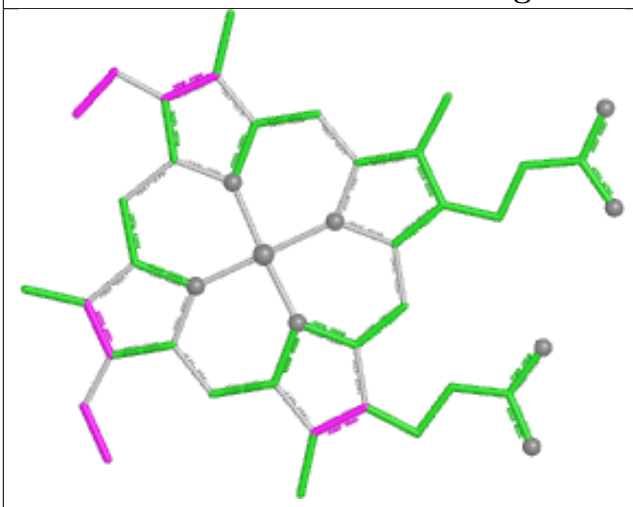
There are no ring outliers.

11 monomers are involved in 61 short contacts:

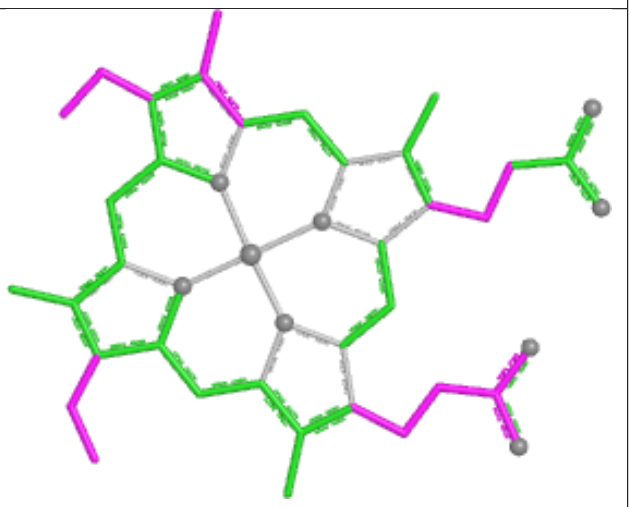
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1333	HEC	2	0
5	C	1336	HEC	3	0
6	M	1325	BCB	7	0
7	M	1326	BPB	5	0
6	M	1324	BCB	3	0
9	M	1328	MQ7	3	0
5	C	1334	HEC	9	0
7	L	1276	BPB	6	0
6	L	1274	BCB	13	0
6	L	1275	BCB	11	0
5	C	1335	HEC	2	0

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.

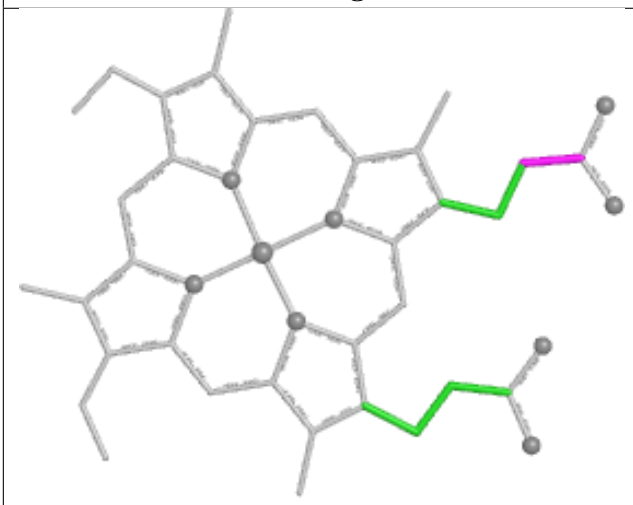
Ligand HEC C 1333



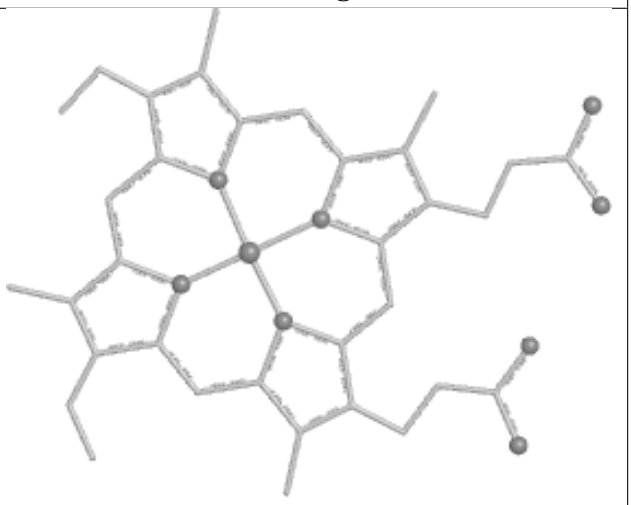
Bond lengths



Bond angles

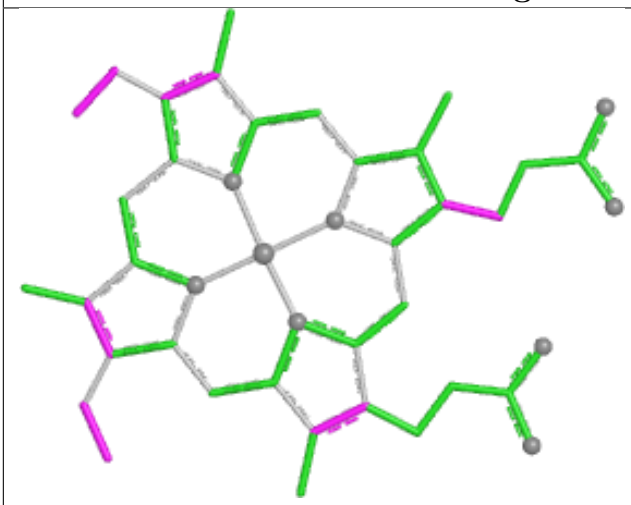


Torsions

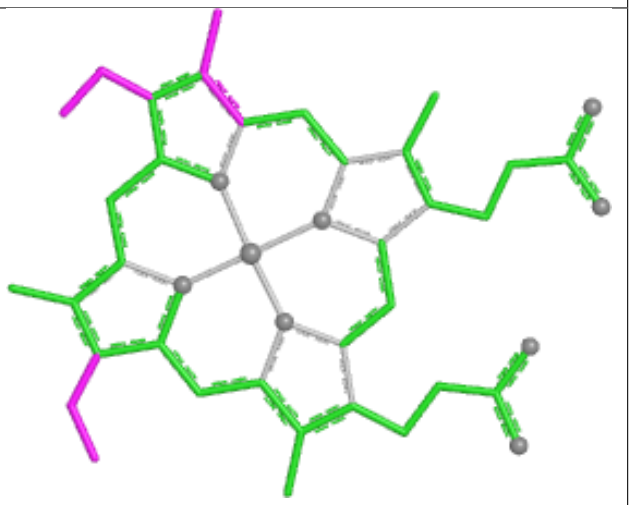


Rings

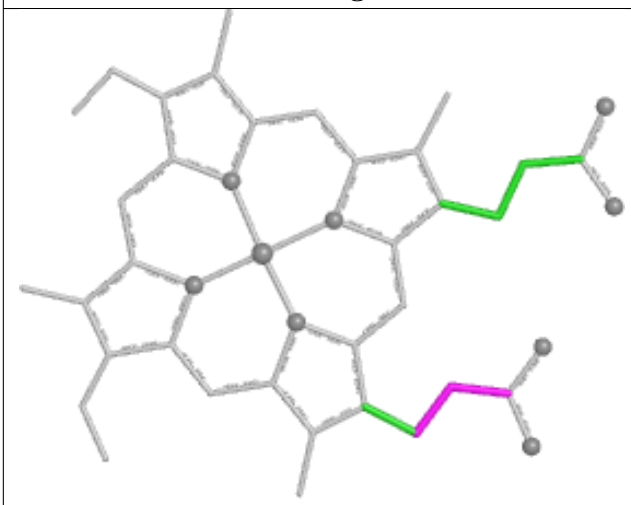
Ligand HEC C 1336



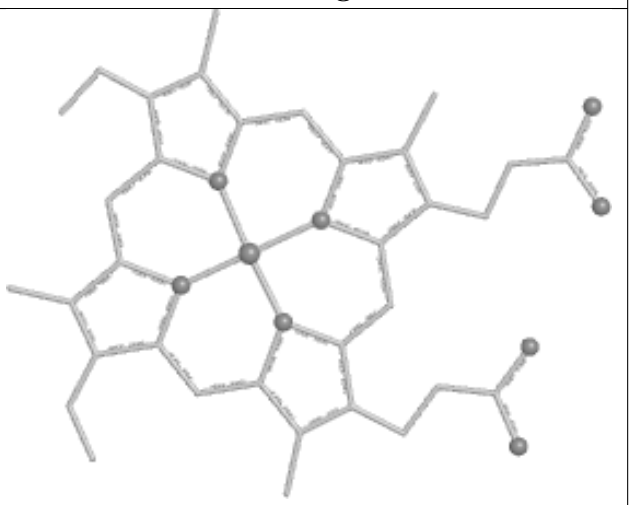
Bond lengths



Bond angles

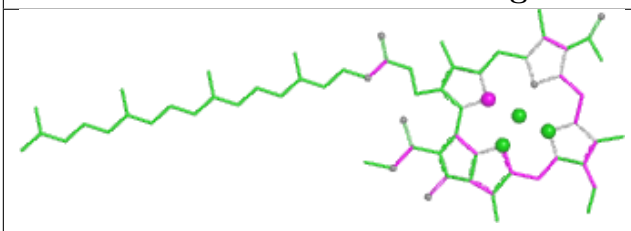


Torsions

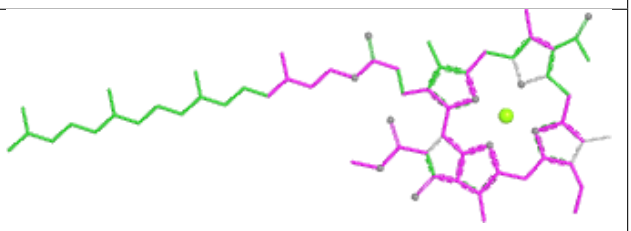


Rings

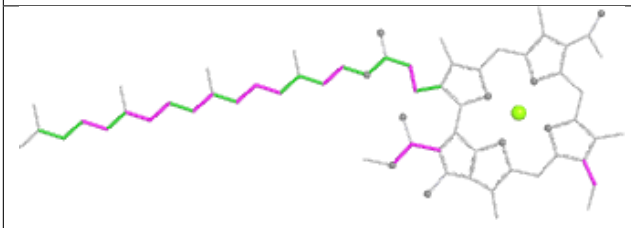
Ligand BCB M 1325



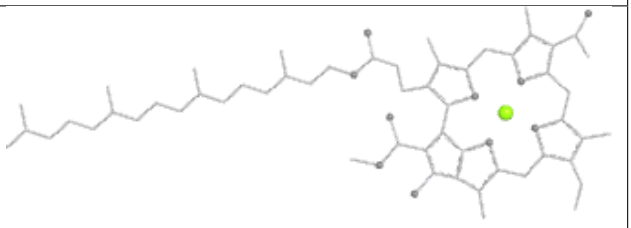
Bond lengths



Bond angles

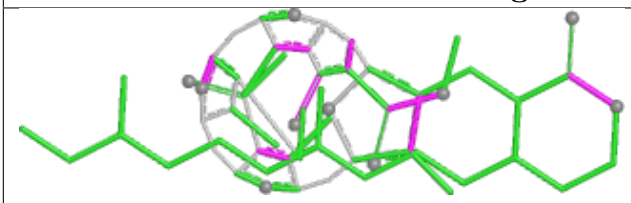


Torsions



Rings

Ligand BPB M 1326



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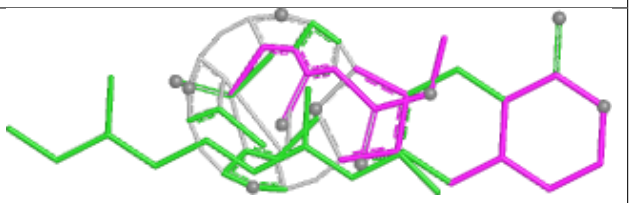
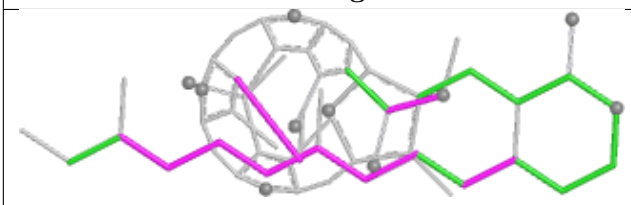


Bond angles



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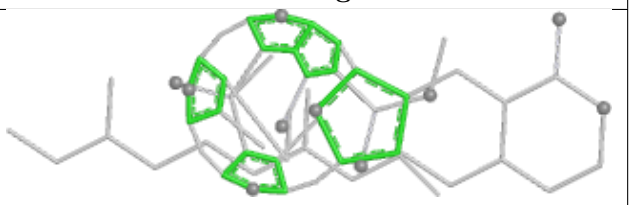
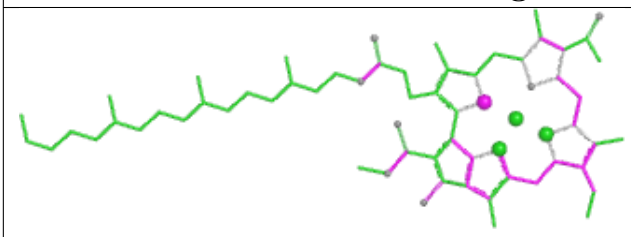


Rings

Ligand BCB M 1324



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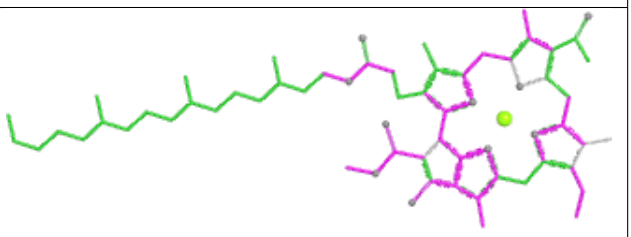
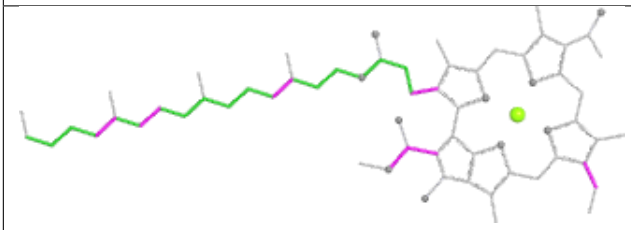


Bond angles



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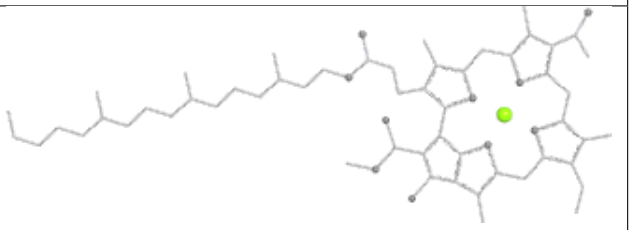
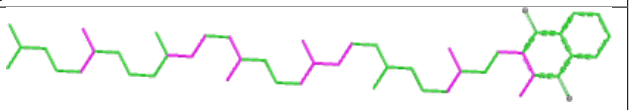


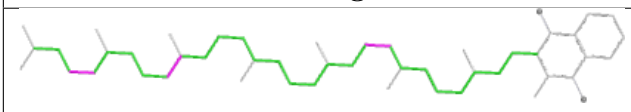
Rings

Ligand MQ7 M 1328

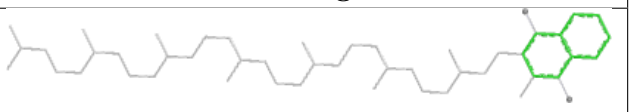
Bond lengths



Bond angles

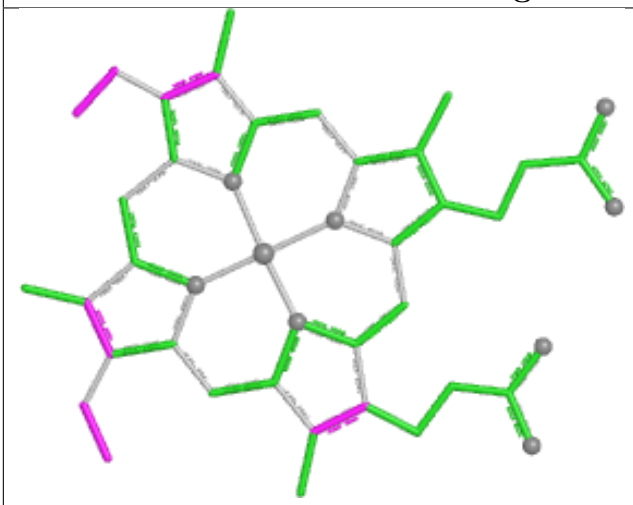


Torsions



Rings

Ligand HEC C 1334



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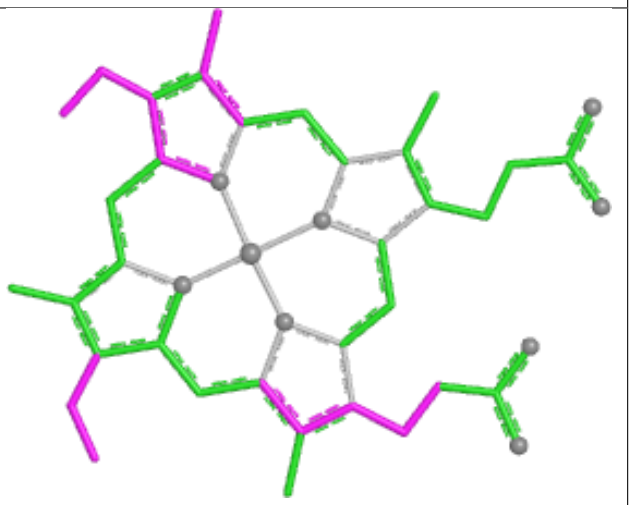
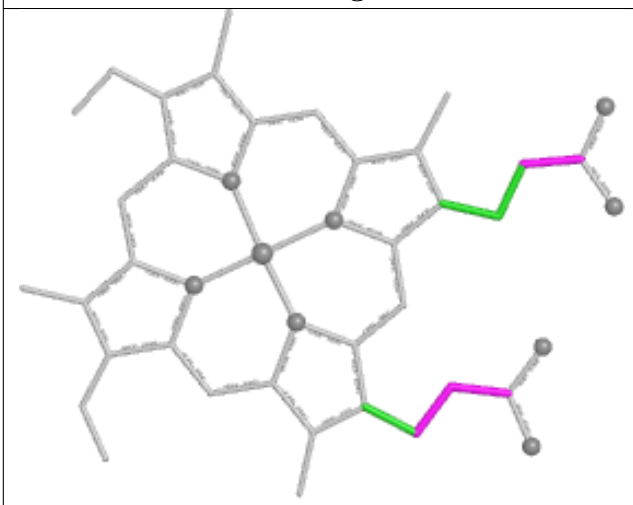


Bond angles



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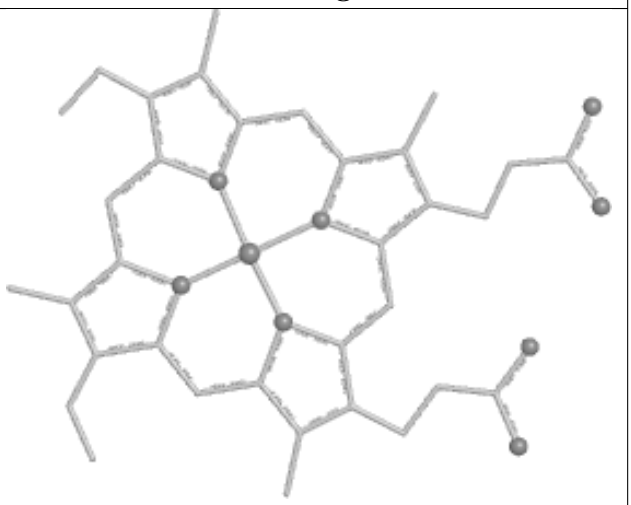
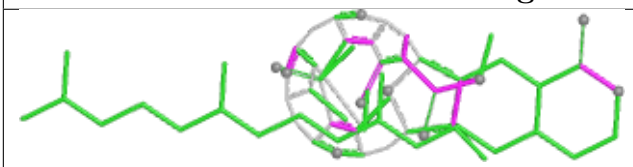
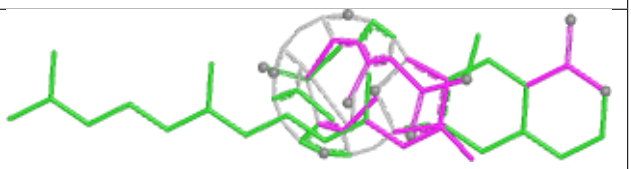


Rings

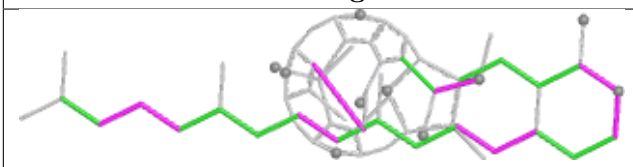
Ligand BPB L 1276



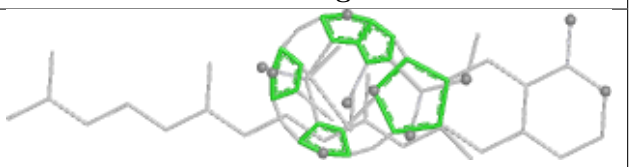
Bond lengths



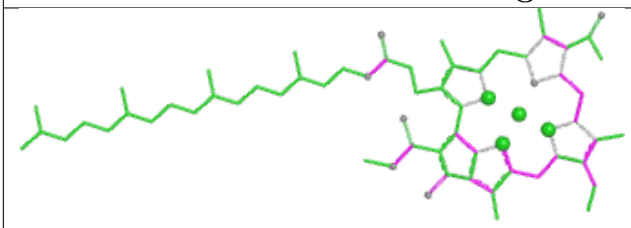
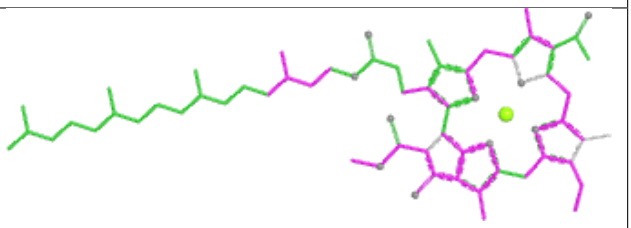
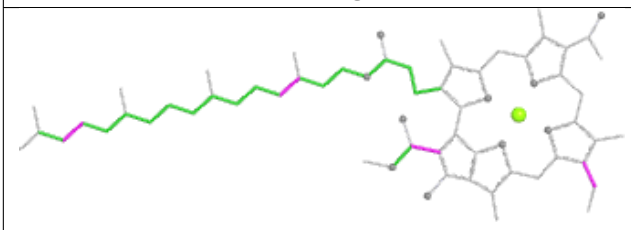
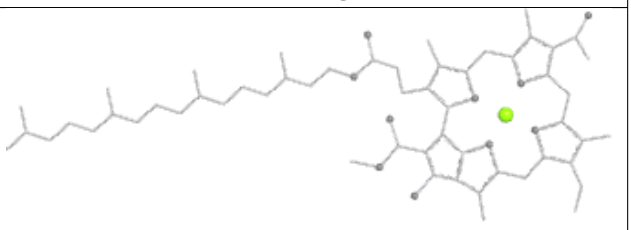
Bond angles



Torsions



Rings

Ligand BCB L 1274	
 Bond lengths	 Bond angles
 Torsions	 Rings

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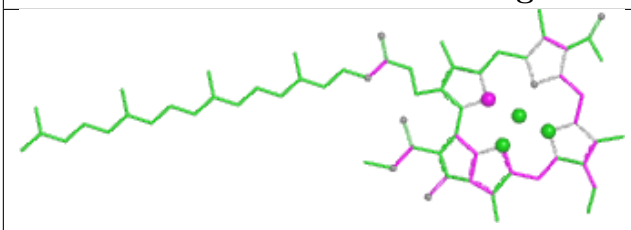
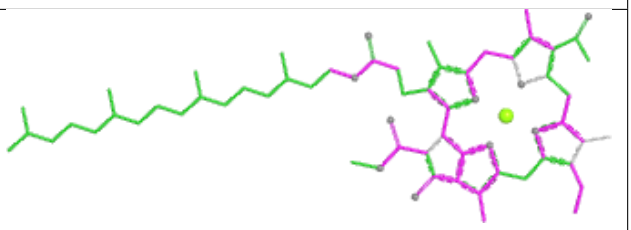
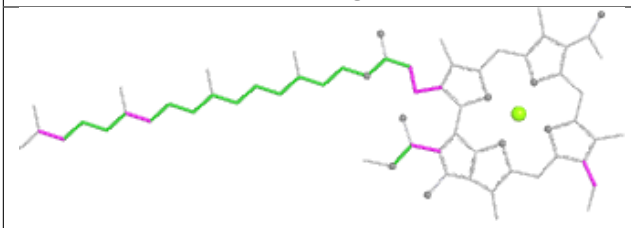
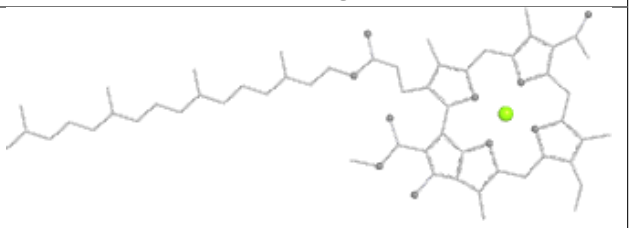
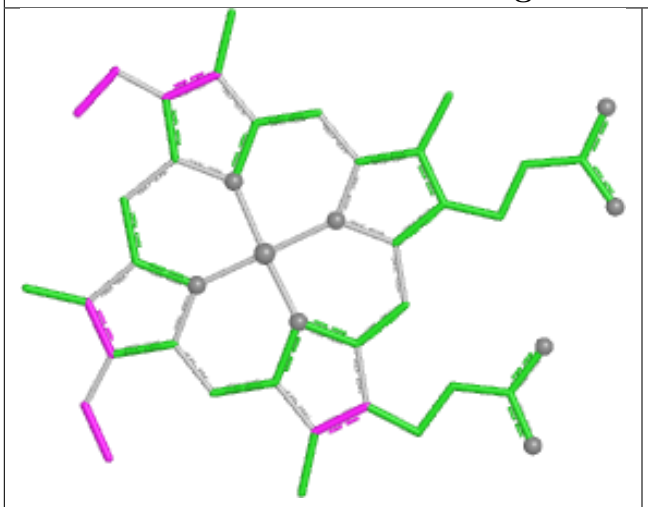
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEC C 1335



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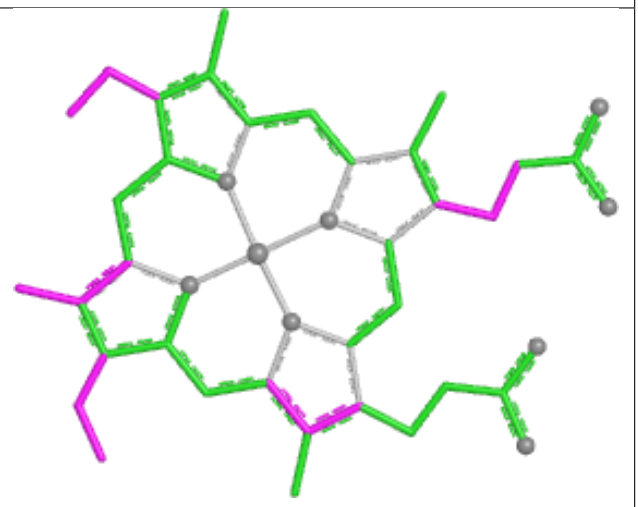
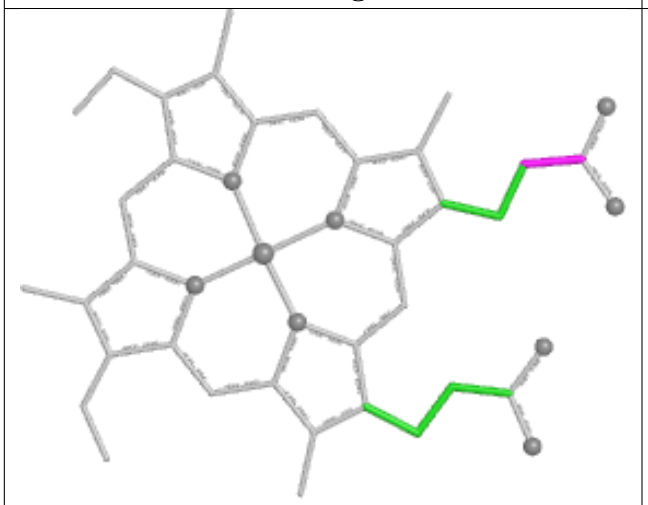
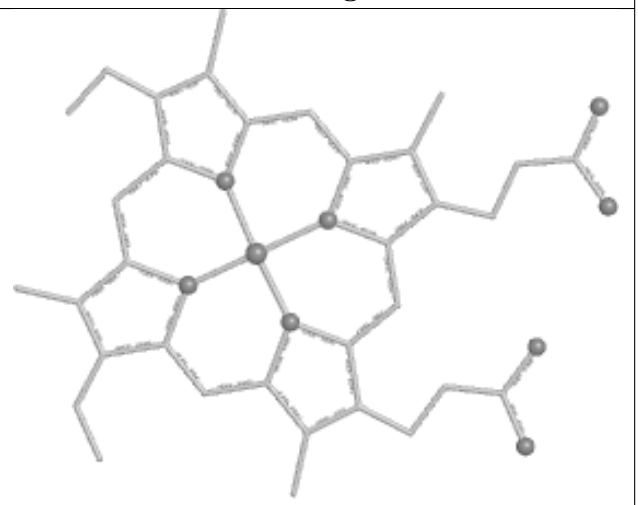


Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	C	332/336 (98%)	-0.25	1 (0%)	94	84	18, 31, 45, 51	1 (0%)
2	H	242/258 (93%)	0.11	9 (3%)	41	17	29, 40, 65, 68	8 (3%)
3	L	273/274 (99%)	-0.26	1 (0%)	92	79	16, 28, 49, 57	2 (0%)
4	M	323/324 (99%)	-0.38	1 (0%)	94	84	16, 26, 41, 44	2 (0%)
All	All	1170/1192 (98%)	-0.21	12 (1%)	82	59	16, 32, 51, 68	13 (1%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	93	THR	3.8
2	H	85	THR	3.8
2	H	83	PRO	3.2
2	H	9	HIS	2.9
3	L	13	GLY	2.9
4	M	16	HIS	2.7
2	H	7	ALA	2.5
2	H	82	ARG	2.3
1	C	218	LYS	2.3
2	H	10	LEU	2.2
2	H	189	GLY	2.1
2	H	96	PHE	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FME	H	1	10/11	0.73	0.35	67,67,68,68	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

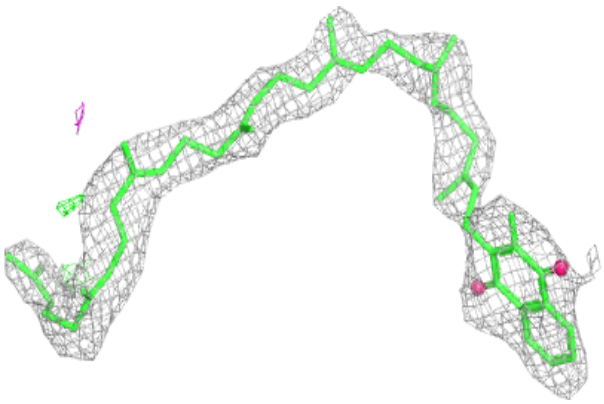
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

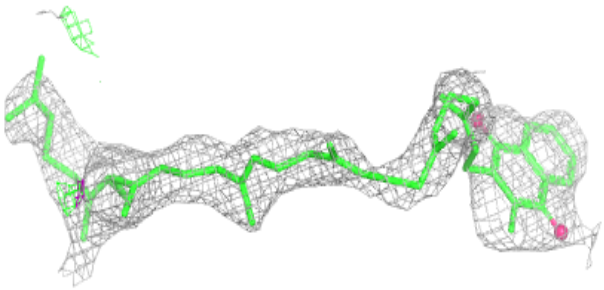
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	MQ7	M	1328	48/48	0.87	0.26	39,41,47,48	0
6	BCB	M	1324	65/66	0.89	0.23	18,20,48,49	0
7	BPB	M	1326	61/65	0.90	0.25	19,24,44,45	0
7	BPB	L	1276	65/65	0.91	0.21	23,28,33,35	0
6	BCB	L	1275	66/66	0.92	0.19	18,21,28,28	0
6	BCB	M	1325	66/66	0.93	0.20	15,18,26,27	0
5	HEC	C	1334	43/43	0.93	0.23	27,29,34,36	0
5	HEC	C	1336	43/43	0.94	0.19	25,28,33,34	0
6	BCB	L	1274	66/66	0.94	0.18	10,12,20,21	0
5	HEC	C	1333	43/43	0.95	0.16	25,32,33,34	0
5	HEC	C	1335	43/43	0.96	0.16	20,21,23,24	0
8	FE2	M	1327	1/1	0.99	0.10	24,24,24,24	0

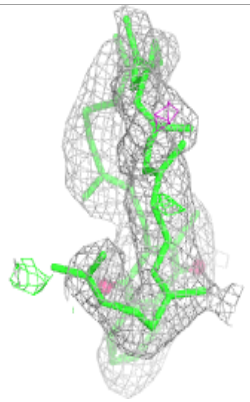
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

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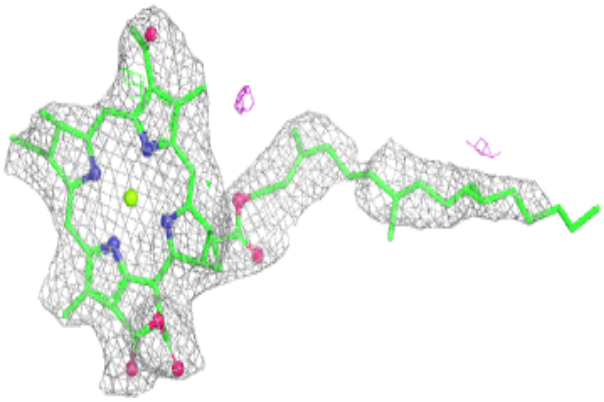
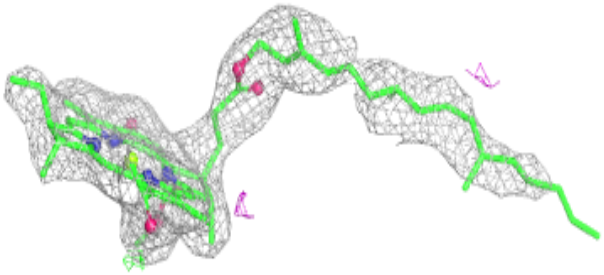
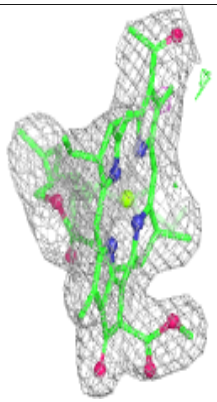
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around BPB M 1326:

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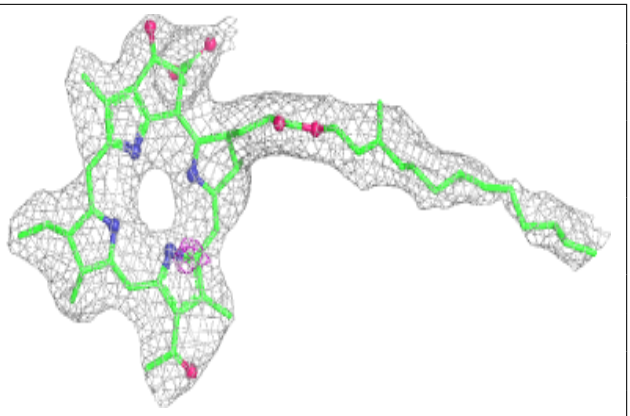
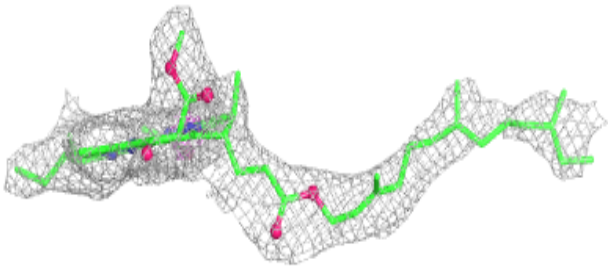
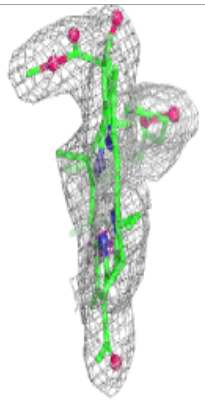
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around BPB L 1276:

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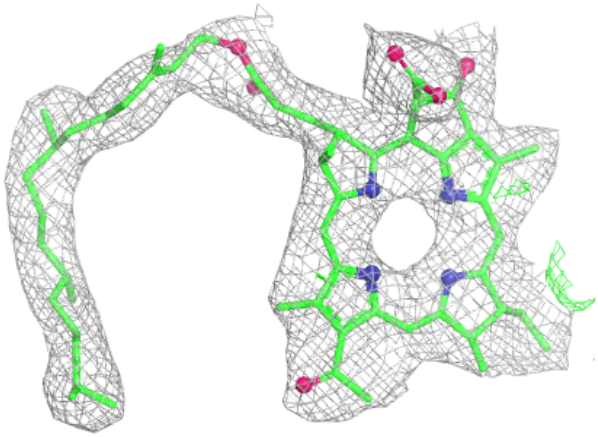
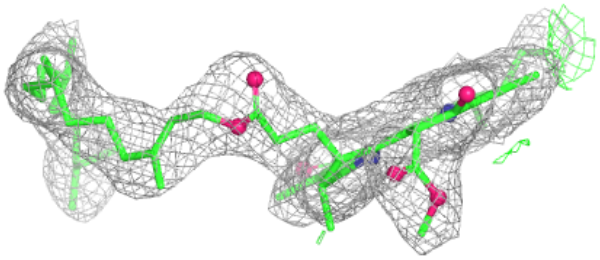
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around BCB L 1275:

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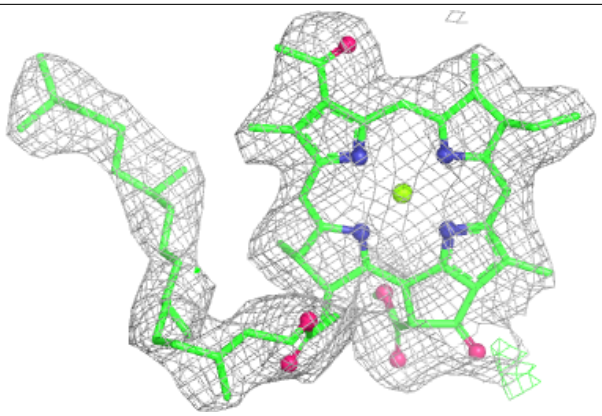
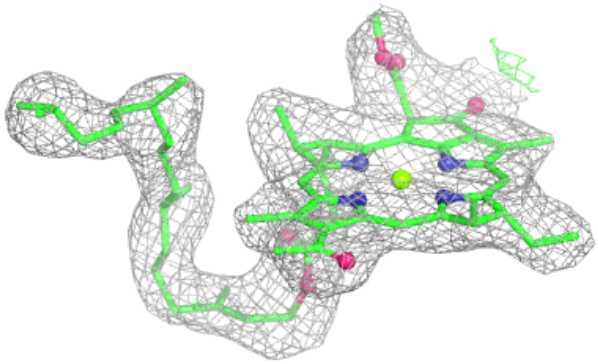
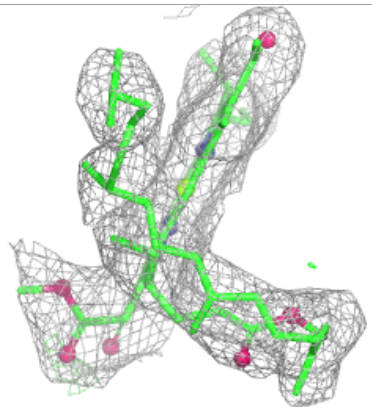
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around BCB M 1325:

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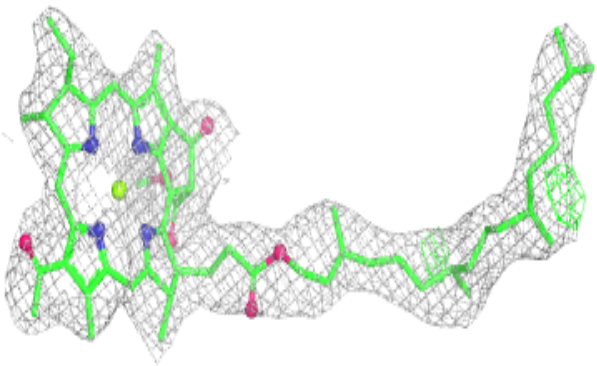
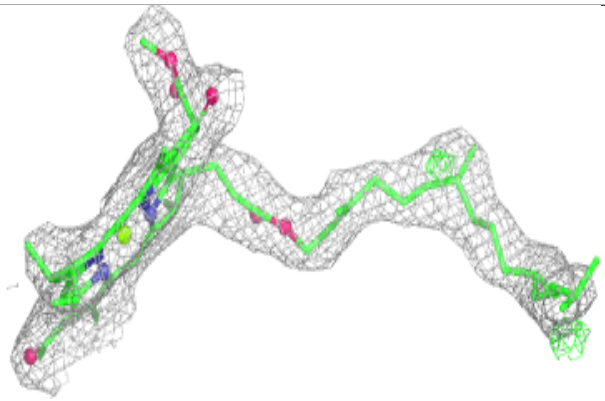
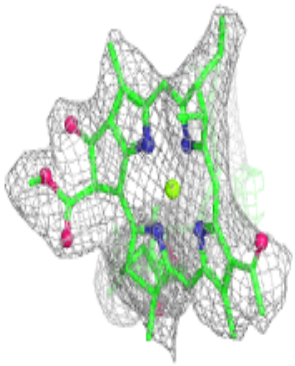
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

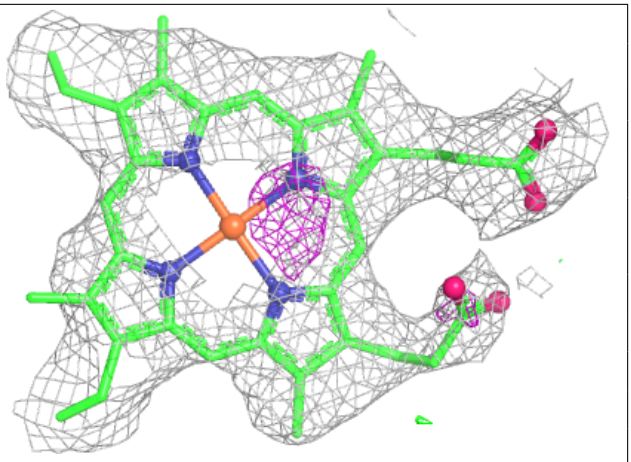


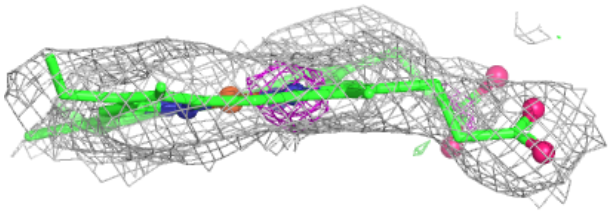


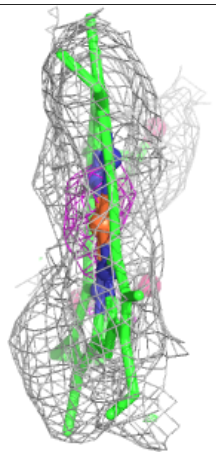


Electron density around HEC C 1334:

$2mF_o$-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 1336:

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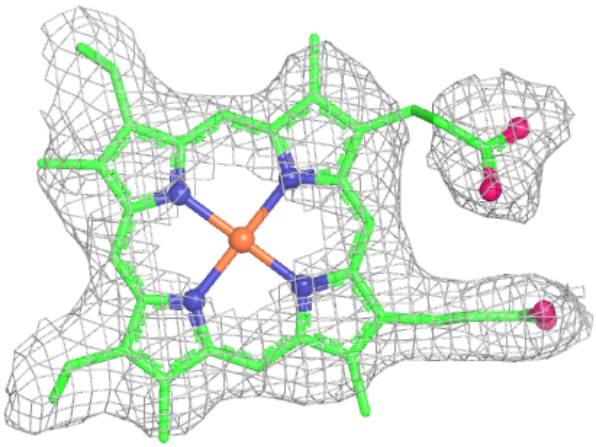
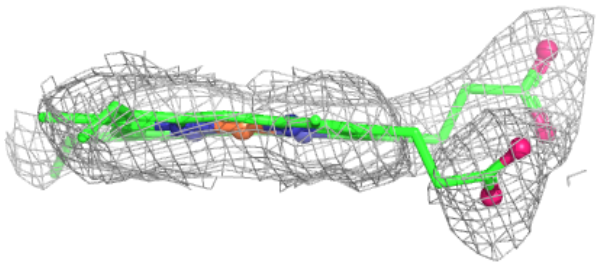
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around BCB L 1274:

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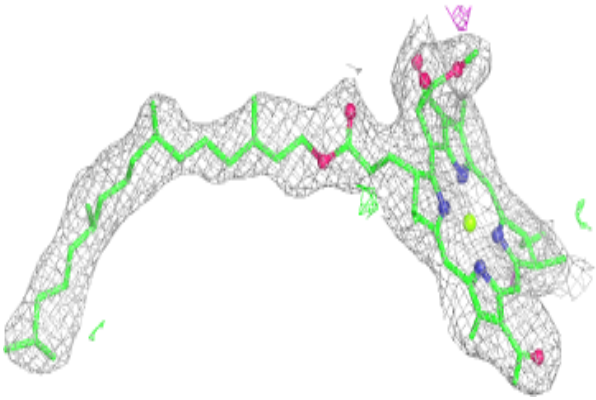
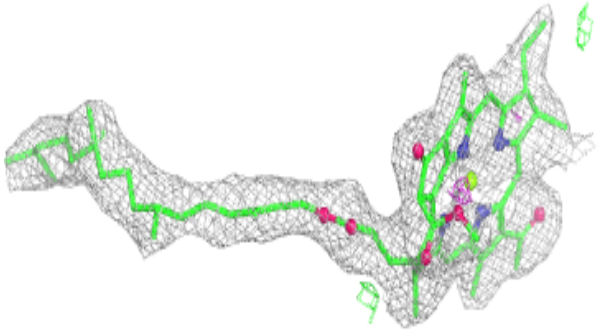
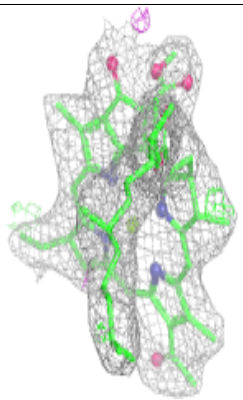
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around HEC C 1333:

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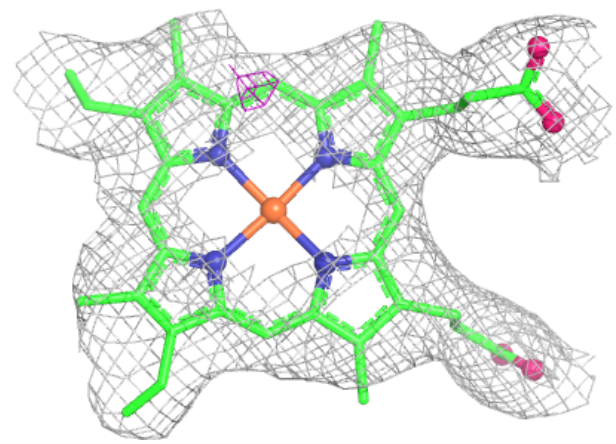
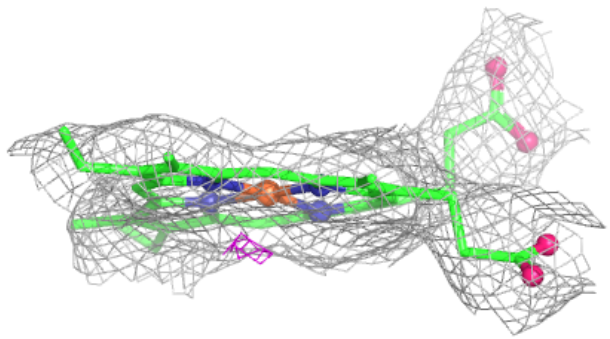
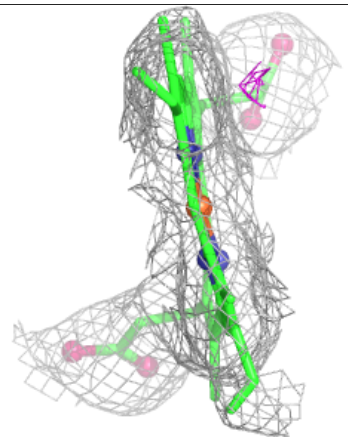
and green (positive)







Electron density around HEC C 1335:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
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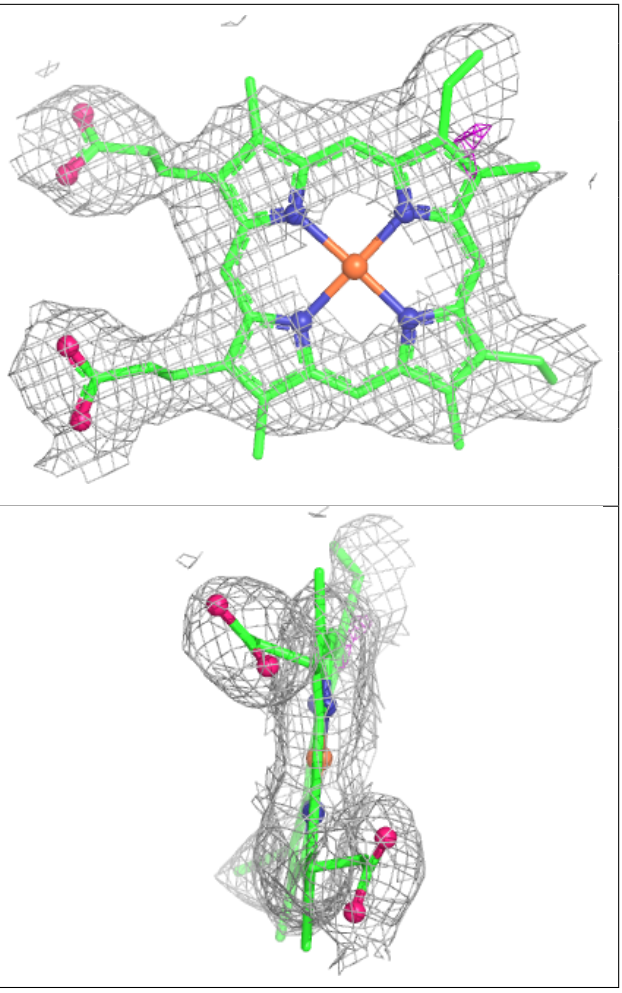

6.5 Other polymers (i)

There are no such residues in this entry.