wwPDB X-ray Structure Validation Summary Report (i)

Jul 31, 2023 – 08:42 PM EDT

PDB ID	:	6PRC
Title	:	PHOTOSYNTHETIC REACTION CENTER FROM RHODOPSEUDOMONAS VIRIDIS (DG-420314 (TRIAZINE) COMPLEX)
Authors	:	Lancaster, C.R.D.; Michel, H.
Deposited on	:	1997-07-31
Resolution	:	2.30 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:

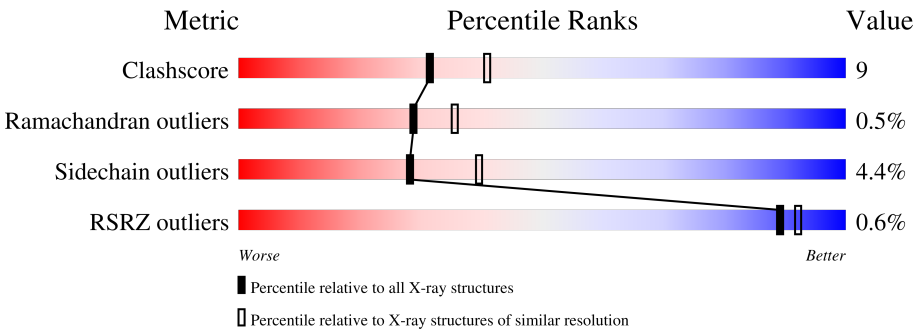
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.30 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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	% 79% 17% • •
2	L	273	85% 14% •
3	M	323	79% 20% •
4	H	258	% 77% 20% •

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
7	BPB	L	402	X	-	-	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 10498 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	51	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	14	0	0

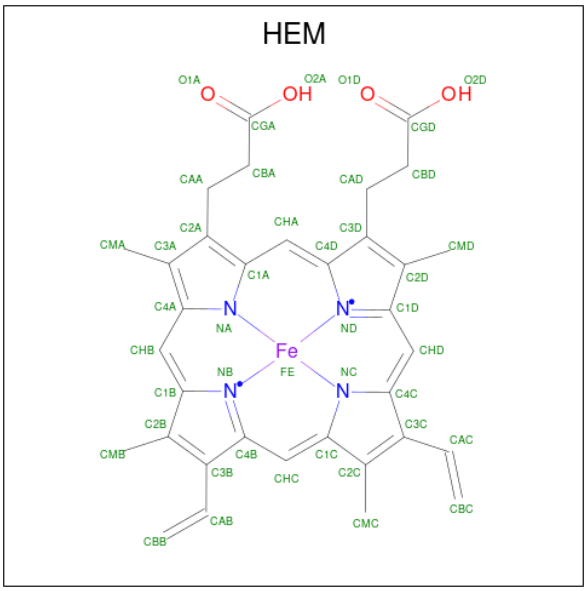
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

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.

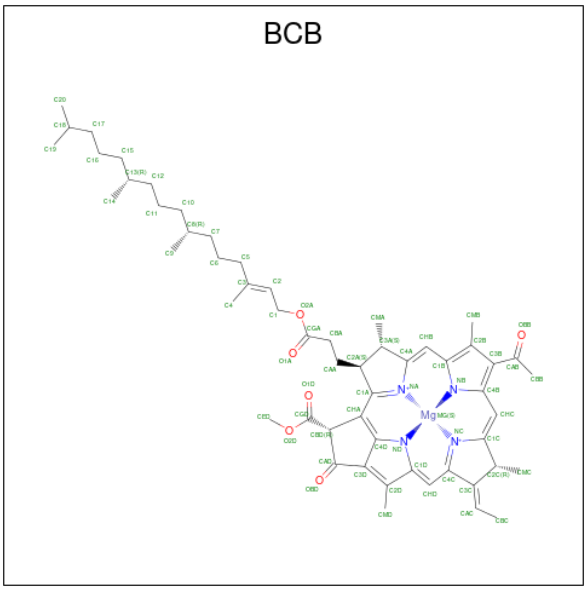
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	258	2018	1292	344	380	2	125	0	0

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



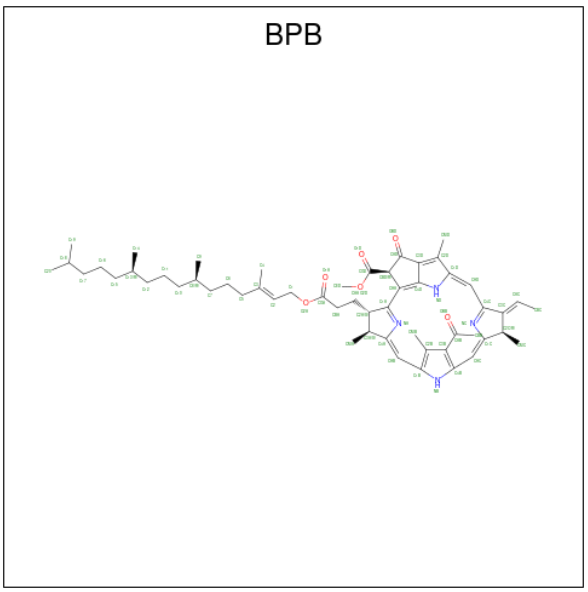
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	C	1	43	34	1	4	4	0	0

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



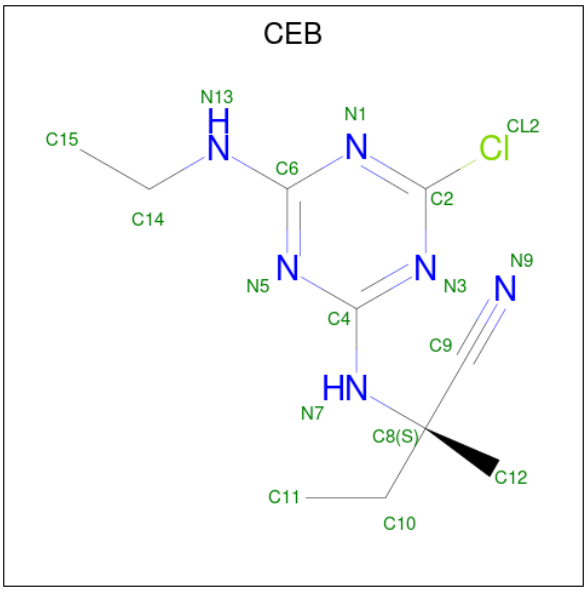
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
6	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
6	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
6	M	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
6	M	1	66	55	1	4	6	0	0

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



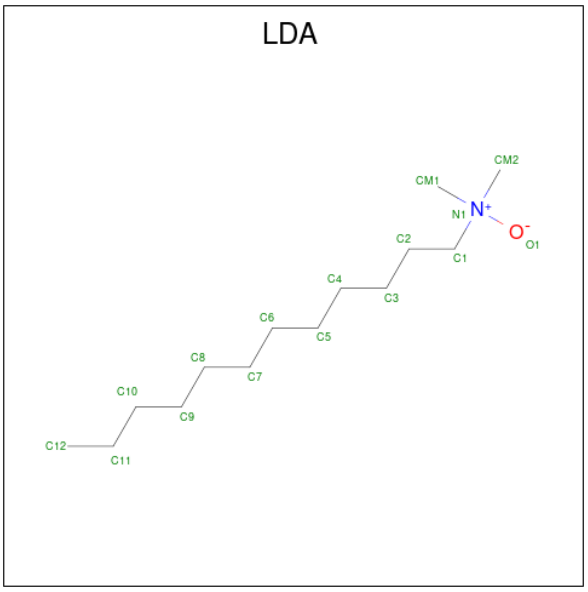
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	L	1	65	55	4	6	0	0
			Total	C	N	O		
7	M	1	65	55	4	6	7	0

- Molecule 8 is 2-CHLORO-4-ETHYLAMINO-6-(S(-)-2'-CYANO-4-BUTYLAMINO)-1,3,5-TRIAZINE (three-letter code: CEB) (formula: $C_{10}H_{15}ClN_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	Cl	N		
8	L	1	17	10	1	6	0	0

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



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

Continued on next page...

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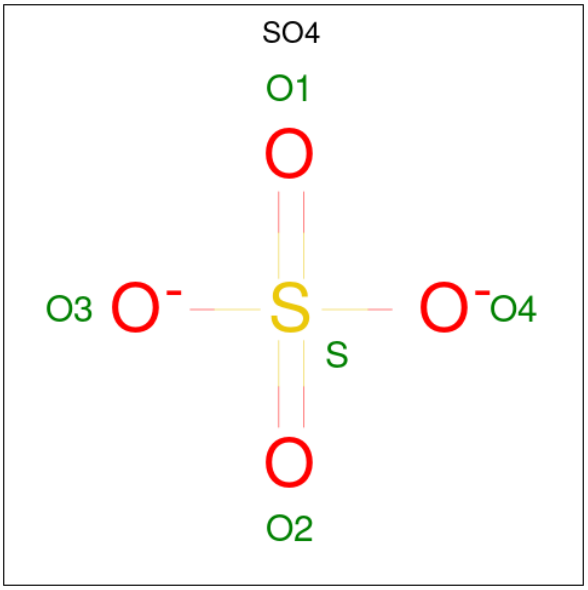
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	M	1	16	14	1	1	5	0
			Total	C	N	O		
9	M	1	16	14	1	1	4	0
			Total	C	N	O		
9	H	1	16	14	1	1	0	0
			Total	C	N	O		
9	H	1	16	14	1	1	0	0

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

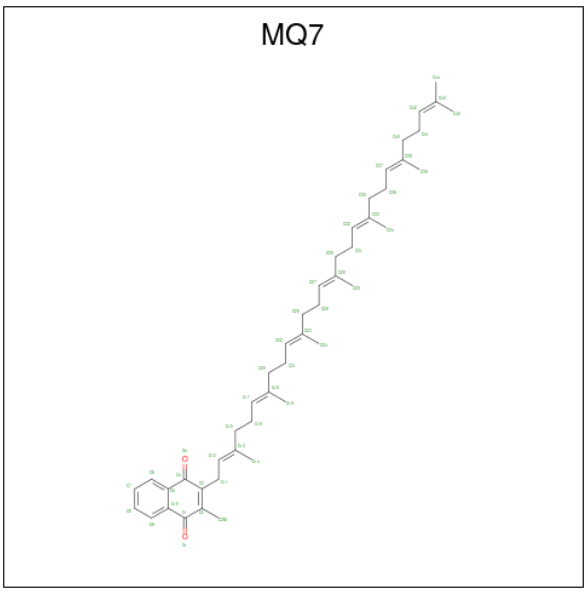
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
10	M	1	1	1	0	0

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



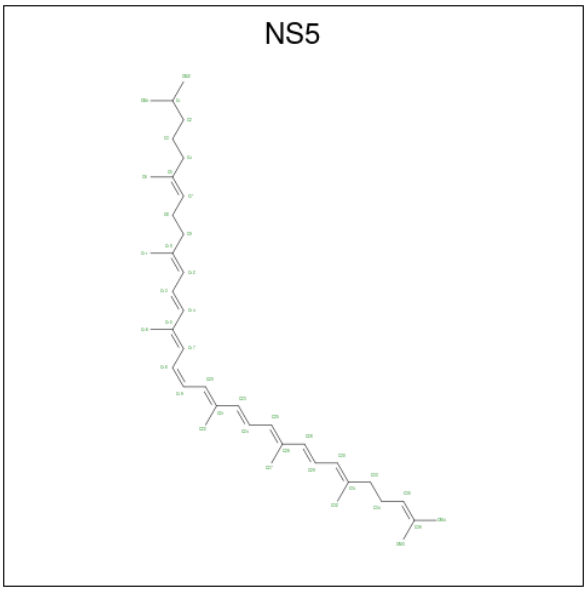
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
11	M	1	5	4	1		0	0
			Total	O	S			
11	M	1	5	4	1		0	0
			Total	O	S			
11	M	1	5	4	1		0	0
			Total	O	S			
11	H	1	5	4	1		0	0

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



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

- Molecule 14 is water.

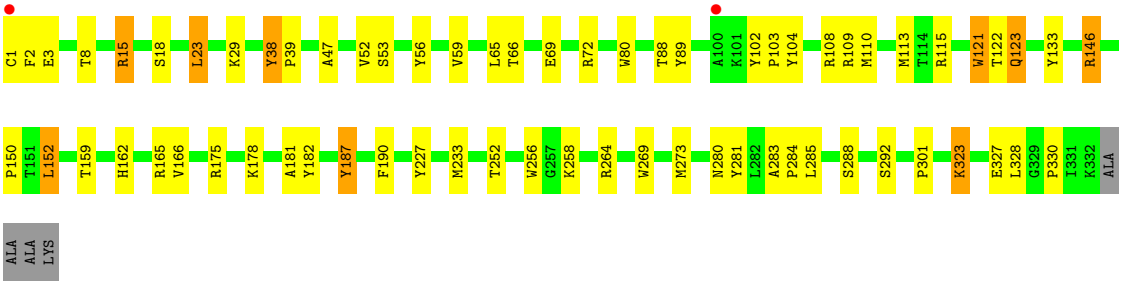
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
14	C	129	129	129	0	0
			Total	O		
14	L	59	59	59	0	0
			Total	O		
14	M	70	70	70	0	0
			Total	O		
14	H	79	79	79	0	0

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.

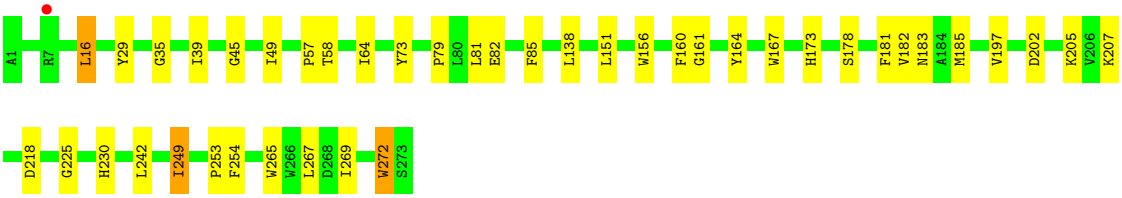
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER

Chain C:



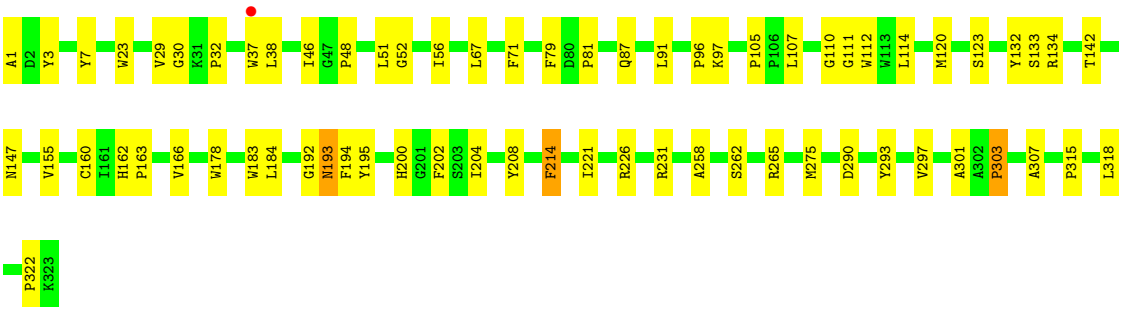
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER

Chain L:



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER

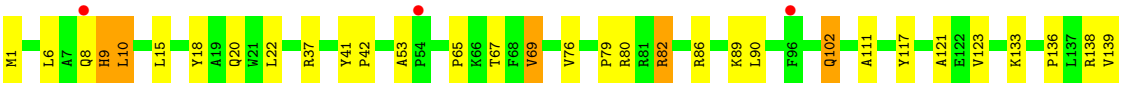
Chain M:

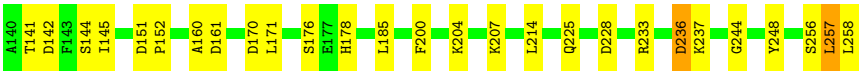


• Molecule 4: PHOTOSYNTHETIC REACTION CENTER

Chain H:

%
77%
20%


M1
L6
A7
Q8
H9
L10
L15
Y18
A19
Q20
W21
L22
R37
Y41
P42
A53
P54
P65
K66
T67
F68
V69
V76
P79
R80
R81
R82
R86
K89
L90
F96
Q102
A111
Y117
A121
E122
V123
K133
P136
L137
R138
V139


A140
T141
D142
F143
S144
I145
D151
P152
A160
D161
D170
L171
S176
E177
H178
L185
F200
K204
K207
L214
Q225
D228
R233
D236
K237
G244
Y248
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 – 2.30 25.84 – 2.30	Depositor EDS
% Data completeness (in resolution range)	81.4 (10.00-2.30) 81.1 (25.84-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.27 (at 2.31Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.184 , 0.225 0.175 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	29.9	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 95.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10498	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FME, MQ7, BCB, BPB, CEB, LDA, SO4, FE2, HEM, NS5

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	0.50	0/2674	0.60	0/3645
2	L	0.53	0/2259	0.56	0/3084
3	M	0.50	0/2683	0.57	0/3669
4	H	0.50	0/2055	0.66	1/2807 (0.0%)
All	All	0.51	0/9671	0.60	1/13205 (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	1
3	M	0	2
4	H	0	1
All	All	0	10

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	53	ALA	CB-CA-C	-7.97	98.15	110.10

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	121	TRP	Mainchain

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Mol	Chain	Res	Type	Group
1	C	15	ARG	Sidechain
1	C	187	TYR	Sidechain
1	C	190	PHE	Sidechain
1	C	89	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2607	0	2575	46	0
2	L	2171	0	2098	33	0
3	M	2577	0	2468	49	0
4	H	2018	0	2020	34	0
5	C	172	0	120	6	0
6	L	132	0	144	9	0
6	M	132	0	144	12	0
7	L	65	0	74	6	0
7	M	65	0	74	9	0
8	L	17	0	15	2	0
9	H	32	0	62	0	0
9	L	16	0	31	3	0
9	M	48	0	93	4	0
10	M	1	0	0	0	0
11	H	5	0	0	0	0
11	M	15	0	0	2	0
12	M	48	0	64	0	0
13	M	40	0	60	5	0
14	C	129	0	0	2	0
14	H	79	0	0	1	0
14	L	59	0	0	0	0
14	M	70	0	0	2	0
All	All	10498	0	10042	176	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 176 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:402:BPB:HBBB	7:L:402:BPB:HHC	1.35	1.09
6:M:805:BCB:HHC	6:M:805:BCB:HBB2	1.57	0.85
9:L:702:LDA:H22	9:L:702:LDA:H62	1.60	0.83
7:L:402:BPB:HHC	7:L:402:BPB:CBB	2.09	0.79
7:M:401:BPB:HBBB	7:M:401:BPB:HHC	1.64	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%)	323 (98%)	8 (2%)	0	100	100
2	L	271/273 (99%)	263 (97%)	6 (2%)	2 (1%)	22	26
3	M	323/323 (100%)	312 (97%)	8 (2%)	3 (1%)	17	20
4	H	256/258 (99%)	242 (94%)	13 (5%)	1 (0%)	34	42
All	All	1181/1190 (99%)	1140 (96%)	35 (3%)	6 (0%)	29	35

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	10	LEU
2	L	57	PRO
3	M	51	LEU
3	M	193	ASN
2	L	202	ASP

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%)	265 (94%)	16 (6%)	20	28
2	L	218/218 (100%)	214 (98%)	4 (2%)	59	75
3	M	251/249 (101%)	245 (98%)	6 (2%)	49	66
4	H	212/212 (100%)	195 (92%)	17 (8%)	12	15
All	All	962/961 (100%)	919 (96%)	43 (4%)	28	39

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	22	LEU
4	H	144	SER
4	H	42	PRO
4	H	89	LYS
4	H	185	LEU

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

Mol	Chain	Res	Type
2	L	183	ASN
2	L	214	GLN
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	0.64	0	7,9,11	2.99	2 (28%)

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	-	3/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	1	FME	CA-N-CN	-6.47	112.86	122.82
4	H	1	FME	O1-CN-N	-3.65	115.65	125.27

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	$\#\|Z\| > 2$
9	LDA	M	704	-	12,15,15	1.84	1 (8%)	14,17,17	0.62	0
13	NS5	M	600	-	39,39,39	0.81	2 (5%)	44,46,46	1.07	5 (11%)
9	LDA	L	702	-	12,15,15	2.42	1 (8%)	14,17,17	0.51	0
11	SO4	M	803	-	4,4,4	0.59	0	6,6,6	0.62	0
7	BPB	L	402	-	49,70,70	1.38	5 (10%)	47,101,101	2.08	10 (21%)
9	LDA	M	705	-	12,15,15	2.21	1 (8%)	14,17,17	0.51	0
6	BCB	L	302	2	54,74,74	1.62	6 (11%)	52,115,115	2.09	12 (23%)
9	LDA	H	703	-	12,15,15	2.25	1 (8%)	14,17,17	0.58	0
11	SO4	M	804	-	4,4,4	0.82	0	6,6,6	0.98	0
5	HEM	C	338	1	41,50,50	1.44	4 (9%)	45,82,82	1.17	3 (6%)
5	HEM	C	340	1	41,50,50	1.53	6 (14%)	45,82,82	1.21	5 (11%)
6	BCB	M	805	3	54,74,74	1.52	10 (18%)	52,115,115	2.52	12 (23%)
6	BCB	L	304	2	54,74,74	1.59	9 (16%)	52,115,115	2.42	13 (25%)
12	MQ7	M	501	-	49,49,49	1.76	11 (22%)	60,63,63	1.36	8 (13%)
9	LDA	H	701	-	12,15,15	2.07	1 (8%)	14,17,17	0.69	0
6	BCB	M	806	3	54,74,74	1.59	6 (11%)	52,115,115	2.51	14 (26%)
11	SO4	H	801	-	4,4,4	0.61	0	6,6,6	0.30	0
11	SO4	M	802	-	4,4,4	0.88	0	6,6,6	0.44	0
5	HEM	C	337	1	41,50,50	1.41	3 (7%)	45,82,82	1.30	7 (15%)
9	LDA	M	706	-	12,15,15	2.32	1 (8%)	14,17,17	0.58	0
5	HEM	C	339	1	41,50,50	1.48	5 (12%)	45,82,82	1.29	5 (11%)
7	BPB	M	401	-	49,70,70	1.47	7 (14%)	47,101,101	2.42	7 (14%)
8	CEB	L	502	-	16,17,17	0.83	1 (6%)	21,23,23	1.74	3 (14%)

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
9	LDA	M	704	-	-	3/13/13/13	-
13	NS5	M	600	-	-	10/43/43/43	-
9	LDA	L	702	-	-	1/13/13/13	-
7	BPB	L	402	-	1/1/18/23	4/37/105/105	0/5/6/6
9	LDA	M	705	-	-	2/13/13/13	-
6	BCB	L	302	2	-	7/37/177/177	-
9	LDA	H	703	-	-	5/13/13/13	-
5	HEM	C	338	1	-	6/12/54/54	-
5	HEM	C	340	1	-	4/12/54/54	-
6	BCB	M	805	3	-	12/37/177/177	-
6	BCB	L	304	2	-	4/37/177/177	-
12	MQ7	M	501	-	-	0/41/61/61	0/2/2/2
9	LDA	H	701	-	-	3/13/13/13	-
6	BCB	M	806	3	-	9/37/177/177	-
5	HEM	C	337	1	-	6/12/54/54	-
9	LDA	M	706	-	-	6/13/13/13	-
5	HEM	C	339	1	-	2/12/54/54	-
7	BPB	M	401	-	-	8/37/105/105	0/5/6/6
8	CEB	L	502	-	-	3/11/14/14	0/1/1/1

The worst 5 of 81 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	702	LDA	O1-N1	-8.33	1.22	1.42
9	M	706	LDA	O1-N1	-8.01	1.23	1.42
9	H	703	LDA	O1-N1	-7.74	1.24	1.42
9	M	705	LDA	O1-N1	-7.62	1.24	1.42
9	H	701	LDA	O1-N1	-7.09	1.25	1.42

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	805	BCB	O2D-CGD-CBD	11.24	125.24	111.00
7	M	401	BPB	O2D-CGD-CBD	11.19	125.18	111.00
6	L	304	BCB	O2D-CGD-CBD	10.80	124.68	111.00
6	M	806	BCB	O2D-CGD-CBD	8.81	122.15	111.00
7	L	402	BPB	O2D-CGD-CBD	7.90	121.01	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	L	402	BPB	C13

5 of 95 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	M	805	BCB	C2C-C3C-CAC-CBC
6	M	805	BCB	C4-C3-C5-C6
6	M	806	BCB	C2A-CAA-CBA-CGA
6	M	806	BCB	CAD-CBD-CGD-O1D
6	M	806	BCB	CAD-CBD-CGD-O2D

There are no ring outliers.

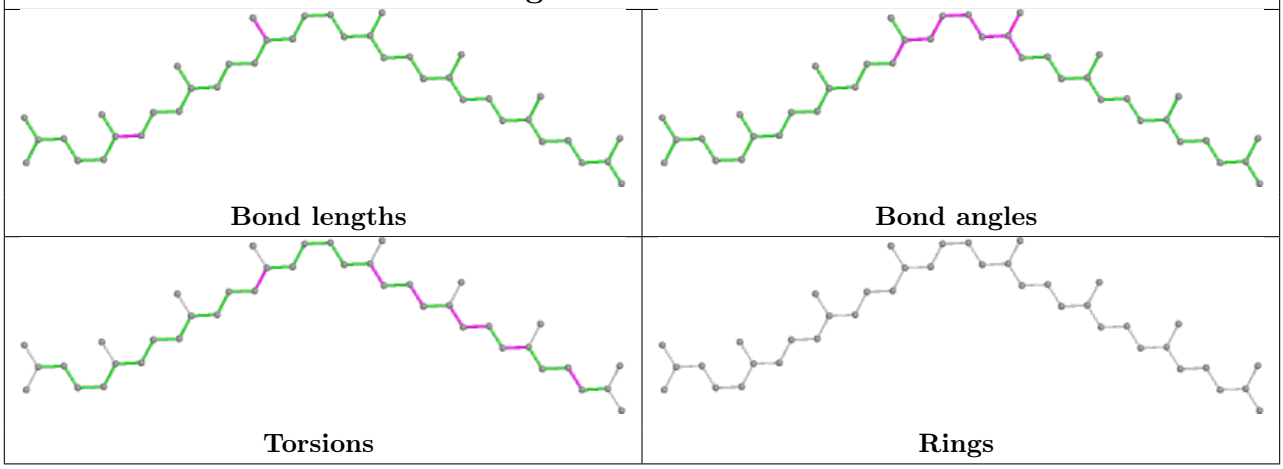
17 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	704	LDA	1	0
13	M	600	NS5	5	0
9	L	702	LDA	3	0
11	M	803	SO4	1	0
7	L	402	BPB	6	0
9	M	705	LDA	1	0
6	L	302	BCB	5	0
11	M	804	SO4	1	0
5	C	338	HEM	3	0
6	M	805	BCB	7	0
6	L	304	BCB	5	0
6	M	806	BCB	5	0
5	C	337	HEM	2	0
9	M	706	LDA	2	0
5	C	339	HEM	1	0
7	M	401	BPB	9	0
8	L	502	CEB	2	0

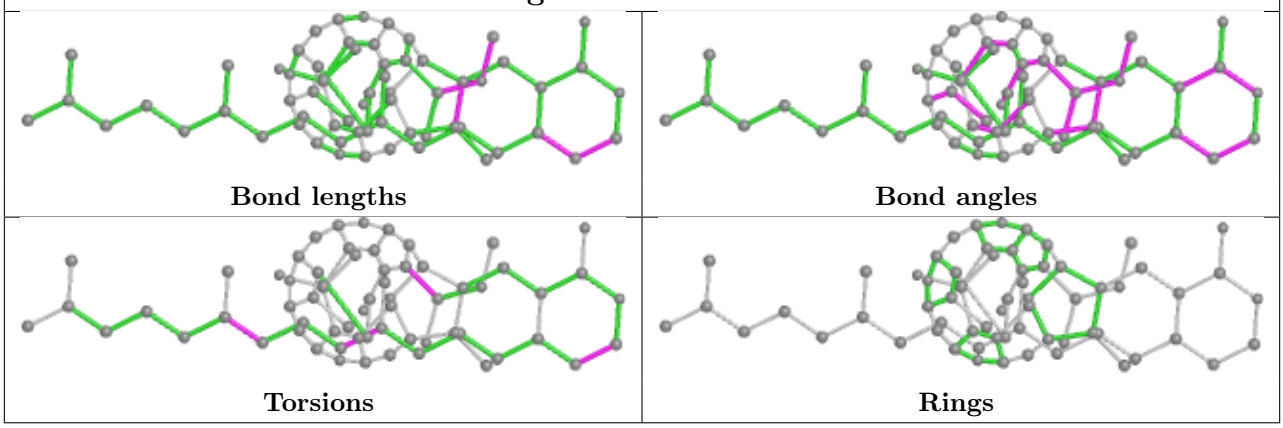
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

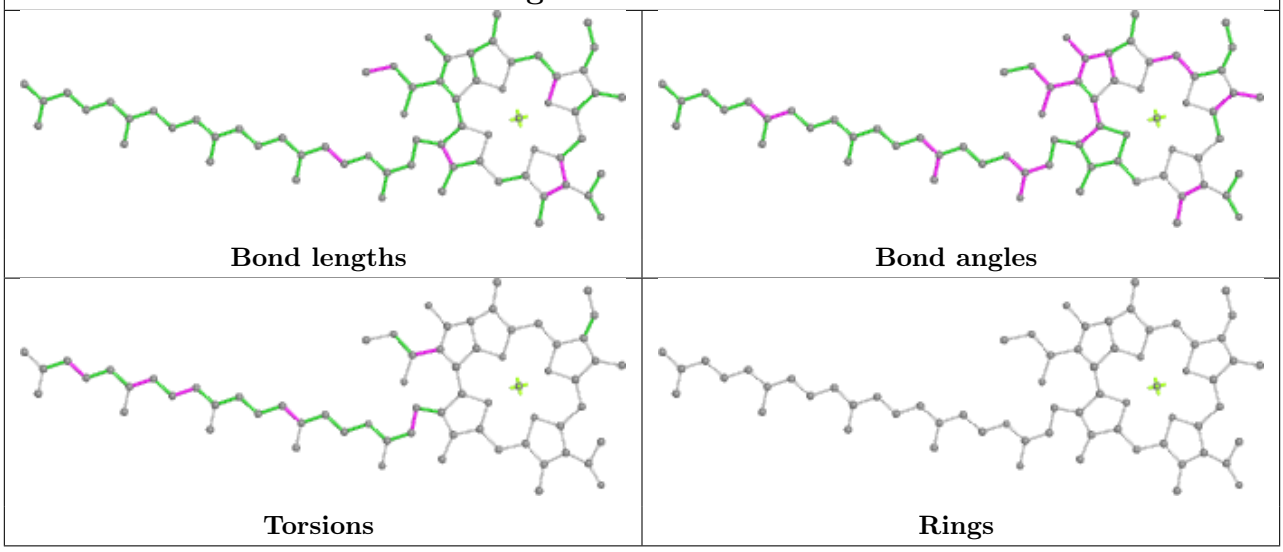
Ligand NS5 M 600



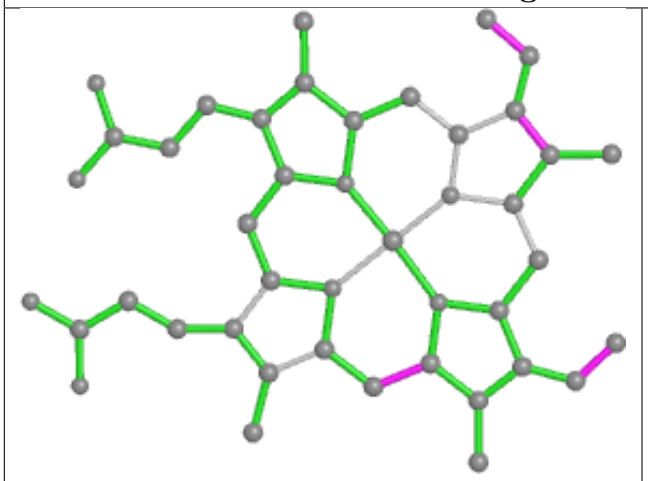
Ligand BPB L 402



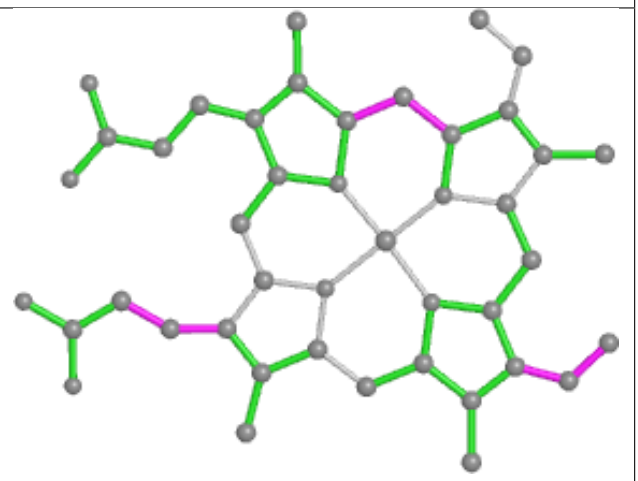
Ligand BCB L 302



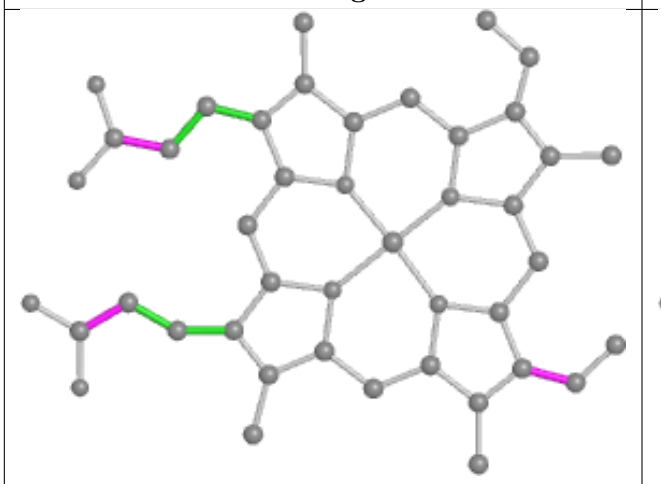
Ligand HEM C 338



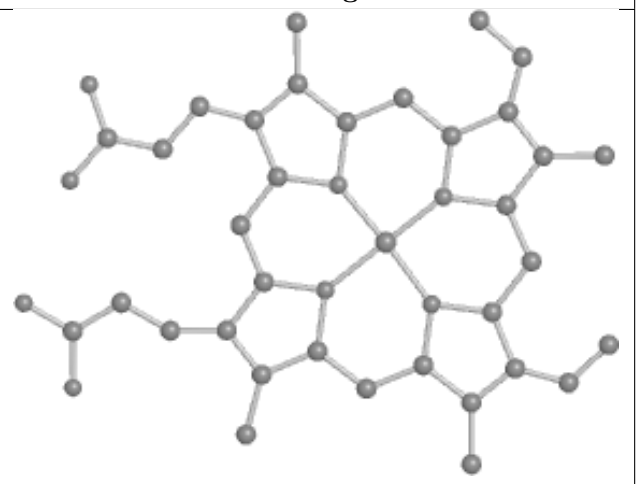
Bond lengths



Bond angles

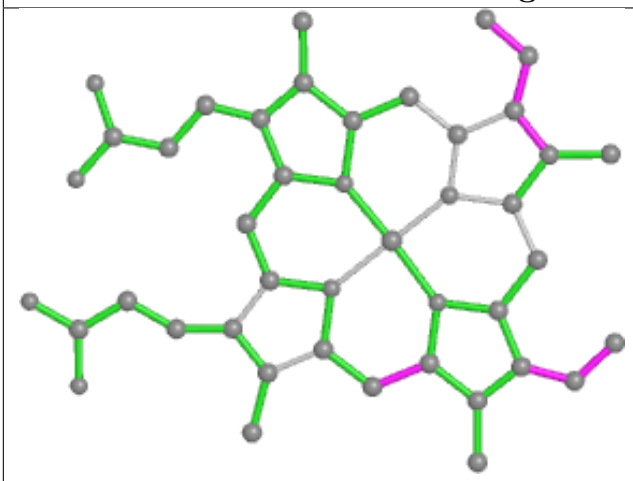


Torsions

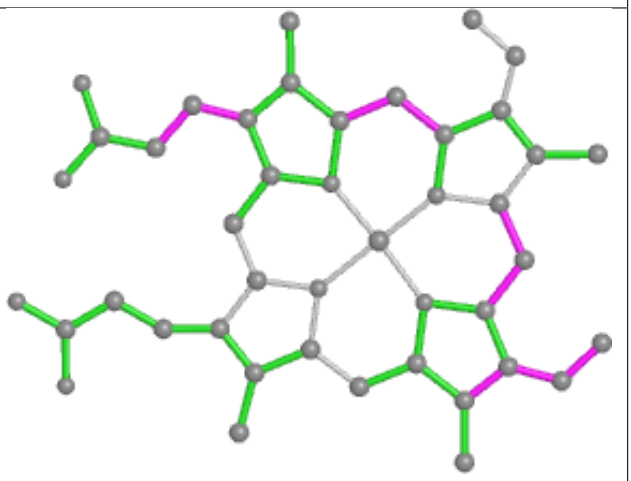


Rings

Ligand HEM C 340



Bond lengths



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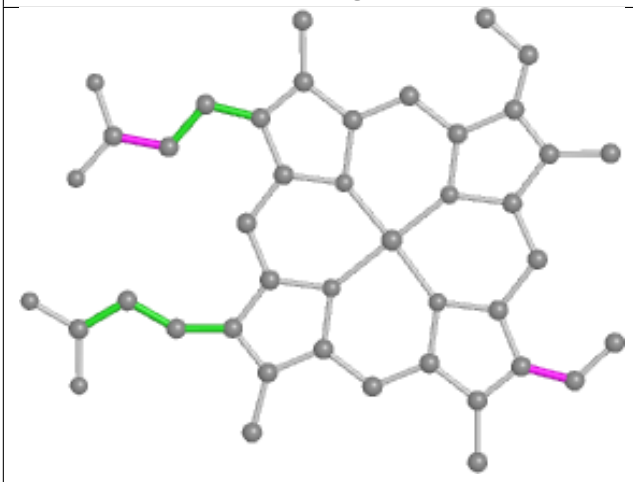
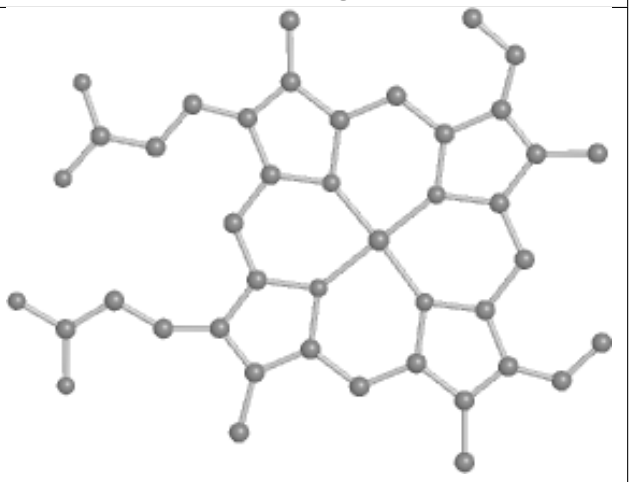
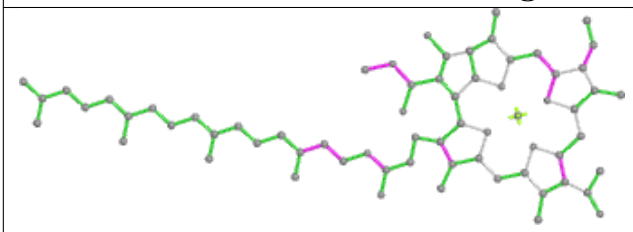


Torsions

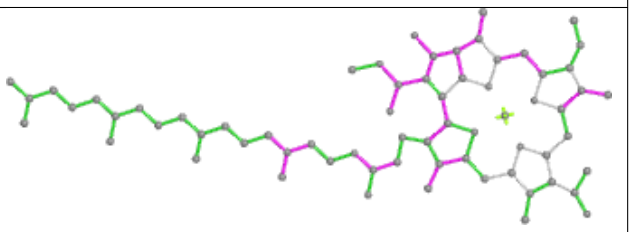


Rings

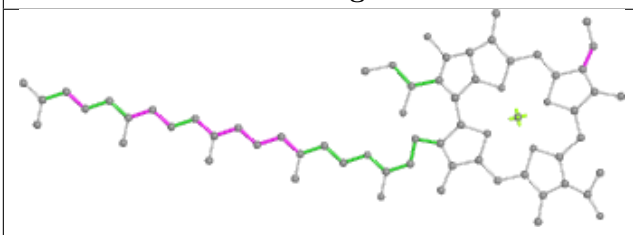
Ligand BCB M 805



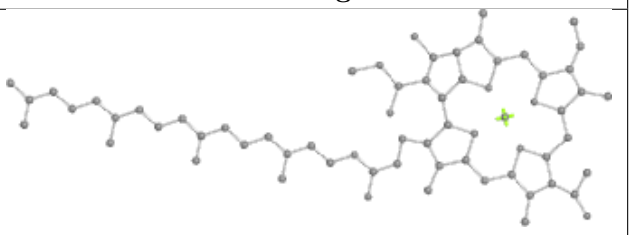
Bond lengths



Bond angles

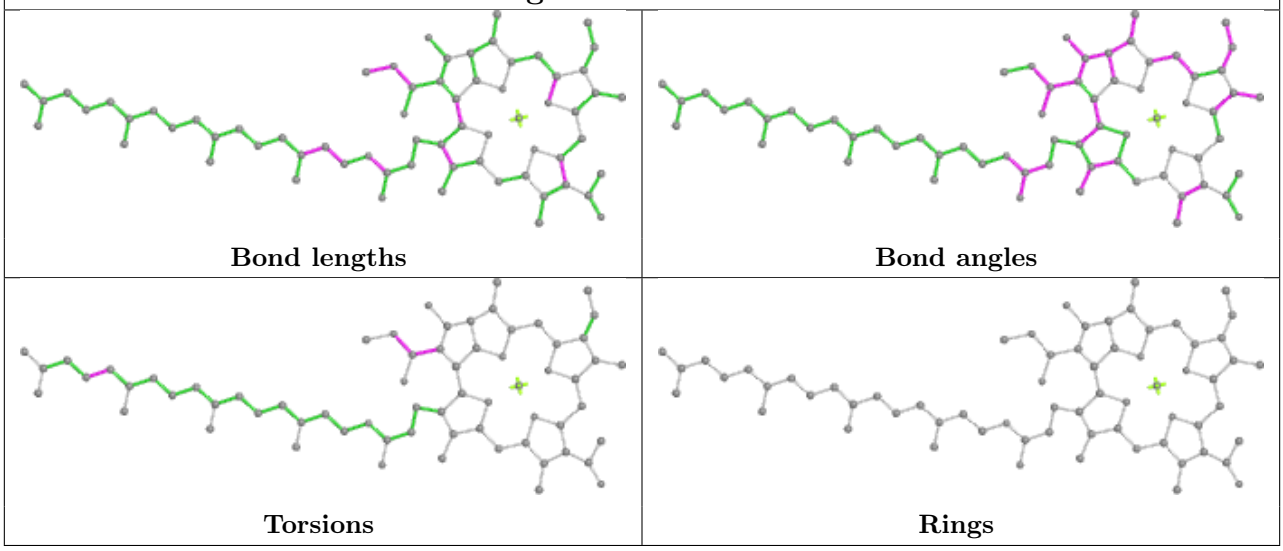


Torsions

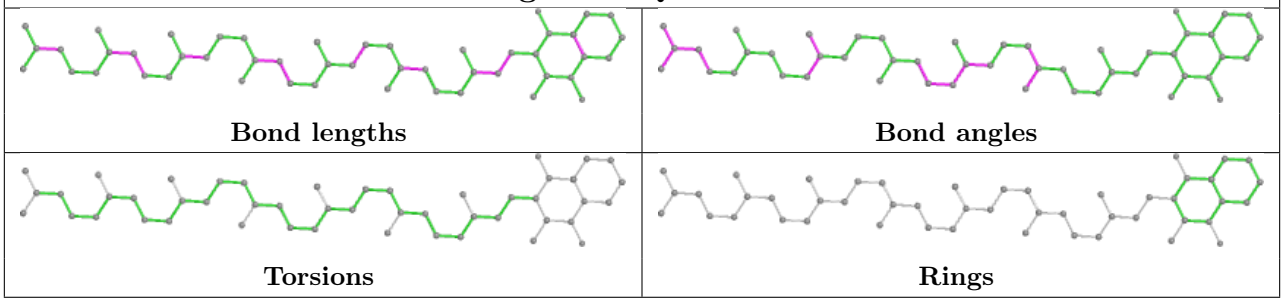


Rings

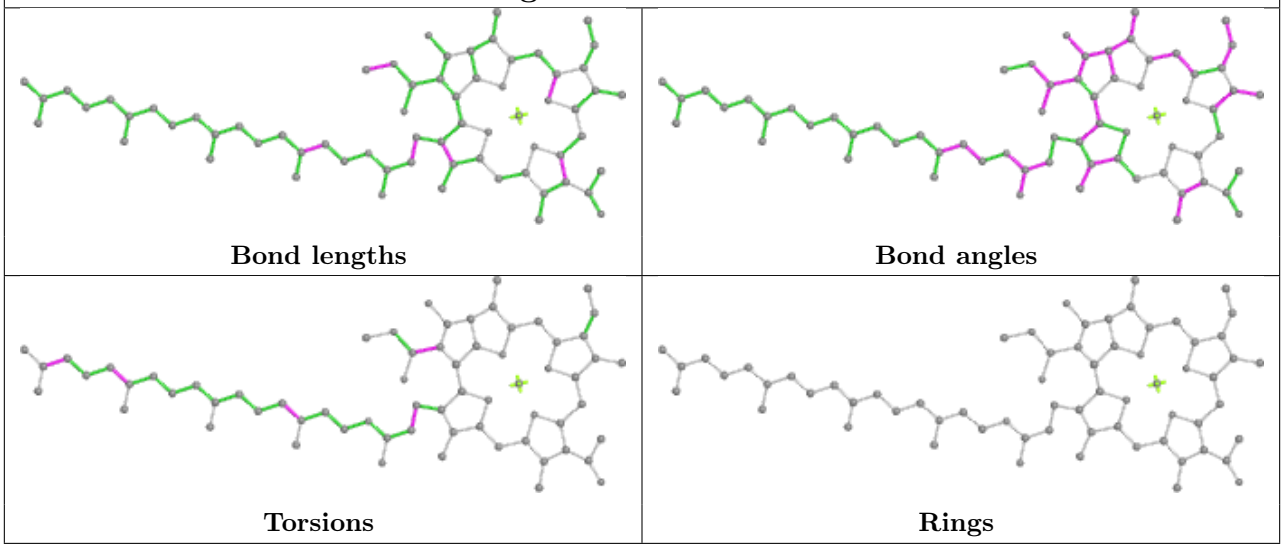
Ligand BCB L 304



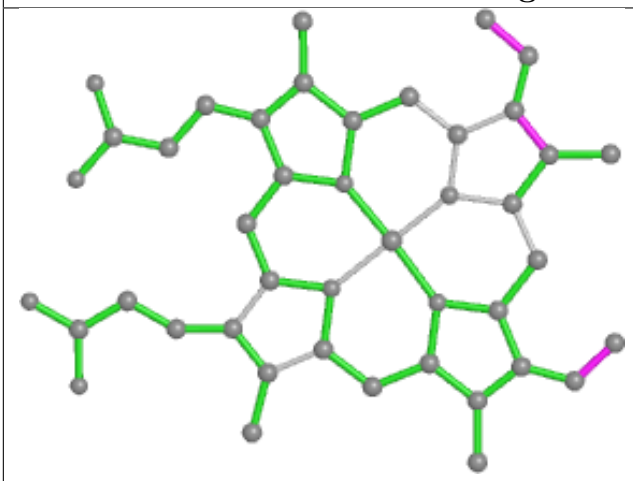
Ligand MQ7 M 501



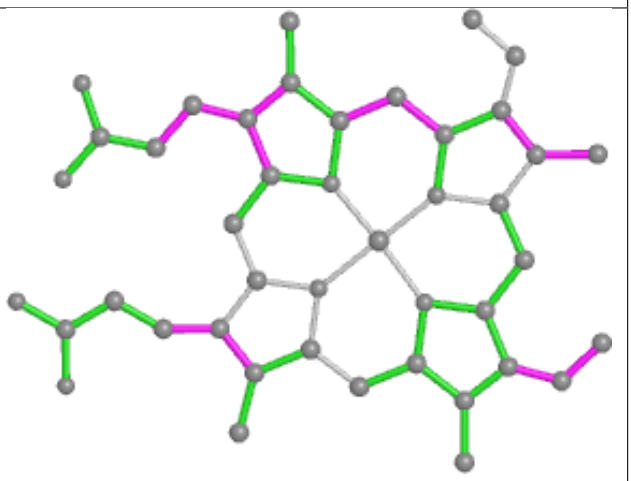
Ligand BCB M 806



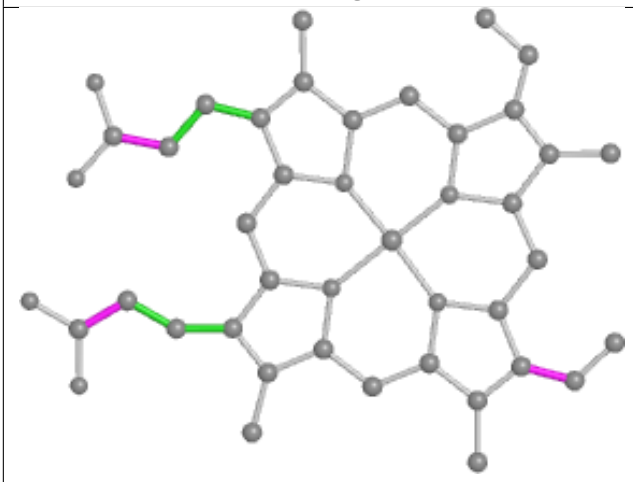
Ligand HEM C 337



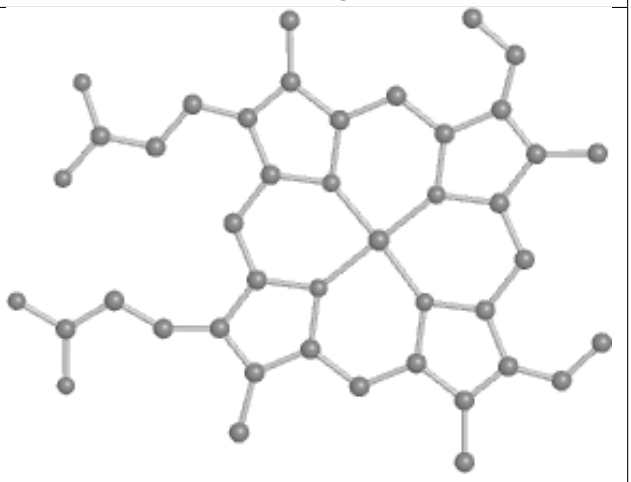
Bond lengths



Bond angles

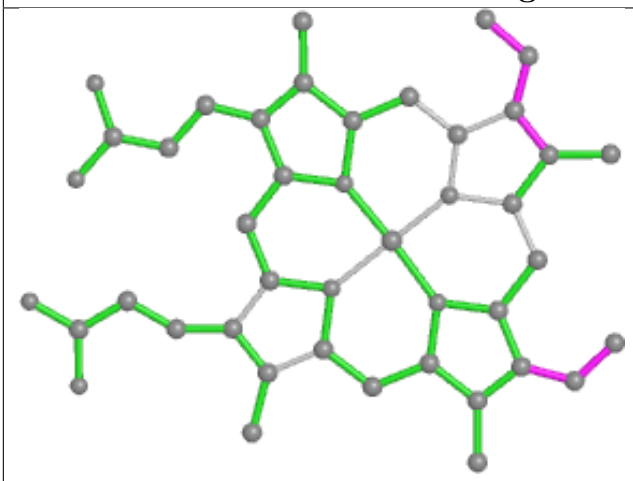


Torsions

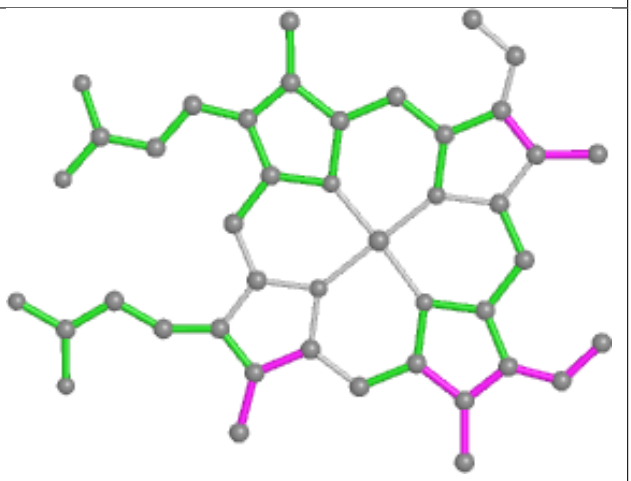


Rings

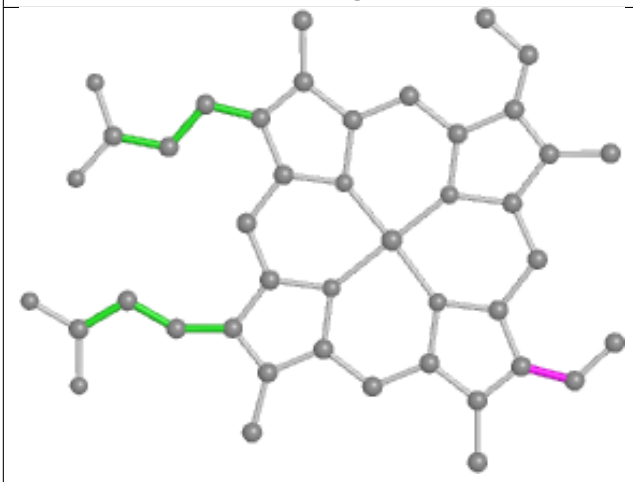
Ligand HEM C 339



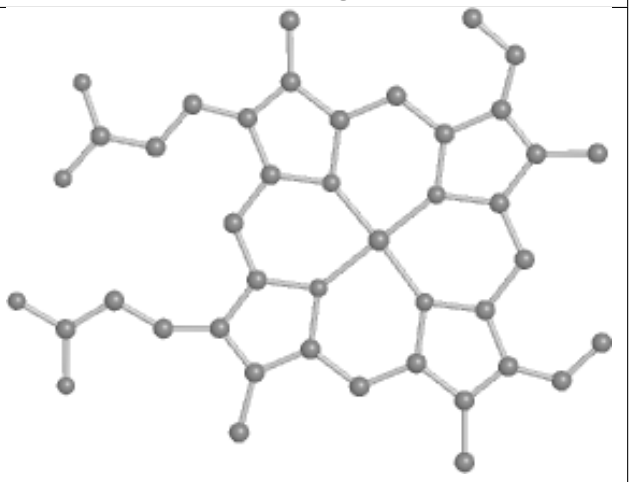
Bond lengths



Bond angles

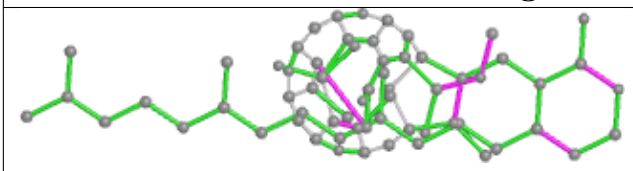


Torsions

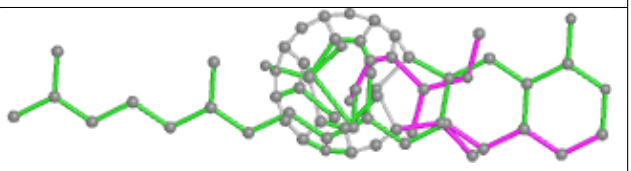


Rings

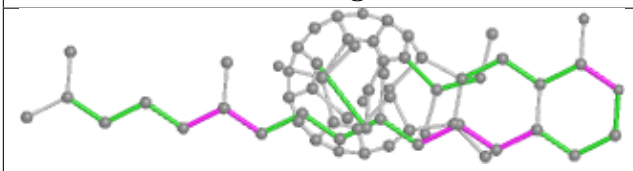
Ligand BPB M 401



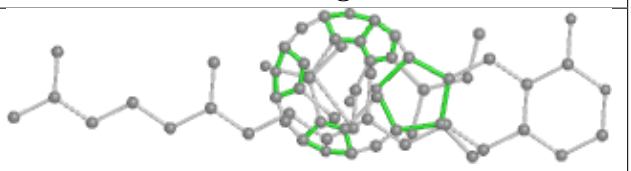
Bond lengths



Bond angles

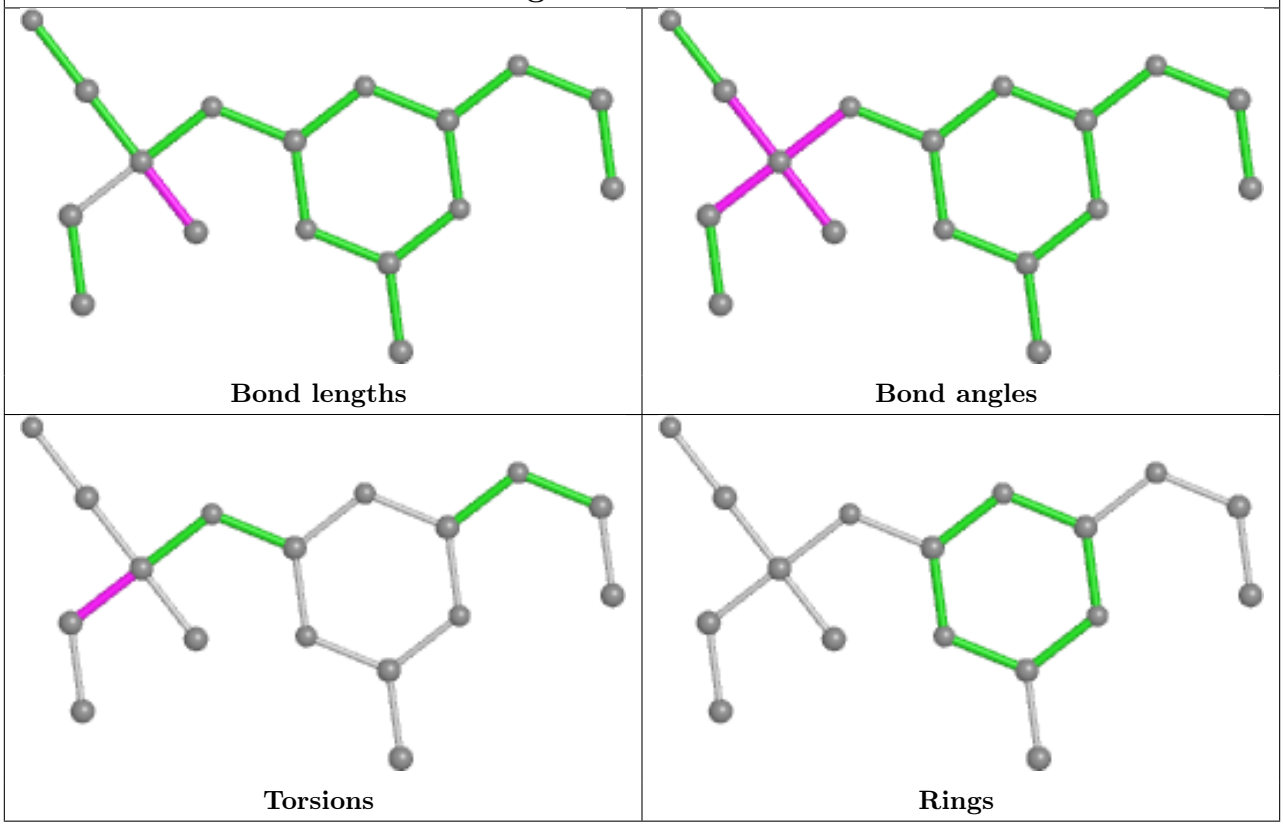


Torsions



Rings

Ligand CEB L 502



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	C	332/336 (98%)	-0.68	2 (0%)	89	92	14, 29, 56, 77	18 (5%)
2	L	273/273 (100%)	-0.84	1 (0%)	92	95	13, 25, 49, 68	7 (2%)
3	M	323/323 (100%)	-0.73	1 (0%)	94	96	12, 27, 57, 72	10 (3%)
4	H	249/258 (96%)	-0.54	3 (1%)	79	83	16, 36, 70, 90	20 (8%)
All	All	1177/1190 (98%)	-0.70	7 (0%)	89	92	12, 29, 59, 90	55 (4%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	8	GLN	4.2
4	H	54	PRO	4.0
1	C	1	CYS	3.4
3	M	37	TRP	3.3
4	H	96	PHE	2.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FME	H	1	10/11	0.97	0.07	32,35,42,52	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

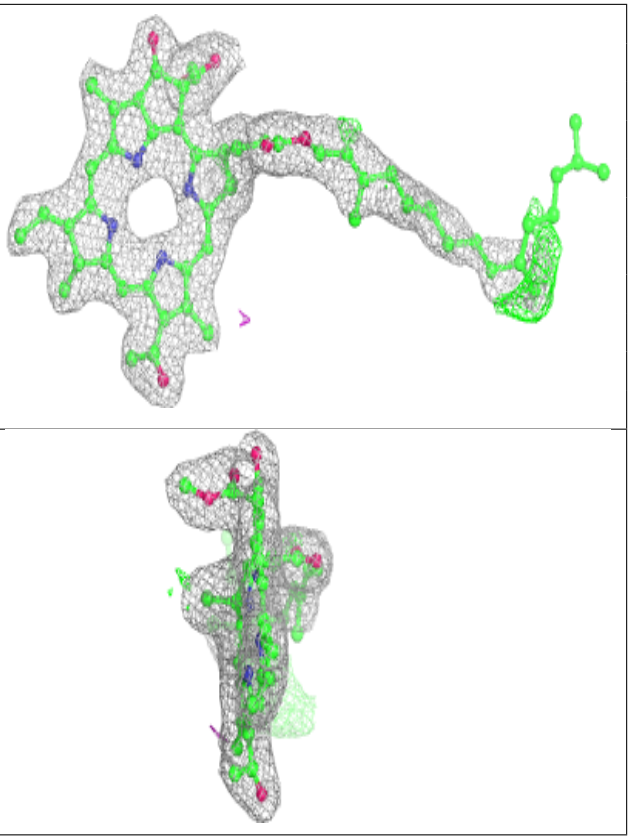
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	LDA	M	706	16/16	0.75	0.29	78,80,83,83	4
9	LDA	L	702	16/16	0.84	0.21	19,60,84,85	0
9	LDA	M	705	16/16	0.87	0.14	65,72,82,82	5
9	LDA	M	704	16/16	0.87	0.25	59,66,88,90	0
9	LDA	H	703	16/16	0.94	0.16	33,48,69,69	0
7	BPB	M	401	65/65	0.95	0.11	15,30,76,78	7
6	BCB	M	805	66/66	0.95	0.10	12,25,56,58	0
13	NS5	M	600	40/40	0.95	0.13	31,45,84,86	14
12	MQ7	M	501	48/48	0.96	0.11	11,19,48,56	0
11	SO4	M	803	5/5	0.96	0.16	83,85,87,90	0
9	LDA	H	701	16/16	0.97	0.09	20,29,33,36	0
7	BPB	L	402	65/65	0.98	0.09	6,17,22,26	0
5	HEM	C	340	43/43	0.98	0.12	13,24,35,49	0
11	SO4	H	801	5/5	0.98	0.08	63,68,69,71	0
8	CEB	L	502	17/17	0.98	0.11	25,32,35,38	0
5	HEM	C	338	43/43	0.98	0.13	14,29,38,39	0
5	HEM	C	339	43/43	0.99	0.06	9,18,23,29	0
11	SO4	M	802	5/5	0.99	0.08	35,42,43,44	0
6	BCB	M	806	66/66	0.99	0.10	7,17,35,37	0
11	SO4	M	804	5/5	0.99	0.13	42,44,49,52	0
5	HEM	C	337	43/43	0.99	0.07	15,31,47,56	0
6	BCB	L	302	66/66	0.99	0.10	9,14,22,25	0
6	BCB	L	304	66/66	0.99	0.10	6,15,34,46	0
10	FE2	M	500	1/1	1.00	0.03	19,19,19,19	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.

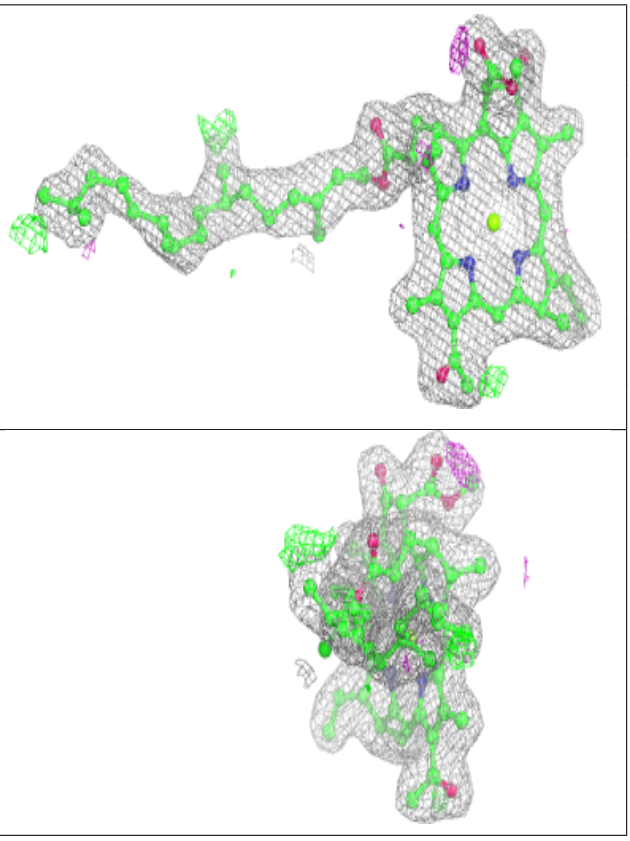
Electron density around BPB M 401:

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



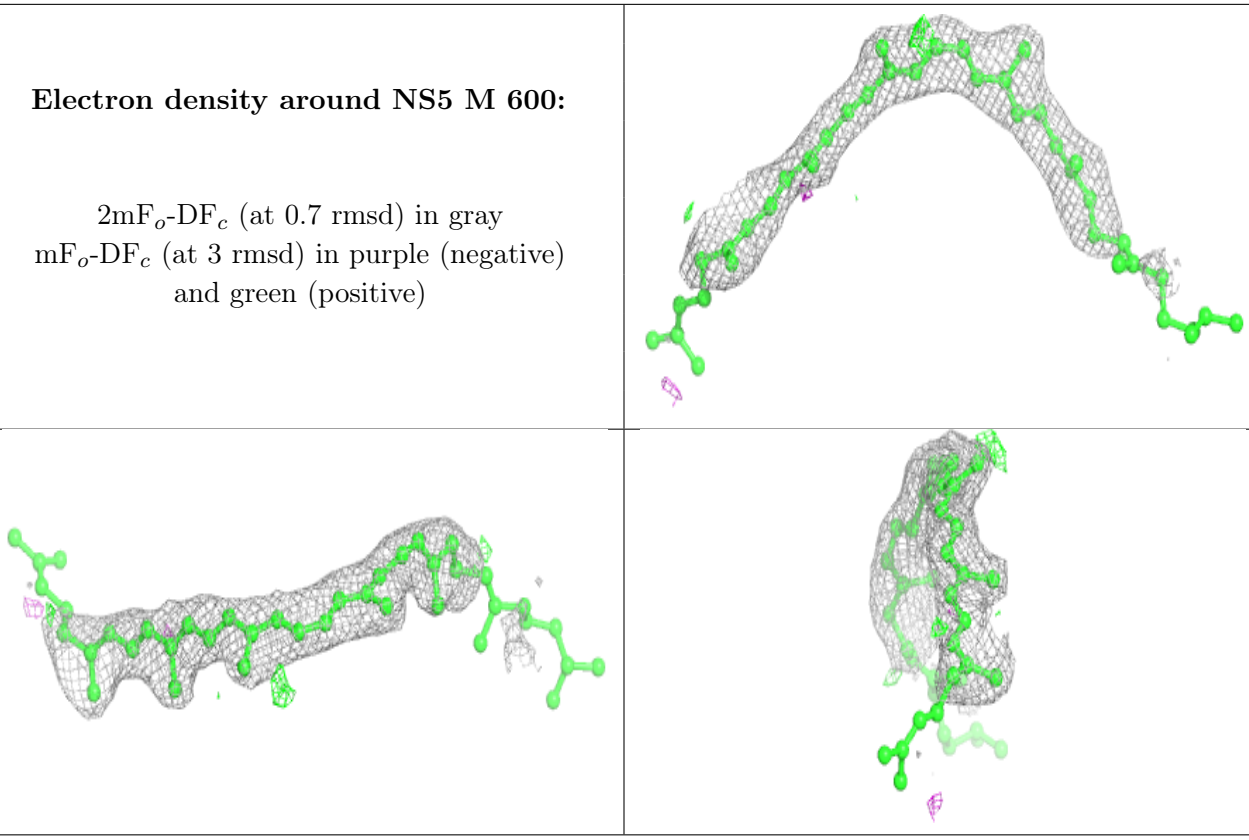
Electron density around BCB M 805:

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



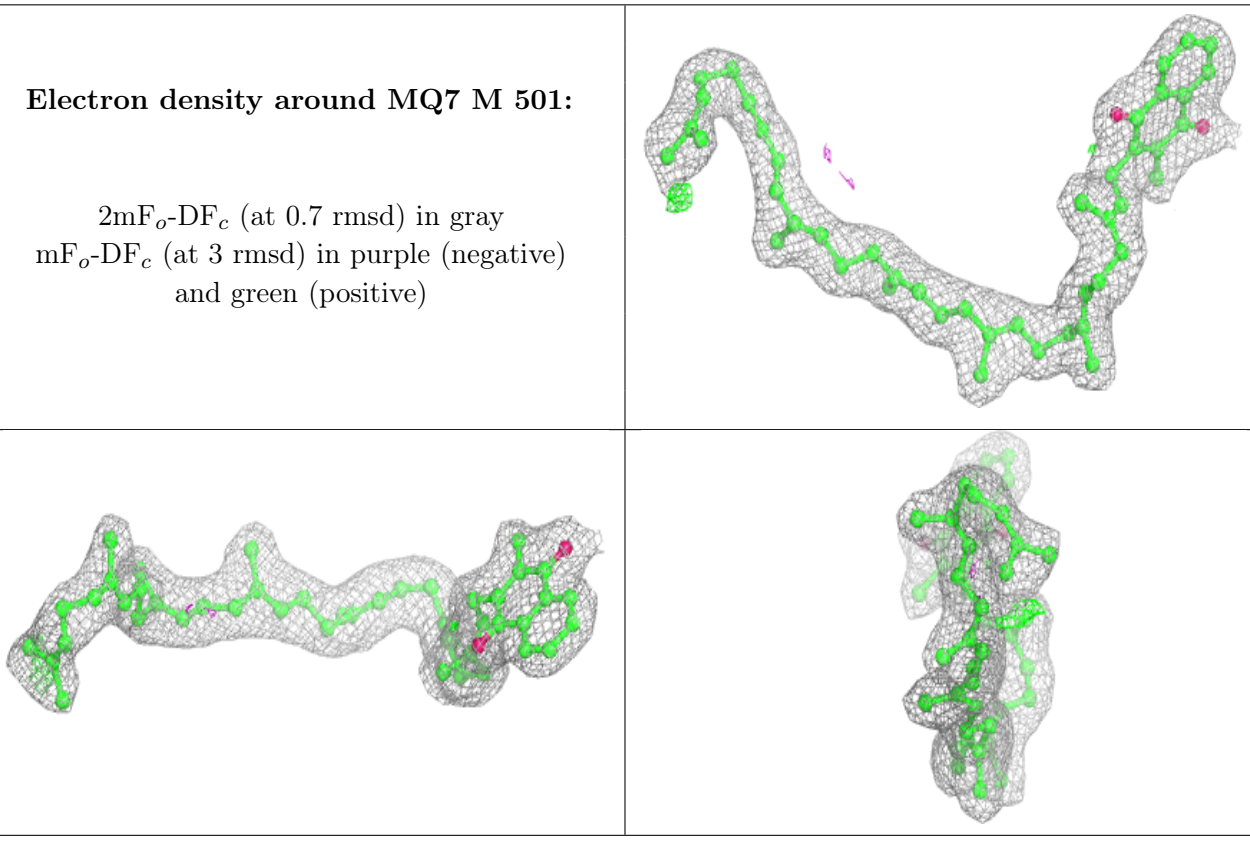
Electron density around NS5 M 600:

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



Electron density around 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 BPB L 402:

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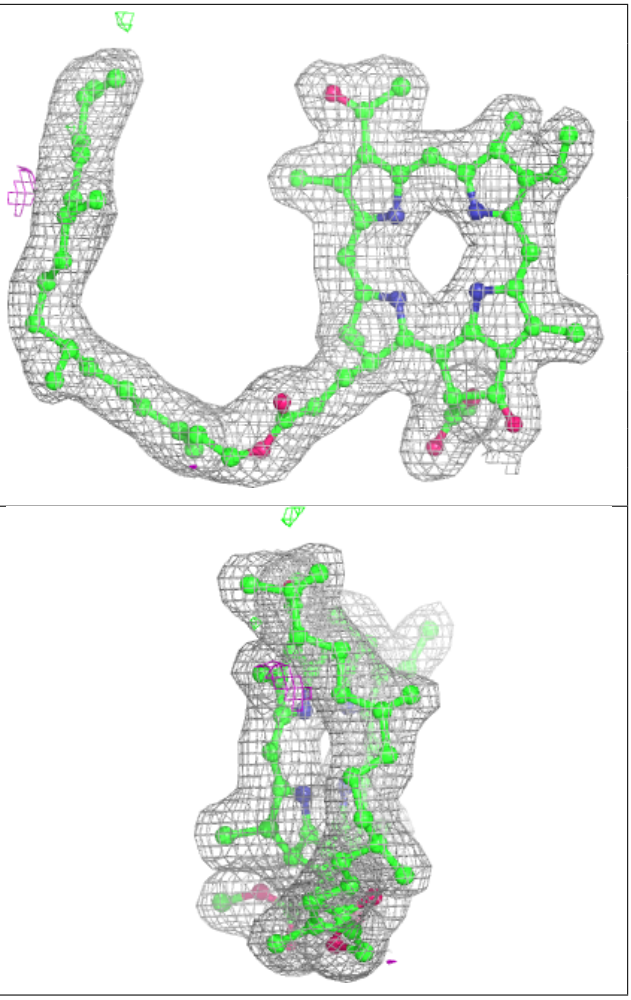
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 340:

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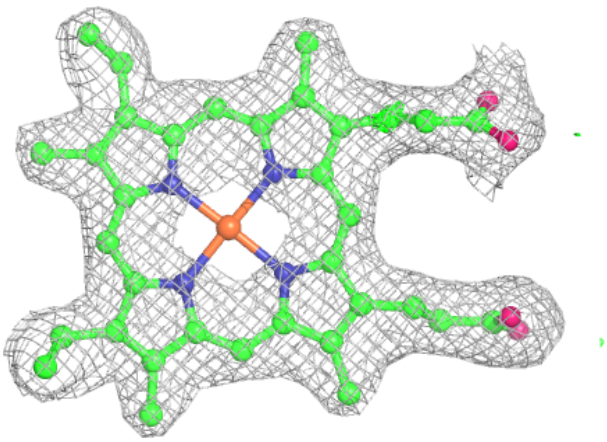
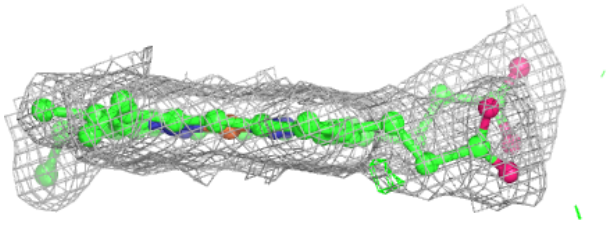
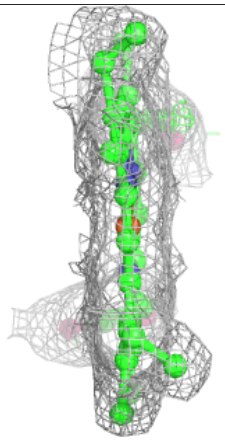
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

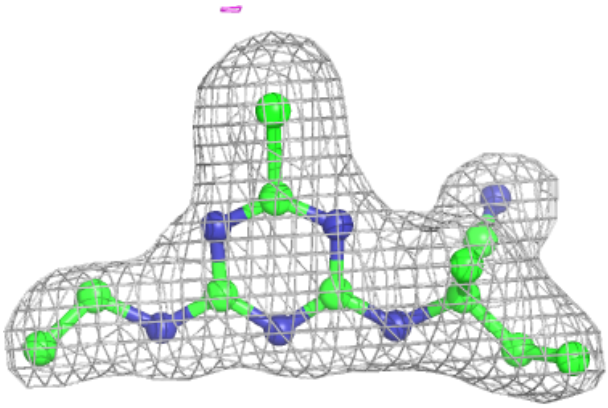


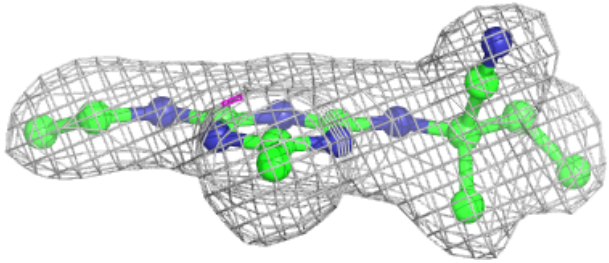


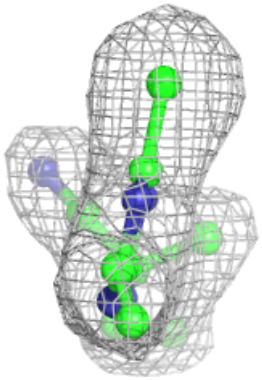


Electron density around CEB L 502:

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

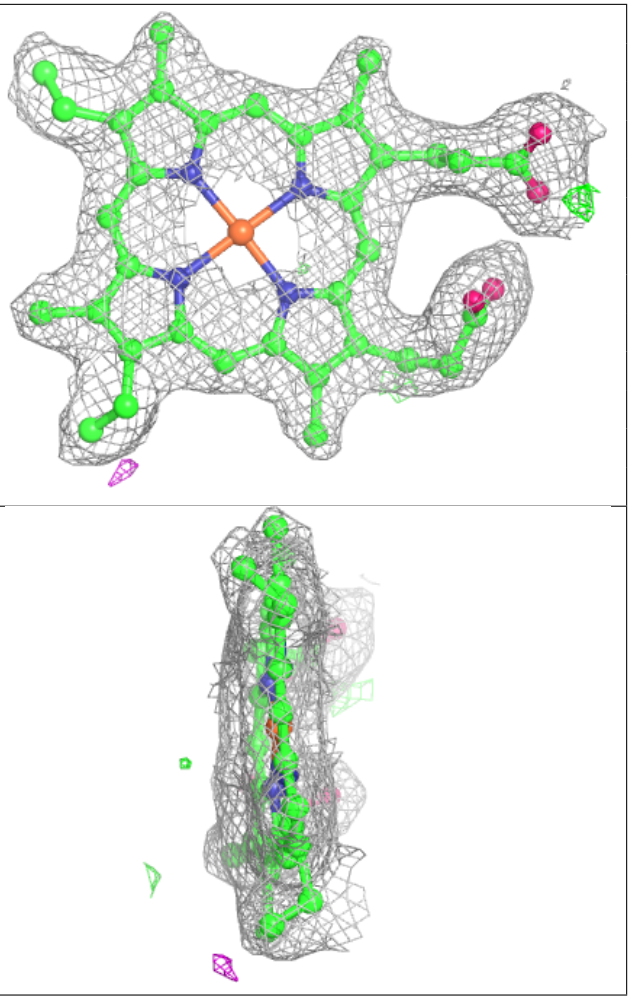






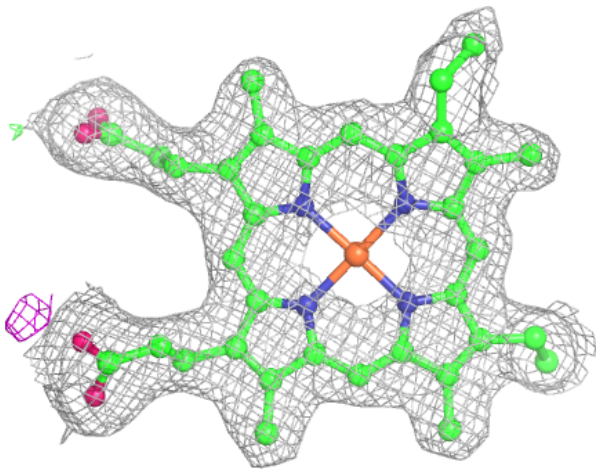
Electron density around HEM C 338:

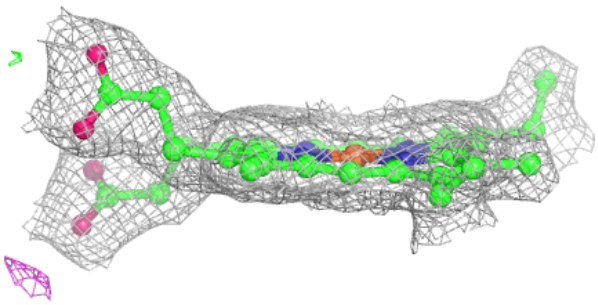
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

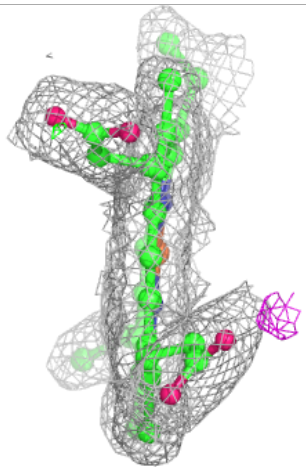


Electron density around HEM C 339:

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

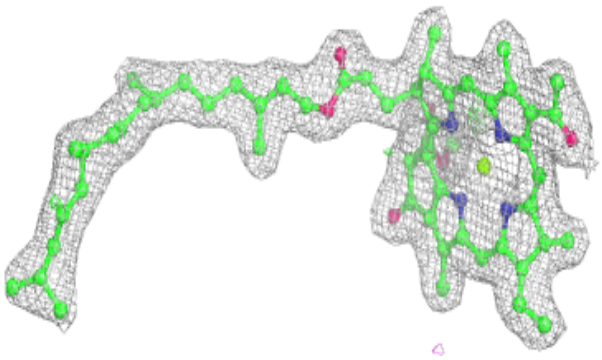


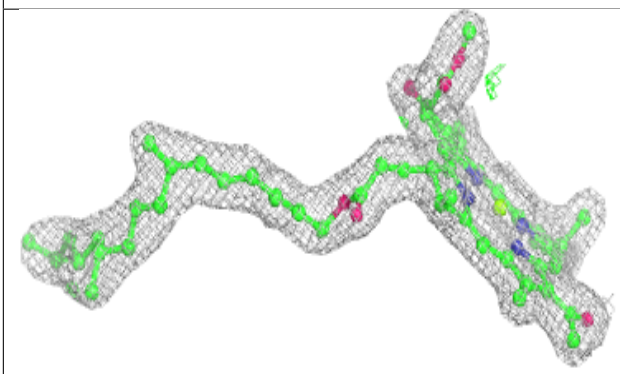


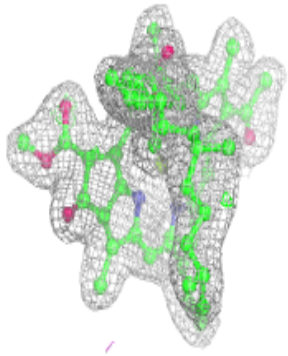


Electron density around BCB M 806:

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

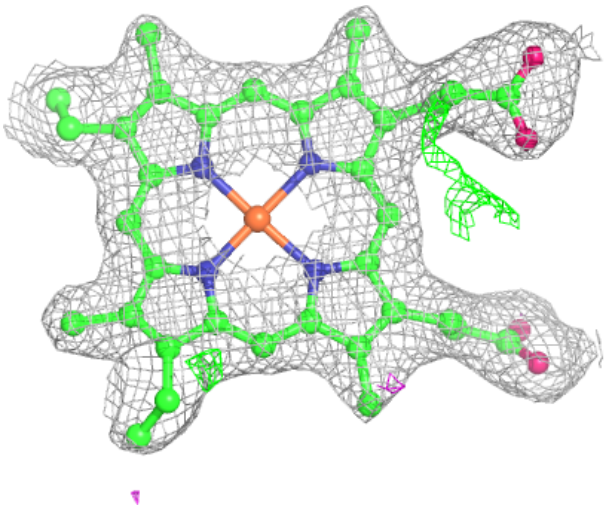


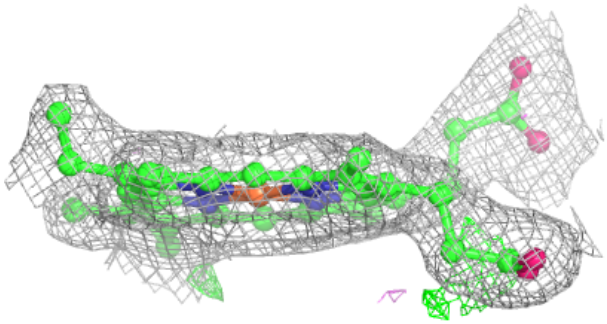


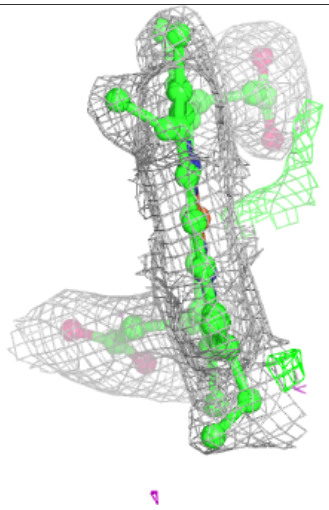


Electron density around HEM C 337:

$2mF_o$-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 L 302:

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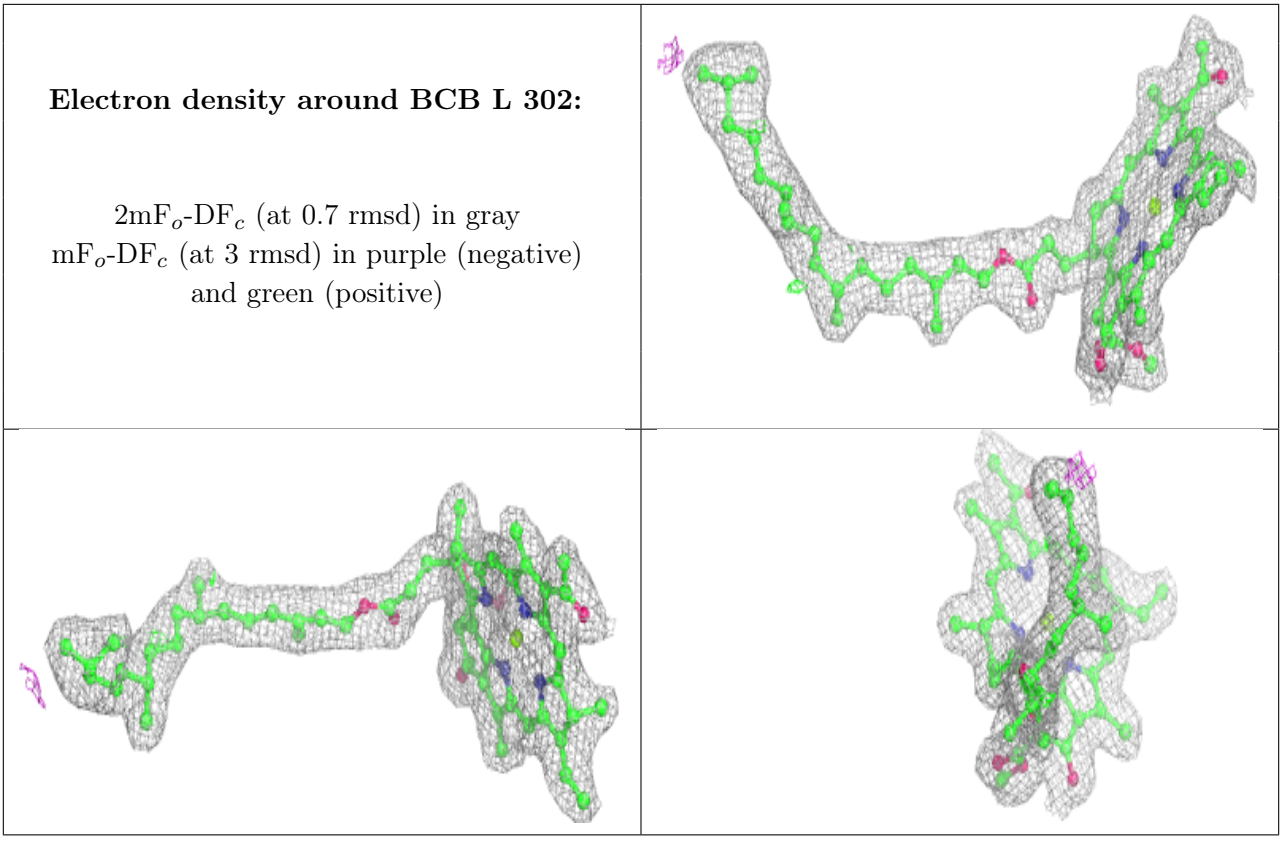
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BCB L 304:

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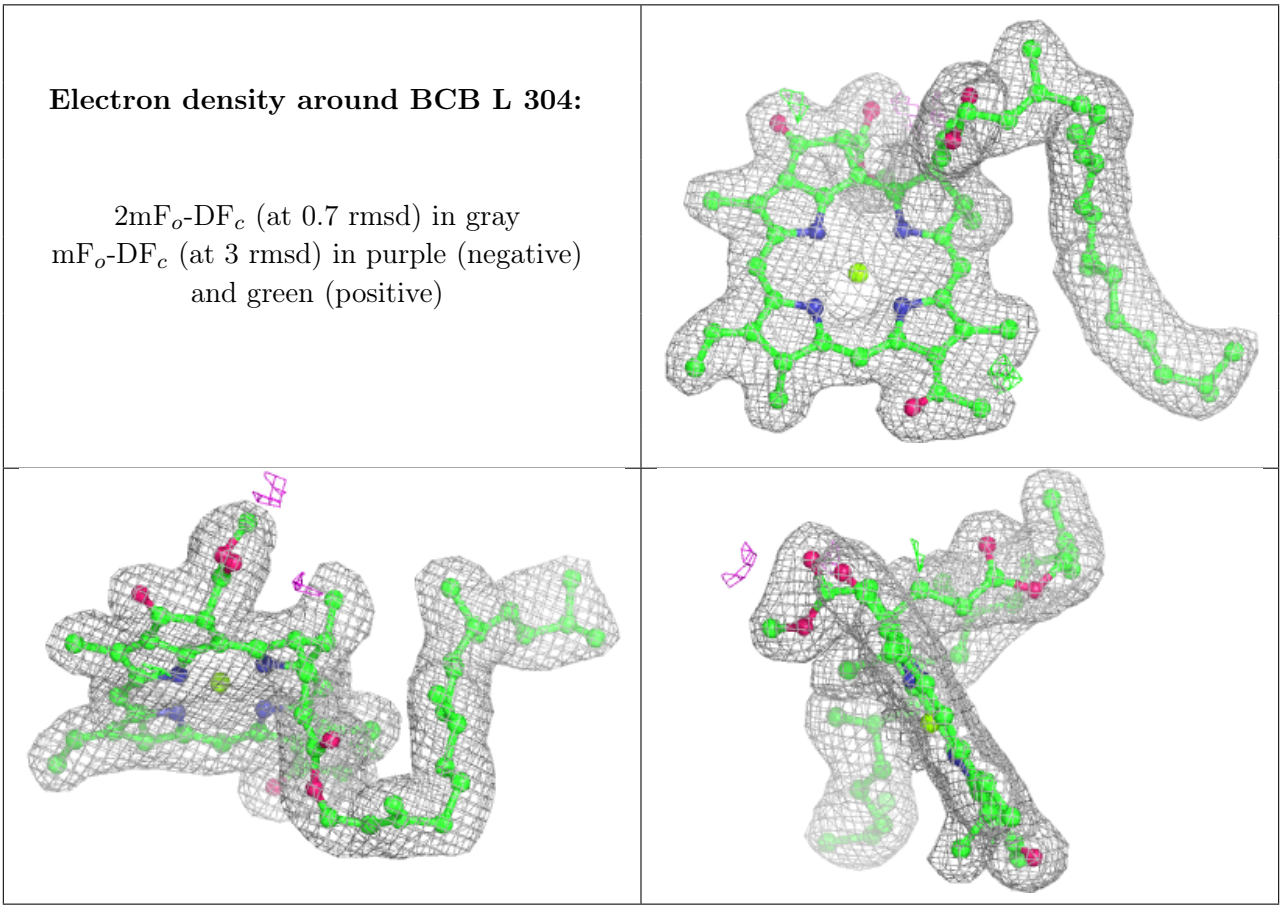
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.