Full wwPDB X-ray Structure Validation Report (i)

Sep 22, 2026 – 06:18 PM EDT

PDB ID	:	3PRC / pdb_00003prc
Title	:	PHOTOSYNTHETIC REACTION CENTER FROM RHODOPSEUDOMONAS VIRIDIS (QB-DEPLETED)
Authors	:	Lancaster, C.R.D.; Michel, H.
Deposited on	:	1997-07-29
Resolution	:	2.40 Å(reported)

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

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

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

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

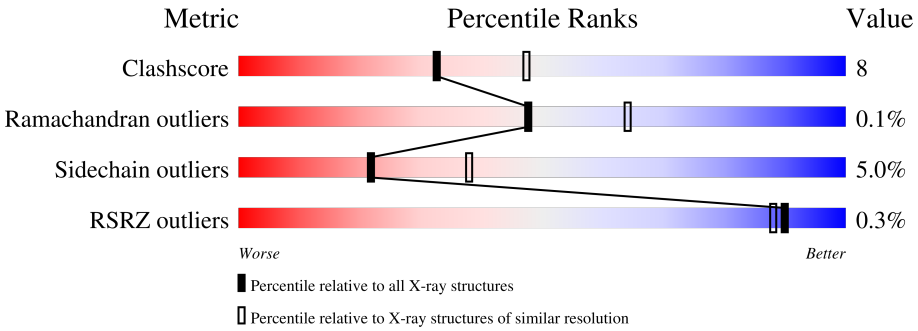
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	82% 15%
2	L	273	85% 13%
3	M	323	83% 16%
4	H	258	% 73% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	HEC	C	337	X	-	-	-
5	HEC	C	338	X	-	-	-
5	HEC	C	339	X	-	-	-
5	HEC	C	340	X	-	-	-
6	BCB	L	302	X	-	-	-
6	BCB	L	304	X	-	-	-
6	BCB	M	805	X	-	-	-
6	BCB	M	806	X	-	-	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 10606 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	332	2607	1642	467	480	18	38	1	0

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	273	2193	1471	358	357	7	14	2	0

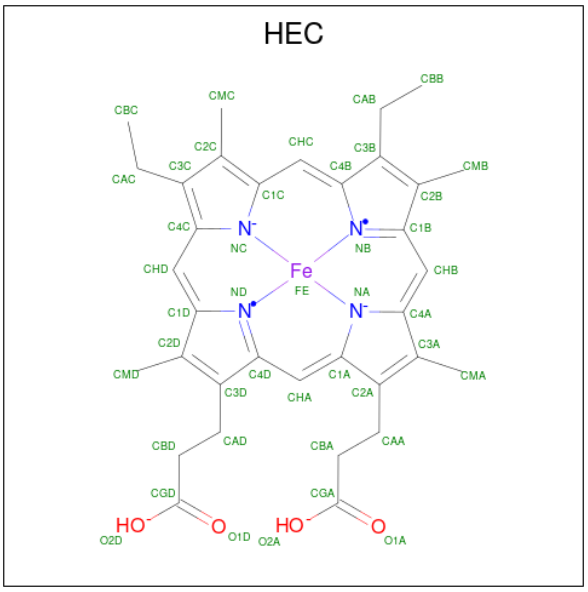
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	323	2566	1711	420	424	11	14	1	0

- Molecule 4 is a protein called PHOTOSYNTHETIC REACTION CENTER.

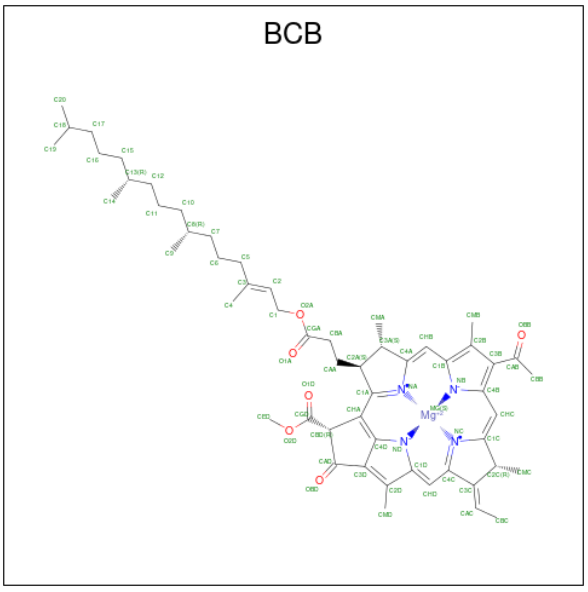
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	258	2028	1298	345	382	3	129	1	0

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



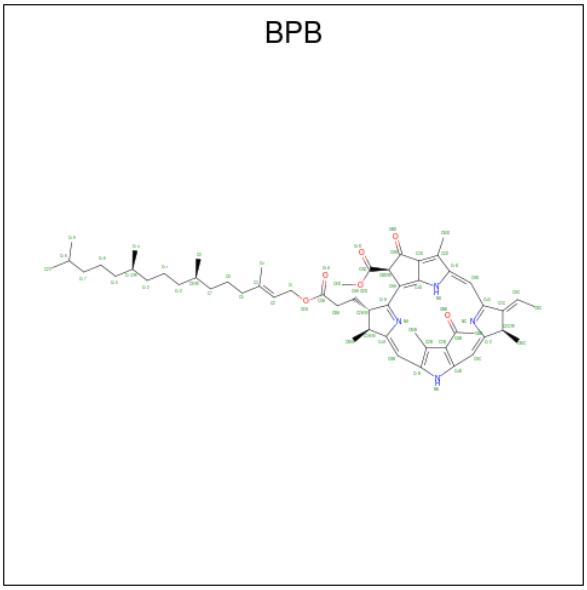
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



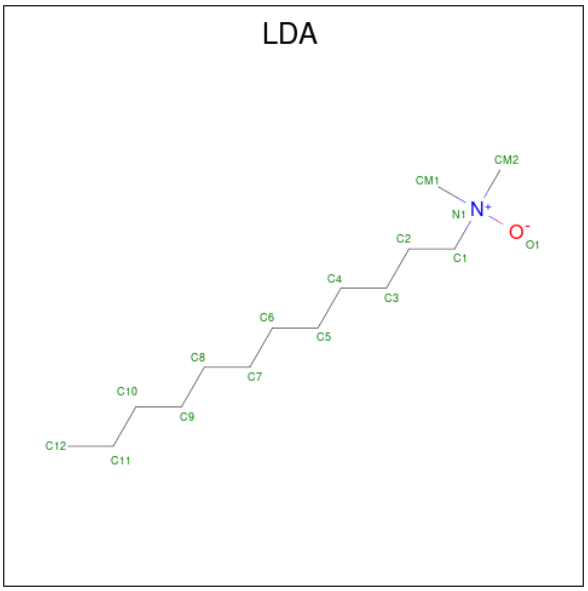
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



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

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

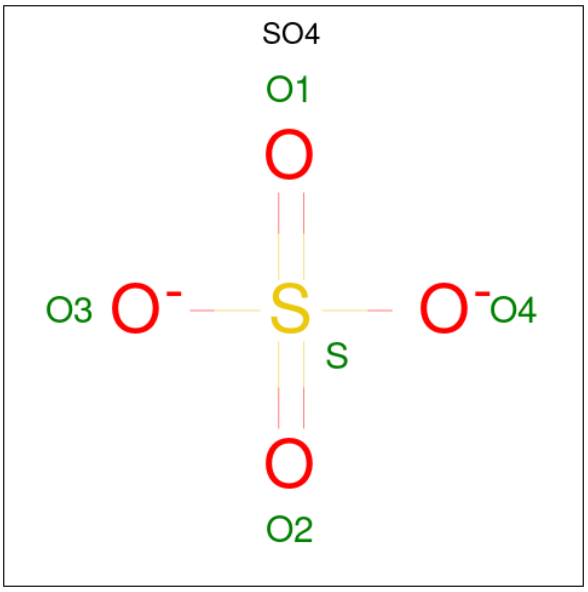


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	1	Total C N O 16 14 1 1	0	0
8	L	1	Total C N O 16 14 1 1	0	0
8	M	1	Total C N O 16 14 1 1	3	0
8	M	1	Total C N O 16 14 1 1	5	0
8	M	1	Total C N O 16 14 1 1	4	0
8	H	1	Total C N O 16 14 1 1	0	0
8	H	1	Total C N O 16 14 1 1	1	0

- Molecule 9 is FE (II) ION (CCD ID: FE2) (formula: Fe).

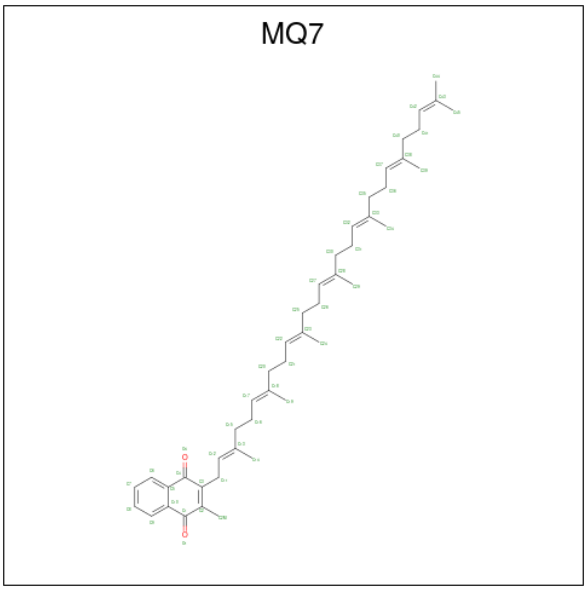
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total Fe 1 1	0	0

- Molecule 10 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



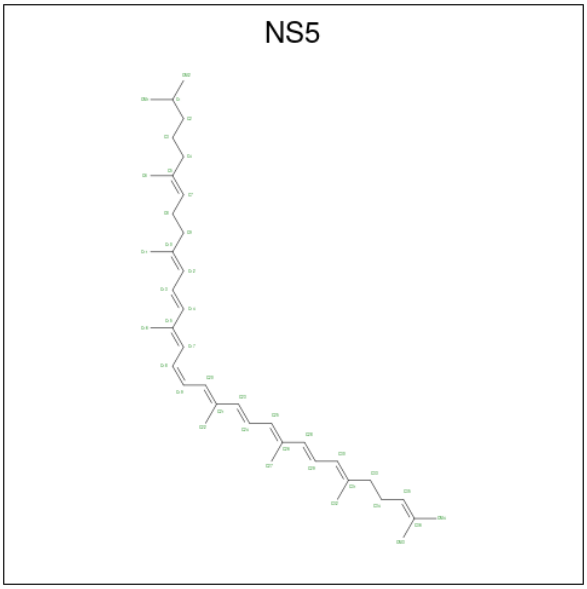
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	M	1	Total O S 5 4 1	0	0
10	M	1	Total O S 5 4 1	0	0
10	M	1	Total O S 5 4 1	0	0
10	H	1	Total O S 5 4 1	0	0

- Molecule 11 is MENAQUINONE-7 (CCD ID: MQ7) (formula: $C_{46}H_{64}O_2$).



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

- Molecule 12 is 15-cis-1,2-dihydroneurosporene (CCD ID: NS5) (formula: $C_{40}H_{60}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	M	1	Total C 40 40	9	0

- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	163	Total O 163 163	0	0
13	L	65	Total O 65 65	0	0
13	M	97	Total O 97 97	0	0
13	H	100	Total O 100 100	0	0

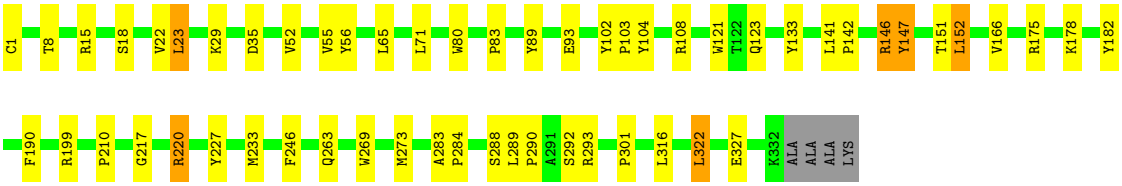
3 Residue-property plots (i)

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

Chain C:

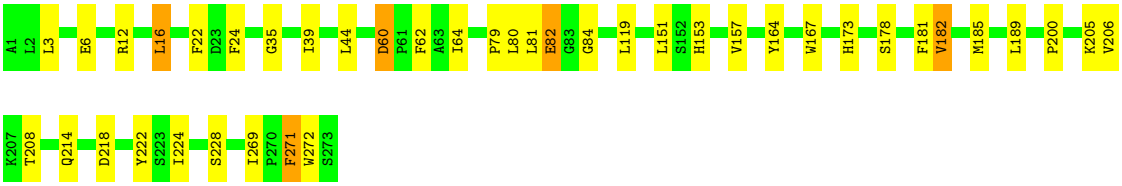




• Molecule 2: PHOTOSYNTHETIC REACTION CENTER

Chain L:

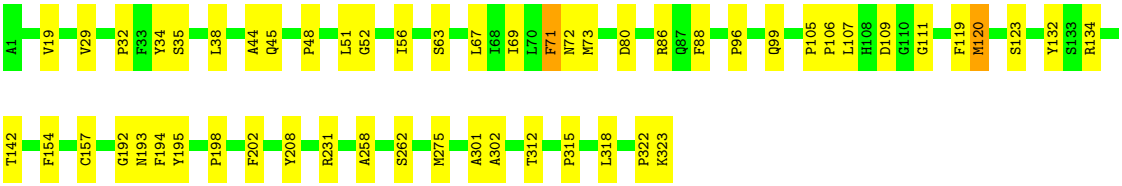




• Molecule 3: PHOTOSYNTHETIC REACTION CENTER

Chain M:



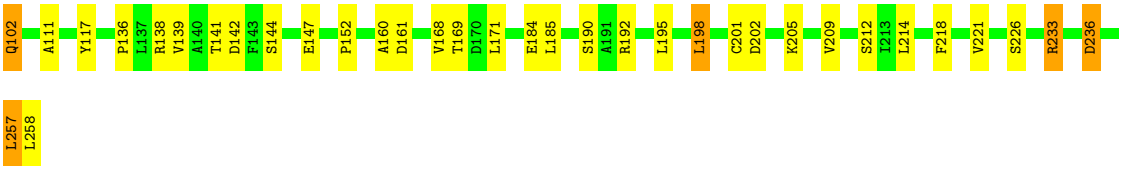


• Molecule 4: PHOTOSYNTHETIC REACTION CENTER

Chain H:






Q102
A111
Y117
P136
L137
R138
V139
A140
T141
D142
F143
S144
E147
P152
A160
D161
V168
T169
D170
L171
E184
L185
S190
A191
R192
L195
L198
C201
D202
K205
V209
S212
I213
L214
F218
V221
S226
R233
D236
L257
L258

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	223.50Å 223.50Å 113.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40 10.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	79.5 (10.00-2.40) 78.2 (10.00-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 2.39Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.178 , 0.215 0.170 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	30.3	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 87.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10606	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, BCB, BPB, HEC, FE2, LDA, NS5, 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	0.64	0/2674	0.84	1/3645 (0.0%)
2	L	0.64	0/2281	0.85	4/3112 (0.1%)
3	M	0.63	0/2671	0.87	5/3653 (0.1%)
4	H	0.67	3/2055 (0.1%)	0.88	4/2807 (0.1%)
All	All	0.64	3/9681 (0.0%)	0.86	14/13217 (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
1	C	0	5
2	L	0	1
3	M	0	1
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	54	PRO	N-CA	-6.81	1.39	1.47
4	H	53	ALA	CA-C	-6.46	1.44	1.52
4	H	53	ALA	C-N	-5.92	1.27	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	53	ALA	N-CA-C	9.72	131.30	109.81
4	H	53	ALA	CB-CA-C	-9.04	92.36	110.17
4	H	45	GLU	CB-CA-C	-7.85	94.70	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	80	ASP	CA-C-N	7.15	126.64	118.85
3	M	80	ASP	C-N-CA	7.15	126.64	118.85
3	M	312	THR	CA-C-N	6.89	126.92	119.89
3	M	312	THR	C-N-CA	6.89	126.92	119.89
4	H	54	PRO	N-CA-C	-6.63	100.09	110.50
2	L	60	ASP	CA-C-N	6.53	126.03	119.24
2	L	60	ASP	C-N-CA	6.53	126.03	119.24
2	L	182	VAL	CB-CA-C	-6.29	103.92	111.97
3	M	302	ALA	N-CA-C	5.89	118.16	109.50
1	C	55	VAL	N-CA-C	5.76	115.95	110.42
2	L	208	THR	N-CA-C	5.25	116.63	109.18

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	147	TYR	Sidechain
1	C	182	TYR	Sidechain
1	C	190	PHE	Sidechain
1	C	227	TYR	Sidechain
1	C	89	TYR	Sidechain
2	L	164	TYR	Sidechain
3	M	119	PHE	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	2607	0	2575	33	0
2	L	2193	0	2122	31	0
3	M	2566	0	2460	36	0
4	H	2028	0	2029	39	0
5	C	172	0	120	3	0
6	L	132	0	144	5	0
6	M	132	0	144	12	0
7	L	65	0	74	4	0
7	M	65	0	74	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	32	0	62	0	0
8	L	32	0	62	10	0
8	M	48	0	93	2	0
9	M	1	0	0	0	0
10	H	5	0	0	0	0
10	M	15	0	0	0	0
11	M	48	0	64	0	0
12	M	40	0	60	0	0
13	C	163	0	0	5	0
13	H	100	0	0	2	0
13	L	65	0	0	2	0
13	M	97	0	0	0	0
All	All	10606	0	10083	155	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 8.

All (155) 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)
7:L:402:BPB:HBBB	7:L:402:BPB:HHC	1.53	0.89
7:M:401:BPB:HBBB	7:M:401:BPB:HHC	1.50	0.89
6:M:805:BCB:HHC	6:M:805:BCB:HBB2	1.58	0.82
1:C:121:TRP:HA	1:C:123[A]:GLN:HE21	1.43	0.81
7:L:402:BPB:HHC	7:L:402:BPB:CBB	2.10	0.81
3:M:29:VAL:HG21	3:M:51:LEU:HD22	1.64	0.79
1:C:152:LEU:HD22	1:C:175:ARG:HA	1.66	0.75
2:L:79:PRO:HG2	2:L:82:GLU:HG3	1.72	0.71
6:M:806:BCB:HAA2	6:M:806:BCB:HBD	1.74	0.69
1:C:123[A]:GLN:HG3	1:C:269:TRP:CE3	2.28	0.69
2:L:178:SER:O	2:L:182:VAL:HG23	1.95	0.67
2:L:181:PHE:HB3	7:M:401:BPB:CBB	2.24	0.66
4:H:55:GLU:HB2	4:H:58:GLN:HG3	1.78	0.65
1:C:217:GLY:O	1:C:220:ARG:HG3	1.97	0.65
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.33	0.64
8:L:707:LDA:HM23	13:L:761:HOH:O	1.99	0.63
3:M:71:PHE:HB3	8:M:706:LDA:H62	1.80	0.63
1:C:290:PRO:HG2	1:C:293:ARG:HG2	1.81	0.62
6:M:805:BCB:HHC	6:M:805:BCB:CBB	2.30	0.62
4:H:160:ALA:HB3	4:H:214:LEU:HD23	1.80	0.62
1:C:152:LEU:HD21	1:C:178:LYS:HG3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:TRP:HA	1:C:123[A]:GLN:NE2	2.13	0.62
4:H:161:ASP:HB3	4:H:214:LEU:HD22	1.81	0.62
8:L:702:LDA:HM23	13:L:772:HOH:O	1.98	0.61
2:L:181:PHE:HB3	7:M:401:BPB:HBBA	1.81	0.61
3:M:315:PRO:HA	3:M:318:LEU:HG	1.82	0.60
2:L:62:PHE:HE2	8:L:702:LDA:HM21	1.66	0.59
4:H:117:TYR:HB2	4:H:236:ASP:HB3	1.85	0.59
1:C:65:LEU:HD11	1:C:327:GLU:HG2	1.85	0.59
2:L:218:ASP:HB3	3:M:134:ARG:HD2	1.85	0.59
3:M:32:PRO:HG3	3:M:48:PRO:HD3	1.83	0.59
3:M:63:SER:O	3:M:67:LEU:HG	2.03	0.58
3:M:29:VAL:CG2	3:M:51:LEU:HD22	2.34	0.58
3:M:231:ARG:HD2	13:H:812:HOH:O	2.03	0.57
7:M:401:BPB:HBBB	7:M:401:BPB:CHC	2.28	0.57
2:L:12:ARG:HD3	4:H:102:GLN:NE2	2.19	0.57
2:L:62:PHE:CE2	8:L:702:LDA:HM21	2.40	0.57
2:L:181:PHE:CD2	7:M:401:BPB:HBB	2.40	0.56
3:M:202:PHE:CE2	4:H:20:GLN:HG2	2.40	0.56
2:L:35:GLY:O	2:L:39:ILE:HG12	2.05	0.56
8:L:702:LDA:H32	13:H:894:HOH:O	2.06	0.56
3:M:96:PRO:HG3	3:M:105:PRO:HB3	1.87	0.56
2:L:153:HIS:O	2:L:157:VAL:HG23	2.06	0.55
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.42	0.55
2:L:80:LEU:HA	2:L:84:GLY:HA3	1.88	0.55
6:M:805:BCB:H61	7:M:401:BPB:HMA	1.89	0.54
4:H:6:LEU:HB2	4:H:10:LEU:HB3	1.89	0.54
4:H:136:PRO:HG2	4:H:139:VAL:HG23	1.90	0.54
2:L:185:MET:SD	6:M:805:BCB:H41	2.47	0.53
6:M:806:BCB:HAA2	6:M:806:BCB:CBD	2.34	0.53
6:M:806:BCB:H203	7:M:401:BPB:H4B	1.91	0.53
2:L:200:PRO:HG3	2:L:205:LYS:O	2.08	0.53
1:C:210:PRO:HB2	4:H:3:HIS:HD2	1.74	0.53
4:H:56:ASP:HB3	4:H:60:TYR:CE2	2.44	0.53
3:M:275:MET:HG2	7:M:401:BPB:HBCA	1.90	0.53
4:H:86:ARG:NH2	4:H:111:ALA:O	2.37	0.53
4:H:136:PRO:HG2	4:H:138:ARG:HG2	1.92	0.52
4:H:233:ARG:O	4:H:233:ARG:HG3	2.09	0.52
1:C:147:TYR:OH	1:C:301:PRO:HG3	2.10	0.52
8:L:702:LDA:H71	3:M:301:ALA:CB	2.40	0.52
6:L:302:BCB:OBB	6:L:302:BCB:HHC	2.09	0.51
4:H:190:SER:HB3	4:H:192:ARG:HG2	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:214:GLN:NE2	3:M:19:VAL:H	2.08	0.51
4:H:86:ARG:NH2	4:H:111:ALA:HB3	2.25	0.51
1:C:289:LEU:HD22	1:C:293:ARG:HG3	1.93	0.50
4:H:152:PRO:O	4:H:168:VAL:HB	2.12	0.50
1:C:93:GLU:HB2	13:C:470:HOH:O	2.10	0.50
2:L:182:VAL:HG22	6:M:805:BCB:H12	1.94	0.50
3:M:99:GLN:HA	3:M:99:GLN:OE1	2.11	0.49
2:L:224:ILE:HG12	2:L:228:SER:HB2	1.93	0.49
1:C:121:TRP:CG	1:C:273:MET:HG3	2.48	0.49
1:C:210:PRO:HB2	4:H:3:HIS:CD2	2.48	0.49
2:L:206:VAL:HG21	4:H:68:PHE:HB3	1.93	0.49
4:H:65:PRO:HA	4:H:79:PRO:HD2	1.94	0.48
4:H:218:PHE:HA	4:H:221:VAL:HG23	1.95	0.48
3:M:34:TYR:HA	3:M:44:ALA:O	2.14	0.48
6:L:304:BCB:HBB2	6:L:304:BCB:HMB3	1.95	0.48
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.48	0.48
3:M:32:PRO:HB3	3:M:45:GLN:HG3	1.95	0.48
3:M:52:GLY:O	3:M:56:ILE:HD12	2.14	0.47
6:L:302:BCB:HMB1	6:L:302:BCB:HBB3	1.96	0.47
3:M:73:MET:HE1	3:M:88:PHE:CE1	2.50	0.47
1:C:220:ARG:NH2	13:C:359:HOH:O	2.47	0.47
2:L:269:ILE:HG22	2:L:271:PHE:HD1	1.79	0.47
3:M:29:VAL:HG21	3:M:51:LEU:CD2	2.40	0.47
7:M:401:BPB:HHC	7:M:401:BPB:CBB	2.31	0.47
1:C:146:ARG:HA	1:C:146:ARG:HD2	1.64	0.47
8:L:702:LDA:H71	3:M:301:ALA:HB2	1.96	0.47
6:M:806:BCB:OBB	6:M:806:BCB:HHC	2.16	0.46
1:C:83:PRO:HD2	13:C:367:HOH:O	2.15	0.46
3:M:132:TYR:CE1	3:M:142:THR:HG21	2.51	0.46
2:L:272:TRP:CE2	3:M:86:ARG:HG3	2.51	0.46
2:L:185:MET:HE2	2:L:189:LEU:HD11	1.98	0.45
1:C:283:ALA:HB3	1:C:284:PRO:HD3	1.98	0.45
2:L:269:ILE:CG2	2:L:271:PHE:HD1	2.30	0.45
4:H:138:ARG:HG3	4:H:139:VAL:HG23	1.99	0.45
4:H:67:THR:HA	4:H:76:VAL:O	2.16	0.45
3:M:107:LEU:HA	3:M:111:GLY:HA3	1.98	0.44
4:H:37:ARG:HG2	4:H:41:TYR:CE1	2.52	0.44
4:H:34:ARG:HG2	4:H:61:GLU:O	2.17	0.44
1:C:283:ALA:N	1:C:284:PRO:CD	2.81	0.44
2:L:60:ASP:O	2:L:64:ILE:HG13	2.16	0.44
1:C:141:LEU:HD12	1:C:142:PRO:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:304:BCB:HHC	6:L:304:BCB:OBB	2.16	0.44
1:C:322:LEU:HA	13:C:469:HOH:O	2.17	0.44
1:C:52:VAL:HB	1:C:56:TYR:CD2	2.53	0.44
2:L:151:LEU:HD21	8:L:702:LDA:H111	2.00	0.44
7:L:402:BPB:NC	7:L:402:BPB:ND	2.66	0.44
4:H:138:ARG:HH22	4:H:184:GLU:CD	2.26	0.44
1:C:104:TYR:HE1	1:C:108:ARG:NH2	2.16	0.44
4:H:33:ARG:HA	4:H:33:ARG:HD2	1.82	0.44
3:M:35:SER:HB3	3:M:38:LEU:HB3	2.00	0.43
3:M:72:ASN:OD1	8:M:706:LDA:H12	2.18	0.43
2:L:3:LEU:HB2	2:L:6:GLU:HB2	1.99	0.43
3:M:120:MET:HG3	6:M:806:BCB:H172	2.00	0.43
4:H:67:THR:CG2	4:H:75:THR:HB	2.47	0.43
1:C:246:PHE:CZ	1:C:263:GLN:HG2	2.54	0.43
2:L:222:TYR:O	8:L:707:LDA:HM13	2.19	0.43
3:M:67:LEU:O	3:M:71:PHE:HB2	2.18	0.43
3:M:195:TYR:CZ	6:M:806:BCB:HMC2	2.53	0.43
2:L:167:TRP:HE1	2:L:173:HIS:CD2	2.37	0.43
2:L:206:VAL:CG2	4:H:68:PHE:HB3	2.48	0.43
3:M:258:ALA:HB1	3:M:262:SER:OG	2.17	0.43
7:L:402:BPB:HBBA	3:M:208:TYR:HB3	2.00	0.43
1:C:8:THR:HB	1:C:23:LEU:HB2	2.01	0.43
1:C:233:MET:HB3	5:C:339:HEC:C4B	2.49	0.43
7:M:401:BPB:H6	7:M:401:BPB:H4	1.77	0.43
4:H:27:VAL:O	4:H:31:TYR:HB3	2.19	0.42
1:C:52:VAL:HB	1:C:56:TYR:HD2	1.83	0.42
4:H:86:ARG:HH21	4:H:111:ALA:HB3	1.84	0.42
5:C:337:HEC:HBB3	5:C:337:HEC:HMB1	2.00	0.42
4:H:138:ARG:CG	4:H:139:VAL:HG23	2.49	0.42
4:H:70:LEU:HD11	4:H:76:VAL:HG23	2.00	0.42
1:C:71:LEU:HD23	1:C:71:LEU:HA	1.88	0.42
2:L:185:MET:SD	6:M:805:BCB:C4	3.07	0.42
3:M:69:ILE:HG22	3:M:73:MET:SD	2.59	0.42
7:M:401:BPB:CBB	7:M:401:BPB:CHC	2.96	0.42
4:H:257:LEU:HD22	4:H:257:LEU:HA	1.80	0.42
5:C:337:HEC:HBC1	5:C:338:HEC:HMA1	2.02	0.42
6:L:302:BCB:H62	6:L:302:BCB:H41	1.90	0.41
2:L:16:LEU:HD12	2:L:16:LEU:HA	1.71	0.41
4:H:37:ARG:HG2	4:H:41:TYR:CZ	2.56	0.41
3:M:192:GLY:O	3:M:193:ASN:HB3	2.20	0.41
4:H:202:ASP:HB3	4:H:209:VAL:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:ASP:HB3	1:C:316:LEU:HA	2.03	0.41
1:C:146:ARG:NH2	13:C:344:HOH:O	2.50	0.41
3:M:198:PRO:HB3	4:H:17:TRP:CZ3	2.56	0.41
4:H:142:ASP:OD1	4:H:142:ASP:N	2.54	0.41
4:H:152:PRO:HD2	4:H:171:LEU:HD11	2.02	0.41
8:L:702:LDA:H62	8:L:702:LDA:H11	2.02	0.40
4:H:198:LEU:O	4:H:201:CYS:HB2	2.21	0.40
2:L:22:PHE:HA	2:L:24:PHE:CE1	2.55	0.40
3:M:106:PRO:HG2	3:M:109:ASP:HB3	2.04	0.40
3:M:120:MET:O	3:M:123:SER:HB3	2.21	0.40
3:M:154:PHE:O	3:M:157:CYS:HB2	2.22	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	331/336 (98%)	320 (97%)	11 (3%)	0	100	100
2	L	273/273 (100%)	264 (97%)	9 (3%)	0	100	100
3	M	322/323 (100%)	308 (96%)	13 (4%)	1 (0%)	36	50
4	H	256/258 (99%)	247 (96%)	9 (4%)	0	100	100
All	All	1182/1190 (99%)	1139 (96%)	42 (4%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	322	PRO

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%)	266 (95%)	15 (5%)	20 36
2	L	220/218 (101%)	214 (97%)	6 (3%)	39 62
3	M	250/249 (100%)	246 (98%)	4 (2%)	55 76
4	H	212/212 (100%)	189 (89%)	23 (11%)	6 9
All	All	963/961 (100%)	915 (95%)	48 (5%)	22 38

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1	CYS
1	C	15	ARG
1	C	18	SER
1	C	22	VAL
1	C	23	LEU
1	C	29	LYS
1	C	146	ARG
1	C	151	THR
1	C	152	LEU
1	C	166	VAL
1	C	199	ARG
1	C	220	ARG
1	C	288	SER
1	C	292	SER
1	C	322	LEU
2	L	16	LEU
2	L	44	LEU
2	L	81	LEU
2	L	82	GLU
2	L	119	LEU
2	L	271	PHE
3	M	71	PHE
3	M	120	MET
3	M	194	PHE

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Mol	Chain	Res	Type
3	M	323	LYS
4	H	9	HIS
4	H	10	LEU
4	H	30	LEU
4	H	69	VAL
4	H	81	ARG
4	H	89	LYS
4	H	94	ASP
4	H	97	GLU
4	H	102	GLN
4	H	141	THR
4	H	144	SER
4	H	147	GLU
4	H	169	THR
4	H	185	LEU
4	H	195	LEU
4	H	198	LEU
4	H	205	LYS
4	H	212	SER
4	H	226	SER
4	H	233	ARG
4	H	236	ASP
4	H	257	LEU
4	H	258	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	37	GLN
1	C	297	GLN
2	L	214	GLN
2	L	239	ASN
3	M	16	HIS
4	H	102	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	FME	H	1[B]	4	8,9,10	0.61	0	8,9,11	2.76	2 (25%)
4	FME	H	1[A]	4	8,9,10	0.67	0	8,9,11	2.09	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FME	H	1[B]	4	-	4/7/9/11	-
4	FME	H	1[A]	4	-	3/7/9/11	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	1[B]	FME	CA-N-CN	-5.33	114.62	122.82
4	H	1[B]	FME	O1-CN-N	-5.12	112.09	125.32
4	H	1[A]	FME	O1-CN-N	-3.90	115.25	125.32
4	H	1[A]	FME	CA-N-CN	-3.81	116.96	122.82

There are no chirality outliers.

All (7) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
4	H	1[B]	FME	CA-CB-CG-SD
4	H	1[A]	FME	CB-CG-SD-CE
4	H	1[B]	FME	C-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 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	BPB	L	402	-	57,70,70	1.73	10 (17%)	55,101,101	2.52	15 (27%)
8	LDA	M	706	-	13,15,15	2.54	2 (15%)	14,17,17	0.50	0
6	BCB	L	302	2	68,74,74	1.41	8 (11%)	77,115,115	1.88	13 (16%)
6	BCB	L	304	2	68,74,74	1.28	8 (11%)	77,115,115	1.85	9 (11%)
8	LDA	M	704	-	13,15,15	2.43	2 (15%)	14,17,17	0.54	0
8	LDA	L	702	-	13,15,15	2.09	2 (15%)	14,17,17	0.69	0
10	SO4	H	801	-	4,4,4	0.65	0	6,6,6	0.37	0
5	HEC	C	338	1	50,50,50	1.10	2 (4%)	68,82,82	1.43	5 (7%)
5	HEC	C	340	1	50,50,50	0.91	2 (4%)	68,82,82	1.39	4 (5%)
5	HEC	C	339	1	50,50,50	1.07	4 (8%)	68,82,82	1.34	6 (8%)
7	BPB	M	401	-	57,70,70	1.63	11 (19%)	55,101,101	2.37	12 (21%)
11	MQ7	M	501	-	49,49,49	1.57	9 (18%)	61,63,63	1.31	8 (13%)
5	HEC	C	337	1	50,50,50	1.10	2 (4%)	68,82,82	1.55	12 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	BCB	M	805	3	68,74,74	1.36	9 (13%)	77,115,115	1.82	12 (15%)
8	LDA	H	701	-	13,15,15	2.42	2 (15%)	14,17,17	0.76	0
10	SO4	M	804	-	4,4,4	0.88	0	6,6,6	0.69	0
8	LDA	M	705	-	13,15,15	2.44	2 (15%)	14,17,17	0.52	0
10	SO4	M	802	-	4,4,4	0.91	0	6,6,6	0.85	0
12	NS5	M	600	-	39,39,39	0.68	0	46,46,46	1.12	5 (10%)
6	BCB	M	806	3	68,74,74	1.12	5 (7%)	77,115,115	2.19	14 (18%)
10	SO4	M	803	-	4,4,4	0.55	0	6,6,6	0.51	0
8	LDA	H	703	-	13,15,15	2.42	2 (15%)	14,17,17	0.59	0
8	LDA	L	707	-	13,15,15	1.84	1 (7%)	14,17,17	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BPB	L	402	-	-	4/37/105/105	0/5/6/6
8	LDA	M	706	-	-	5/13/13/13	-
6	BCB	L	302	2	3/3/21/26	4/41/137/137	-
6	BCB	L	304	2	2/2/21/26	5/41/137/137	-
8	LDA	M	704	-	-	4/13/13/13	-
8	LDA	L	702	-	-	3/13/13/13	-
5	HEC	C	338	1	1/1/3/7	8/14/54/54	-
5	HEC	C	340	1	1/1/3/7	5/14/54/54	-
5	HEC	C	339	1	1/1/3/7	4/14/54/54	-
7	BPB	M	401	-	-	6/37/105/105	0/5/6/6
11	MQ7	M	501	-	-	1/41/61/61	0/2/2/2
5	HEC	C	337	1	1/1/3/7	8/14/54/54	-
6	BCB	M	805	3	3/3/21/26	10/41/137/137	-
8	LDA	H	701	-	-	4/13/13/13	-
8	LDA	M	705	-	-	2/13/13/13	-
12	NS5	M	600	-	-	11/43/43/43	-
6	BCB	M	806	3	3/3/21/26	3/41/137/137	-
8	LDA	H	703	-	-	5/13/13/13	-
8	LDA	L	707	-	-	5/13/13/13	-

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	701	LDA	O1-N1	-8.26	1.21	1.42
8	H	703	LDA	O1-N1	-7.53	1.23	1.42
8	M	704	LDA	O1-N1	-7.35	1.24	1.42
8	M	706	LDA	O1-N1	-7.33	1.24	1.42
8	L	702	LDA	O1-N1	-7.04	1.24	1.42
8	M	705	LDA	O1-N1	-6.94	1.25	1.42
8	L	707	LDA	O1-N1	-6.13	1.27	1.42
6	L	302	BCB	MG-NA	5.42	2.19	2.06
6	M	805	BCB	MG-NA	5.41	2.19	2.06
8	M	706	LDA	C1-N1	-5.39	1.45	1.51
8	M	705	LDA	C1-N1	-5.30	1.46	1.51
7	L	402	BPB	C1D-C2D	5.20	1.45	1.39
7	M	401	BPB	C1D-C2D	5.02	1.45	1.39
6	L	304	BCB	MG-NA	5.00	2.18	2.06
7	L	402	BPB	C1B-C2B	4.97	1.45	1.39
8	M	704	LDA	C1-N1	-4.68	1.46	1.51
6	L	302	BCB	MG-ND	-4.49	1.96	2.05
5	C	337	HEC	FE-NB	4.48	2.08	1.94
11	M	501	MQ7	C11-C12	-4.45	1.43	1.50
7	L	402	BPB	C3A-C2A	-4.45	1.50	1.54
6	L	302	BCB	O2D-CED	-4.44	1.35	1.45
6	M	806	BCB	MG-NA	4.32	2.16	2.06
8	H	703	LDA	C1-N1	-4.28	1.47	1.51
7	M	401	BPB	C1B-C2B	4.19	1.44	1.39
7	L	402	BPB	O2D-CGD	4.15	1.43	1.33
7	M	401	BPB	C3A-C2A	-4.15	1.51	1.54
6	L	302	BCB	C1-C2	-4.02	1.37	1.49
5	C	338	HEC	FE-NC	4.01	2.08	1.95
7	M	401	BPB	O2A-CGA	3.86	1.44	1.33
6	L	304	BCB	O2D-CED	-3.81	1.36	1.45
6	M	805	BCB	O2A-CGA	3.69	1.44	1.33
5	C	339	HEC	FE-NA	3.61	2.07	1.95
7	L	402	BPB	O2D-CED	-3.57	1.37	1.45
7	L	402	BPB	C3B-C4B	3.37	1.46	1.41
5	C	338	HEC	FE-NB	3.32	2.05	1.94
6	M	806	BCB	CAA-CBA	-3.22	1.43	1.52
11	M	501	MQ7	C26-C27	-3.21	1.40	1.50
11	M	501	MQ7	C32-C33	3.18	1.40	1.33
7	M	401	BPB	C3B-C2B	-3.07	1.34	1.39
6	M	805	BCB	O2D-CGD	3.07	1.40	1.33
6	M	805	BCB	O2D-CED	-3.06	1.38	1.45
5	C	340	HEC	FE-NA	3.03	2.05	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	304	BCB	C2-C3	2.97	1.39	1.33
5	C	337	HEC	FE-NA	2.97	2.05	1.95
5	C	339	HEC	FE-NB	2.95	2.04	1.94
7	M	401	BPB	C2-C3	2.92	1.39	1.33
11	M	501	MQ7	C17-C18	2.89	1.39	1.33
6	L	304	BCB	C3B-C4B	2.88	1.46	1.41
6	M	806	BCB	C2-C3	2.87	1.39	1.33
6	M	805	BCB	C3B-C4B	2.87	1.46	1.41
11	M	501	MQ7	C37-C38	2.85	1.39	1.33
7	L	402	BPB	C2-C3	2.82	1.39	1.33
6	M	805	BCB	C2-C3	2.77	1.39	1.33
8	H	701	LDA	C1-N1	-2.74	1.48	1.51
7	M	401	BPB	O2D-CGD	2.73	1.39	1.33
7	M	401	BPB	O2D-CED	-2.71	1.39	1.45
6	M	806	BCB	C3B-C4B	2.67	1.46	1.41
7	M	401	BPB	CHA-CBD	2.56	1.54	1.51
8	L	702	LDA	C1-N1	-2.55	1.48	1.51
5	C	340	HEC	FE-NB	2.54	2.02	1.94
6	M	805	BCB	C5-C3	2.53	1.56	1.51
6	L	304	BCB	CAC-C3C	2.49	1.39	1.33
11	M	501	MQ7	C27-C28	2.44	1.38	1.33
11	M	501	MQ7	C42-C43	2.43	1.39	1.32
7	M	401	BPB	C3B-C4B	2.42	1.45	1.41
6	L	302	BCB	C2-C3	2.40	1.38	1.33
7	L	402	BPB	CMD-C2D	2.39	1.56	1.51
7	L	402	BPB	C1-C2	-2.31	1.42	1.49
6	L	304	BCB	C1-C2	-2.30	1.42	1.49
11	M	501	MQ7	C10-C5	-2.30	1.37	1.40
6	L	302	BCB	CAC-C3C	2.29	1.39	1.33
6	L	302	BCB	CMB-C2B	2.28	1.55	1.50
6	L	302	BCB	C3B-C4B	2.24	1.45	1.41
5	C	339	HEC	CAB-C3B	2.21	1.56	1.51
6	M	806	BCB	C1-C2	-2.18	1.43	1.49
7	M	401	BPB	CBC-CAC	2.18	1.57	1.49
6	L	304	BCB	MG-ND	-2.15	2.01	2.05
11	M	501	MQ7	C22-C23	2.15	1.38	1.33
7	L	402	BPB	C1D-ND	-2.10	1.34	1.38
6	M	805	BCB	CAC-C3C	2.09	1.38	1.33
5	C	339	HEC	O2D-CGD	-2.05	1.24	1.30
6	L	304	BCB	O2D-CGD	2.02	1.38	1.33
6	M	805	BCB	MG-NC	2.01	2.11	2.06

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	401	BPB	O2D-CGD-CBD	12.03	124.16	110.95
7	L	402	BPB	O2D-CGD-CBD	10.58	122.57	110.95
6	M	806	BCB	C4A-NA-C1A	9.34	110.94	106.68
6	L	302	BCB	C4A-NA-C1A	8.45	110.53	106.68
6	L	304	BCB	C4A-NA-C1A	7.42	110.06	106.68
6	M	805	BCB	C4A-NA-C1A	7.40	110.06	106.68
6	L	304	BCB	O2D-CGD-CBD	7.10	123.64	111.23
6	M	805	BCB	O2D-CGD-CBD	6.88	123.26	111.23
7	L	402	BPB	O1D-CGD-CBD	-6.44	114.96	124.72
7	M	401	BPB	O1D-CGD-CBD	-6.38	115.06	124.72
6	M	806	BCB	O2D-CGD-CBD	6.24	122.14	111.23
7	L	402	BPB	C4D-CHA-CBD	-6.12	105.52	108.45
5	C	338	HEC	CAC-C3C-C4C	-5.96	116.71	124.91
5	C	338	HEC	CAC-C3C-C2C	5.72	135.94	126.89
6	M	806	BCB	CMB-C2B-C1B	-5.56	116.96	125.42
5	C	340	HEC	CAB-C3B-C4B	-5.43	117.73	124.79
6	M	806	BCB	C1C-NC-C4C	4.97	108.95	106.68
7	L	402	BPB	C2D-C1D-ND	4.95	113.01	109.43
5	C	340	HEC	CAC-C3C-C2C	4.93	134.69	126.89
6	M	806	BCB	OBB-CAB-C3B	4.91	129.12	120.43
7	M	401	BPB	C4D-CHA-CBD	-4.91	106.10	108.45
5	C	339	HEC	CAC-C3C-C2C	4.91	134.65	126.89
5	C	340	HEC	CAC-C3C-C4C	-4.86	118.23	124.91
5	C	338	HEC	CAB-C3B-C4B	-4.79	118.56	124.79
6	M	805	BCB	O1D-CGD-CBD	-4.78	115.08	124.52
6	L	304	BCB	O1D-CGD-CBD	-4.78	115.08	124.52
5	C	339	HEC	CAB-C3B-C4B	-4.71	118.66	124.79
6	L	302	BCB	O2D-CGD-CBD	4.65	119.36	111.23
5	C	339	HEC	CAC-C3C-C4C	-4.58	118.61	124.91
6	L	302	BCB	C1C-NC-C4C	4.55	108.75	106.68
5	C	337	HEC	CAC-C3C-C4C	-4.45	118.78	124.91
5	C	337	HEC	CAC-C3C-C2C	4.41	133.87	126.89
6	M	805	BCB	C1C-NC-C4C	4.40	108.69	106.68
5	C	340	HEC	CAB-C3B-C2B	4.39	135.62	127.56
6	M	806	BCB	O2A-CGA-CBA	4.28	124.89	111.83
7	L	402	BPB	OBD-CAD-CBD	-4.24	119.61	125.82
6	L	304	BCB	C1C-NC-C4C	4.11	108.56	106.68
6	M	806	BCB	O1D-CGD-CBD	-4.04	116.56	124.52
7	M	401	BPB	C1-C2-C3	3.99	132.74	126.20
5	C	339	HEC	CAB-C3B-C2B	3.91	134.75	127.56
5	C	337	HEC	CMD-C2D-C1D	3.69	130.79	125.03
7	L	402	BPB	C2B-C1B-NB	3.68	112.09	109.43
6	L	302	BCB	OBB-CAB-C3B	3.65	126.88	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	338	HEC	CAB-C3B-C2B	3.65	134.25	127.56
7	M	401	BPB	OBD-CAD-CBD	-3.64	120.48	125.82
6	M	806	BCB	CAA-C2A-C1A	-3.63	100.08	111.97
6	L	302	BCB	O1D-CGD-CBD	-3.62	117.38	124.52
5	C	337	HEC	CAB-C3B-C4B	-3.58	120.14	124.79
12	M	600	NS5	C19-C18-C17	3.54	130.76	123.52
6	M	806	BCB	O2A-CGA-O1A	-3.49	114.90	123.63
7	M	401	BPB	CMA-C3A-C4A	-3.31	107.49	114.61
6	M	806	BCB	CBB-CAB-C3B	-3.29	113.46	120.40
7	L	402	BPB	C4B-NB-C1B	-3.27	104.05	108.82
7	M	401	BPB	CED-O2D-CGD	3.26	123.32	115.92
5	C	337	HEC	CMA-C3A-C4A	3.20	130.36	124.73
7	L	402	BPB	CMD-C2D-C3D	3.19	131.06	124.68
6	M	806	BCB	CMB-C2B-C3B	3.06	135.32	125.67
11	M	501	MQ7	C41-C42-C43	3.06	137.83	127.64
5	C	337	HEC	CAA-C2A-C3A	-3.05	122.16	127.87
6	L	302	BCB	O2A-CGA-CBA	3.01	121.00	111.83
7	L	402	BPB	C4D-ND-C1D	-2.97	105.31	108.87
5	C	337	HEC	CAB-C3B-C2B	2.97	133.01	127.56
6	L	304	BCB	CAB-C3B-C2B	2.95	133.87	127.74
6	M	806	BCB	CAB-C3B-C2B	2.94	133.84	127.74
5	C	337	HEC	CAD-C3D-C4D	2.93	129.80	124.70
6	L	304	BCB	C4-C3-C5	-2.86	110.26	115.23
11	M	501	MQ7	C35-C33-C32	2.86	127.59	121.17
6	L	302	BCB	CAB-C3B-C2B	2.81	133.57	127.74
6	L	302	BCB	C2A-C1A-CHA	2.80	128.72	123.87
6	L	302	BCB	C15-C13-C12	-2.79	97.94	112.07
6	L	302	BCB	CBB-CAB-C3B	-2.78	114.54	120.40
11	M	501	MQ7	C34-C33-C35	-2.76	110.44	115.23
12	M	600	NS5	C18-C19-C20	2.74	129.13	123.52
6	L	302	BCB	CMB-C2B-C1B	-2.73	121.25	125.42
7	M	401	BPB	CMD-C2D-C3D	2.73	130.13	124.68
5	C	337	HEC	CAA-C2A-C1A	2.69	130.33	124.85
11	M	501	MQ7	C26-C25-C23	-2.67	104.33	113.19
12	M	600	NS5	C19-C20-C21	-2.67	123.53	127.28
11	M	501	MQ7	C39-C38-C40	-2.62	110.68	115.23
6	L	302	BCB	O2A-CGA-O1A	-2.61	117.09	123.63
6	M	805	BCB	CBB-CAB-C3B	2.59	125.87	120.40
6	M	806	BCB	CBC-CAC-C3C	-2.58	119.70	126.70
11	M	501	MQ7	C25-C23-C22	2.57	126.93	121.17
6	M	805	BCB	C6-C5-C3	2.54	119.66	113.47
6	M	805	BCB	CMB-C2B-C1B	-2.51	121.60	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	M	600	NS5	C16-C15-C14	-2.44	114.36	118.09
6	L	304	BCB	CBB-CAB-C3B	-2.44	115.27	120.40
7	L	402	BPB	O2A-CGA-CBA	2.43	119.26	111.83
11	M	501	MQ7	C36-C35-C33	-2.43	105.13	113.19
7	L	402	BPB	CMA-C3A-C4A	-2.37	109.50	114.61
6	M	805	BCB	C1-C2-C3	2.37	130.08	126.20
5	C	338	HEC	CBA-CAA-C2A	-2.37	105.98	112.53
7	L	402	BPB	C3D-C4D-ND	2.37	110.75	107.71
5	C	337	HEC	CAD-C3D-C2D	-2.36	123.45	127.87
6	L	304	BCB	O2A-CGA-CBA	2.34	118.95	111.83
6	L	304	BCB	C15-C13-C12	-2.33	100.27	112.07
6	M	805	BCB	OBB-CAB-C3B	-2.32	116.33	120.43
5	C	339	HEC	CMB-C2B-C1B	-2.32	121.41	125.03
7	M	401	BPB	C4D-ND-C1D	-2.31	106.10	108.87
5	C	337	HEC	CMC-C2C-C3C	2.27	130.44	125.62
6	L	302	BCB	CHB-C1B-NB	2.23	127.39	124.05
6	M	805	BCB	CHB-C1B-NB	2.21	127.36	124.05
6	M	806	BCB	CHD-C1D-ND	-2.20	121.70	124.80
7	L	402	BPB	CED-O2D-CGD	2.20	120.92	115.92
11	M	501	MQ7	C11-C3-C2	-2.20	121.12	124.89
12	M	600	NS5	C22-C21-C23	-2.20	114.73	118.09
7	M	401	BPB	C3D-C4D-ND	2.19	110.51	107.71
5	C	339	HEC	CMB-C2B-C3B	2.16	131.99	126.15
7	M	401	BPB	OBD-CAD-C3D	2.15	131.24	127.89
6	M	805	BCB	C2A-C1A-CHA	2.10	127.50	123.87
6	M	805	BCB	C4-C3-C2	-2.09	118.27	123.63
7	M	401	BPB	OBB-CAB-C3B	2.08	123.47	119.99
7	L	402	BPB	C1-C2-C3	2.03	129.51	126.20
5	C	337	HEC	CBD-CAD-C3D	-2.01	106.99	112.53
7	L	402	BPB	OBD-CAD-C3D	2.00	131.02	127.89

All (15) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	337	HEC	NA
5	C	338	HEC	NA
5	C	339	HEC	NA
5	C	340	HEC	NA
6	L	302	BCB	NA
6	L	302	BCB	NC
6	L	302	BCB	ND
6	L	304	BCB	NA

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Mol	Chain	Res	Type	Atom
6	L	304	BCB	NC
6	M	805	BCB	NA
6	M	805	BCB	NC
6	M	805	BCB	ND
6	M	806	BCB	NA
6	M	806	BCB	NC
6	M	806	BCB	ND

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	M	806	BCB	CAD-CBD-CGD-O1D
6	M	806	BCB	CAD-CBD-CGD-O2D
12	M	600	NS5	C9-C10-C12-C13
12	M	600	NS5	C11-C10-C12-C13
12	M	600	NS5	C10-C12-C13-C14
12	M	600	NS5	C20-C21-C23-C24
5	C	337	HEC	C2B-C3B-CAB-CBB
6	L	302	BCB	C4-C3-C5-C6
12	M	600	NS5	C3-C4-C5-C7
5	C	337	HEC	C4B-C3B-CAB-CBB
5	C	338	HEC	C4B-C3B-CAB-CBB
5	C	338	HEC	C2B-C3B-CAB-CBB
7	M	401	BPB	C4-C3-C5-C6
6	L	302	BCB	C2-C3-C5-C6
6	M	805	BCB	C2-C3-C5-C6
7	M	401	BPB	C2-C3-C5-C6
5	C	339	HEC	C2C-C3C-CAC-CBC
12	M	600	NS5	C6-C5-C7-C8
6	M	805	BCB	C4-C3-C5-C6
6	M	805	BCB	C11-C12-C13-C14
12	M	600	NS5	C22-C21-C23-C24
5	C	338	HEC	C2C-C3C-CAC-CBC
5	C	339	HEC	C4C-C3C-CAC-CBC
6	M	806	BCB	C2A-CAA-CBA-CGA
5	C	340	HEC	C2B-C3B-CAB-CBB
5	C	338	HEC	C4C-C3C-CAC-CBC
6	M	805	BCB	C15-C16-C17-C18
7	L	402	BPB	O2A-C1-C2-C3
5	C	337	HEC	C2C-C3C-CAC-CBC
8	L	702	LDA	C2-C3-C4-C5
8	L	702	LDA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
8	L	707	LDA	C4-C5-C6-C7
5	C	339	HEC	C2B-C3B-CAB-CBB
8	L	707	LDA	C3-C4-C5-C6
8	M	706	LDA	C3-C4-C5-C6
8	H	703	LDA	C11-C10-C9-C8
8	H	703	LDA	C3-C4-C5-C6
8	M	706	LDA	C5-C6-C7-C8
8	L	702	LDA	C1-C2-C3-C4
5	C	337	HEC	C4C-C3C-CAC-CBC
6	M	805	BCB	C3-C5-C6-C7
8	M	704	LDA	C4-C5-C6-C7
7	M	401	BPB	C12-C13-C15-C16
12	M	600	NS5	C3-C4-C5-C6
6	M	805	BCB	C10-C11-C12-C13
8	H	703	LDA	C5-C6-C7-C8
8	H	701	LDA	C7-C8-C9-C10
5	C	339	HEC	C4B-C3B-CAB-CBB
8	M	706	LDA	C4-C5-C6-C7
7	M	401	BPB	C5-C6-C7-C8
7	M	401	BPB	C13-C15-C16-C17
8	M	704	LDA	C5-C6-C7-C8
7	M	401	BPB	C14-C13-C15-C16
6	L	304	BCB	O1D-CGD-O2D-CED
5	C	340	HEC	C2C-C3C-CAC-CBC
8	M	705	LDA	C1-C2-C3-C4
6	L	304	BCB	CBD-CGD-O2D-CED
12	M	600	NS5	C19-C20-C21-C22
8	L	707	LDA	C2-C3-C4-C5
7	L	402	BPB	C16-C17-C18-C20
5	C	340	HEC	C4B-C3B-CAB-CBB
8	H	703	LDA	C9-C10-C11-C12
8	M	704	LDA	C7-C8-C9-C10
6	L	302	BCB	CAD-CBD-CGD-O1D
12	M	600	NS5	C29-C30-C31-C33
8	L	707	LDA	C11-C10-C9-C8
6	L	304	BCB	C14-C13-C15-C16
8	M	706	LDA	C1-C2-C3-C4
6	M	805	BCB	C4B-C3B-CAB-CBB
8	M	705	LDA	C2-C3-C4-C5
8	H	703	LDA	C2-C3-C4-C5
7	L	402	BPB	C8-C10-C11-C12
5	C	337	HEC	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
8	H	701	LDA	C4-C5-C6-C7
5	C	337	HEC	CAA-CBA-CGA-O1A
8	L	707	LDA	C6-C7-C8-C9
5	C	338	HEC	CAA-CBA-CGA-O1A
5	C	337	HEC	CAA-CBA-CGA-O2A
8	M	704	LDA	C6-C7-C8-C9
6	L	304	BCB	C12-C13-C15-C16
12	M	600	NS5	C12-C10-C9-C8
7	L	402	BPB	C13-C15-C16-C17
5	C	338	HEC	CAA-CBA-CGA-O2A
8	M	706	LDA	C11-C10-C9-C8
5	C	338	HEC	CAD-CBD-CGD-O2D
6	L	304	BCB	C13-C15-C16-C17
8	H	701	LDA	C5-C6-C7-C8
5	C	338	HEC	CAD-CBD-CGD-O1D
5	C	340	HEC	C4C-C3C-CAC-CBC
8	H	701	LDA	C3-C4-C5-C6
11	M	501	MQ7	C38-C40-C41-C42
6	M	805	BCB	C2C-C3C-CAC-CBC
6	M	805	BCB	C2B-C3B-CAB-CBB
6	L	302	BCB	C15-C16-C17-C18
6	M	805	BCB	C4B-C3B-CAB-OBB
5	C	337	HEC	CAD-CBD-CGD-O2D
5	C	340	HEC	CAD-CBD-CGD-O2D

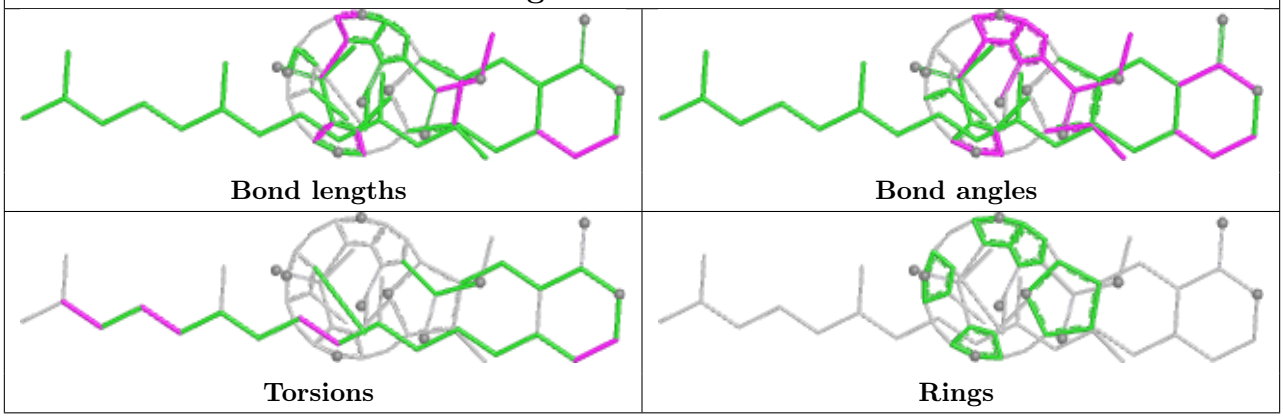
There are no ring outliers.

12 monomers are involved in 45 short contacts:

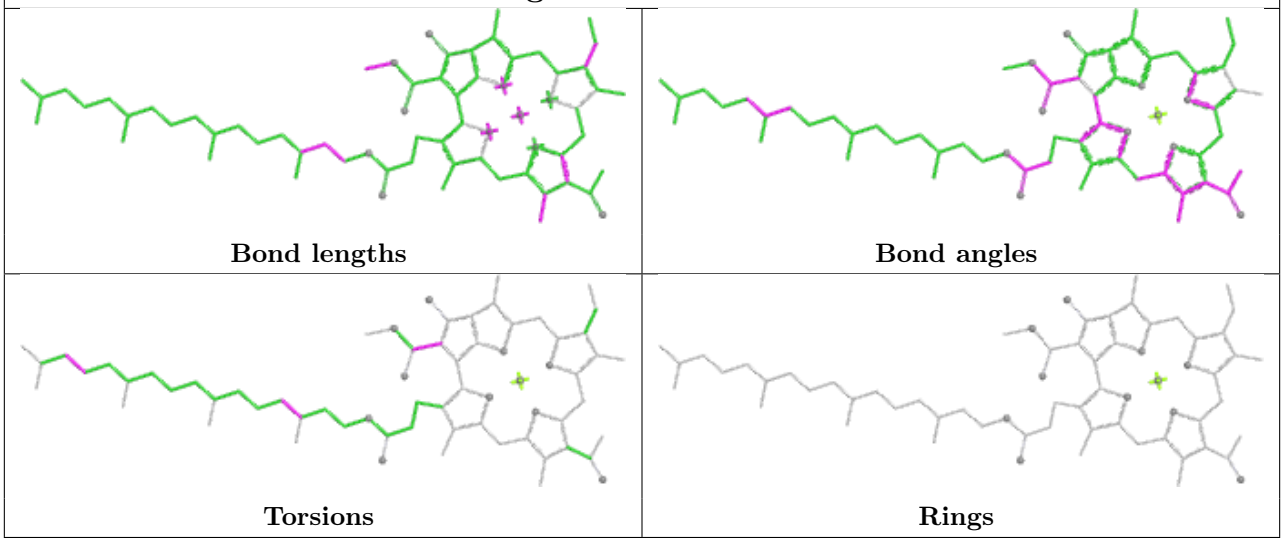
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	402	BPB	4	0
8	M	706	LDA	2	0
6	L	302	BCB	3	0
6	L	304	BCB	2	0
8	L	702	LDA	8	0
5	C	338	HEC	1	0
5	C	339	HEC	1	0
7	M	401	BPB	11	0
5	C	337	HEC	2	0
6	M	805	BCB	6	0
6	M	806	BCB	6	0
8	L	707	LDA	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

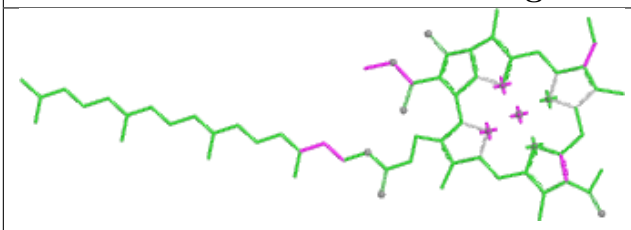
Ligand BPB L 402



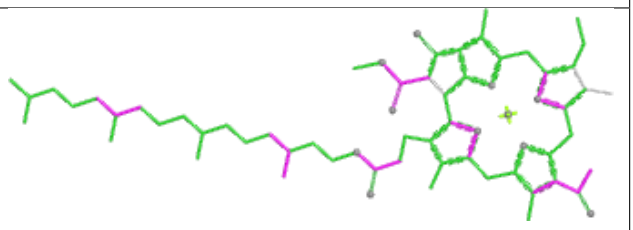
Ligand BCB L 302



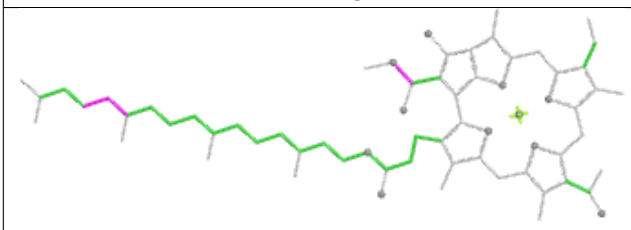
Ligand BCB L 304



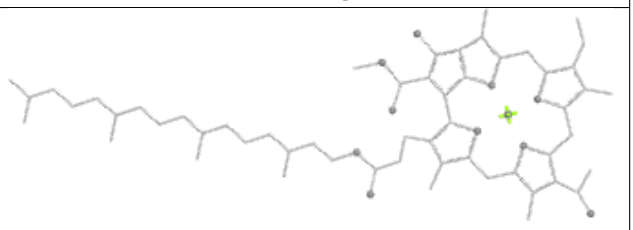
Bond lengths



Bond angles

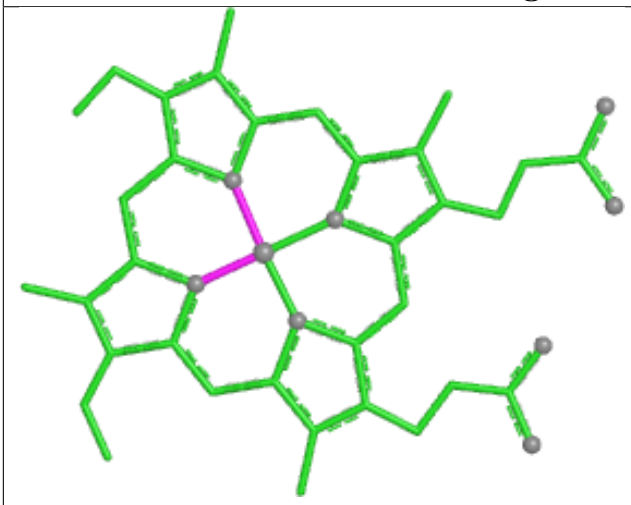


Torsions

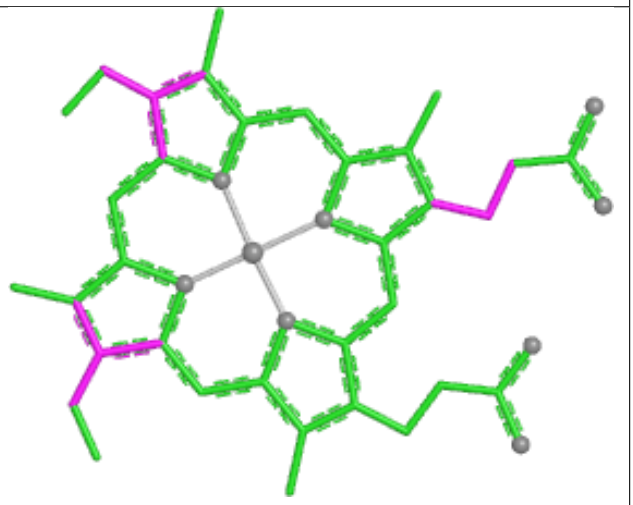


Rings

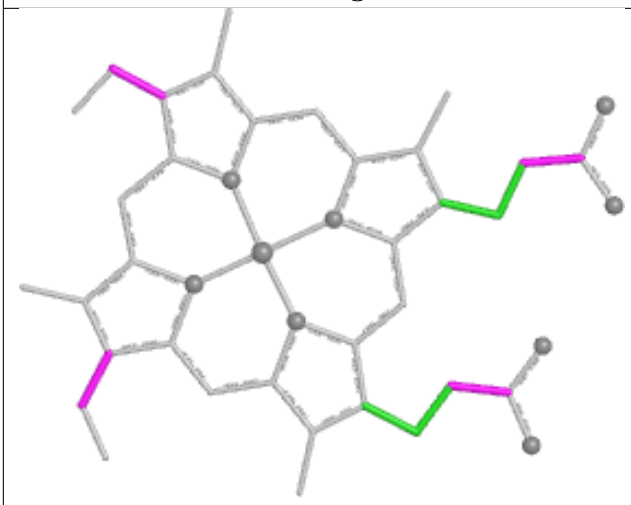
Ligand HEC C 338



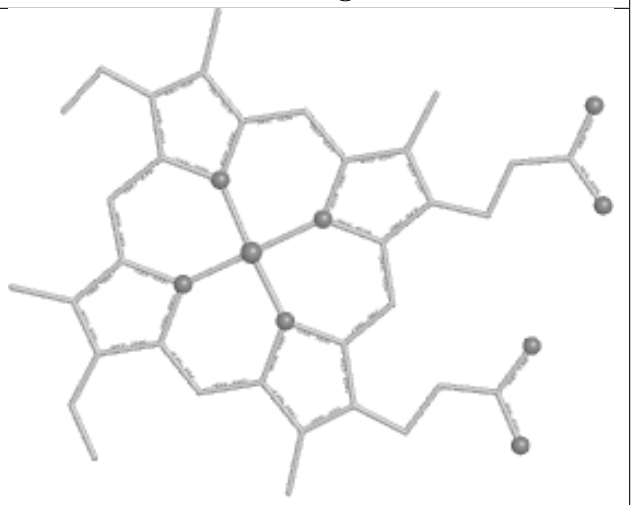
Bond lengths



Bond angles

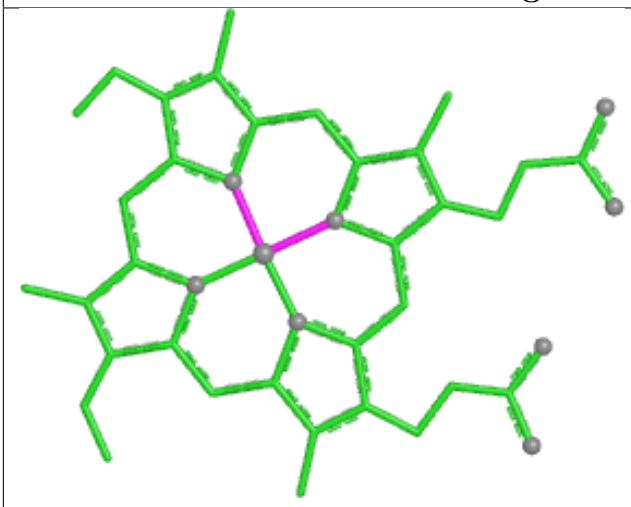


Torsions

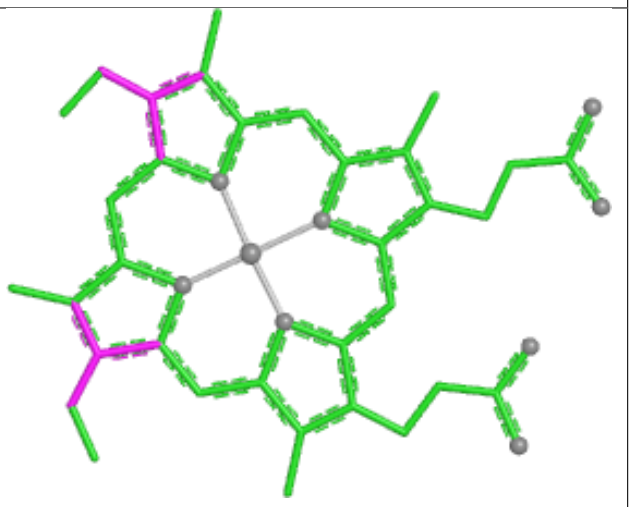


Rings

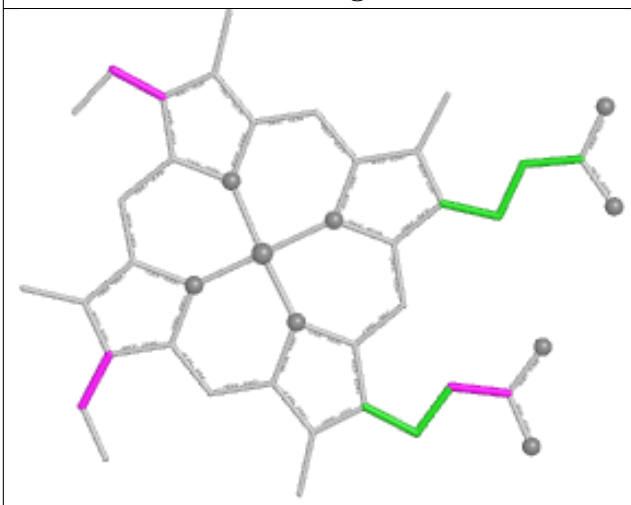
Ligand HEC C 340



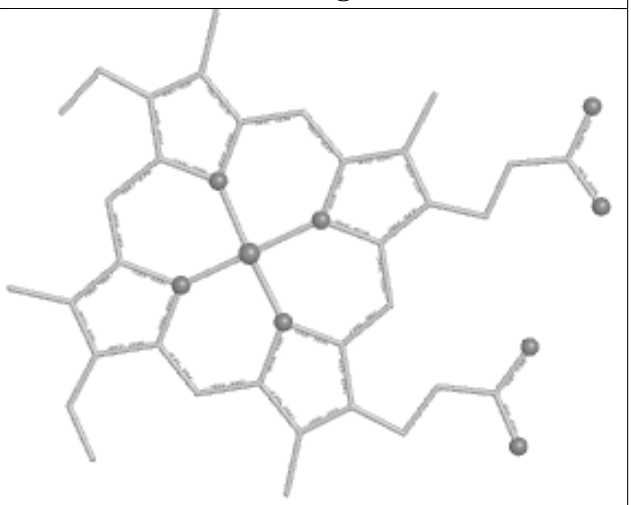
Bond lengths



Bond angles

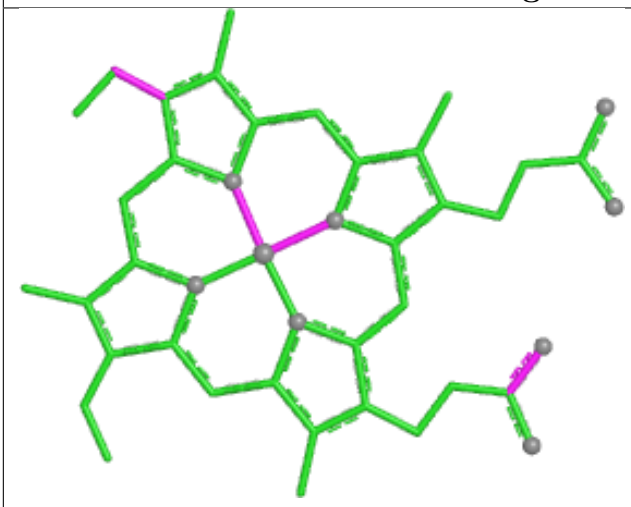


Torsions

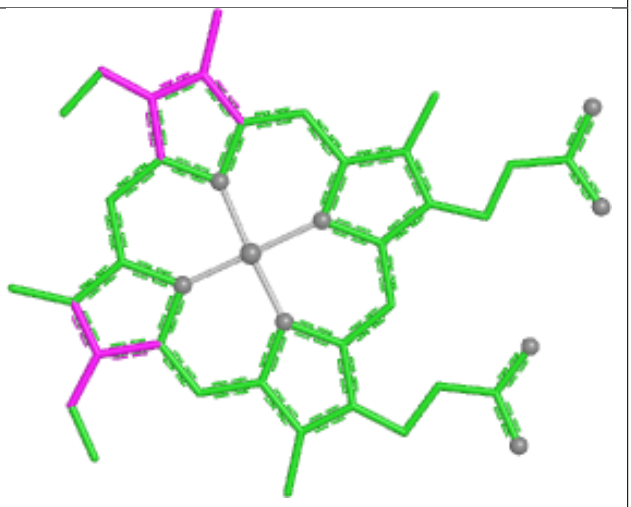


Rings

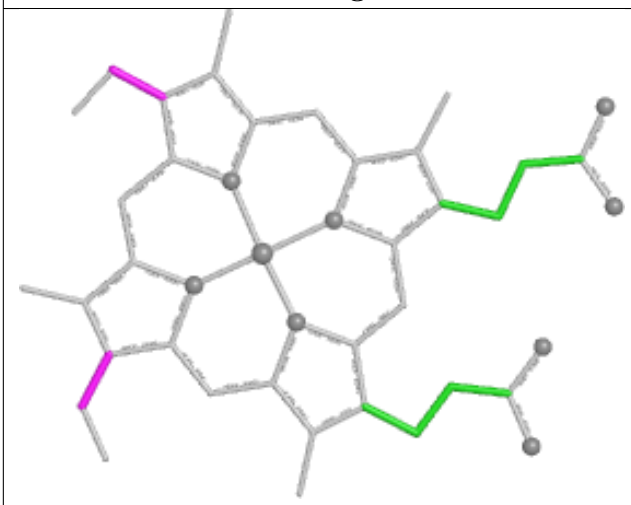
Ligand HEC C 339



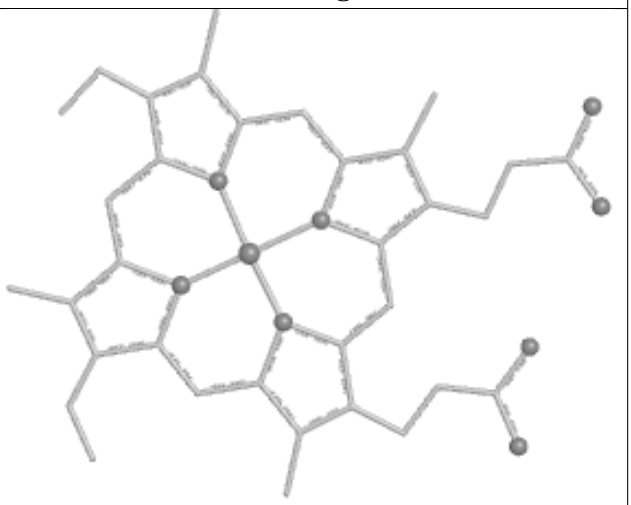
Bond lengths



Bond angles

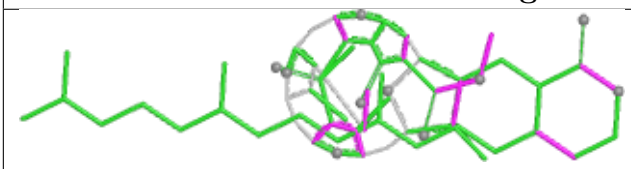


Torsions



Rings

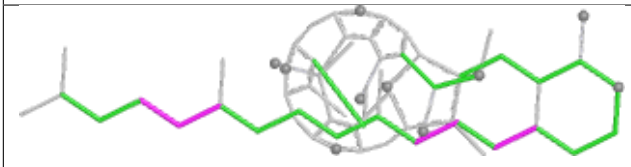
Ligand BPB M 401



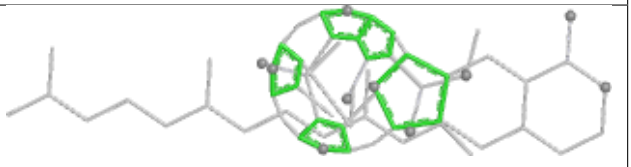
Bond lengths



Bond angles

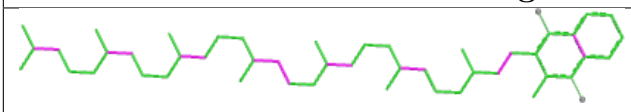


Torsions

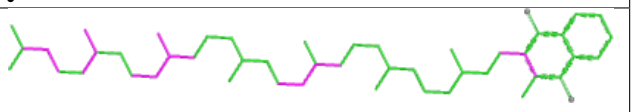


Rings

Ligand MQ7 M 501



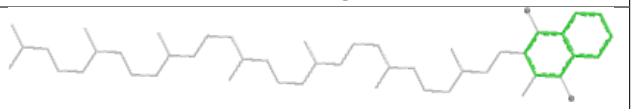
Bond lengths



Bond angles

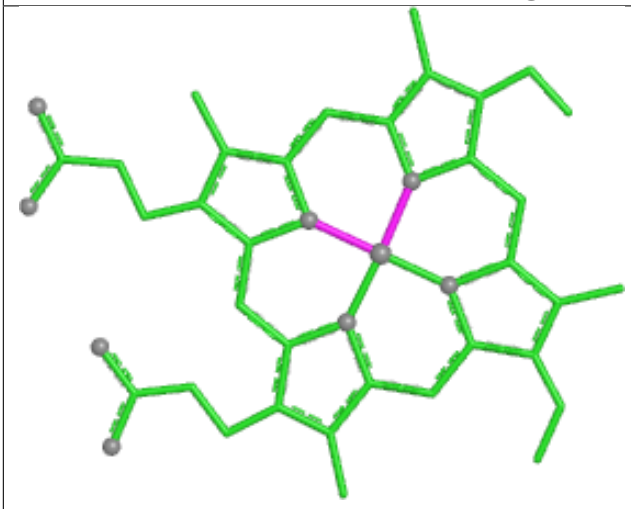


Torsions

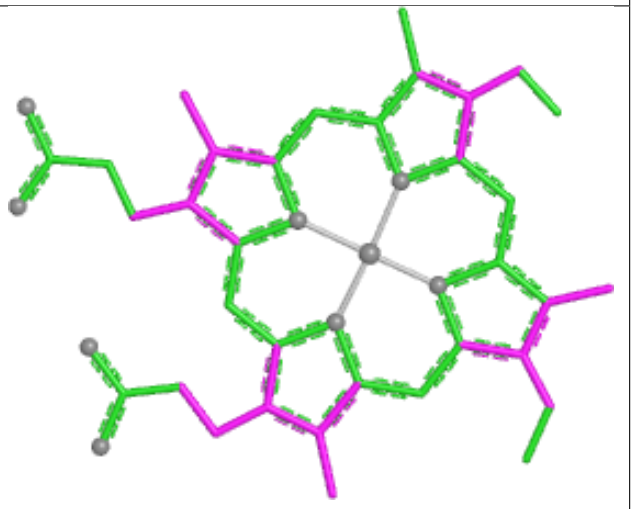


Rings

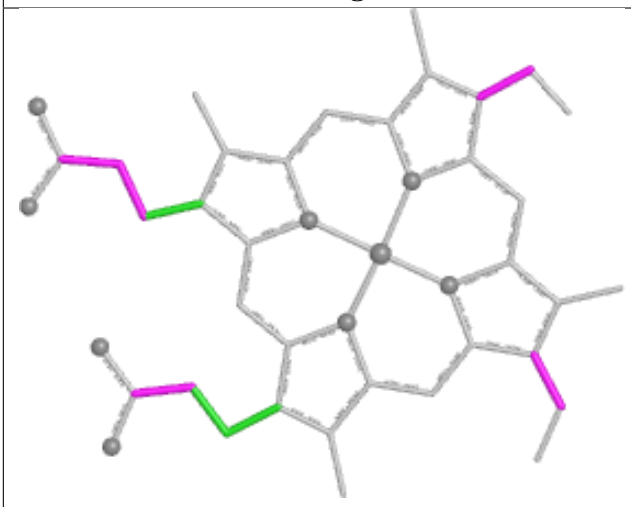
Ligand HEC C 337



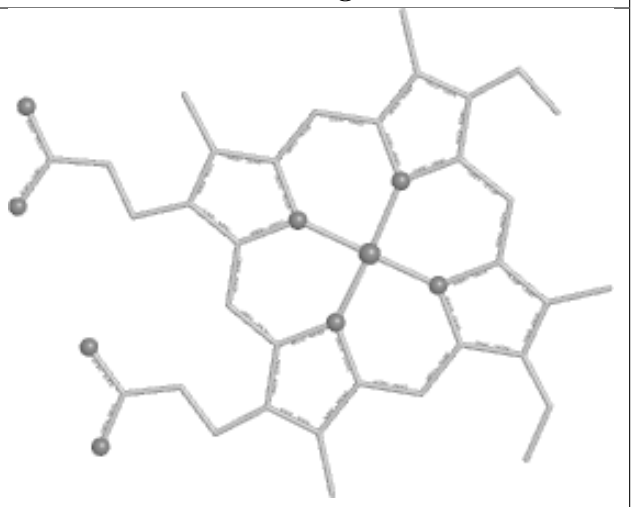
Bond lengths



Bond angles

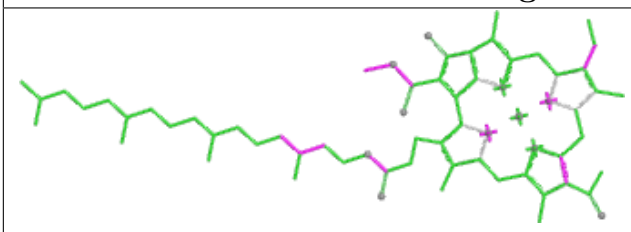


Torsions

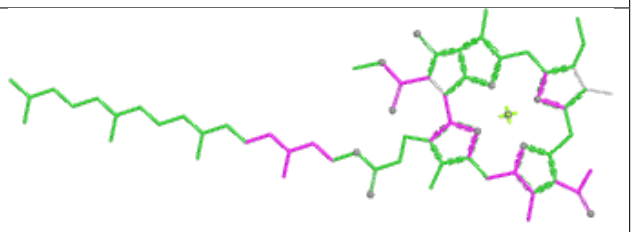


Rings

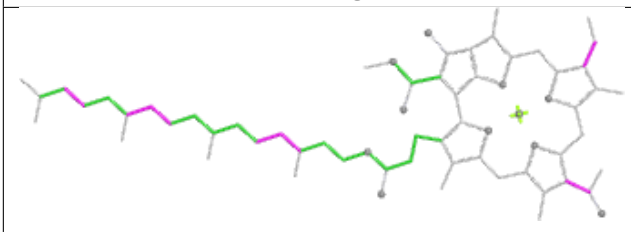
Ligand BCB M 805



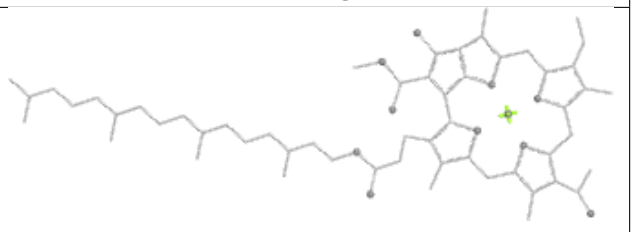
Bond lengths



Bond angles

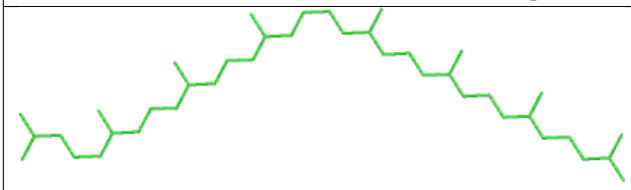


Torsions

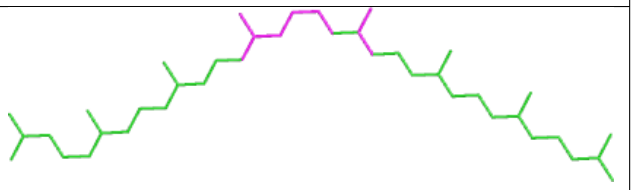


Rings

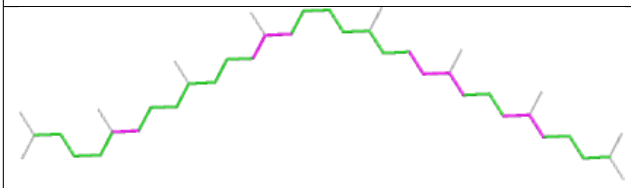
Ligand NS5 M 600



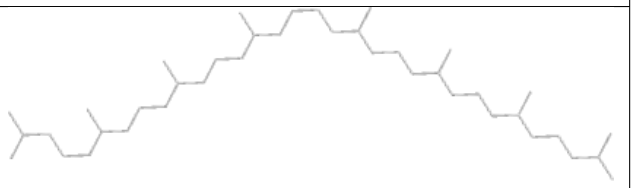
Bond lengths



Bond angles

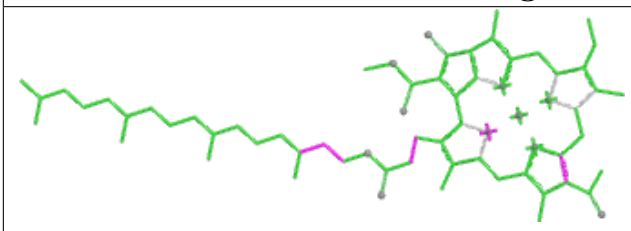


Torsions

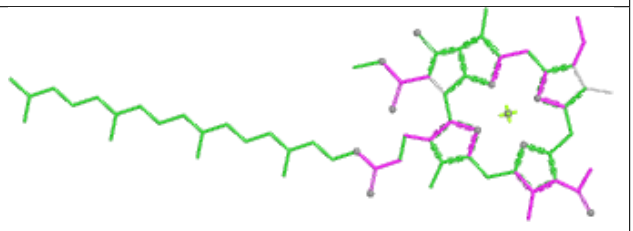


Rings

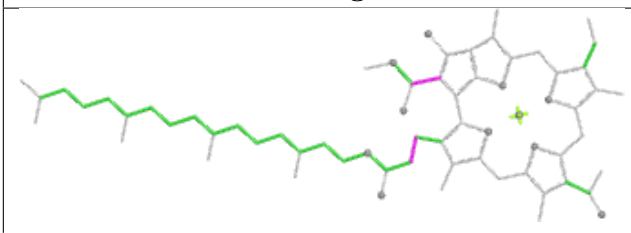
Ligand BCB M 806



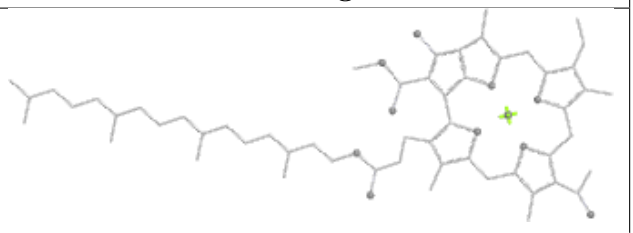
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.90	0	100	100	11, 25, 46, 67	16 (4%)
2	L	273/273 (100%)	-0.99	0	100	100	9, 19, 39, 50	9 (3%)
3	M	323/323 (100%)	-0.91	0	100	100	9, 22, 50, 61	9 (2%)
4	H	249/258 (96%)	-0.65	3 (1%)	76	73	12, 28, 46, 61	22 (8%)
All	All	1177/1190 (98%)	-0.87	3 (0%)	90	88	9, 23, 46, 67	56 (4%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	45	GLU	3.0
4	H	8	GLN	2.8
4	H	7	ALA	2.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	FME	H	1[A]	10/11	0.94	0.08	22,25,27,27	10
4	FME	H	1[B]	10/11	0.94	0.08	27,30,30,30	10

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands (i)

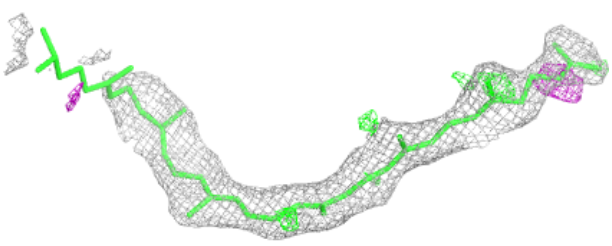
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

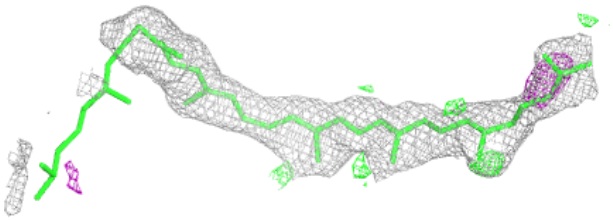
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	LDA	L	707	16/16	0.72	0.13	54,64,65,66	0
8	LDA	M	705	16/16	0.74	0.11	51,55,59,59	5
8	LDA	M	706	16/16	0.77	0.15	69,70,72,72	4
8	LDA	M	704	16/16	0.82	0.11	53,59,61,62	3
12	NS5	M	600	40/40	0.87	0.09	31,49,68,68	9
8	LDA	H	703	16/16	0.91	0.08	30,41,52,52	1
10	SO4	M	803	5/5	0.92	0.10	85,85,86,86	0
6	BCB	M	805	66/66	0.94	0.08	8,18,37,38	20
8	LDA	H	701	16/16	0.95	0.05	28,30,31,32	0
8	LDA	L	702	16/16	0.95	0.09	19,44,66,66	0
10	SO4	H	801	5/5	0.96	0.07	64,65,65,67	0
7	BPB	M	401	65/65	0.97	0.05	10,24,61,62	7
7	BPB	L	402	65/65	0.98	0.04	7,12,18,20	0
6	BCB	L	304	66/66	0.98	0.04	6,13,26,36	0
10	SO4	M	804	5/5	0.98	0.07	40,41,42,43	0
6	BCB	L	302	66/66	0.98	0.03	7,11,18,19	0
11	MQ7	M	501	48/48	0.98	0.04	11,17,43,49	0
6	BCB	M	806	66/66	0.98	0.04	4,12,30,31	0
5	HEC	C	338	43/43	0.99	0.04	16,25,32,38	0
5	HEC	C	339	43/43	0.99	0.04	8,14,18,25	0
5	HEC	C	340	43/43	0.99	0.05	11,19,34,42	0
5	HEC	C	337	43/43	0.99	0.05	21,27,38,43	0
10	SO4	M	802	5/5	0.99	0.06	30,30,32,39	0
9	FE2	M	500	1/1	1.00	0.01	14,14,14,14	0

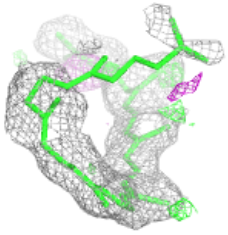
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NS5 M 600:

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

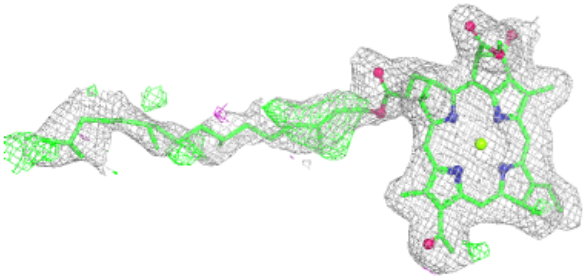


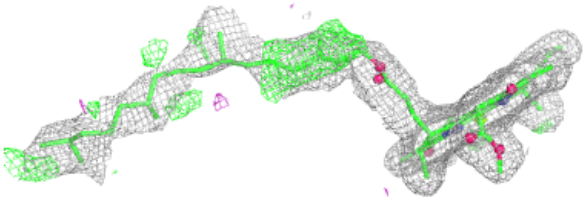


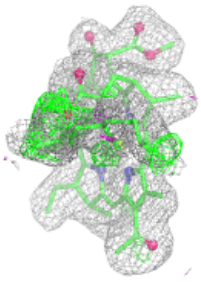


Electron density around BCB M 805:

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

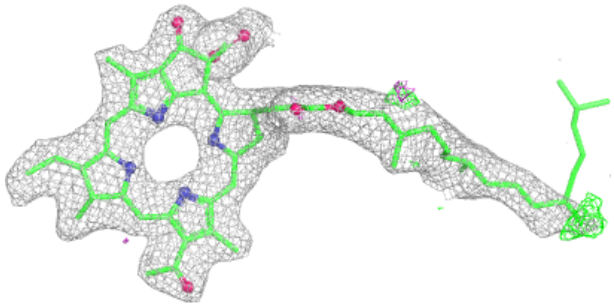


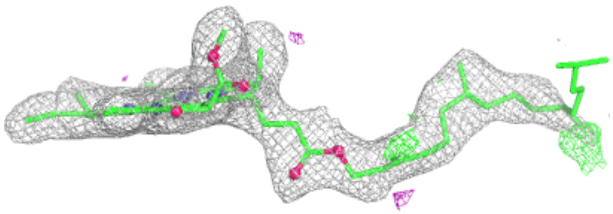




Electron density around BPB M 401:

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

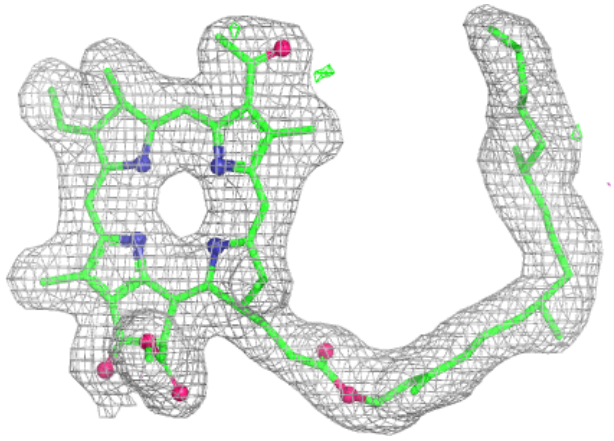


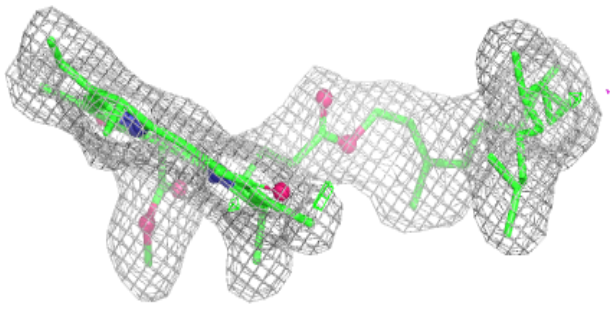


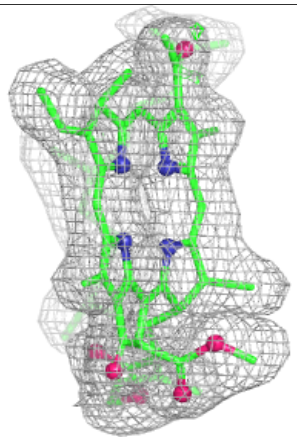


Electron density around BPB L 402:

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

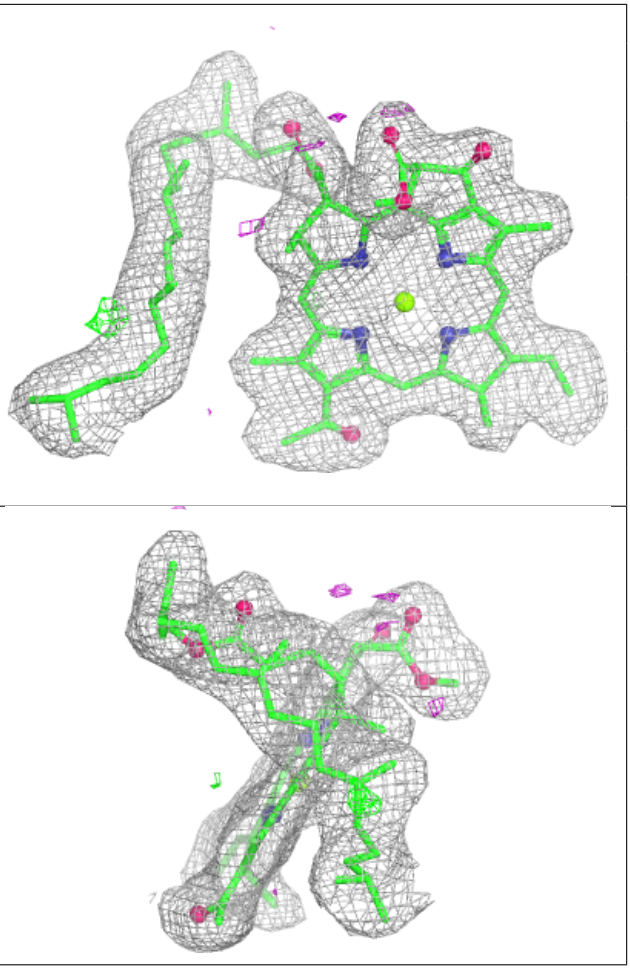


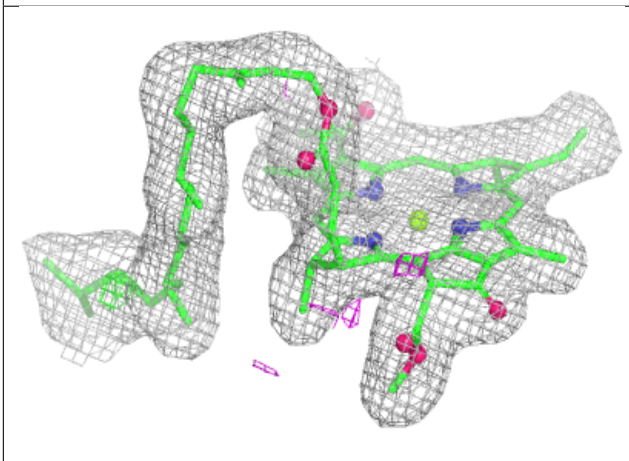




Electron density around BCB L 304:

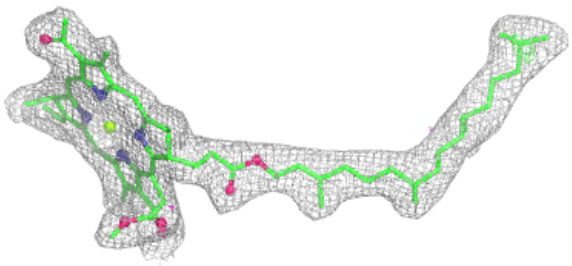
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

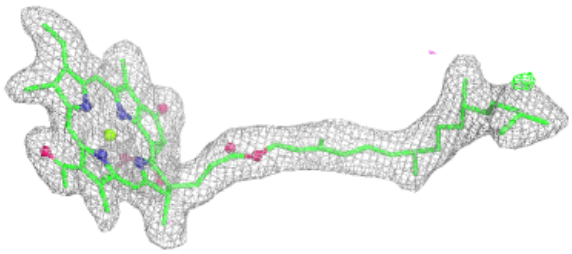


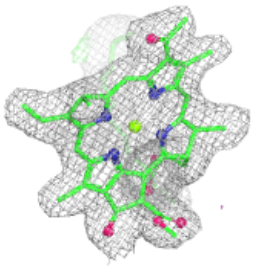


Electron density around BCB L 302:

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

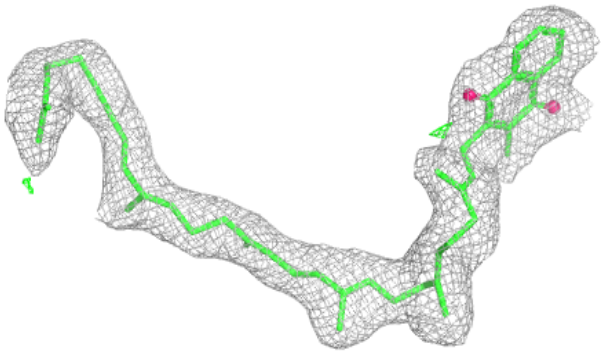


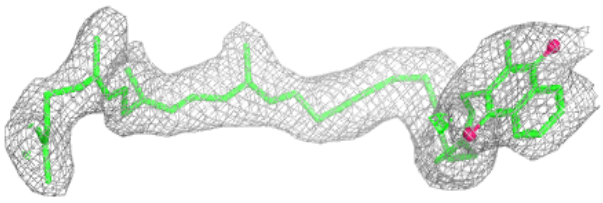


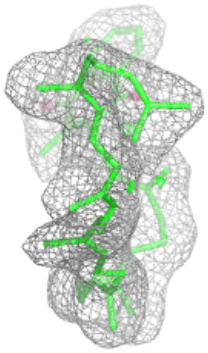


Electron density around MQ7 M 501:

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

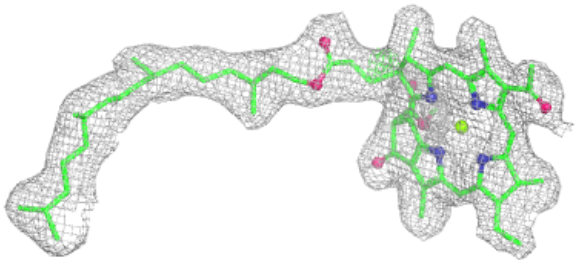


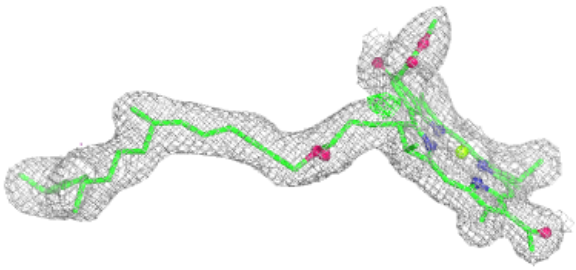


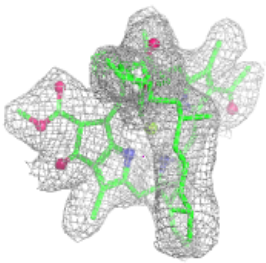


Electron density around BCB M 806:

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

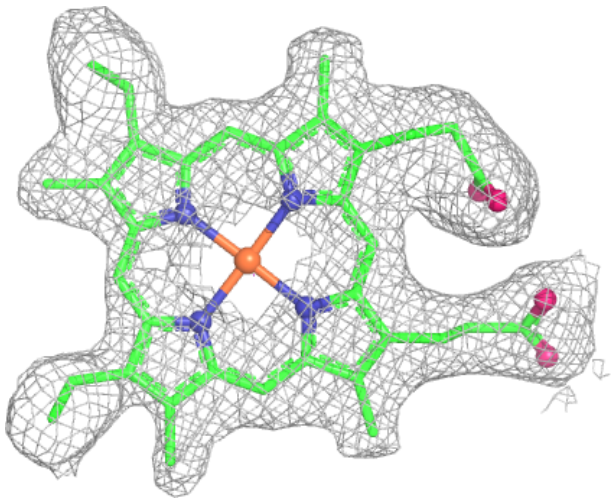


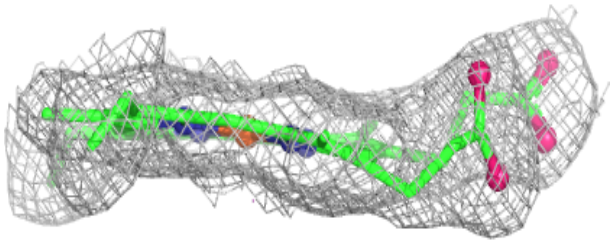


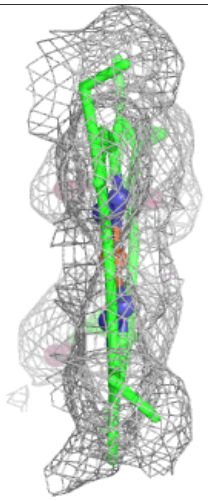


Electron density around HEC C 338:

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

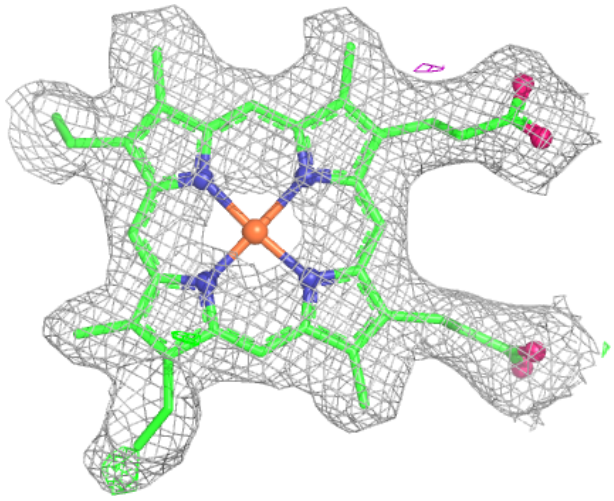


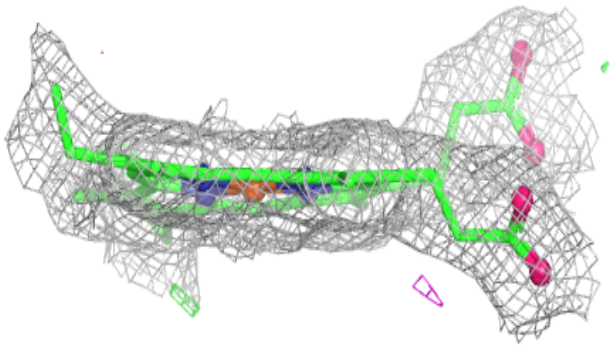


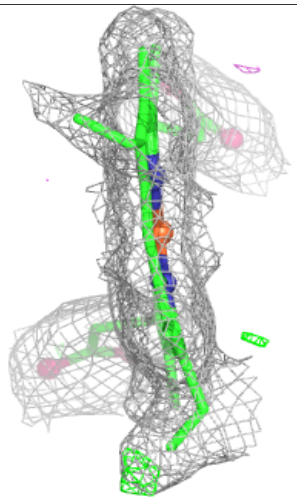


Electron density around HEC C 339:

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

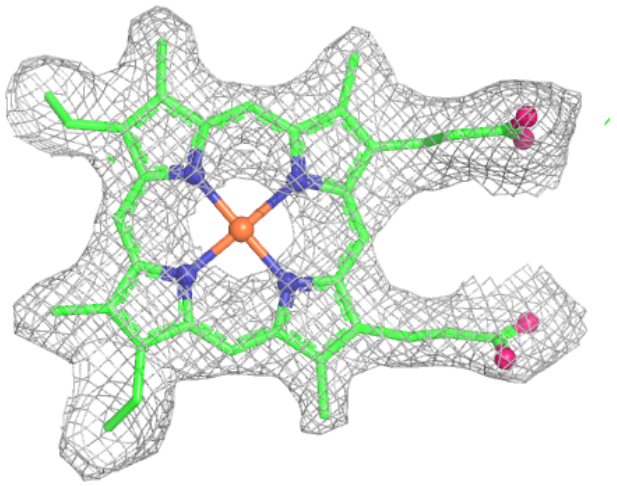


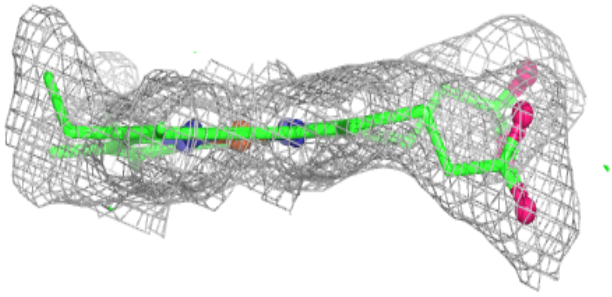


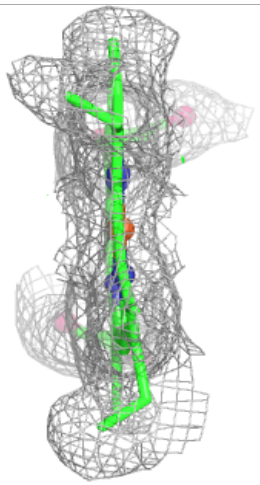


Electron density around HEC C 340:

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

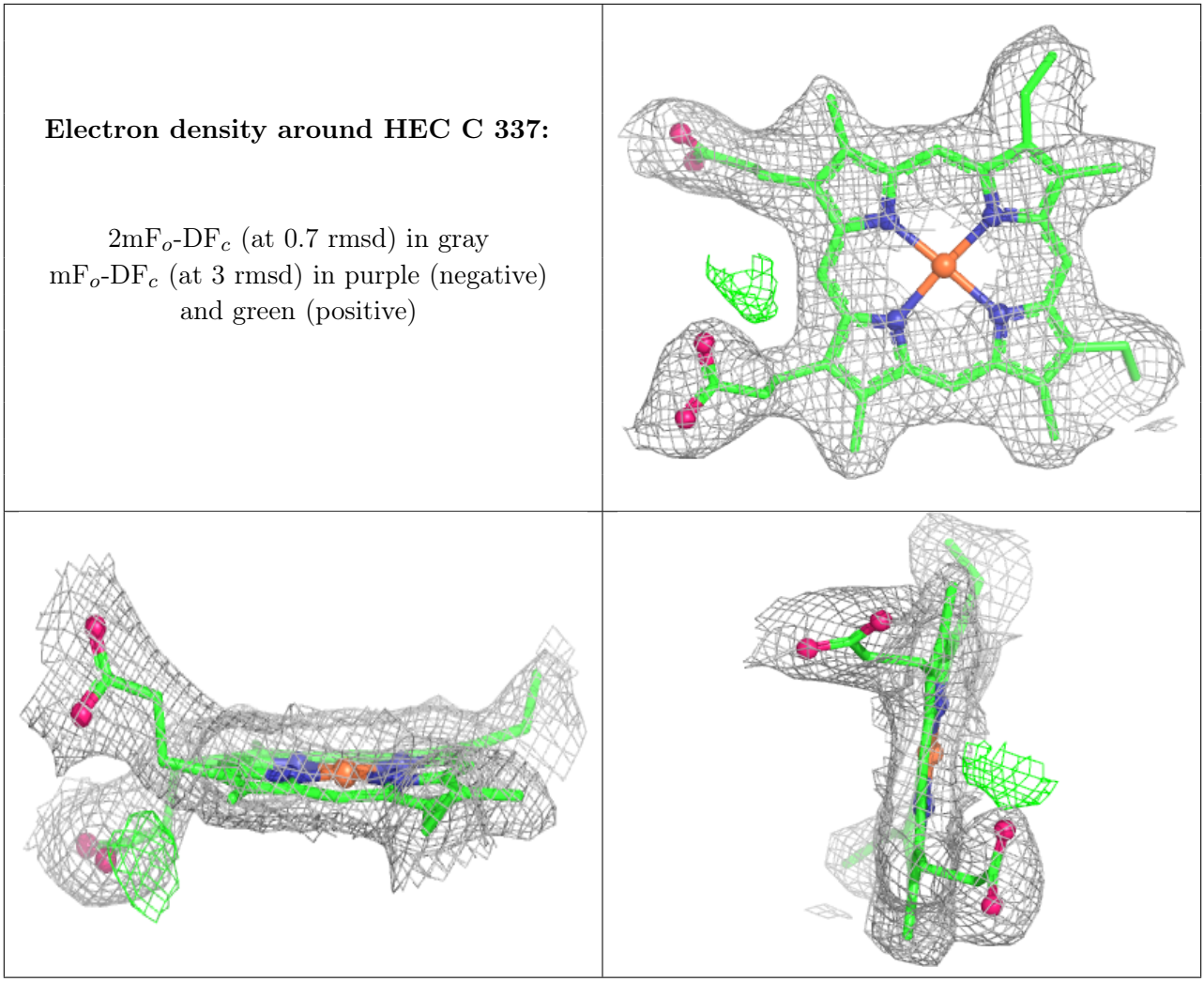






Electron density around HEC C 337:

$2mF_o$-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.