



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 18, 2024 – 03:19 PM EDT

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

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

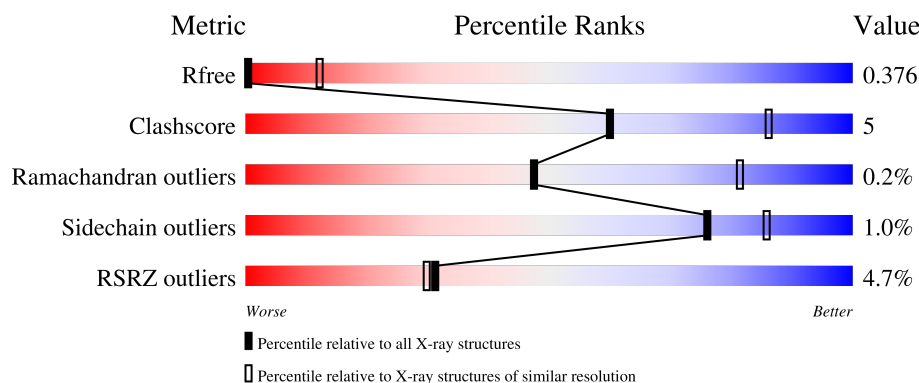
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 8.20 Å.





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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1005 (11.50-3.90)
Clashscore	141614	1070 (11.50-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
Sidechain outliers	138945	1003 (11.50-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NS5	M	1329	-	-	-	X
6	BCB	L	1274	X	-	-	-
6	BCB	L	1275	X	-	-	-
6	BCB	M	1324	X	-	-	X
6	BCB	M	1325	X	-	-	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9835 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	332	Total	C	N	O	S	0	0	0
			2590	1632	464	476	18			

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

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

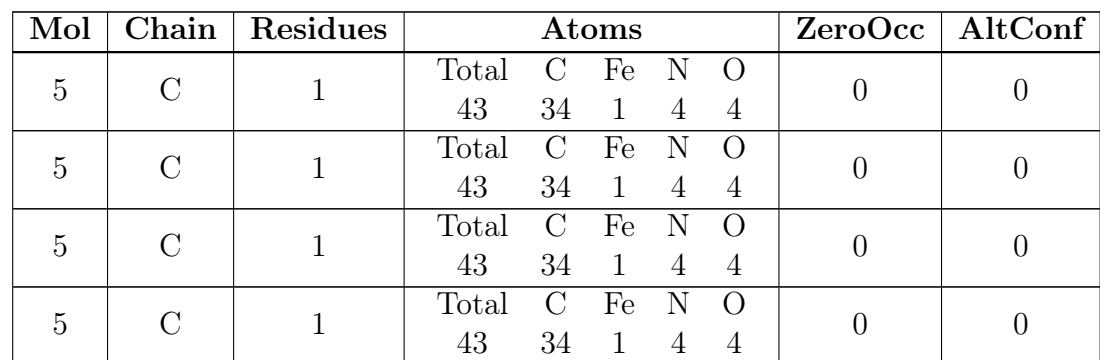
- Molecule 3 is a protein called REACTION CENTER PROTEIN L CHAIN.

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

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

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

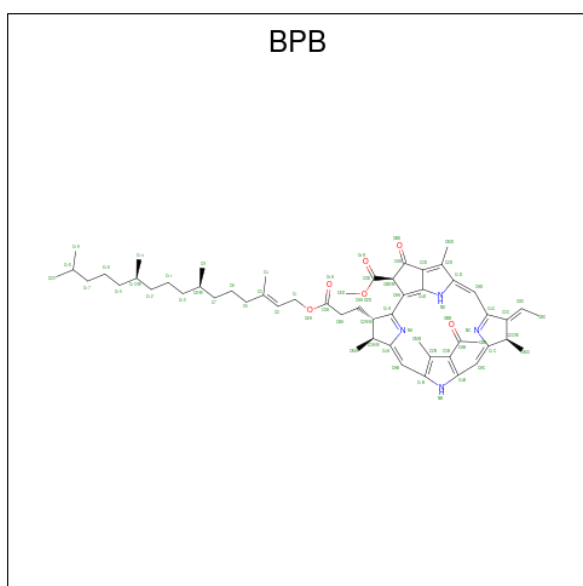
- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



- # BCB

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

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

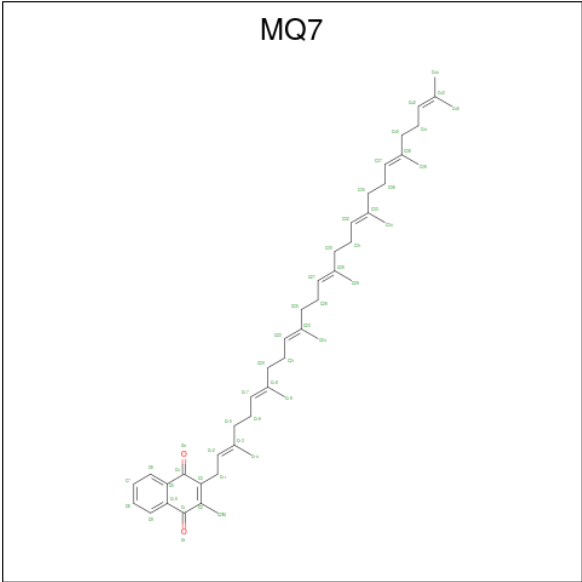


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			61	51	4	6		

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

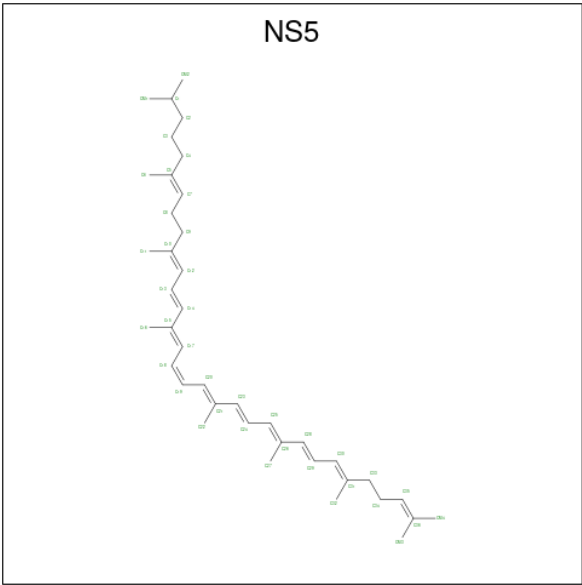
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

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



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

- Molecule 10 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: C<sub>40</sub>H<sub>60</sub>).

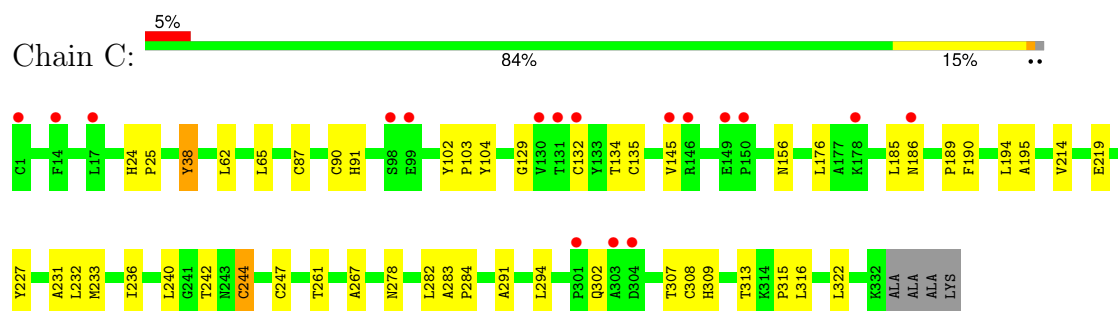


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	1	Total	C	0	0
			40	40		

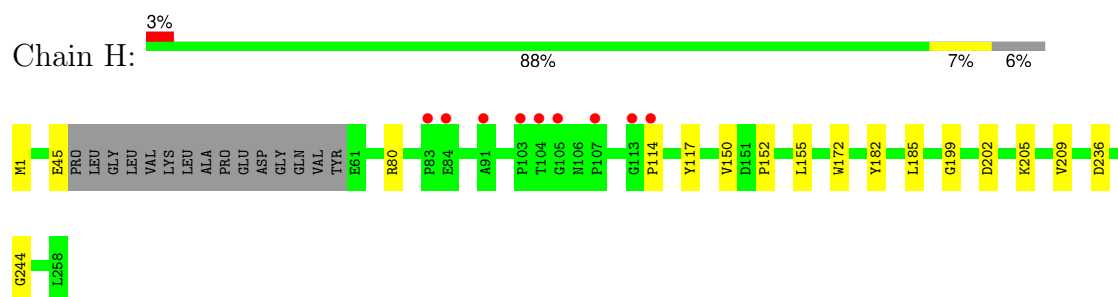
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

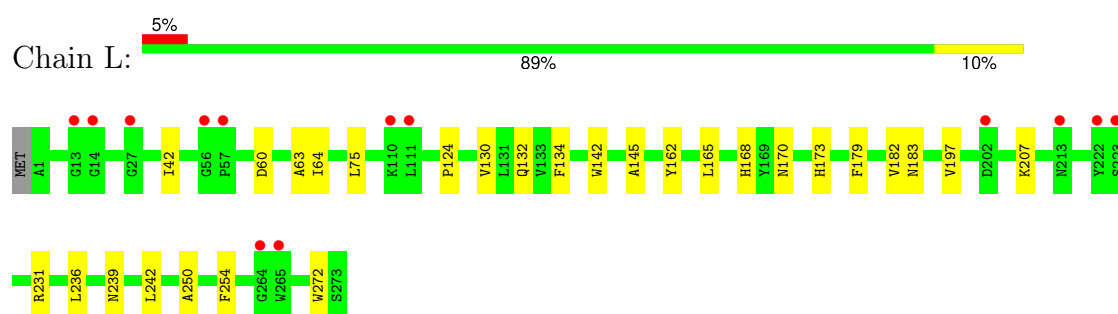
#### • Molecule 1: PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT



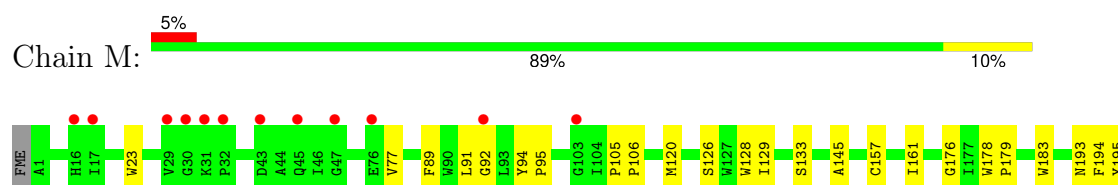
#### • Molecule 2: REACTION CENTER PROTEIN H CHAIN



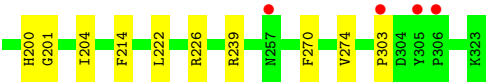
#### • Molecule 3: REACTION CENTER PROTEIN L CHAIN



#### • Molecule 4: REACTION CENTER PROTEIN M CHAIN







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.50Å 84.60Å 375.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.10 – 8.20 56.84 – 8.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (46.10-8.20) 97.3 (56.84-8.20)	Depositor EDS
$R_{merge}$	0.50	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 8.36Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.351 , 0.384 0.344 , 0.376	Depositor DCC
$R_{free}$ test set	95 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	-2.7	Xtriage
Anisotropy	-13.102	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 211.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.67	EDS
Total number of atoms	9835	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.09% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: HEM, NS5, FE2, BPB, MQ7, BCB, FME

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	C	0.31	0/2657	0.46	0/3624
2	H	0.32	0/1919	0.46	0/2621
3	L	0.34	0/2248	0.42	0/3069
4	M	0.33	0/2652	0.40	0/3630
All	All	0.33	0/9476	0.44	0/12944

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	2590	0	2561	34	0
2	H	1886	0	1880	8	0
3	L	2161	0	2089	16	0
4	M	2548	0	2432	22	0
5	C	172	0	120	10	0
6	L	132	0	144	12	0
6	M	131	0	140	5	0
7	L	65	0	74	4	0
7	M	61	0	63	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	M	1	0	0	0	0
9	M	48	0	64	0	0
10	M	40	0	60	3	0
All	All	9835	0	9627	90	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 5.

The worst 5 of 90 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:1325:BCB:HBD	6:M:1325:BCB:HAA1	1.62	0.80
1:C:247:CYS:SG	5:C:1335:HEM:HAC	2.24	0.78
1:C:308:CYS:SG	5:C:1336:HEM:HAC	2.25	0.76
7:L:1276:BPB:HHC	7:L:1276:BPB:HBBB	1.69	0.73
3:L:239:ASN:HA	3:L:242:LEU:HB2	1.76	0.66

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	330/336 (98%)	311 (94%)	19 (6%)	0	100	100
2	H	239/258 (93%)	229 (96%)	10 (4%)	0	100	100
3	L	271/274 (99%)	253 (93%)	17 (6%)	1 (0%)	34	72
4	M	321/324 (99%)	309 (96%)	11 (3%)	1 (0%)	41	77
All	All	1161/1192 (97%)	1102 (95%)	57 (5%)	2 (0%)	47	81

All (2) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	278/282 (99%)	274 (99%)	4 (1%)	67	80
2	H	194/212 (92%)	192 (99%)	2 (1%)	76	86
3	L	216/219 (99%)	215 (100%)	1 (0%)	88	93
4	M	247/249 (99%)	245 (99%)	2 (1%)	81	89
All	All	935/962 (97%)	926 (99%)	9 (1%)	76	86

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	M	194	PHE
4	M	214	PHE
1	C	307	THR
2	H	45	GLU
2	H	185	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	278	ASN
4	M	72	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	FME	H	1	2	8,9,10	0.74	0	8,9,11	3.18	3 (37%)

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

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	FME	CA-N-CN	-8.28	110.09	122.82
2	H	1	FME	O1-CN-N	-2.11	119.86	125.32
2	H	1	FME	CE-SD-CG	2.01	110.70	100.32

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	HEM	C	1334	1	42,50,50	1.95	7 (16%)	46,82,82	1.56	6 (13%)
5	HEM	C	1336	1	42,50,50	1.98	8 (19%)	46,82,82	1.55	4 (8%)
6	BCB	M	1324	-	62,73,74	2.85	15 (24%)	70,113,115	2.70	22 (31%)
10	NS5	M	1329	-	39,39,39	2.07	5 (12%)	46,46,46	2.39	17 (36%)
6	BCB	M	1325	4	63,74,74	2.89	16 (25%)	72,115,115	2.66	20 (27%)
7	BPB	L	1276	-	49,70,70	1.91	8 (16%)	48,101,101	1.92	11 (22%)
5	HEM	C	1333	1	42,50,50	1.98	8 (19%)	46,82,82	1.66	6 (13%)
6	BCB	L	1275	-	63,74,74	2.94	17 (26%)	72,115,115	2.58	20 (27%)
7	BPB	M	1326	-	45,66,70	1.97	8 (17%)	43,96,101	2.06	10 (23%)
6	BCB	L	1274	3	63,74,74	2.87	16 (25%)	72,115,115	2.71	22 (30%)
5	HEM	C	1335	1	42,50,50	1.95	7 (16%)	46,82,82	1.63	7 (15%)
9	MQ7	M	1328	-	49,49,49	1.54	2 (4%)	61,63,63	1.21	8 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	C	1334	1	-	7/12/54/54	-
5	HEM	C	1336	1	-	3/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BCB	M	1324	-	3/3/20/26	21/36/136/137	-
10	NS5	M	1329	-	-	16/43/43/43	-
6	BCB	M	1325	4	3/3/21/26	22/37/137/137	-
7	BPB	L	1276	-	-	19/37/105/105	0/5/6/6
5	HEM	C	1333	1	-	7/12/54/54	-
6	BCB	L	1275	-	3/3/21/26	14/37/137/137	-
7	BPB	M	1326	-	-	13/33/101/105	0/5/6/6
6	BCB	L	1274	3	3/3/21/26	16/37/137/137	-
5	HEM	C	1335	1	-	6/12/54/54	-
9	MQ7	M	1328	-	-	3/41/61/61	0/2/2/2

The worst 5 of 117 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1275	BCB	CHC-C1C	16.86	1.48	1.33
6	M	1325	BCB	CHC-C1C	16.59	1.48	1.33
6	L	1274	BCB	CHC-C1C	16.29	1.48	1.33
6	M	1324	BCB	CHC-C1C	16.17	1.48	1.33
9	M	1328	MQ7	C3-C2	8.35	1.50	1.35

The worst 5 of 153 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1274	BCB	C1C-NC-C4C	-14.59	100.02	106.68
6	M	1324	BCB	C1C-NC-C4C	-13.98	100.30	106.68
6	M	1325	BCB	C1C-NC-C4C	-13.32	100.60	106.68
6	L	1275	BCB	C1C-NC-C4C	-12.55	100.95	106.68
7	M	1326	BPB	O2D-CGD-CBD	8.66	120.46	110.95

5 of 12 chirality outliers are listed below:

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

5 of 147 torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
5	C	1333	HEM	C3D-CAD-CBD-CGD
5	C	1335	HEM	C2B-C3B-CAB-CBB
6	L	1274	BCB	C2C-C3C-CAC-CBC
6	L	1274	BCB	C4C-C3C-CAC-CBC
6	L	1274	BCB	CBD-CGD-O2D-CED

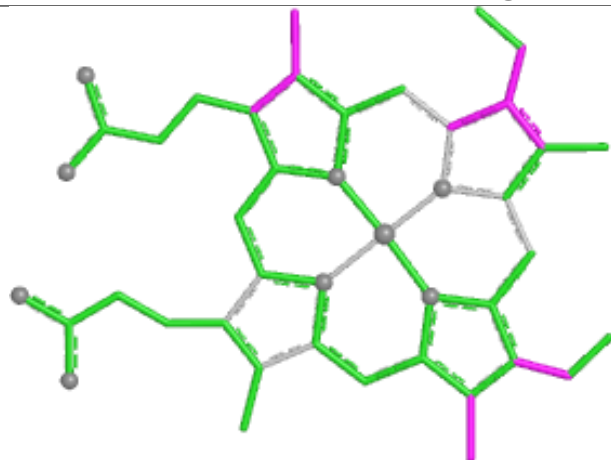
There are no ring outliers.

10 monomers are involved in 34 short contacts:

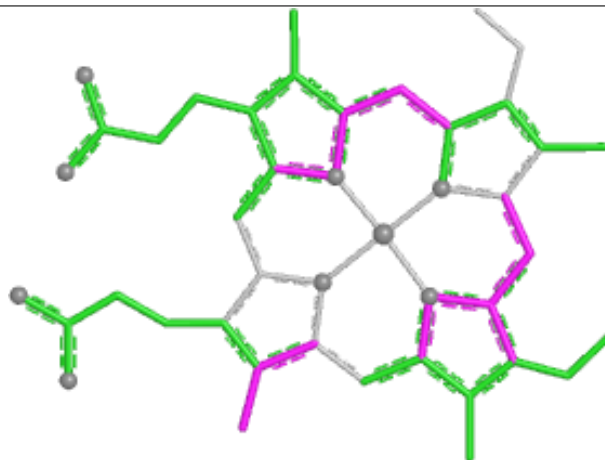
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1334	HEM	2	0
5	C	1336	HEM	2	0
10	M	1329	NS5	3	0
6	M	1325	BCB	5	0
7	L	1276	BPB	4	0
5	C	1333	HEM	1	0
6	L	1275	BCB	7	0
7	M	1326	BPB	1	0
6	L	1274	BCB	6	0
5	C	1335	HEM	5	0

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 than 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.

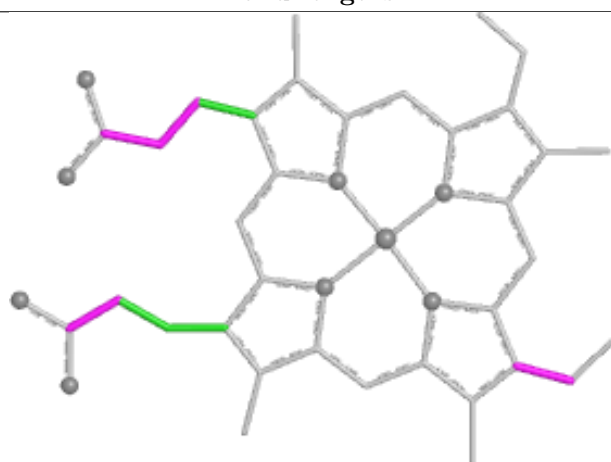
## Ligand HEM C 1334



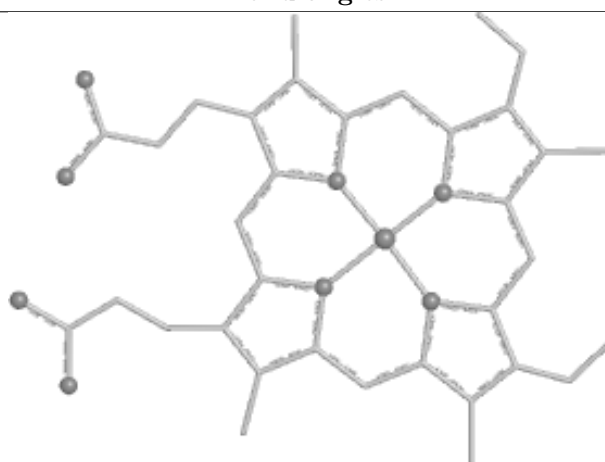
Bond lengths



Bond angles

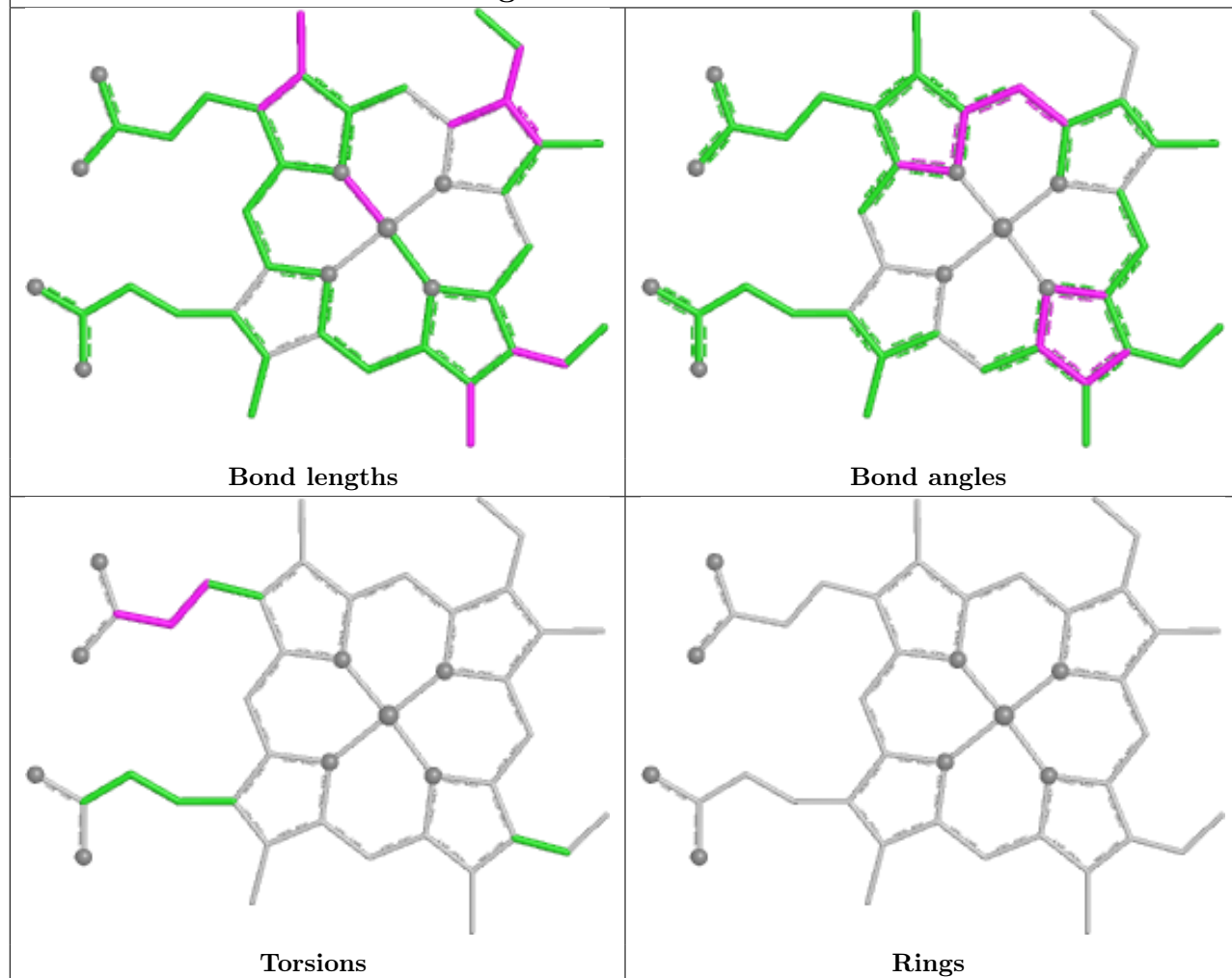


Torsions

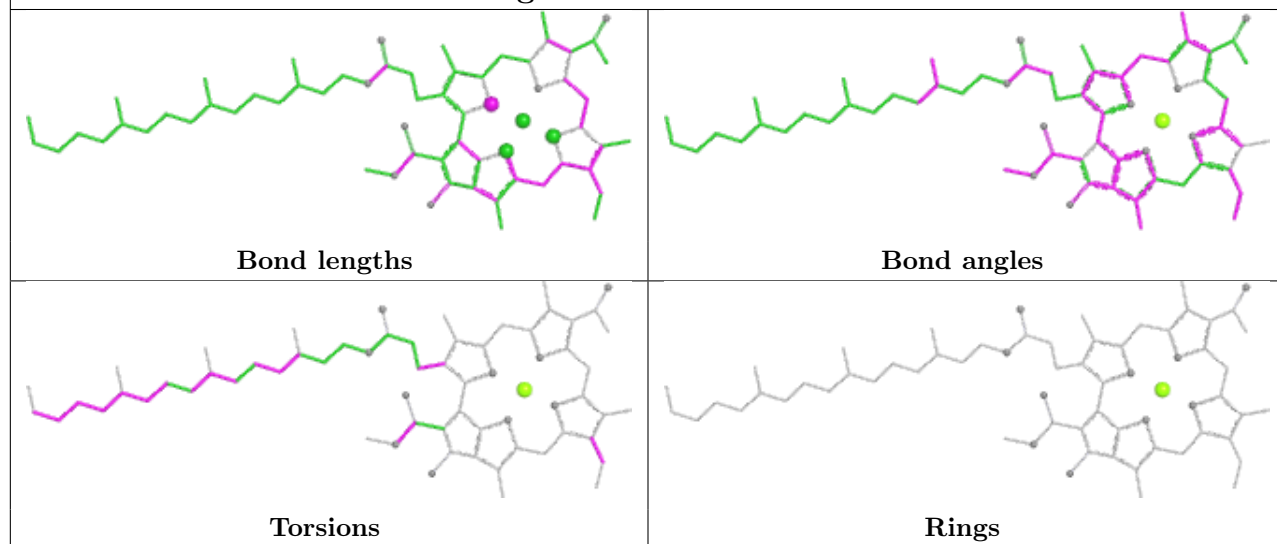


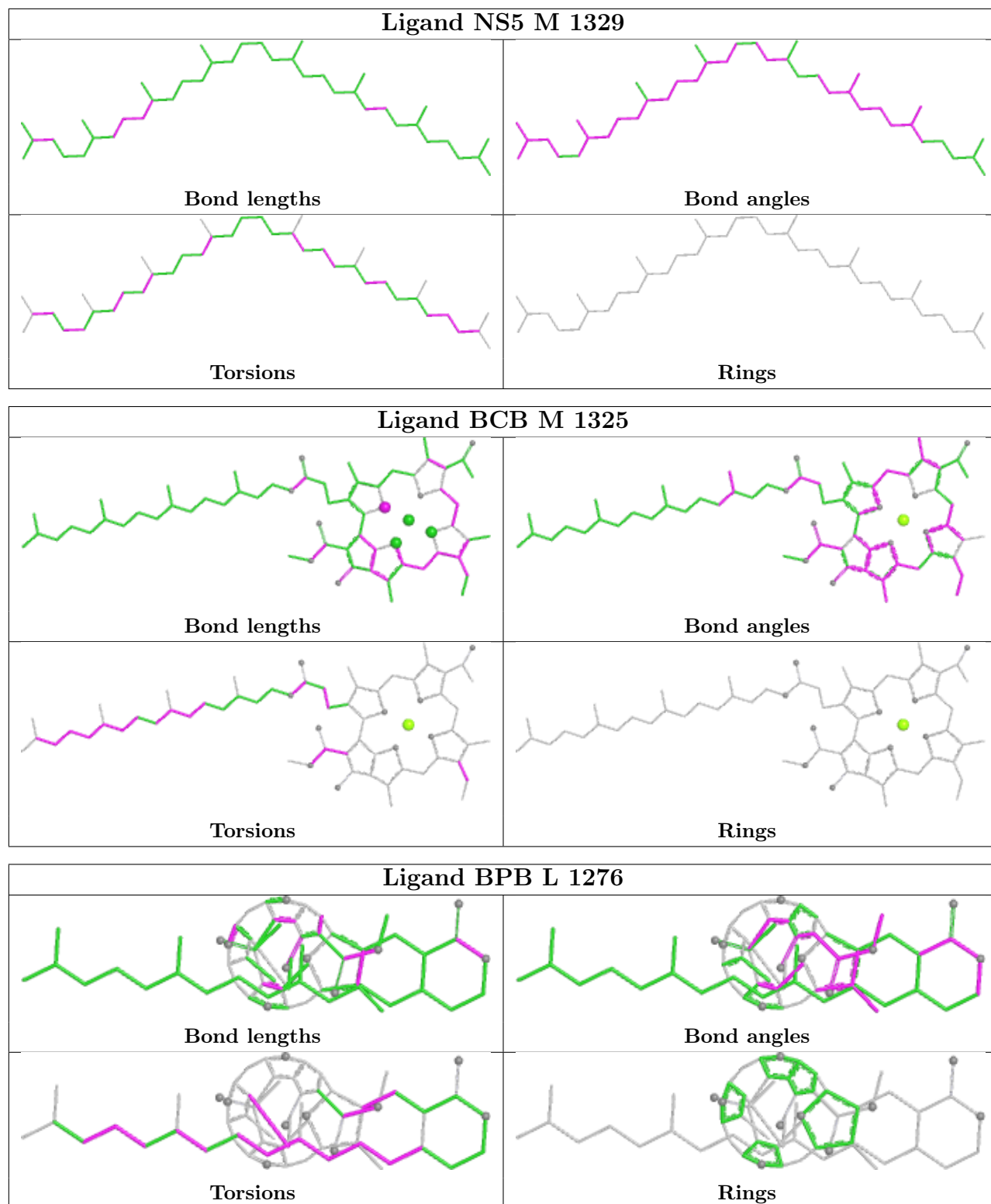
Rings

## Ligand HEM C 1336

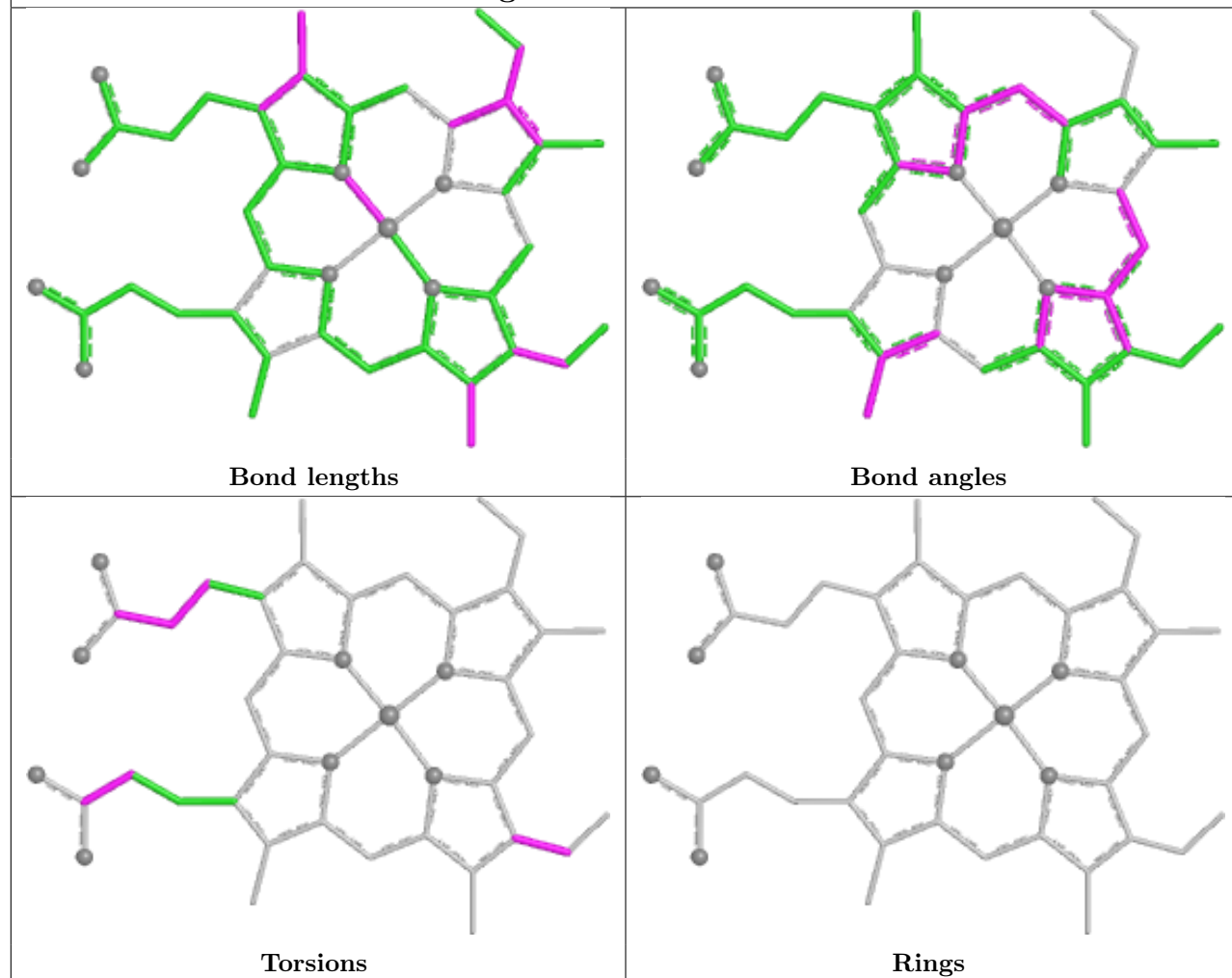


## Ligand BCB M 1324

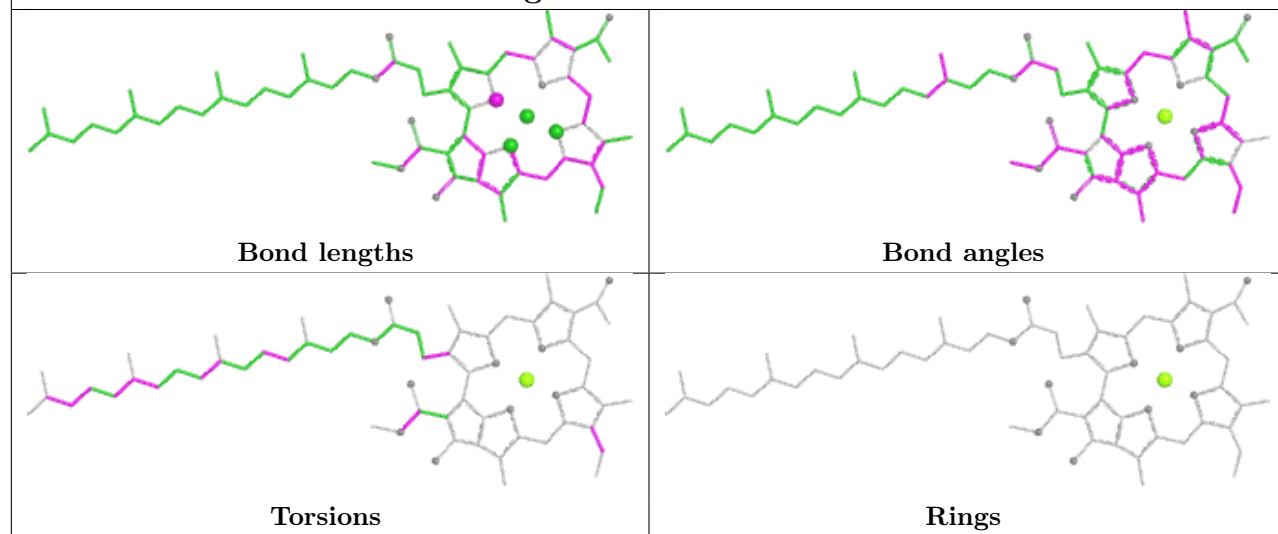


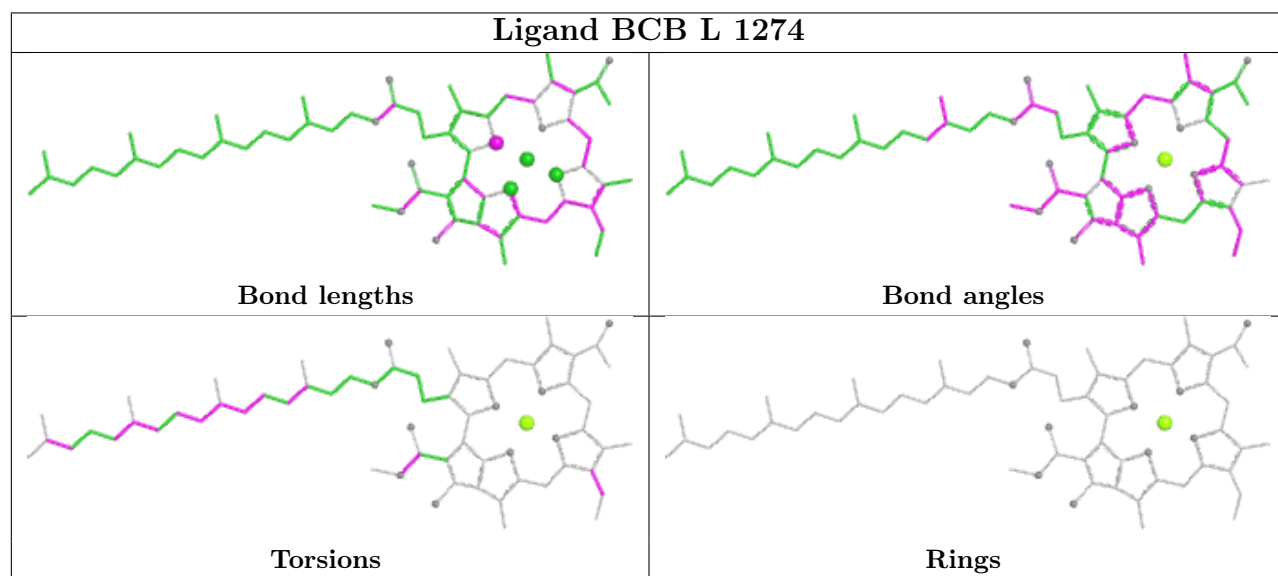
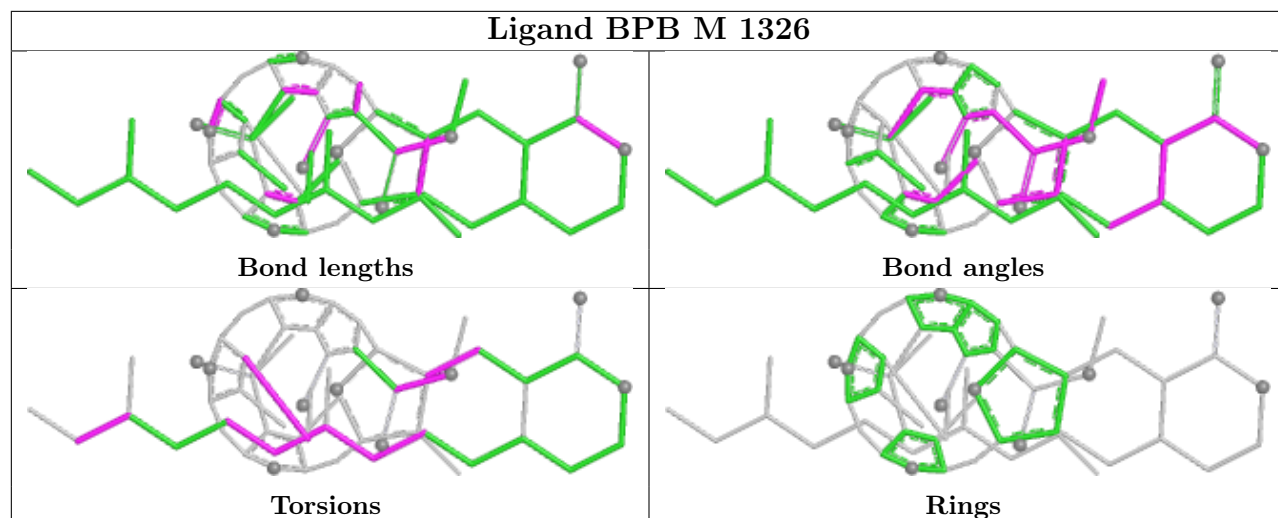


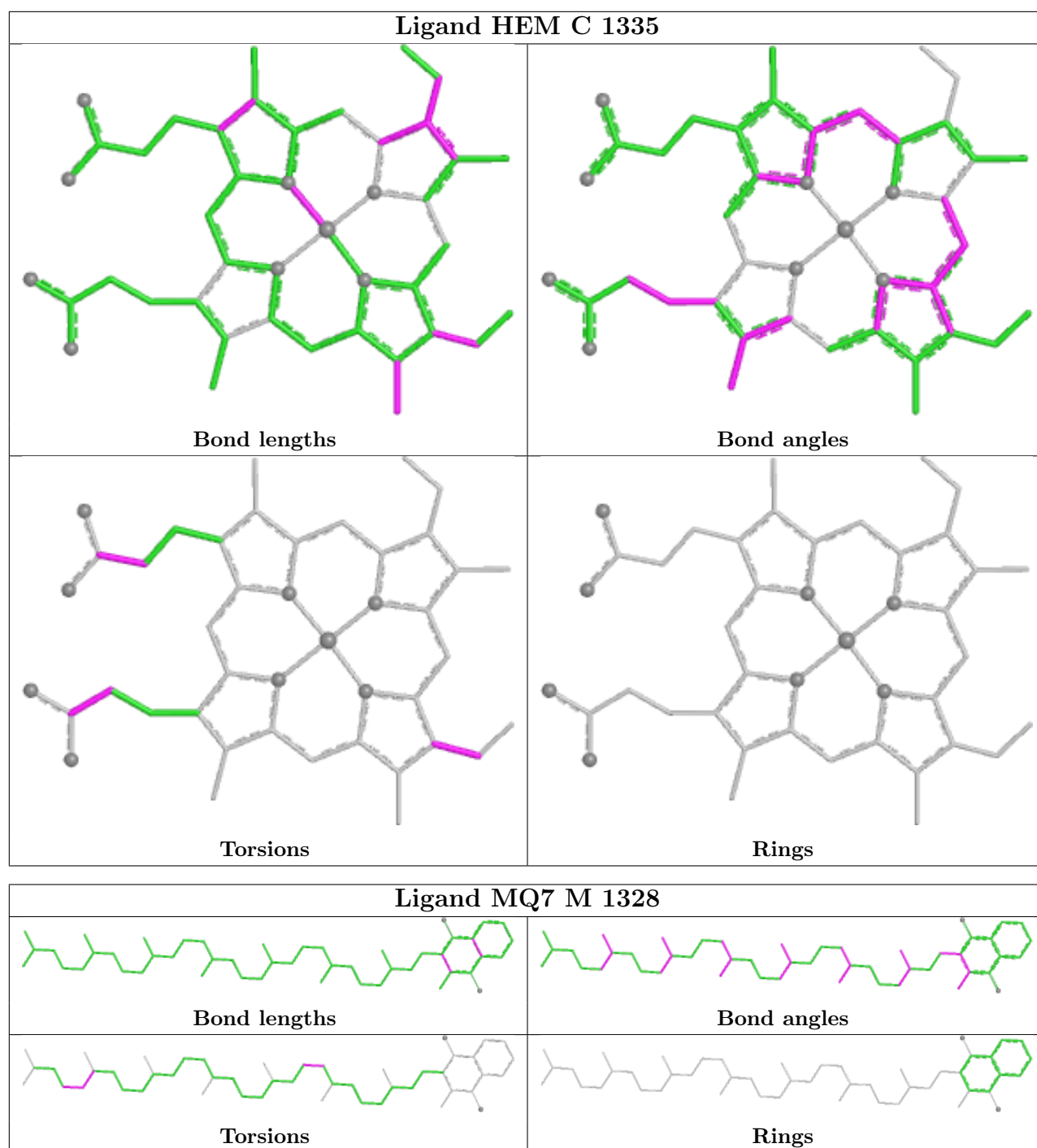
## Ligand HEM C 1333



## Ligand BCB L 1275







## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	C	332/336 (98%)	0.31	17 (5%) 28 27	12, 15, 19, 21	0
2	H	242/258 (93%)	0.20	9 (3%) 41 37	12, 16, 25, 26	0
3	L	273/274 (99%)	0.18	13 (4%) 30 29	10, 15, 21, 22	0
4	M	323/324 (99%)	0.18	16 (4%) 28 28	11, 15, 20, 20	0
All	All	1170/1192 (98%)	0.22	55 (4%) 31 30	10, 15, 21, 26	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	131	THR	4.9
1	C	186	ASN	4.5
2	H	83	PRO	4.4
2	H	84	GLU	4.3
3	L	223	SER	4.2

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	FME	H	1	10/11	0.71	0.38	18,18,18,18	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 6.4 Ligands ⓘ

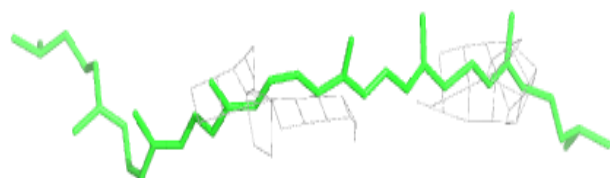
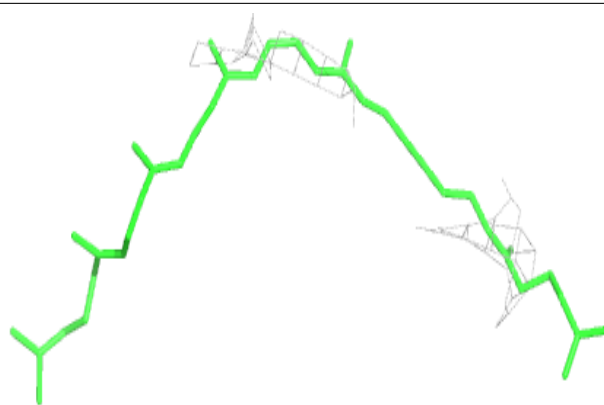
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
10	NS5	M	1329	40/40	0.59	0.65	27,28,30,30	0
6	BCB	M	1324	65/66	0.76	0.45	16,16,16,17	0
6	BCB	L	1275	66/66	0.81	0.46	19,20,21,21	0
7	BPB	M	1326	61/65	0.82	0.53	26,26,27,27	0
9	MQ7	M	1328	48/48	0.86	0.58	9,9,10,10	0
6	BCB	M	1325	66/66	0.87	0.45	12,12,15,15	0
5	HEM	C	1333	43/43	0.89	0.37	15,16,16,16	0
8	FE2	M	1327	1/1	0.90	0.33	2,2,2,2	0
7	BPB	L	1276	65/65	0.90	0.46	2,2,4,4	0
6	BCB	L	1274	66/66	0.90	0.42	29,29,30,30	0
5	HEM	C	1336	43/43	0.91	0.38	2,2,2,2	0
5	HEM	C	1334	43/43	0.92	0.67	2,2,2,2	0
5	HEM	C	1335	43/43	0.93	0.33	4,4,4,4	0

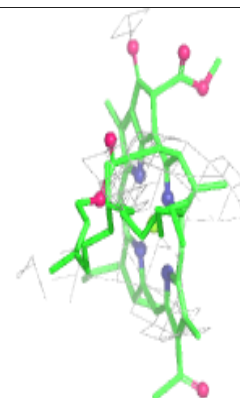
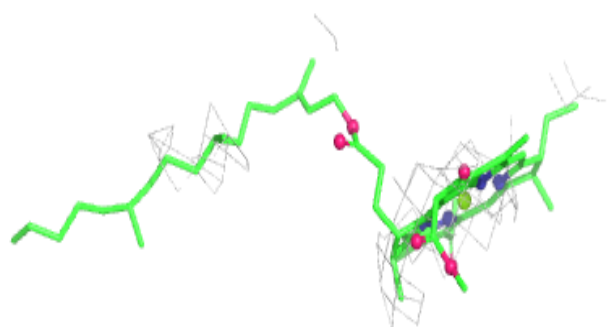
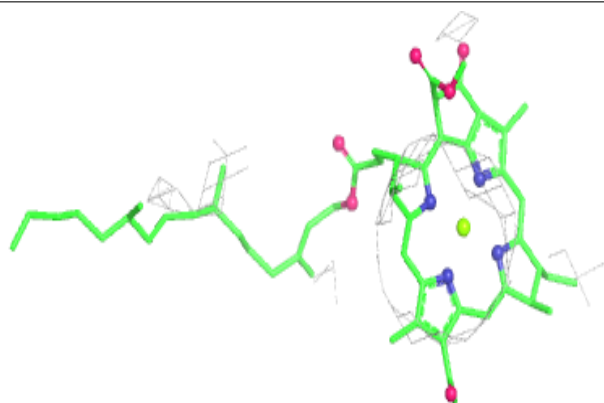
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NS5 M 1329:**

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

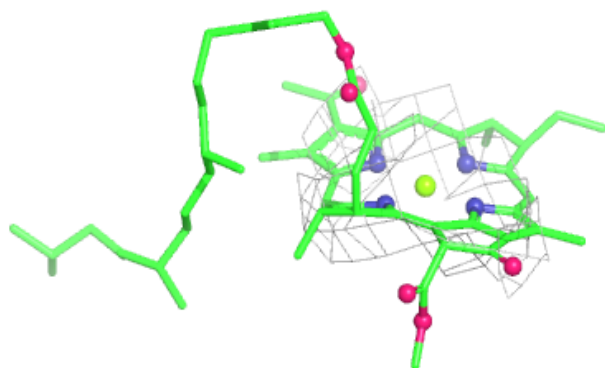
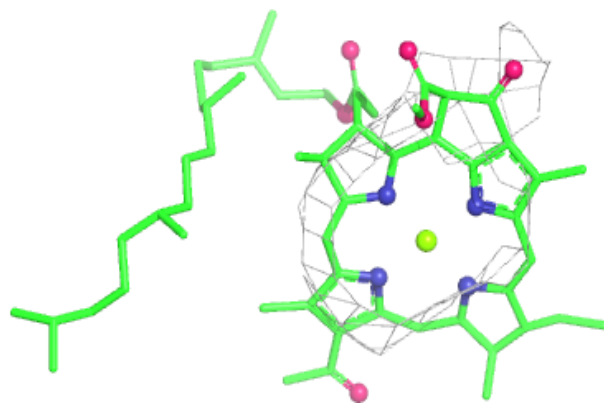
**Electron density around BCB M 1324:**

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

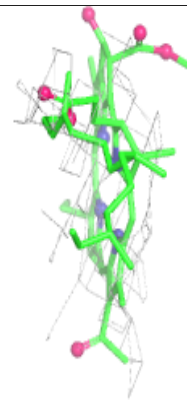
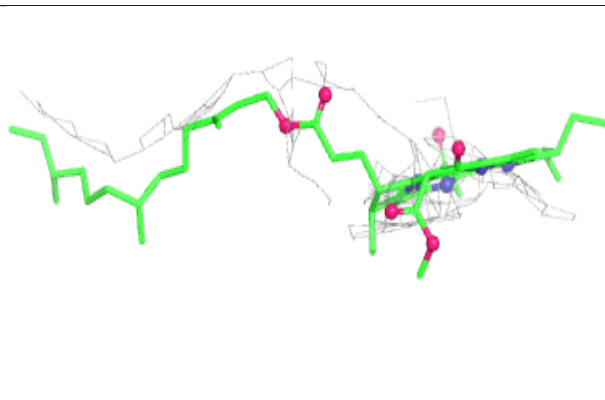
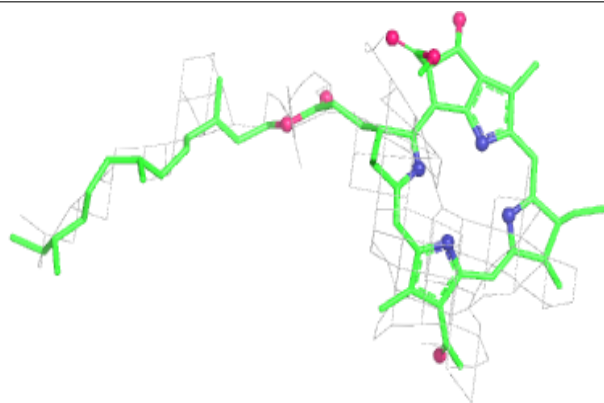


**Electron density around BCB L 1275:**

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

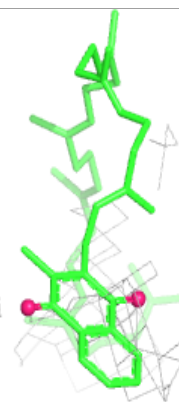
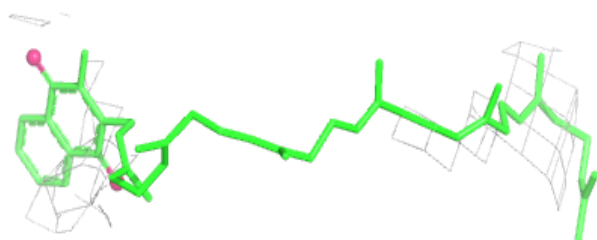
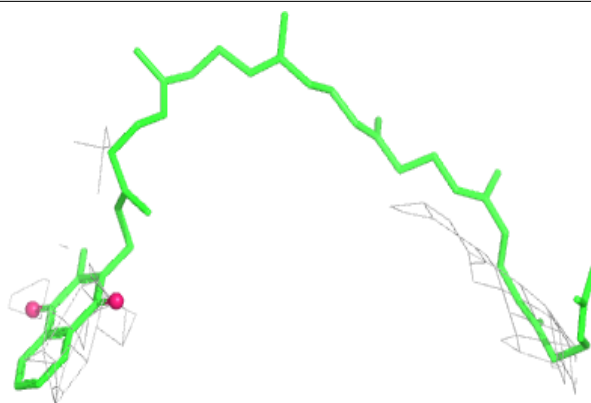
**Electron density around BPB M 1326:**

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and green (positive)

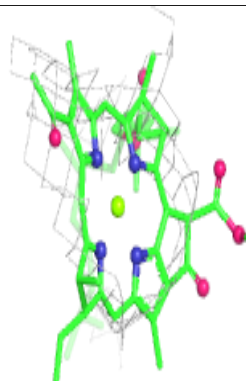
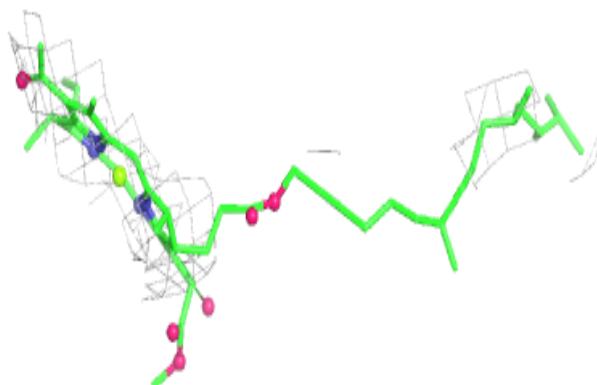
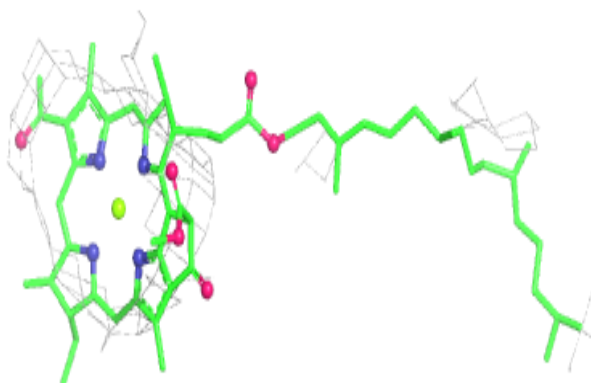


**Electron density around MQ7 M 1328:**

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

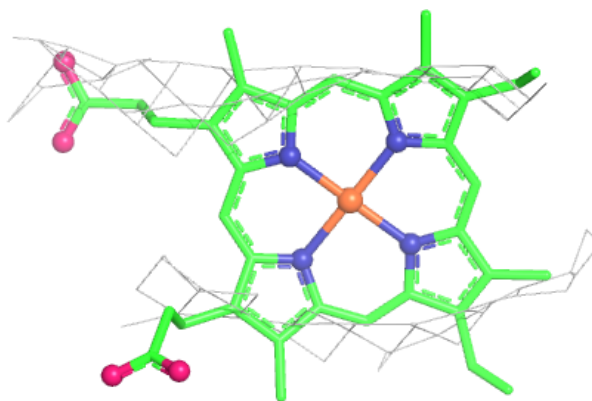
**Electron density around BCB M 1325:**

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

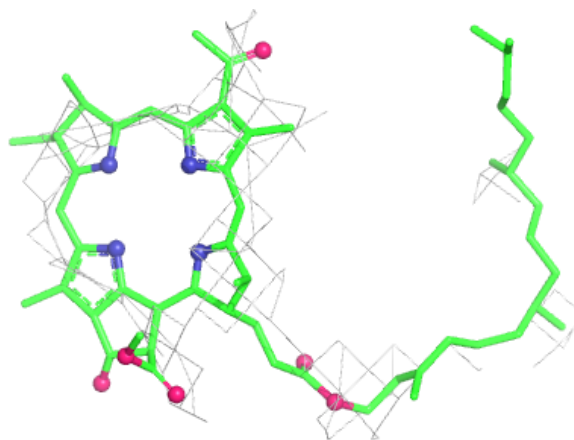


**Electron density around HEM C 1333:**

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

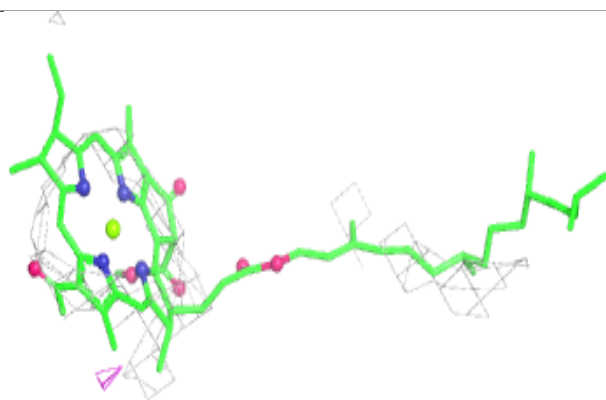
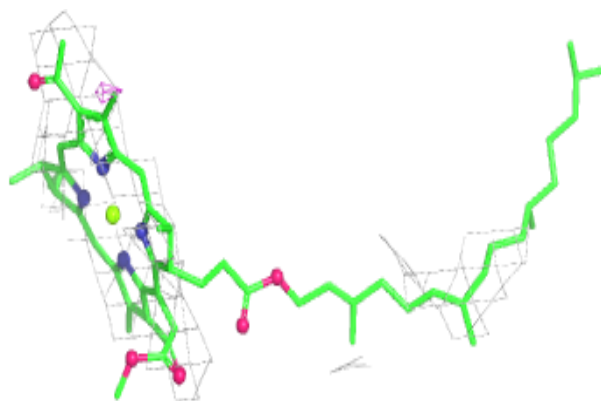
**Electron density around BPB L 1276:**

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and green (positive)



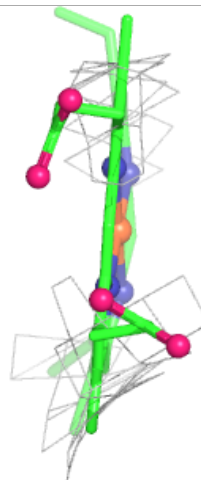
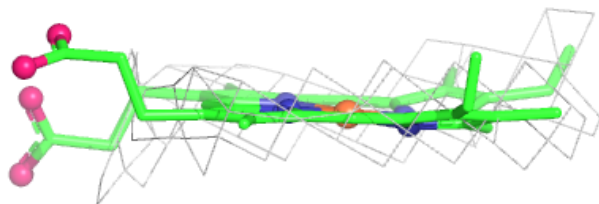
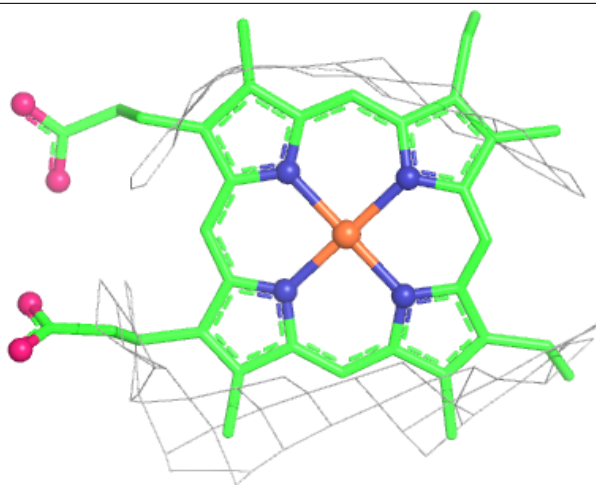
**Electron density around BCB L 1274:**

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



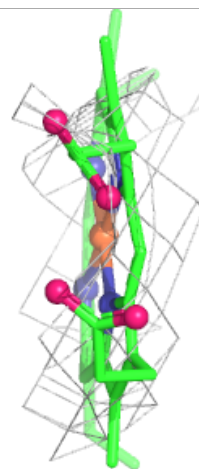
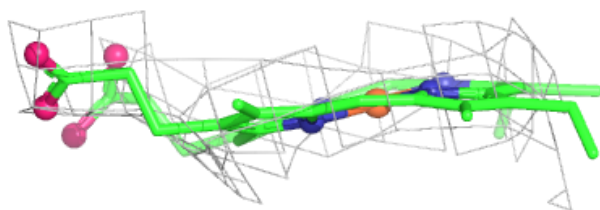
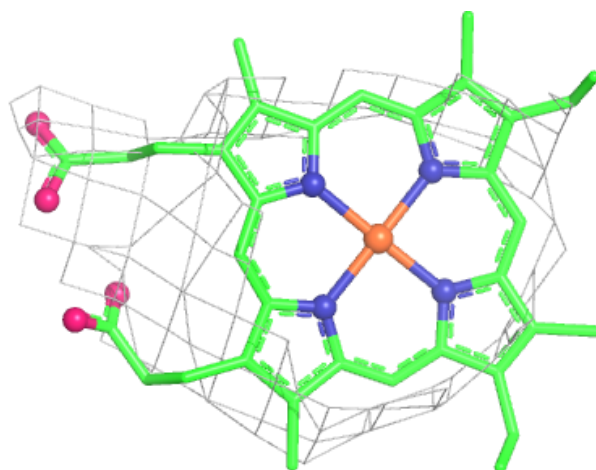
**Electron density around HEM C 1336:**

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and green (positive)



**Electron density around HEM C 1334:**

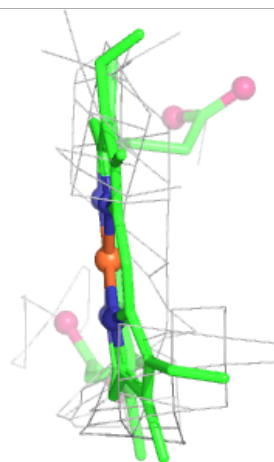
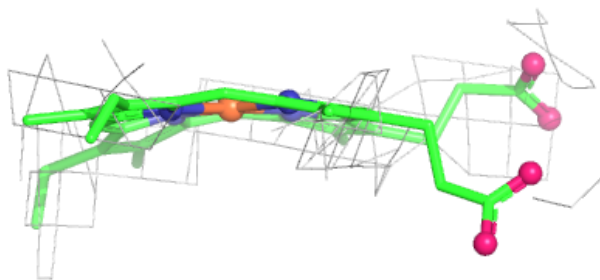
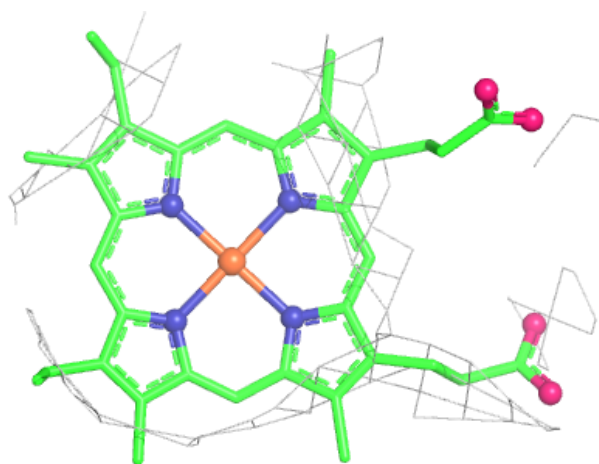
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM C 1335:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.