wwPDB X-ray Structure Validation Summary Report (i)

Aug 26, 2026 – 04:51 am BST

PDB ID	:	4AC5 / pdb_00004ac5
Title	:	Lipidic sponge phase crystal structure of the Bl. viridis reaction centre solved using serial femtosecond crystallography
Authors	:	Johansson, L.C.; Arnlund, D.; White, T.A.; Katona, G.; DePonte, D.P.; Weierstall, U.; Doak, R.B.; Shoeman, R.L.; Lomb, L.; Malmerberg, E.; Davidsson, J.; Nass, K.; Liang, M.; Andreasson, J.; Aquila, A.; Bajt, S.; Barthelmess, M.; Barty, A.; Bogan, M.J.; Bostedt, C.; Bozek, J.D.; Caleman, C.; Coffee, R.; Coppola, N.; Ekeberg, T.; Epp, S.W.; Erk, B.; Fleckenstein, H.; Foucar, L.; Graafsma, H.; Gumprecht, L.; Hajdu, J.; Hampton, C.Y.; Hartmann, R.; Hartmann, A.; Hauser, G.; Hirsemann, H.; Holl, P.; Hunter, M.S.; Kassemeyer, S.; Kimmel, N.; Kirian, R.A.; Maia, F.R.N.C.; Marchesini, S.; Martin, A.V.; Reich, C.; Rolles, D.; Rudek, B.; Rudenko, A.; Schlichting, I.; Schulz, J.; Seibert, M.M.; Sierra, R.; Soltau, H.; Starodub, D.; Stellato, F.; Stern, S.; Struder, L.; Timneanu, N.; Ullrich, J.; Wahlgren, W.Y.; Wang, X.; Weidenspointner, G.; Wunderer, C.; Fromme, P.; Chapman, H.N.; Spence, J.C.H.; Neutze, R.
Deposited on	:	2011-12-14
Resolution	:	8.20 Å(reported)

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

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

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

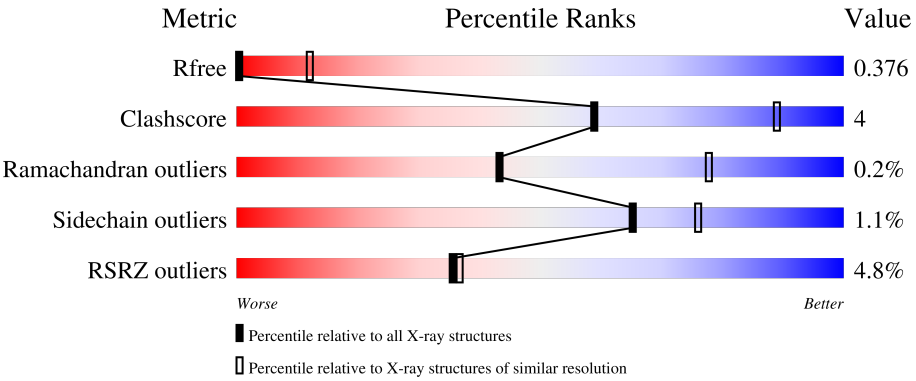
The following versions of software and data (see references (1)) were used in the production of this report:

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 8.20 Å.

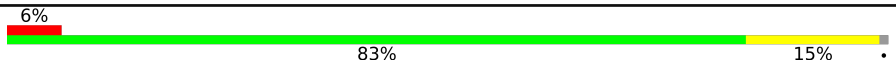
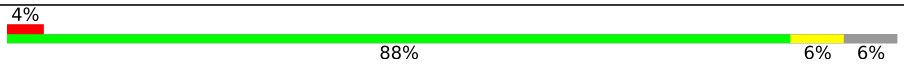
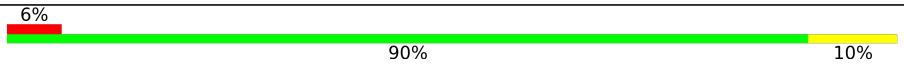
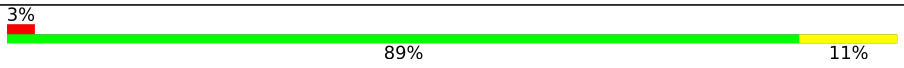
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1168 (11.50-4.00)
Clashscore	190562	1001 (11.50-4.06)
Ramachandran outliers	187476	1055 (11.50-4.00)
Sidechain outliers	187428	1018 (11.50-4.00)
RSRZ outliers	180081	1162 (11.50-4.00)

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.

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

Mol	Chain	Length	Quality of chain
1	C	336	
2	H	258	
3	L	274	
4	M	324	

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 9835 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	2590	1632	464	476	18	0	0	0

- Molecule 2 is a protein called REACTION CENTER PROTEIN H CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	243	1886	1209	326	349	2	0	0	0

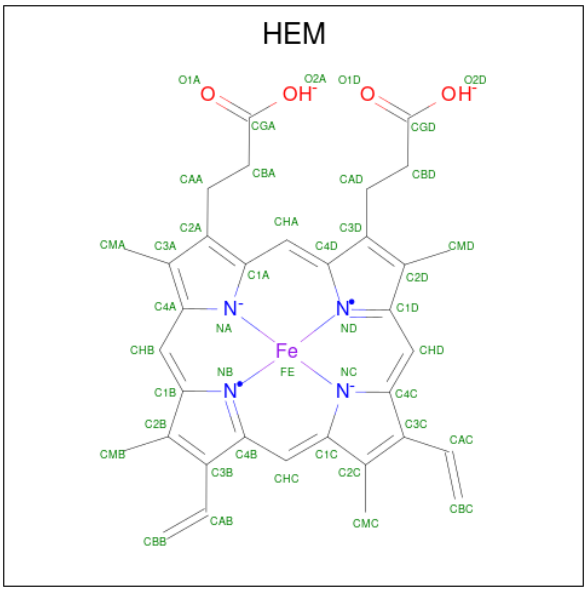
- Molecule 3 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	273	2161	1452	350	352	7	0	0	0

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

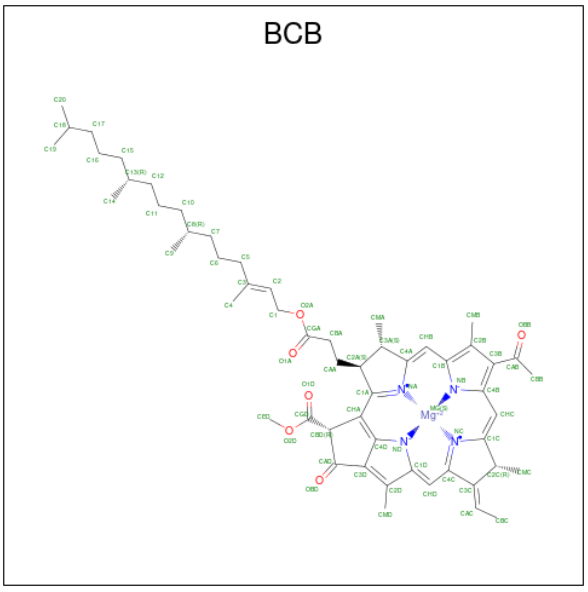
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	M	323	2548	1697	417	423	11	0	0	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



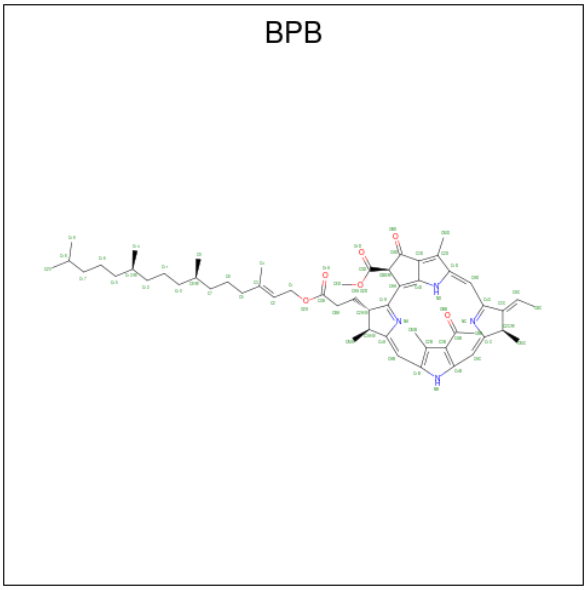
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



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

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

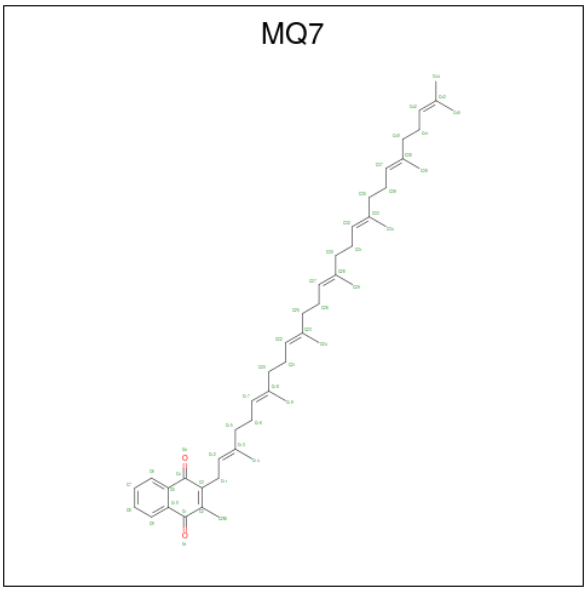


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			61	51	4	6		

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

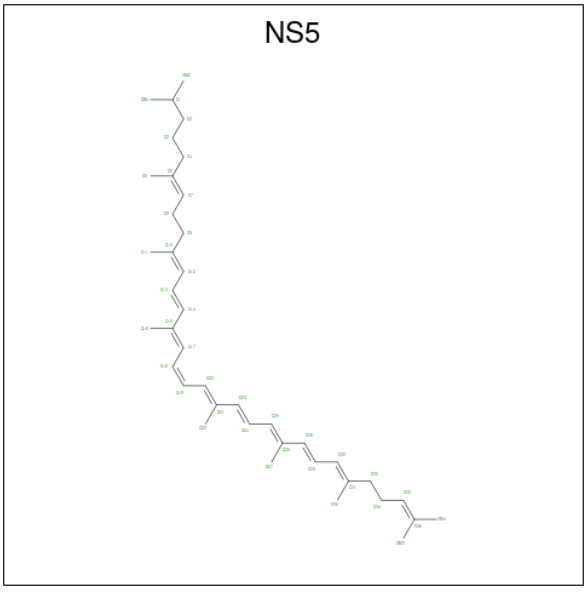
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

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



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

- Molecule 10 is 15-cis-1,2-dihydroneurosporene (CCD ID: NS5) (formula: $C_{40}H_{60}$).

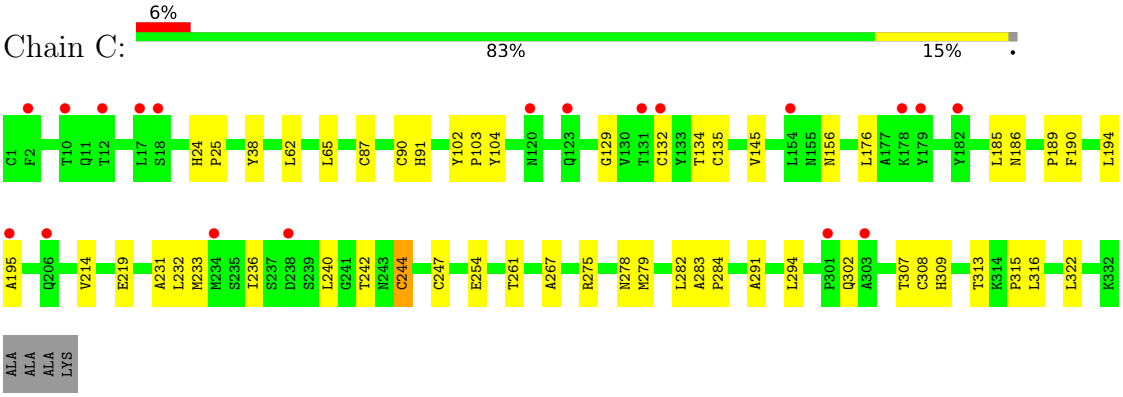


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	M	1	Total C 40 40	0	0

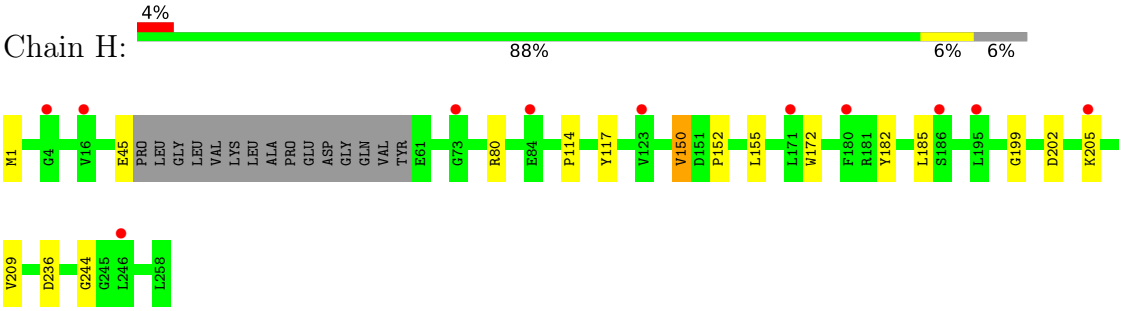
3 Residue-property plots (i)

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.

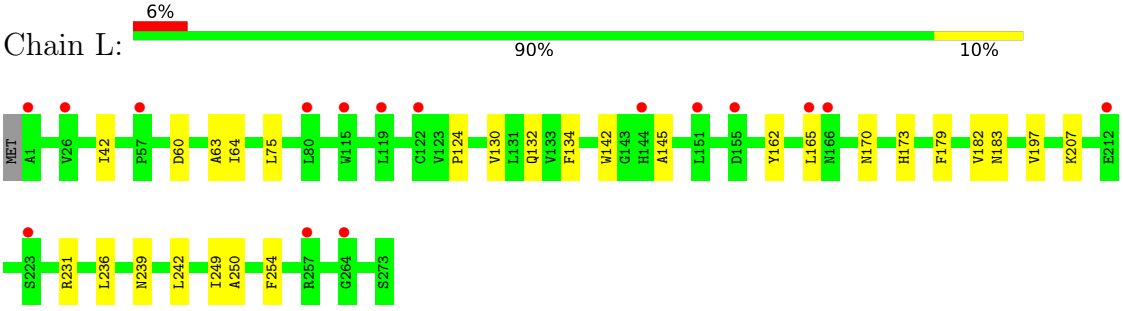
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT



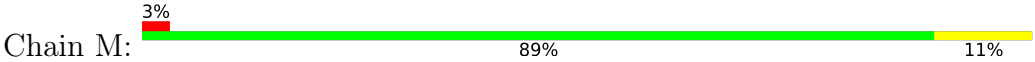
• Molecule 2: REACTION CENTER PROTEIN H CHAIN

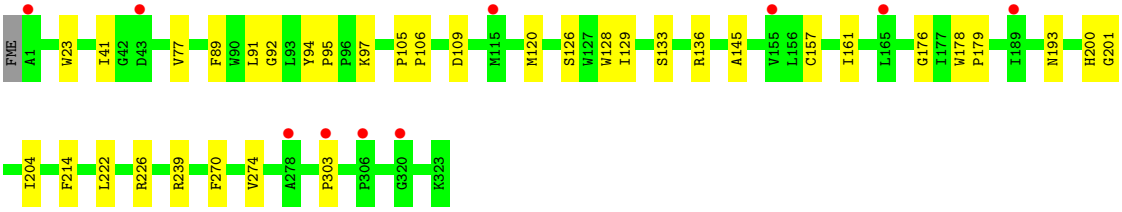


• Molecule 3: REACTION CENTER PROTEIN L CHAIN



• Molecule 4: REACTION CENTER PROTEIN M CHAIN




FME
A1
W23
I41
G42
D43
V77
F89
W90
L91
G92
L93
Y94
P95
P96
K97
P105
P106
D109
M115
M120
S126
W127
W128
I129
S133
R136
A145
V155
L156
C157
I161
L165
G176
I177
W178
P179
I189
N193
H200
G201
I204
F214
L222
R226
R239
F270
V274
A278
P303
P306
G320
K323

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.50Å 84.60Å 375.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.10 – 8.20 46.10 – 8.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (46.10-8.20) 96.5 (46.10-8.20)	Depositor EDS
R_{merge}	0.50	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 8.36Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.351 , 0.384 0.344 , 0.376	Depositor DCC
R_{free} test set	95 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å^2)	-2.7	Xtriage
Anisotropy	-13.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 192.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.69	EDS
Total number of atoms	9835	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.09% 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: BCB, HEM, MQ7, BPB, FE2, NS5, FME

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	0.43	0/2657	0.78	0/3624
2	H	0.46	0/1919	0.73	0/2621
3	L	0.42	0/2248	0.78	0/3069
4	M	0.43	0/2652	0.77	0/3630
All	All	0.44	0/9476	0.77	0/12944

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2590	0	2561	35	0
2	H	1886	0	1880	8	0
3	L	2161	0	2089	15	0
4	M	2548	0	2432	20	0
5	C	172	0	120	10	0
6	L	132	0	144	7	0
6	M	131	0	140	4	0
7	L	65	0	74	4	0
7	M	61	0	63	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	M	1	0	0	0	0
9	M	48	0	64	0	0
10	M	40	0	60	3	0
All	All	9835	0	9627	86	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 4.

The worst 5 of 86 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)
6:M:1325:BCB:HBD	6:M:1325:BCB:HAA1	1.62	0.80
1:C:247:CYS:SG	5:C:1335:HEM:HAC	2.24	0.78
1:C:308:CYS:SG	5:C:1336:HEM:HAC	2.25	0.76
7:L:1276:BPB:HHC	7:L:1276:BPB:HBBB	1.69	0.73
3:L:239:ASN:HA	3:L:242:LEU:HB2	1.76	0.66

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%)	311 (94%)	19 (6%)	0	100	100
2	H	239/258 (93%)	229 (96%)	10 (4%)	0	100	100
3	L	271/274 (99%)	253 (93%)	17 (6%)	1 (0%)	30	67
4	M	321/324 (99%)	309 (96%)	11 (3%)	1 (0%)	36	72
All	All	1161/1192 (97%)	1102 (95%)	57 (5%)	2 (0%)	43	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	165	LEU
4	M	193	ASN

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	278/282 (99%)	275 (99%)	3 (1%)	65	76
2	H	194/212 (92%)	191 (98%)	3 (2%)	57	72
3	L	216/219 (99%)	215 (100%)	1 (0%)	81	83
4	M	247/249 (99%)	244 (99%)	3 (1%)	63	75
All	All	935/962 (97%)	925 (99%)	10 (1%)	65	76

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	M	41	ILE
4	M	136	ARG
4	M	214	PHE
2	H	45	GLU
2	H	150	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	217	GLN
2	H	178	HIS
1	C	278	ASN
1	C	263	GLN
2	H	8	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)

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	0.72	0	7,9,11	3.49	3 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	H	1	2	-	5/7/9/11	-

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	-8.28	110.09	122.82
2	H	1	FME	CE-SD-CG	3.00	110.70	100.40
2	H	1	FME	O1-CN-N	-2.05	119.86	125.27

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

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 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	$\#\|Z\| > 2$
10	NS5	M	1329	-	39,39,39	2.10	5 (12%)	44,46,46	2.42	15 (34%)
7	BPB	M	1326	-	53,66,70	2.82	14 (26%)	51,96,101	2.90	17 (33%)
7	BPB	L	1276	-	57,70,70	2.71	14 (24%)	56,101,101	2.81	18 (32%)
6	BCB	L	1275	3	68,74,74	2.13	19 (27%)	79,115,115	2.76	24 (30%)
9	MQ7	M	1328	-	49,49,49	1.51	2 (4%)	60,63,63	1.21	7 (11%)
5	HEM	C	1333	1	50,50,50	2.01	10 (20%)	66,82,82	1.42	4 (6%)
5	HEM	C	1334	1	50,50,50	1.91	10 (20%)	66,82,82	1.38	4 (6%)
5	HEM	C	1336	1	50,50,50	1.98	10 (20%)	66,82,82	1.39	6 (9%)
5	HEM	C	1335	1	50,50,50	1.94	10 (20%)	66,82,82	1.40	4 (6%)
6	BCB	L	1274	3	68,74,74	2.12	18 (26%)	79,115,115	2.93	26 (32%)
6	BCB	M	1325	4	68,74,74	2.11	19 (27%)	79,115,115	2.87	24 (30%)
6	BCB	M	1324	-	67,73,74	2.08	18 (26%)	77,113,115	2.92	26 (33%)

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
10	NS5	M	1329	-	-	16/43/43/43	-
7	BPB	M	1326	-	-	13/33/101/105	0/5/6/6

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BPB	L	1276	-	-	20/37/105/105	0/5/6/6
6	BCB	L	1275	3	3/3/21/26	16/41/137/137	-
9	MQ7	M	1328	-	-	3/41/61/61	0/2/2/2
5	HEM	C	1333	1	-	7/14/54/54	-
5	HEM	C	1334	1	-	9/14/54/54	-
5	HEM	C	1336	1	-	5/14/54/54	-
5	HEM	C	1335	1	-	8/14/54/54	-
6	BCB	L	1274	3	3/3/21/26	18/41/137/137	-
6	BCB	M	1325	4	3/3/21/26	23/41/137/137	-
6	BCB	M	1324	-	3/3/20/26	26/40/136/137	-

The worst 5 of 149 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1326	BPB	C1B-C2B	8.95	1.49	1.39
7	L	1276	BPB	C1B-C2B	8.76	1.49	1.39
7	M	1326	BPB	C1D-C2D	8.50	1.49	1.39
9	M	1328	MQ7	C3-C2	8.19	1.50	1.35
5	C	1336	HEM	C3D-C2D	8.19	1.54	1.36

The worst 5 of 175 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	1274	BCB	C1C-NC-C4C	-14.87	100.02	106.71
6	M	1324	BCB	C1C-NC-C4C	-14.24	100.30	106.71
6	M	1325	BCB	C1C-NC-C4C	-13.58	100.60	106.71
6	L	1275	BCB	C1C-NC-C4C	-12.79	100.95	106.71
6	L	1274	BCB	C2B-C1B-NB	9.90	116.87	110.23

5 of 12 chirality outliers are listed below:

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

5 of 164 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1333	HEM	C3D-CAD-CBD-CGD
5	C	1334	HEM	C2C-C3C-CAC-CBC
5	C	1334	HEM	C4C-C3C-CAC-CBC
5	C	1335	HEM	C2B-C3B-CAB-CBB
5	C	1336	HEM	C2C-C3C-CAC-CBC

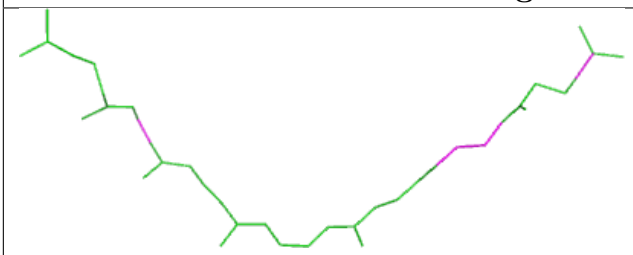
There are no ring outliers.

10 monomers are involved in 28 short contacts:

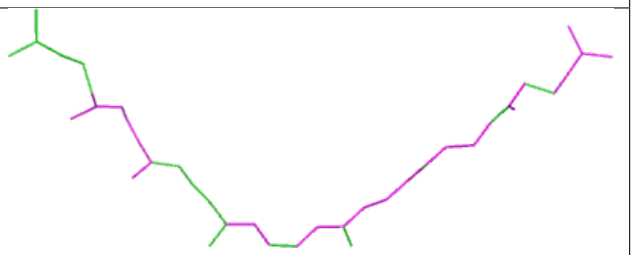
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	M	1329	NS5	3	0
7	M	1326	BPB	1	0
7	L	1276	BPB	4	0
6	L	1275	BCB	4	0
5	C	1333	HEM	1	0
5	C	1334	HEM	2	0
5	C	1336	HEM	2	0
5	C	1335	HEM	5	0
6	L	1274	BCB	4	0
6	M	1325	BCB	4	0

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.

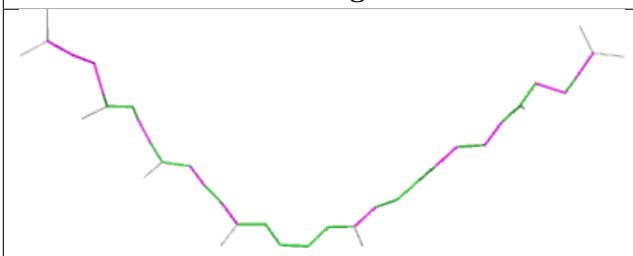
Ligand NS5 M 1329



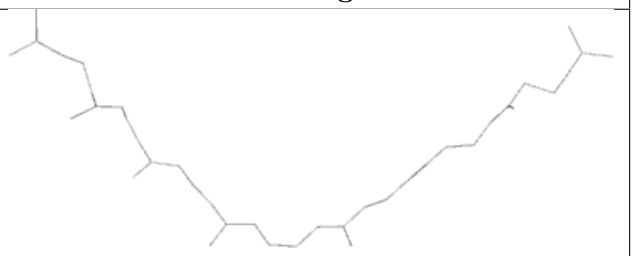
Bond lengths



Bond angles

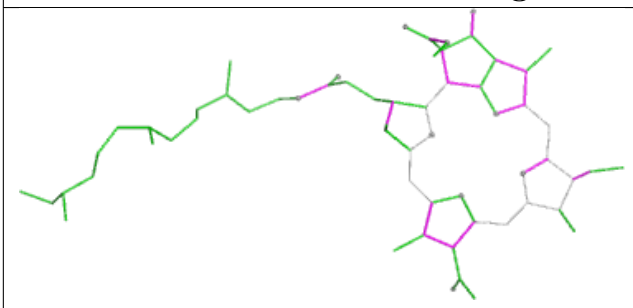


Torsions

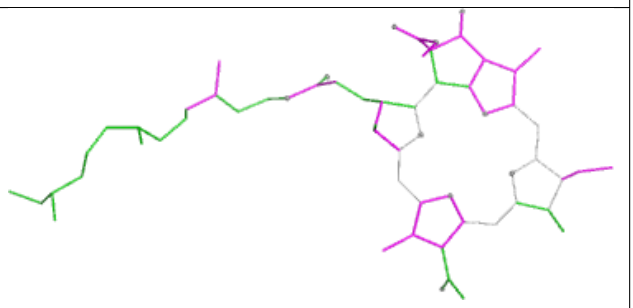


Rings

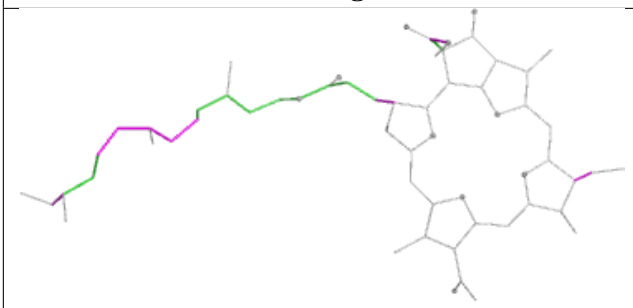
Ligand BPB M 1326



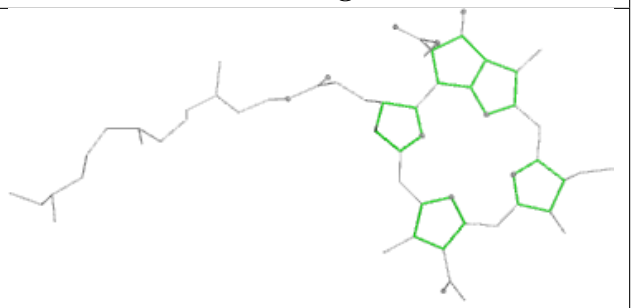
Bond lengths



Bond angles

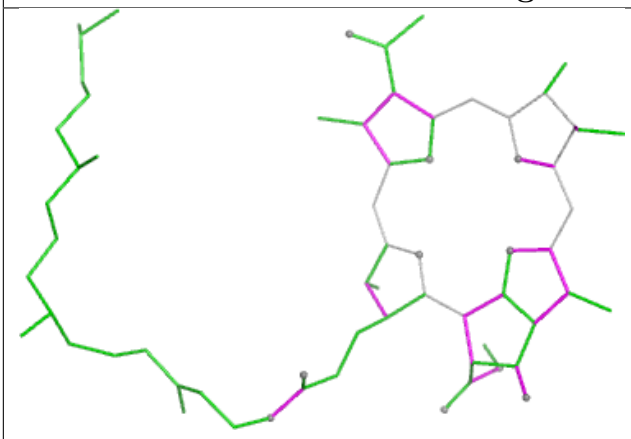


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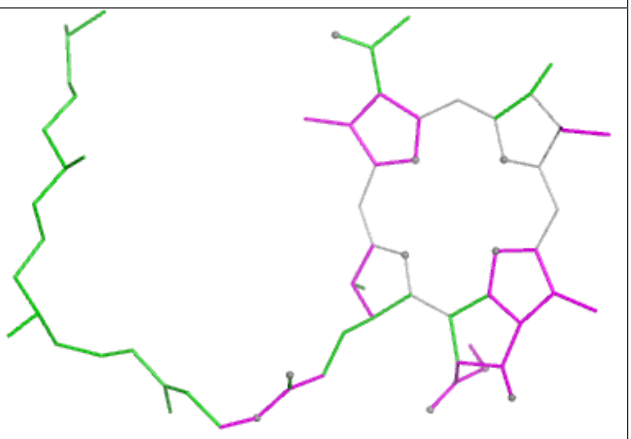


Rings

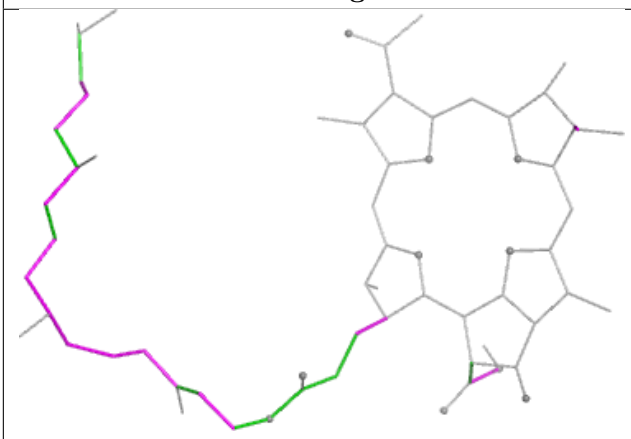
Ligand BPB L 1276



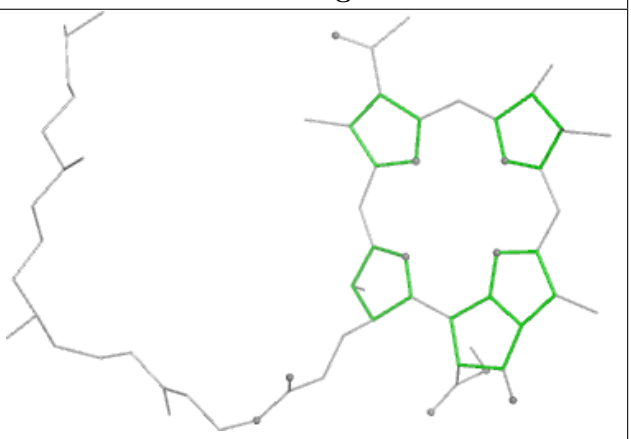
Bond lengths



Bond angles

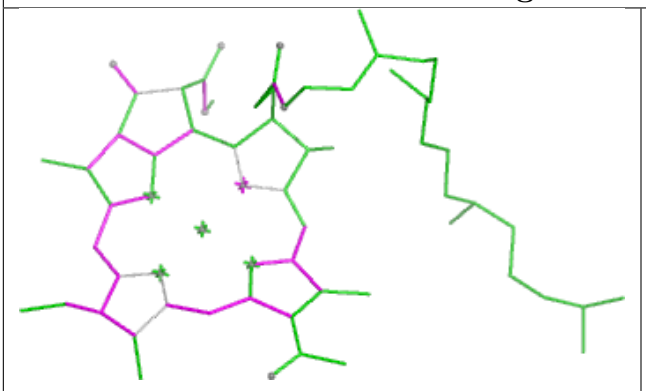


Torsions

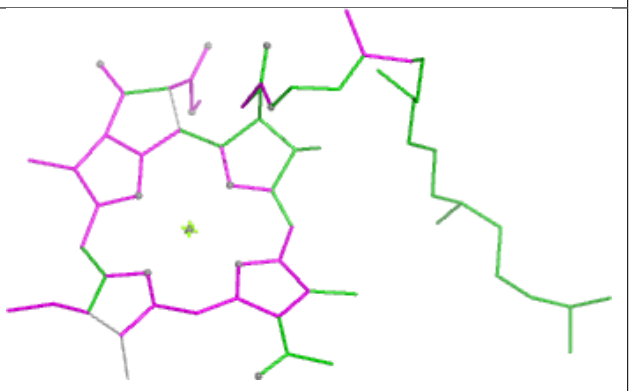


Rings

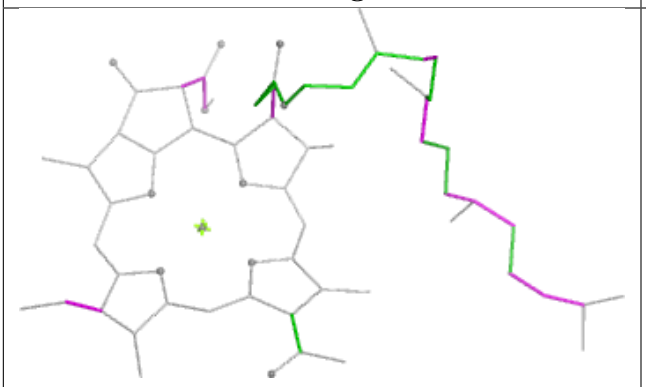
Ligand BCB L 1275



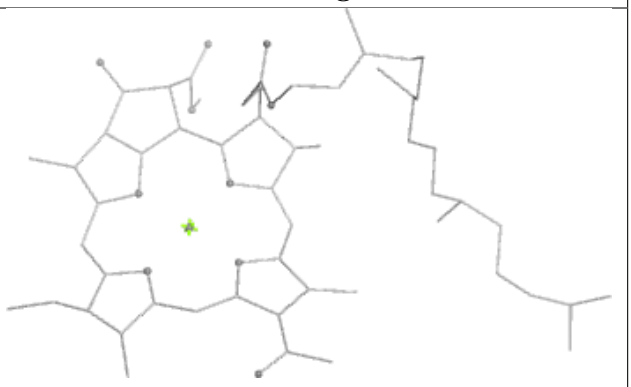
Bond lengths



Bond angles

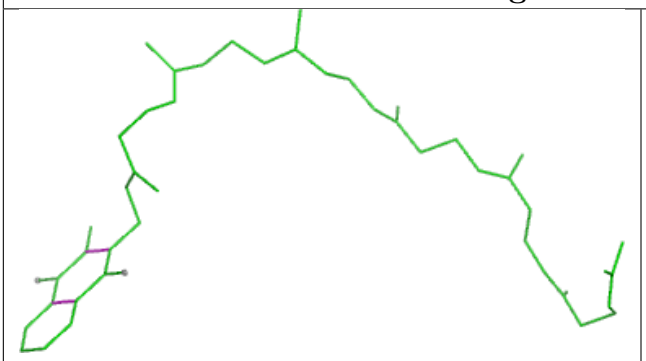


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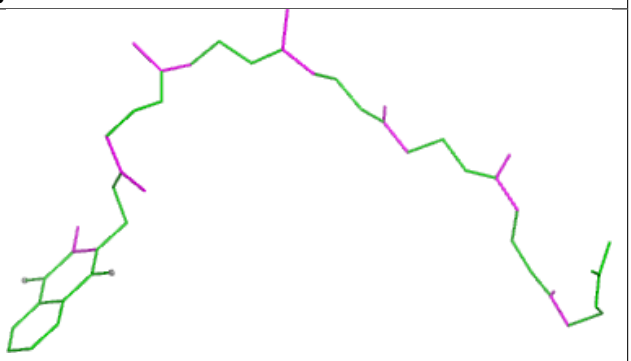


Rings

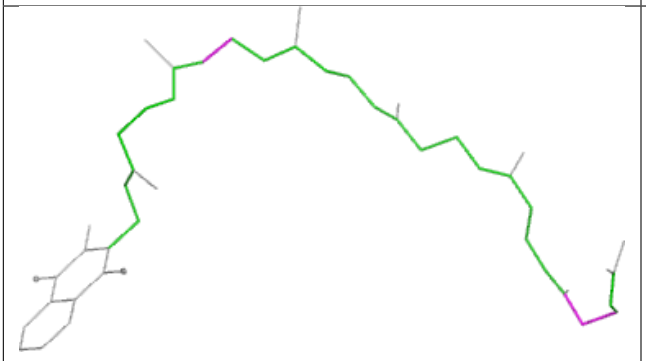
Ligand MQ7 M 1328



Bond lengths



Bond angles

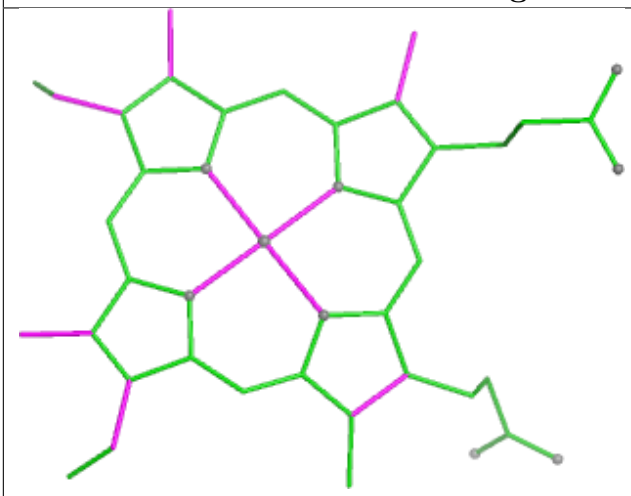


Torsions

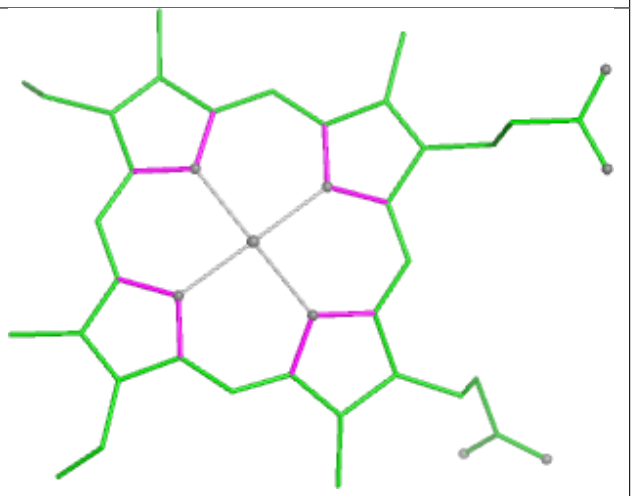


Rings

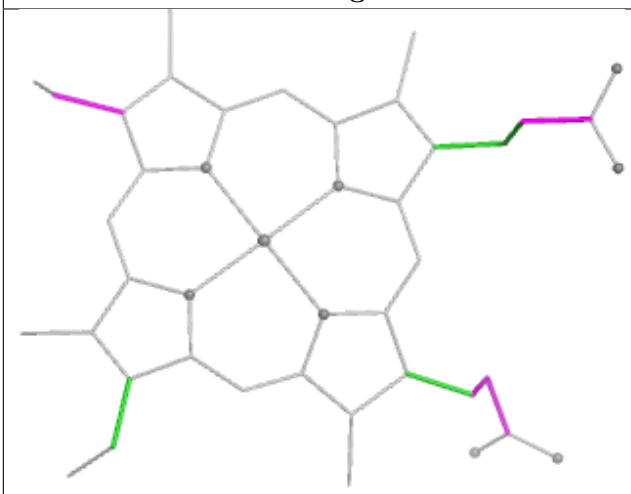
Ligand HEM C 1333



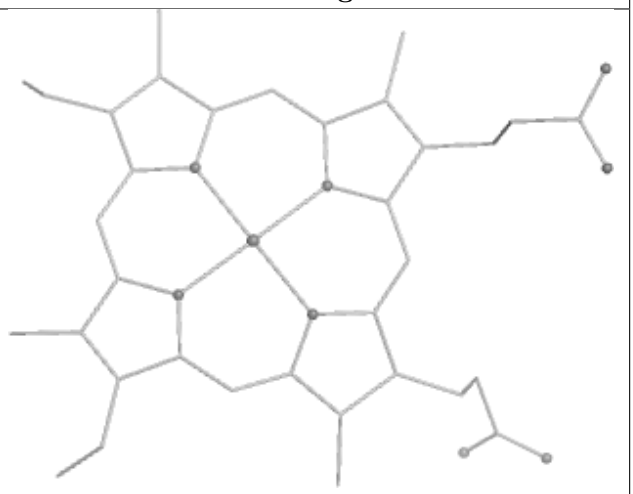
Bond lengths



Bond angles

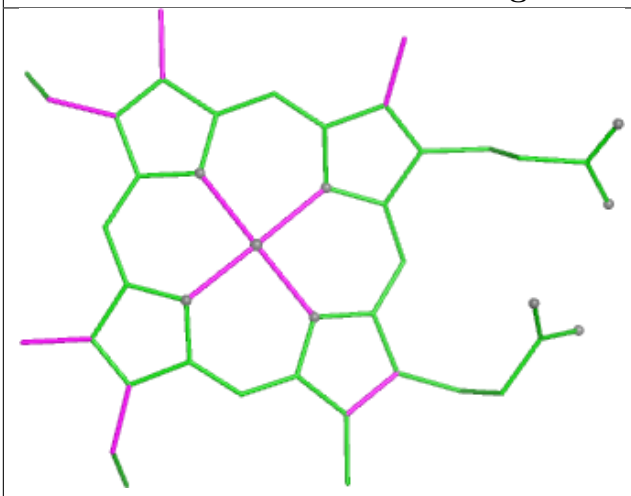


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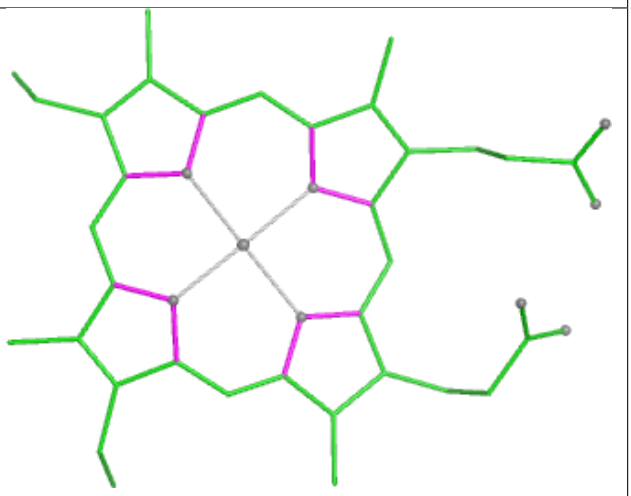


Rings

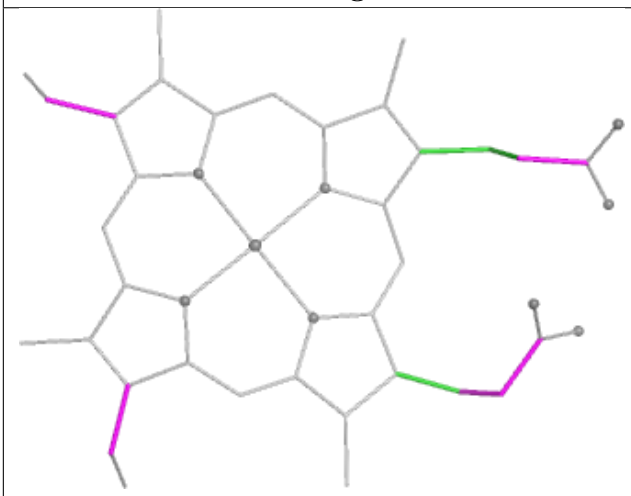
Ligand HEM C 1334



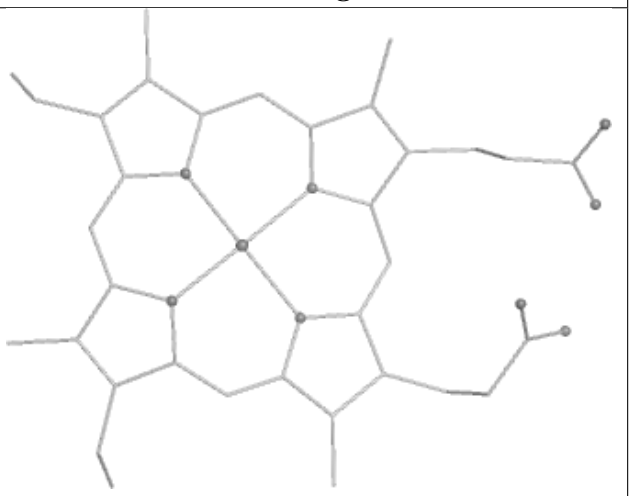
Bond lengths



Bond angles

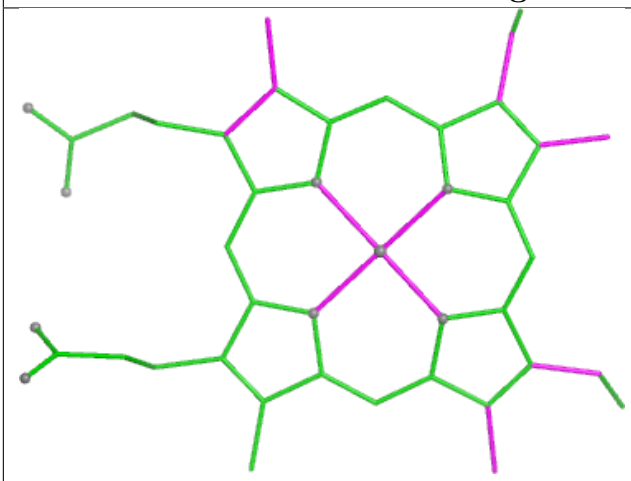


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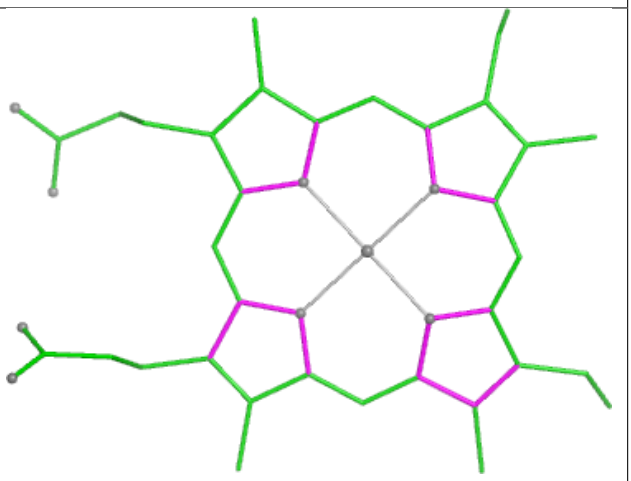


Rings

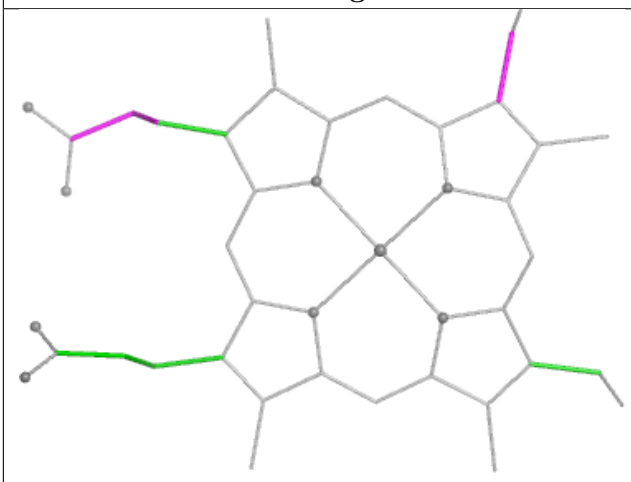
Ligand HEM C 1336



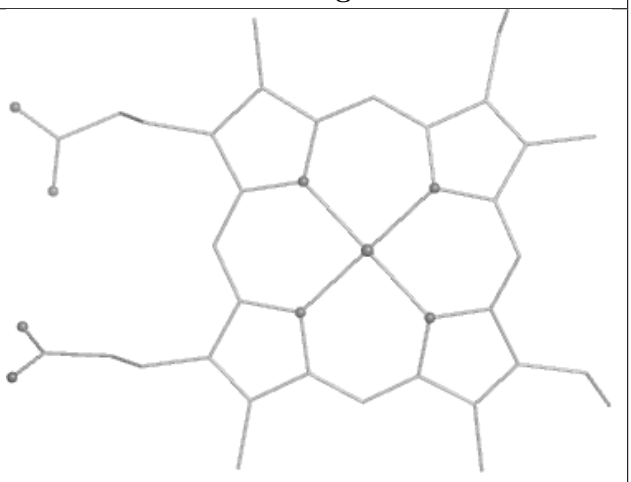
Bond lengths



Bond angles

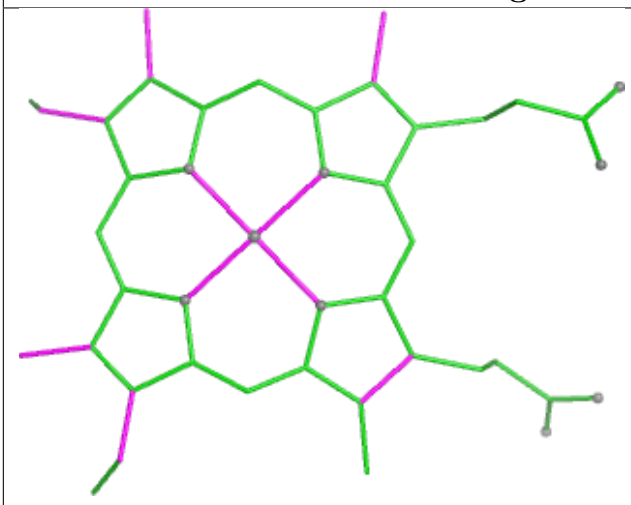


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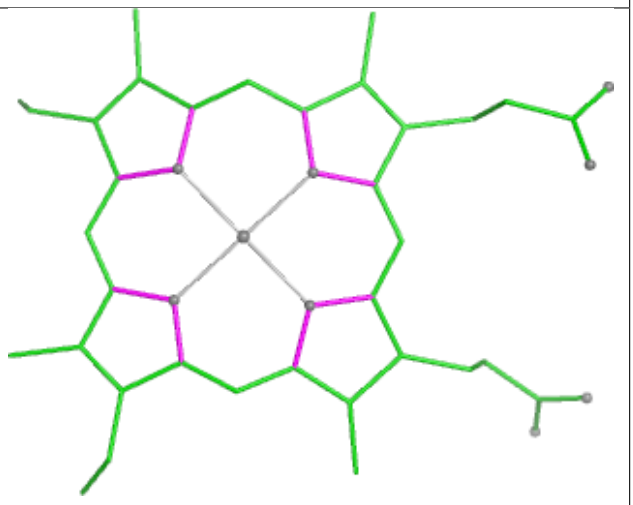


Rings

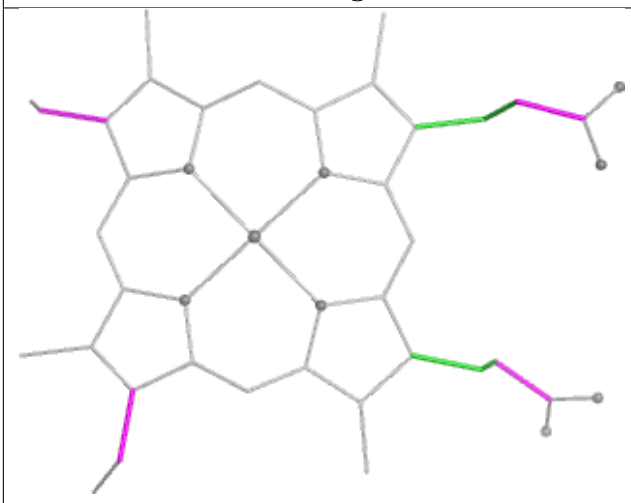
Ligand HEM C 1335



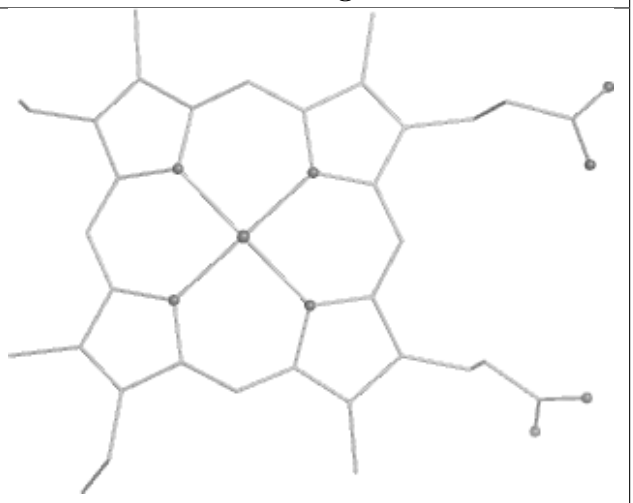
Bond lengths



Bond angles

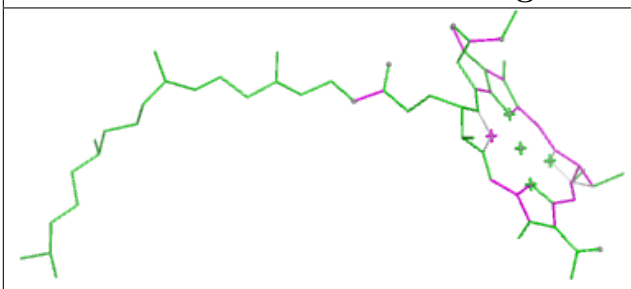


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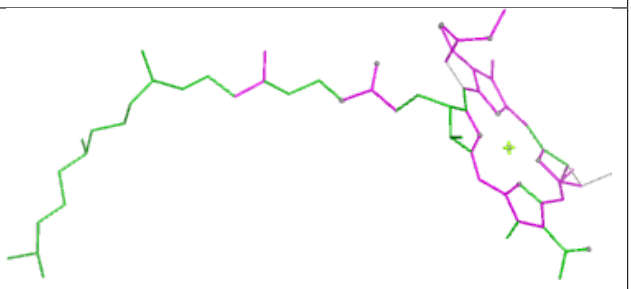


Rings

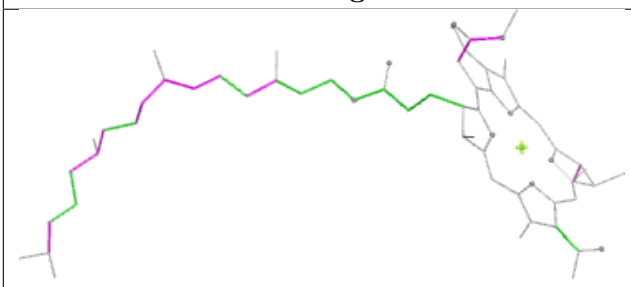
Ligand BCB L 1274



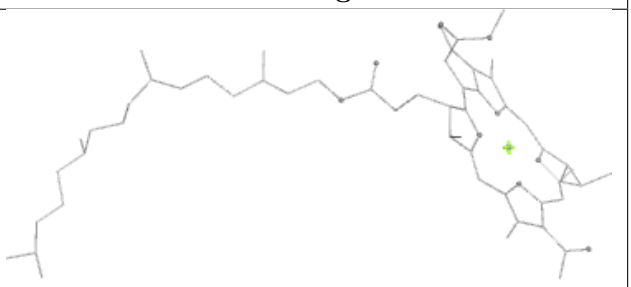
Bond lengths



Bond angles

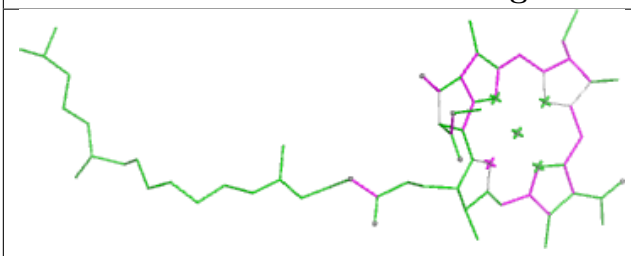


Torsions

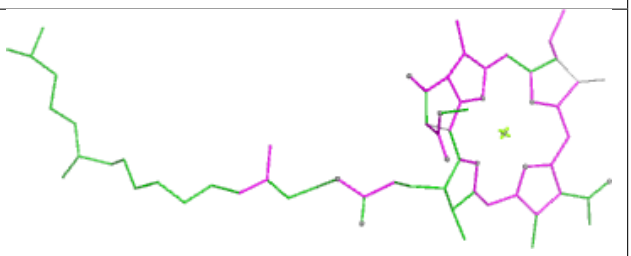


Rings

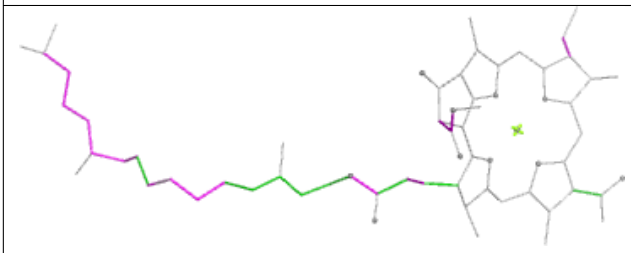
Ligand BCB M 1325



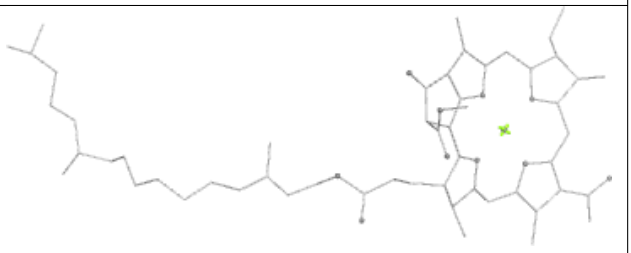
Bond lengths



Bond angles

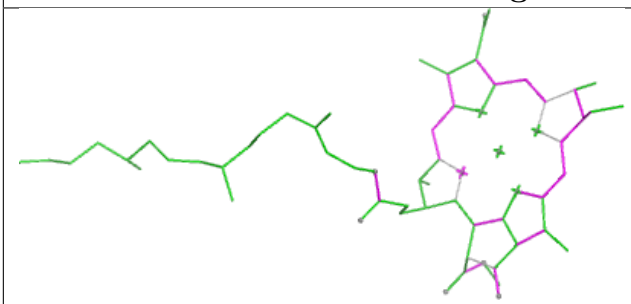


Torsions

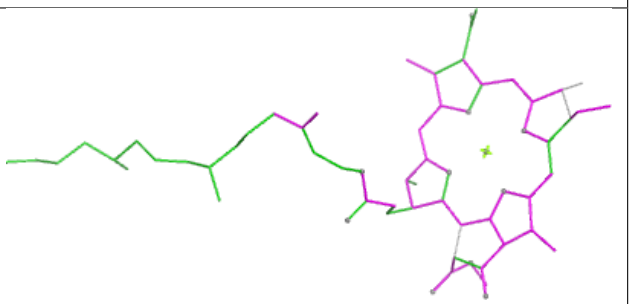


Rings

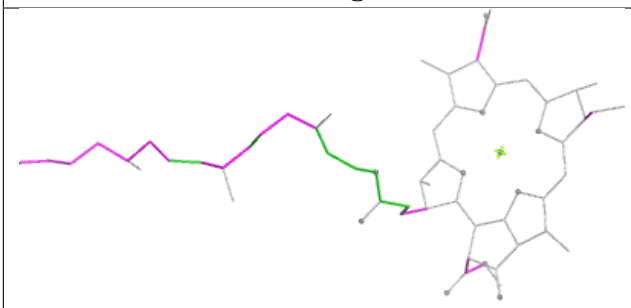
Ligand BCB M 1324



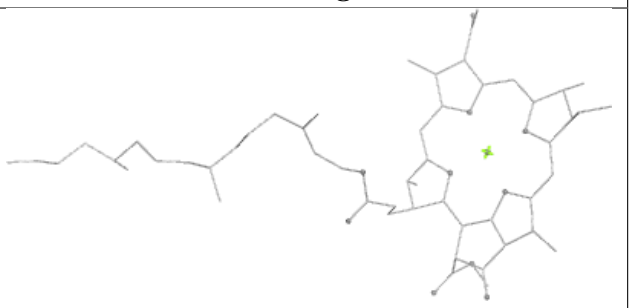
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	C	332/336 (98%)	0.14	19 (5%)	29	33	12, 15, 19, 21	0
2	H	242/258 (93%)	0.14	11 (4%)	38	38	12, 16, 25, 26	0
3	L	273/274 (99%)	0.31	16 (5%)	28	33	10, 15, 21, 22	0
4	M	323/324 (99%)	-0.12	10 (3%)	51	46	11, 15, 20, 20	0
All	All	1170/1192 (98%)	0.11	56 (4%)	35	37	10, 15, 21, 26	0

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	178	LYS	8.9
2	H	195	LEU	7.5
3	L	144	HIS	6.3
1	C	179	TYR	6.2
3	L	115	TRP	5.8

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FME	H	1	10/11	0.76	0.18	18,18,18,18	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands (i)

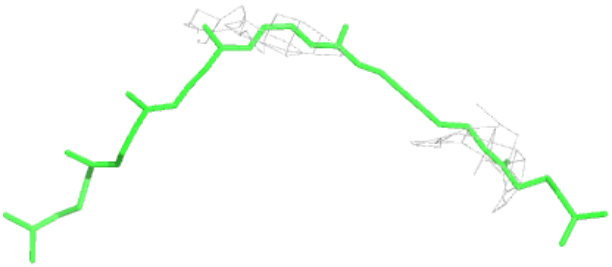
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

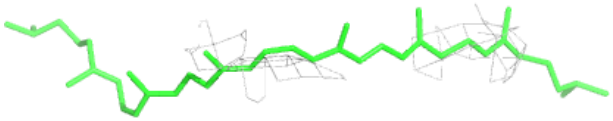
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	NS5	M	1329	40/40	0.85	0.18	27,28,30,30	0
6	BCB	M	1324	65/66	0.86	0.14	16,16,16,17	0
6	BCB	L	1275	66/66	0.87	0.18	19,20,21,21	0
9	MQ7	M	1328	48/48	0.90	0.19	9,9,10,10	0
7	BPB	M	1326	61/65	0.91	0.13	26,26,27,27	0
7	BPB	L	1276	65/65	0.92	0.17	2,2,4,4	0
6	BCB	M	1325	66/66	0.92	0.12	12,12,15,15	0
6	BCB	L	1274	66/66	0.93	0.14	29,29,30,30	0
5	HEM	C	1334	43/43	0.95	0.13	2,2,2,2	0
5	HEM	C	1336	43/43	0.96	0.11	2,2,2,2	0
5	HEM	C	1333	43/43	0.96	0.09	15,16,16,16	0
5	HEM	C	1335	43/43	0.96	0.11	4,4,4,4	0
8	FE2	M	1327	1/1	1.00	0.00	2,2,2,2	0

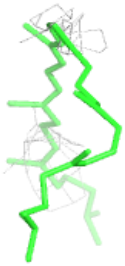
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NS5 M 1329:

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

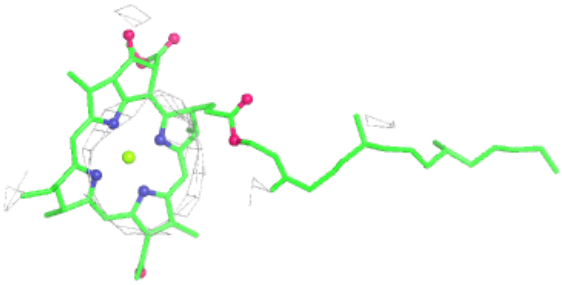




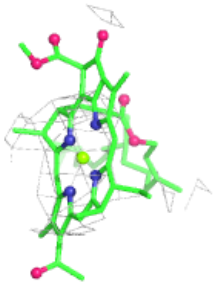


Electron density around BCB M 1324:

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

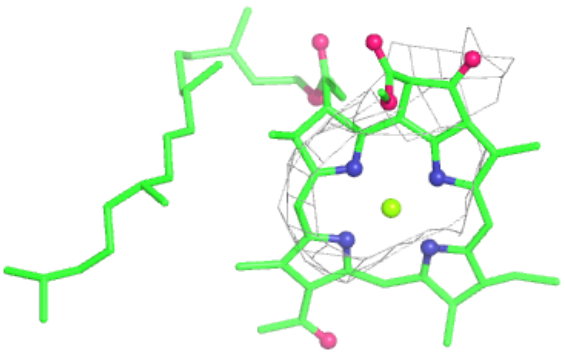


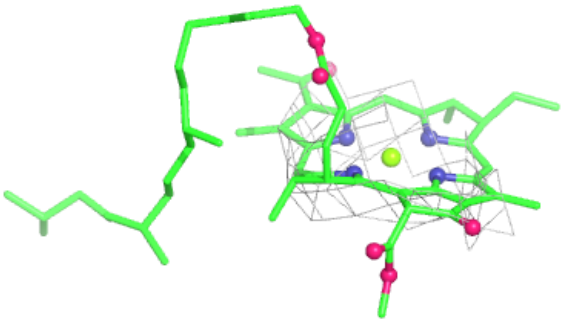


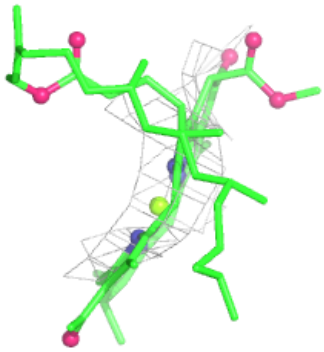


Electron density around BCB L 1275:

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

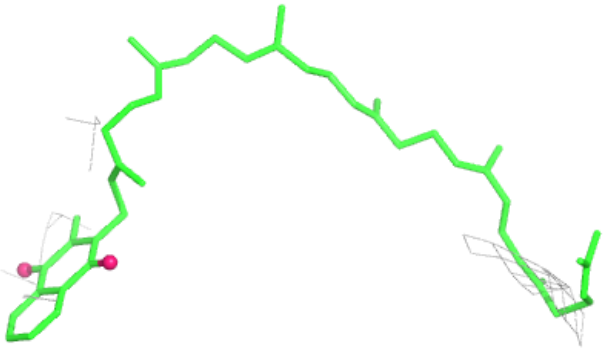


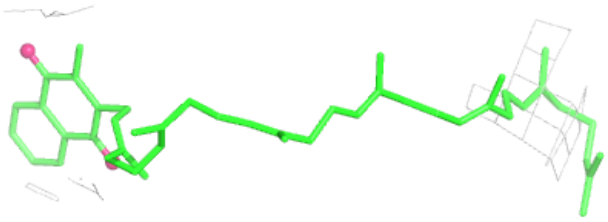


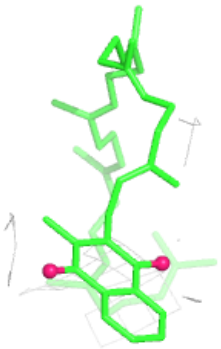


Electron density around MQ7 M 1328:

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

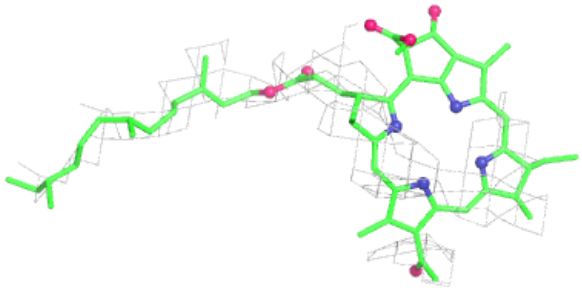






Electron density around BPB M 1326:

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

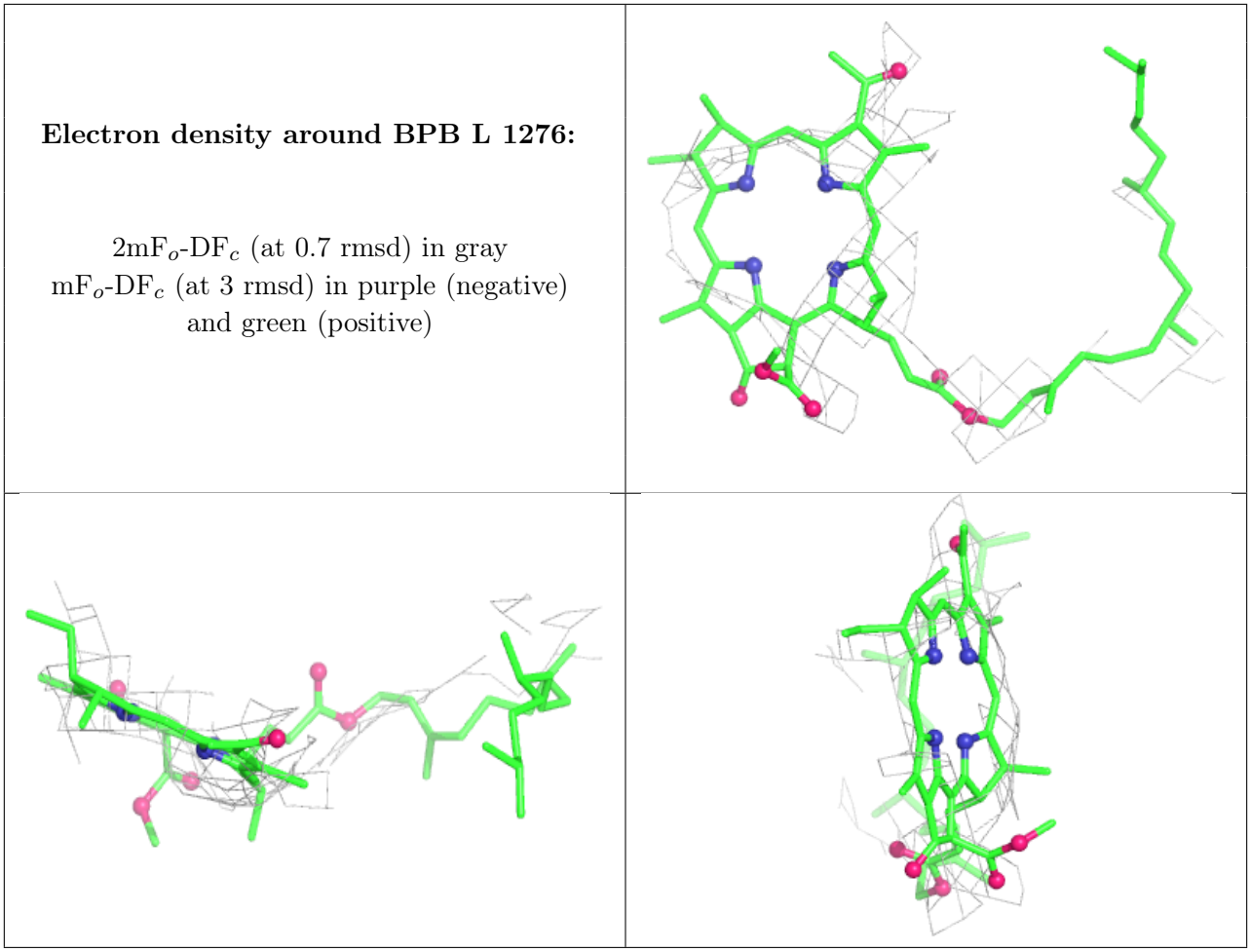






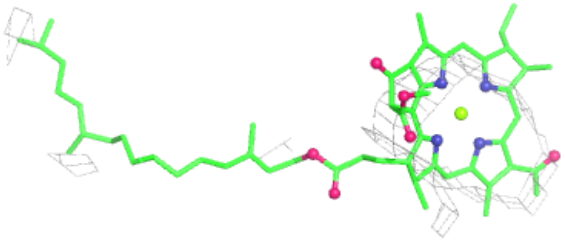
Electron density around BPB L 1276:

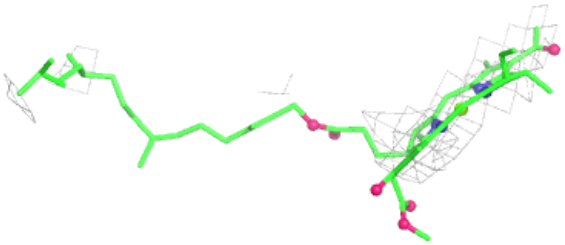
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

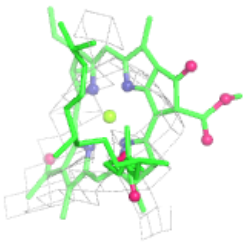


Electron density around BCB M 1325:

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

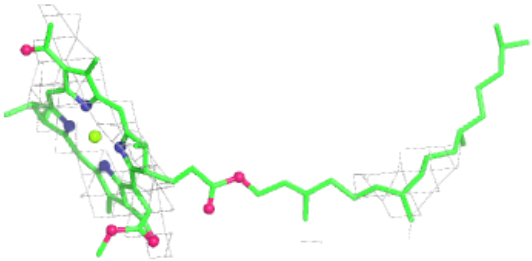


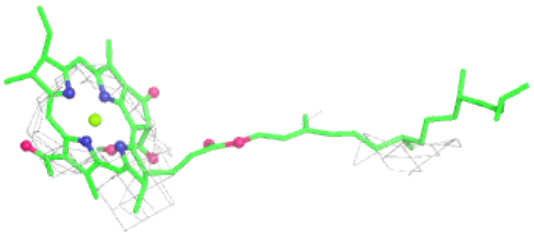


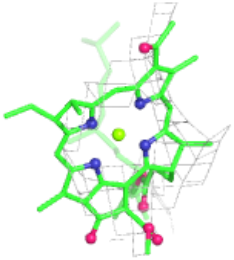


Electron density around BCB L 1274:

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

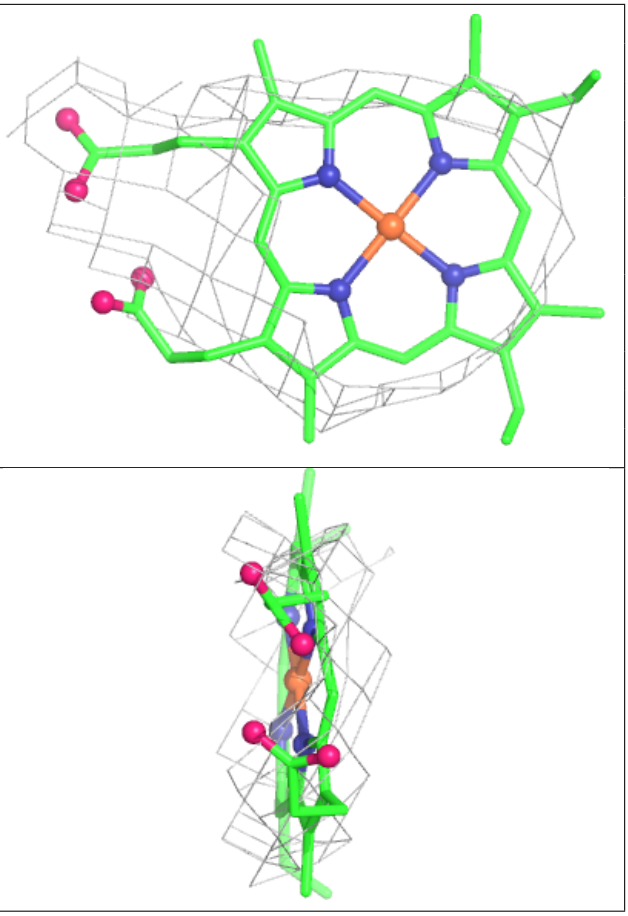


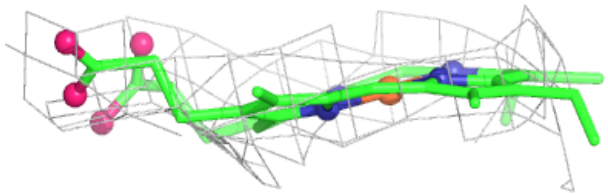




Electron density around HEM C 1334:

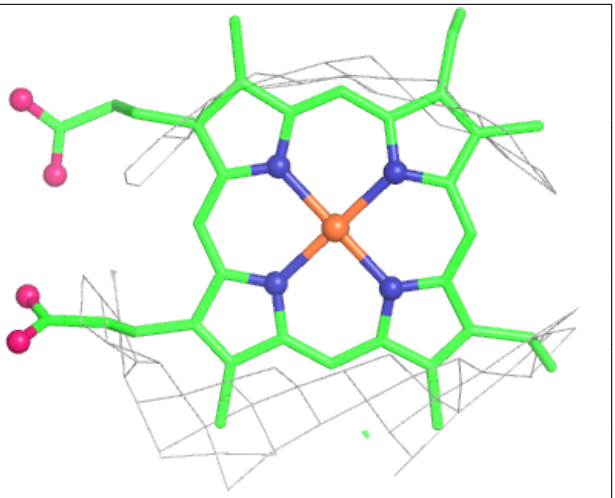
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

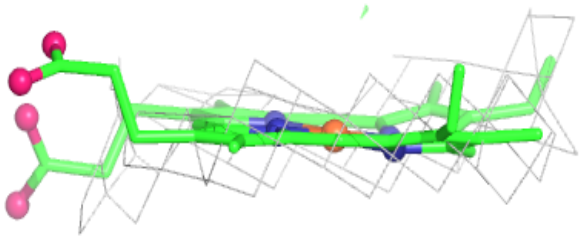


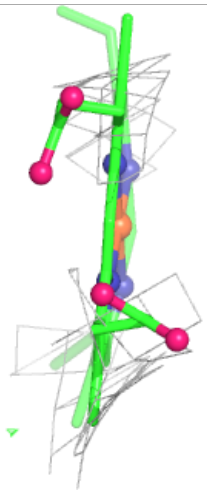


Electron density around HEM C 1336:

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

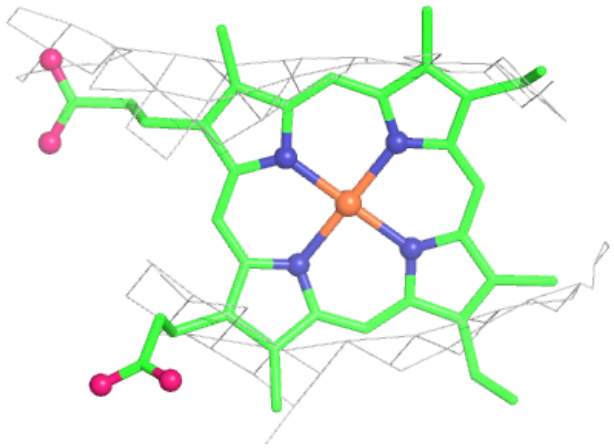


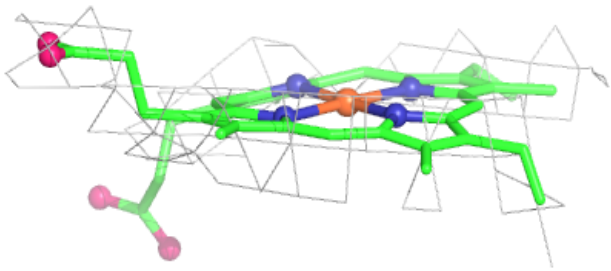


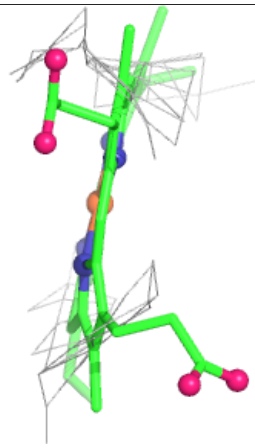


Electron density around HEM C 1333:

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

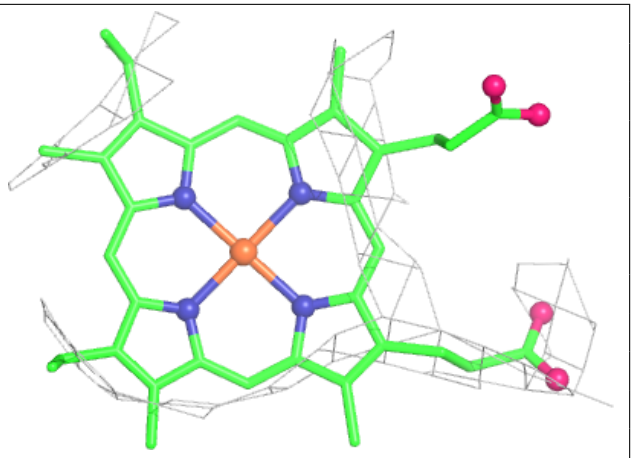


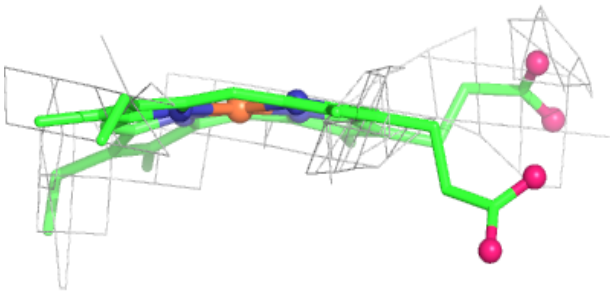


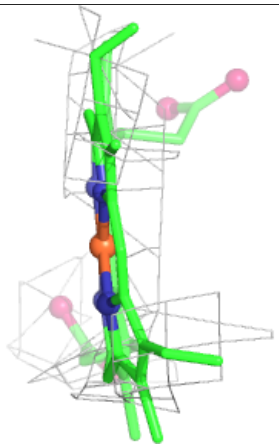


Electron density around HEM C 1335:

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







6.5 Other polymers (i)

There are no such residues in this entry.