



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:34 am BST

PDB ID : 3PRC  
Title : PHOTOSYNTHETIC REACTION CENTER FROM RHODOPSEUDOMONAS VIRIDIS (QB-DEPLETED)  
Authors : Lancaster, C.R.D.; Michel, H.  
Deposited on : 1997-07-29  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.11  
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) : 2.11

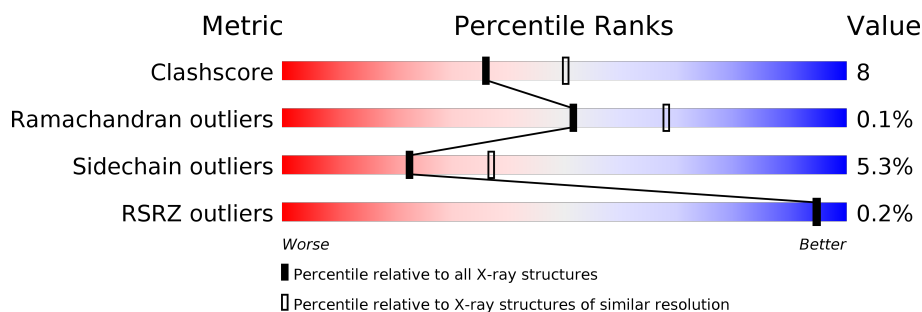
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on 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	
2	L	273	
3	M	323	
4	H	258	

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 10606 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	38	1	0
			2607	1642	467	480	18			

- 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	14	1	0
			2566	1711	420	424	11			

- Molecule 4 is a protein called PHOTOSYNTHETIC REACTION CENTER.

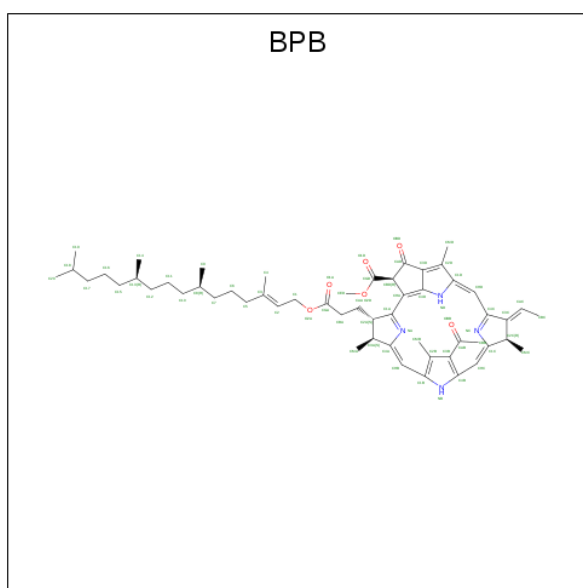
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	258	Total	C	N	O	S	129	1	0
			2028	1298	345	382	3			

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



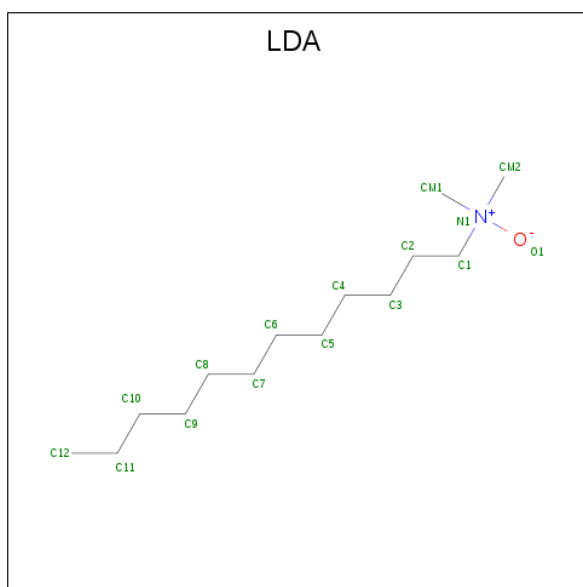
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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

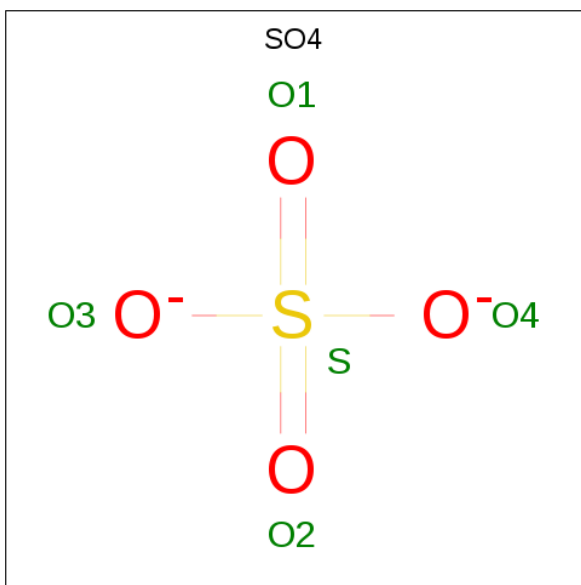


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	L	1	Total	C	N	O	0	0
			16	14	1	1		
8	L	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	3	0
			16	14	1	1		
8	M	1	Total	C	N	O	5	0
			16	14	1	1		
8	M	1	Total	C	N	O	4	0
			16	14	1	1		
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	H	1	Total	C	N	O	1	0
			16	14	1	1		

- Molecule 9 is FE (II) ION (three-letter code: FE2) (formula: Fe).

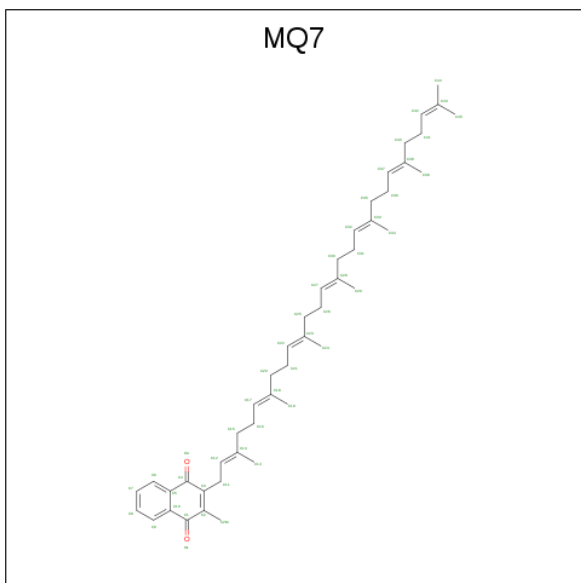
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	1	Total	Fe	0	0
			1	1		

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



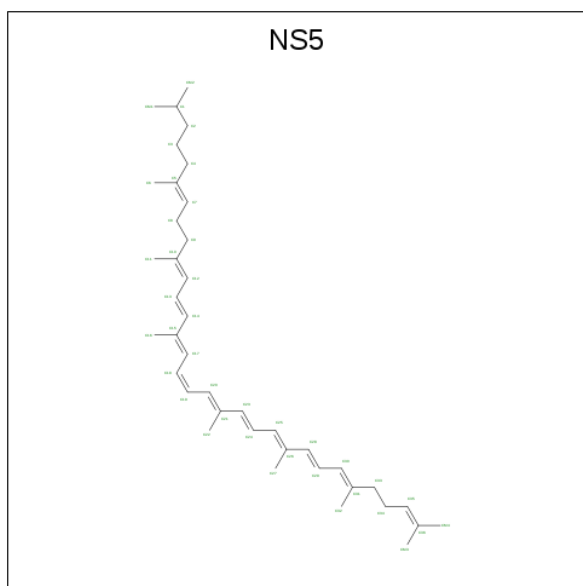
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	O	S	0	0
			5	4	1		
10	M	1	Total	O	S	0	0
			5	4	1		
10	M	1	Total	O	S	0	0
			5	4	1		
10	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 11 is MENAQUINONE-7 (three-letter code: MQ7) (formula:  $C_{46}H_{64}O_2$ ).



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

- Molecule 12 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
12	M	1	Total	C	9	0
			40	40		

- Molecule 13 is water.

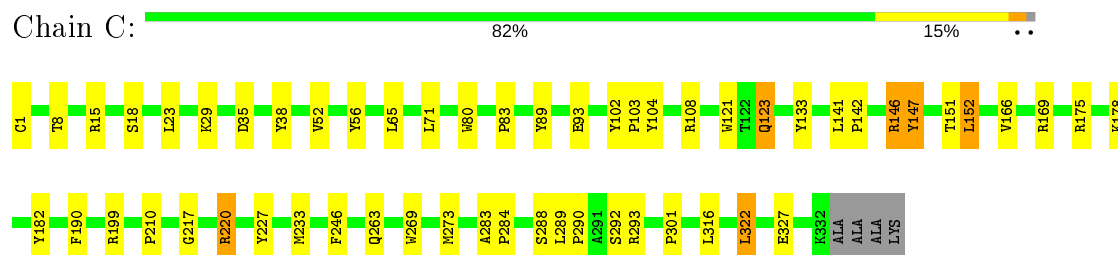
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	C	163	Total	O	0	0
			163	163		
13	L	65	Total	O	0	0
			65	65		
13	M	97	Total	O	0	0
			97	97		
13	H	100	Total	O	0	0
			100	100		



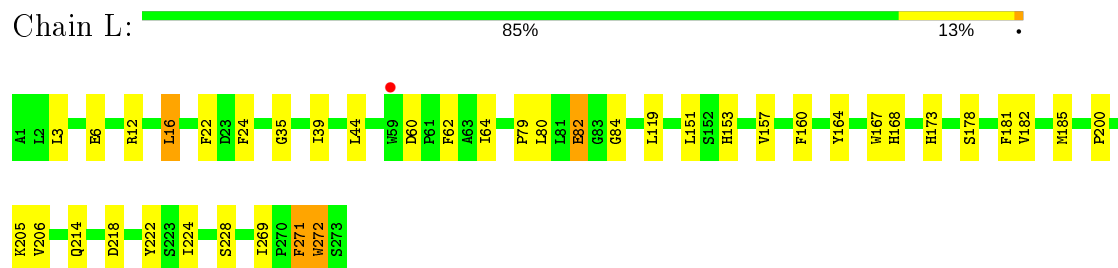
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

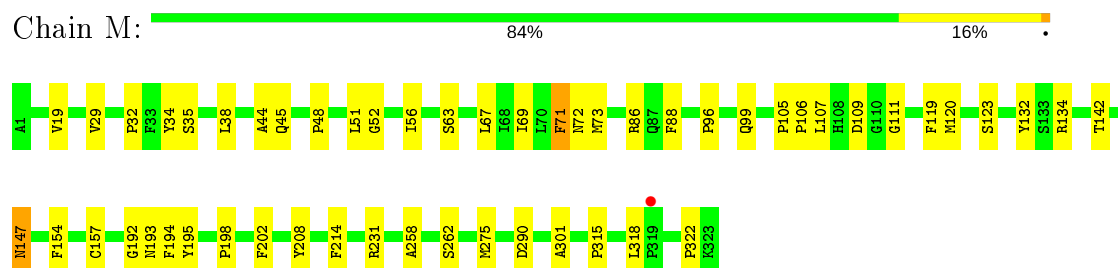
#### • Molecule 1: PHOTOSYNTHETIC REACTION CENTER



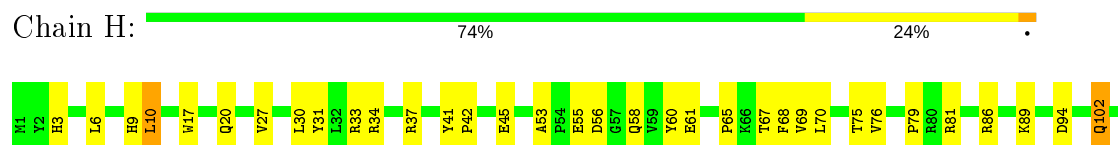
#### • Molecule 2: PHOTOSYNTHETIC REACTION CENTER



#### • 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, $\alpha$ , $\beta$ , $\gamma$	223.50 Å   223.50 Å   113.60 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	10.00 – 2.40 27.62 – 2.40	Depositor EDS
% Data completeness (in resolution range)	79.5 (10.00-2.40) 79.5 (27.62-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 2.39 Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.178 ,   0.215 0.170 ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.3	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 89.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10606	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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: LDA, BPB, BCB, FE2, SO4, MQ7, HEM, FME, 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	0.51	0/2674	0.60	0/3645
2	L	0.53	0/2281	0.57	0/3112
3	M	0.52	0/2671	0.58	0/3653
4	H	0.53	0/2055	0.71	3/2807 (0.1%)
All	All	0.52	0/9681	0.61	3/13217 (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	5
2	L	0	1
3	M	0	1
All	All	0	7

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	53	ALA	CB-CA-C	-11.82	92.36	110.10
4	H	45	GLU	CB-CA-C	-7.85	94.70	110.40
4	H	53	ALA	N-CA-C	7.52	131.30	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	147	TYR	Sidechain
1	C	182	TYR	Sidechain
1	C	190	PHE	Sidechain
1	C	227	TYR	Sidechain
1	C	89	TYR	Sidechain
2	L	164	TYR	Sidechain
3	M	119	PHE	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	33	0
2	L	2193	0	2122	31	0
3	M	2566	0	2460	37	0
4	H	2028	0	2029	38	0
5	C	172	0	120	1	0
6	L	132	0	144	9	0
6	M	132	0	144	13	0
7	L	65	0	74	5	0
7	M	65	0	74	12	0
8	H	32	0	62	0	0
8	L	32	0	62	10	0
8	M	48	0	93	2	0
9	M	1	0	0	0	0
10	H	5	0	0	0	0
10	M	15	0	0	0	0
11	M	48	0	64	0	0
12	M	40	0	60	0	0
13	C	163	0	0	5	0
13	H	100	0	0	2	0
13	L	65	0	0	2	0
13	M	97	0	0	0	0
All	All	10606	0	10083	157	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 8.

All (157) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:402:BPB:HHC	7:L:402:BPB:HBBB	1.53	0.89
7:M:401:BPB:HHC	7:M:401:BPB:HBBB	1.50	0.89
6:M:805:BCB:HHC	6:M:805:BCB:HBB2	1.58	0.82
1:C:121:TRP:HA	1:C:123[A]:GLN:HE21	1.43	0.81
7:L:402:BPB:HHC	7:L:402:BPB:CBB	2.10	0.81
3:M:29:VAL:HG21	3:M:51:LEU:HD22	1.64	0.79
1:C:152:LEU:HD22	1:C:175:ARG:HA	1.66	0.75
2:L:79:PRO:HG2	2:L:82:GLU:HG3	1.72	0.71
6:M:806:BCB:HBD	6:M:806:BCB:HAA2	1.74	0.69
1:C:123[A]:GLN:HG3	1:C:269:TRP:CE3	2.28	0.69
2:L:178:SER:O	2:L:182:VAL:HG23	1.95	0.67
2:L:181:PHE:HB3	7:M:401:BPB:CBB	2.24	0.66
4:H:55:GLU:HB2	4:H:58:GLN:HG3	1.78	0.65
1:C:217:GLY:O	1:C:220:ARG:HG3	1.97	0.65
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.33	0.64
8:L:707:LDA:HM23	13:L:761:HOH:O	1.99	0.63
3:M:71:PHE:HB3	8:M:706:LDA:H62	1.80	0.63
1:C:290:PRO:HG2	1:C:293:ARG:HG2	1.81	0.62
6:M:805:BCB:CBB	6:M:805:BCB:HHC	2.30	0.62
4:H:160:ALA:HB3	4:H:214:LEU:HD23	1.80	0.62
1:C:152:LEU:HD21	1:C:178:LYS:HG3	1.82	0.62
1:C:121:TRP:HA	1:C:123[A]:GLN:NE2	2.13	0.62
4:H:161:ASP:HB3	4:H:214:LEU:HD22	1.81	0.62
8:L:702:LDA:HM23	13:L:772:HOH:O	1.98	0.61
2:L:181:PHE:HB3	7:M:401:BPB:HBBA	1.81	0.61
3:M:315:PRO:HA	3:M:318:LEU:HG	1.82	0.60
4:H:117:TYR:HB2	4:H:236:ASP:HB3	1.85	0.59
2:L:62:PHE:HE2	8:L:702:LDA:HM21	1.66	0.59
1:C:65:LEU:HD11	1:C:327:GLU:HG2	1.85	0.59
2:L:218:ASP:HB3	3:M:134:ARG:HD2	1.85	0.59
3:M:32:PRO:HG3	3:M:48:PRO:HD3	1.83	0.59
3:M:63:SER:O	3:M:67:LEU:HG	2.03	0.58
3:M:29:VAL:CG2	3:M:51:LEU:HD22	2.34	0.58
3:M:231:ARG:HD2	13:H:812:HOH:O	2.03	0.57
7:M:401:BPB:CHC	7:M:401:BPB:HBBB	2.28	0.57
2:L:12:ARG:HD3	4:H:102:GLN:NE2	2.19	0.57
2:L:62:PHE:CE2	8:L:702:LDA:HM21	2.40	0.57
2:L:181:PHE:CD2	7:M:401:BPB:HBB	2.40	0.56
6:L:304:BCB:HMB1	6:L:304:BCB:HBB2	1.87	0.56
3:M:202:PHE:CE2	4:H:20:GLN:HG2	2.40	0.56
6:L:304:BCB:HMB2	7:L:402:BPB:HMBA	1.88	0.56
2:L:35:GLY:O	2:L:39:ILE:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:702:LDA:H32	13:H:894:HOH:O	2.06	0.56
3:M:96:PRO:HG3	3:M:105:PRO:HB3	1.87	0.56
2:L:153:HIS:O	2:L:157:VAL:HG23	2.06	0.55
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.42	0.55
2:L:80:LEU:HA	2:L:84:GLY:HA3	1.88	0.55
6:M:805:BCB:H61	7:M:401:BPB:HMA	1.89	0.54
4:H:136:PRO:HG2	4:H:139:VAL:HG23	1.90	0.54
4:H:6:LEU:HB2	4:H:10:LEU:HB3	1.89	0.54
2:L:185:MET:SD	6:M:805:BCB:H41	2.47	0.53
6:M:806:BCB:H203	7:M:401:BPB:H4B	1.91	0.53
6:M:806:BCB:HAA2	6:M:806:BCB:CBD	2.34	0.53
2:L:200:PRO:HG3	2:L:205:LYS:O	2.08	0.53
1:C:210:PRO:HB2	4:H:3:HIS:HD2	1.74	0.53
4:H:56:ASP:HB3	4:H:60:TYR:CE2	2.44	0.53
3:M:275:MET:HG2	7:M:401:BPB:HBCA	1.90	0.53
4:H:86:ARG:NH2	4:H:111:ALA:O	2.37	0.53
6:L:302:BCB:HBB3	6:L:302:BCB:HMB1	1.89	0.53
4:H:136:PRO:HG2	4:H:138:ARG:HG2	1.92	0.52
4:H:233:ARG:HG3	4:H:233:ARG:O	2.09	0.52
1:C:147:TYR:OH	1:C:301:PRO:HG3	2.10	0.52
8:L:702:LDA:H71	3:M:301:ALA:CB	2.40	0.52
4:H:190:SER:HB3	4:H:192:ARG:HG2	1.90	0.51
6:L:302:BCB:OBB	6:L:302:BCB:HHC	2.09	0.51
2:L:214:GLN:NE2	3:M:19:VAL:H	2.08	0.51
4:H:86:ARG:NH2	4:H:111:ALA:HB3	2.25	0.51
6:L:304:BCB:HMB1	6:L:304:BCB:CBB	2.41	0.50
1:C:289:LEU:HD22	1:C:293:ARG:HG3	1.93	0.50
4:H:152:PRO:O	4:H:168:VAL:HB	2.12	0.50
1:C:93:GLU:HB2	13:C:470:HOH:O	2.10	0.50
2:L:182:VAL:HG22	6:M:805:BCB:H12	1.94	0.50
6:L:302:BCB:HMB1	6:L:302:BCB:CBB	2.42	0.49
3:M:99:GLN:OE1	3:M:99:GLN:HA	2.11	0.49
2:L:224:ILE:HG12	2:L:228:SER:HB2	1.93	0.49
1:C:121:TRP:CG	1:C:273:MET:HG3	2.48	0.49
1:C:210:PRO:HB2	4:H:3:HIS:CD2	2.48	0.49
2:L:206:VAL:HG21	4:H:68:PHE:HB3	1.93	0.49
3:M:147:ASN:HD22	7:M:401:BPB:HMDA	1.77	0.49
4:H:65:PRO:HA	4:H:79:PRO:HD2	1.94	0.48
4:H:218:PHE:HA	4:H:221:VAL:HG23	1.95	0.48
3:M:34:TYR:HA	3:M:44:ALA:O	2.14	0.48
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:32:PRO:HB3	3:M:45:GLN:HG3	1.95	0.48
1:C:233:MET:HB3	5:C:339:HEM:C4B	2.49	0.48
3:M:52:GLY:O	3:M:56:ILE:HD12	2.14	0.47
2:L:168:HIS:CE1	6:L:302:BCB:HMC2	2.50	0.47
1:C:220:ARG:NH2	13:C:359:HOH:O	2.47	0.47
3:M:29:VAL:HG21	3:M:51:LEU:CD2	2.40	0.47
2:L:269:ILE:HG22	2:L:271:PHE:HD1	1.79	0.47
7:M:401:BPB:HHC	7:M:401:BPB:CBB	2.31	0.47
1:C:146:ARG:HA	1:C:146:ARG:HD2	1.64	0.47
8:L:702:LDA:H71	3:M:301:ALA:HB2	1.96	0.47
6:M:806:BCB:OBB	6:M:806:BCB:HHC	2.16	0.46
1:C:83:PRO:HD2	13:C:367:HOH:O	2.15	0.46
3:M:132:TYR:CE1	3:M:142:THR:HG21	2.51	0.46
2:L:272:TRP:CE2	3:M:86:ARG:HG3	2.51	0.46
1:C:283:ALA:HB3	1:C:284:PRO:HD3	1.98	0.45
2:L:269:ILE:CG2	2:L:271:PHE:HD1	2.30	0.45
4:H:138:ARG:HG3	4:H:139:VAL:HG23	1.99	0.45
4:H:67:THR:HA	4:H:76:VAL:O	2.16	0.45
4:H:37:ARG:HG2	4:H:41:TYR:CE1	2.52	0.44
3:M:107:LEU:HA	3:M:111:GLY:HA3	1.98	0.44
4:H:34:ARG:HG2	4:H:61:GLU:O	2.17	0.44
1:C:283:ALA:N	1:C:284:PRO:CD	2.81	0.44
2:L:60:ASP:O	2:L:64:ILE:HG13	2.16	0.44
1:C:141:LEU:HD12	1:C:142:PRO:HD2	1.98	0.44
6:L:304:BCB:HHC	6:L:304:BCB:OBB	2.16	0.44
1:C:322:LEU:HA	13:C:469:HOH:O	2.17	0.44
1:C:52:VAL:HB	1:C:56:TYR:CD2	2.53	0.44
7:L:402:BPB:ND	7:L:402:BPB:NC	2.66	0.44
2:L:151:LEU:HD21	8:L:702:LDA:H111	2.00	0.44
1:C:104:TYR:HE1	1:C:108:ARG:NH2	2.16	0.44
4:H:33:ARG:HA	4:H:33:ARG:HD2	1.82	0.44
3:M:35:SER:HB3	3:M:38:LEU:HB3	2.00	0.43
3:M:72:ASN:OD1	8:M:706:LDA:H12	2.18	0.43
4:H:67:THR:CG2	4:H:75:THR:HB	2.47	0.43
2:L:3:LEU:HB2	2:L:6:GLU:HB2	1.99	0.43
3:M:120:MET:HG3	6:M:806:BCB:H172	2.00	0.43
1:C:246:PHE:CZ	1:C:263:GLN:HG2	2.54	0.43
2:L:222:TYR:O	8:L:707:LDA:HM13	2.19	0.43
3:M:195:TYR:CZ	6:M:806:BCB:HMC2	2.53	0.43
3:M:67:LEU:O	3:M:71:PHE:HB2	2.18	0.43
2:L:167:TRP:HE1	2:L:173:HIS:CD2	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:206:VAL:CG2	4:H:68:PHE:HB3	2.48	0.43
3:M:258:ALA:HB1	3:M:262:SER:OG	2.17	0.43
7:L:402:BPB:HBBA	3:M:208:TYR:HB3	2.00	0.43
6:M:805:BCB:H203	6:M:805:BCB:H162	1.92	0.43
1:C:8:THR:HB	1:C:23:LEU:HB2	2.01	0.43
7:M:401:BPB:H4	7:M:401:BPB:H6	1.77	0.43
4:H:27:VAL:O	4:H:31:TYR:HB3	2.19	0.42
1:C:52:VAL:HB	1:C:56:TYR:HD2	1.83	0.42
4:H:86:ARG:HH21	4:H:111:ALA:HB3	1.84	0.42
4:H:138:ARG:CG	4:H:139:VAL:HG23	2.49	0.42
4:H:70:LEU:HD11	4:H:76:VAL:HG23	2.00	0.42
1:C:71:LEU:HD23	1:C:71:LEU:HA	1.88	0.42
3:M:69:ILE:HG22	3:M:73:MET:SD	2.59	0.42
2:L:185:MET:SD	6:M:805:BCB:C4	3.07	0.42
7:M:401:BPB:CHC	7:M:401:BPB:CBB	2.96	0.42
4:H:257:LEU:HA	4:H:257:LEU:HD22	1.80	0.42
6:L:302:BCB:H41	6:L:302:BCB:H62	1.90	0.41
4:H:37:ARG:HG2	4:H:41:TYR:CZ	2.56	0.41
2:L:16:LEU:HA	2:L:16:LEU:HD12	1.71	0.41
4:H:202:ASP:HB3	4:H:209:VAL:HB	2.01	0.41
3:M:192:GLY:O	3:M:193:ASN:HB3	2.20	0.41
1:C:146:ARG:NH2	13:C:344:HOH:O	2.50	0.41
1:C:35:ASP:HB3	1:C:316:LEU:HA	2.03	0.41
3:M:73:MET:HE1	3:M:88:PHE:CE1	2.56	0.41
3:M:198:PRO:HB3	4:H:17:TRP:CZ3	2.56	0.41
4:H:142:ASP:N	4:H:142:ASP:OD1	2.54	0.41
4:H:152:PRO:HD2	4:H:171:LEU:HD11	2.02	0.41
8:L:702:LDA:H62	8:L:702:LDA:H11	2.02	0.40
4:H:198:LEU:O	4:H:201:CYS:HB2	2.21	0.40
2:L:22:PHE:HA	2:L:24:PHE:CE1	2.55	0.40
3:M:106:PRO:HG2	3:M:109:ASP:HB3	2.04	0.40
3:M:120:MET:O	3:M:123:SER:HB3	2.21	0.40
3:M:154:PHE:O	3:M:157:CYS:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	320 (97%)	11 (3%)	0	100	100
2	L	273/273 (100%)	264 (97%)	9 (3%)	0	100	100
3	M	322/323 (100%)	308 (96%)	13 (4%)	1 (0%)	41	55
4	H	256/258 (99%)	247 (96%)	9 (4%)	0	100	100
All	All	1182/1190 (99%)	1139 (96%)	42 (4%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	322	PRO

### 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	281/282 (100%)	264 (94%)	17 (6%)	19	31
2	L	220/218 (101%)	213 (97%)	7 (3%)	39	59
3	M	250/249 (100%)	245 (98%)	5 (2%)	55	74
4	H	212/212 (100%)	189 (89%)	23 (11%)	6	9
All	All	963/961 (100%)	911 (95%)	52 (5%)	22	36

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1	CYS
1	C	15	ARG
1	C	18	SER
1	C	29	LYS
1	C	38	TYR
1	C	123[A]	GLN
1	C	123[B]	GLN
1	C	146	ARG
1	C	151	THR
1	C	152	LEU
1	C	166	VAL
1	C	169	ARG
1	C	199	ARG
1	C	220	ARG
1	C	288	SER
1	C	292	SER
1	C	322	LEU
2	L	16	LEU
2	L	44	LEU
2	L	82	GLU
2	L	119	LEU
2	L	160	PHE
2	L	271	PHE
2	L	272	TRP
3	M	71	PHE
3	M	147	ASN
3	M	194	PHE
3	M	214	PHE
3	M	290	ASP
4	H	9	HIS
4	H	10	LEU
4	H	30	LEU
4	H	42	PRO
4	H	69	VAL
4	H	81	ARG
4	H	89	LYS
4	H	94	ASP
4	H	102	GLN
4	H	141	THR
4	H	147	GLU
4	H	169	THR
4	H	178	HIS
4	H	185	LEU

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Mol	Chain	Res	Type
4	H	198	LEU
4	H	205	LYS
4	H	212	SER
4	H	226	SER
4	H	227	ARG
4	H	233	ARG
4	H	236	ASP
4	H	257	LEU
4	H	258	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	37	GLN
1	C	302	GLN
2	L	183	ASN
2	L	214	GLN
2	L	239	ASN
3	M	16	HIS
3	M	147	ASN
4	H	102	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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[B]	4	8,9,10	0.60	0	7,9,11	2.95	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FME	H	1[A]	4	8,9,10	0.68	0	7,9,11	2.23	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[B]	4	-	4/7/9/11	-
4	FME	H	1[A]	4	-	3/7/9/11	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1[B]	FME	CA-N-CN	-5.33	114.62	122.82
4	H	1[B]	FME	O1-CN-N	-5.01	112.09	125.27
4	H	1[A]	FME	CA-N-CN	-3.81	116.96	122.82
4	H	1[A]	FME	O1-CN-N	-3.81	115.25	125.27

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1[B]	FME	O1-CN-N-CA
4	H	1[A]	FME	O1-CN-N-CA
4	H	1[B]	FME	CB-CG-SD-CE
4	H	1[A]	FME	N-CA-CB-CG
4	H	1[B]	FME	CA-CB-CG-SD
4	H	1[A]	FME	CB-CG-SD-CE
4	H	1[B]	FME	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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
10	SO4	M	804	-	4,4,4	1.03	0	6,6,6	0.68	0
6	BCB	L	302	2	60,74,74	3.72	21 (35%)	48,115,115	2.47	16 (33%)
8	LDA	L	707	-	12,15,15	1.97	1 (8%)	14,17,17	0.60	0
10	SO4	M	802	-	4,4,4	1.02	0	6,6,6	0.85	0
6	BCB	M	805	3	60,74,74	3.64	24 (40%)	48,115,115	2.81	17 (35%)
7	BPB	L	402	-	64,70,70	1.31	7 (10%)	64,101,101	1.64	12 (18%)
10	SO4	H	801	-	4,4,4	0.64	0	6,6,6	0.40	0
7	BPB	M	401	-	64,70,70	1.21	8 (12%)	64,101,101	1.67	8 (12%)
12	NS5	M	600	-	39,39,39	0.73	0	44,46,46	1.15	5 (11%)
5	HEM	C	339	1	27,50,50	1.86	6 (22%)	17,82,82	1.13	1 (5%)
8	LDA	H	701	-	12,15,15	2.51	1 (8%)	14,17,17	0.75	0
11	MQ7	M	501	-	49,49,49	1.57	9 (18%)	60,63,63	1.37	9 (15%)
8	LDA	M	704	-	12,15,15	2.24	1 (8%)	14,17,17	0.54	0
6	BCB	M	806	3	60,74,74	3.53	22 (36%)	48,115,115	2.81	16 (33%)
5	HEM	C	340	1	27,50,50	1.76	7 (25%)	17,82,82	1.32	3 (17%)
5	HEM	C	338	1	27,50,50	1.58	5 (18%)	17,82,82	1.37	2 (11%)
8	LDA	M	705	-	12,15,15	2.12	1 (8%)	14,17,17	0.53	0
8	LDA	H	703	-	12,15,15	2.29	1 (8%)	14,17,17	0.59	0
5	HEM	C	337	1	27,50,50	1.70	5 (18%)	17,82,82	1.48	2 (11%)
8	LDA	L	702	-	12,15,15	2.14	1 (8%)	14,17,17	0.69	0
8	LDA	M	706	-	12,15,15	2.23	1 (8%)	14,17,17	0.51	0
6	BCB	L	304	2	60,74,74	3.74	23 (38%)	48,115,115	2.47	15 (31%)
10	SO4	M	803	-	4,4,4	0.63	0	6,6,6	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BCB	M	806	3	-	5/41/177/177	-
5	HEM	C	340	1	-	0/6/54/54	-
6	BCB	M	805	3	-	8/41/177/177	-
5	HEM	C	338	1	-	0/6/54/54	-
8	LDA	M	705	-	-	2/13/13/13	-
6	BCB	L	302	2	-	7/41/177/177	-
8	LDA	L	707	-	-	5/13/13/13	-
5	HEM	C	337	1	-	0/6/54/54	-
7	BPB	L	402	-	-	5/47/105/105	0/5/6/6
5	HEM	C	339	1	-	0/6/54/54	-
8	LDA	M	706	-	-	5/13/13/13	-
12	NS5	M	600	-	-	11/43/43/43	-
8	LDA	H	701	-	-	4/13/13/13	-
11	MQ7	M	501	-	-	1/41/61/61	0/2/2/2
6	BCB	L	304	2	-	8/41/177/177	-
8	LDA	H	703	-	-	5/13/13/13	-
7	BPB	M	401	-	-	7/47/105/105	0/5/6/6
8	LDA	M	704	-	-	5/13/13/13	-
8	LDA	L	702	-	-	3/13/13/13	-

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	302	BCB	CHD-C1D	-9.39	1.38	1.53
6	L	304	BCB	CHB-C1B	-9.17	1.39	1.53
6	M	805	BCB	CHD-C1D	-9.07	1.39	1.53
6	L	304	BCB	C1A-CHA	-8.99	1.40	1.54
6	M	805	BCB	C1A-CHA	-8.80	1.40	1.54
8	H	701	LDA	O1-N1	-8.65	1.21	1.42
6	M	806	BCB	CHB-C1B	-8.63	1.40	1.53
6	L	304	BCB	CHD-C1D	-8.63	1.40	1.53
6	M	805	BCB	CHB-C1B	-8.61	1.40	1.53
6	M	806	BCB	CHD-C1D	-8.51	1.40	1.53
6	L	302	BCB	CHB-C1B	-8.23	1.40	1.53
6	L	302	BCB	CHC-C4B	-8.22	1.40	1.53
6	M	806	BCB	CHC-C4B	-8.08	1.40	1.53
6	L	304	BCB	CHC-C4B	-8.06	1.40	1.53
6	M	805	BCB	CHC-C4B	-8.00	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	302	BCB	CHD-C4C	-8.00	1.39	1.53
6	L	302	BCB	C1A-CHA	-7.96	1.41	1.54
6	L	304	BCB	CHD-C4C	-7.90	1.40	1.53
8	H	703	LDA	O1-N1	-7.89	1.23	1.42
8	M	704	LDA	O1-N1	-7.70	1.24	1.42
6	M	805	BCB	CHD-C4C	-7.70	1.40	1.53
8	M	706	LDA	O1-N1	-7.68	1.24	1.42
8	L	702	LDA	O1-N1	-7.38	1.24	1.42
6	L	304	BCB	C3D-C2D	-7.29	1.36	1.55
8	M	705	LDA	O1-N1	-7.28	1.25	1.42
6	M	806	BCB	C1A-CHA	-7.23	1.42	1.54
6	L	304	BCB	C3B-C2B	-7.11	1.36	1.55
6	L	302	BCB	C3D-C2D	-7.11	1.36	1.55
6	M	806	BCB	C3B-C2B	-7.07	1.36	1.55
6	L	302	BCB	C3B-C2B	-7.07	1.36	1.55
6	M	805	BCB	C3B-C2B	-6.99	1.36	1.55
6	M	806	BCB	CHD-C4C	-6.94	1.41	1.53
6	M	806	BCB	C3D-C2D	-6.80	1.37	1.55
6	L	304	BCB	C4D-ND	-6.59	1.36	1.50
6	M	806	BCB	C4D-ND	-6.59	1.36	1.50
6	L	302	BCB	C4D-ND	-6.49	1.36	1.50
6	L	302	BCB	C3B-CAB	-6.48	1.45	1.52
8	L	707	LDA	O1-N1	-6.43	1.27	1.42
6	M	805	BCB	C4D-ND	-6.16	1.37	1.50
6	L	304	BCB	CHB-C4A	-6.14	1.38	1.52
6	L	302	BCB	CHB-C4A	-6.10	1.38	1.52
6	M	805	BCB	C3D-C2D	-6.07	1.39	1.55
6	L	302	BCB	C1D-ND	-5.98	1.37	1.50
6	M	806	BCB	C4B-NB	-5.98	1.37	1.50
6	L	302	BCB	C4B-NB	-5.96	1.37	1.50
6	L	304	BCB	C1D-ND	-5.90	1.37	1.50
6	M	806	BCB	C1D-ND	-5.88	1.37	1.50
6	L	304	BCB	C3B-CAB	-5.81	1.45	1.52
6	M	805	BCB	CHB-C4A	-5.77	1.39	1.52
6	M	805	BCB	CHC-C1C	-5.76	1.39	1.52
6	M	805	BCB	C1D-ND	-5.72	1.38	1.50
6	L	304	BCB	CHC-C1C	-5.72	1.39	1.52
6	M	806	BCB	C1B-NB	-5.68	1.38	1.50
6	L	304	BCB	C4B-NB	-5.65	1.38	1.50
6	M	805	BCB	C4B-NB	-5.55	1.38	1.50
6	L	304	BCB	C1B-NB	-5.51	1.38	1.50
6	M	806	BCB	CHB-C4A	-5.50	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	302	BCB	C1B-NB	-5.50	1.38	1.50
6	M	806	BCB	CHC-C1C	-5.44	1.40	1.52
6	M	805	BCB	C1B-NB	-5.37	1.38	1.50
6	M	805	BCB	C3B-CAB	-5.33	1.46	1.52
6	M	806	BCB	C3B-CAB	-5.15	1.46	1.52
6	L	302	BCB	CHC-C1C	-5.13	1.41	1.52
6	M	806	BCB	C2B-C1B	-5.04	1.44	1.53
6	L	302	BCB	C2B-C1B	-4.92	1.44	1.53
11	M	501	MQ7	C11-C12	-4.90	1.43	1.50
6	M	805	BCB	C2B-C1B	-4.78	1.44	1.53
6	L	302	BCB	C2D-C1D	-4.67	1.44	1.53
6	L	304	BCB	C2B-C1B	-4.61	1.45	1.53
7	L	402	BPB	C3B-C4B	4.39	1.46	1.41
5	C	337	HEM	C3B-C2B	-4.36	1.34	1.40
5	C	339	HEM	C3B-CAB	4.32	1.56	1.47
6	L	304	BCB	C2D-C1D	-4.24	1.45	1.53
6	L	302	BCB	O2D-CED	-4.21	1.35	1.45
7	L	402	BPB	O2D-CGD	4.19	1.43	1.33
6	M	805	BCB	C2D-C1D	-4.07	1.45	1.53
5	C	339	HEM	CBC-CAC	3.97	1.55	1.29
5	C	339	HEM	CBB-CAB	3.93	1.55	1.29
7	M	401	BPB	O2A-CGA	3.85	1.44	1.33
6	L	304	BCB	C3D-CAD	-3.82	1.44	1.51
6	M	806	BCB	C2D-C1D	-3.81	1.46	1.53
5	C	340	HEM	CBC-CAC	3.81	1.54	1.29
6	L	302	BCB	C1-C2	-3.78	1.37	1.49
5	C	337	HEM	CBC-CAC	3.72	1.54	1.29
6	M	805	BCB	O2A-CGA	3.69	1.44	1.33
6	L	304	BCB	O2D-CED	-3.62	1.36	1.45
5	C	337	HEM	CBB-CAB	3.58	1.53	1.29
5	C	339	HEM	C3C-C2C	-3.55	1.35	1.40
5	C	338	HEM	CBB-CAB	3.47	1.52	1.29
5	C	340	HEM	CBB-CAB	3.44	1.52	1.29
6	M	806	BCB	C3D-CAD	-3.44	1.45	1.51
5	C	340	HEM	C3C-C2C	-3.42	1.35	1.40
5	C	338	HEM	CBC-CAC	3.41	1.51	1.29
7	L	402	BPB	O2D-CED	-3.39	1.37	1.45
5	C	339	HEM	C3C-CAC	3.37	1.54	1.47
6	L	302	BCB	C3D-CAD	-3.34	1.45	1.51
5	C	340	HEM	C3B-C2B	-3.30	1.35	1.40
5	C	338	HEM	C3C-C2C	-3.24	1.35	1.40
6	L	302	BCB	C4C-C3C	-3.19	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	401	BPB	C3B-C4B	3.19	1.45	1.41
5	C	340	HEM	C3C-CAC	3.14	1.54	1.47
6	M	805	BCB	O2D-CGD	3.11	1.40	1.33
6	L	304	BCB	C4C-C3C	-3.10	1.41	1.50
6	M	805	BCB	C4C-C3C	-3.10	1.41	1.50
11	M	501	MQ7	C32-C33	3.08	1.40	1.33
6	M	806	BCB	C4C-C3C	-3.07	1.41	1.50
6	M	806	BCB	CAA-CBA	-3.07	1.43	1.52
5	C	337	HEM	C3C-C2C	-3.07	1.36	1.40
5	C	337	HEM	C3C-CAC	2.98	1.53	1.47
11	M	501	MQ7	C26-C27	-2.97	1.40	1.50
6	M	805	BCB	C3D-CAD	-2.92	1.46	1.51
6	M	805	BCB	O2D-CED	-2.91	1.38	1.45
6	L	304	BCB	C2-C3	2.89	1.39	1.33
5	C	339	HEM	C3B-C2B	-2.88	1.36	1.40
5	C	338	HEM	C3B-CAB	2.87	1.53	1.47
7	M	401	BPB	C2-C3	2.84	1.39	1.33
5	C	338	HEM	C3B-C2B	-2.83	1.36	1.40
7	M	401	BPB	C3B-C2B	-2.81	1.34	1.39
11	M	501	MQ7	C17-C18	2.81	1.39	1.33
6	M	806	BCB	C2-C3	2.79	1.39	1.33
7	L	402	BPB	C4C-C3C	-2.78	1.39	1.45
11	M	501	MQ7	C37-C38	2.77	1.39	1.33
7	M	401	BPB	O2D-CGD	2.76	1.39	1.33
6	L	304	BCB	C2A-C3A	-2.74	1.49	1.54
7	L	402	BPB	C2-C3	2.74	1.39	1.33
6	M	805	BCB	C2-C3	2.69	1.39	1.33
7	L	402	BPB	CMD-C2D	2.64	1.56	1.50
6	M	805	BCB	C2A-C3A	-2.59	1.50	1.54
7	M	401	BPB	O2D-CED	-2.58	1.39	1.45
11	M	501	MQ7	C42-C43	2.57	1.39	1.32
6	M	805	BCB	C5-C3	2.51	1.56	1.51
11	M	501	MQ7	C27-C28	2.38	1.38	1.33
5	C	340	HEM	C3B-CAB	2.36	1.52	1.47
6	L	302	BCB	C2-C3	2.34	1.38	1.33
5	C	340	HEM	CAA-C2A	-2.31	1.48	1.52
6	M	806	BCB	C4A-C3A	-2.30	1.51	1.53
7	M	401	BPB	CAC-C3C	2.25	1.39	1.33
11	M	501	MQ7	C10-C5	-2.23	1.37	1.40
7	L	402	BPB	C1-C2	-2.15	1.42	1.49
6	L	304	BCB	C1-C2	-2.15	1.42	1.49
7	M	401	BPB	CBC-CAC	2.13	1.57	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	501	MQ7	C22-C23	2.09	1.38	1.33
6	L	304	BCB	O2D-CGD	2.05	1.38	1.33
6	M	806	BCB	C1-C2	-2.04	1.43	1.49

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	805	BCB	CBB-CAB-C3B	8.89	125.87	116.80
6	M	806	BCB	CMB-C2B-C3B	8.47	135.32	114.29
6	L	304	BCB	C1D-CHD-C4C	7.39	128.11	112.37
7	M	401	BPB	O2D-CGD-CBD	7.26	124.16	111.27
6	M	806	BCB	OBB-CAB-C3B	7.21	129.12	121.52
6	L	302	BCB	C1D-CHD-C4C	7.19	127.70	112.37
6	M	805	BCB	C1D-CHD-C4C	7.15	127.60	112.37
6	M	806	BCB	C1D-CHD-C4C	7.09	127.48	112.37
6	L	302	BCB	CMB-C2B-C3B	6.86	131.34	114.29
6	M	805	BCB	CMB-C2B-C3B	6.50	130.42	114.29
6	L	304	BCB	CMB-C2B-C3B	6.40	130.18	114.29
7	L	402	BPB	O2D-CGD-CBD	6.36	122.57	111.27
6	M	806	BCB	CMD-C2D-C3D	6.33	130.00	114.29
6	M	805	BCB	CMD-C2D-C3D	5.86	128.83	114.29
6	L	302	BCB	CMD-C2D-C3D	5.82	128.74	114.29
6	L	304	BCB	CMD-C2D-C3D	5.69	128.41	114.29
6	L	304	BCB	O2D-CGD-CBD	5.34	123.64	111.11
6	M	805	BCB	O2D-CGD-CBD	5.17	123.26	111.11
6	L	302	BCB	OBB-CAB-C3B	5.09	126.88	121.52
6	M	805	BCB	OBB-CAB-C3B	-4.92	116.33	121.52
6	M	805	BCB	O1D-CGD-CBD	-4.78	115.08	124.54
6	L	304	BCB	O1D-CGD-CBD	-4.77	115.08	124.54
6	M	806	BCB	O2D-CGD-CBD	4.70	122.14	111.11
7	L	402	BPB	O1D-CGD-CBD	-4.65	114.96	124.48
7	M	401	BPB	O1D-CGD-CBD	-4.61	115.06	124.48
6	M	806	BCB	CHA-CBD-CGD	-4.50	104.83	115.02
6	L	302	BCB	CHA-CBD-CGD	-4.49	104.87	115.02
6	M	805	BCB	CHA-CBD-CGD	-4.37	105.13	115.02
6	M	806	BCB	O2A-CGA-CBA	4.14	124.89	111.91
6	M	806	BCB	O1D-CGD-CBD	-4.03	116.56	124.54
6	L	304	BCB	CHA-CBD-CGD	-3.92	106.15	115.02
5	C	339	HEM	CMB-C2B-C3B	3.91	131.99	124.68
7	M	401	BPB	C1-C2-C3	3.87	132.74	126.04
6	L	302	BCB	O1D-CGD-CBD	-3.62	117.38	124.54
12	M	600	NS5	C19-C18-C17	3.56	130.76	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	338	HEM	CBA-CAA-C2A	-3.53	105.98	112.49
7	L	402	BPB	C3C-C2C-C1C	3.52	105.51	100.72
6	L	302	BCB	O2D-CGD-CBD	3.51	119.36	111.11
6	M	806	BCB	O2A-CGA-O1A	-3.44	114.90	123.59
7	M	401	BPB	C4B-C3B-CAB	-3.40	119.81	127.19
6	M	806	BCB	CHC-C4B-C3B	3.39	126.48	118.17
6	M	805	BCB	CHC-C4B-C3B	3.28	126.21	118.17
6	M	806	BCB	CBB-CAB-C3B	-3.27	113.46	116.80
7	M	401	BPB	CED-O2D-CGD	3.26	123.32	115.94
6	M	806	BCB	CHC-C1C-C2C	3.23	126.94	117.19
6	L	302	BCB	CHC-C4B-C3B	3.22	126.05	118.17
11	M	501	MQ7	C35-C33-C32	3.20	127.59	121.12
6	L	304	BCB	CHC-C1C-C2C	3.11	126.60	117.19
6	L	304	BCB	CHC-C4B-C3B	3.11	125.79	118.17
5	C	337	HEM	CMC-C2C-C3C	3.08	130.44	124.68
7	M	401	BPB	C3C-C2C-C1C	3.06	104.88	100.72
6	M	805	BCB	CHC-C1C-C2C	3.05	126.40	117.19
6	M	806	BCB	OBD-CAD-CBD	-3.04	120.20	127.49
5	C	340	HEM	CMB-C2B-C3B	3.02	130.34	124.68
5	C	337	HEM	CBD-CAD-C3D	-2.98	106.99	112.48
6	L	304	BCB	C4-C3-C5	-2.98	110.26	115.27
6	L	302	BCB	CHC-C1C-C2C	2.97	126.16	117.19
11	M	501	MQ7	C41-C42-C43	2.95	137.83	127.75
6	L	302	BCB	O2A-CGA-CBA	2.90	121.00	111.91
11	M	501	MQ7	C25-C23-C22	2.87	126.93	121.12
11	M	501	MQ7	C34-C33-C35	-2.87	110.44	115.27
6	M	805	BCB	OBD-CAD-CBD	-2.84	120.67	127.49
6	L	304	BCB	OBD-CAD-CBD	-2.78	120.82	127.49
12	M	600	NS5	C18-C19-C20	2.76	129.13	123.47
7	L	402	BPB	C4B-C3B-CAB	-2.76	121.20	127.19
11	M	501	MQ7	C39-C38-C40	-2.73	110.68	115.27
6	L	302	BCB	C15-C13-C12	-2.70	97.94	112.13
7	L	402	BPB	CBD-CHA-C4D	-2.68	105.52	108.54
12	M	600	NS5	C19-C20-C21	-2.65	123.53	127.31
6	M	805	BCB	CBA-CAA-C2A	-2.63	112.14	115.72
11	M	501	MQ7	C26-C25-C23	-2.63	104.33	112.98
5	C	340	HEM	CBD-CAD-C3D	2.63	117.32	112.48
6	L	302	BCB	O2A-CGA-O1A	-2.58	117.09	123.59
6	M	806	BCB	C3B-C4B-NB	2.57	108.44	103.75
6	L	302	BCB	OBD-CAD-CBD	-2.57	121.34	127.49
6	L	304	BCB	C3B-C4B-NB	2.55	108.39	103.75
6	L	304	BCB	CBA-CAA-C2A	-2.54	112.27	115.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	805	BCB	C3B-C4B-NB	2.48	108.27	103.75
6	L	302	BCB	C3B-C4B-NB	2.46	108.24	103.75
11	M	501	MQ7	C40-C41-C42	-2.45	103.84	111.88
6	M	805	BCB	OBD-CAD-C3D	2.44	131.03	126.73
7	M	401	BPB	CBD-CHA-C1A	2.42	130.71	126.84
6	L	302	BCB	OBD-CAD-C3D	2.42	130.99	126.73
11	M	501	MQ7	C36-C35-C33	-2.39	105.13	112.98
6	M	805	BCB	C6-C5-C3	2.37	119.66	113.45
12	M	600	NS5	C16-C15-C14	-2.36	114.36	118.08
7	L	402	BPB	O2A-CGA-CBA	2.34	119.26	111.91
6	M	805	BCB	C1-C2-C3	2.34	130.08	126.04
6	L	304	BCB	C15-C13-C12	-2.25	100.27	112.13
6	L	304	BCB	O2A-CGA-CBA	2.25	118.95	111.91
7	L	402	BPB	C3A-C2A-C1A	2.23	104.68	101.34
6	M	806	BCB	OBD-CAD-C3D	2.22	130.65	126.73
5	C	340	HEM	CBA-CAA-C2A	-2.22	108.39	112.49
6	L	302	BCB	CBB-CAB-C3B	-2.21	114.54	116.80
7	L	402	BPB	CHD-C1D-ND	-2.21	119.98	124.58
7	L	402	BPB	CED-O2D-CGD	2.20	120.92	115.94
5	C	338	HEM	CMA-C3A-C4A	-2.18	125.11	128.46
7	M	401	BPB	CBD-CHA-C4D	-2.17	106.10	108.54
6	L	304	BCB	OBD-CAD-C3D	2.16	130.54	126.73
6	M	806	BCB	OBB-CAB-CBB	-2.13	117.36	121.15
7	L	402	BPB	C2D-C1D-ND	2.13	113.01	109.79
12	M	600	NS5	C22-C21-C23	-2.12	114.73	118.08
6	M	805	BCB	C4-C3-C2	-2.11	118.27	123.68
11	M	501	MQ7	C44-C43-C42	2.05	128.57	122.65
7	L	402	BPB	CMB-C2B-C3B	2.01	128.44	124.68
7	L	402	BPB	C1-C2-C3	2.01	129.51	126.04

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	302	BCB	C2B-C3B-CAB-OBB
6	L	302	BCB	C2B-C3B-CAB-CBB
6	L	302	BCB	C4-C3-C5-C6
7	L	402	BPB	O2A-C1-C2-C3
12	M	600	NS5	C3-C4-C5-C7
12	M	600	NS5	C9-C10-C12-C13
12	M	600	NS5	C11-C10-C12-C13
12	M	600	NS5	C10-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
12	M	600	NS5	C20-C21-C23-C24
12	M	600	NS5	C22-C21-C23-C24
6	M	806	BCB	C2B-C3B-CAB-OBB
6	M	806	BCB	C2B-C3B-CAB-CBB
6	M	806	BCB	CAD-CBD-CGD-O1D
6	M	806	BCB	CAD-CBD-CGD-O2D
6	L	304	BCB	C2B-C3B-CAB-CBB
6	L	302	BCB	C2-C3-C5-C6
6	M	805	BCB	C2-C3-C5-C6
6	M	806	BCB	C2A-CAA-CBA-CGA
6	M	805	BCB	C4-C3-C5-C6
7	M	401	BPB	C4-C3-C5-C6
7	M	401	BPB	C2-C3-C5-C6
12	M	600	NS5	C6-C5-C7-C8
6	M	805	BCB	C11-C12-C13-C14
6	M	805	BCB	C15-C16-C17-C18
8	L	702	LDA	C2-C3-C4-C5
8	L	702	LDA	C5-C6-C7-C8
8	L	707	LDA	C3-C4-C5-C6
8	L	707	LDA	C4-C5-C6-C7
8	M	706	LDA	C3-C4-C5-C6
8	H	703	LDA	C3-C4-C5-C6
8	H	703	LDA	C11-C10-C9-C8
8	M	706	LDA	C5-C6-C7-C8
8	M	704	LDA	C4-C5-C6-C7
8	L	702	LDA	C1-C2-C3-C4
6	M	805	BCB	C3-C5-C6-C7
8	H	703	LDA	C5-C6-C7-C8
8	H	701	LDA	C7-C8-C9-C10
8	M	706	LDA	C4-C5-C6-C7
6	M	805	BCB	C10-C11-C12-C13
7	M	401	BPB	C5-C6-C7-C8
7	M	401	BPB	C13-C15-C16-C17
6	L	304	BCB	O1D-CGD-O2D-CED
12	M	600	NS5	C3-C4-C5-C6
7	M	401	BPB	C12-C13-C15-C16
8	M	704	LDA	C5-C6-C7-C8
6	M	805	BCB	C4B-C3B-CAB-OBB
6	M	805	BCB	C4B-C3B-CAB-CBB
7	M	401	BPB	C14-C13-C15-C16
8	M	705	LDA	C1-C2-C3-C4
6	L	304	BCB	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	M	600	NS5	C19-C20-C21-C22
7	M	401	BPB	CAD-CBD-CGD-O2D
8	L	707	LDA	C2-C3-C4-C5
7	L	402	BPB	C16-C17-C18-C20
12	M	600	NS5	C29-C30-C31-C33
8	M	704	LDA	C7-C8-C9-C10
8	H	703	LDA	C9-C10-C11-C12
8	L	707	LDA	C11-C10-C9-C8
6	L	302	BCB	CAD-CBD-CGD-O1D
8	M	706	LDA	C1-C2-C3-C4
8	M	705	LDA	C2-C3-C4-C5
6	L	304	BCB	C14-C13-C15-C16
8	H	703	LDA	C2-C3-C4-C5
8	H	701	LDA	C4-C5-C6-C7
8	L	707	LDA	C6-C7-C8-C9
8	M	704	LDA	C6-C7-C8-C9
6	L	304	BCB	C12-C13-C15-C16
7	L	402	BPB	C8-C10-C11-C12
6	L	304	BCB	C2B-C3B-CAB-OBB
7	L	402	BPB	C13-C15-C16-C17
8	M	706	LDA	C11-C10-C9-C8
11	M	501	MQ7	C38-C40-C41-C42
12	M	600	NS5	C12-C10-C9-C8
7	L	402	BPB	CAD-CBD-CGD-O2D
8	H	701	LDA	C5-C6-C7-C8
6	L	304	BCB	C13-C15-C16-C17
8	H	701	LDA	C3-C4-C5-C6
6	L	302	BCB	CAD-CBD-CGD-O2D
6	L	302	BCB	C15-C16-C17-C18
6	L	304	BCB	CHA-CBD-CGD-O1D
8	M	704	LDA	C11-C10-C9-C8

There are no ring outliers.

10 monomers are involved in 49 short contacts:

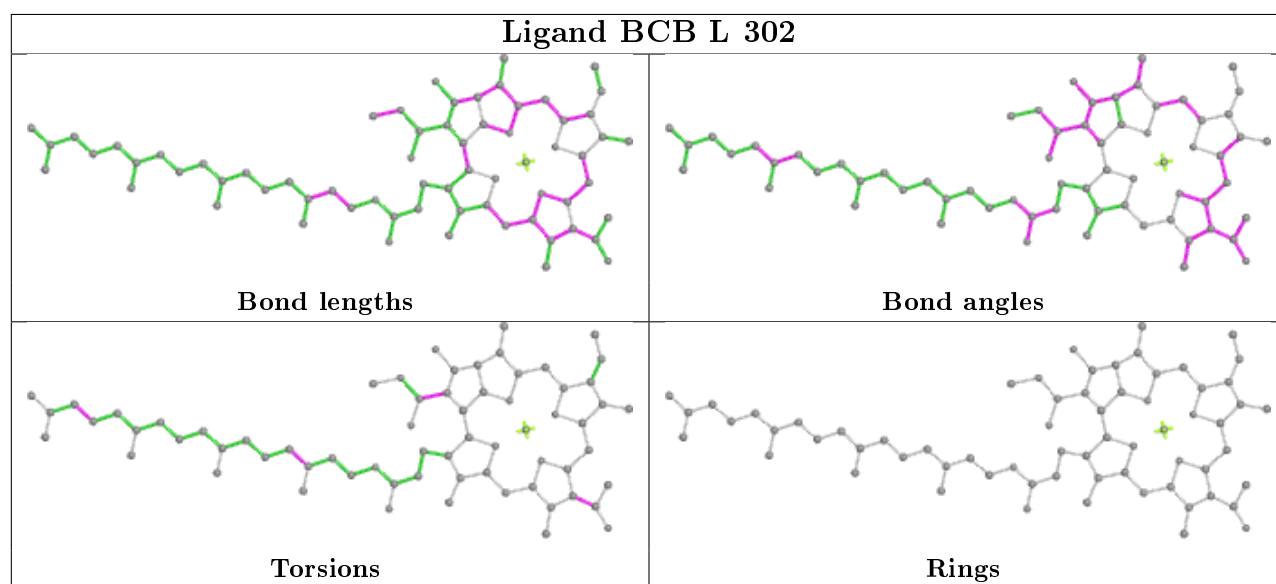
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	302	BCB	5	0
8	L	707	LDA	2	0
6	M	805	BCB	7	0
7	L	402	BPB	5	0
7	M	401	BPB	12	0
5	C	339	HEM	1	0

*Continued on next page...*

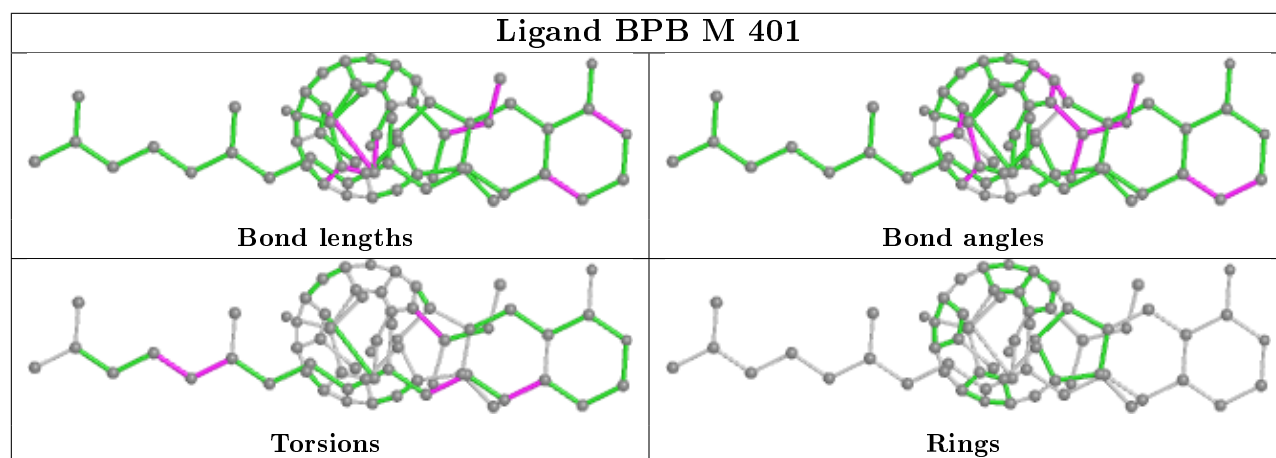
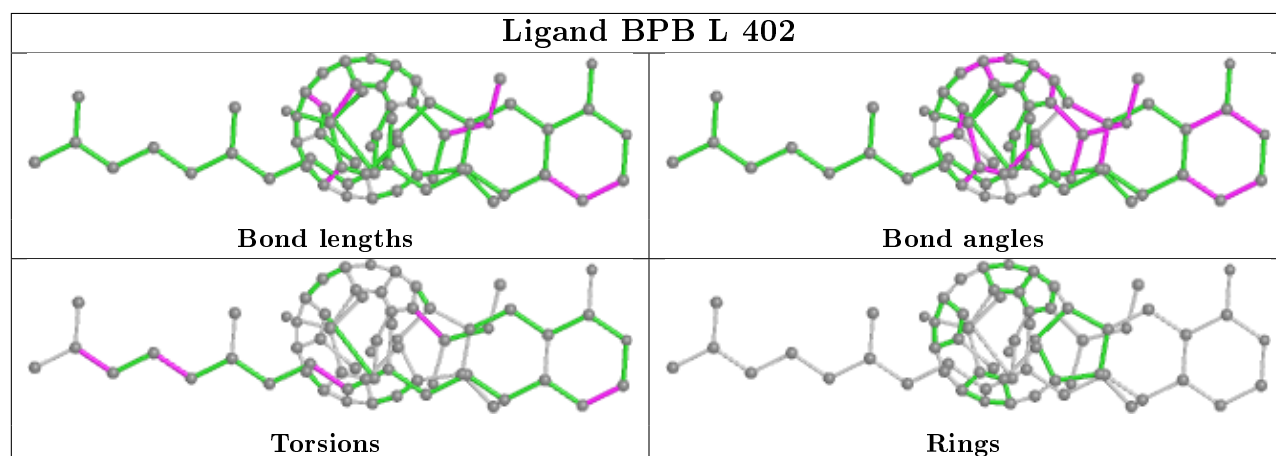
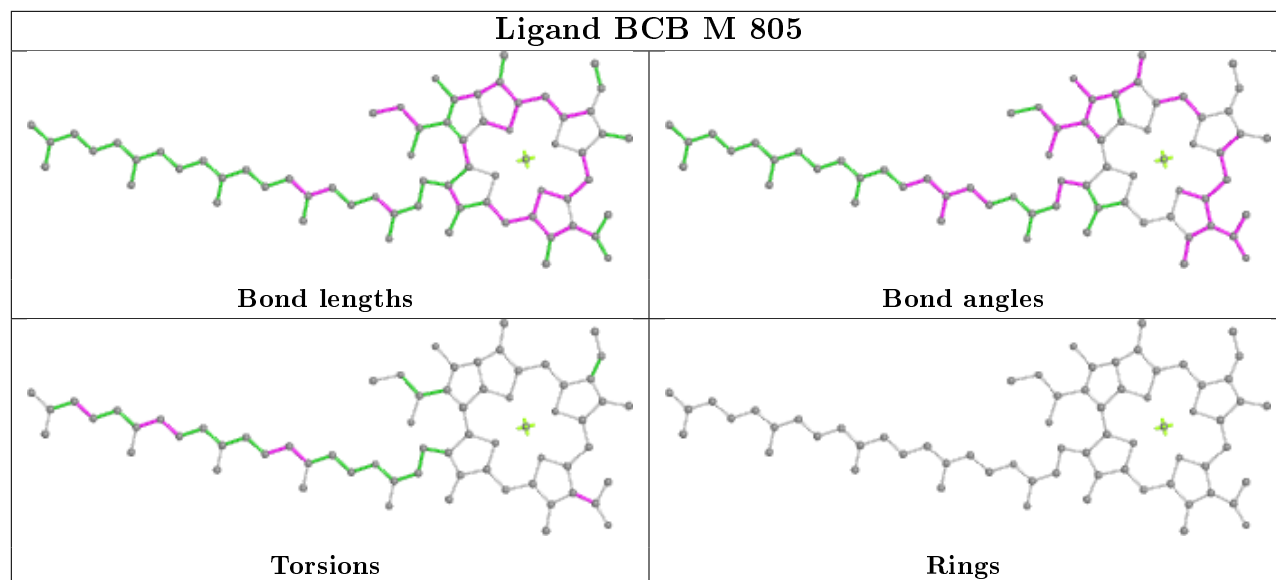
*Continued from previous page...*

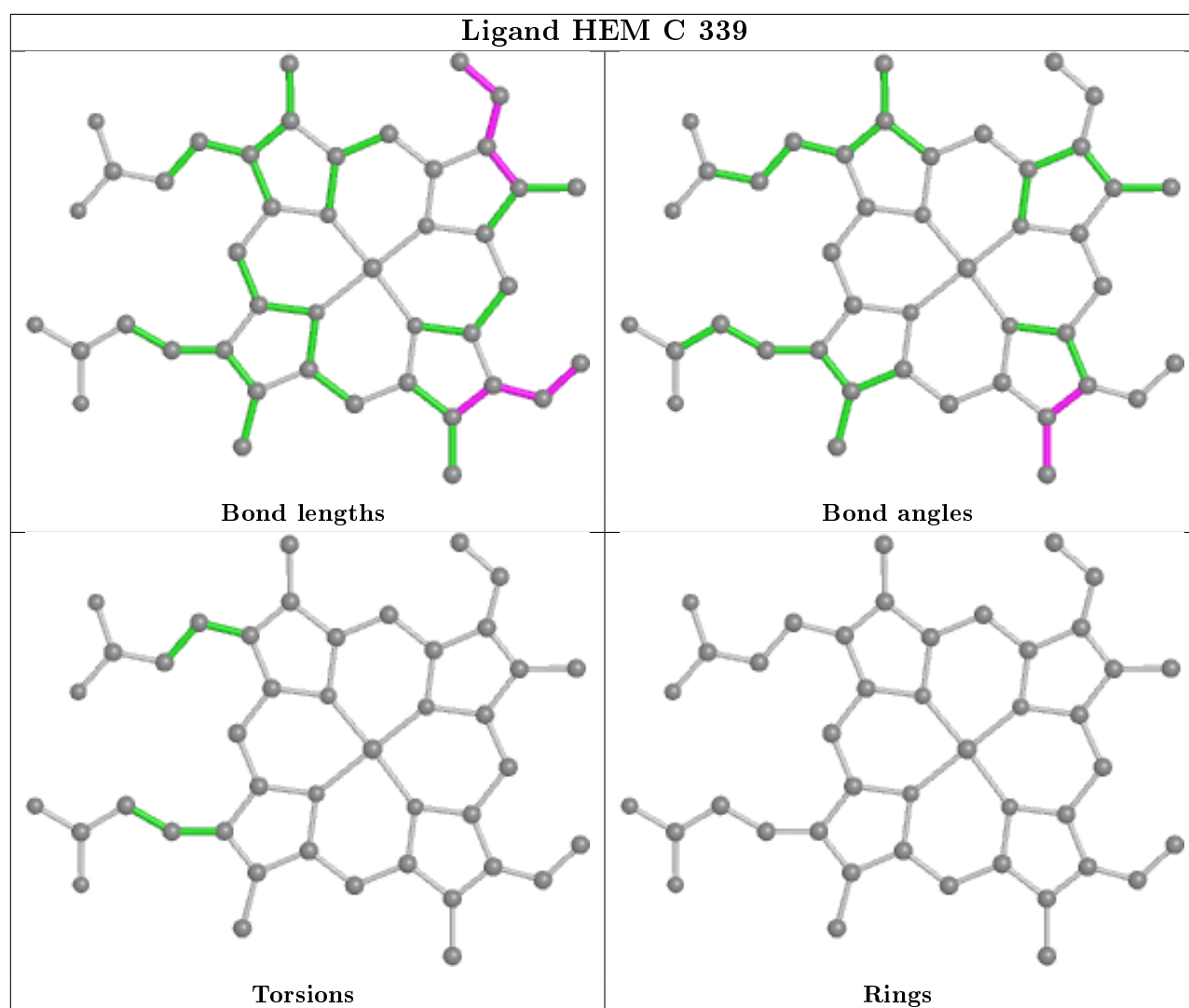
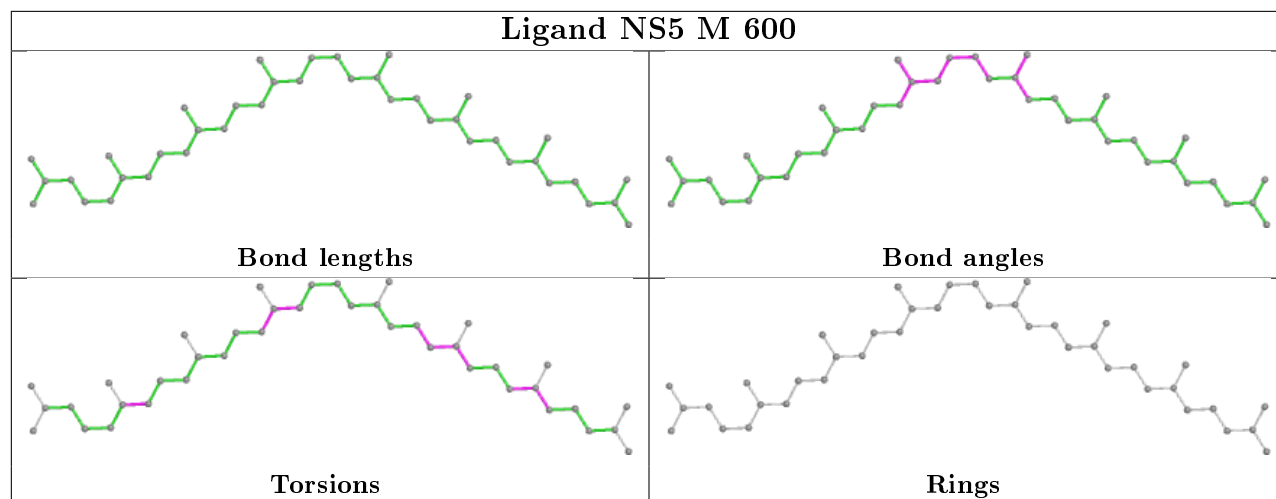
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	806	BCB	6	0
8	L	702	LDA	8	0
8	M	706	LDA	2	0
6	L	304	BCB	4	0

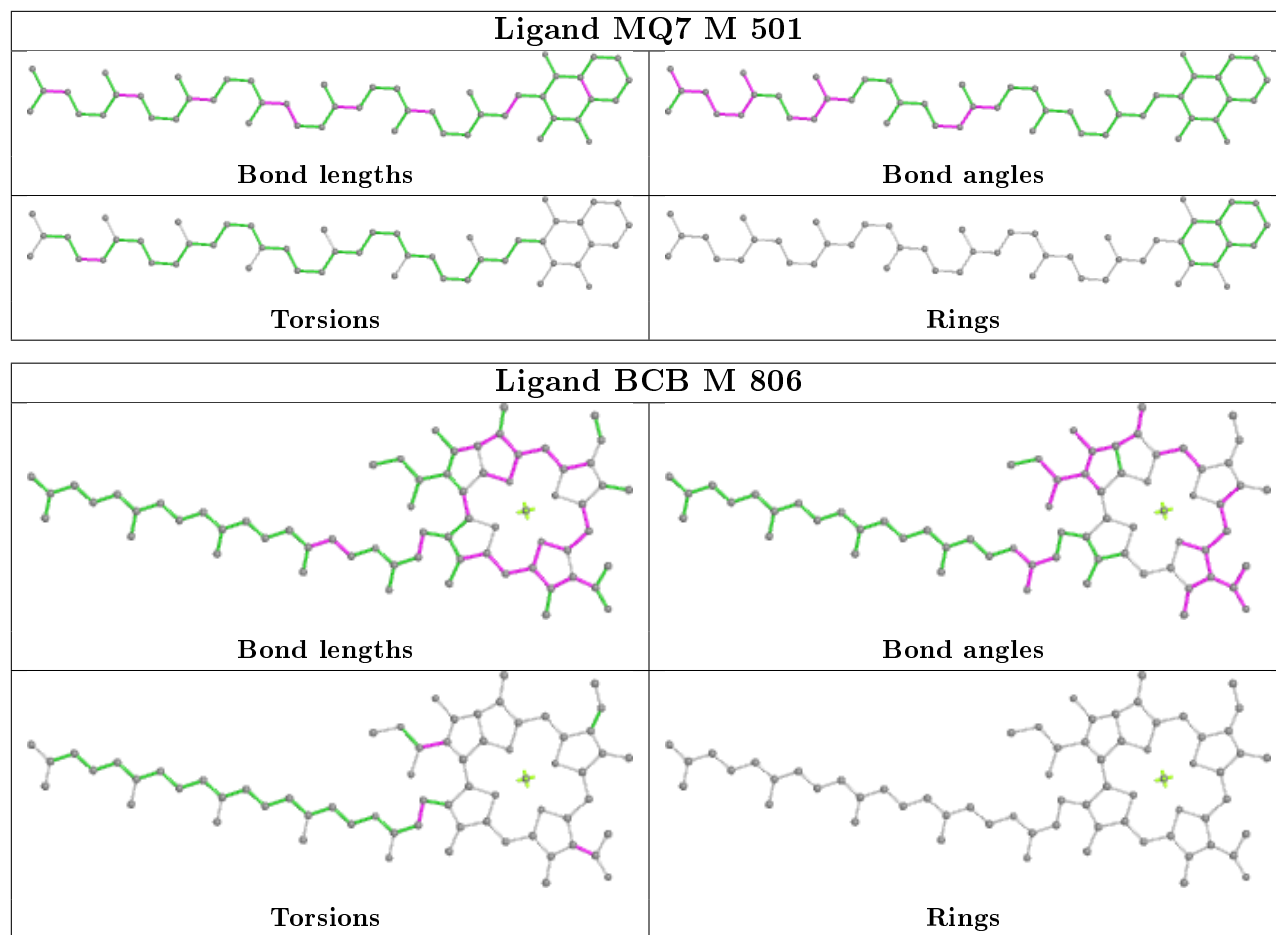
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

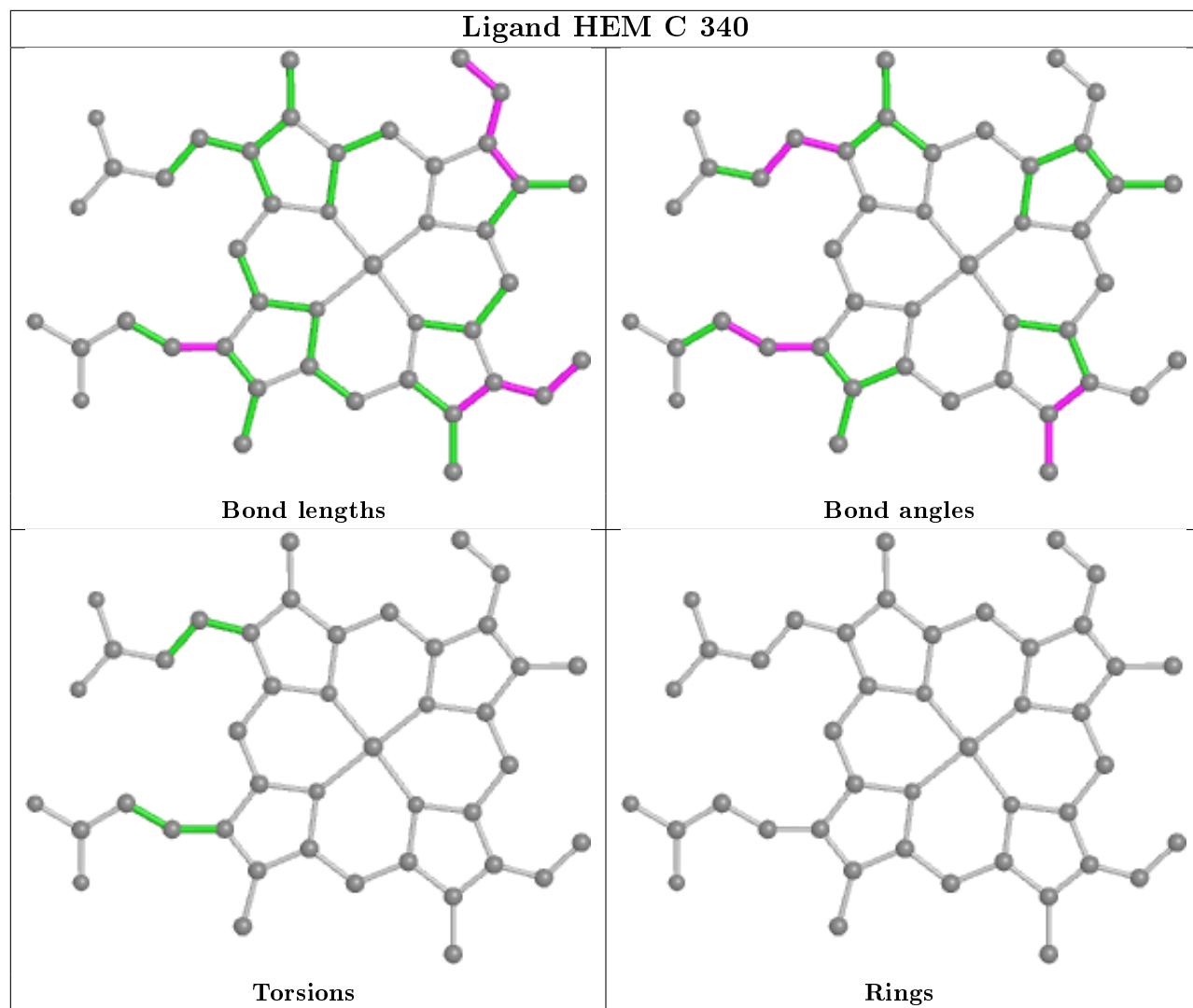


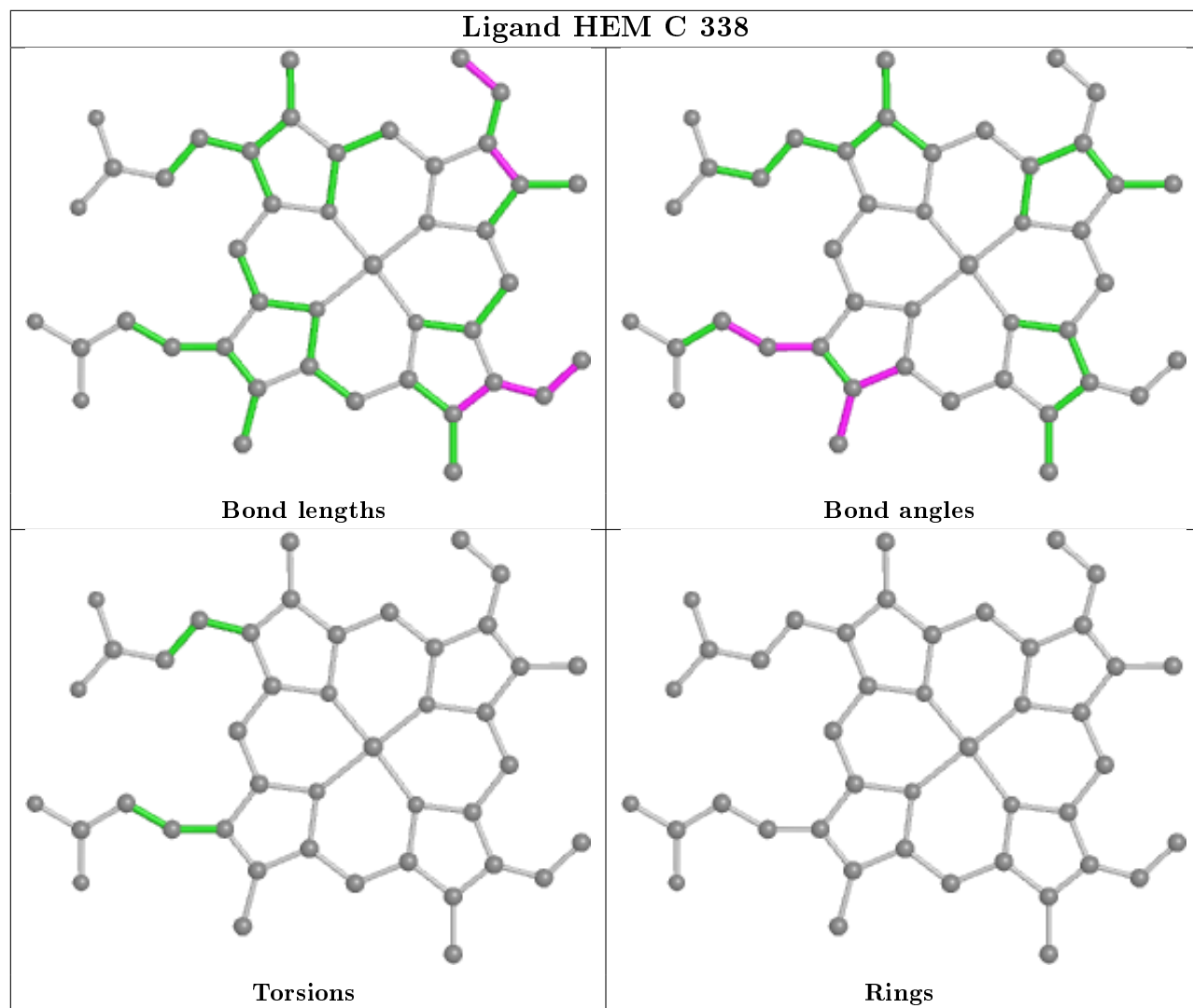


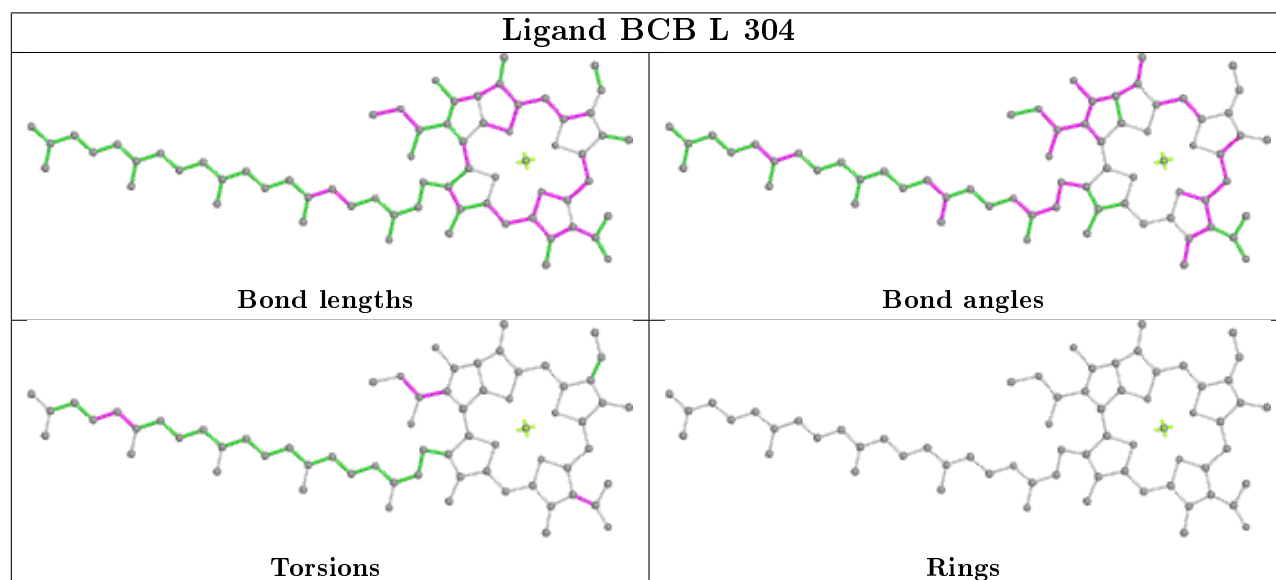
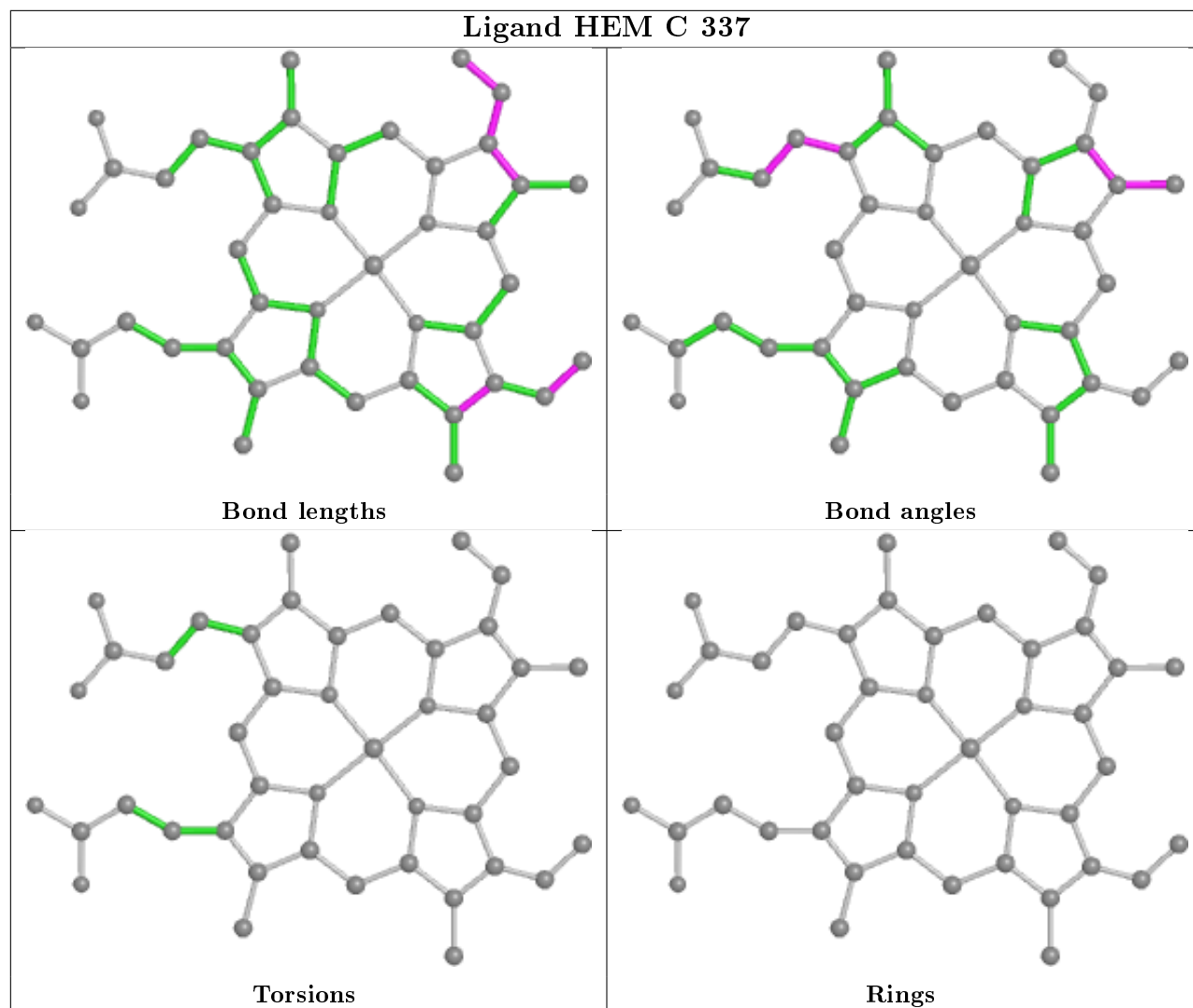












## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [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%)	-0.86	0 <a href="#">100</a>   <a href="#">100</a>	11, 25, 47, 67	15 (4%)
2	L	273/273 (100%)	-1.02	1 (0%) <a href="#">92</a>   <a href="#">91</a>	9, 19, 41, 50	7 (2%)
3	M	323/323 (100%)	-0.97	1 (0%) <a href="#">94</a>   <a href="#">93</a>	9, 22, 50, 61	8 (2%)
4	H	249/258 (96%)	-0.83	0 <a href="#">100</a>   <a href="#">100</a>	12, 30, 54, 64	22 (8%)
All	All	1177/1190 (98%)	-0.92	2 (0%) <a href="#">95</a>   <a href="#">94</a>	9, 24, 49, 67	52 (4%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	59	TRP	2.1
3	M	319	PRO	2.0

### 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[B]	10/11	0.97	0.09	27,30,30,30	10
4	FME	H	1[A]	10/11	0.97	0.09	22,25,27,27	10

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.



## 6.4 Ligands ⓘ

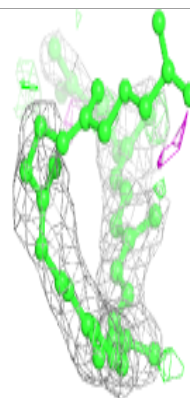
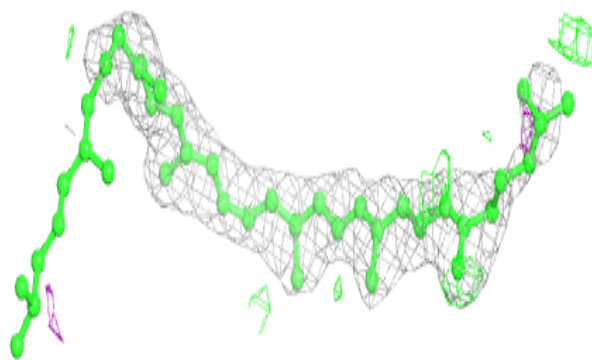
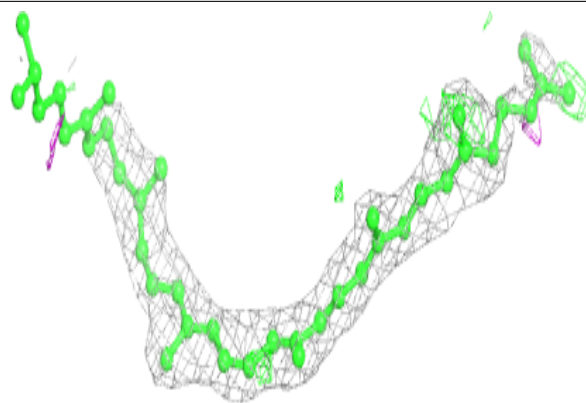
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
8	LDA	L	707	16/16	0.64	0.27	54,64,65,66	0
8	LDA	M	706	16/16	0.74	0.28	69,70,72,72	4
8	LDA	L	702	16/16	0.81	0.25	19,44,66,66	0
8	LDA	M	704	16/16	0.83	0.22	53,59,61,62	3
12	NS5	M	600	40/40	0.88	0.19	31,49,68,68	9
8	LDA	M	705	16/16	0.90	0.15	51,55,59,59	5
8	LDA	H	703	16/16	0.94	0.16	30,41,52,52	1
11	MQ7	M	501	48/48	0.95	0.11	11,17,43,49	0
6	BCB	M	805	66/66	0.96	0.12	8,18,37,38	20
8	LDA	H	701	16/16	0.96	0.10	28,30,31,32	0
10	SO4	M	803	5/5	0.96	0.11	85,85,86,86	0
7	BPB	M	401	65/65	0.97	0.10	10,24,61,62	7
10	SO4	H	801	5/5	0.98	0.09	64,65,65,67	0
7	BPB	L	402	65/65	0.98	0.08	7,12,18,20	0
5	HEM	C	337	43/43	0.98	0.08	21,27,38,43	0
6	BCB	M	806	66/66	0.98	0.10	4,12,30,31	0
5	HEM	C	340	43/43	0.98	0.10	11,19,34,42	0
6	BCB	L	304	66/66	0.98	0.12	6,13,26,36	0
5	HEM	C	338	43/43	0.98	0.13	16,25,32,38	0
6	BCB	L	302	66/66	0.99	0.10	7,11,18,19	0
10	SO4	M	804	5/5	0.99	0.14	40,41,42,43	0
5	HEM	C	339	43/43	0.99	0.06	8,14,18,25	0
10	SO4	M	802	5/5	0.99	0.08	30,30,32,39	0
9	FE2	M	500	1/1	1.00	0.04	14,14,14,14	0

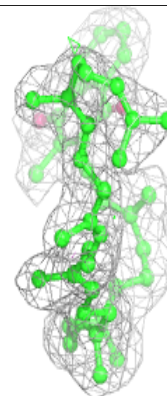
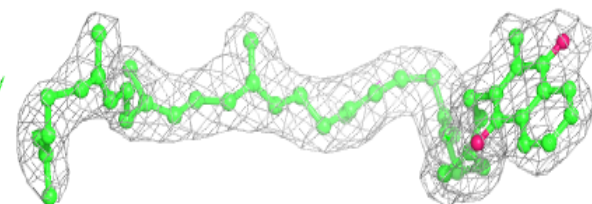
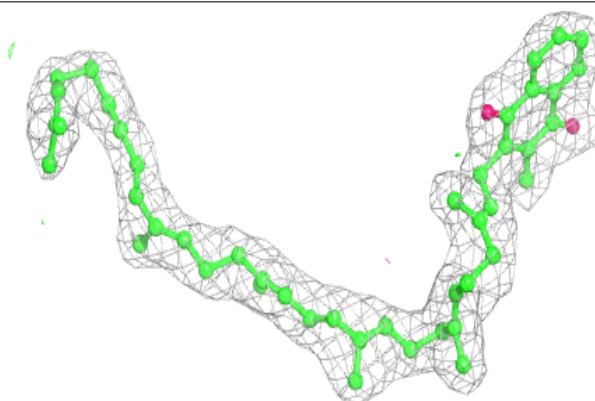
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

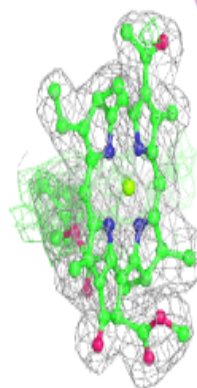
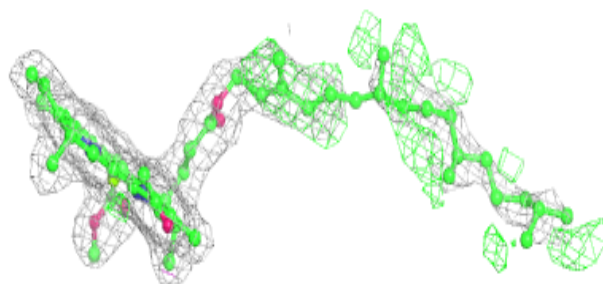
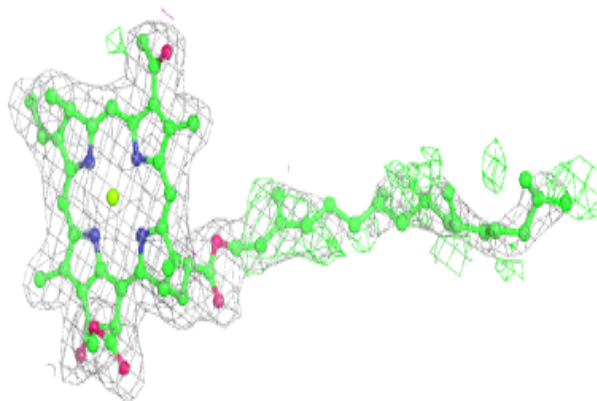
**Electron density around MQ7 M 501:**

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

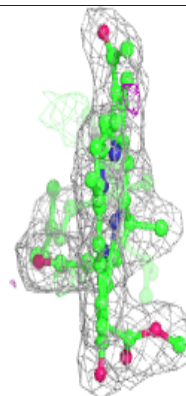
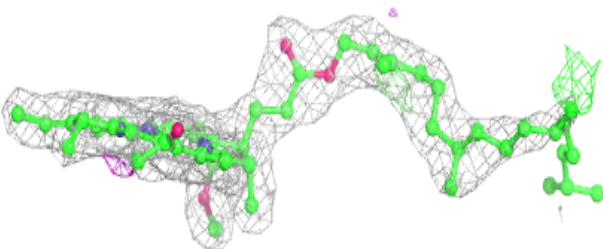
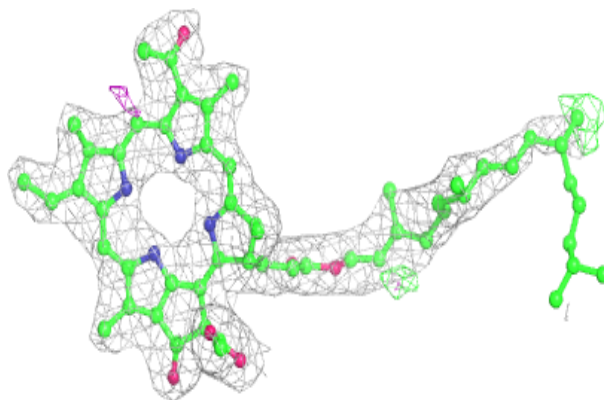


**Electron density around BCB M 805:**

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

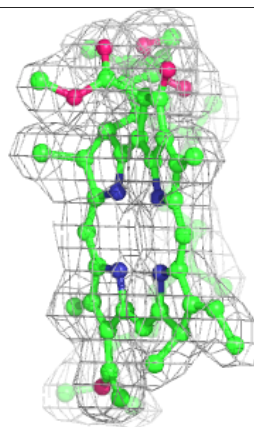
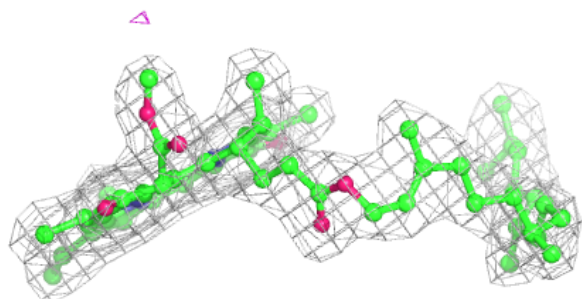
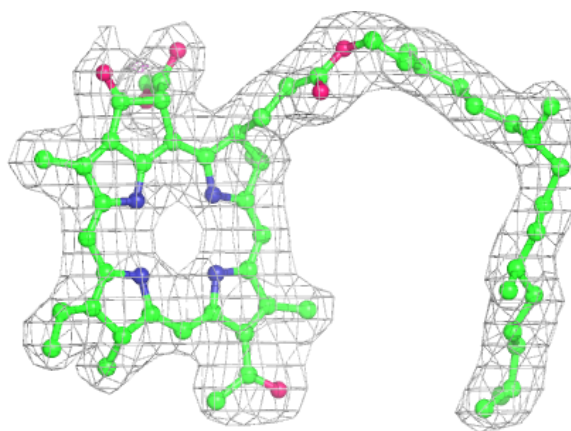
**Electron density around BPB M 401:**

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



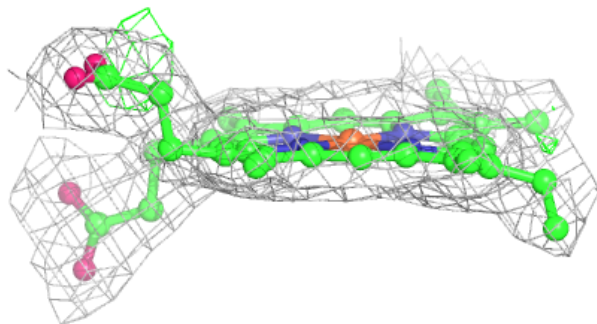
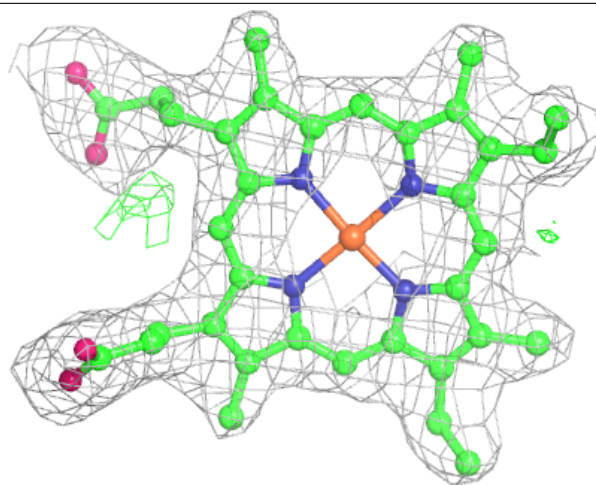
**Electron density around BPB L 402:**

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



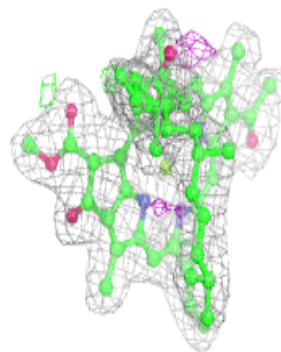
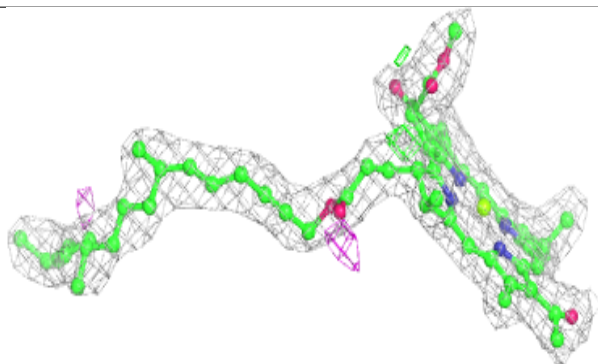
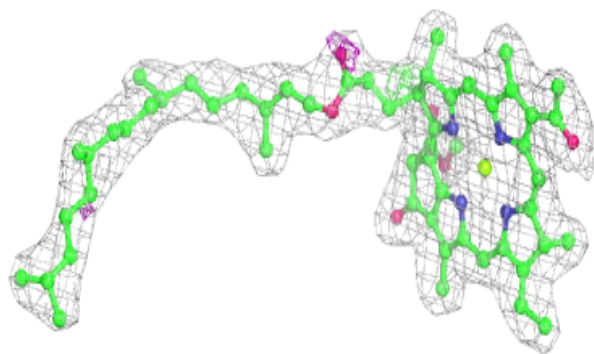
**Electron density around HEM C 337:**

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



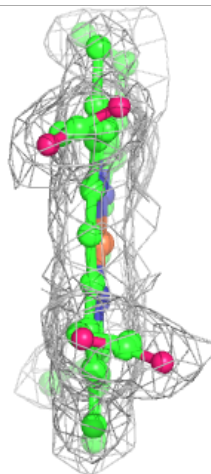
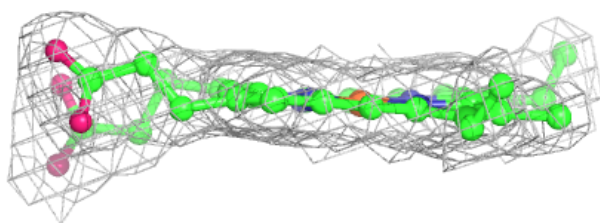
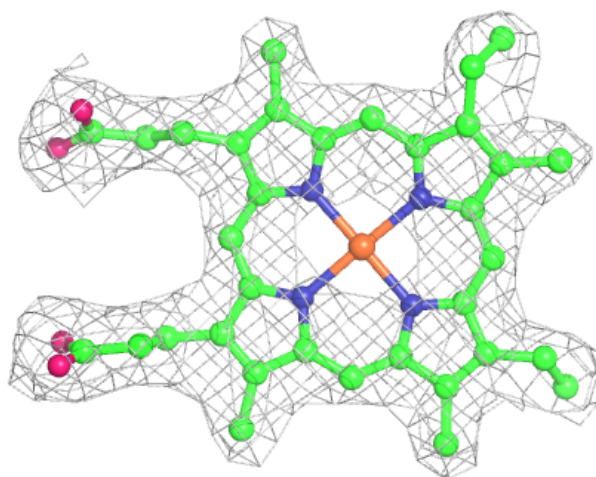
**Electron density around BCB M 806:**

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



**Electron density around HEM C 340:**

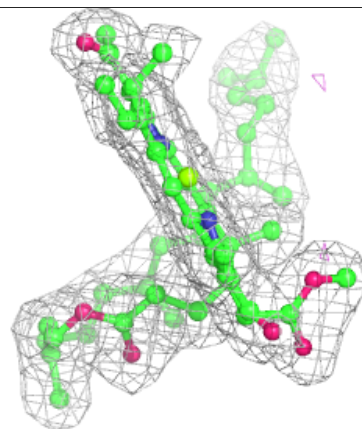
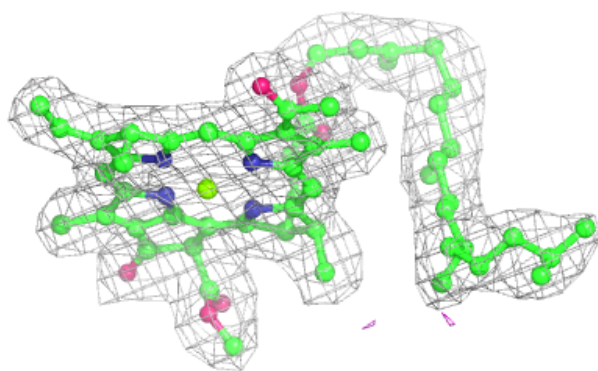
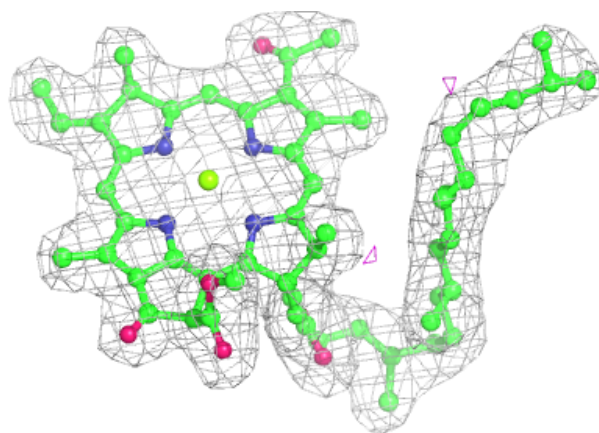
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around BCB L 304:**

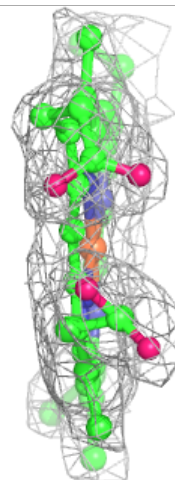
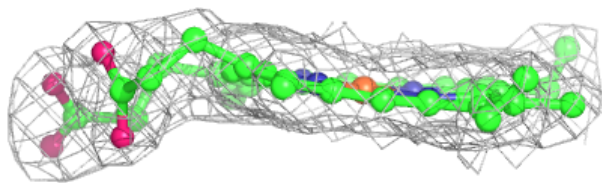
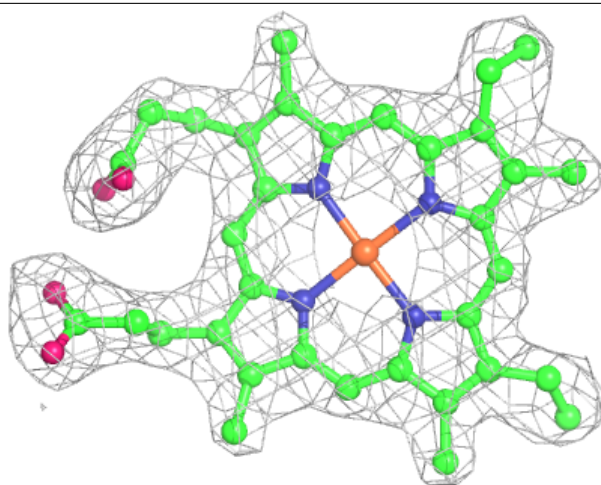
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





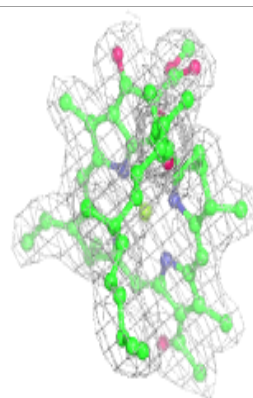
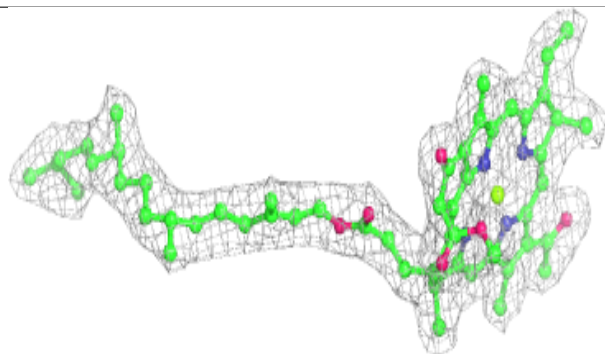
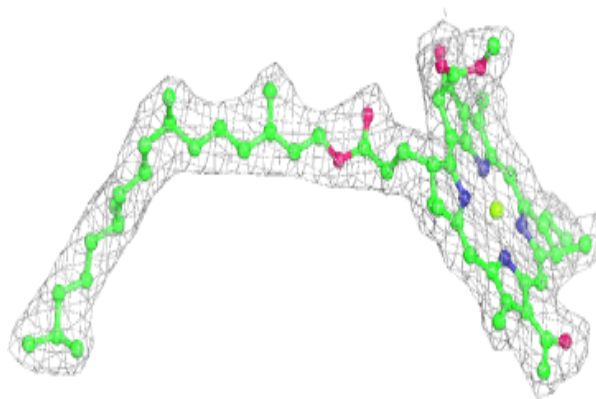
**Electron density around HEM C 338:**

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



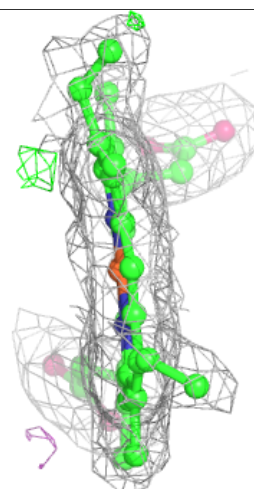
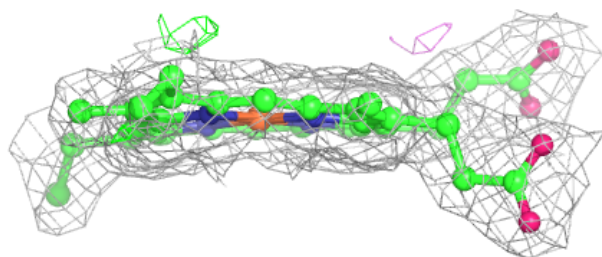
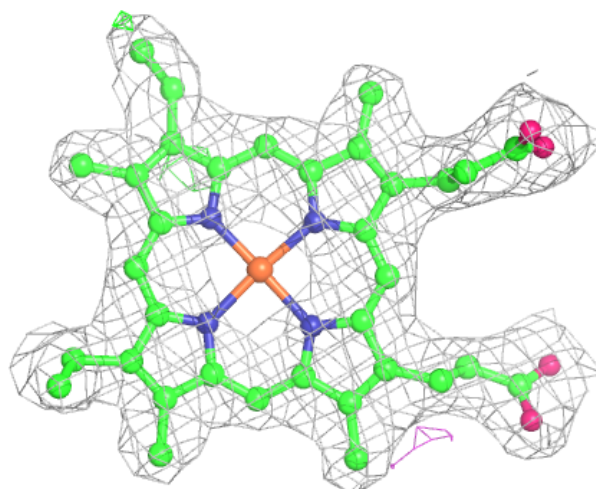
**Electron density around BCB L 302:**

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



**Electron density around HEM C 339:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.