



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 5, 2024 – 08:01 AM EDT

PDB ID : 2PRC  
Title : PHOTOSYNTHETIC REACTION CENTER FROM RHODOPSEUDOMONAS VIRIDIS (UBIQUINONE-2 COMPLEX)  
Authors : Lancaster, C.R.D.; Michel, H.  
Deposited on : 1997-07-29  
Resolution : 2.45 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>.

---

The following versions of software and data (see [references ⓘ](#)) 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

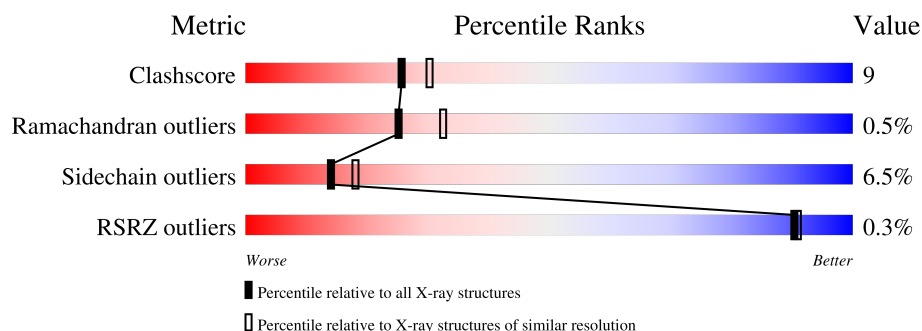
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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	1178 (2.46-2.46)
Ramachandran outliers	177936	1170 (2.46-2.46)
Sidechain outliers	177891	1170 (2.46-2.46)
RSRZ outliers	164620	1096 (2.46-2.46)

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.

Mol	Chain	Length	Quality of chain
1	C	336	<div> <div>77%</div> <div>20%</div> <div>..</div> </div>
2	L	273	<div> <div>82%</div> <div>17%</div> <div>.</div> </div>
3	M	323	<div> <div>78%</div> <div>19%</div> <div>.</div> </div>
4	H	258	<div> <div>2%</div> <div>71%</div> <div>28%</div> <div>.</div> </div>

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	-	-	-

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 10528 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
1	C	332	Total	C	N	O	S	53	4	0
			2630	1655	470	485	20			

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

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

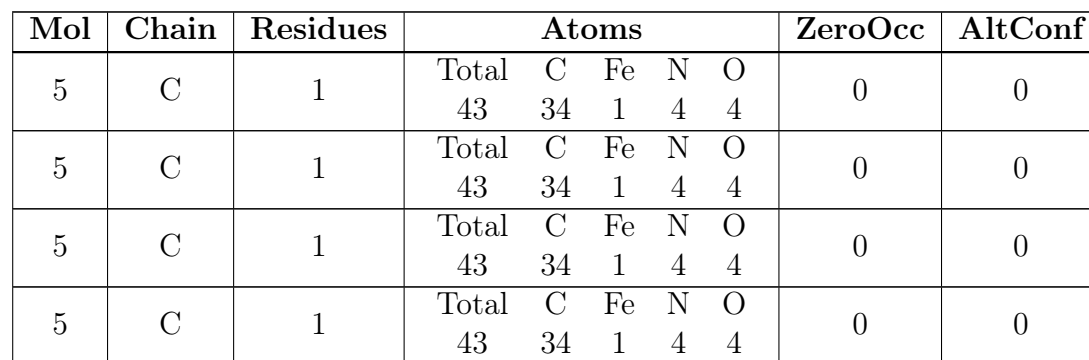
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

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

- Molecule 4 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	258	Total	C	N	O	S	124	0	0
			2018	1292	344	380	2			

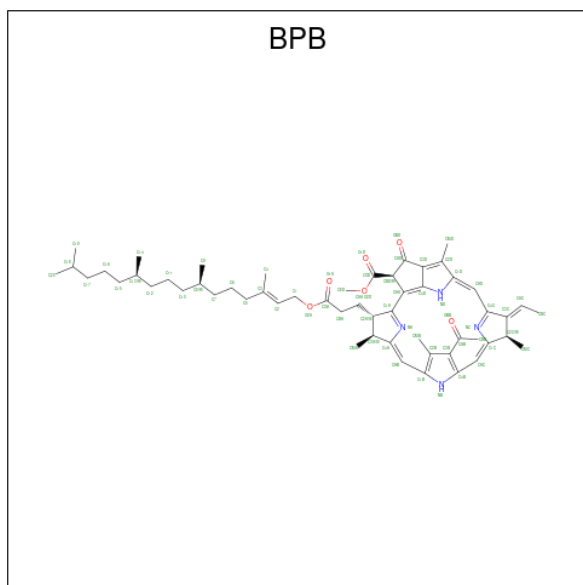
- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



- # BCB

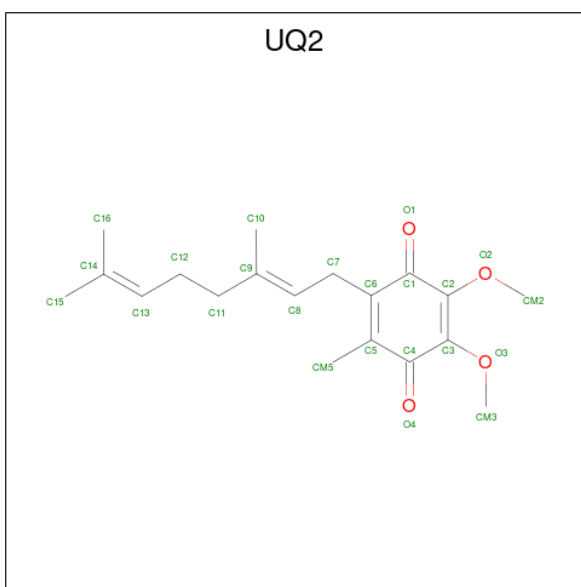
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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



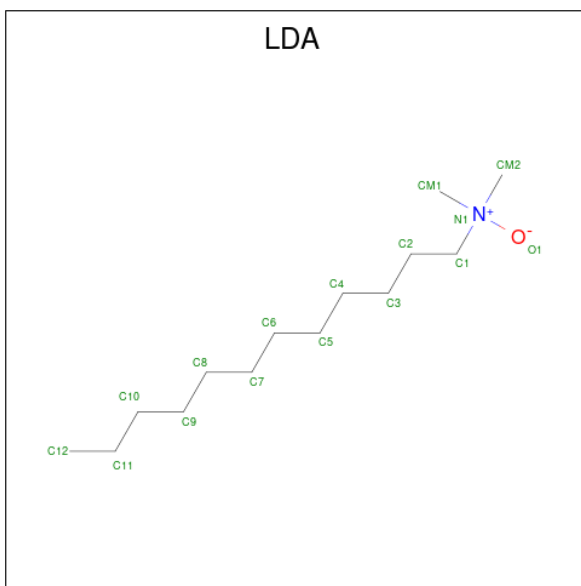
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	7	0
			65	55	4	6		

- Molecule 8 is UBIQUINONE-2 (three-letter code: UQ2) (formula:  $C_{19}H_{26}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			23	19	4		

- 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	5	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		

*Continued on next page...*

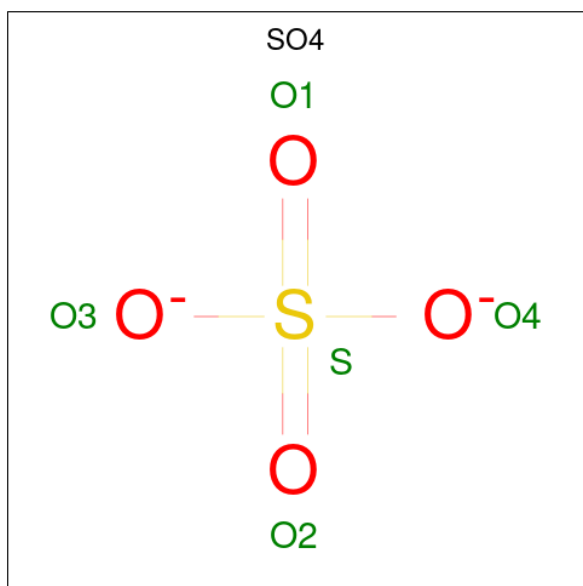
Continued from previous page...

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

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

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

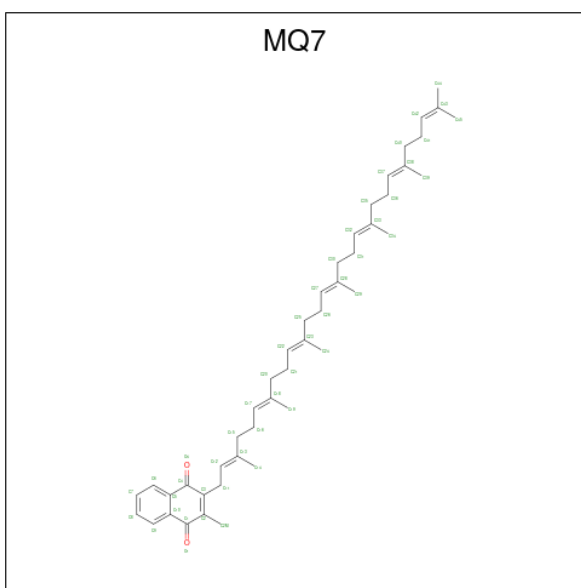
- Molecule 11 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

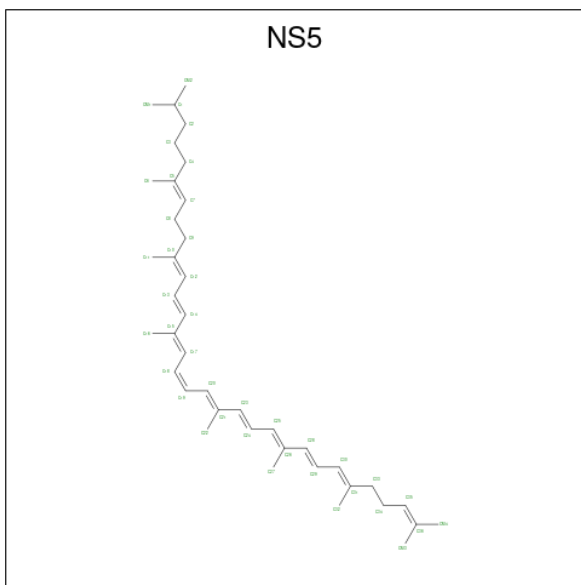


- Molecule 12 is MENAQUINONE-7 (three-letter code: MQ7) (formula:  $C_{46}H_{64}O_2$ ).



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

- 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	14	0
			40	40		

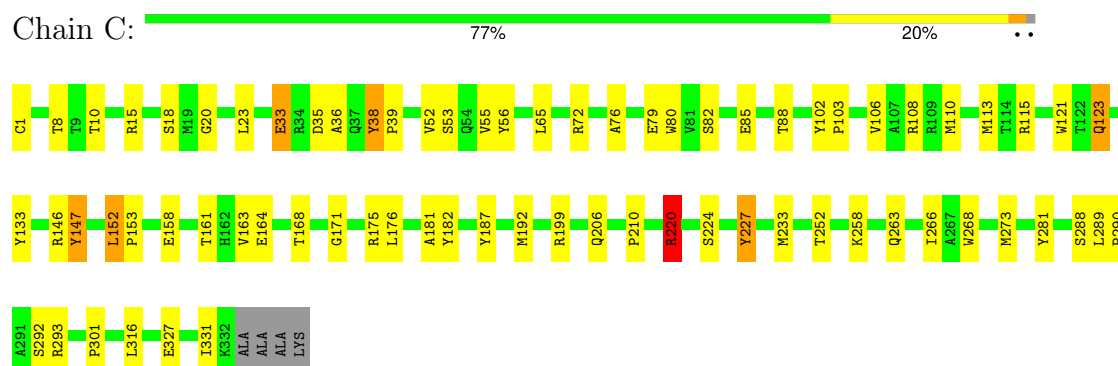
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	121	Total 121	O 121	0	0
14	L	48	Total 48	O 48	0	0
14	M	76	Total 76	O 76	0	0
14	H	71	Total 71	O 71	0	0

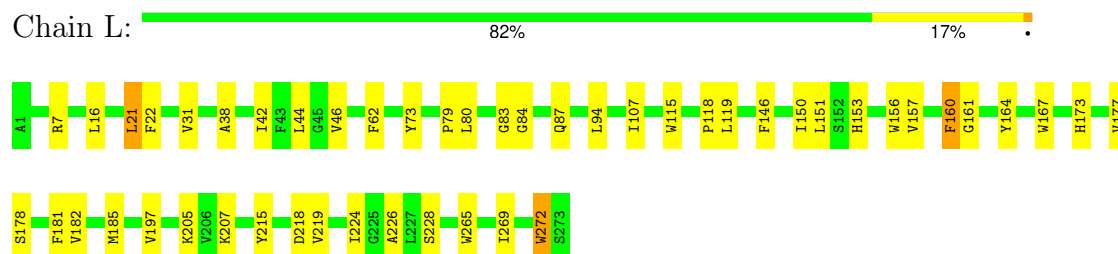
### 3 Residue-property plots

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.

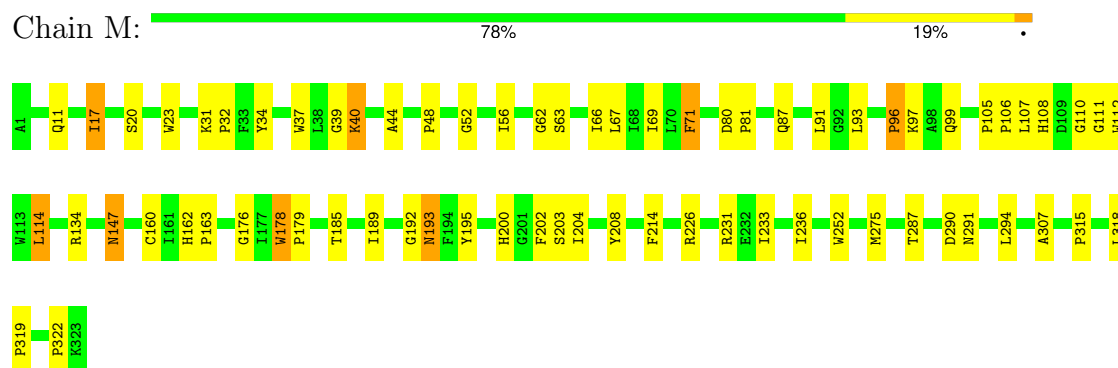
#### • Molecule 1: PHOTOSYNTHETIC REACTION CENTER



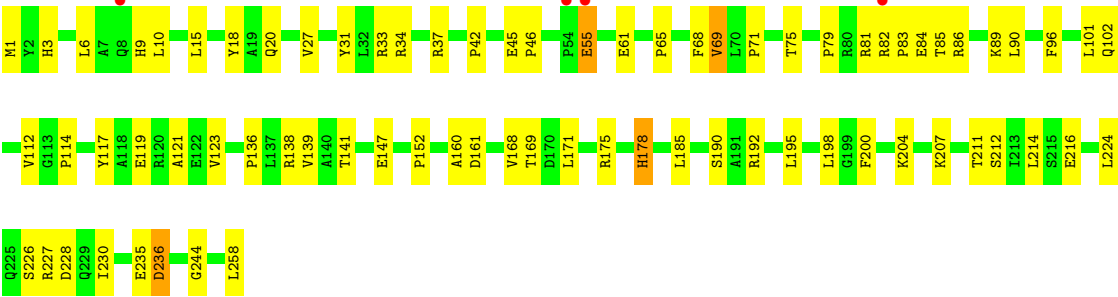
#### • Molecule 2: PHOTOSYNTHETIC REACTION CENTER



#### • Molecule 3: PHOTOSYNTHETIC REACTION CENTER



#### • Molecule 4: PHOTOSYNTHETIC REACTION CENTER



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	223.50Å 223.50Å 113.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.45 10.00 – 2.45	Depositor EDS
% Data completeness (in resolution range)	76.5 (10.00-2.45) 75.3 (10.00-2.45)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 2.44Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.182 , 0.229 0.174 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 93.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10528	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, LDA, FME, MQ7, FE2, BCB, SO4, NS5, UQ2, BPB

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	0.53	0/2697	0.62	0/3675
2	L	0.55	0/2281	0.57	0/3112
3	M	0.54	0/2683	0.59	0/3669
4	H	0.52	0/2055	0.64	1/2807 (0.0%)
All	All	0.53	0/9716	0.60	1/13263 (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	3
2	L	0	2
4	H	0	1
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	45	GLU	CB-CA-C	-5.62	99.17	110.40

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	147	TYR	Sidechain
1	C	220	ARG	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	C	227	TYR	Sidechain
2	L	160	PHE	Sidechain
2	L	164	TYR	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2630	0	2594	49	0
2	L	2193	0	2122	34	0
3	M	2577	0	2468	52	0
4	H	2018	0	2020	39	0
5	C	172	0	120	3	0
6	L	132	0	144	13	0
6	M	132	0	144	12	0
7	L	65	0	74	6	0
7	M	65	0	74	8	0
8	L	23	0	26	2	0
9	H	16	0	31	1	0
9	L	16	0	31	0	0
9	M	64	0	124	2	0
10	M	1	0	0	0	0
11	H	5	0	0	0	0
11	M	15	0	0	0	0
12	M	48	0	64	1	0
13	M	40	0	60	6	0
14	C	121	0	0	1	0
14	H	71	0	0	0	0
14	L	48	0	0	0	0
14	M	76	0	0	0	0
All	All	10528	0	10096	185	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 185 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	1.42	1.02
7:M:401:BPB:HBBB	7:M:401:BPB:HHC	1.59	0.84
6:M:805:BCB:HHC	6:M:805:BCB:HBB2	1.60	0.84
4:H:161:ASP:HB3	4:H:214:LEU:HD22	1.59	0.83
7:L:402:BPB:HHC	7:L:402:BPB:CBB	2.12	0.79

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	333/336 (99%)	320 (96%)	13 (4%)	0	100	100
2	L	273/273 (100%)	256 (94%)	16 (6%)	1 (0%)	30	38
3	M	323/323 (100%)	310 (96%)	10 (3%)	3 (1%)	14	18
4	H	256/258 (99%)	243 (95%)	11 (4%)	2 (1%)	16	21
All	All	1185/1190 (100%)	1129 (95%)	50 (4%)	6 (0%)	25	32

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	46	PRO
3	M	322	PRO
4	H	55	GLU
3	M	193	ASN
2	L	31	VAL

### 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	284/282 (101%)	267 (94%)	17 (6%)	16	22
2	L	220/218 (101%)	213 (97%)	7 (3%)	34	48
3	M	251/249 (101%)	236 (94%)	15 (6%)	16	22
4	H	212/212 (100%)	188 (89%)	24 (11%)	4	4
All	All	967/961 (101%)	904 (94%)	63 (6%)	14	18

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	40	LYS
4	H	198	LEU
3	M	203	SER
4	H	195	LEU
4	H	226	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	239	ASN
3	M	147	ASN
4	H	58	GLN
1	C	206	GLN
1	C	37	GLN

### 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	$\# Z  > 2$
4	FME	H	1	4	8,9,10	0.66	0	8,9,11	2.95	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	-	3/7/9/11	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	H	1	FME	CA-N-CN	-6.31	113.11	122.82
4	H	1	FME	O1-CN-N	-4.50	113.69	125.32
4	H	1	FME	CE-SD-CG	2.13	111.35	100.32

There are no chirality outliers.

All (3) 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

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	$\# Z  > 2$
5	HEM	C	338	1	42,50,50	1.52	6 (14%)	46,82,82	1.49	8 (17%)
5	HEM	C	340	1	42,50,50	1.64	8 (19%)	46,82,82	1.39	5 (10%)
5	HEM	C	337	1	42,50,50	1.53	7 (16%)	46,82,82	1.27	5 (10%)
6	BCB	L	302	2	63,74,74	1.95	9 (14%)	72,115,115	2.02	17 (23%)
6	BCB	L	304	2	63,74,74	1.84	8 (12%)	72,115,115	2.10	16 (22%)
8	UQ2	L	502	-	23,23,23	2.84	6 (26%)	30,31,31	1.38	5 (16%)
9	LDA	M	702	-	13,15,15	2.21	1 (7%)	14,17,17	0.49	0
11	SO4	M	803	-	4,4,4	0.53	0	6,6,6	0.59	0
7	BPB	L	402	-	49,70,70	1.50	7 (14%)	48,101,101	2.41	10 (20%)
11	SO4	M	802	-	4,4,4	0.59	0	6,6,6	0.97	0
11	SO4	M	804	-	4,4,4	0.85	0	6,6,6	0.68	0
11	SO4	H	801	-	4,4,4	0.56	0	6,6,6	0.18	0
7	BPB	M	401	-	49,70,70	1.25	5 (10%)	48,101,101	2.52	9 (18%)
9	LDA	H	703	-	13,15,15	2.49	2 (15%)	14,17,17	0.60	0
9	LDA	M	701	-	13,15,15	2.43	2 (15%)	14,17,17	0.69	0
5	HEM	C	339	1	42,50,50	1.50	6 (14%)	46,82,82	1.09	3 (6%)
9	LDA	L	705	-	13,15,15	2.49	2 (15%)	14,17,17	0.58	0
12	MQ7	M	501	-	49,49,49	1.71	17 (34%)	61,63,63	1.31	5 (8%)
13	NS5	M	600	-	39,39,39	0.76	0	46,46,46	1.27	6 (13%)
9	LDA	M	706	-	13,15,15	2.60	2 (15%)	14,17,17	0.54	0
6	BCB	M	806	3	63,74,74	1.83	10 (15%)	72,115,115	2.38	17 (23%)
9	LDA	M	704	-	13,15,15	1.88	2 (15%)	14,17,17	0.74	0
6	BCB	M	805	3	63,74,74	1.73	10 (15%)	72,115,115	1.90	12 (16%)

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
6	BCB	L	304	2	3/3/21/26	8/37/137/137	-
5	HEM	C	338	1	-	6/12/54/54	-
6	BCB	L	302	2	3/3/21/26	6/37/137/137	-
5	HEM	C	337	1	-	7/12/54/54	-
5	HEM	C	340	1	-	3/12/54/54	-
8	UQ2	L	502	-	-	4/15/39/39	0/1/1/1
9	LDA	M	702	-	-	3/13/13/13	-
7	BPB	L	402	-	-	5/37/105/105	0/5/6/6
7	BPB	M	401	-	-	6/37/105/105	0/5/6/6
9	LDA	H	703	-	-	4/13/13/13	-
9	LDA	M	701	-	-	2/13/13/13	-
5	HEM	C	339	1	-	2/12/54/54	-
9	LDA	L	705	-	-	1/13/13/13	-
12	MQ7	M	501	-	-	2/41/61/61	0/2/2/2
13	NS5	M	600	-	-	15/43/43/43	-
9	LDA	M	706	-	-	5/13/13/13	-
6	BCB	M	806	3	3/3/21/26	7/37/137/137	-
9	LDA	M	704	-	-	3/13/13/13	-
6	BCB	M	805	3	3/3/21/26	14/37/137/137	-

The worst 5 of 110 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	502	UQ2	C7-C8	-11.73	1.32	1.50
6	M	806	BCB	CHC-C1C	8.43	1.40	1.33
9	M	702	LDA	O1-N1	-7.72	1.23	1.42
6	L	304	BCB	CHC-C1C	7.65	1.40	1.33
6	L	302	BCB	CHC-C1C	7.57	1.40	1.33

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	401	BPB	O2D-CGD-CBD	12.75	124.96	110.95
7	L	402	BPB	O2D-CGD-CBD	11.87	123.99	110.95
6	M	806	BCB	CMB-C2B-C1B	-8.99	115.28	128.46
6	M	805	BCB	C4A-NA-C1A	7.78	110.23	106.68
6	L	302	BCB	C4A-NA-C1A	7.67	110.18	106.68

5 of 12 chirality outliers are listed below:

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

5 of 103 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	M	805	BCB	C2C-C3C-CAC-CBC
6	M	806	BCB	CAD-CBD-CGD-O1D
6	M	806	BCB	CAD-CBD-CGD-O2D
6	M	806	BCB	C14-C13-C15-C16
13	M	600	NS5	C3-C4-C5-C6

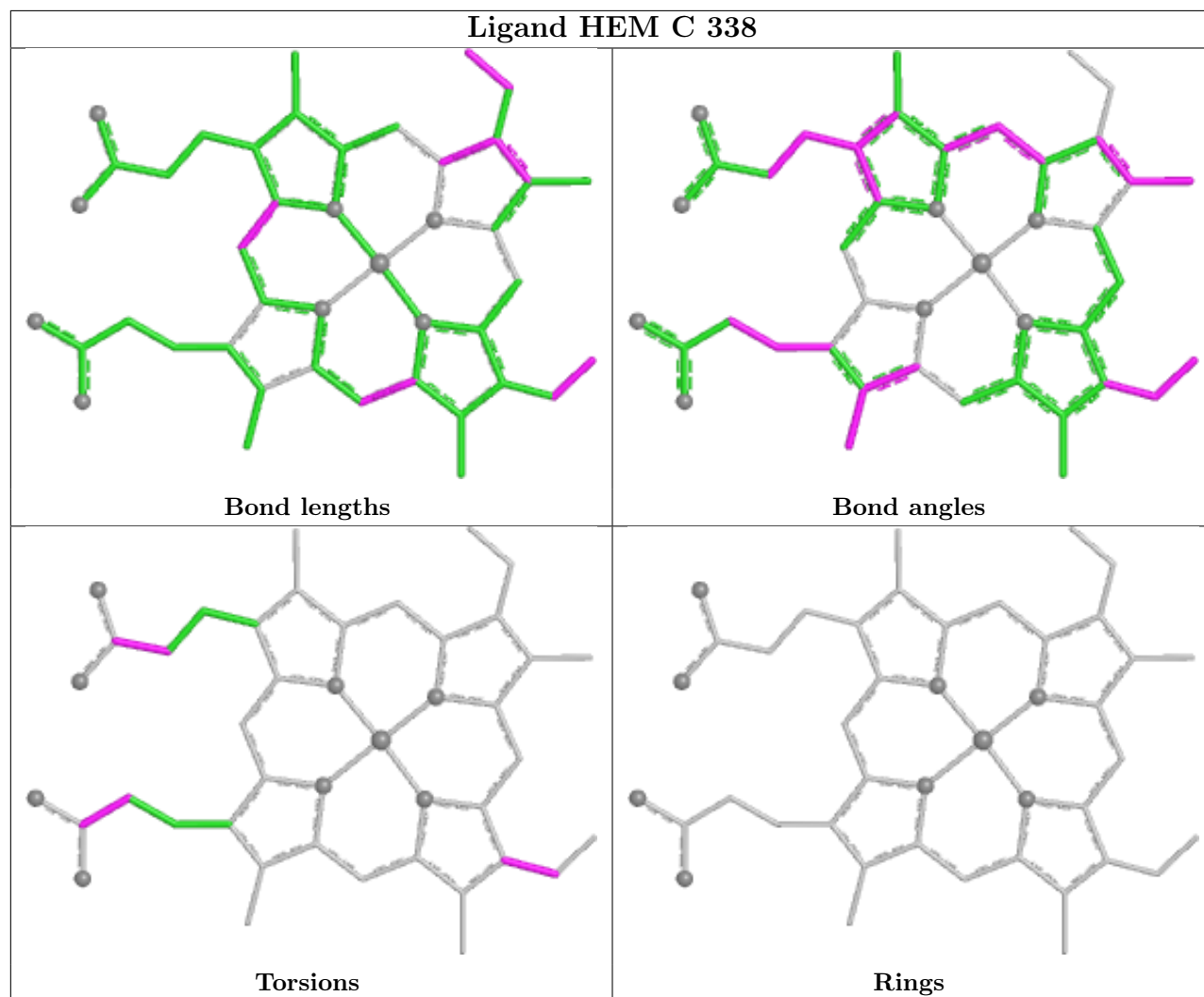
There are no ring outliers.

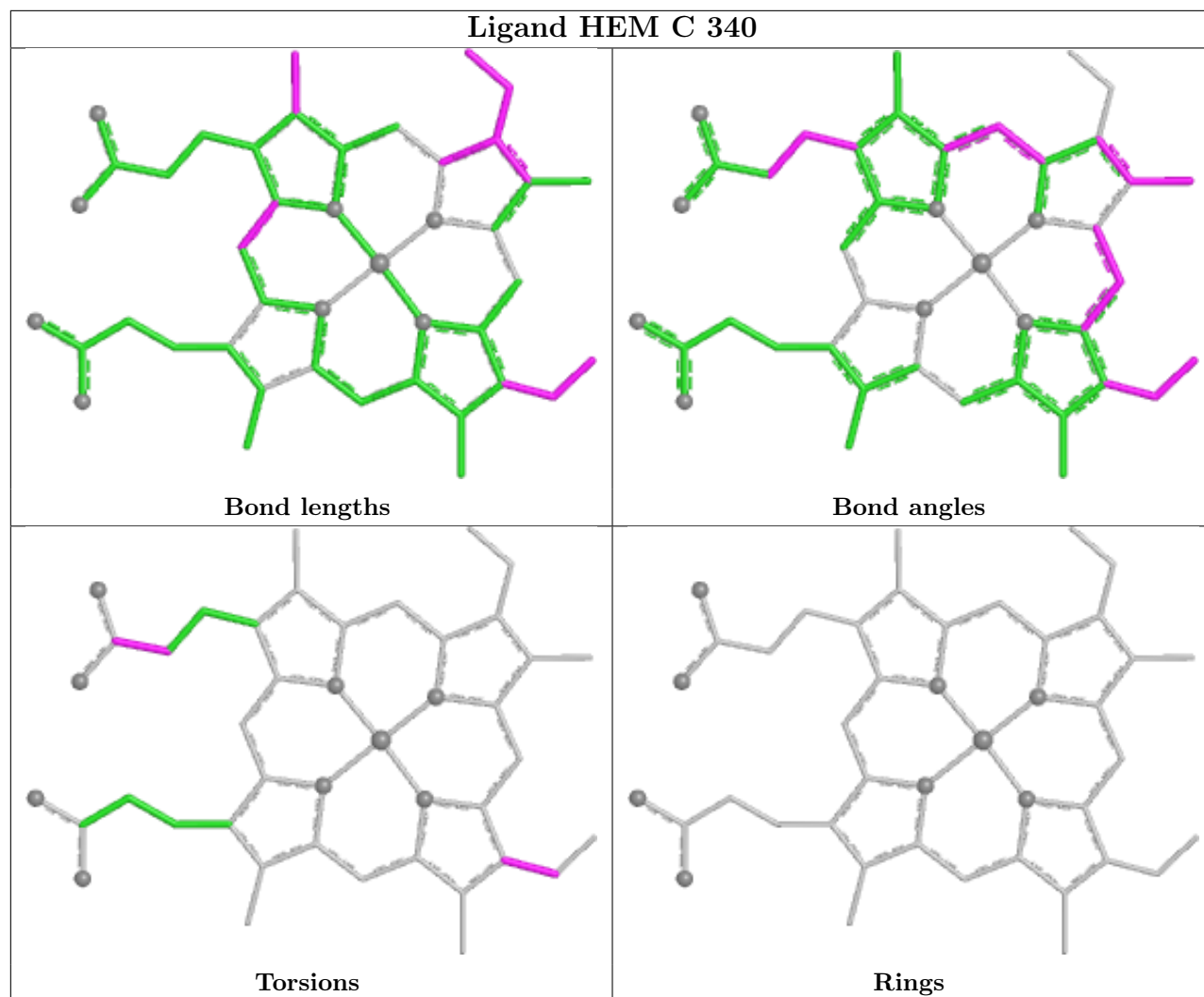
14 monomers are involved in 51 short contacts:

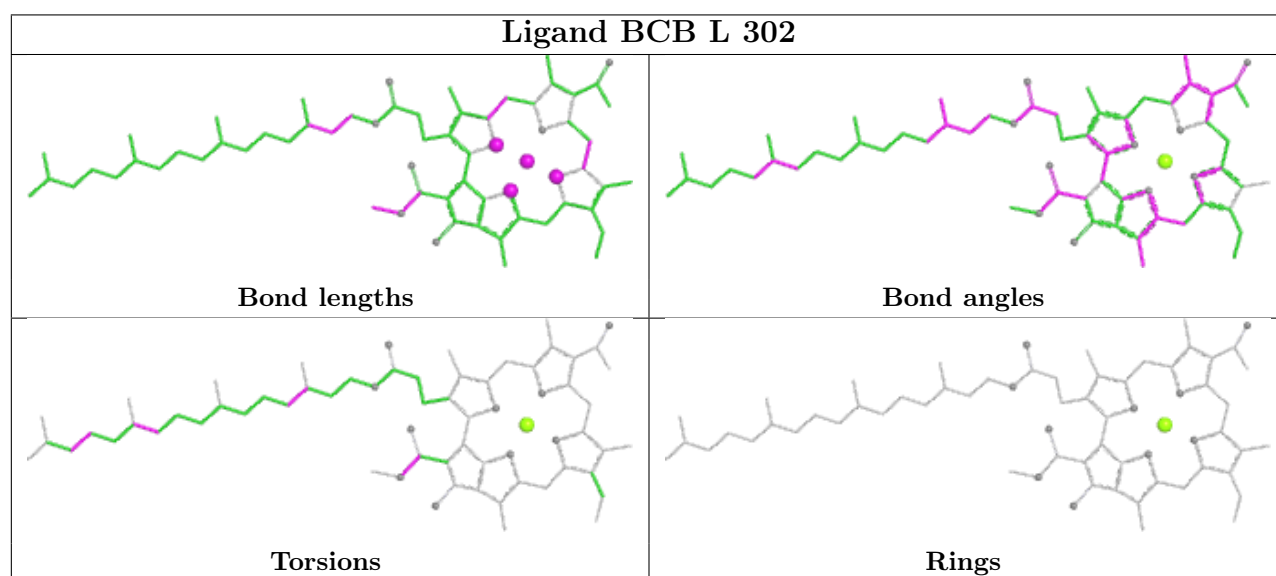
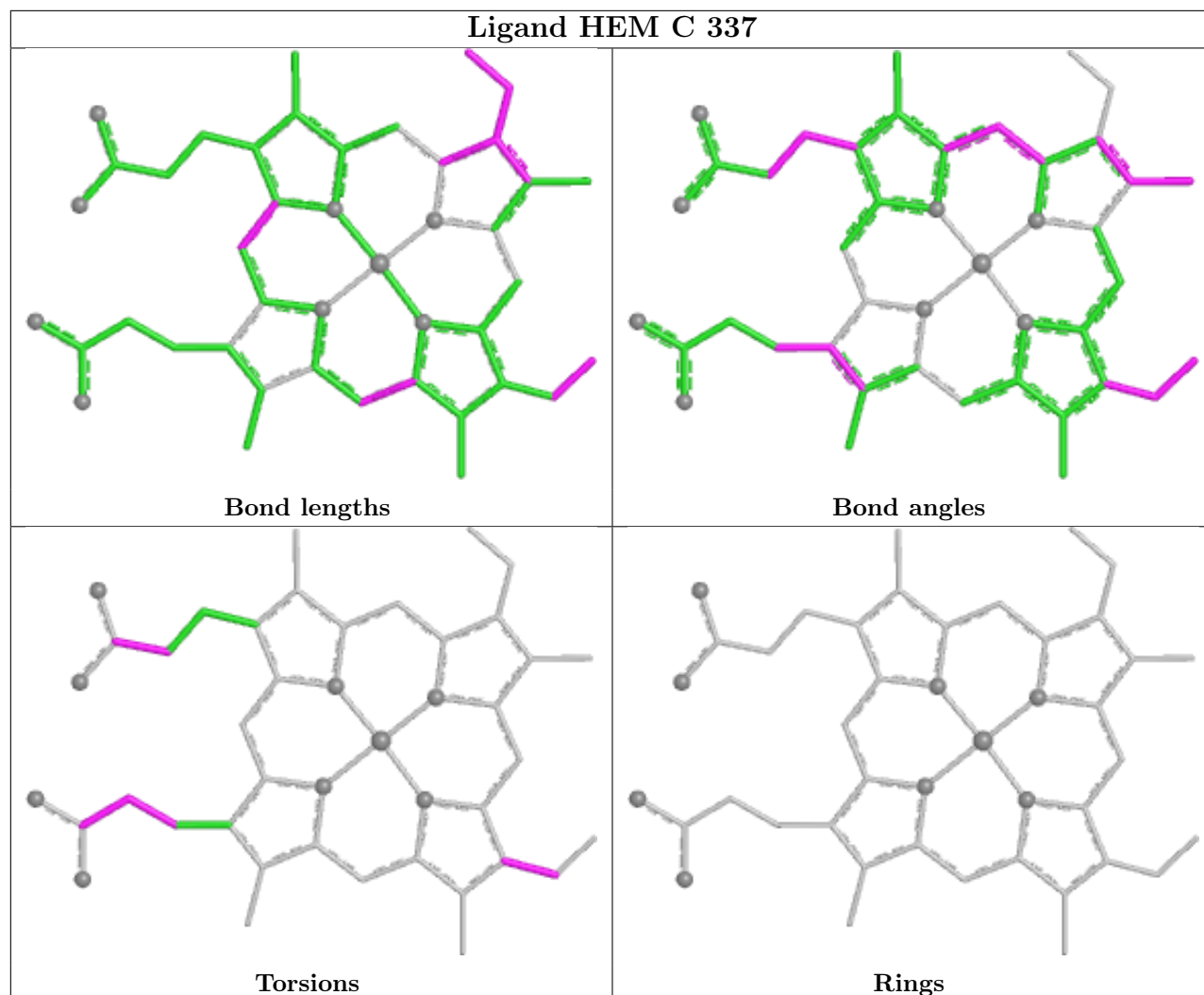
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	338	HEM	2	0
6	L	302	BCB	6	0
6	L	304	BCB	7	0
8	L	502	UQ2	2	0
7	L	402	BPB	6	0
7	M	401	BPB	8	0
9	H	703	LDA	1	0
5	C	339	HEM	1	0
12	M	501	MQ7	1	0
13	M	600	NS5	6	0
9	M	706	LDA	1	0
6	M	806	BCB	7	0
9	M	704	LDA	1	0
6	M	805	BCB	6	0

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

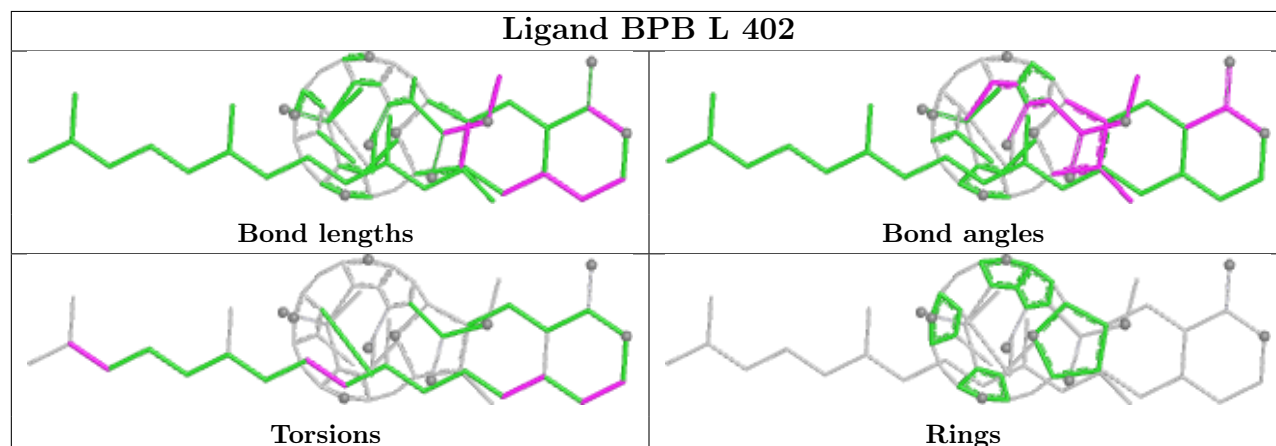
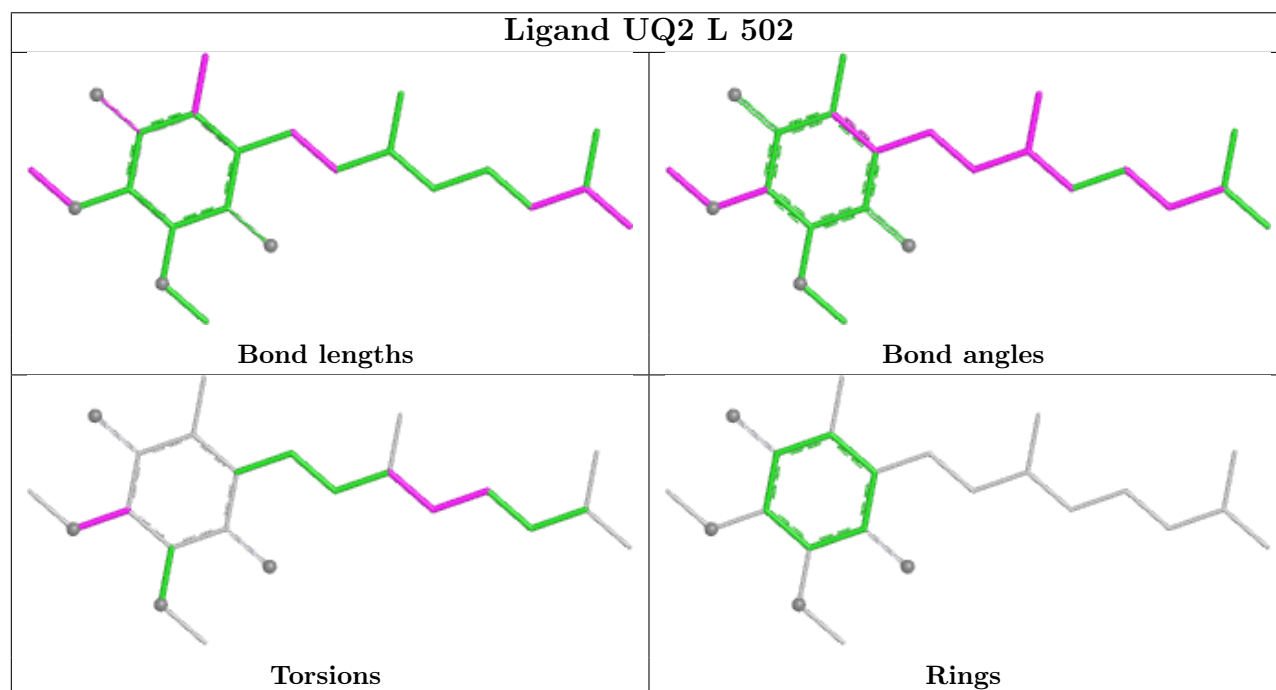
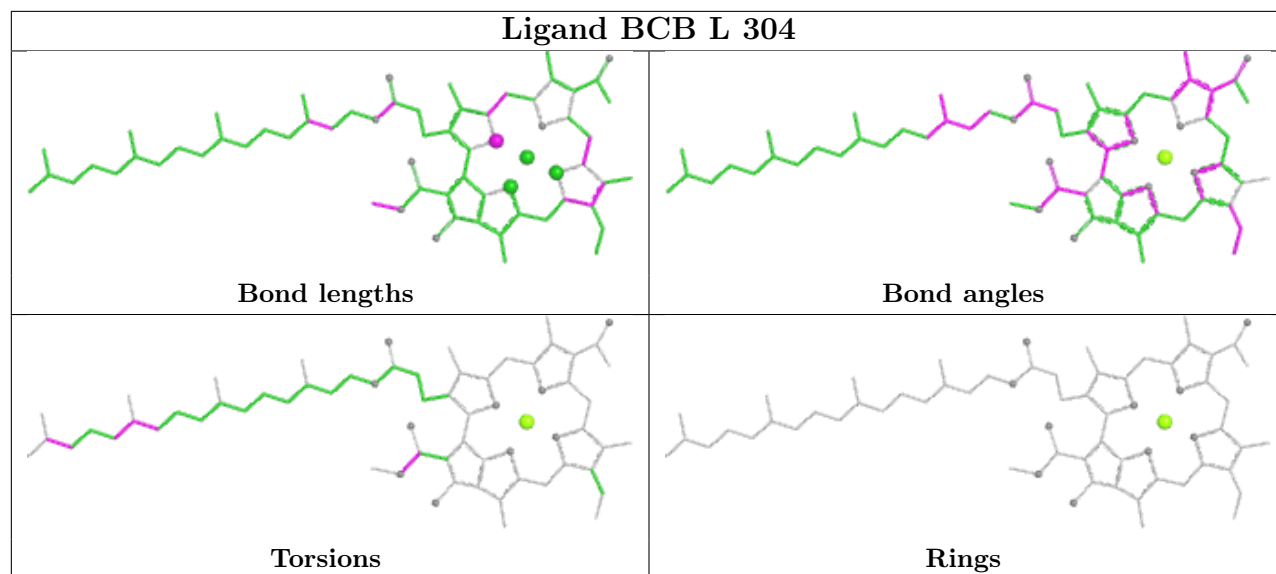
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

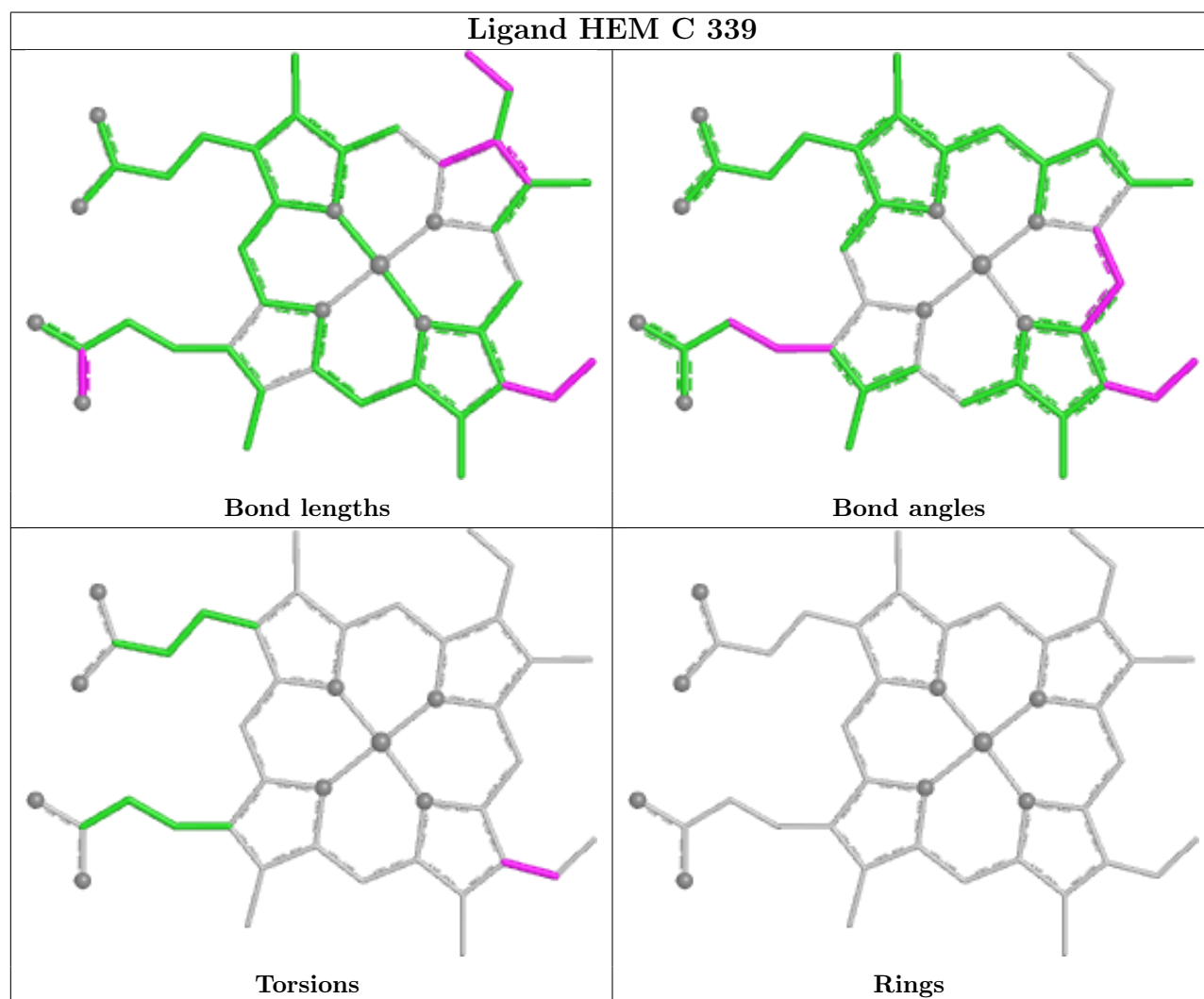
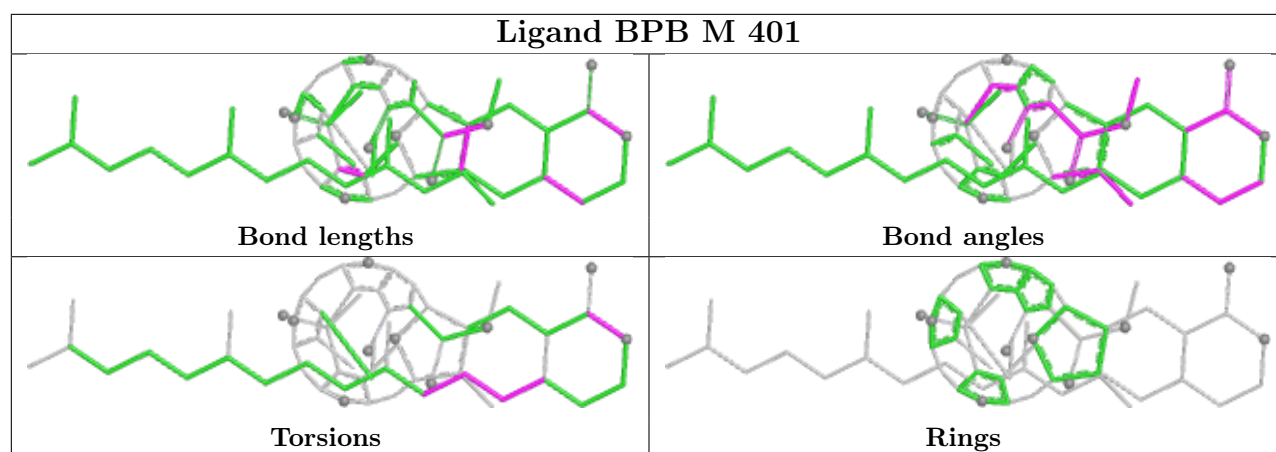



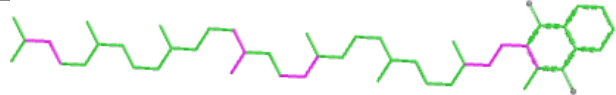

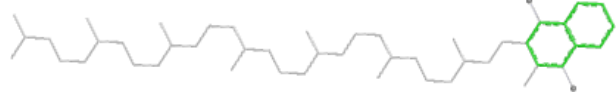
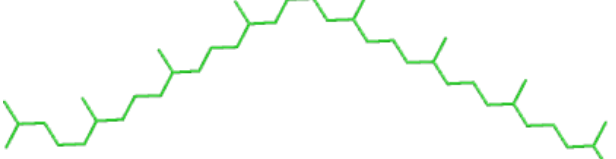
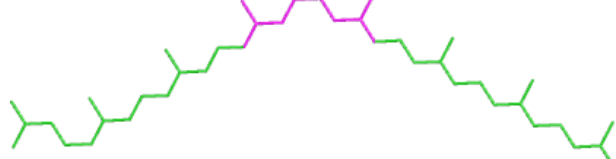
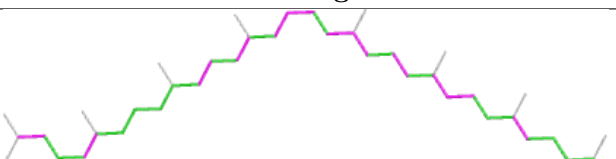
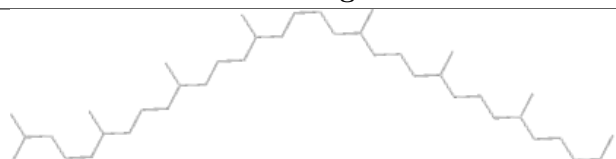
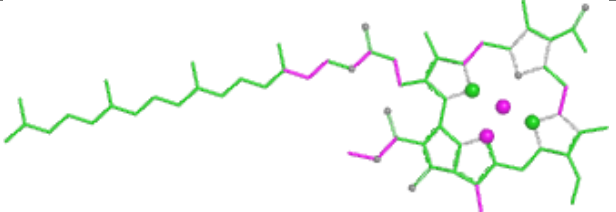
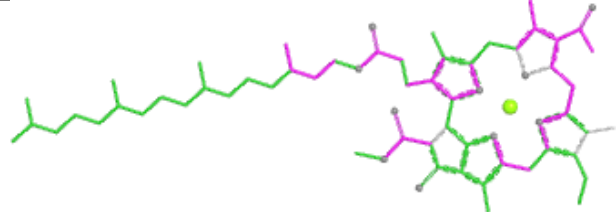
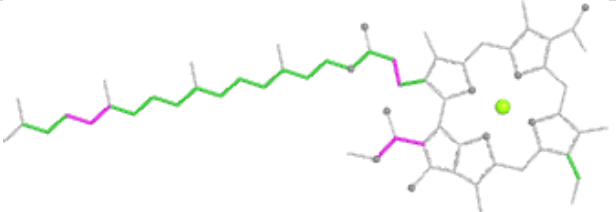
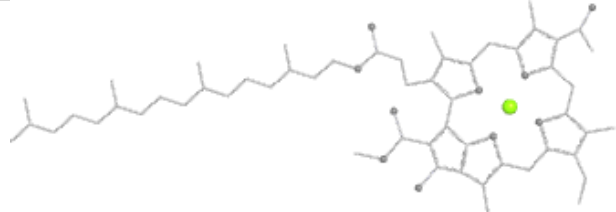


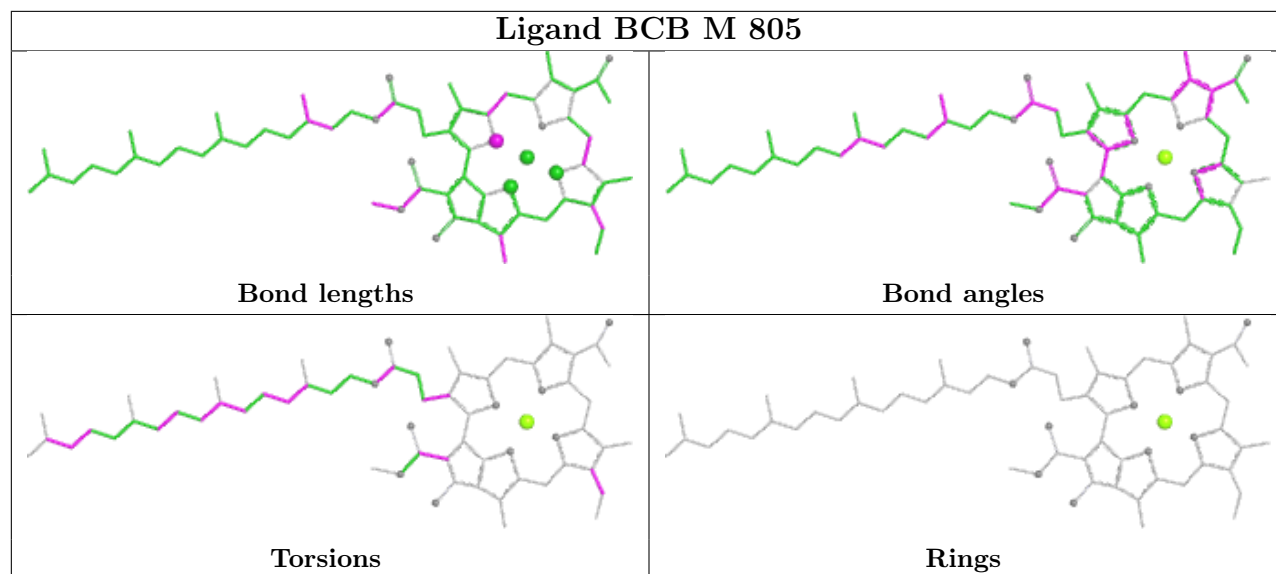








Ligand MQ7 M 501	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand NS5 M 600	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCB M 806	
 Bond lengths	 Bond angles
 Torsions	 Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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%)	-0.93	0	100 100	9, 26, 46, 65	23 (6%)
2	L	273/273 (100%)	-1.04	0	100 100	10, 21, 43, 60	8 (2%)
3	M	323/323 (100%)	-0.93	0	100 100	8, 23, 50, 65	12 (3%)
4	H	249/258 (96%)	-0.68	4 (1%)	70 72	12, 31, 52, 64	21 (8%)
All	All	1177/1190 (98%)	-0.90	4 (0%)	90 91	8, 25, 48, 65	64 (5%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	54	PRO	3.7
4	H	82	ARG	3.4
4	H	55	GLU	2.3
4	H	8	GLN	2.1

### 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
4	FME	H	1	10/11	0.97	0.05	30,34,36,40	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

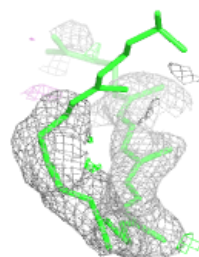
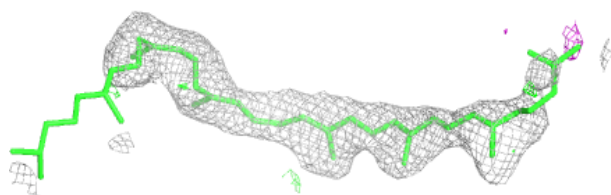
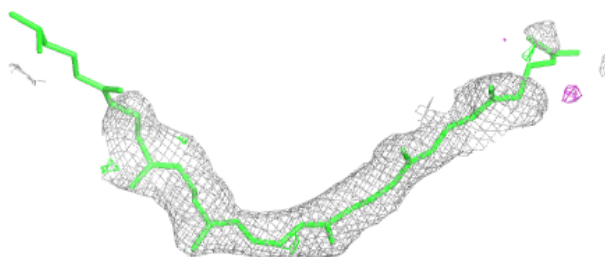
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
9	LDA	L	705	16/16	0.79	0.11	54,55,60,62	5
9	LDA	M	704	16/16	0.83	0.14	56,60,79,79	0
9	LDA	M	706	16/16	0.86	0.11	60,64,68,68	4
9	LDA	M	702	16/16	0.91	0.10	17,49,67,67	0
9	LDA	H	703	16/16	0.92	0.09	33,39,60,61	0
11	SO4	M	803	5/5	0.92	0.10	77,77,79,79	0
13	NS5	M	600	40/40	0.92	0.08	32,42,52,53	14
8	UQ2	L	502	23/23	0.93	0.06	21,25,38,40	0
11	SO4	H	801	5/5	0.94	0.07	61,62,64,64	0
9	LDA	M	701	16/16	0.95	0.05	26,29,31,31	0
6	BCB	M	805	66/66	0.96	0.06	11,19,48,49	0
12	MQ7	M	501	48/48	0.97	0.05	13,19,39,42	0
7	BPB	M	401	65/65	0.97	0.06	8,24,59,61	7
5	HEM	C	337	43/43	0.98	0.05	23,29,34,41	0
6	BCB	M	806	66/66	0.98	0.04	3,13,30,32	0
11	SO4	M	804	5/5	0.98	0.05	46,48,48,48	0
7	BPB	L	402	65/65	0.98	0.04	2,10,17,20	0
6	BCB	L	302	66/66	0.98	0.04	2,12,17,22	0
6	BCB	L	304	66/66	0.98	0.04	7,14,29,34	0
5	HEM	C	340	43/43	0.99	0.05	13,21,30,39	0
5	HEM	C	338	43/43	0.99	0.04	15,27,31,32	0
11	SO4	M	802	5/5	0.99	0.05	34,34,36,38	0
5	HEM	C	339	43/43	0.99	0.04	10,17,25,30	0
10	FE2	M	500	1/1	1.00	0.01	18,18,18,18	0

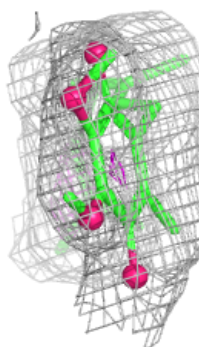
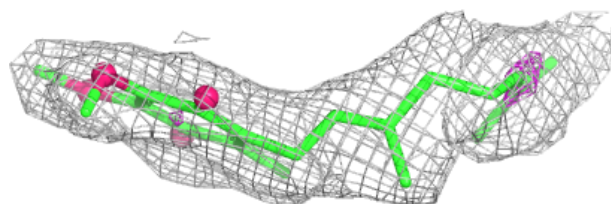
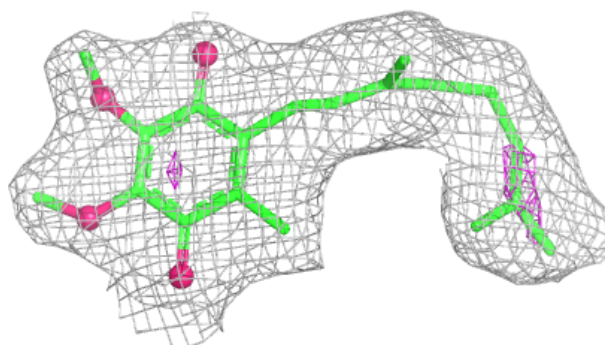
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

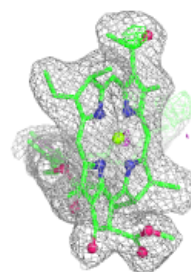
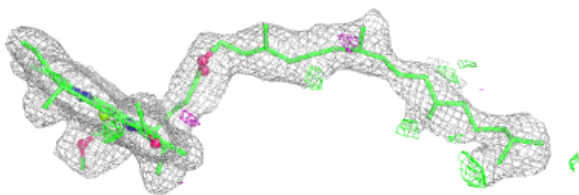
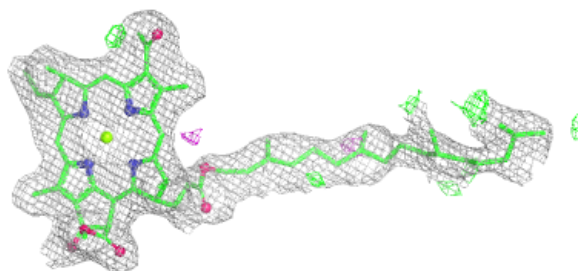
**Electron density around UQ2 L 502:**

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

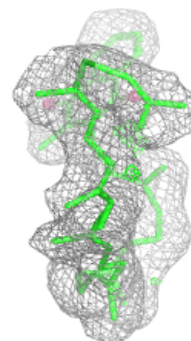
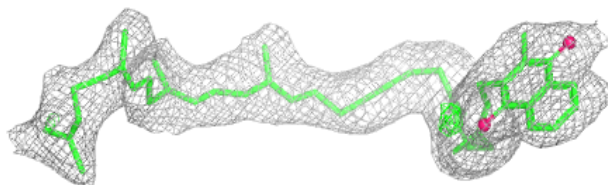
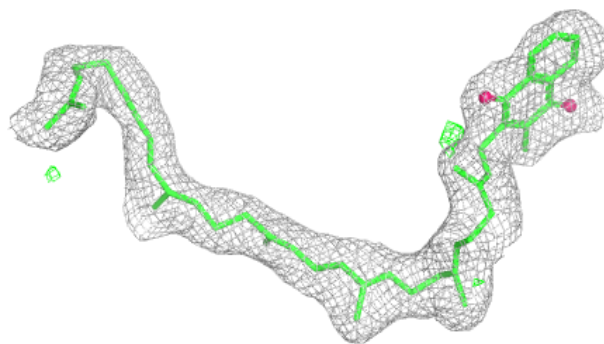


**Electron density around BCB M 805:**

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

**Electron density around MQ7 M 501:**

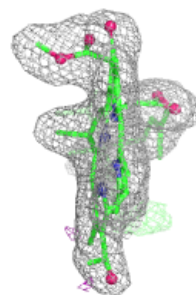
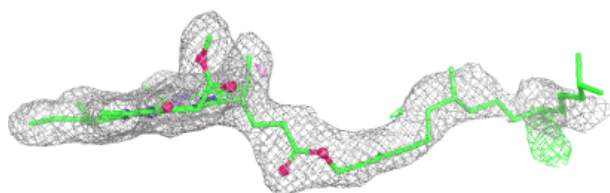
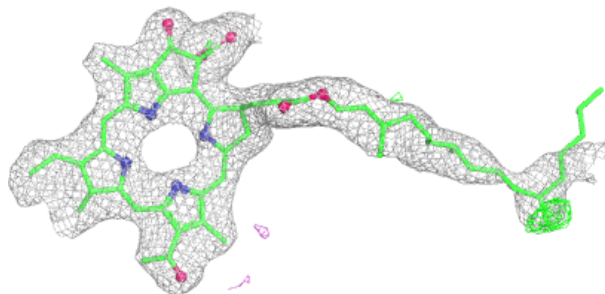
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





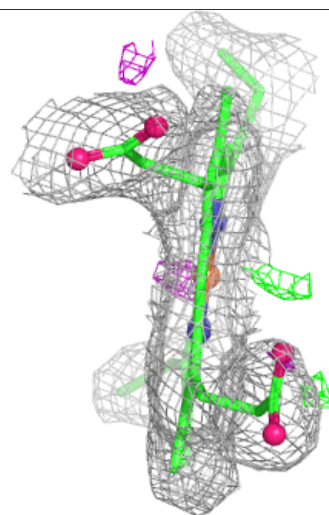
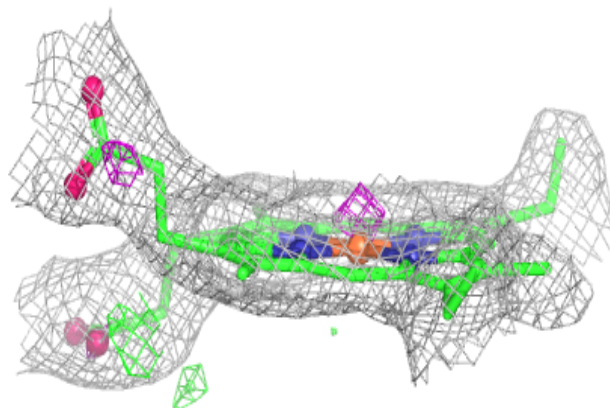
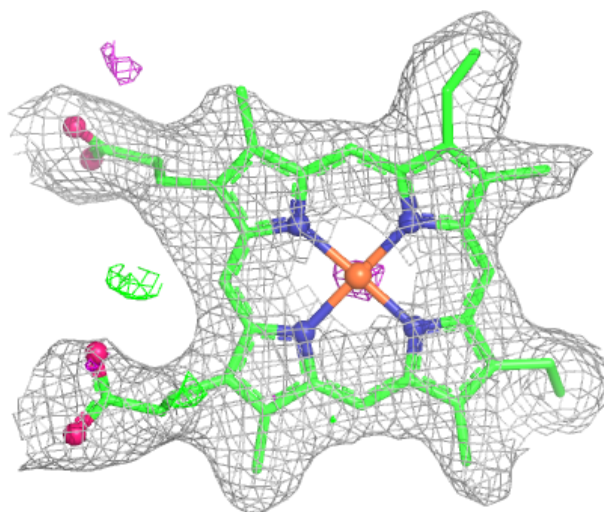
**Electron density around BPB M 401:**

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



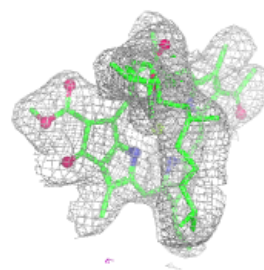
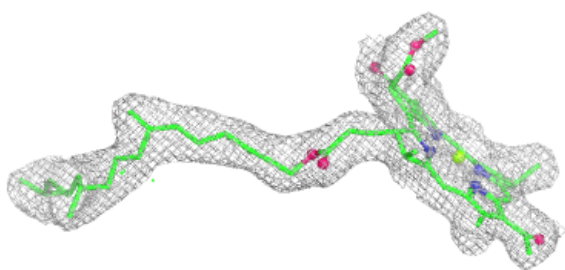
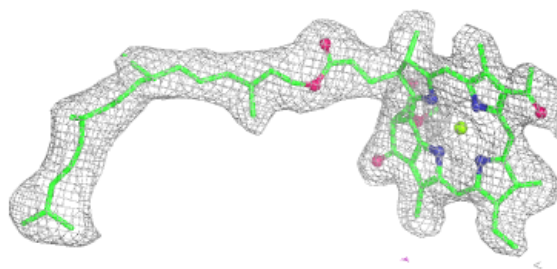
**Electron density around HEM C 337:**

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



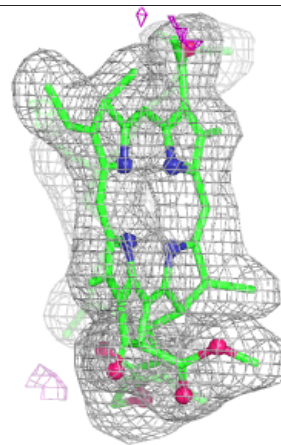
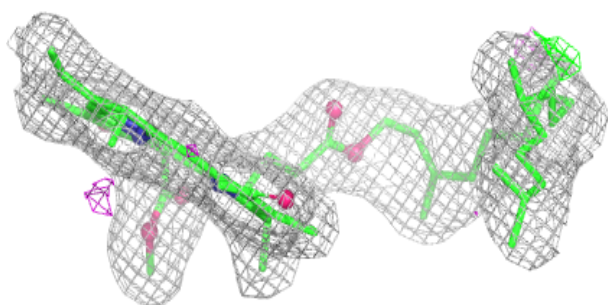
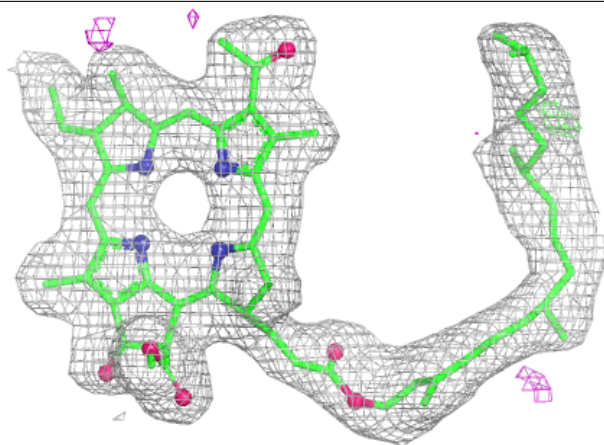
**Electron density around BCB M 806:**

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



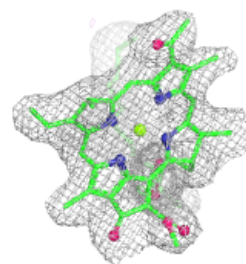
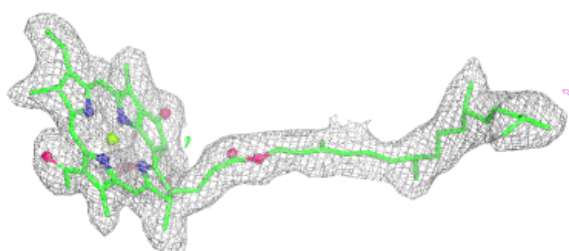
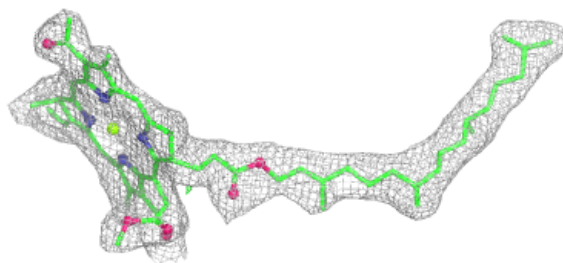
**Electron density around BPB L 402:**

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

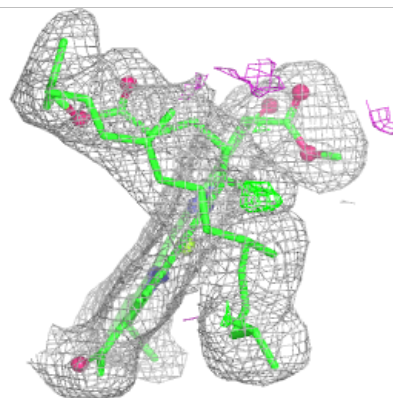
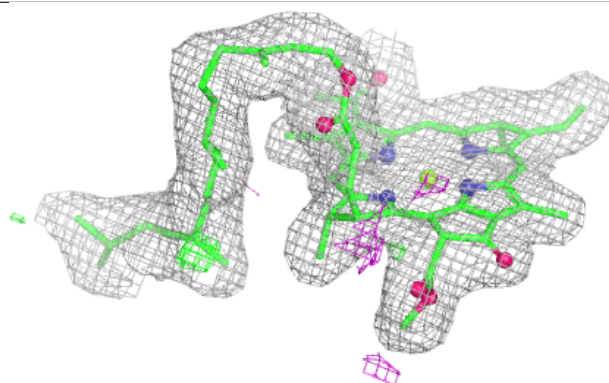
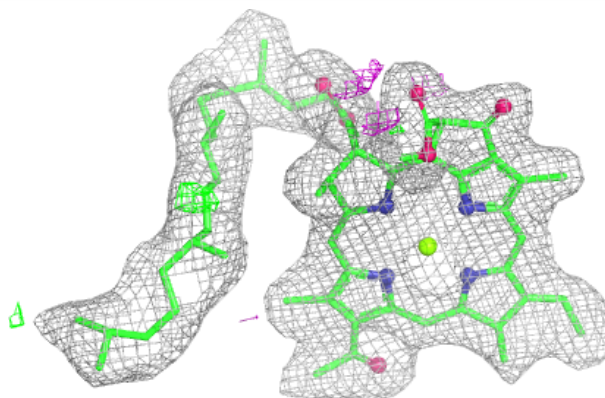


**Electron density around BCB L 302:**

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

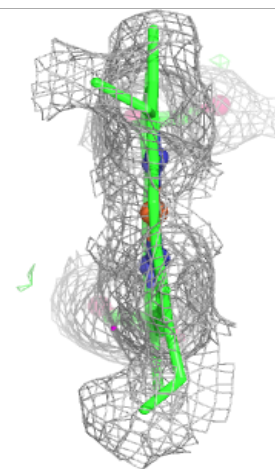
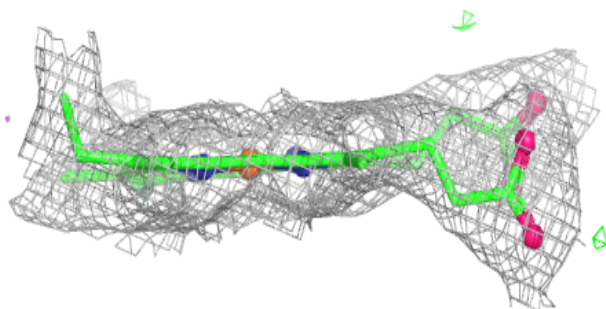
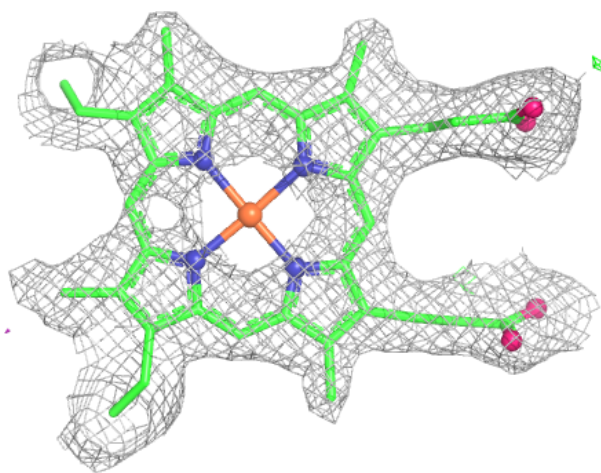
**Electron density around BCB L 304:**

$2mF_o-DF_c$  (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:**

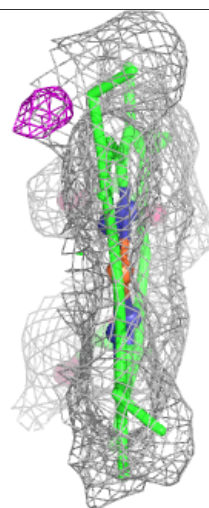
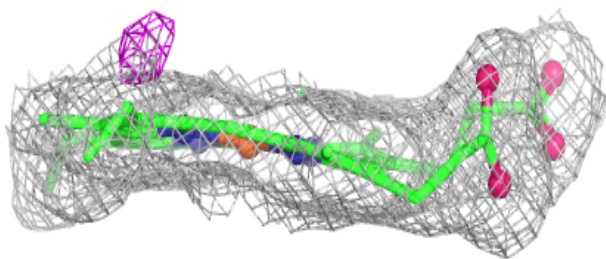
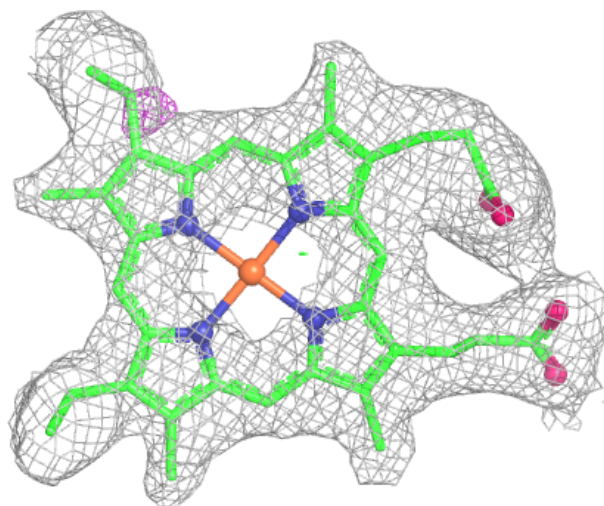
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

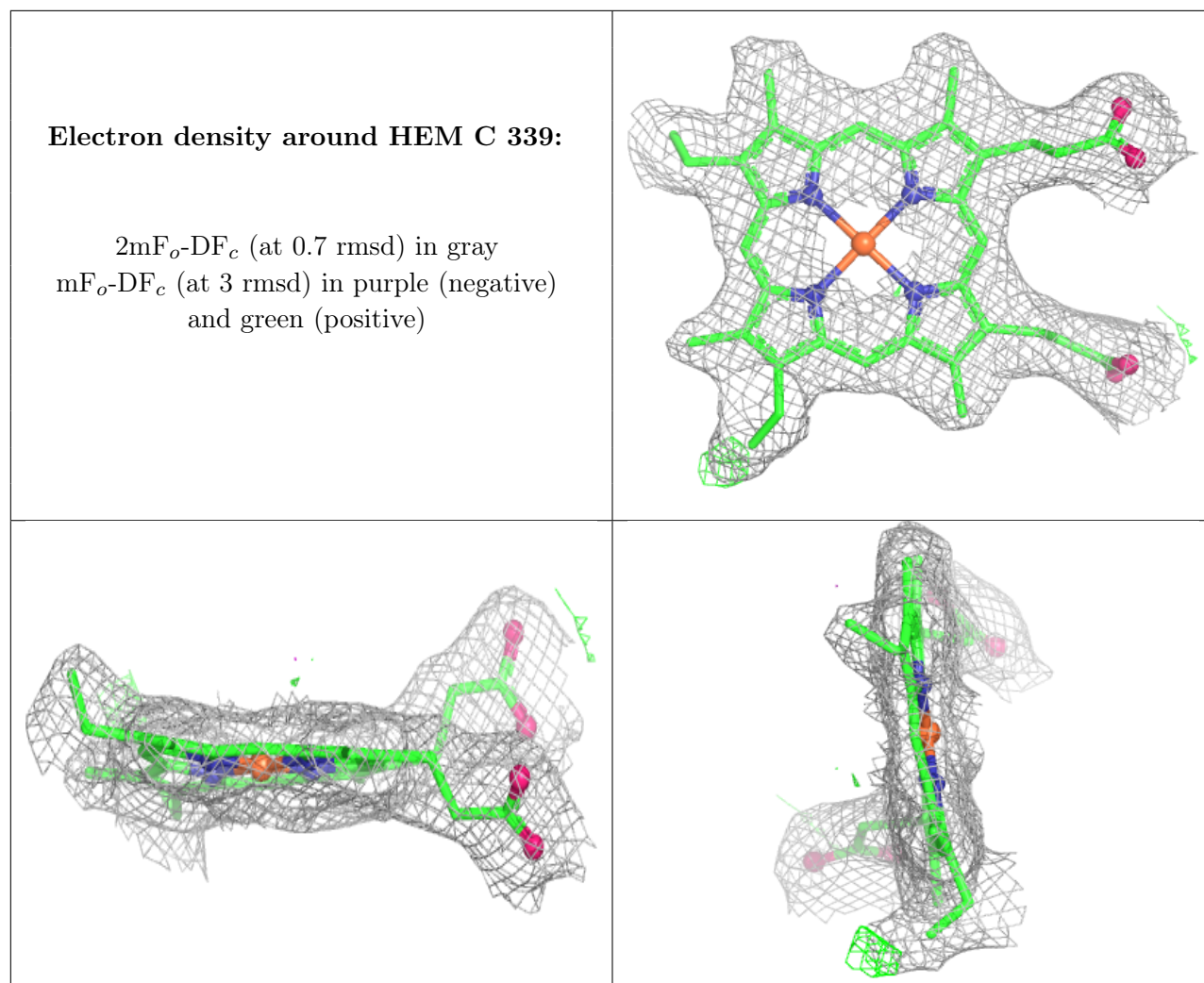




**Electron density around HEM C 338:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.