



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:10 PM UTC

PDB ID : 7PRC / pdb\_00007prc  
Title : PHOTOSYNTHETIC REACTION CENTER FROM RHODOPSEU-  
DOMONAS VIRIDIS (DG-420315 (TRIAZINE) COMPLEX)  
Authors : Lancaster, C.R.D.; Michel, H.  
Deposited on : 1997-08-01  
Resolution : 2.65 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.

The types of validation reports are described at

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

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

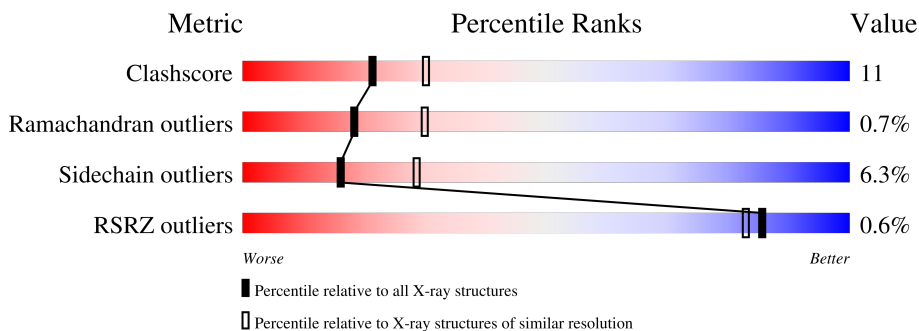
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 2.65 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	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	 75% 20%
2	L	273	 77% 20%
3	M	323	 75% 23%
4	H	258	 2% 69% 28%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	BCB	L	302	X	-	-	-
6	BCB	L	304	X	-	-	-
6	BCB	M	805	X	-	-	-
6	BCB	M	806	X	-	-	-
7	BPB	L	402	X	-	-	-

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 10476 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	332	2607	1642	467	480	18	51	1	0

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	273	2171	1459	350	355	7	14	0	0

- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

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

- Molecule 4 is a protein called PHOTOSYNTHETIC REACTION CENTER.

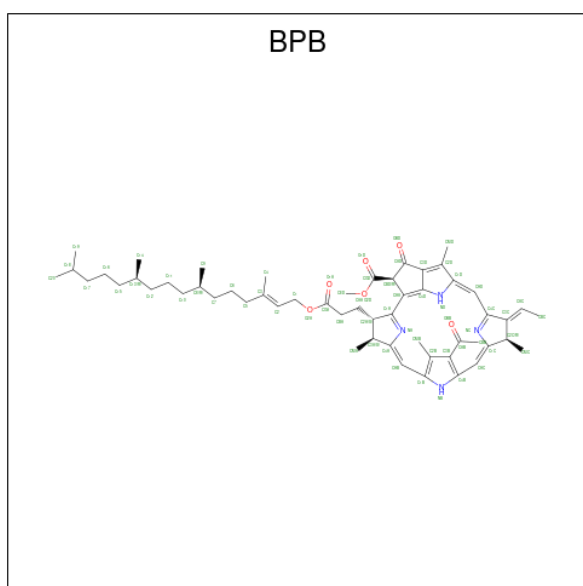
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	258	2018	1292	344	380	2	122	0	0

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



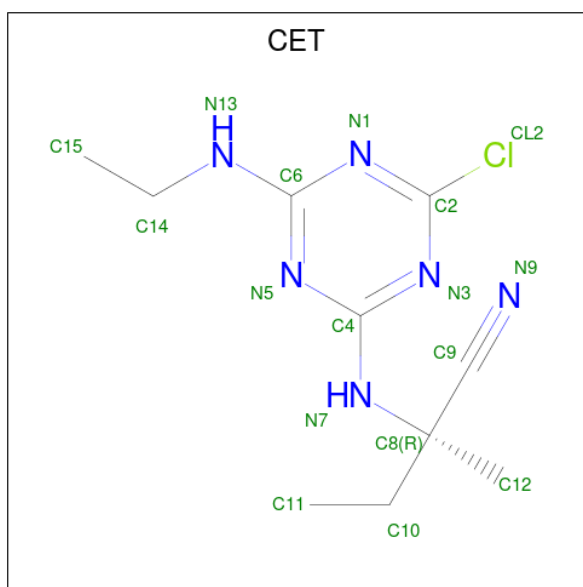
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



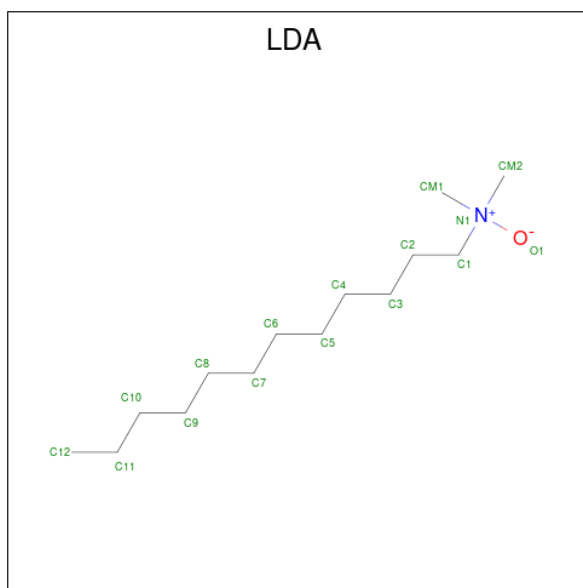
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	7	0
			65	55	4	6		
7	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 8 is 2-CHLORO-4-ETHYLAMINO-6-(R(+)-2'-CYANO-4-BUTYLAMINO)-1,3,5-TRIAZINE (CCD ID: CET) (formula:  $C_{10}H_{15}ClN_6$ ).



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

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



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

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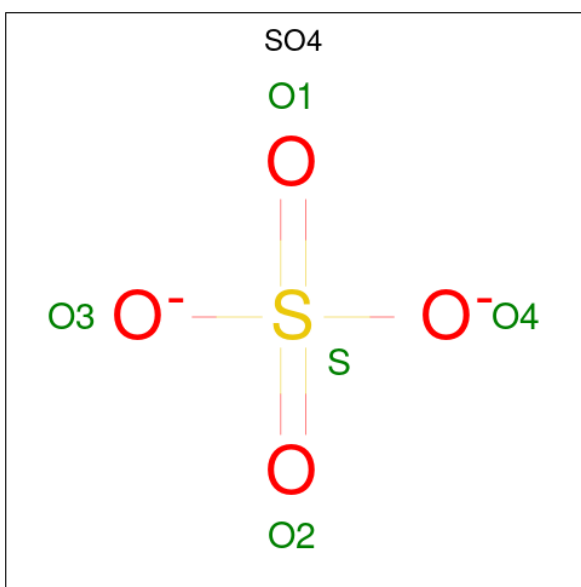
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	M	1	Total	C	N	O	5	0
			16	14	1	1		
9	M	1	Total	C	N	O	4	0
			16	14	1	1		
9	H	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 10 is FE (II) ION (CCD ID: FE2) (formula: Fe).

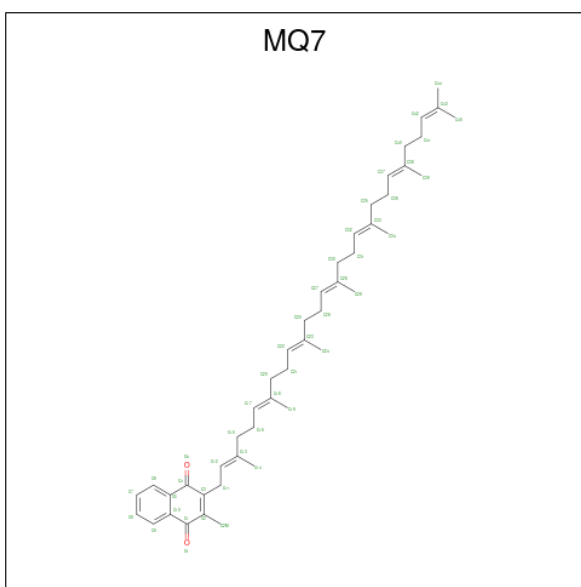
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	1	Total	Fe	0	0
			1	1		

- Molecule 11 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



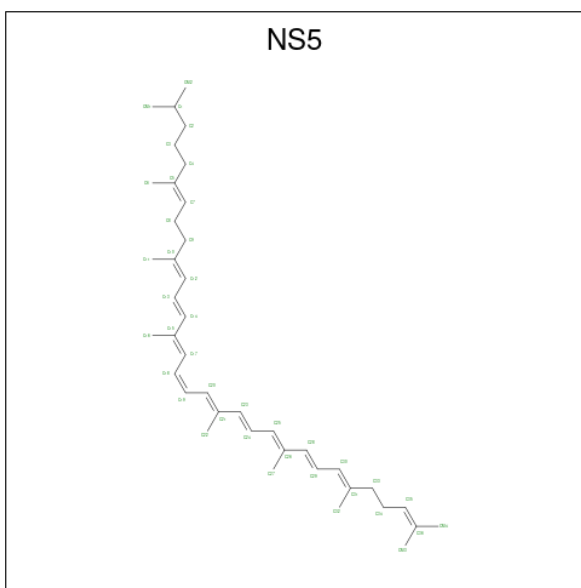
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	M	1	Total	O	S	0	0
			5	4	1		
11	M	1	Total	O	S	0	0
			5	4	1		
11	M	1	Total	O	S	0	0
			5	4	1		
11	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 12 is MENAQUINONE-7 (CCD ID: MQ7) (formula: C<sub>46</sub>H<sub>64</sub>O<sub>2</sub>).



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 (CCD ID: NS5) (formula: C<sub>40</sub>H<sub>60</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	M	1	Total	C	4	0
			40	40		

- Molecule 14 is water.

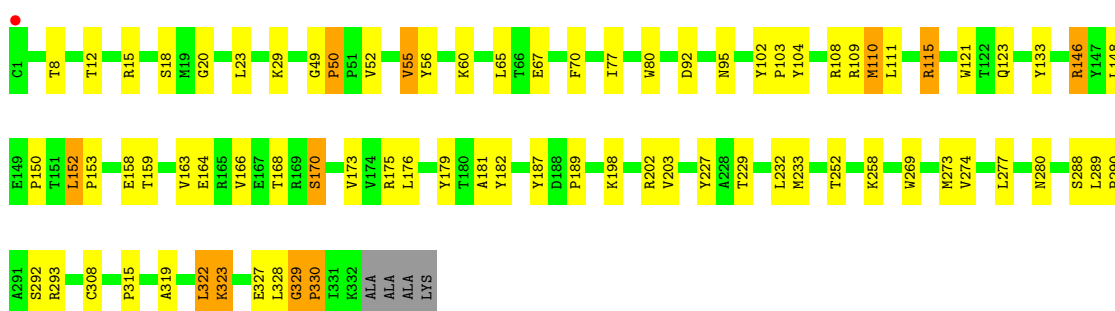
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
14	C	118	Total 118	O 118	0	0
14	L	55	Total 55	O 55	0	0
14	M	78	Total 78	O 78	0	0
14	H	64	Total 64	O 64	0	0

### 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.

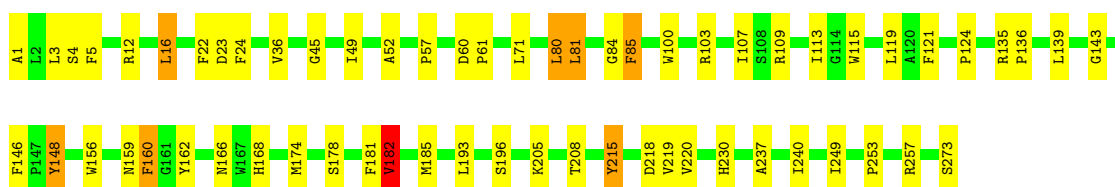
- Molecule 1: PHOTOSYNTHETIC REACTION CENTER

Chain C: 



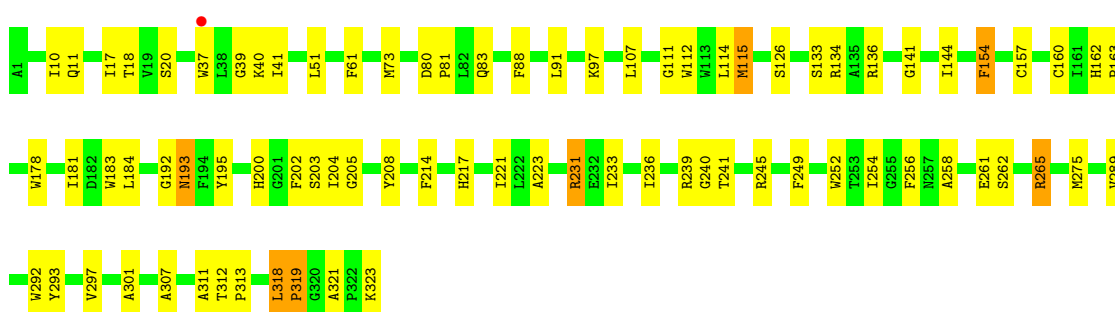
- Molecule 2: PHOTOSYNTHETIC REACTION CENTER

Chain L: 

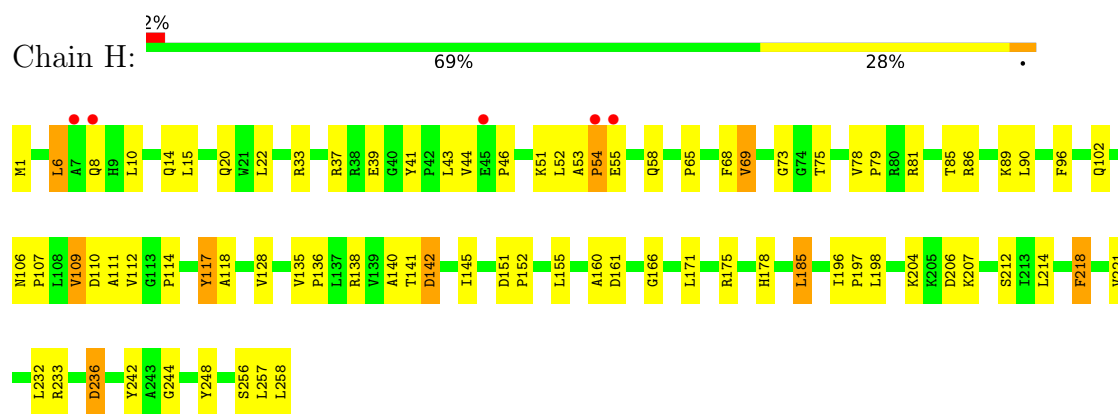


- Molecule 3: PHOTOSYNTHETIC REACTION CENTER

Chain M: 



- 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 – 2.65 10.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	88.3 (10.00-2.65) 86.5 (10.00-2.65)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.59 (at 2.61Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.184 , 0.231 0.180 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtrriage
Anisotropy	0.039	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 88.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10476	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.70	0/2674	0.96	4/3645 (0.1%)
2	L	0.71	0/2259	0.89	1/3084 (0.0%)
3	M	0.70	0/2683	0.93	5/3669 (0.1%)
4	H	0.92	3/2055 (0.1%)	1.05	8/2807 (0.3%)
All	All	0.75	3/9671 (0.0%)	0.96	18/13205 (0.1%)

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	4
2	L	0	7
3	M	0	5
4	H	0	2
All	All	0	18

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	54	PRO	C-N	24.52	1.68	1.33
4	H	52	LEU	C-N	-8.88	1.19	1.33
4	H	46	PRO	C-N	6.88	1.42	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	52	LEU	O-C-N	-21.21	93.41	122.04
1	C	50	PRO	CB-CA-C	-10.64	97.93	110.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	52	LEU	CA-C-N	7.62	144.09	122.21
4	H	52	LEU	C-N-CA	7.62	144.09	122.21
3	M	312	THR	CA-C-N	7.46	127.46	119.78
3	M	312	THR	C-N-CA	7.46	127.46	119.78
1	C	55	VAL	N-CA-C	6.98	117.69	110.36
1	C	50	PRO	N-CA-C	6.38	118.49	110.70
4	H	44	VAL	O-C-N	6.34	129.97	122.36
2	L	182	VAL	CB-CA-C	-6.27	103.57	112.22
4	H	53	ALA	CB-CA-C	-5.97	99.92	108.88
4	H	73	GLY	N-CA-C	5.96	117.62	111.95
3	M	301	ALA	N-CA-C	5.95	117.44	111.07
3	M	318	LEU	CA-C-N	5.87	127.18	119.84
3	M	318	LEU	C-N-CA	5.87	127.18	119.84
4	H	68	PHE	CA-C-N	-5.39	116.00	122.90
4	H	68	PHE	C-N-CA	-5.39	116.00	122.90
1	C	329	GLY	C-N-CD	-5.03	109.53	120.60

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	15	ARG	Sidechain
1	C	187	TYR	Sidechain
1	C	202	ARG	Sidechain
1	C	227	TYR	Sidechain
4	H	117	TYR	Sidechain
4	H	218	PHE	Sidechain
2	L	103	ARG	Sidechain
2	L	148	TYR	Sidechain
2	L	160	PHE	Sidechain
2	L	162	TYR	Sidechain
2	L	215	TYR	Sidechain
2	L	257	ARG	Sidechain
2	L	85	PHE	Sidechain
3	M	154	PHE	Sidechain
3	M	231	ARG	Sidechain
3	M	249	PHE	Sidechain
3	M	265	ARG	Sidechain
3	M	61	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	54	0
2	L	2171	0	2098	48	0
3	M	2577	0	2468	60	0
4	H	2018	0	2019	51	0
5	C	172	0	120	6	0
6	L	132	0	144	8	0
6	M	132	0	144	13	0
7	L	130	0	148	18	0
8	L	17	0	15	1	0
9	H	16	0	31	1	0
9	L	16	0	31	0	0
9	M	64	0	124	5	0
10	M	1	0	0	0	0
11	H	5	0	0	0	0
11	M	15	0	0	1	0
12	M	48	0	64	1	0
13	M	40	0	60	7	0
14	C	118	0	0	3	0
14	H	64	0	0	0	0
14	L	55	0	0	1	0
14	M	78	0	0	2	0
All	All	10476	0	10041	215	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (215) 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)
4:H:54:PRO:C	4:H:55:GLU:N	1.68	1.48
7:L:402:BPB:HHC	7:L:402:BPB:HBBB	1.54	0.90
6:M:805:BCB:HBB2	6:M:805:BCB:HHC	1.57	0.85
7:L:402:BPB:HHC	7:L:402:BPB:CBB	2.09	0.83
2:L:181:PHE:HB3	7:L:401:BPB:CBB	2.10	0.81
1:C:65:LEU:HD11	1:C:327:GLU:HG2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:152:PRO:HA	4:H:155:LEU:HD12	1.67	0.76
1:C:152:LEU:HB3	1:C:164:GLU:HG2	1.69	0.75
7:L:401:BPB:H4B	6:M:806:BCB:H172	1.69	0.75
9:M:701:LDA:HM21	9:M:705:LDA:H22	1.71	0.73
1:C:123[A]:GLN:HG3	1:C:269:TRP:CE3	2.24	0.73
3:M:107:LEU:HD22	3:M:112:TRP:CE2	2.26	0.71
2:L:178:SER:O	2:L:182:VAL:HG23	1.91	0.70
3:M:160:CYS:SG	13:M:600:NS5:C31	2.80	0.69
3:M:160:CYS:SG	13:M:600:NS5:H332	2.34	0.68
4:H:160:ALA:HB3	4:H:214:LEU:HD23	1.76	0.68
2:L:80:LEU:HA	2:L:84:GLY:HA3	1.73	0.67
4:H:161:ASP:HB3	4:H:214:LEU:HD22	1.77	0.67
1:C:258:LYS:HG2	3:M:307:ALA:HB2	1.77	0.66
1:C:52:VAL:HB	1:C:56:TYR:HD2	1.60	0.65
1:C:323:LYS:H	1:C:323:LYS:HD3	1.62	0.65
6:M:805:BCB:HHC	6:M:805:BCB:CBB	2.26	0.64
2:L:208:THR:HG21	4:H:128:VAL:HG23	1.79	0.64
4:H:117:TYR:HB2	4:H:236:ASP:HB3	1.80	0.64
1:C:52:VAL:HG13	1:C:65:LEU:O	1.98	0.64
1:C:290:PRO:HG2	1:C:293:ARG:HG2	1.79	0.64
3:M:202:PHE:CE2	4:H:20:GLN:HG2	2.32	0.63
3:M:195:TYR:CE2	6:M:806:BCB:HMC2	2.34	0.63
7:L:401:BPB:HBBB	7:L:401:BPB:HHC	1.80	0.63
6:L:302:BCB:OBB	6:L:302:BCB:HHC	1.99	0.63
3:M:107:LEU:HA	3:M:111:GLY:HA3	1.80	0.63
2:L:205:LYS:HA	4:H:69:VAL:HG22	1.80	0.63
1:C:152:LEU:HD22	1:C:175:ARG:HA	1.81	0.62
4:H:107:PRO:HA	4:H:110:ASP:HB2	1.82	0.62
3:M:160:CYS:SG	13:M:600:NS5:H322	2.40	0.61
1:C:323:LYS:H	1:C:323:LYS:CD	2.14	0.61
3:M:195:TYR:CZ	6:M:806:BCB:HMC2	2.36	0.61
3:M:178:TRP:HA	3:M:178:TRP:CE3	2.36	0.60
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.36	0.60
2:L:185:MET:SD	6:M:805:BCB:H41	2.41	0.60
6:M:805:BCB:HBB3	6:M:806:BCB:H41	1.83	0.60
3:M:231:ARG:HD2	14:M:1013:HOH:O	2.02	0.59
2:L:230:HIS:CD2	3:M:221:ILE:HG13	2.37	0.59
3:M:73:MET:HE1	3:M:88:PHE:CE1	2.37	0.58
7:L:401:BPB:HBBB	7:L:401:BPB:CHC	2.33	0.58
3:M:136:ARG:HE	3:M:136:ARG:HA	1.69	0.58
1:C:8:THR:HB	1:C:23:LEU:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:54:PRO:C	4:H:55:GLU:CA	2.73	0.58
2:L:215:TYR:O	2:L:219:VAL:HG23	2.03	0.57
4:H:37:ARG:HG2	4:H:41:TYR:CZ	2.39	0.57
4:H:86:ARG:NH2	4:H:111:ALA:O	2.36	0.57
1:C:56:TYR:HB3	5:C:337:HEM:O2A	2.04	0.57
2:L:181:PHE:HB3	7:L:401:BPB:HBB	1.86	0.57
7:L:402:BPB:HBB	3:M:208:TYR:CD2	2.40	0.57
1:C:121:TRP:HA	1:C:123[A]:GLN:HE21	1.70	0.57
4:H:136:PRO:HG2	4:H:138:ARG:HG2	1.86	0.57
1:C:189:PRO:HB3	1:C:232:LEU:HA	1.86	0.56
2:L:181:PHE:CD2	7:L:401:BPB:HBB	2.41	0.56
8:L:502:CET:N3	8:L:502:CET:H101	2.21	0.56
4:H:55:GLU:HB3	4:H:58:GLN:HG3	1.88	0.55
4:H:90:LEU:HA	4:H:102:GLN:O	2.06	0.55
1:C:52:VAL:HB	1:C:56:TYR:CD2	2.41	0.55
4:H:155:LEU:HD22	4:H:206:ASP:C	2.32	0.55
2:L:124:PRO:HB2	6:L:302:BCB:H93	1.89	0.54
6:L:304:BCB:OBB	6:L:304:BCB:HHC	2.07	0.54
3:M:192:GLY:O	3:M:193:ASN:HB3	2.06	0.54
4:H:166:GLY:HA3	4:H:185:LEU:HD12	1.89	0.54
2:L:220:VAL:HG11	7:L:401:BPB:HEDA	1.89	0.54
4:H:218:PHE:HA	4:H:221:VAL:HG23	1.89	0.54
2:L:109:ARG:HD2	14:L:1243:HOH:O	2.08	0.53
3:M:178:TRP:HA	3:M:178:TRP:HE3	1.72	0.53
4:H:114:PRO:HB2	4:H:244:GLY:HA2	1.90	0.53
7:L:401:BPB:HBCA	3:M:275:MET:HG2	1.90	0.53
4:H:152:PRO:HD2	4:H:171:LEU:HD11	1.90	0.53
1:C:170:SER:HB2	3:M:83:GLN:HG3	1.90	0.53
3:M:160:CYS:C	3:M:163:PRO:HD2	2.35	0.52
2:L:185:MET:SD	6:M:805:BCB:C4	2.97	0.52
1:C:323:LYS:HD3	1:C:323:LYS:N	2.25	0.52
2:L:139:LEU:HD21	2:L:253:PRO:HD3	1.92	0.52
2:L:12:ARG:HD3	4:H:102:GLN:NE2	2.26	0.51
1:C:319:ALA:HB2	14:C:1169:HOH:O	2.11	0.51
4:H:233:ARG:O	4:H:233:ARG:HG2	2.11	0.50
1:C:50:PRO:HB2	1:C:55:VAL:HG23	1.91	0.50
2:L:22:PHE:HA	2:L:24:PHE:CE1	2.47	0.50
2:L:193:LEU:HB2	3:M:144:ILE:HD11	1.94	0.50
4:H:78:VAL:HA	4:H:79:PRO:C	2.36	0.50
2:L:81:LEU:HD23	2:L:85:PHE:CE2	2.47	0.50
3:M:160:CYS:SG	13:M:600:NS5:C30	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:289:VAL:HG11	3:M:292:TRP:CD2	2.47	0.50
2:L:124:PRO:HB2	6:L:302:BCB:C9	2.42	0.50
3:M:160:CYS:SG	13:M:600:NS5:C32	2.99	0.50
1:C:252:THR:HG23	1:C:252:THR:O	2.11	0.49
2:L:166:ASN:OD1	2:L:168:HIS:HB2	2.12	0.49
1:C:123[A]:GLN:HG3	1:C:269:TRP:CD2	2.47	0.49
4:H:106:ASN:ND2	4:H:109:VAL:HG23	2.28	0.49
4:H:145:ILE:HD13	4:H:151:ASP:HA	1.95	0.49
3:M:160:CYS:SG	13:M:600:NS5:C33	2.99	0.49
4:H:65:PRO:HA	4:H:79:PRO:HD2	1.95	0.49
2:L:205:LYS:HA	4:H:69:VAL:CG2	2.42	0.49
3:M:256:PHE:HB2	4:H:33:ARG:NH2	2.27	0.49
1:C:146:ARG:NH2	1:C:150:PRO:HA	2.28	0.48
4:H:65:PRO:HG3	9:H:703:LDA:H82	1.95	0.48
4:H:37:ARG:HG2	4:H:41:TYR:CE1	2.48	0.48
4:H:96:PHE:HD1	4:H:96:PHE:H	1.61	0.48
4:H:204:LYS:HB2	4:H:207:LYS:O	2.13	0.48
1:C:65:LEU:HD11	1:C:327:GLU:CG	2.40	0.48
7:L:402:BPB:HBBA	3:M:208:TYR:HB3	1.95	0.48
4:H:106:ASN:CG	4:H:109:VAL:HG23	2.39	0.48
2:L:148:TYR:CE1	7:L:402:BPB:H14	2.48	0.48
3:M:200:HIS:CE1	3:M:204:ILE:HD11	2.48	0.48
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.49	0.47
6:M:806:BCB:HAA2	6:M:806:BCB:HBD	1.97	0.47
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.97	0.47
4:H:145:ILE:CD1	4:H:151:ASP:HA	2.45	0.47
1:C:52:VAL:HA	1:C:55:VAL:HB	1.97	0.47
2:L:22:PHE:HA	2:L:24:PHE:HE1	1.79	0.47
2:L:1:ALA:N	4:H:43:LEU:HB3	2.30	0.47
6:L:302:BCB:HBB3	6:M:805:BCB:HMD2	1.96	0.47
2:L:16:LEU:HD12	2:L:16:LEU:HA	1.63	0.47
3:M:154:PHE:O	3:M:157:CYS:HB2	2.14	0.47
3:M:289:VAL:HG11	3:M:292:TRP:CE3	2.50	0.46
1:C:115:ARG:HA	1:C:328:LEU:O	2.15	0.46
3:M:293:TYR:O	3:M:297:VAL:HG23	2.16	0.46
2:L:196:SER:HB2	3:M:141:GLY:O	2.15	0.46
2:L:237:ALA:HA	2:L:240:ILE:HD12	1.97	0.46
1:C:123[A]:GLN:H	1:C:123[A]:GLN:NE2	2.14	0.46
1:C:179:TYR:HB2	14:C:914:HOH:O	2.14	0.46
2:L:113:ILE:HB	3:M:223:ALA:O	2.16	0.46
1:C:233:MET:HB3	5:C:339:HEM:C4B	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:GLY:HA2	1:C:330:PRO:C	2.41	0.46
2:L:45:GLY:O	2:L:49:ILE:HG13	2.16	0.46
7:L:401:BPB:C1B	6:M:805:BCB:H42	2.46	0.46
2:L:3:LEU:HD13	2:L:5:PHE:CZ	2.51	0.46
3:M:133:SER:OG	9:M:704:LDA:HM12	2.17	0.45
1:C:49:GLY:HA3	1:C:50:PRO:HD3	1.63	0.45
1:C:273:MET:O	1:C:277:LEU:HG	2.16	0.45
2:L:81:LEU:HD23	2:L:85:PHE:HE2	1.80	0.45
2:L:159:ASN:O	2:L:160:PHE:C	2.58	0.45
4:H:96:PHE:N	4:H:96:PHE:CD1	2.85	0.45
1:C:50:PRO:HB2	1:C:55:VAL:CG2	2.47	0.45
2:L:71:LEU:HD23	2:L:143:GLY:HA3	1.98	0.45
1:C:104:TYR:HE1	1:C:108:ARG:NH2	2.15	0.45
4:H:90:LEU:HD21	4:H:112:VAL:HB	1.99	0.45
1:C:110:MET:HB3	5:C:338:HEM:C4B	2.52	0.44
1:C:70:PHE:HE2	5:C:337:HEM:C2A	2.35	0.44
1:C:108:ARG:NH1	5:C:337:HEM:O2D	2.50	0.44
1:C:163:VAL:HB	2:L:273:SER:O	2.17	0.44
2:L:218:ASP:HB3	3:M:134:ARG:HD2	1.99	0.44
4:H:6:LEU:HD23	4:H:6:LEU:HA	1.77	0.44
1:C:123[A]:GLN:H	1:C:123[A]:GLN:CD	2.24	0.44
1:C:181:ALA:O	1:C:182:TYR:HB2	2.18	0.44
3:M:10:ILE:CG2	4:H:145:ILE:HG23	2.48	0.44
2:L:107:ILE:HG23	3:M:252:TRP:HE3	1.83	0.44
6:M:805:BCB:HBA2	6:M:805:BCB:C4A	2.47	0.44
1:C:18:SER:HB2	2:L:156:TRP:CD1	2.53	0.44
1:C:92:ASP:HB3	1:C:95:ASN:O	2.18	0.43
3:M:112:TRP:CZ2	9:M:706:LDA:H51	2.53	0.43
3:M:241:THR:O	3:M:245:ARG:HG3	2.18	0.43
1:C:173:VAL:HG13	14:C:1137:HOH:O	2.18	0.43
3:M:262:SER:O	3:M:265:ARG:HB2	2.18	0.43
4:H:196:ILE:HD12	4:H:242:TYR:CE1	2.53	0.43
1:C:109:ARG:NH2	1:C:280:ASN:O	2.52	0.43
2:L:115:TRP:CD1	2:L:115:TRP:N	2.86	0.43
1:C:308:CYS:O	1:C:315:PRO:HB3	2.18	0.43
13:M:600:NS5:H271	13:M:600:NS5:H29	1.71	0.43
4:H:114:PRO:HD2	4:H:248:TYR:CE2	2.53	0.43
7:L:401:BPB:H7A	7:L:401:BPB:H4	2.00	0.43
3:M:162:HIS:HD2	14:M:913:HOH:O	2.02	0.43
2:L:174:MET:HE3	6:M:805:BCB:HED3	2.01	0.43
3:M:183:TRP:CE3	3:M:184:LEU:HD23	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:239:ARG:HD3	4:H:39:GLU:OE1	2.18	0.43
3:M:240:GLY:HA2	4:H:118:ALA:CB	2.49	0.43
4:H:142:ASP:OD1	4:H:142:ASP:N	2.50	0.43
1:C:111:LEU:HD23	5:C:338:HEM:CBB	2.49	0.43
2:L:52:ALA:HB2	2:L:85:PHE:CG	2.53	0.43
3:M:112:TRP:O	3:M:115:MET:HB2	2.19	0.43
3:M:233:ILE:O	3:M:236:ILE:HB	2.19	0.42
4:H:10:LEU:HD21	4:H:15:LEU:HD21	2.01	0.42
1:C:12:THR:OG1	1:C:20:GLY:HA2	2.19	0.42
3:M:115:MET:HE2	3:M:115:MET:HA	2.01	0.42
2:L:80:LEU:HA	2:L:80:LEU:HD12	1.85	0.42
1:C:322:LEU:HD11	1:C:330:PRO:HD3	2.00	0.42
3:M:217:HIS:CE1	3:M:221:ILE:HD11	2.55	0.42
4:H:69:VAL:HA	4:H:75:THR:HG22	2.01	0.42
4:H:135:VAL:HG23	4:H:140:ALA:HB2	2.01	0.42
2:L:60:ASP:HA	2:L:61:PRO:HD3	1.80	0.42
3:M:11:GLN:OE1	3:M:39:GLY:HA3	2.20	0.42
2:L:100:TRP:CH2	12:M:501:MQ7:H301	2.55	0.42
2:L:160:PHE:C	2:L:160:PHE:CD1	2.98	0.42
6:L:304:BCB:H92	6:L:304:BCB:H62	1.75	0.42
11:M:804:SO4:O4	9:M:704:LDA:H22	2.20	0.42
2:L:121:PHE:O	2:L:124:PRO:HG2	2.19	0.42
3:M:17:ILE:HG13	4:H:178:HIS:CE1	2.55	0.42
3:M:318:LEU:HB2	3:M:321:ALA:HB2	2.02	0.42
6:L:304:BCB:HMB1	6:L:304:BCB:HBB3	2.02	0.41
1:C:77:ILE:HD11	1:C:111:LEU:HD21	2.02	0.41
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.55	0.41
2:L:146:PHE:HB3	2:L:156:TRP:CD2	2.56	0.41
3:M:236:ILE:HG12	3:M:261:GLU:HB2	2.01	0.41
3:M:311:ALA:O	3:M:313:PRO:HD3	2.20	0.41
1:C:153:PRO:HG2	1:C:158:GLU:HB2	2.03	0.41
7:L:401:BPB:H4	7:L:401:BPB:C7	2.50	0.41
3:M:275:MET:HE2	3:M:275:MET:HA	2.01	0.41
3:M:73:MET:HE3	3:M:91:LEU:HB2	2.02	0.41
1:C:289:LEU:HD22	1:C:293:ARG:HG3	2.01	0.41
3:M:258:ALA:HB1	3:M:262:SER:OG	2.21	0.41
3:M:205:GLY:HA3	9:M:701:LDA:H121	2.03	0.40
4:H:232:LEU:HD23	4:H:232:LEU:HA	1.89	0.40
3:M:80:ASP:HA	3:M:81:PRO:HD2	1.87	0.40
3:M:318:LEU:HA	3:M:319:PRO:HD2	1.64	0.40
7:L:401:BPB:H4	7:L:401:BPB:H6	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:304:BCB:HMB2	7:L:402:BPB:HMBA	2.04	0.40
4:H:196:ILE:HG13	4:H:197:PRO:HD2	2.03	0.40
1:C:60:LYS:HB2	1:C:108:ARG:NH1	2.36	0.40
3:M:202:PHE:CZ	4:H:20:GLN:HG2	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	331/336 (98%)	314 (95%)	14 (4%)	3 (1%)	14	24
2	L	271/273 (99%)	255 (94%)	14 (5%)	2 (1%)	18	30
3	M	323/323 (100%)	308 (95%)	12 (4%)	3 (1%)	14	24
4	H	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
All	All	1181/1190 (99%)	1118 (95%)	55 (5%)	8 (1%)	18	30

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	51	LEU
3	M	193	ASN
2	L	57	PRO
1	C	67	GLU
2	L	23	ASP
1	C	148	LEU
3	M	319	PRO
1	C	330	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	281/282 (100%)	263 (94%)	18 (6%)	16	28
2	L	218/218 (100%)	210 (96%)	8 (4%)	30	50
3	M	251/249 (101%)	237 (94%)	14 (6%)	19	32
4	H	212/212 (100%)	192 (91%)	20 (9%)	8	13
All	All	962/961 (100%)	902 (94%)	60 (6%)	16	29

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	29	LYS
1	C	110	MET
1	C	115	ARG
1	C	146	ARG
1	C	152	LEU
1	C	159	THR
1	C	166	VAL
1	C	168	THR
1	C	170	SER
1	C	176	LEU
1	C	198	LYS
1	C	203	VAL
1	C	229	THR
1	C	274	VAL
1	C	288	SER
1	C	292	SER
1	C	322	LEU
1	C	323	LYS
2	L	4	SER
2	L	16	LEU
2	L	36	VAL
2	L	80	LEU
2	L	81	LEU
2	L	119	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	L	182	VAL
2	L	249	ILE
3	M	18	THR
3	M	20	SER
3	M	37	TRP
3	M	40	LYS
3	M	41	ILE
3	M	97	LYS
3	M	114	LEU
3	M	115	MET
3	M	126	SER
3	M	181	ILE
3	M	203	SER
3	M	214	PHE
3	M	254	ILE
3	M	323	LYS
4	H	6	LEU
4	H	8	GLN
4	H	14	GLN
4	H	22	LEU
4	H	51	LYS
4	H	69	VAL
4	H	81	ARG
4	H	85	THR
4	H	89	LYS
4	H	109	VAL
4	H	141	THR
4	H	142	ASP
4	H	175	ARG
4	H	185	LEU
4	H	198	LEU
4	H	212	SER
4	H	236	ASP
4	H	256	SER
4	H	257	LEU
4	H	258	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	297	GLN
2	L	239	ASN

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Mol	Chain	Res	Type
3	M	147	ASN
4	H	102	GLN
4	H	178	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FME	H	1	4	8,9,10	0.63	0	8,9,11	2.64	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FME	H	1	4	-	3/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	FME	O1-CN-N	-5.76	110.45	125.32
4	H	1	FME	CA-N-CN	-4.04	116.60	122.82

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

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
6	BCB	L	302	2	60,74,74	1.75	9 (15%)	59,115,115	2.37	16 (27%)
6	BCB	L	304	2	60,74,74	1.74	9 (15%)	59,115,115	2.99	18 (30%)
9	LDA	M	701	-	13,15,15	3.17	2 (15%)	14,17,17	0.72	0
11	SO4	M	804	-	4,4,4	0.73	0	6,6,6	0.67	0
6	BCB	M	806	3	60,74,74	1.73	12 (20%)	59,115,115	2.98	17 (28%)
9	LDA	M	706	-	13,15,15	2.43	2 (15%)	14,17,17	0.49	0
5	HEM	C	339	1	50,50,50	1.40	5 (10%)	67,82,82	1.20	8 (11%)
5	HEM	C	338	1	50,50,50	1.34	3 (6%)	67,82,82	1.04	4 (5%)
8	CET	L	502	-	16,17,17	1.36	2 (12%)	21,23,23	0.88	1 (4%)
11	SO4	H	801	-	4,4,4	0.51	0	6,6,6	0.31	0
9	LDA	H	703	-	13,15,15	2.71	2 (15%)	14,17,17	0.68	0
5	HEM	C	337	1	50,50,50	1.43	6 (12%)	67,82,82	1.12	6 (8%)
7	BPB	L	401	-	57,70,70	1.77	10 (17%)	55,101,101	2.75	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	BPB	L	402	-	57,70,70	1.88	11 (19%)	55,101,101	2.44	14 (25%)
12	MQ7	M	501	-	49,49,49	1.51	12 (24%)	61,63,63	1.65	14 (22%)
9	LDA	M	704	-	13,15,15	1.99	2 (15%)	14,17,17	0.54	0
13	NS5	M	600	-	39,39,39	0.73	1 (2%)	46,46,46	1.17	7 (15%)
11	SO4	M	803	-	4,4,4	0.58	0	6,6,6	0.73	0
9	LDA	L	702	-	13,15,15	2.27	2 (15%)	14,17,17	0.53	0
11	SO4	M	802	-	4,4,4	0.54	0	6,6,6	0.80	0
6	BCB	M	805	3	60,74,74	1.72	11 (18%)	59,115,115	2.65	17 (28%)
5	HEM	C	340	1	50,50,50	1.56	8 (16%)	67,82,82	1.28	9 (13%)
9	LDA	M	705	-	13,15,15	2.55	2 (15%)	14,17,17	0.50	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	L	302	2	3/3/21/26	7/37/137/137	-
6	BCB	L	304	2	2/2/21/26	6/37/137/137	-
9	LDA	M	701	-	-	5/13/13/13	-
6	BCB	M	806	3	3/3/21/26	12/37/137/137	-
9	LDA	M	706	-	-	4/13/13/13	-
5	HEM	C	339	1	-	5/14/54/54	-
5	HEM	C	338	1	-	8/14/54/54	-
8	CET	L	502	-	-	0/11/14/14	0/1/1/1
9	LDA	H	703	-	-	3/13/13/13	-
5	HEM	C	337	1	-	6/14/54/54	-
7	BPB	L	401	-	-	7/37/105/105	0/5/6/6
7	BPB	L	402	-	1/1/18/23	4/37/105/105	0/5/6/6
12	MQ7	M	501	-	-	2/41/61/61	0/2/2/2
9	LDA	M	704	-	-	6/13/13/13	-
9	LDA	L	702	-	-	4/13/13/13	-
6	BCB	M	805	3	3/3/21/26	11/37/137/137	-
5	HEM	C	340	1	-	5/14/54/54	-
9	LDA	M	705	-	-	1/13/13/13	-
13	NS5	M	600	-	-	14/43/43/43	-

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	701	LDA	O1-N1	-8.18	1.22	1.42
9	M	701	LDA	C1-N1	-7.87	1.43	1.51
9	H	703	LDA	O1-N1	-7.46	1.23	1.42
9	L	702	LDA	O1-N1	-7.43	1.23	1.42
9	M	705	LDA	O1-N1	-7.21	1.24	1.42
9	M	706	LDA	O1-N1	-7.19	1.24	1.42
6	M	806	BCB	C1D-C2D	6.61	1.47	1.39
6	M	805	BCB	C1D-C2D	6.42	1.46	1.39
9	M	704	LDA	O1-N1	-6.31	1.26	1.42
9	H	703	LDA	C1-N1	-6.25	1.45	1.51
7	L	402	BPB	C1B-C2B	6.09	1.46	1.39
6	L	302	BCB	C1D-C2D	6.07	1.46	1.39
9	M	705	LDA	C1-N1	-5.69	1.45	1.51
6	L	304	BCB	C1B-C2B	5.68	1.46	1.39
7	L	401	BPB	C1B-C2B	5.67	1.45	1.39
6	L	304	BCB	C1D-C2D	5.67	1.46	1.39
7	L	401	BPB	C1D-C2D	5.50	1.45	1.39
5	C	340	HEM	CBC-CAC	5.46	1.56	1.30
7	L	402	BPB	C1D-C2D	5.38	1.45	1.39
7	L	402	BPB	C3A-C2A	-5.32	1.50	1.54
5	C	339	HEM	CBC-CAC	5.16	1.55	1.30
5	C	339	HEM	CBB-CAB	5.03	1.54	1.30
6	L	304	BCB	C3A-C2A	-5.02	1.50	1.54
9	M	706	LDA	C1-N1	-4.90	1.46	1.51
7	L	402	BPB	O2D-CED	-4.88	1.34	1.45
5	C	337	HEM	CBB-CAB	4.75	1.53	1.30
5	C	337	HEM	CBC-CAC	4.65	1.52	1.30
5	C	338	HEM	CBC-CAC	4.59	1.52	1.30
7	L	401	BPB	O2A-CGA	4.57	1.46	1.33
6	M	805	BCB	C1-C2	-4.51	1.36	1.49
6	L	302	BCB	C1B-C2B	4.49	1.44	1.39
6	M	805	BCB	O2D-CED	-4.35	1.35	1.45
6	L	302	BCB	O2D-CED	-4.32	1.35	1.45
5	C	340	HEM	CBB-CAB	4.28	1.51	1.30
5	C	338	HEM	CBB-CAB	4.15	1.50	1.30
7	L	402	BPB	C3B-C4B	4.12	1.48	1.41
6	M	805	BCB	C3A-C2A	-4.07	1.51	1.54
6	L	302	BCB	C3A-C2A	-4.02	1.51	1.54
6	L	302	BCB	MG-ND	-3.88	1.98	2.05
6	L	304	BCB	C3B-C4B	3.87	1.47	1.41
8	L	502	CET	C9-N9	3.74	1.19	1.14
6	M	806	BCB	C1B-C2B	3.71	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	806	BCB	C3A-C2A	-3.59	1.51	1.54
6	M	806	BCB	C3B-C4B	3.45	1.46	1.41
6	L	302	BCB	C1-C2	-3.35	1.39	1.49
7	L	401	BPB	C3A-C2A	-3.35	1.51	1.54
6	M	805	BCB	C1B-C2B	3.29	1.43	1.39
6	L	302	BCB	O2D-CGD	3.29	1.41	1.33
12	M	501	MQ7	C32-C33	3.28	1.40	1.33
9	M	704	LDA	C1-N1	-3.26	1.48	1.51
9	L	702	LDA	C1-N1	-3.19	1.48	1.51
5	C	340	HEM	FE-NA	3.18	2.05	1.95
6	L	304	BCB	MG-ND	-3.16	1.99	2.05
12	M	501	MQ7	C11-C12	-3.11	1.45	1.50
12	M	501	MQ7	C21-C22	-3.09	1.41	1.50
7	L	402	BPB	CMD-C2D	2.99	1.57	1.51
5	C	338	HEM	FE-NC	2.99	2.05	1.95
6	M	806	BCB	CHC-C1C	2.98	1.42	1.38
6	M	805	BCB	C3B-C4B	2.98	1.46	1.41
6	M	806	BCB	MG-ND	-2.94	2.00	2.05
7	L	401	BPB	C2-C3	2.89	1.39	1.33
6	M	805	BCB	O2A-CGA	2.88	1.41	1.33
6	L	304	BCB	C3D-C2D	-2.88	1.34	1.39
5	C	340	HEM	FE-NB	2.83	2.03	1.94
6	M	806	BCB	CAA-CBA	-2.80	1.44	1.52
7	L	401	BPB	CHA-CBD	2.77	1.54	1.51
5	C	339	HEM	CAC-C3C	2.75	1.54	1.47
7	L	402	BPB	O2D-CGD	2.74	1.40	1.33
7	L	401	BPB	O2D-CGD	2.71	1.39	1.33
13	M	600	NS5	C22-C21	-2.70	1.45	1.50
7	L	402	BPB	C2-C3	2.69	1.39	1.33
6	L	304	BCB	O2D-CGD	2.68	1.39	1.33
5	C	340	HEM	CAC-C3C	2.68	1.54	1.47
5	C	340	HEM	FE-NC	2.68	2.04	1.95
5	C	337	HEM	FE-ND	2.66	2.03	1.94
5	C	337	HEM	FE-NB	2.64	2.03	1.94
5	C	339	HEM	CAB-C3B	2.60	1.54	1.47
5	C	340	HEM	CAB-C3B	2.59	1.54	1.47
6	M	806	BCB	C2-C3	2.57	1.39	1.33
8	L	502	CET	C8-C9	-2.57	1.47	1.49
12	M	501	MQ7	C37-C38	2.56	1.39	1.33
6	L	304	BCB	O2D-CED	-2.56	1.39	1.45
5	C	340	HEM	CAD-C3D	-2.53	1.44	1.51
5	C	337	HEM	CMD-C2D	2.52	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	401	BPB	C1B-NB	2.52	1.43	1.38
12	M	501	MQ7	C27-C28	2.52	1.38	1.33
6	M	806	BCB	CHA-CBD	2.51	1.54	1.51
12	M	501	MQ7	C10-C5	-2.49	1.36	1.40
12	M	501	MQ7	C17-C18	2.48	1.38	1.33
6	L	304	BCB	C2-C3	2.45	1.38	1.33
6	M	805	BCB	MG-NB	-2.40	2.01	2.05
5	C	337	HEM	CMA-C3A	2.40	1.55	1.50
7	L	402	BPB	O2A-CGA	2.38	1.40	1.33
12	M	501	MQ7	C16-C17	-2.34	1.43	1.50
12	M	501	MQ7	C19-C18	2.34	1.56	1.50
12	M	501	MQ7	C42-C43	2.33	1.39	1.32
7	L	402	BPB	CMB-C2B	2.31	1.56	1.51
7	L	401	BPB	C3B-C4B	2.30	1.45	1.41
6	M	805	BCB	O2D-CGD	2.28	1.38	1.33
7	L	402	BPB	C1-C2	-2.28	1.42	1.49
7	L	401	BPB	C3B-C2B	-2.24	1.35	1.39
6	M	806	BCB	CMD-C2D	2.23	1.56	1.51
6	M	806	BCB	O2D-CGD	2.23	1.38	1.33
6	L	302	BCB	C3B-C4B	2.18	1.44	1.41
6	M	805	BCB	C2-C3	2.17	1.38	1.33
5	C	339	HEM	FE-NB	2.14	2.01	1.94
6	M	805	BCB	CHA-CBD	2.10	1.54	1.51
6	M	806	BCB	O2D-CED	-2.08	1.40	1.45
12	M	501	MQ7	C22-C23	2.08	1.37	1.33
12	M	501	MQ7	C12-C13	2.06	1.37	1.33
6	L	302	BCB	C2-C3	2.05	1.37	1.33

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	401	BPB	O2D-CGD-CBD	12.45	124.63	110.95
6	L	304	BCB	O2D-CGD-CBD	11.96	124.09	110.95
7	L	402	BPB	O2D-CGD-CBD	10.76	122.77	110.95
6	M	806	BCB	O2D-CGD-CBD	10.05	121.99	110.95
6	L	304	BCB	C1B-CHB-C4A	9.39	127.36	121.32
6	L	304	BCB	C4B-CHC-C1C	9.39	127.36	121.32
6	M	806	BCB	C1B-CHB-C4A	9.24	127.27	121.32
6	M	805	BCB	O2D-CGD-CBD	8.98	120.82	110.95
6	M	806	BCB	C4B-CHC-C1C	8.45	126.76	121.32
6	M	805	BCB	C4B-CHC-C1C	8.32	126.67	121.32
6	L	302	BCB	C4B-CHC-C1C	7.88	126.39	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	805	BCB	C1B-CHB-C4A	7.44	126.11	121.32
6	L	302	BCB	C1B-CHB-C4A	7.03	125.85	121.32
6	L	304	BCB	O1D-CGD-CBD	-6.98	114.14	124.72
7	L	402	BPB	O1D-CGD-CBD	-6.97	114.15	124.72
7	L	401	BPB	OBB-CAB-C3B	6.93	131.56	119.99
7	L	401	BPB	O1D-CGD-CBD	-6.69	114.58	124.72
6	L	302	BCB	O2D-CGD-CBD	6.64	118.24	110.95
6	M	806	BCB	O1D-CGD-CBD	-6.10	115.47	124.72
6	M	806	BCB	CMB-C2B-C3B	5.93	136.54	124.68
6	M	806	BCB	OBB-CAB-C3B	5.59	129.34	119.99
6	M	805	BCB	O1D-CGD-CBD	-5.55	116.31	124.72
6	L	302	BCB	O1D-CGD-CBD	-5.52	116.36	124.72
7	L	401	BPB	CED-O2D-CGD	5.33	128.01	115.92
7	L	401	BPB	C4D-CHA-CBD	-5.33	105.90	108.45
7	L	402	BPB	C4D-CHA-CBD	-5.25	105.94	108.45
12	M	501	MQ7	C41-C42-C43	4.76	143.52	127.64
6	M	805	BCB	C1-C2-C3	4.55	133.65	126.20
12	M	501	MQ7	C29-C28-C30	-4.53	107.36	115.23
7	L	402	BPB	OBD-CAD-CBD	-4.37	119.41	125.82
6	M	806	BCB	O2A-CGA-CBA	4.35	125.10	111.83
6	M	806	BCB	C3D-C4D-CHA	4.24	114.99	108.54
13	M	600	NS5	C19-C20-C21	-4.22	121.36	127.28
7	L	401	BPB	CBB-CAB-C3B	-4.20	107.77	120.34
6	M	805	BCB	C4-C3-C5	4.17	122.47	115.23
6	M	805	BCB	C3D-C4D-CHA	4.14	114.84	108.54
6	M	806	BCB	C1-C2-C3	-4.11	119.46	126.20
6	L	304	BCB	C3D-C4D-CHA	4.07	114.73	108.54
6	L	302	BCB	C3D-C4D-CHA	4.07	114.72	108.54
6	L	302	BCB	CED-O2D-CGD	-3.68	107.56	115.92
7	L	401	BPB	OBD-CAD-CBD	-3.67	120.44	125.82
5	C	339	HEM	CAA-C2A-C1A	3.61	131.99	124.94
12	M	501	MQ7	C25-C23-C22	3.60	129.24	121.17
12	M	501	MQ7	C35-C33-C32	3.59	129.23	121.17
6	L	302	BCB	OBD-CAD-CBD	-3.53	120.64	125.82
6	L	304	BCB	O2A-CGA-CBA	3.51	122.53	111.83
6	M	805	BCB	OBD-CAD-CBD	-3.43	120.78	125.82
6	M	806	BCB	O2A-CGA-O1A	-3.43	115.05	123.63
6	L	304	BCB	OBD-CAD-CBD	-3.40	120.83	125.82
6	M	805	BCB	CMB-C2B-C3B	3.39	131.46	124.68
12	M	501	MQ7	C34-C33-C35	-3.38	109.36	115.23
5	C	340	HEM	CAD-C3D-C4D	-3.38	118.81	124.70
6	M	805	BCB	C4C-CHD-C1D	3.38	128.16	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	806	BCB	OBD-CAD-CBD	-3.38	120.87	125.82
5	C	339	HEM	CBB-CAB-C3B	-3.32	110.95	127.53
5	C	338	HEM	CAC-C3C-C4C	-3.32	116.90	124.82
6	L	302	BCB	OBB-CAB-C3B	3.30	125.50	119.99
6	L	304	BCB	CMA-C3A-C4A	-3.29	107.53	114.61
6	M	806	BCB	C4D-CHA-CBD	-3.27	105.67	108.97
6	L	304	BCB	C4C-CHD-C1D	3.26	127.73	116.07
6	M	806	BCB	C4C-CHD-C1D	3.24	127.67	116.07
6	M	805	BCB	O2A-CGA-CBA	3.22	121.66	111.83
12	M	501	MQ7	C24-C23-C25	-3.20	109.68	115.23
6	M	805	BCB	CMA-C3A-C4A	-3.18	107.76	114.61
5	C	338	HEM	CBC-CAC-C3C	-3.17	111.70	127.53
5	C	339	HEM	CBC-CAC-C3C	-3.07	112.17	127.53
5	C	337	HEM	CBB-CAB-C3B	-3.06	112.24	127.53
7	L	401	BPB	C4D-ND-C1D	-3.05	105.22	108.87
6	L	302	BCB	C4C-CHD-C1D	3.02	126.87	116.07
5	C	339	HEM	CAC-C3C-C4C	-3.02	117.61	124.82
6	L	304	BCB	CMB-C2B-C3B	3.01	130.70	124.68
7	L	402	BPB	C2D-C1D-ND	2.99	111.59	109.43
7	L	402	BPB	C4D-ND-C1D	-2.98	105.30	108.87
6	L	302	BCB	C1A-CHA-C4D	2.98	123.95	118.98
5	C	340	HEM	CMA-C3A-C4A	2.97	129.94	125.42
5	C	340	HEM	CMB-C2B-C1B	2.97	129.67	125.03
6	L	302	BCB	CMB-C2B-C3B	2.96	130.60	124.68
5	C	340	HEM	CAD-C3D-C2D	2.95	133.39	127.87
7	L	402	BPB	C4B-NB-C1B	-2.92	104.56	108.82
7	L	402	BPB	CMA-C3A-C4A	-2.89	108.38	114.61
6	L	304	BCB	C4D-CHA-CBD	-2.89	106.06	108.97
5	C	339	HEM	CAA-C2A-C3A	-2.89	120.60	127.07
5	C	337	HEM	CAD-C3D-C4D	2.86	129.69	124.70
6	L	304	BCB	OBB-CAB-C3B	2.86	124.78	119.99
7	L	401	BPB	CMA-C3A-C4A	-2.81	108.55	114.61
6	M	805	BCB	CHA-C1A-C2A	-2.80	126.74	133.31
7	L	401	BPB	C6-C5-C3	2.78	120.25	113.47
5	C	338	HEM	CBB-CAB-C3B	-2.77	113.67	127.53
5	C	340	HEM	CAC-C3C-C4C	-2.76	118.23	124.82
6	L	304	BCB	C1-C2-C3	-2.76	121.68	126.20
12	M	501	MQ7	C30-C28-C27	2.73	127.31	121.17
12	M	501	MQ7	C21-C20-C18	-2.70	104.23	113.19
6	M	805	BCB	C5-C3-C2	-2.69	115.13	121.17
6	M	805	BCB	C4D-CHA-CBD	-2.68	106.27	108.97
6	M	806	BCB	C1A-CHA-C4D	2.66	123.42	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	302	BCB	C4D-CHA-CBD	-2.66	106.28	108.97
13	M	600	NS5	C23-C21-C20	2.65	123.18	119.01
12	M	501	MQ7	C31-C32-C33	2.65	133.69	127.62
13	M	600	NS5	C22-C21-C23	-2.65	114.05	118.09
6	M	806	BCB	CBB-CAB-C3B	-2.62	112.48	120.34
5	C	340	HEM	CBD-CAD-C3D	2.62	119.78	112.53
7	L	402	BPB	C3D-C4D-ND	2.60	111.04	107.71
6	L	304	BCB	CHA-C1A-C2A	-2.58	127.25	133.31
6	L	302	BCB	CHA-C1A-C2A	-2.57	127.26	133.31
7	L	402	BPB	O2A-CGA-O1A	-2.54	117.28	123.63
5	C	337	HEM	CMD-C2D-C1D	2.53	128.99	125.03
7	L	402	BPB	O2A-CGA-CBA	2.53	119.55	111.83
6	L	302	BCB	OBD-CAD-C3D	2.51	131.80	127.89
7	L	402	BPB	CMD-C2D-C3D	2.47	129.62	124.68
6	M	806	BCB	CMA-C3A-C4A	-2.47	109.29	114.61
13	M	600	NS5	C19-C18-C17	2.46	128.56	123.52
5	C	337	HEM	CBC-CAC-C3C	-2.45	115.30	127.53
6	M	806	BCB	CHA-C1A-C2A	-2.44	127.57	133.31
7	L	402	BPB	C4-C3-C5	-2.44	111.00	115.23
7	L	401	BPB	C10-C8-C7	2.41	124.30	112.07
8	L	502	CET	C11-C10-C8	-2.40	108.98	115.07
6	M	805	BCB	C1A-CHA-C4D	2.37	122.94	118.98
5	C	338	HEM	CAC-C3C-C2C	2.33	135.99	128.43
5	C	340	HEM	CBB-CAB-C3B	-2.32	115.92	127.53
13	M	600	NS5	C18-C19-C20	2.31	128.24	123.52
12	M	501	MQ7	C44-C43-C42	2.30	129.56	122.66
6	L	304	BCB	C1A-CHA-C4D	2.29	122.80	118.98
5	C	337	HEM	CAA-C2A-C1A	2.25	129.34	124.94
5	C	340	HEM	CAB-C3B-C2B	2.25	135.75	128.43
12	M	501	MQ7	C40-C41-C42	-2.24	100.96	112.02
12	M	501	MQ7	C21-C22-C23	-2.20	122.59	127.62
5	C	340	HEM	CMB-C2B-C3B	-2.19	123.12	128.43
7	L	402	BPB	C4A-C3A-C2A	2.18	104.91	102.84
5	C	337	HEM	CAD-C3D-C2D	-2.16	123.82	127.87
6	L	304	BCB	O2A-CGA-O1A	-2.16	118.23	123.63
6	M	805	BCB	OBD-CAD-C3D	2.14	131.23	127.89
6	L	302	BCB	C15-C13-C12	-2.13	101.29	112.07
7	L	401	BPB	C2D-C1D-ND	2.12	110.97	109.43
7	L	401	BPB	C1-C2-C3	2.10	129.63	126.20
13	M	600	NS5	C16-C15-C14	-2.09	114.89	118.09
5	C	339	HEM	CAC-C3C-C2C	2.08	135.19	128.43
13	M	600	NS5	C27-C26-C28	-2.07	114.93	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	401	BPB	C4B-NB-C1B	-2.06	105.81	108.82
6	L	304	BCB	C4-C3-C5	-2.06	111.66	115.23
5	C	339	HEM	CAB-C3B-C2B	2.06	135.11	128.43
12	M	501	MQ7	C26-C25-C23	-2.04	106.41	113.19
12	M	501	MQ7	C36-C37-C38	-2.04	122.95	127.62
5	C	339	HEM	O2D-CGD-CBD	2.03	120.40	114.00
6	L	302	BCB	O2A-CGA-CBA	2.01	117.97	111.83
6	L	304	BCB	CMD-C2D-C3D	2.00	128.69	124.68

All (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	NC
6	M	805	BCB	NA
6	M	805	BCB	ND
6	M	805	BCB	NC
6	M	806	BCB	NA
6	M	806	BCB	ND
6	M	806	BCB	NC
7	L	402	BPB	C13

All (110) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	M	805	BCB	C3A-C2A-CAA-CBA
6	M	806	BCB	CAD-CBD-CGD-O1D
6	M	806	BCB	CAD-CBD-CGD-O2D
9	M	704	LDA	C2-C1-N1-CM1
9	M	704	LDA	N1-C1-C2-C3
9	M	706	LDA	N1-C1-C2-C3
13	M	600	NS5	C20-C21-C23-C24
13	M	600	NS5	C29-C30-C31-C33
6	L	302	BCB	O1D-CGD-O2D-CED
6	L	302	BCB	CBD-CGD-O2D-CED
6	L	302	BCB	C4-C3-C5-C6
6	M	805	BCB	C4-C3-C5-C6
6	M	805	BCB	C2-C3-C5-C6
13	M	600	NS5	C30-C31-C33-C34

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
13	M	600	NS5	C7-C8-C9-C10
7	L	401	BPB	CBD-CGD-O2D-CED
7	L	401	BPB	C4-C3-C5-C6
6	L	302	BCB	C2-C3-C5-C6
7	L	401	BPB	C2-C3-C5-C6
13	M	600	NS5	C22-C21-C23-C24
6	M	806	BCB	C13-C15-C16-C17
13	M	600	NS5	C2-C3-C4-C5
9	H	703	LDA	C3-C4-C5-C6
6	M	806	BCB	O1D-CGD-O2D-CED
6	M	806	BCB	C8-C10-C11-C12
6	L	302	BCB	C15-C16-C17-C18
13	M	600	NS5	C16-C15-C17-C18
13	M	600	NS5	C24-C25-C26-C27
6	M	806	BCB	C2A-CAA-CBA-CGA
6	L	304	BCB	C16-C17-C18-C20
6	M	805	BCB	C15-C16-C17-C18
7	L	401	BPB	O1A-CGA-O2A-C1
7	L	401	BPB	CBA-CGA-O2A-C1
6	M	805	BCB	C3-C5-C6-C7
6	M	806	BCB	CBD-CGD-O2D-CED
13	M	600	NS5	C12-C13-C14-C15
7	L	401	BPB	O1D-CGD-O2D-CED
9	M	706	LDA	C1-C2-C3-C4
6	M	806	BCB	C15-C16-C17-C18
5	C	340	HEM	C2B-C3B-CAB-CBB
6	L	304	BCB	C16-C17-C18-C19
9	M	706	LDA	C6-C7-C8-C9
6	L	304	BCB	C12-C13-C15-C16
9	M	704	LDA	C4-C5-C6-C7
7	L	402	BPB	O2A-C1-C2-C3
9	L	702	LDA	C3-C4-C5-C6
9	M	701	LDA	C2-C3-C4-C5
9	M	704	LDA	C5-C6-C7-C8
13	M	600	NS5	C3-C4-C5-C6
6	M	805	BCB	C10-C11-C12-C13
6	L	304	BCB	C14-C13-C15-C16
7	L	401	BPB	C5-C6-C7-C8
6	M	805	BCB	C11-C12-C13-C15
7	L	402	BPB	C4-C3-C5-C6
9	H	703	LDA	C11-C10-C9-C8
9	M	701	LDA	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
5	C	338	HEM	C2B-C3B-CAB-CBB
5	C	338	HEM	C2C-C3C-CAC-CBC
5	C	339	HEM	C2B-C3B-CAB-CBB
5	C	339	HEM	C2C-C3C-CAC-CBC
5	C	340	HEM	C2C-C3C-CAC-CBC
6	L	304	BCB	C8-C10-C11-C12
9	M	701	LDA	C9-C10-C11-C12
9	L	702	LDA	C1-C2-C3-C4
6	M	806	BCB	C11-C10-C8-C7
9	H	703	LDA	C7-C8-C9-C10
9	L	702	LDA	C2-C3-C4-C5
9	M	704	LDA	C6-C7-C8-C9
6	L	302	BCB	CAD-CBD-CGD-O1D
13	M	600	NS5	C28-C29-C30-C31
5	C	339	HEM	C1A-C2A-CAA-CBA
9	M	701	LDA	C7-C8-C9-C10
7	L	402	BPB	C10-C11-C12-C13
9	L	702	LDA	N1-C1-C2-C3
13	M	600	NS5	C31-C33-C34-C35
6	M	805	BCB	C11-C12-C13-C14
6	M	806	BCB	C11-C10-C8-C9
5	C	337	HEM	C4C-C3C-CAC-CBC
5	C	340	HEM	C4B-C3B-CAB-CBB
6	M	806	BCB	C6-C7-C8-C10
12	M	501	MQ7	C34-C33-C35-C36
13	M	600	NS5	C3-C4-C5-C7
9	M	701	LDA	C1-C2-C3-C4
6	M	805	BCB	C1A-C2A-CAA-CBA
5	C	337	HEM	CAA-CBA-CGA-O2A
12	M	501	MQ7	C32-C33-C35-C36
5	C	337	HEM	CAD-CBD-CGD-O2D
5	C	338	HEM	CAA-CBA-CGA-O1A
9	M	706	LDA	C7-C8-C9-C10
5	C	338	HEM	CAD-CBD-CGD-O2D
5	C	337	HEM	C2C-C3C-CAC-CBC
5	C	337	HEM	CAA-CBA-CGA-O1A
9	M	705	LDA	C9-C10-C11-C12
5	C	338	HEM	C4B-C3B-CAB-CBB
5	C	338	HEM	C4C-C3C-CAC-CBC
5	C	339	HEM	C4B-C3B-CAB-CBB
5	C	339	HEM	C4C-C3C-CAC-CBC
5	C	340	HEM	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
5	C	337	HEM	CAD-CBD-CGD-O1D
5	C	338	HEM	CAD-CBD-CGD-O1D
6	M	805	BCB	C6-C7-C8-C10
6	M	806	BCB	C11-C12-C13-C15
7	L	402	BPB	C2-C3-C5-C6
5	C	338	HEM	CAA-CBA-CGA-O2A
13	M	600	NS5	C32-C31-C33-C34
6	L	302	BCB	C16-C17-C18-C20
6	M	805	BCB	C6-C7-C8-C9
9	M	704	LDA	C2-C1-N1-O1
6	L	304	BCB	C13-C15-C16-C17
5	C	340	HEM	CAD-CBD-CGD-O2D

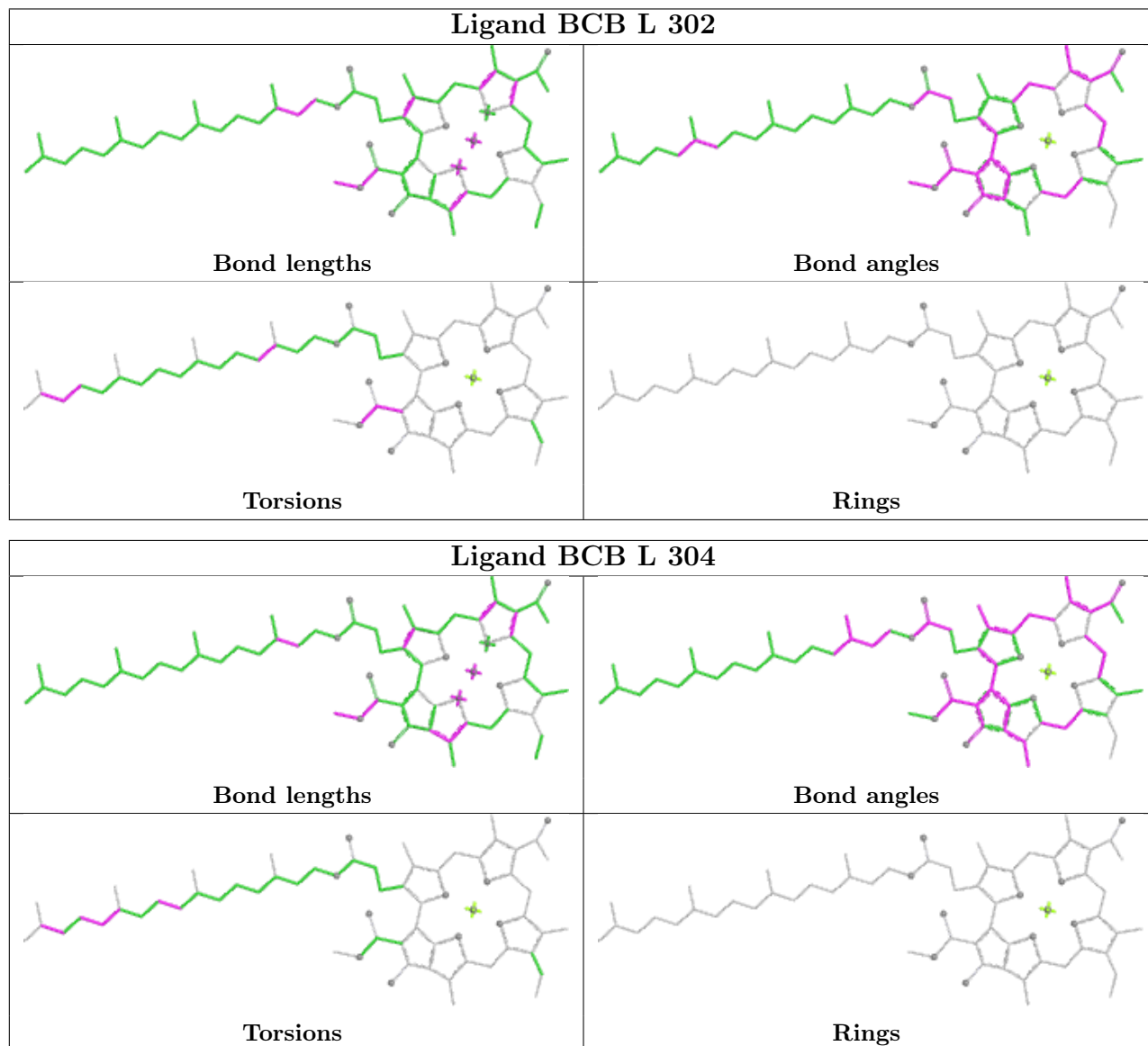
There are no ring outliers.

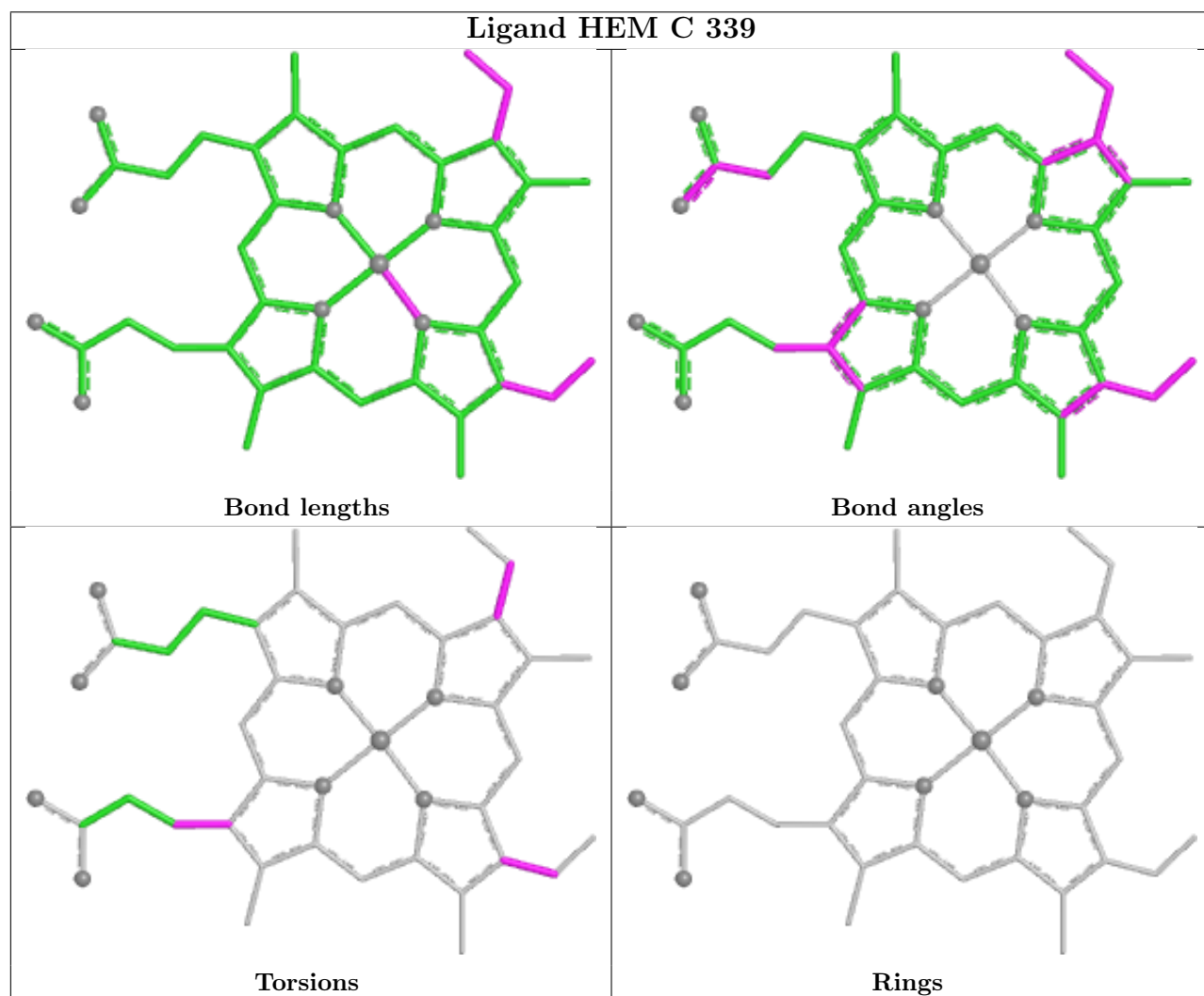
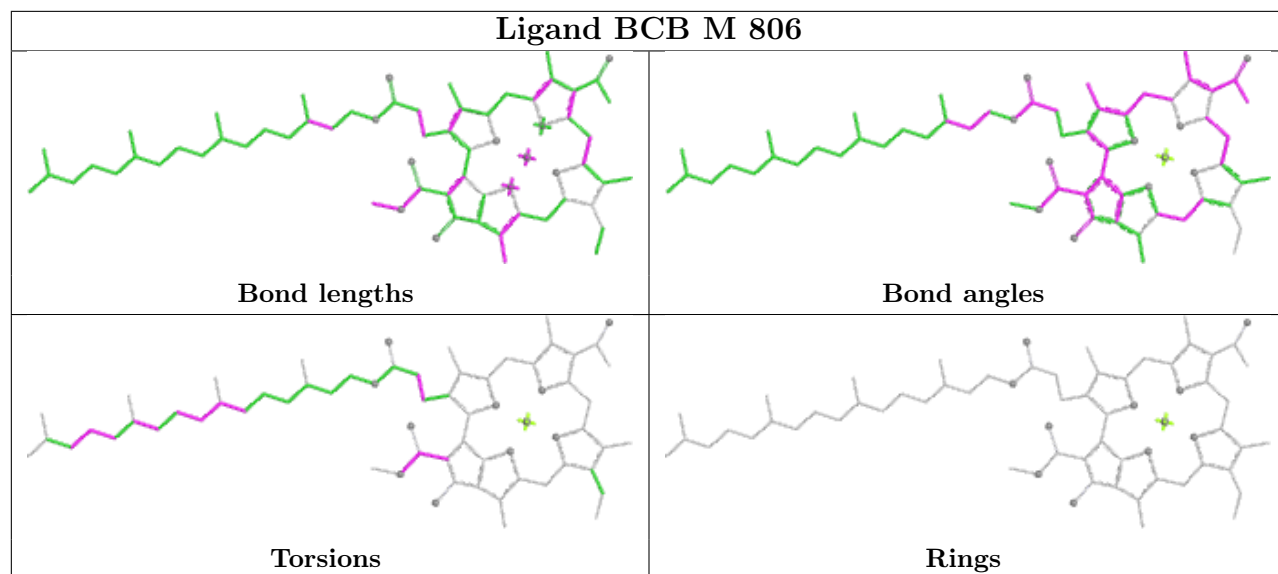
18 monomers are involved in 56 short contacts:

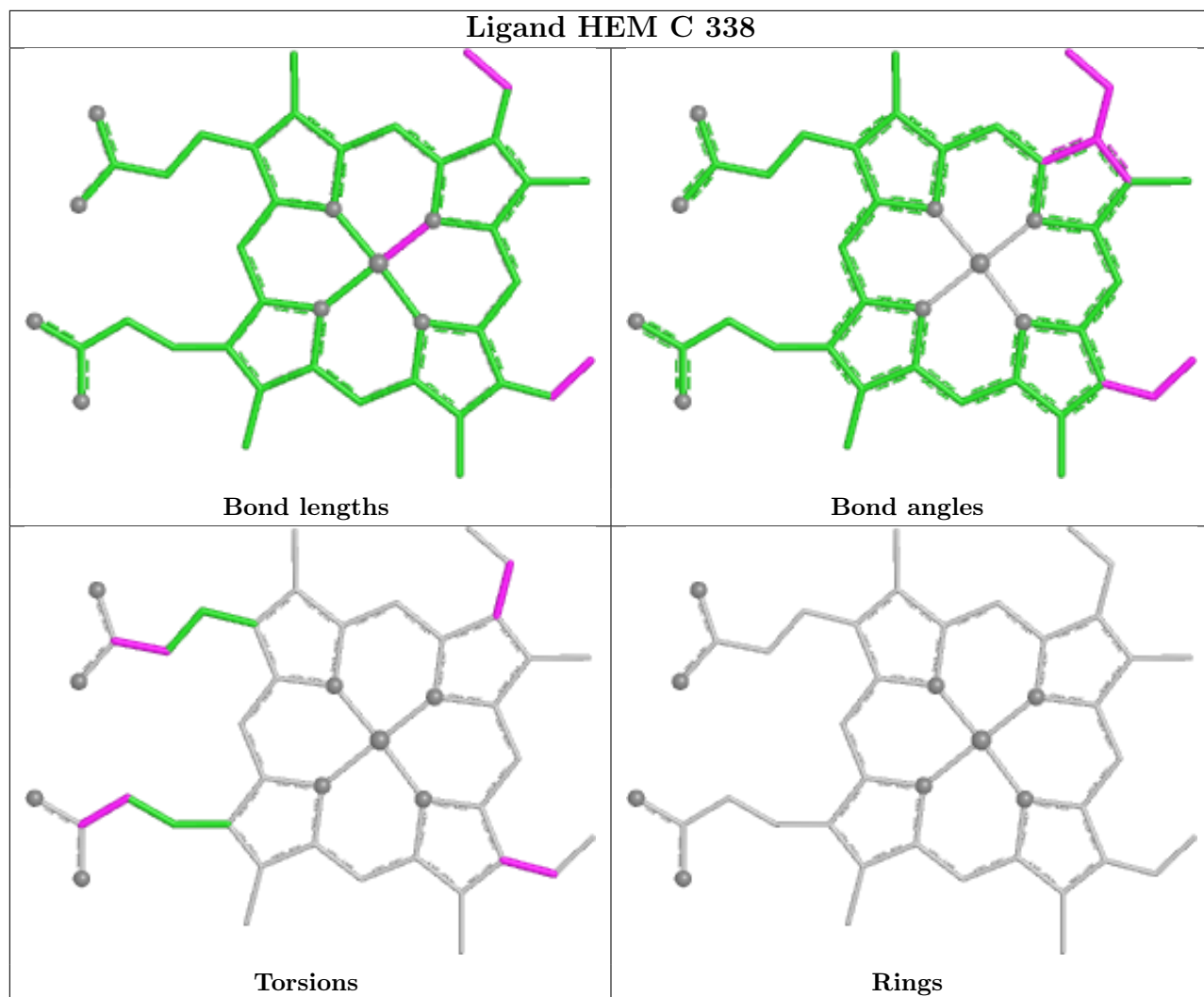
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	302	BCB	4	0
6	L	304	BCB	4	0
9	M	701	LDA	2	0
11	M	804	SO4	1	0
6	M	806	BCB	5	0
9	M	706	LDA	1	0
5	C	339	HEM	1	0
5	C	338	HEM	2	0
8	L	502	CET	1	0
9	H	703	LDA	1	0
5	C	337	HEM	3	0
7	L	401	BPB	12	0
7	L	402	BPB	6	0
12	M	501	MQ7	1	0
9	M	704	LDA	2	0
13	M	600	NS5	7	0
6	M	805	BCB	9	0
9	M	705	LDA	1	0

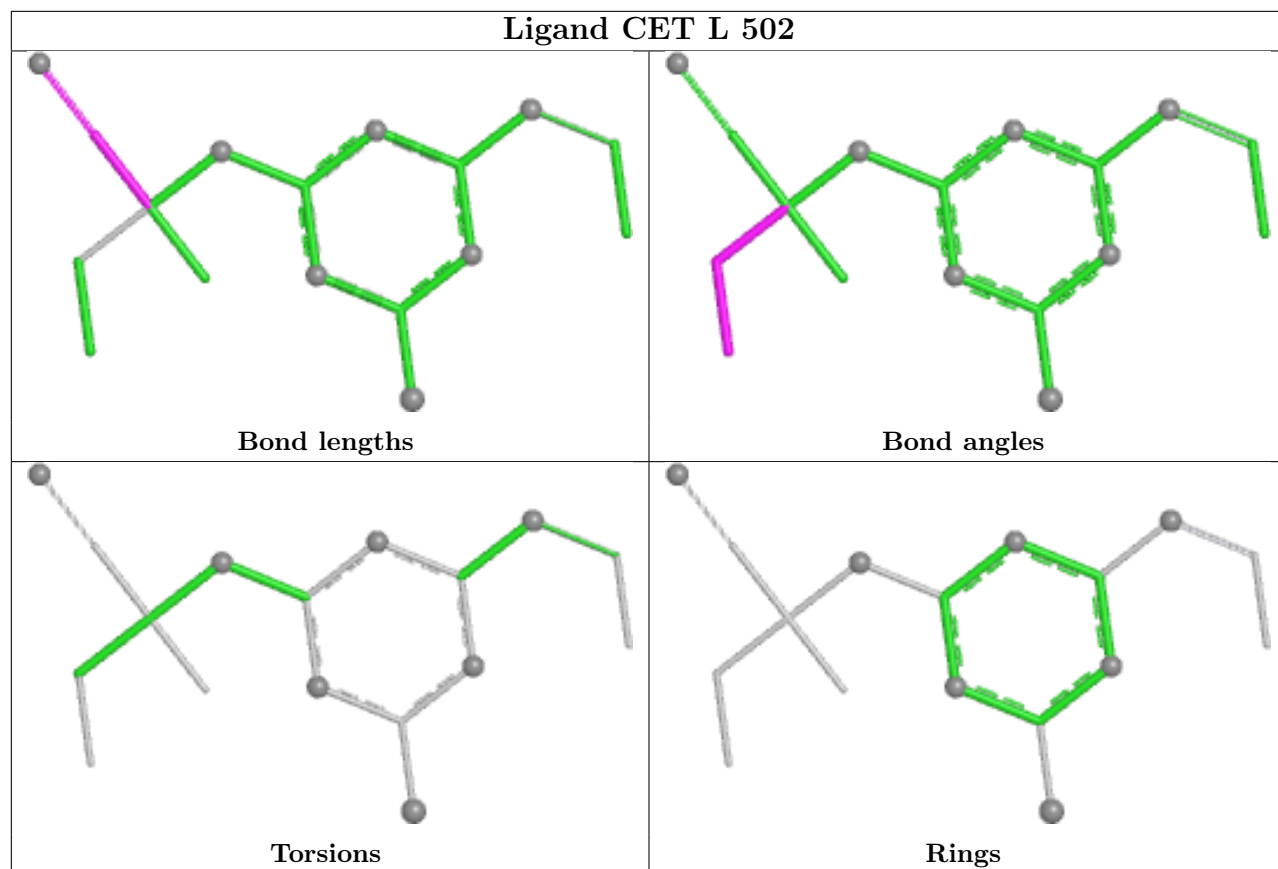
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

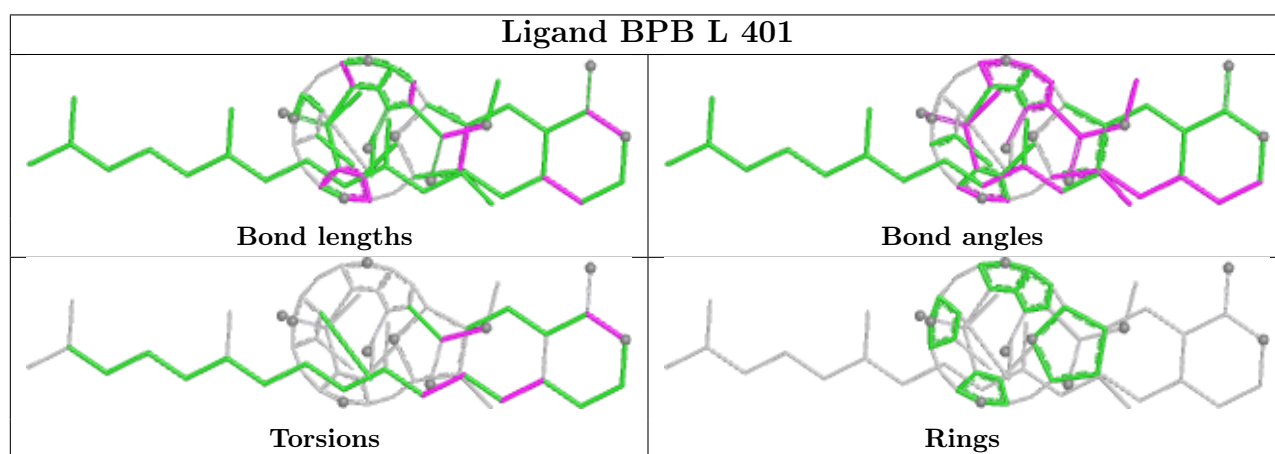
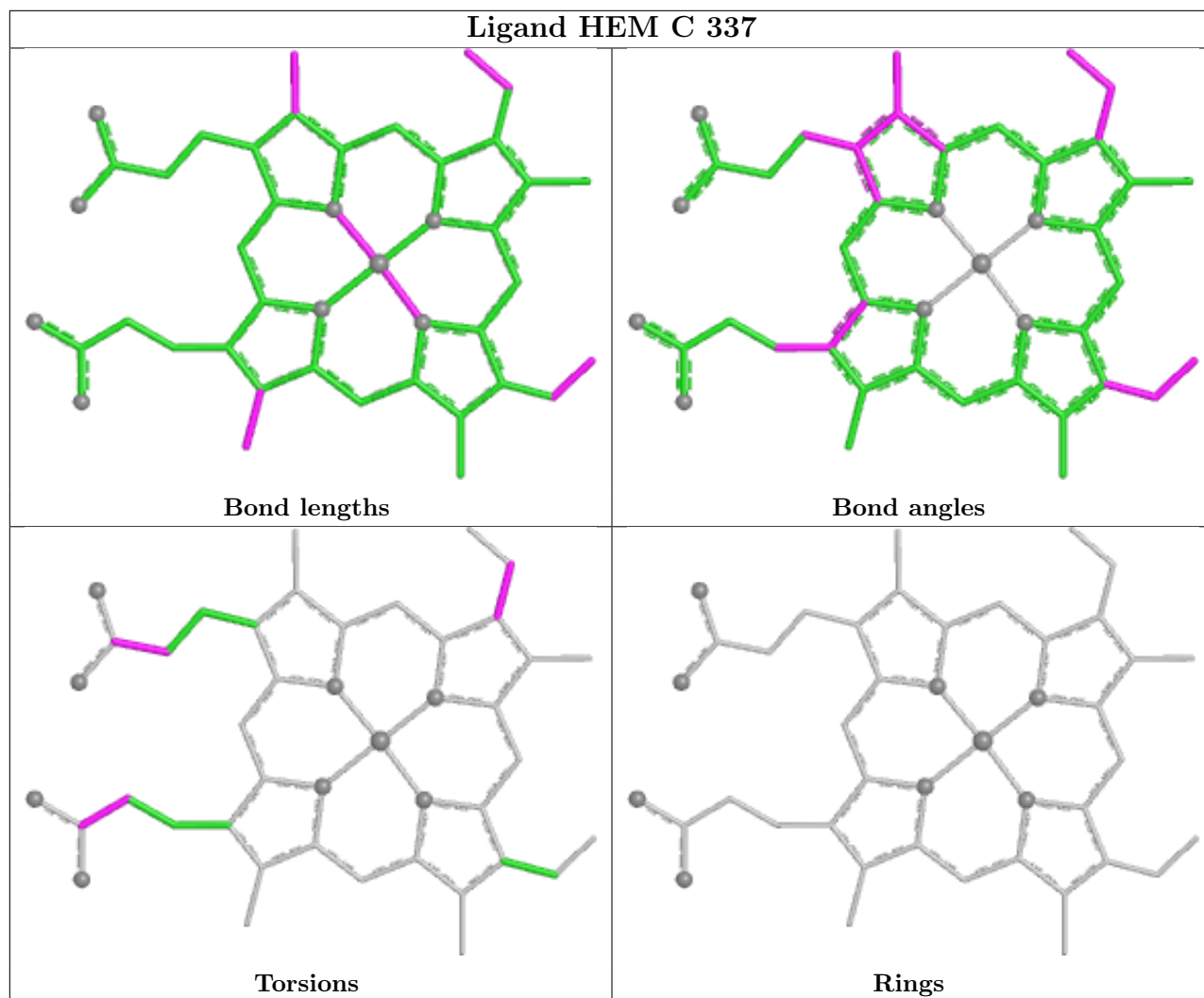
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

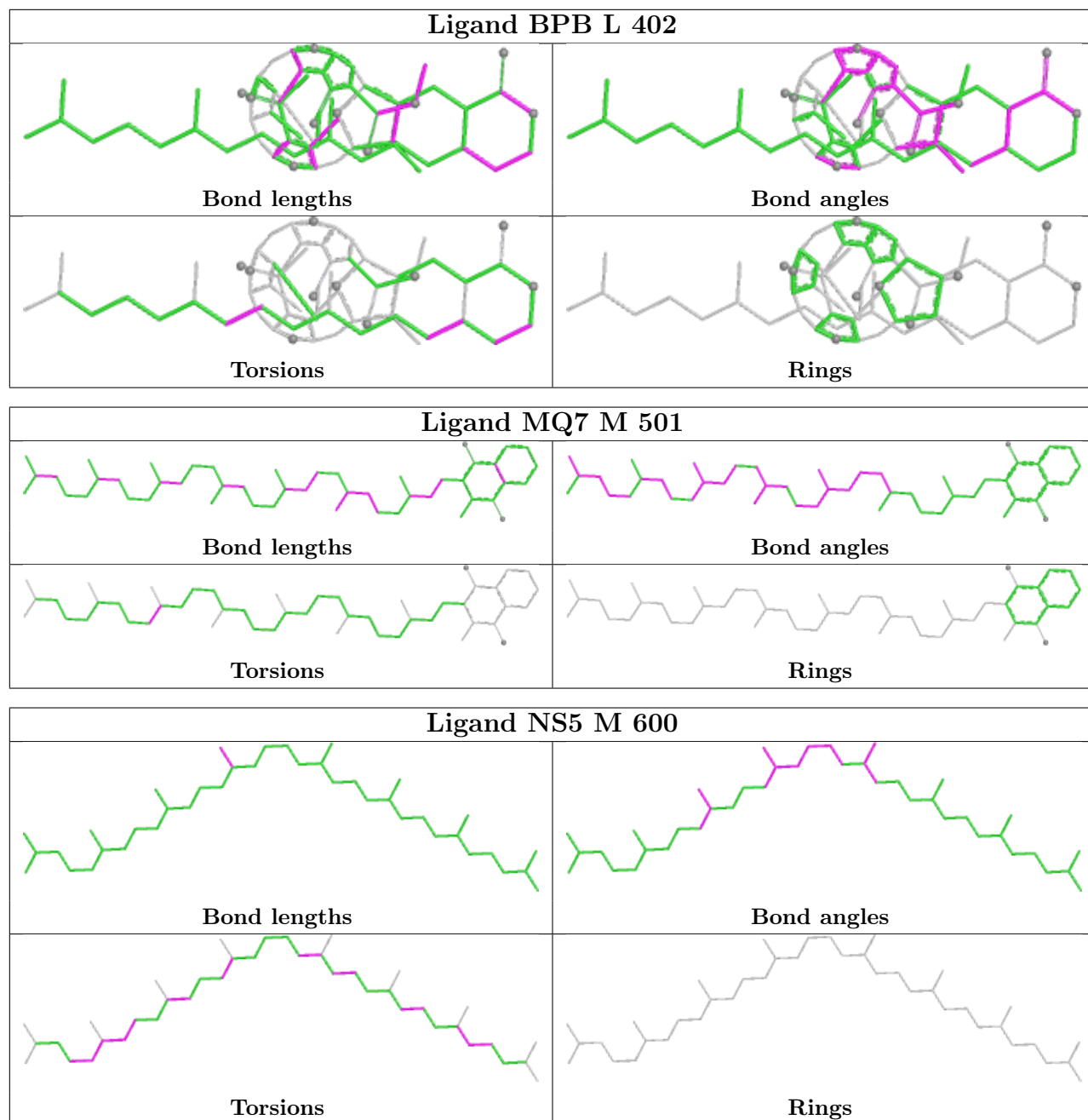


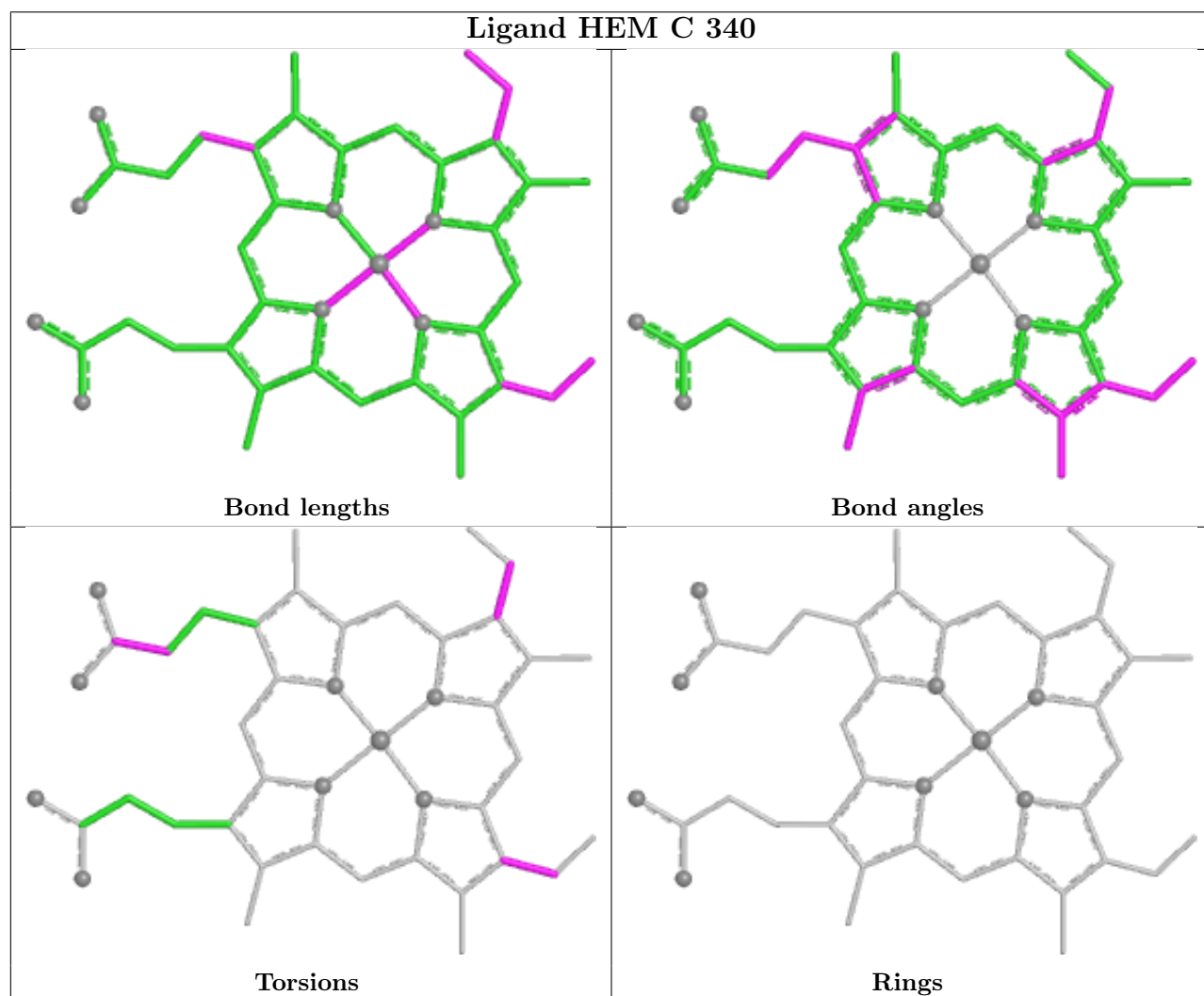
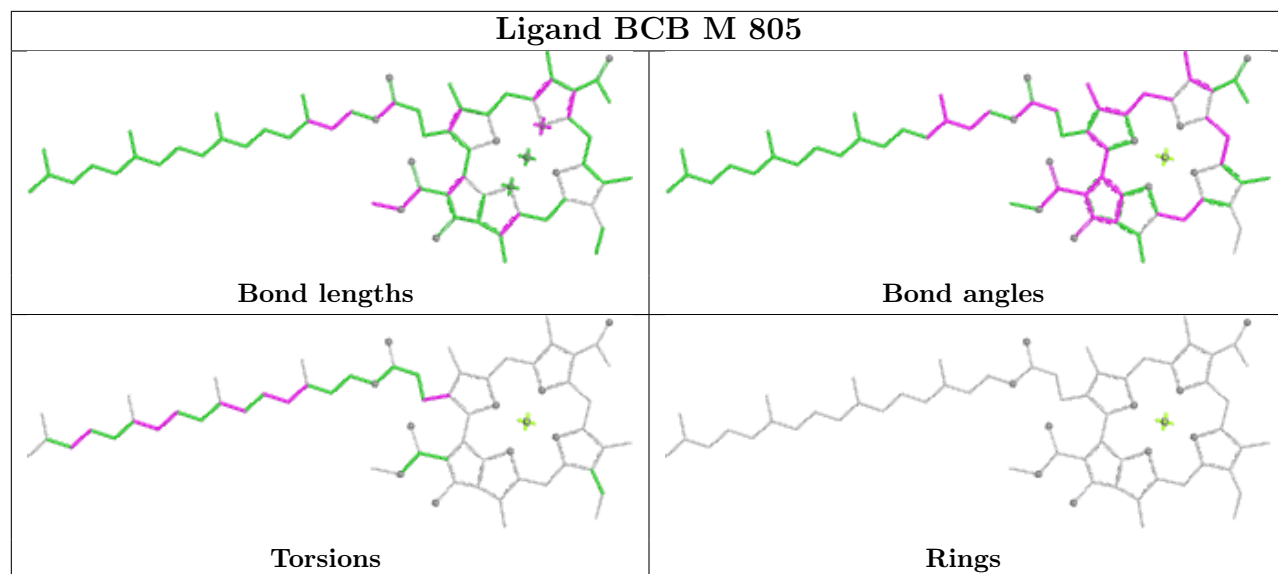












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	H	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	54:PRO	C	55:GLU	N	1.68
1	H	52:LEU	C	53:ALA	N	1.19

## 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%)	-0.72	1 (0%) 90   89	4, 20, 42, 66	19 (5%)
2	L	273/273 (100%)	-0.80	0 100   100	4, 16, 40, 61	6 (2%)
3	M	323/323 (100%)	-0.70	1 (0%) 90   89	4, 18, 45, 60	12 (3%)
4	H	249/258 (96%)	-0.38	5 (2%) 65   59	6, 26, 51, 76	19 (7%)
All	All	1177/1190 (98%)	-0.66	7 (0%) 85   83	4, 20, 44, 76	56 (4%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	54	PRO	3.8
4	H	45	GLU	2.7
4	H	8	GLN	2.7
3	M	37	TRP	2.6
4	H	7	ALA	2.5
4	H	55	GLU	2.4
1	C	1	CYS	2.3

### 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	0.93	0.07	23,30,40,42	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

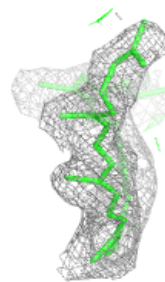
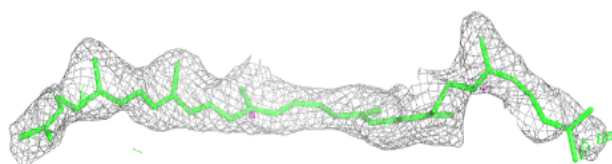
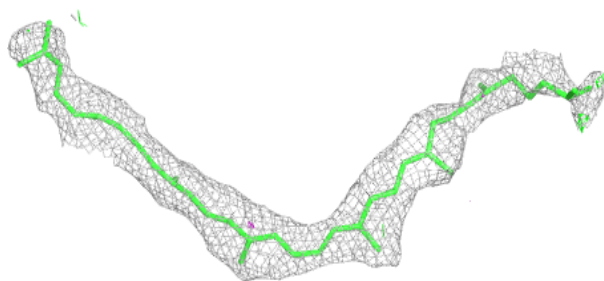
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	M	705	16/16	0.72	0.14	53,58,69,69	5
9	LDA	M	704	16/16	0.75	0.18	55,59,79,81	0
9	LDA	M	706	16/16	0.75	0.19	68,71,72,73	4
13	NS5	M	600	40/40	0.86	0.11	23,40,76,76	4
9	LDA	H	703	16/16	0.91	0.11	27,38,57,58	0
9	LDA	M	701	16/16	0.92	0.06	11,21,24,27	0
11	SO4	M	803	5/5	0.93	0.12	73,74,76,77	0
9	LDA	L	702	16/16	0.93	0.11	17,45,71,72	0
6	BCB	M	805	66/66	0.95	0.07	2,15,44,46	0
11	SO4	H	801	5/5	0.96	0.06	56,56,57,57	0
7	BPB	L	401	65/65	0.96	0.07	2,21,70,70	7
6	BCB	M	806	66/66	0.97	0.05	2,10,25,29	0
11	SO4	M	804	5/5	0.97	0.07	39,39,44,44	0
7	BPB	L	402	65/65	0.97	0.05	2,6,13,17	0
12	MQ7	M	501	48/48	0.97	0.05	3,15,34,38	0
8	CET	L	502	17/17	0.97	0.06	10,18,21,25	0
5	HEM	C	338	43/43	0.98	0.05	11,22,28,33	0
5	HEM	C	340	43/43	0.98	0.06	5,13,30,44	0
6	BCB	L	302	66/66	0.98	0.04	2,8,15,19	0
6	BCB	L	304	66/66	0.98	0.04	2,6,21,27	0
5	HEM	C	337	43/43	0.98	0.07	8,21,30,39	0
11	SO4	M	802	5/5	0.99	0.05	21,24,27,28	0
5	HEM	C	339	43/43	0.99	0.04	2,10,15,23	0
10	FE2	M	500	1/1	0.99	0.02	16,16,16,16	0

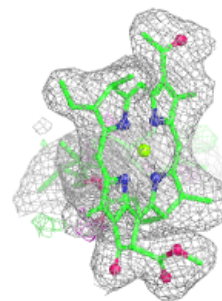
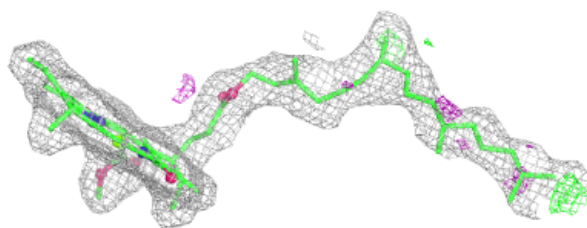
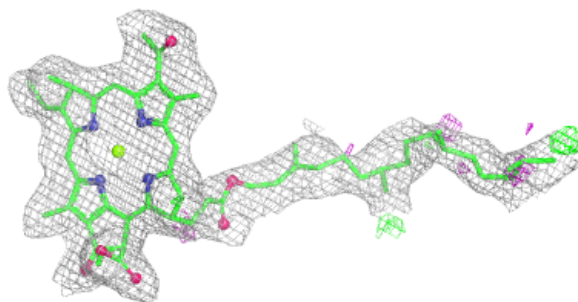
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

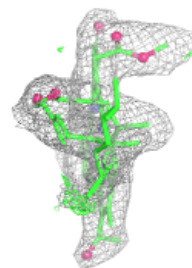
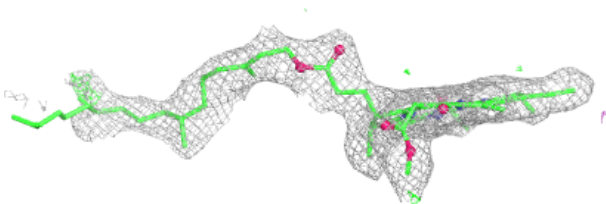
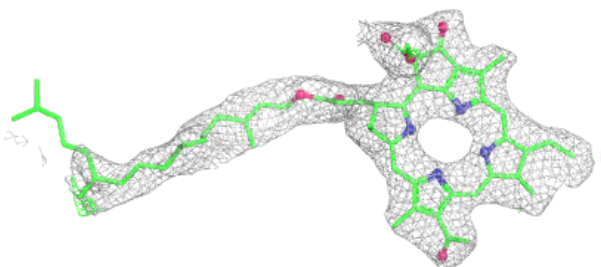
**Electron density around BCB M 805:**

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

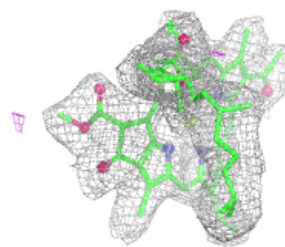
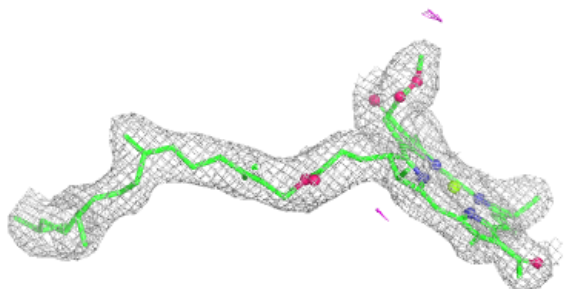
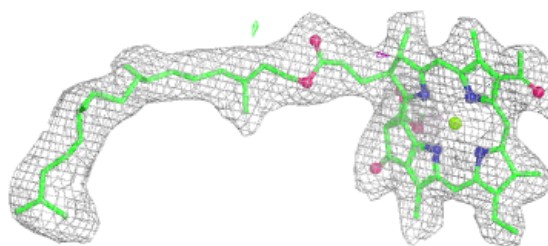


**Electron density around BPB L 401:**

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

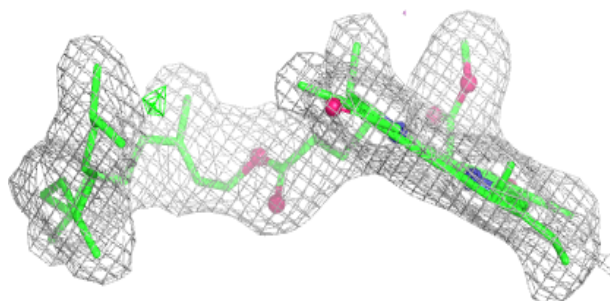
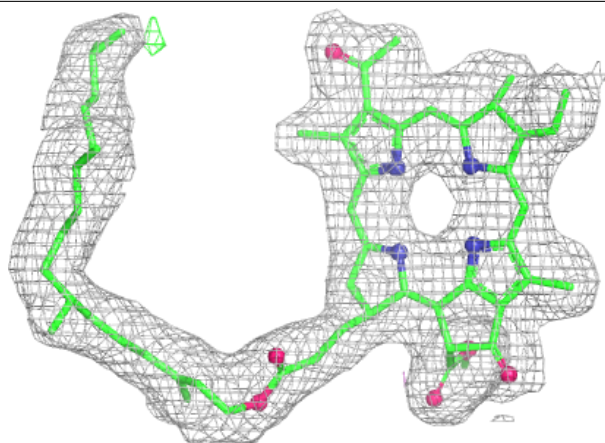
**Electron density around BCB M 806:**

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

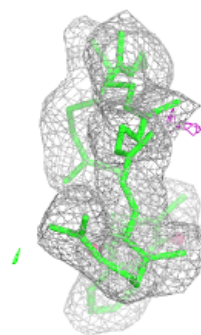
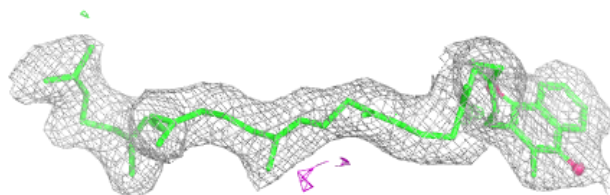
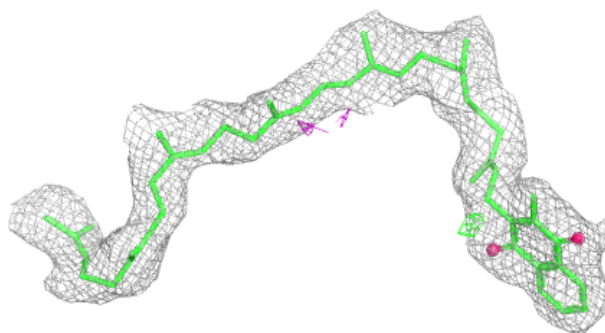


**Electron density around BPB L 402:**

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

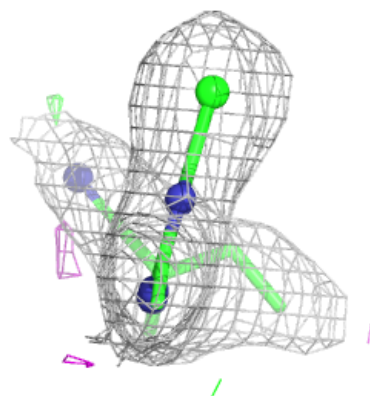
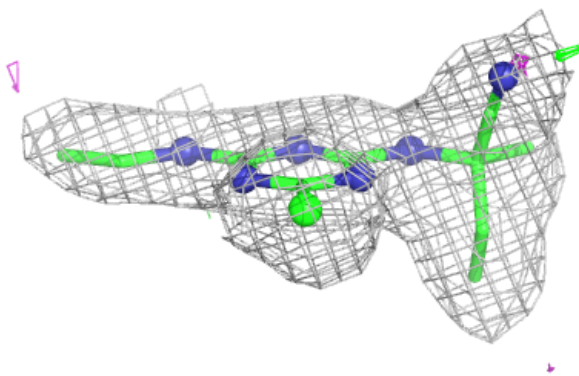
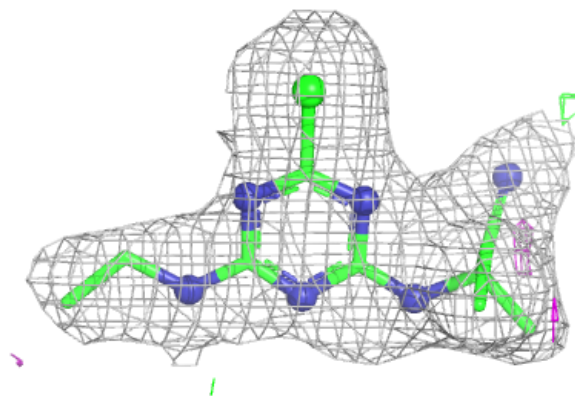
**Electron density around MQ7 M 501:**

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



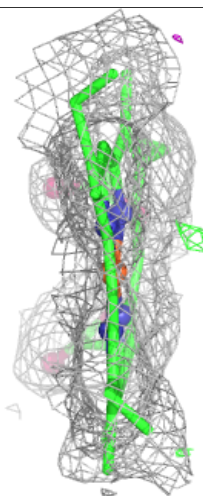
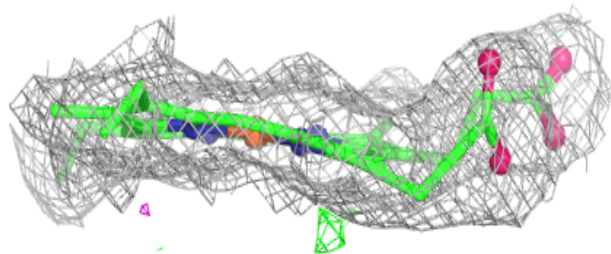
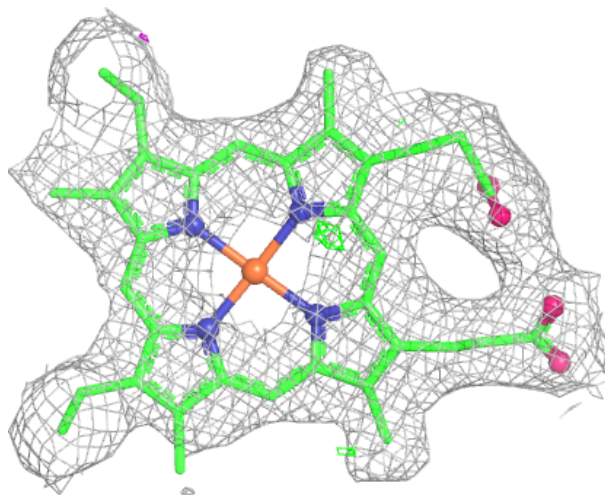
**Electron density around CET L 502:**

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



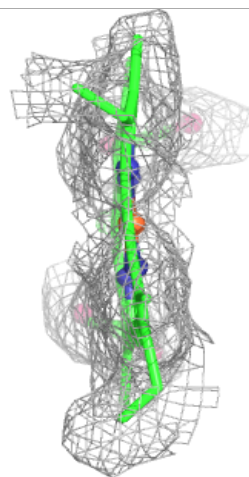
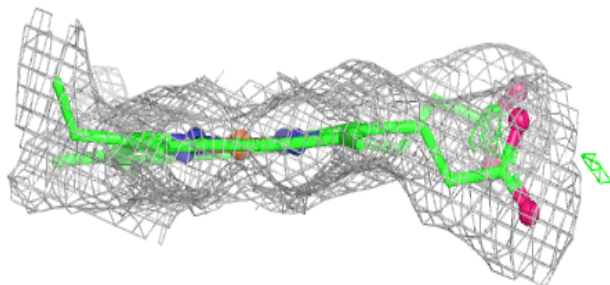
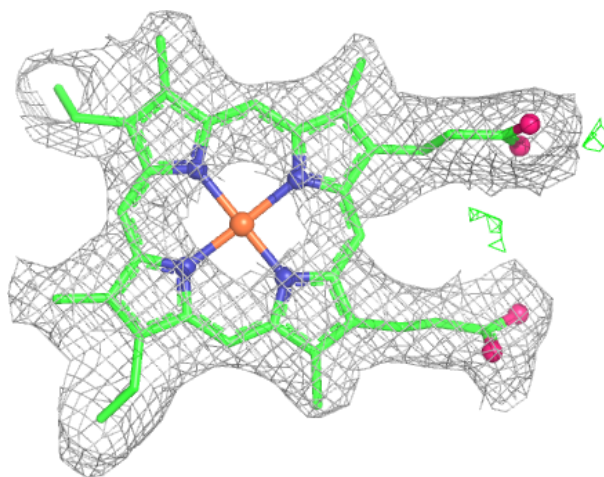
**Electron density around HEM C 338:**

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



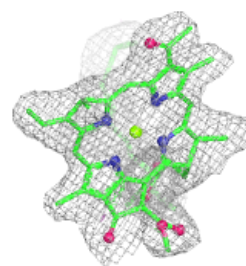
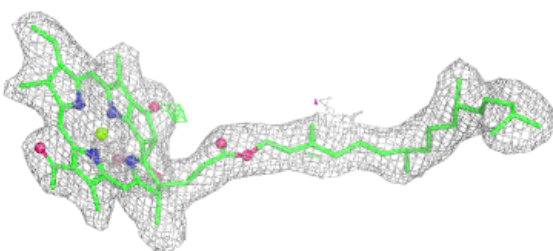
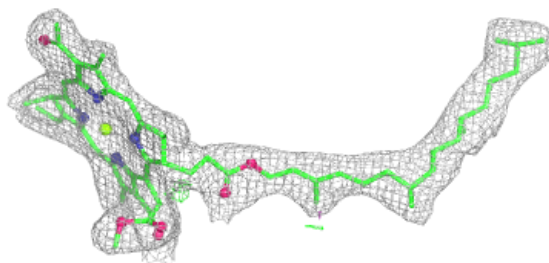
**Electron density around HEM C 340:**

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

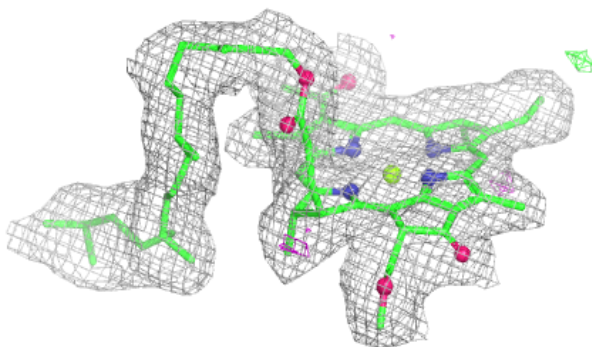
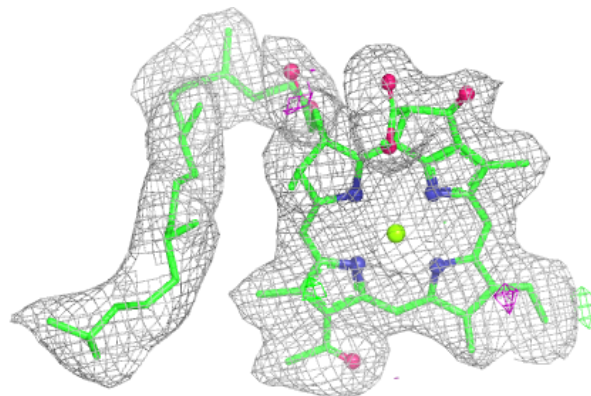


**Electron density around BCB L 302:**

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

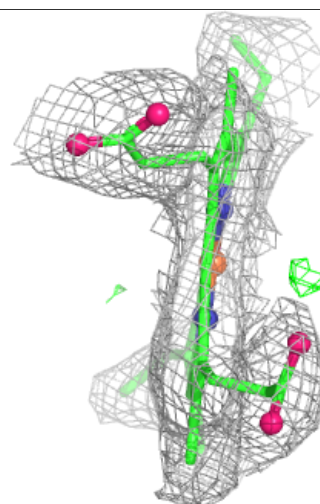
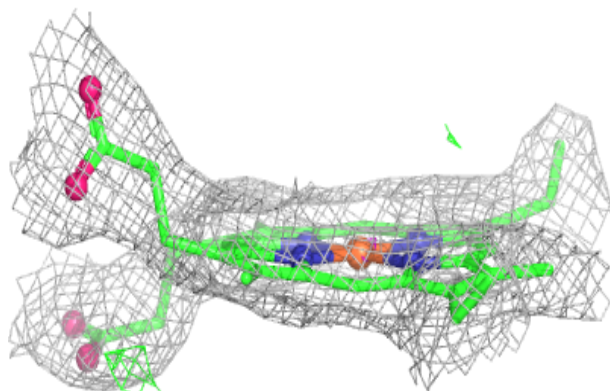
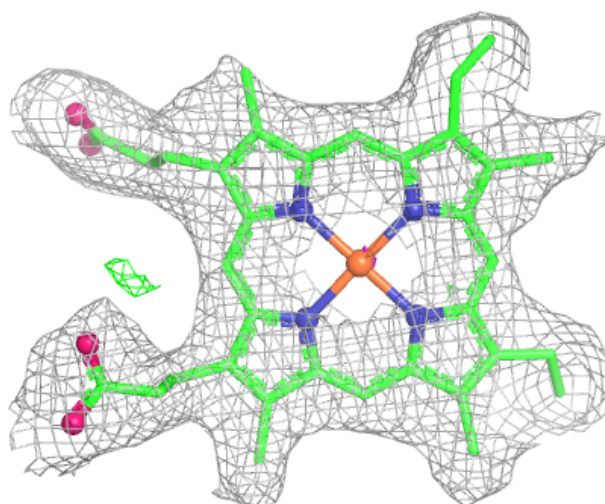
**Electron density around BCB L 304:**

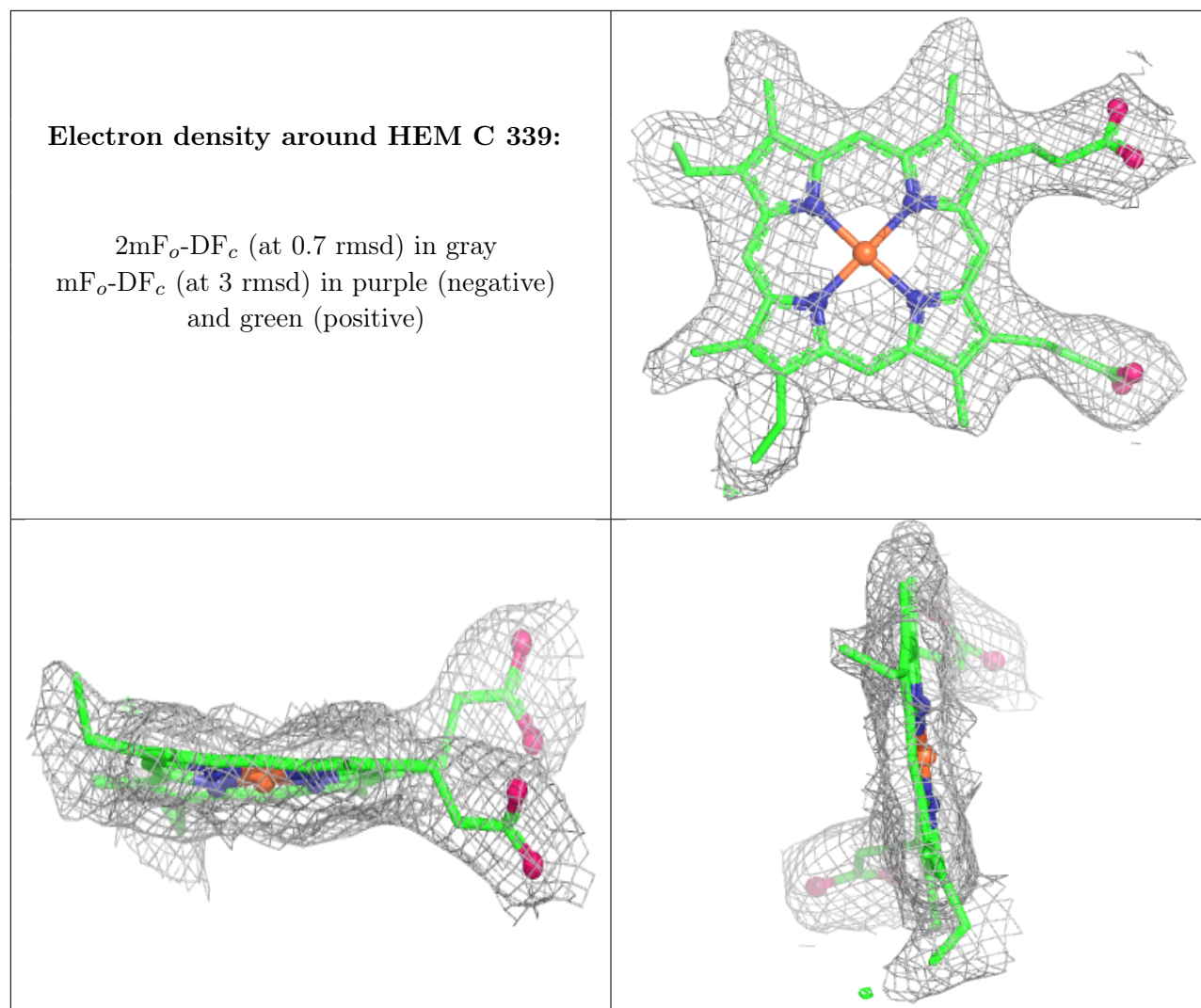
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM C 337:**

$2mF_o-DF_c$  (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.