wwPDB X-ray Structure Validation Summary Report (i)

Oct 19, 2024 – 01:26 PM EDT

PDB ID	:	5PRC
Title	:	PHOTOSYNTHETIC REACTION CENTER FROM RHODOPSEUDOMONAS VIRIDIS (ATRAZINE COMPLEX)
Authors	:	Lancaster, C.R.D.; Michel, H.
Deposited on	:	1997-08-01
Resolution	:	2.35 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 (i)) were used in the production of this report:

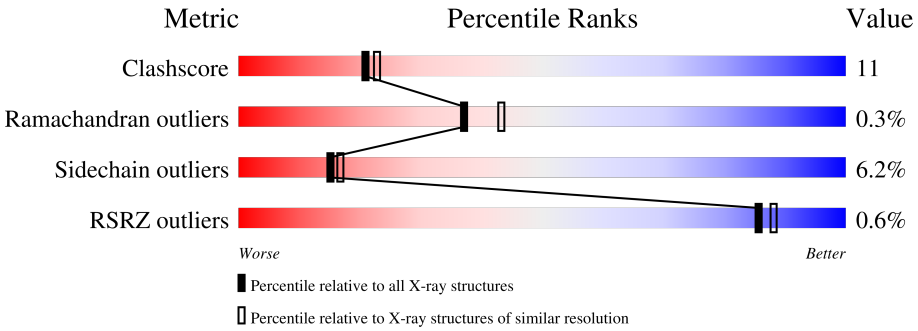
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.35 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	180529	1571 (2.36-2.36)
Ramachandran outliers	177936	1559 (2.36-2.36)
Sidechain outliers	177891	1559 (2.36-2.36)
RSRZ outliers	164620	1460 (2.36-2.36)

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	78% 18%
2	L	273	82% 16%
3	M	323	72% 24%
4	H	258	2% 73% 24%

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	302	X	-	-	-
6	BCB	L	304	X	-	-	-
6	BCB	M	805	X	-	-	-
6	BCB	M	806	X	-	-	-
7	BPB	L	402	X	-	-	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 10501 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	50	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	2171	1459	350	355	7	15	0	0

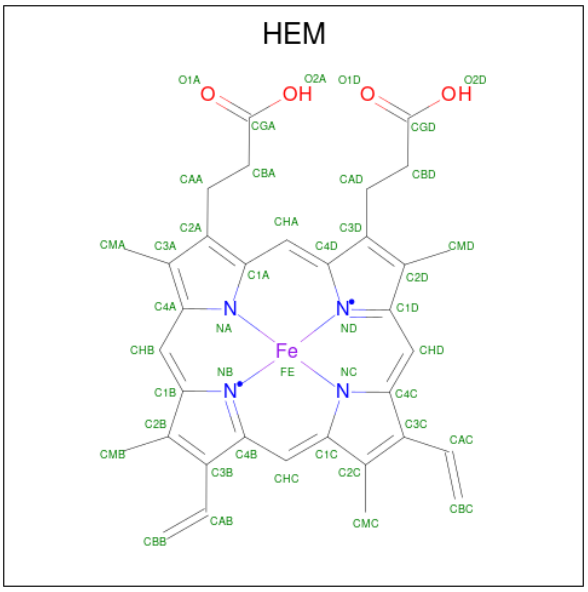
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	323	2577	1720	421	425	11	19	2	0

- Molecule 4 is a protein called PHOTOSYNTHETIC REACTION CENTER.

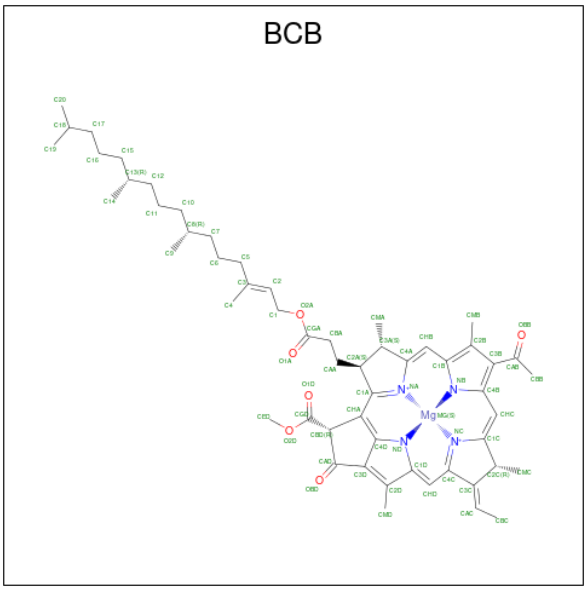
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	258	2018	1292	344	380	2	122	0	0

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



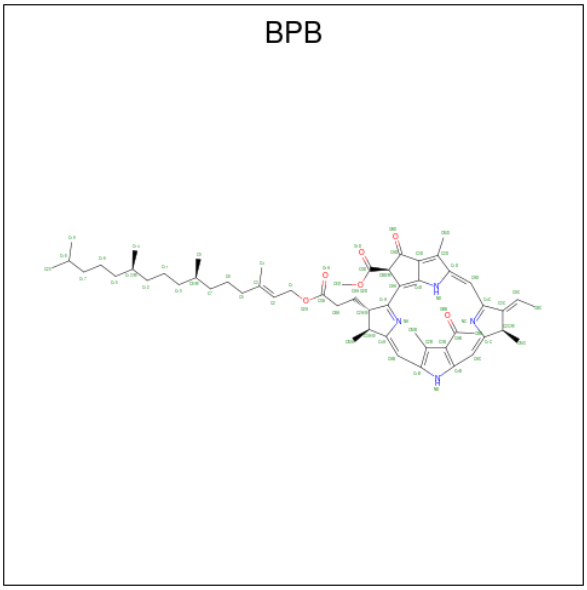
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



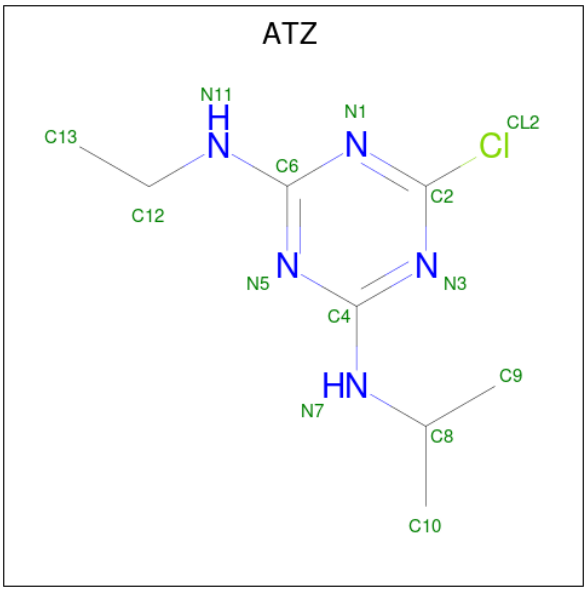
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



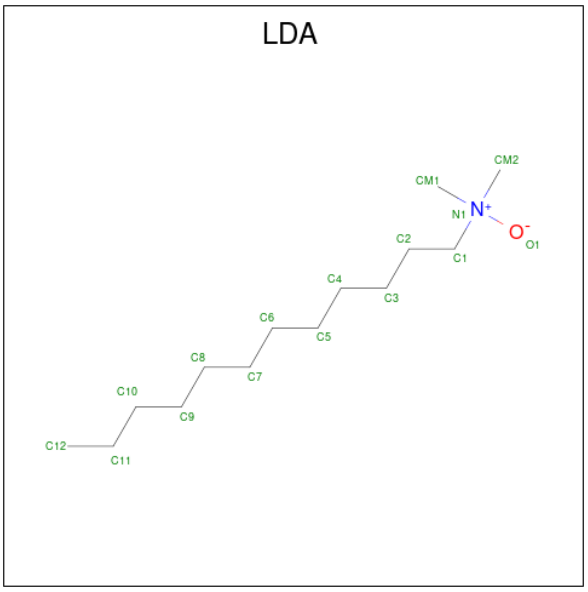
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	7	0
			65	55	4	6		

- Molecule 8 is 2-CHLORO-4-ISOPROPYLAMINO-6-ETHYLAMINO -1,3,5-TRIAZINE (three-letter code: ATZ) (formula: $C_8H_{14}ClN_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	L	1	Total	C	Cl	N	0	0
			14	8	1	5		

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



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

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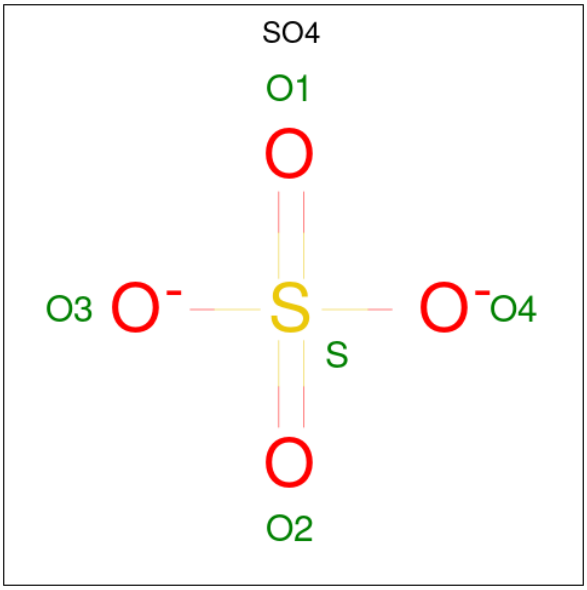
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total C N O 16 14 1 1	0	0
9	M	1	Total C N O 16 14 1 1	4	0
9	H	1	Total C N O 16 14 1 1	0	0
9	H	1	Total C N O 16 14 1 1	0	0

- Molecule 10 is FE (II) ION (three-letter code: FE2) (formula: Fe).

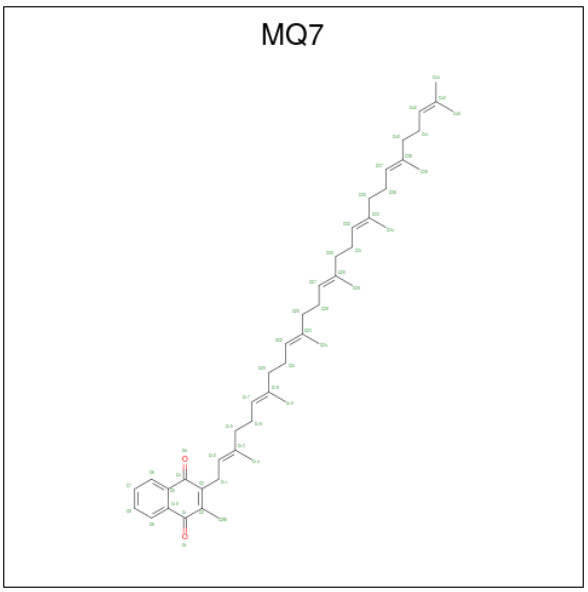
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	M	1	Total Fe 1 1	0	0

- Molecule 11 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



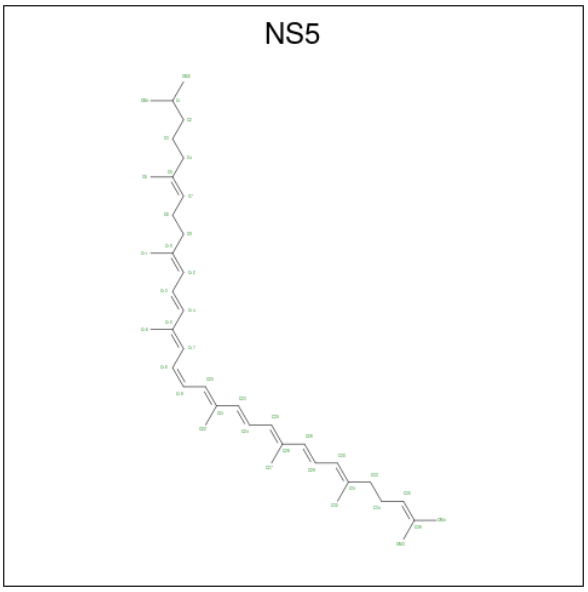
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total O S 5 4 1	0	0
11	M	1	Total O S 5 4 1	0	0
11	M	1	Total O S 5 4 1	0	0
11	H	1	Total O S 5 4 1	0	0

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



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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	M	1	Total C 40 40	14	0

- Molecule 14 is water.

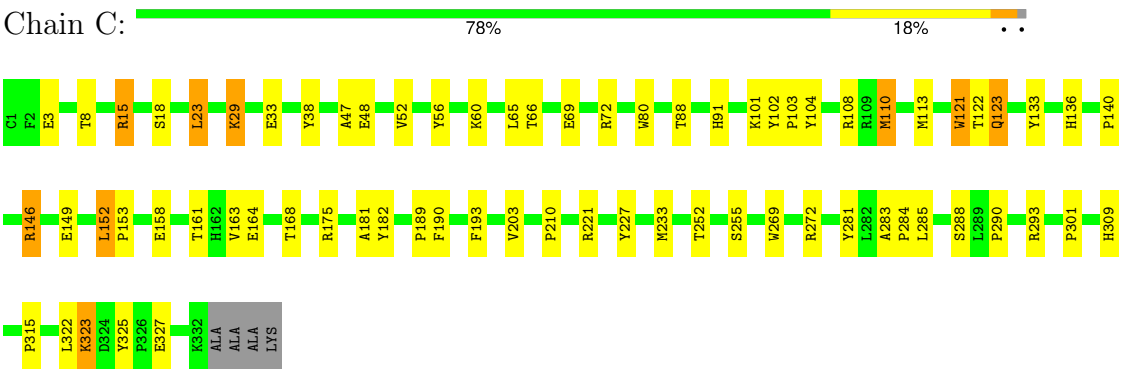
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	134	Total O 134 134	0	0
14	L	57	Total O 57 57	0	0
14	M	71	Total O 71 71	0	0
14	H	81	Total O 81 81	0	0

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.

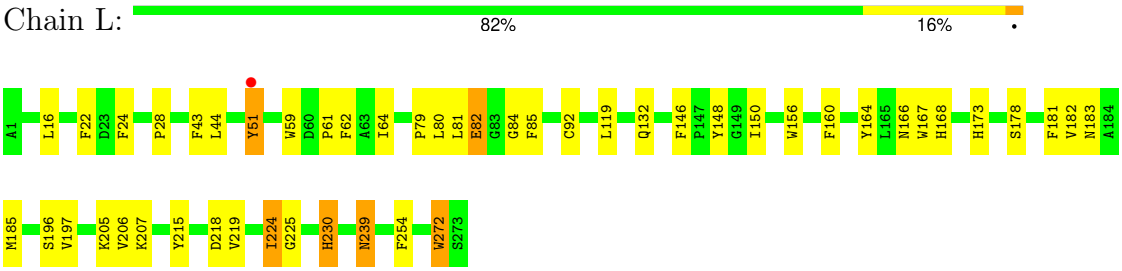
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER

Chain C:



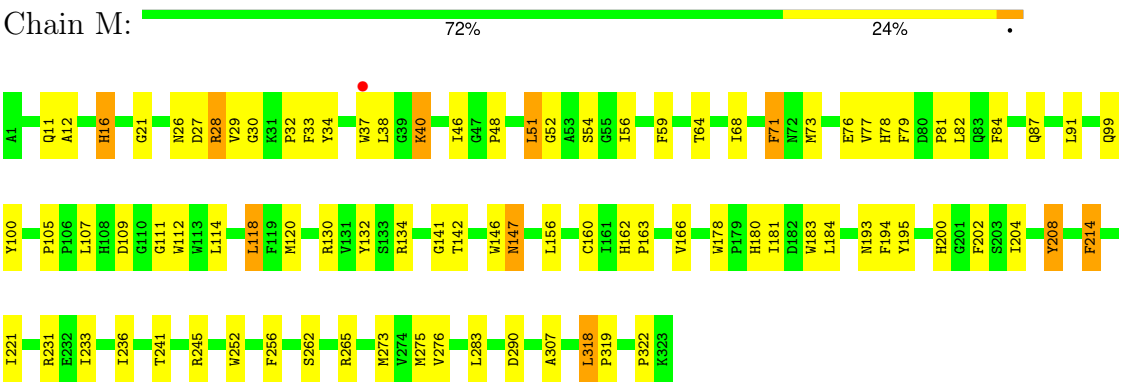
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER

Chain L:



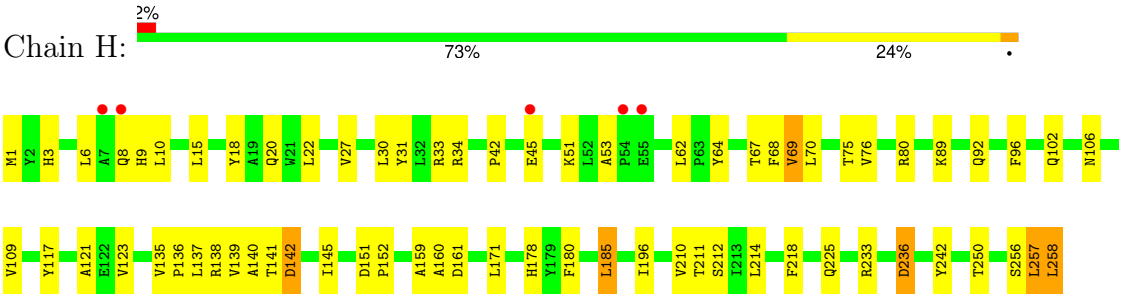
• Molecule 3: PHOTOSYNTHETIC REACTION CENTER

Chain M:



• Molecule 4: PHOTOSYNTHETIC REACTION CENTER

Chain H:


2%
73%
24%
M1 Y2 H3 L6 A7 Q8 H9 L10 L15 Y18 A19 Q20 W21 L22 V27 L30 Y31 L32 R33 R34 P42 E45 K51 L52 A53 P54 E55 L62 P63 Y64 T67 F68 V69 L70 T75 V76 R80 K89 Q92 F96 Q102 N106
V109 Y117 A121 E122 V123 V135 P136 L137 R138 V139 A140 T141 D142 I145 D151 P152 A159 A160 D161 L171 H178 Y179 F180 L185 I196 V210 T211 S212 I213 L214 F218 Q225 R233 D236 Y242 T250 S256 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 – 2.35 10.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	78.5 (10.00-2.35) 77.4 (10.00-2.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 2.31Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.190 , 0.236 0.183 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 84.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10501	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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: FE2, BCB, MQ7, NS5, SO4, BPB, LDA, FME, ATZ, HEM

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	0.52	0/2674	0.62	0/3645
2	L	0.54	0/2259	0.58	0/3084
3	M	0.55	0/2683	0.61	1/3669 (0.0%)
4	H	0.53	0/2055	0.69	2/2807 (0.1%)
All	All	0.53	0/9671	0.62	3/13205 (0.0%)

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	6
2	L	0	4
3	M	0	2
4	H	0	3
All	All	0	15

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	53	ALA	CB-CA-C	-10.63	94.16	110.10
3	M	318	LEU	O-C-N	6.16	132.81	121.10
4	H	45	GLU	CB-CA-C	-5.25	99.89	110.40

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	121	TRP	Mainchain
1	C	15	ARG	Sidechain
1	C	190	PHE	Sidechain
1	C	227	TYR	Sidechain
1	C	272	ARG	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	41	0
2	L	2171	0	2098	41	0
3	M	2577	0	2468	74	0
4	H	2018	0	2020	42	0
5	C	172	0	120	3	0
6	L	132	0	144	10	0
6	M	132	0	144	20	0
7	L	65	0	74	9	0
7	M	65	0	74	10	0
8	L	14	0	14	2	0
9	H	32	0	62	2	0
9	L	32	0	62	4	0
9	M	32	0	62	2	0
10	M	1	0	0	0	0
11	H	5	0	0	0	0
11	M	15	0	0	1	0
12	M	48	0	64	1	0
13	M	40	0	60	6	0
14	C	134	0	0	1	0
14	H	81	0	0	1	0
14	L	57	0	0	0	0
14	M	71	0	0	2	0
All	All	10501	0	10041	214	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 11.

The worst 5 of 214 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:HHC	7:L:402:BPB:HBBB	1.32	1.09
1:C:52:VAL:HB	1:C:56:TYR:HD2	1.31	0.92
1:C:152:LEU:HD22	1:C:175:ARG:HA	1.53	0.91
7:L:402:BPB:HBBA	3:M:208:TYR:HB3	1.60	0.83
7:L:402:BPB:HHC	7:L:402:BPB:CBB	2.12	0.78

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%)	313 (95%)	18 (5%)	0	100 100
2	L	271/273 (99%)	257 (95%)	14 (5%)	0	100 100
3	M	323/323 (100%)	309 (96%)	11 (3%)	3 (1%)	14 14
4	H	256/258 (99%)	237 (93%)	19 (7%)	0	100 100
All	All	1181/1190 (99%)	1116 (94%)	62 (5%)	3 (0%)	37 43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	51	LEU
3	M	322	PRO
3	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	281/282 (100%)	264 (94%)	17 (6%)	16 18
2	L	218/218 (100%)	210 (96%)	8 (4%)	29 38
3	M	251/249 (101%)	236 (94%)	15 (6%)	16 18
4	H	212/212 (100%)	192 (91%)	20 (9%)	7 6
All	All	962/961 (100%)	902 (94%)	60 (6%)	15 17

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	33	PHE
4	H	236	ASP
3	M	156	LEU
4	H	225	GLN
4	H	258	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	58	ASN
2	L	183	ASN
2	L	239	ASN
3	M	147	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	FME	H	1	4	8,9,10	0.62	0	8,9,11	2.85	3 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FME	H	1	4	-	4/7/9/11	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	1	FME	CA-N-CN	-6.20	113.28	122.82
4	H	1	FME	O1-CN-N	-4.52	113.65	125.32
4	H	1	FME	O-C-CA	-2.07	119.43	124.77

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

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	$\#\|Z\| > 2$
8	ATZ	L	502	-	14,14,14	0.64	0	18,18,18	1.76	1 (5%)
9	LDA	L	705	-	13,15,15	2.56	2 (15%)	14,17,17	0.53	0
11	SO4	M	803	-	4,4,4	0.48	0	6,6,6	0.62	0
13	NS5	M	600	-	39,39,39	0.69	0	46,46,46	1.37	6 (13%)
5	HEM	C	340	1	42,50,50	1.66	8 (19%)	46,82,82	1.17	4 (8%)
11	SO4	M	802	-	4,4,4	0.43	0	6,6,6	0.45	0
9	LDA	M	704	-	13,15,15	2.05	2 (15%)	14,17,17	0.58	0
11	SO4	M	804	-	4,4,4	0.57	0	6,6,6	0.96	0
9	LDA	H	701	-	13,15,15	2.65	2 (15%)	14,17,17	0.78	1 (7%)
6	BCB	M	805	3	63,74,74	1.70	9 (14%)	72,115,115	2.05	11 (15%)
6	BCB	L	304	2	63,74,74	1.65	8 (12%)	72,115,115	2.09	12 (16%)
12	MQ7	M	501	-	49,49,49	1.72	12 (24%)	61,63,63	1.52	10 (16%)
9	LDA	M	706	-	13,15,15	2.48	2 (15%)	14,17,17	0.46	0
6	BCB	M	806	3	63,74,74	1.77	9 (14%)	72,115,115	2.35	18 (25%)
7	BPB	M	401	-	49,70,70	1.54	7 (14%)	48,101,101	2.40	9 (18%)
6	BCB	L	302	2	63,74,74	1.65	10 (15%)	72,115,115	2.08	16 (22%)
5	HEM	C	339	1	42,50,50	1.49	4 (9%)	46,82,82	1.24	6 (13%)
7	BPB	L	402	-	49,70,70	1.23	6 (12%)	48,101,101	2.25	7 (14%)
11	SO4	H	801	-	4,4,4	0.55	0	6,6,6	0.56	0
5	HEM	C	338	1	42,50,50	1.51	6 (14%)	46,82,82	1.28	5 (10%)
9	LDA	H	703	-	13,15,15	3.08	2 (15%)	14,17,17	0.56	0
5	HEM	C	337	1	42,50,50	1.49	4 (9%)	46,82,82	1.35	6 (13%)
9	LDA	L	702	-	13,15,15	2.70	2 (15%)	14,17,17	0.53	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
8	ATZ	L	502	-	-	1/7/7/7	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	LDA	L	705	-	-	6/13/13/13	-
13	NS5	M	600	-	-	10/43/43/43	-
5	HEM	C	340	1	-	3/12/54/54	-
9	LDA	M	704	-	-	4/13/13/13	-
9	LDA	H	701	-	-	2/13/13/13	-
6	BCB	M	805	3	3/3/21/26	8/37/137/137	-
6	BCB	L	304	2	3/3/21/26	6/37/137/137	-
12	MQ7	M	501	-	-	1/41/61/61	0/2/2/2
9	LDA	M	706	-	-	5/13/13/13	-
6	BCB	M	806	3	3/3/21/26	10/37/137/137	-
7	BPB	M	401	-	-	10/37/105/105	0/5/6/6
6	BCB	L	302	2	3/3/21/26	8/37/137/137	-
5	HEM	C	339	1	-	3/12/54/54	-
7	BPB	L	402	-	1/1/18/23	5/37/105/105	0/5/6/6
5	HEM	C	338	1	-	6/12/54/54	-
9	LDA	H	703	-	-	5/13/13/13	-
5	HEM	C	337	1	-	5/12/54/54	-
9	LDA	L	702	-	-	1/13/13/13	-

The worst 5 of 95 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	702	LDA	O1-N1	-8.29	1.21	1.42
9	H	703	LDA	O1-N1	-7.84	1.22	1.42
9	H	703	LDA	C1-N1	-7.78	1.43	1.51
9	H	701	LDA	O1-N1	-7.75	1.23	1.42
9	L	705	LDA	O1-N1	-7.63	1.23	1.42

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	401	BPB	O2D-CGD-CBD	11.40	123.47	110.95
7	L	402	BPB	O2D-CGD-CBD	10.69	122.69	110.95
6	M	806	BCB	C4A-NA-C1A	8.75	110.67	106.68
6	L	302	BCB	C4A-NA-C1A	8.33	110.48	106.68
6	M	805	BCB	C4A-NA-C1A	8.07	110.36	106.68

5 of 13 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	L	302	BCB	ND
6	L	302	BCB	NA
6	L	302	BCB	NC
6	L	304	BCB	ND
6	L	304	BCB	NA

5 of 99 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
9	L	705	LDA	N1-C1-C2-C3
13	M	600	NS5	C10-C12-C13-C14
13	M	600	NS5	C13-C14-C15-C17

There are no ring outliers.

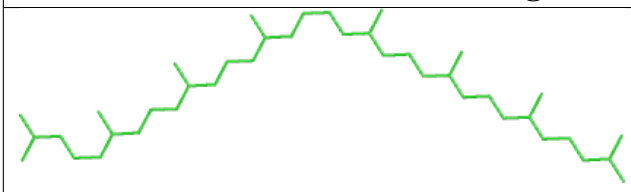
17 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	502	ATZ	2	0
9	L	705	LDA	1	0
13	M	600	NS5	6	0
9	M	704	LDA	1	0
11	M	804	SO4	1	0
6	M	805	BCB	9	0
6	L	304	BCB	5	0
12	M	501	MQ7	1	0
9	M	706	LDA	1	0
6	M	806	BCB	13	0
7	M	401	BPB	10	0
6	L	302	BCB	5	0
5	C	339	HEM	1	0
7	L	402	BPB	9	0
5	C	338	HEM	2	0
9	H	703	LDA	2	0
9	L	702	LDA	3	0

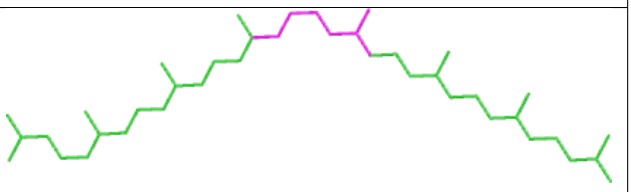
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

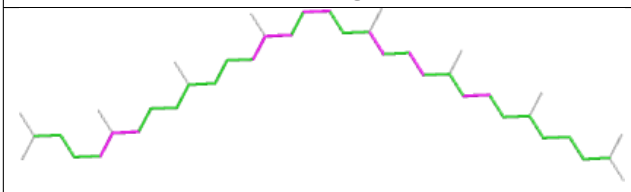
Ligand NS5 M 600



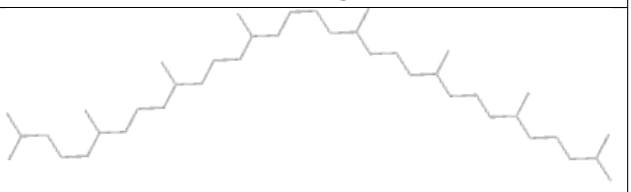
Bond lengths



Bond angles

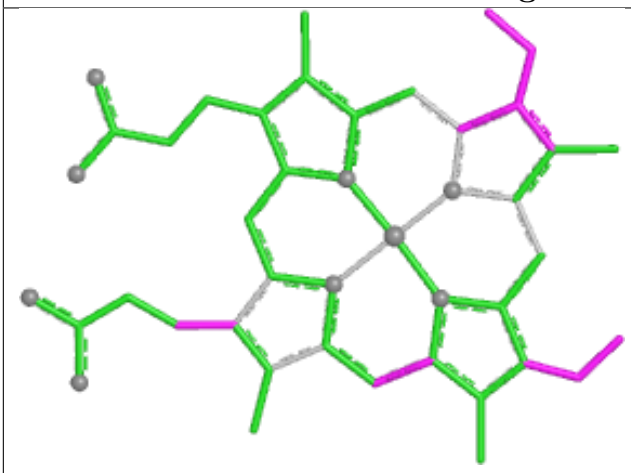


Torsions

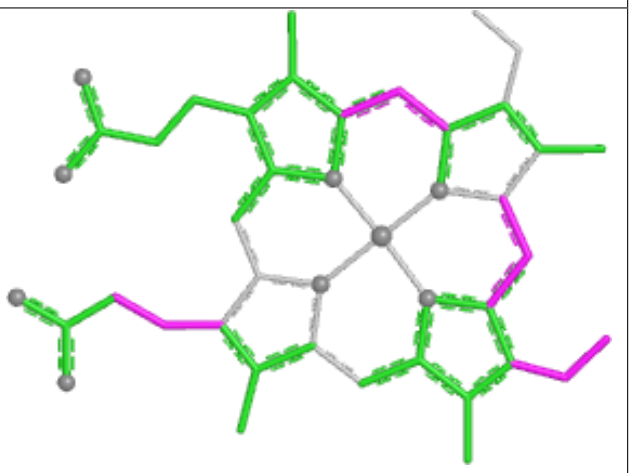


Rings

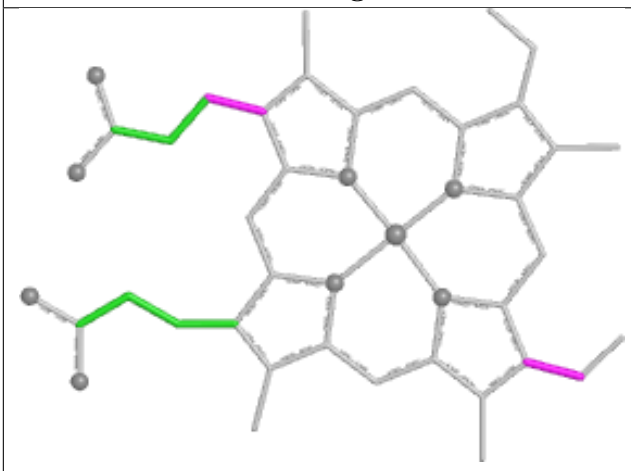
Ligand HEM C 340



Bond lengths



Bond angles



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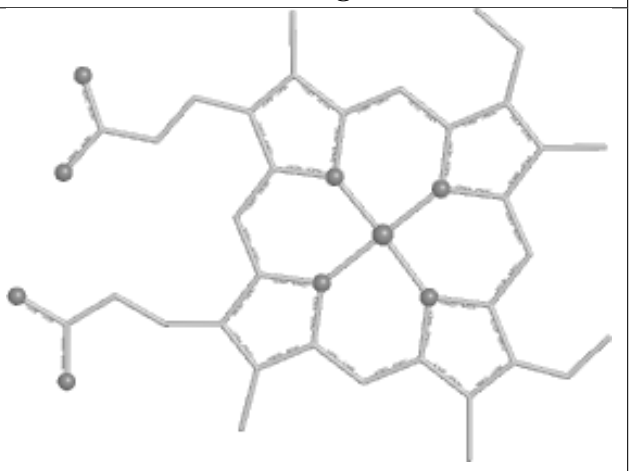
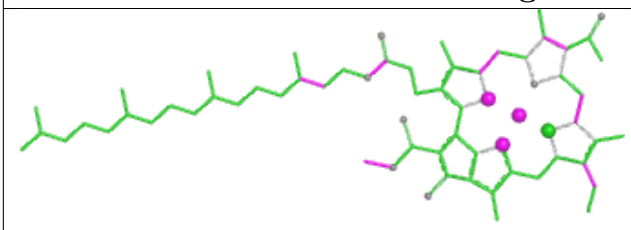


Rings

Ligand BCB M 805



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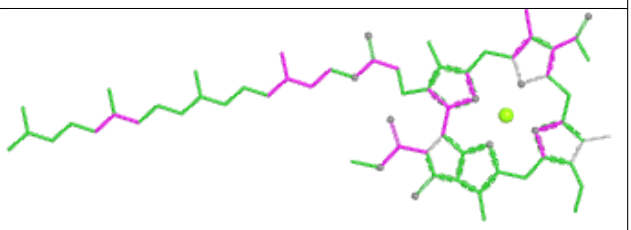
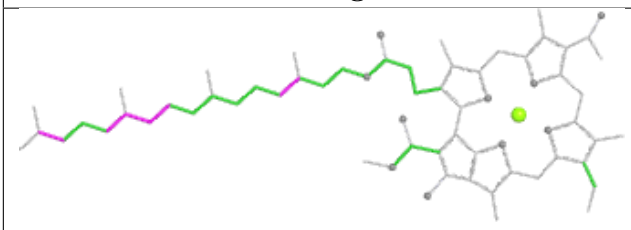
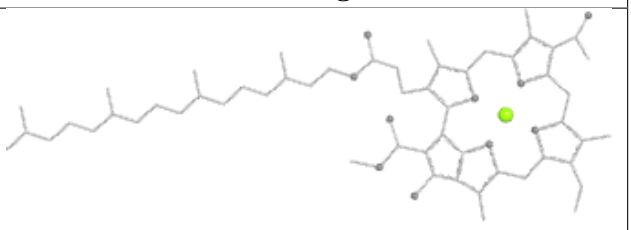


Bond angles

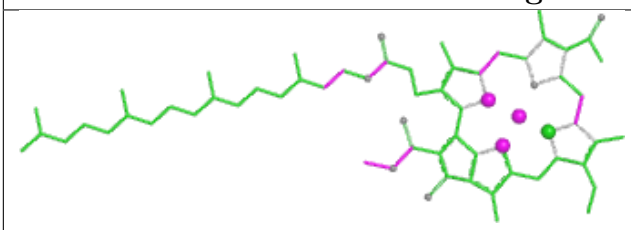


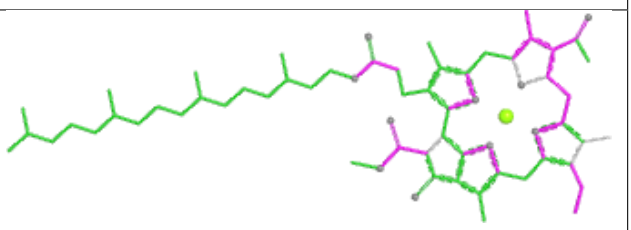
Torsions

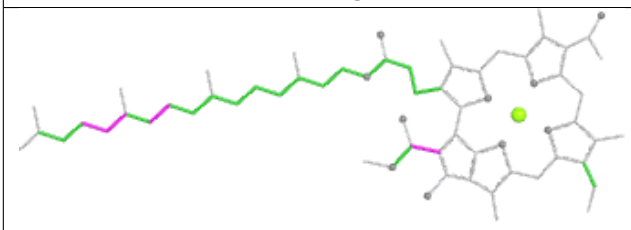


Rings

Ligand BCB L 304


Bond lengths


Bond angles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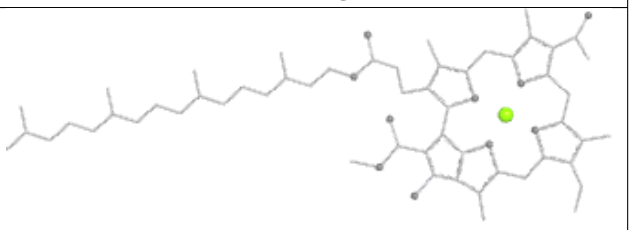
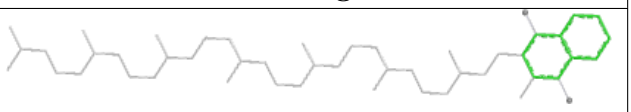

Rings

Ligand MQ7 M 501

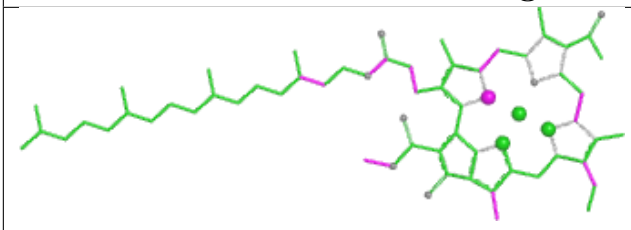

Bond lengths

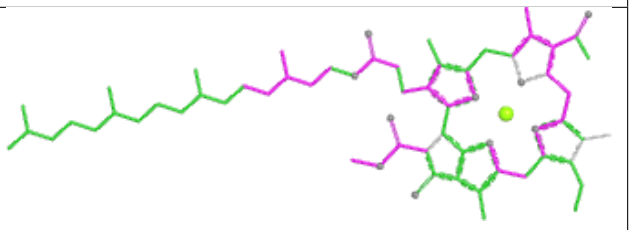

Bond angles

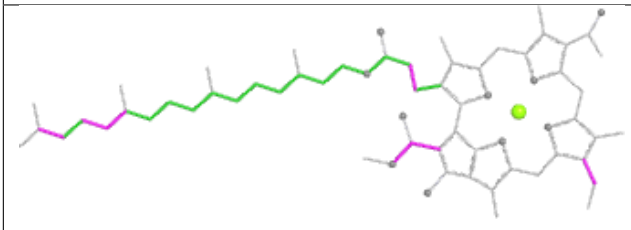

Torsions

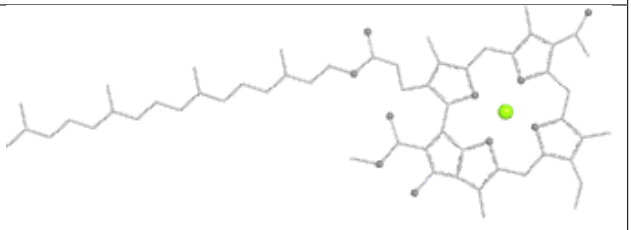

Rings

Ligand BCB M 806

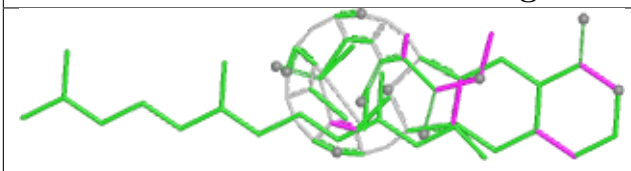

Bond lengths


Bond angles

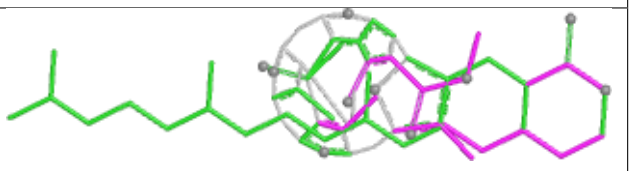

Torsions


Rings

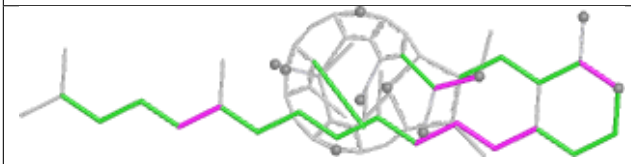
Ligand BPB M 401



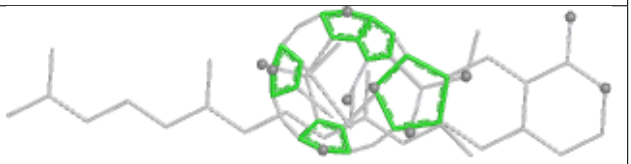
Bond lengths



Bond angles

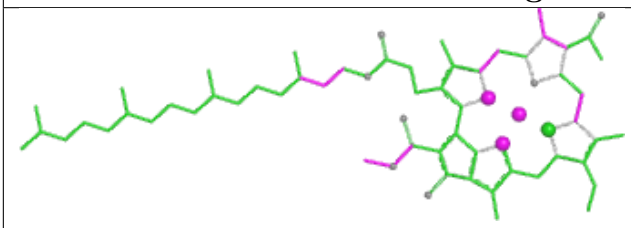


Torsions



Rings

Ligand BCB L 302



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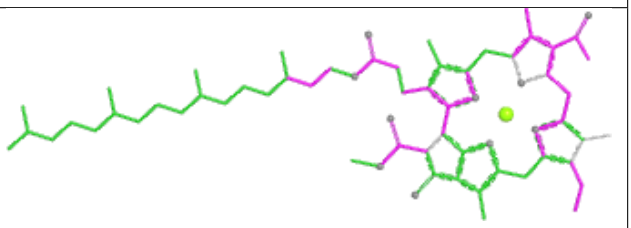
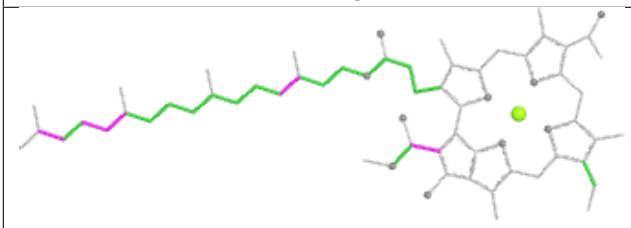


Bond angles



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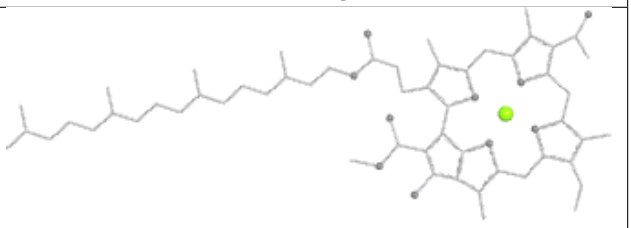
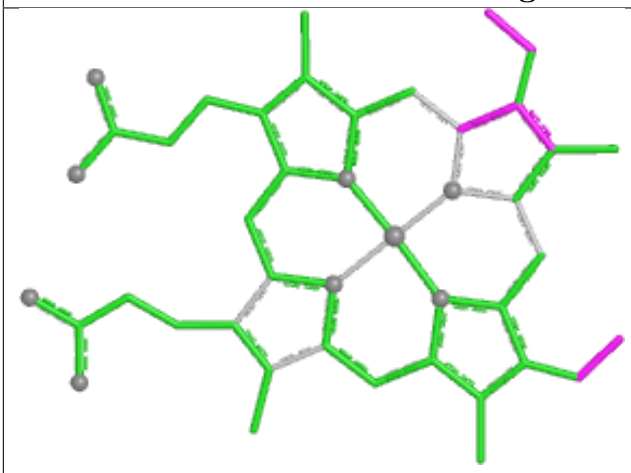


Rings

Ligand HEM C 339



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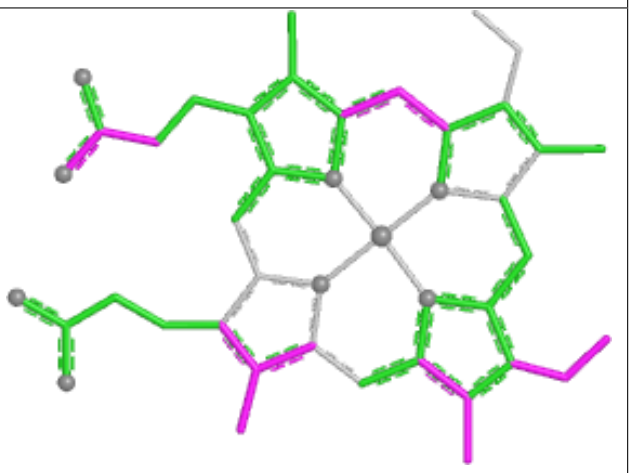
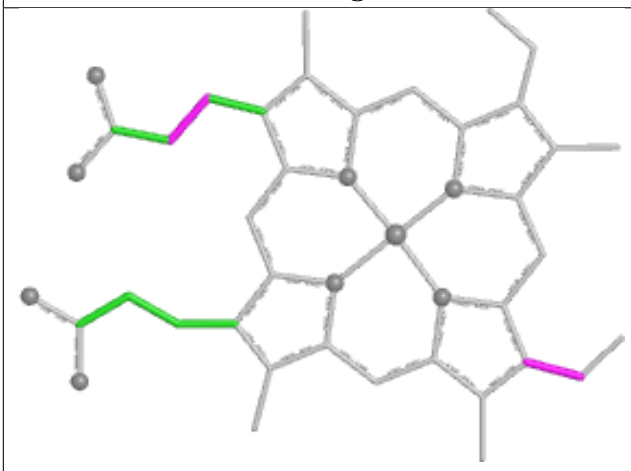
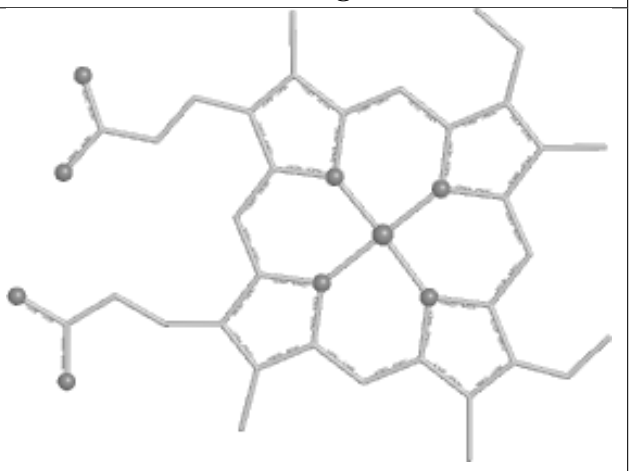


Bond angles

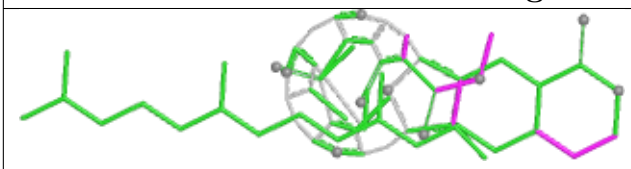


Torsions

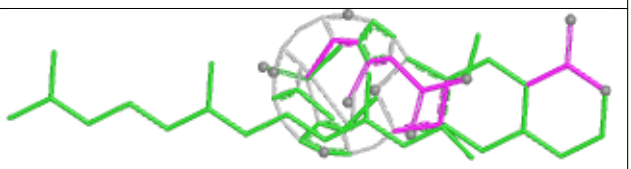


Rings

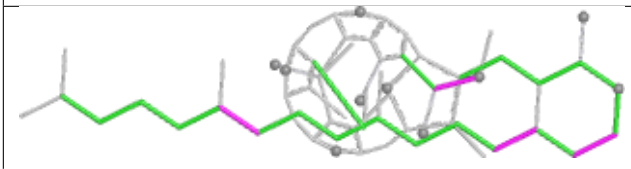
Ligand BPB L 402



Bond lengths



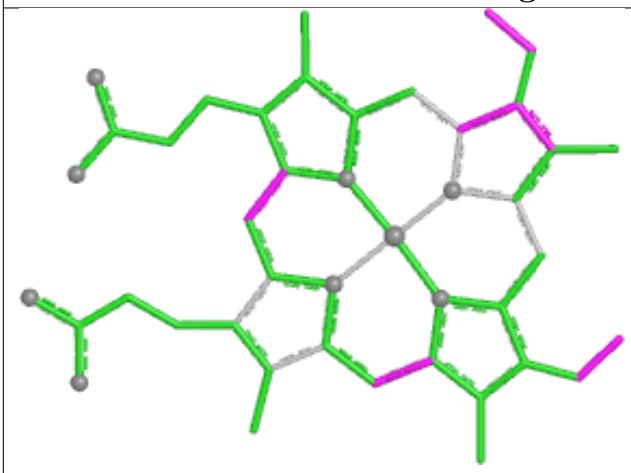
Bond angles



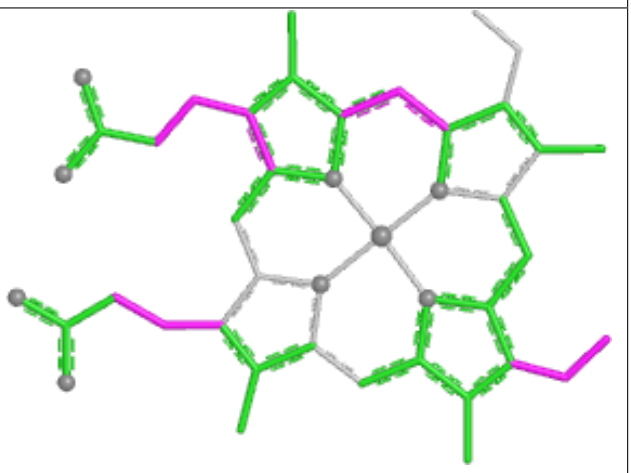
Torsions

Rings

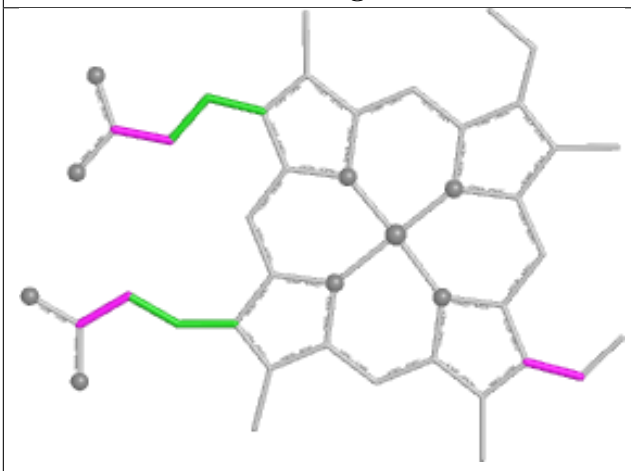
Ligand HEM C 338



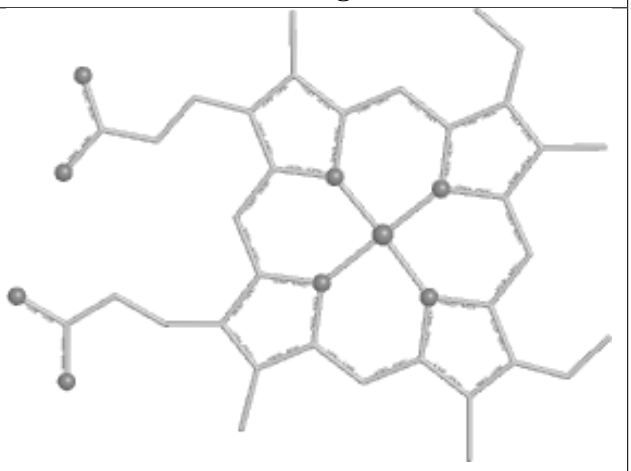
Bond lengths



Bond angles

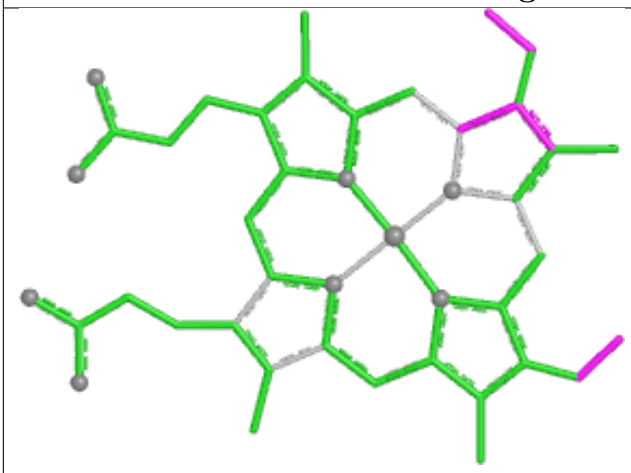


Torsions

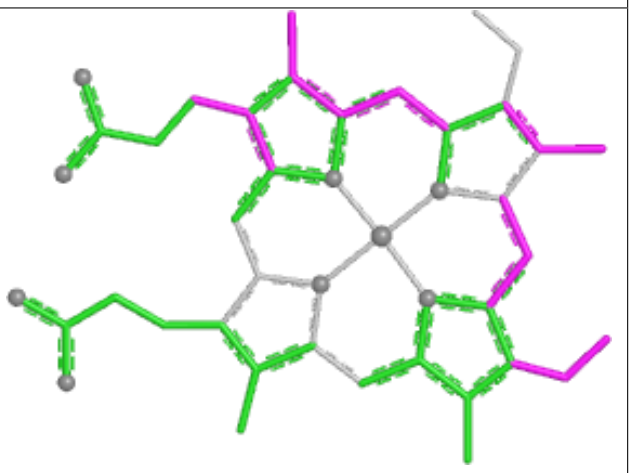


Rings

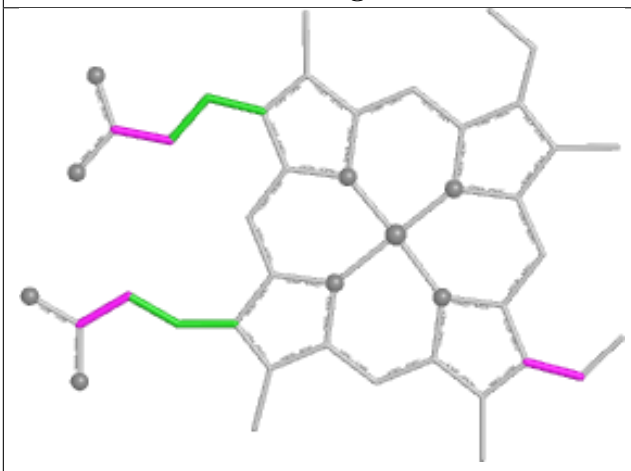
Ligand HEM C 337



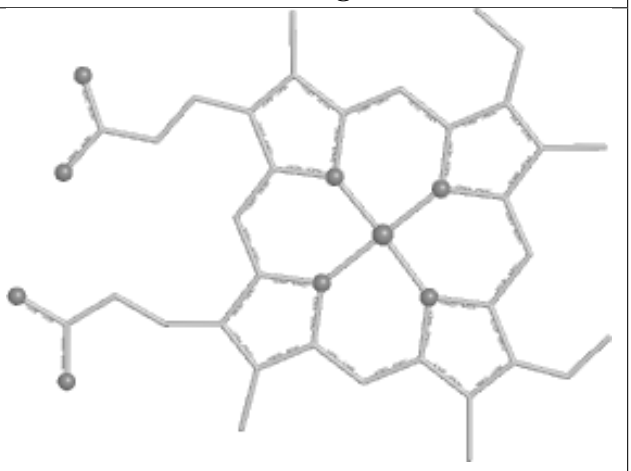
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	C	332/336 (98%)	-0.90	0 100 100	13, 29, 53, 82	19 (5%)
2	L	273/273 (100%)	-0.96	1 (0%) 89 90	11, 25, 48, 67	7 (2%)
3	M	323/323 (100%)	-0.82	1 (0%) 90 91	10, 28, 55, 72	12 (3%)
4	H	249/258 (96%)	-0.44	5 (2%) 64 69	16, 38, 65, 90	19 (7%)
All	All	1177/1190 (98%)	-0.79	7 (0%) 85 88	10, 30, 56, 90	57 (4%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	54	PRO	4.0
4	H	8	GLN	3.1
4	H	45	GLU	2.5
3	M	37	TRP	2.5
4	H	7	ALA	2.4

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
4	FME	H	1	10/11	0.95	0.06	34,38,46,54	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

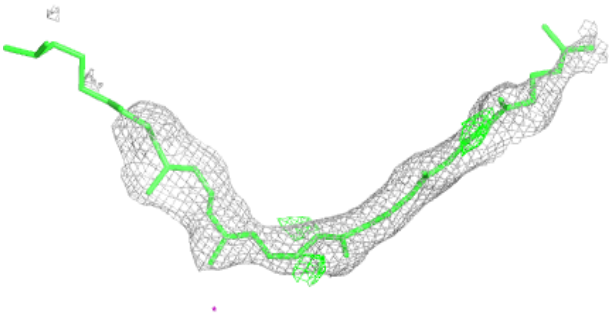
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

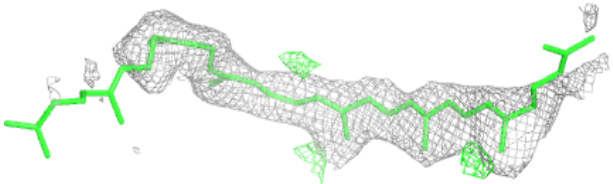
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	LDA	M	706	16/16	0.82	0.15	77,82,87,87	4
9	LDA	M	704	16/16	0.83	0.14	67,73,102,103	0
9	LDA	L	705	16/16	0.83	0.10	62,70,78,79	3
13	NS5	M	600	40/40	0.89	0.09	34,51,70,70	14
11	SO4	M	803	5/5	0.92	0.11	84,88,90,90	0
9	LDA	H	703	16/16	0.92	0.08	30,40,65,67	0
9	LDA	H	701	16/16	0.95	0.05	18,28,36,37	0
11	SO4	H	801	5/5	0.95	0.06	62,65,65,66	0
9	LDA	L	702	16/16	0.95	0.08	34,54,73,75	0
7	BPB	M	401	65/65	0.96	0.06	14,32,81,82	7
6	BCB	M	805	66/66	0.96	0.06	8,27,61,62	0
8	ATZ	L	502	14/14	0.97	0.05	21,33,35,36	0
11	SO4	M	804	5/5	0.97	0.06	45,49,53,54	0
5	HEM	C	337	43/43	0.98	0.05	25,31,44,49	0
6	BCB	M	806	66/66	0.98	0.04	6,16,31,36	0
7	BPB	L	402	65/65	0.98	0.04	2,17,22,26	0
6	BCB	L	302	66/66	0.98	0.03	3,13,21,24	0
12	MQ7	M	501	48/48	0.98	0.04	12,18,46,48	0
6	BCB	L	304	66/66	0.98	0.03	8,17,29,44	0
5	HEM	C	340	43/43	0.99	0.04	10,23,36,53	0
5	HEM	C	338	43/43	0.99	0.05	15,30,38,47	0
11	SO4	M	802	5/5	0.99	0.06	37,41,47,51	0
5	HEM	C	339	43/43	0.99	0.04	6,19,24,34	0
10	FE2	M	500	1/1	1.00	0.01	24,24,24,24	0

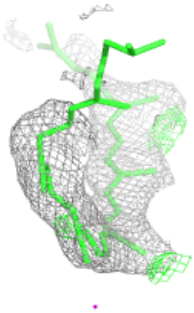
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NS5 M 600:

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

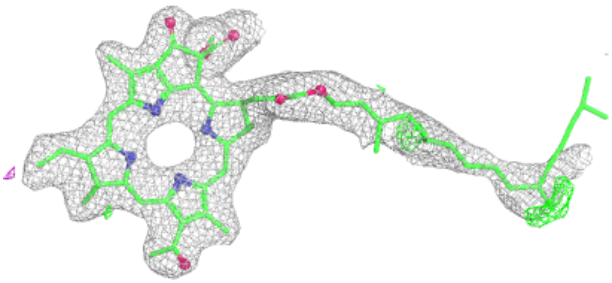


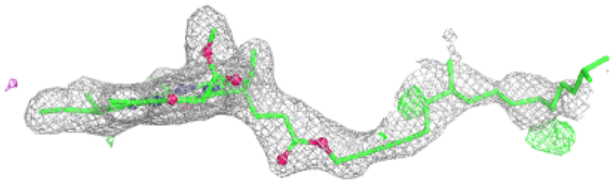


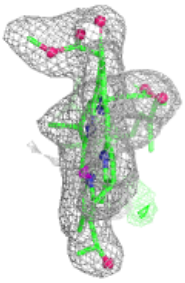


Electron density around BPB M 401:

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

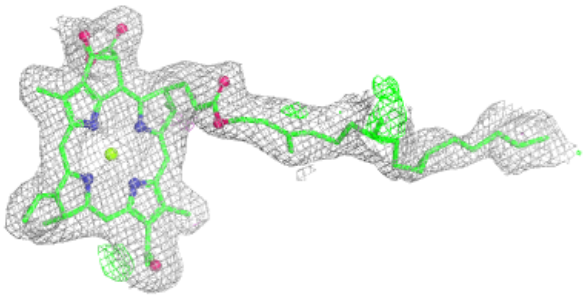


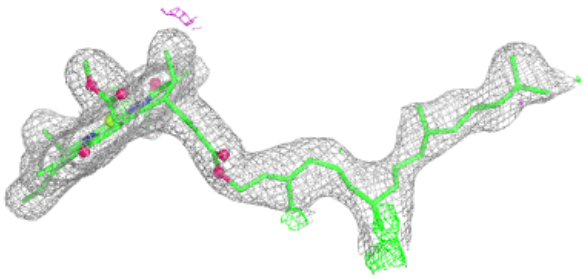


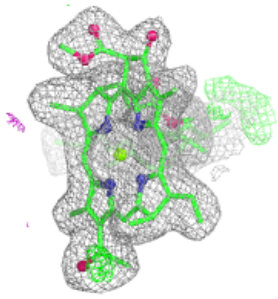


Electron density around BCB M 805:

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

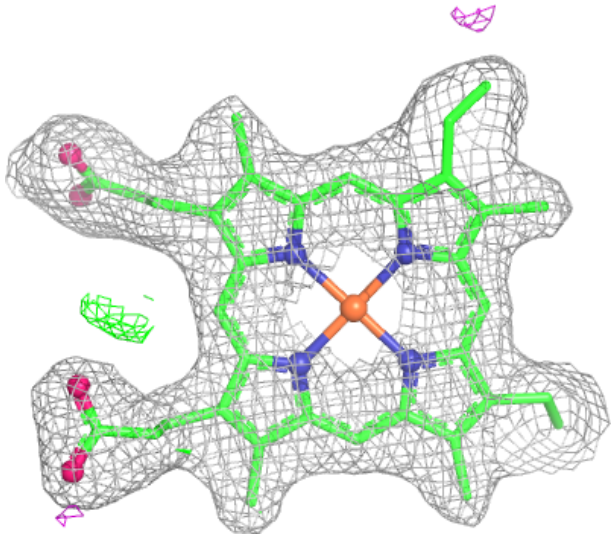


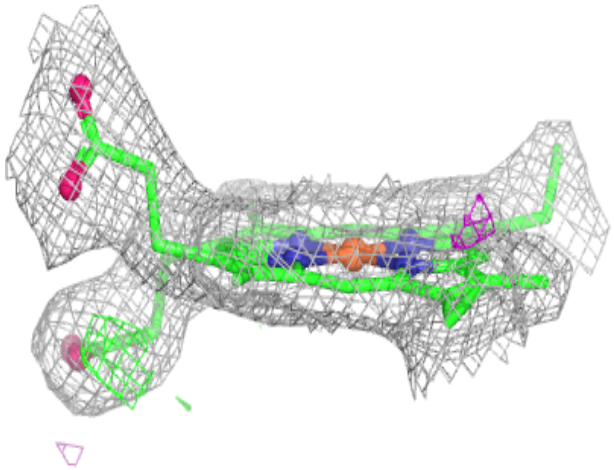


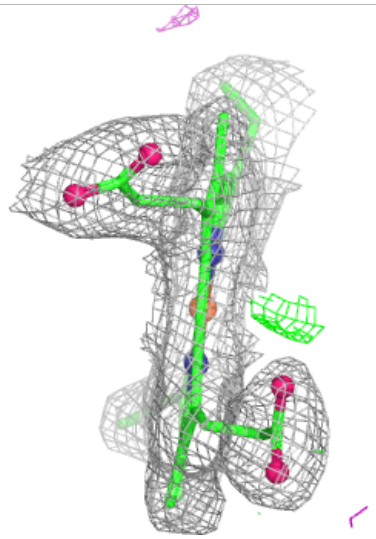


Electron density around HEM C 337:

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

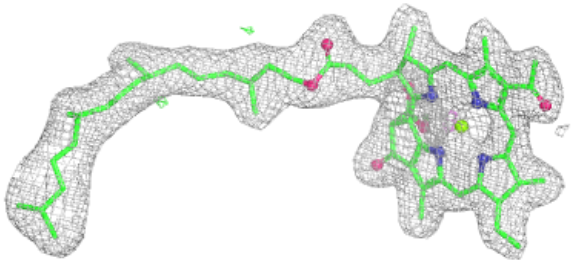


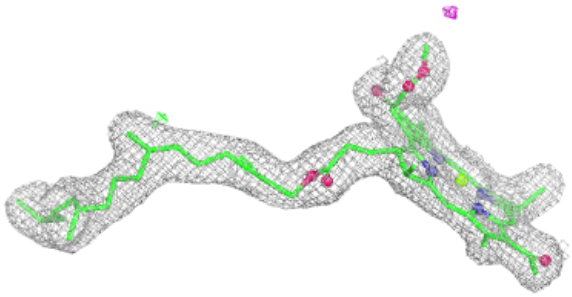


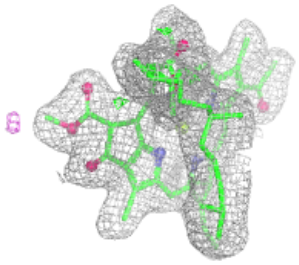


Electron density around BCB M 806:

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

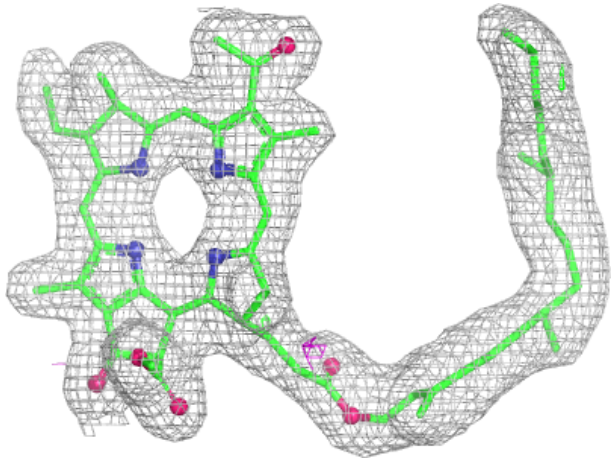


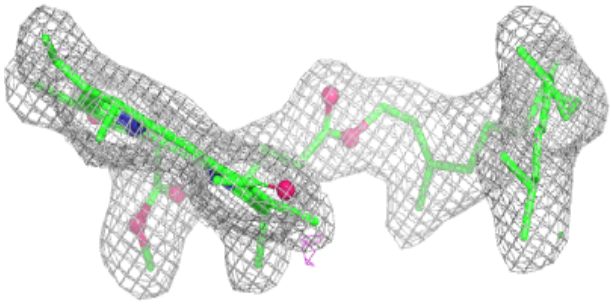


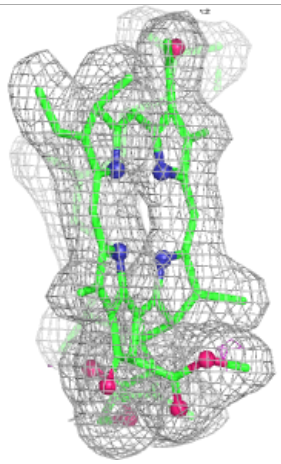


Electron density around BPB L 402:

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

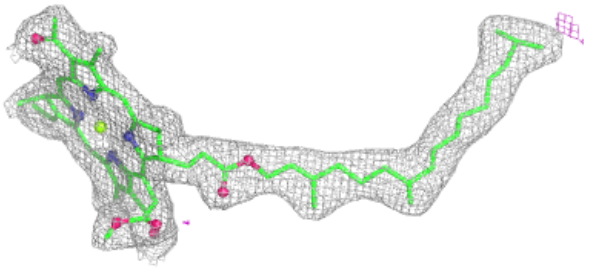


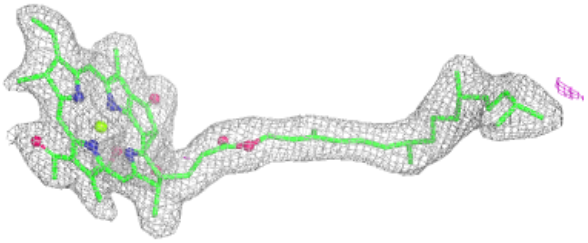


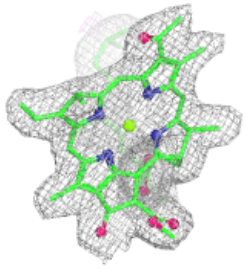


Electron density around BCB L 302:

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

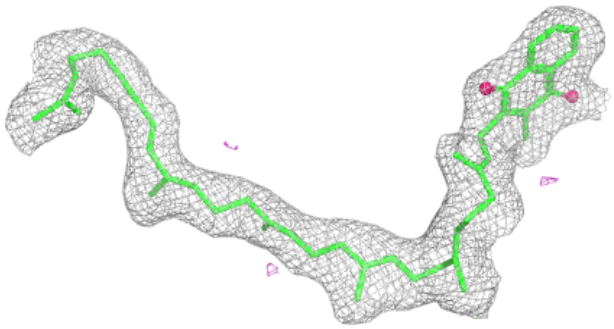


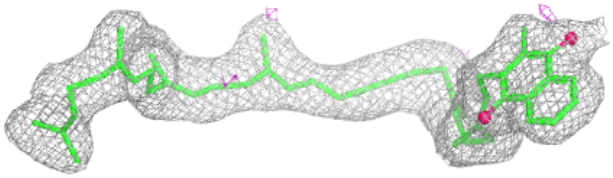


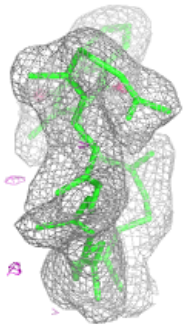


Electron density around MQ7 M 501:

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

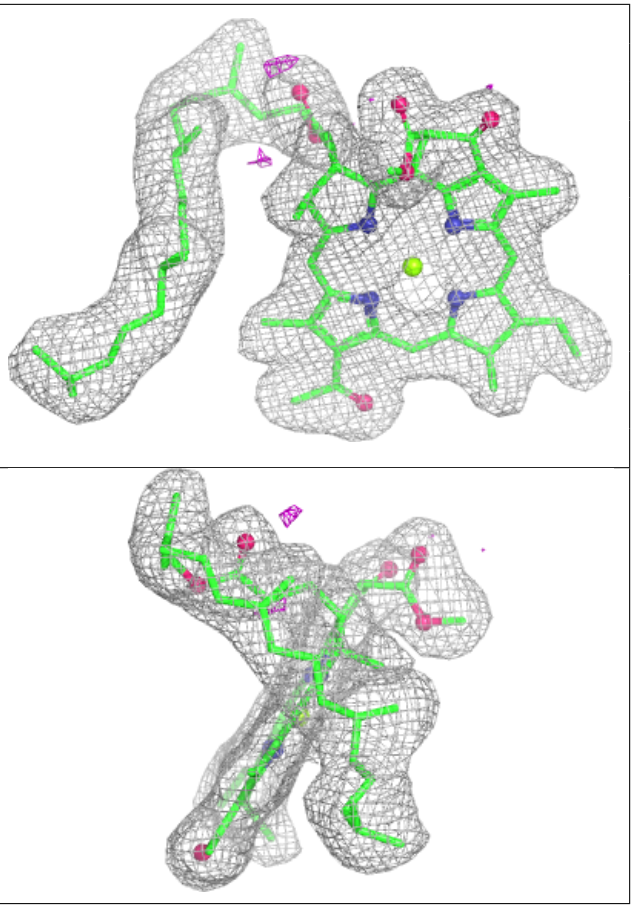


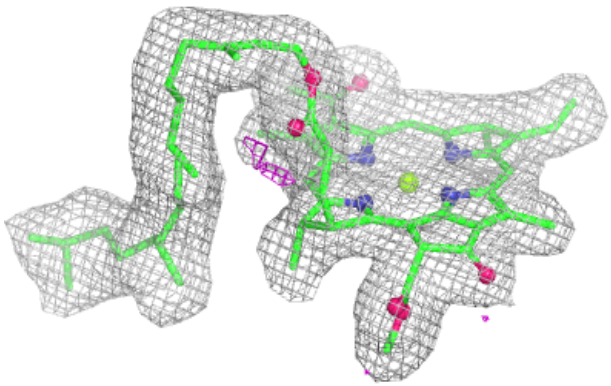




Electron density around BCB L 304:

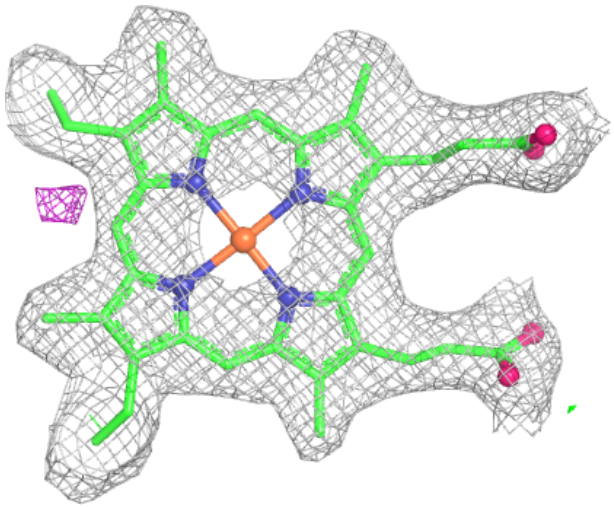
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

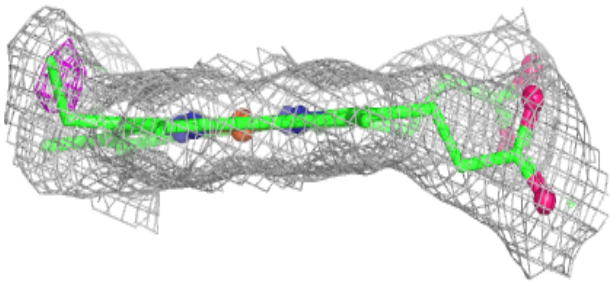


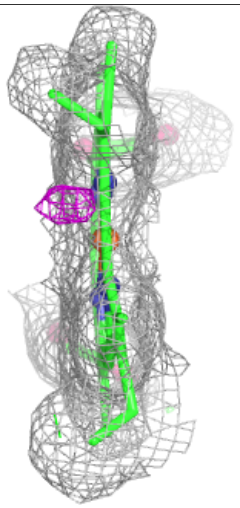


Electron density around HEM C 340:

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

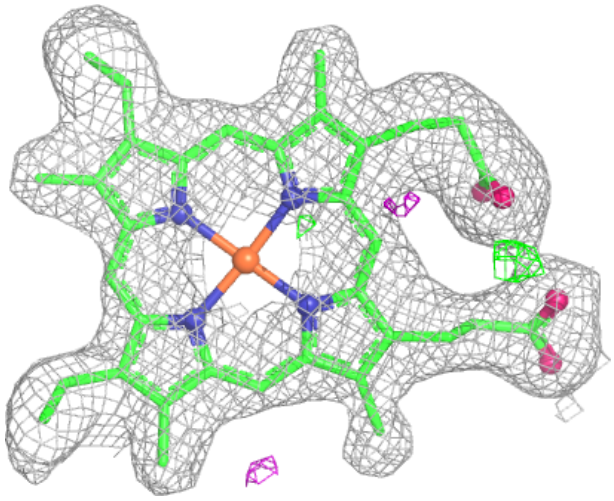


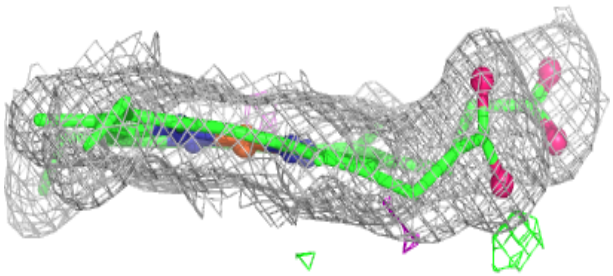


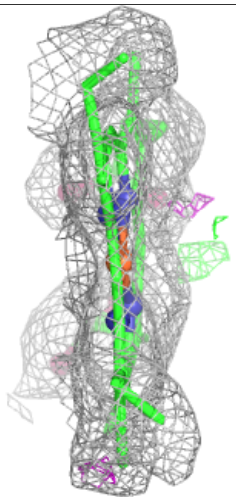


Electron density around HEM C 338:

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

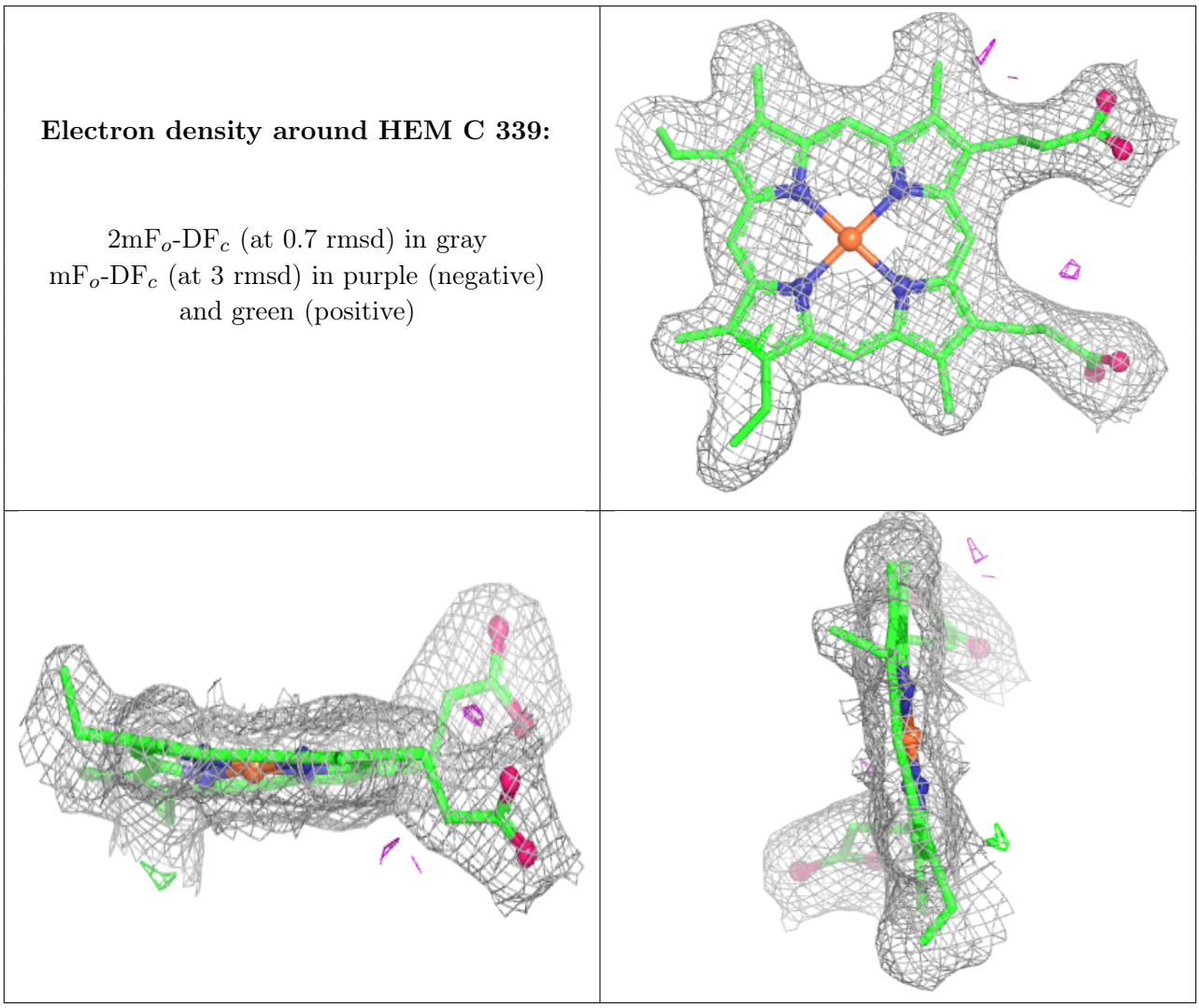






Electron density around HEM C 339:

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



6.5 Other polymers

There are no such residues in this entry.