



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 12:43 pm BST

PDB ID : 2JBL  
Title : PHOTOSYNTHETIC REACTION CENTER FROM BLASTOCHLORIS VIRIDIS  
Authors : Lancaster, C.R.D.  
Deposited on : 2006-12-08  
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

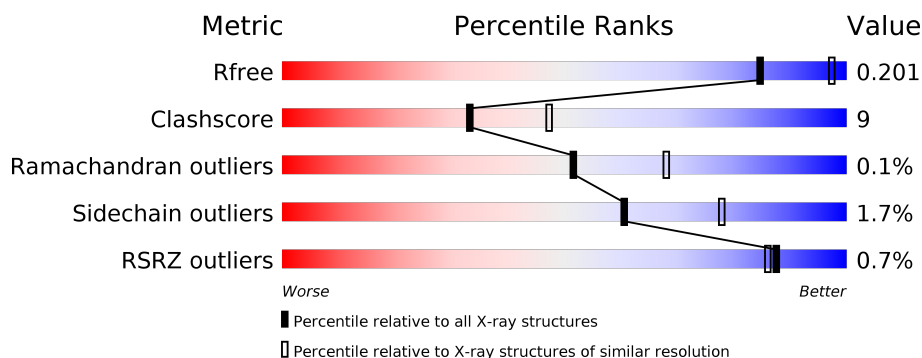
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3907 (2.40-2.40)
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	356	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">%</div> <div style="position: absolute; top: 10px; left: 0;">78%</div> <div style="position: absolute; top: 10px; right: 0;">15%</div> <div style="position: absolute; top: 10px; right: 0;">7%</div> </div> </div>
2	H	258	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 10px; left: 0;">83%</div> <div style="position: absolute; top: 10px; right: 0;">16%</div> </div> </div>
3	L	273	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 10px; left: 0;">87%</div> <div style="position: absolute; top: 10px; right: 0;">13%</div> </div> </div>
4	M	323	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">%</div> <div style="position: absolute; top: 10px; left: 0;">82%</div> <div style="position: absolute; top: 10px; right: 0;">17%</div> </div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	LDA	M	1331	-	-	-	X
8	BCB	M	1324	X	-	-	-

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 10512 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	332	Total	C	N	O	S	51	2	0
			2618	1648	471	481	18			

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

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

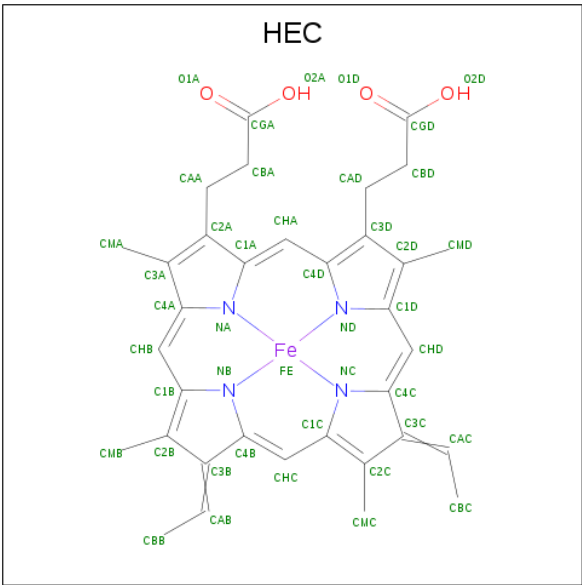
- Molecule 3 is a protein called REACTION CENTER PROTEIN L CHAIN.

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

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

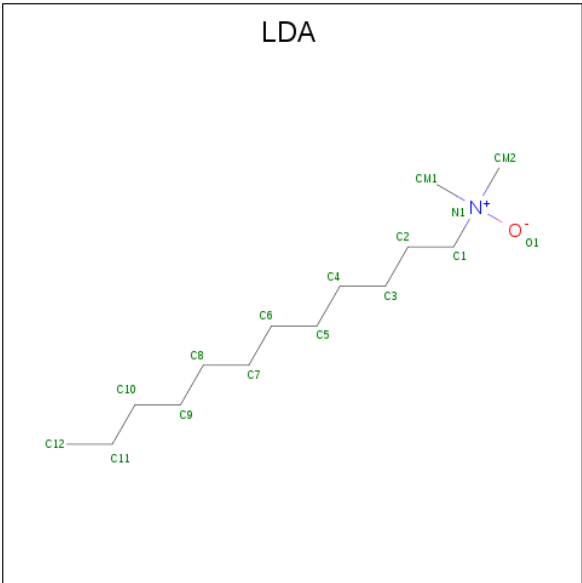
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	19	0	0
			2555	1702	419	423	11			

- Molecule 5 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



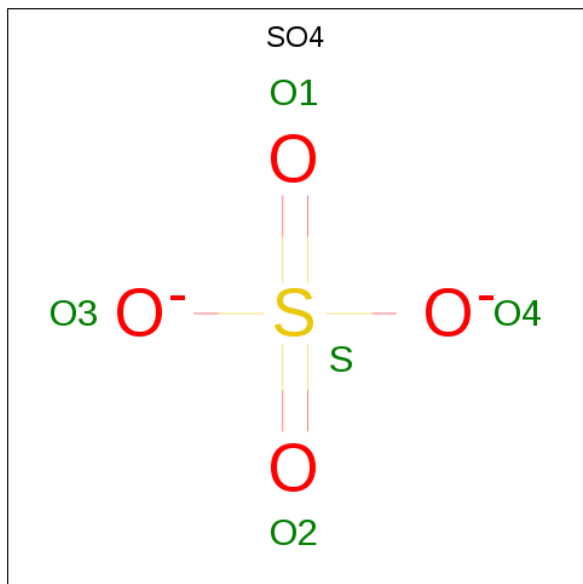
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



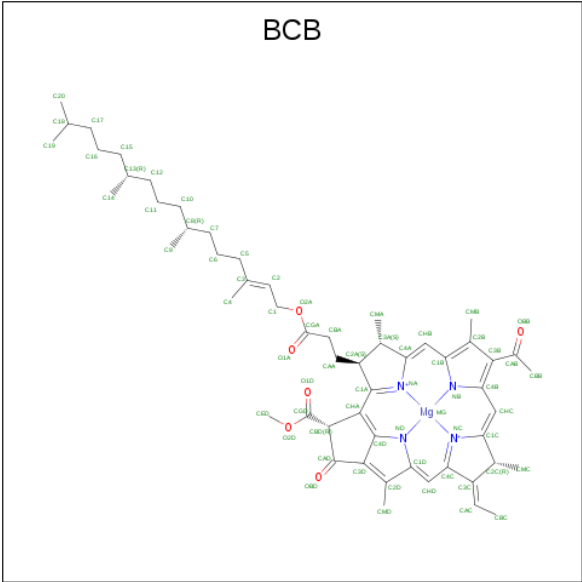
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	5	0
			16	14	1	1		
6	M	1	Total	C	N	O	4	0
			16	14	1	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



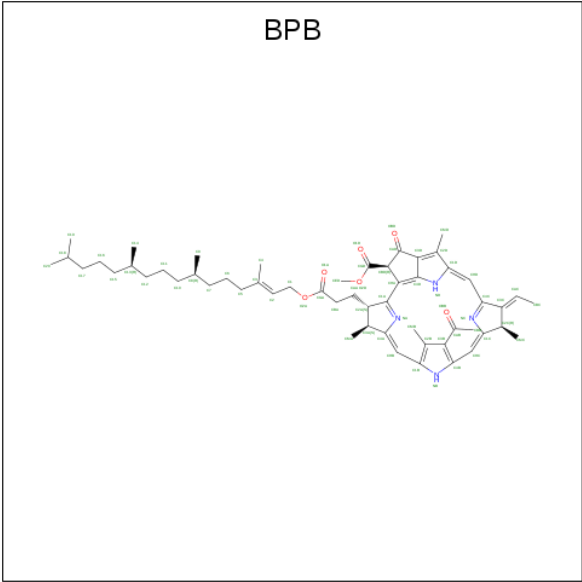
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	H	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>6</sub>).



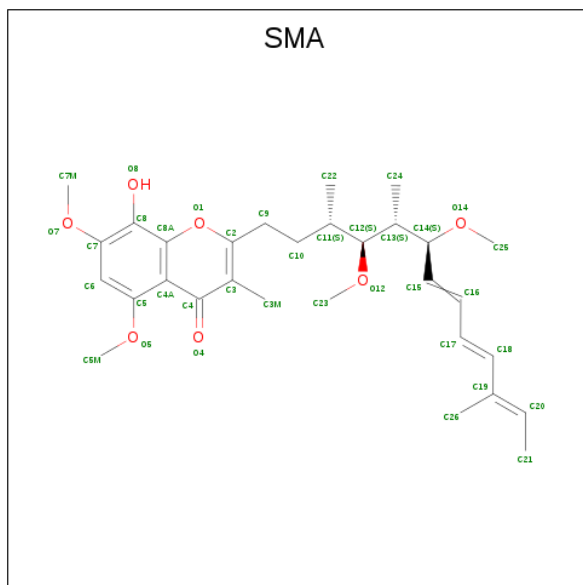
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 9 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>6</sub>).



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

- Molecule 10 is STIGMATELLIN A (three-letter code: SMA) (formula:  $C_{30}H_{42}O_7$ ).

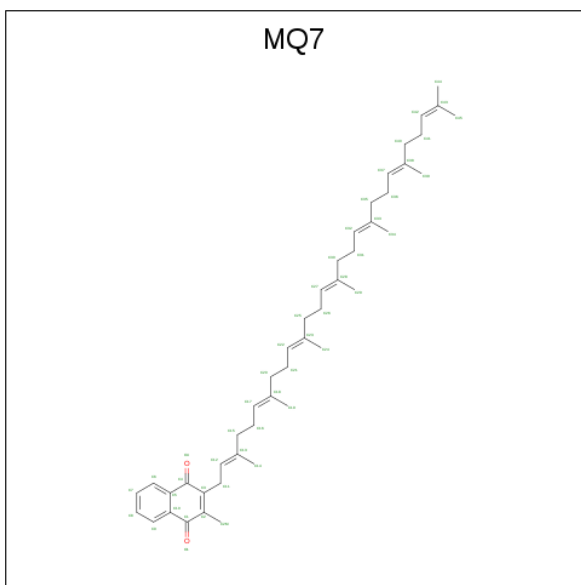


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			37	30	7		

- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).

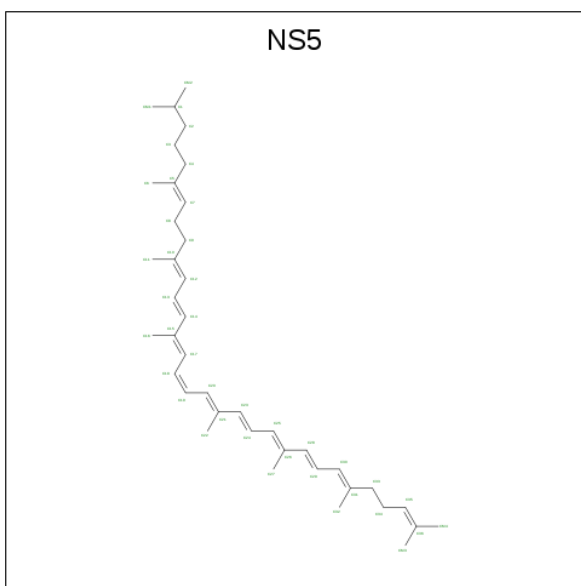
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

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



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

- Molecule 13 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: C<sub>40</sub>H<sub>60</sub>).



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

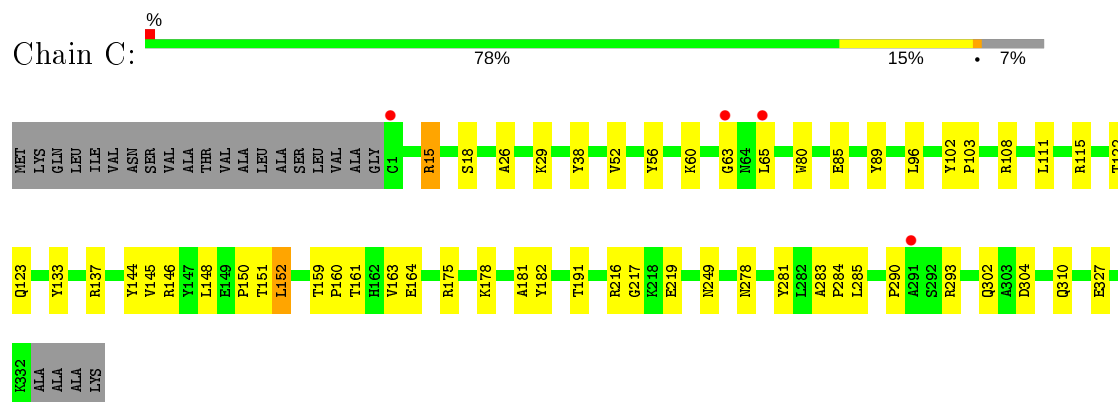
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	124	Total 124	O 124	0	0
14	H	76	Total 76	O 76	0	0
14	L	66	Total 66	O 66	0	0
14	M	76	Total 76	O 76	0	0

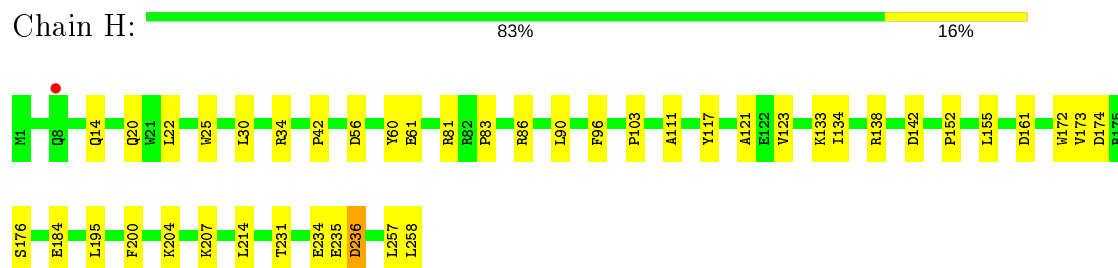
### 3 Residue-property plots [i](#)

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.

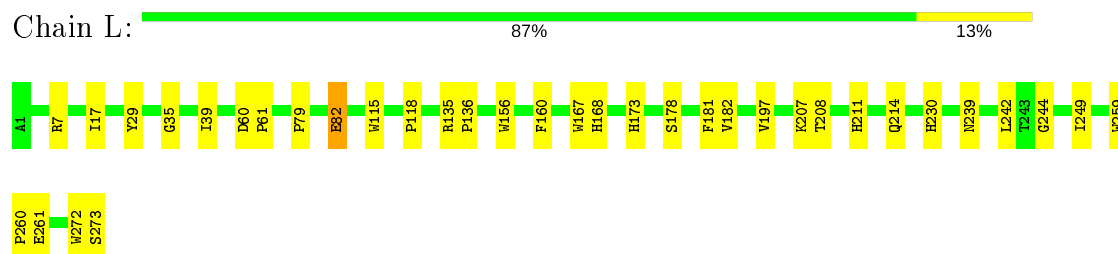
- Molecule 1: PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT



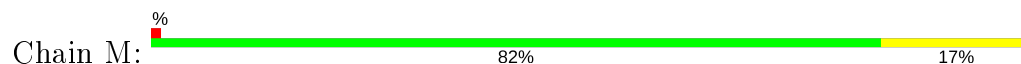
- Molecule 2: REACTION CENTER PROTEIN H CHAIN

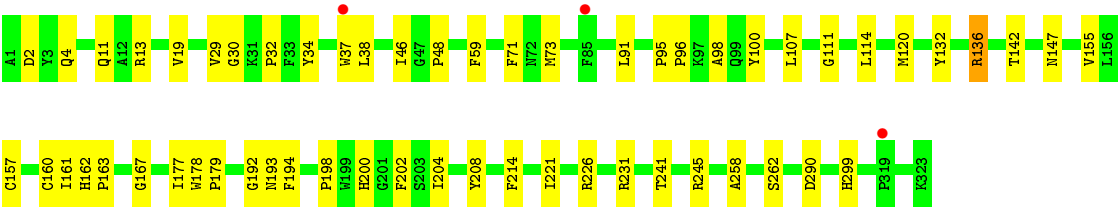


- Molecule 3: REACTION CENTER PROTEIN L CHAIN



- Molecule 4: REACTION CENTER PROTEIN M CHAIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 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)	26.56 – 2.40 47.79 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.3 (26.56-2.40) 92.4 (47.79-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 2.39 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.190   ,   0.206 0.182   ,   0.201	Depositor DCC
$R_{free}$ test set	1500 reflections (1.45%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.5	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 55.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10512	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% 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: LDA, BPB, BCB, FE, MQ7, HEC, FME, NS5, SMA, SO4

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	0.32	0/2685	0.60	1/3659 (0.0%)
2	H	0.31	0/2055	0.59	0/2807
3	L	0.39	0/2259	0.58	0/3084
4	M	0.37	0/2659	0.55	0/3637
All	All	0.35	0/9658	0.58	1/13187 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	249	ASN	N-CA-C	-6.31	93.97	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2618	0	2587	43	0
2	H	2018	0	2020	31	0
3	L	2171	0	2098	34	0
4	M	2555	0	2452	45	0
5	C	172	0	120	4	0
6	H	16	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	80	0	155	7	0
7	H	5	0	0	0	0
7	M	15	0	0	0	0
8	L	198	0	216	23	0
8	M	66	0	72	10	0
9	L	65	0	74	5	0
9	M	65	0	74	7	0
10	L	37	0	42	2	0
11	M	1	0	0	0	0
12	M	48	0	64	0	0
13	M	40	0	60	3	0
14	C	124	0	0	1	0
14	H	76	0	0	1	0
14	L	66	0	0	1	0
14	M	76	0	0	1	0
All	All	10512	0	10065	170	0

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

All (170) 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:M:32:PRO:HG3	4:M:48:PRO:HD3	1.49	0.95
8:L:1278:BCB:H91	8:L:1278:BCB:H122	1.52	0.87
9:L:1276:BPB:HHC	9:L:1276:BPB:HBBB	1.59	0.84
8:L:1278:BCB:H141	8:L:1278:BCB:H172	1.60	0.82
4:M:136:ARG:HA	4:M:136:ARG:HE	1.45	0.81
3:L:178:SER:O	3:L:182:VAL:HG23	1.79	0.81
6:M:1331:LDA:H91	6:M:1331:LDA:H52	1.67	0.76
9:L:1276:BPB:HBBA	4:M:208:TYR:HB3	1.70	0.74
2:H:81:ARG:HG2	2:H:83:PRO:HD3	1.71	0.72
1:C:65:LEU:HD11	1:C:327:GLU:HG2	1.73	0.71
3:L:181:PHE:HB3	9:M:1325:BPB:CBB	2.21	0.71
1:C:146[B]:ARG:HB3	1:C:146[B]:ARG:HH11	1.57	0.70
1:C:152:LEU:HD21	1:C:178:LYS:HG3	1.73	0.69
3:L:181:PHE:CD2	9:M:1325:BPB:HBB	2.28	0.68
1:C:152:LEU:HD22	1:C:175:ARG:HA	1.76	0.66
2:H:42:PRO:HD3	6:H:1259:LDA:H121	1.78	0.66
2:H:86:ARG:NH2	2:H:111:ALA:HB3	2.12	0.65
4:M:38:LEU:CD2	4:M:46:ILE:HD11	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:LEU:O	1:C:115:ARG:HG3	1.97	0.64
2:H:14:GLN:HE21	6:M:1330:LDA:HM13	1.61	0.64
3:L:182:VAL:HG13	8:L:1278:BCB:H42	1.80	0.64
8:L:1278:BCB:HHC	8:L:1278:BCB:HBB2	1.80	0.64
5:C:1335:HEC:HBC3	5:C:1335:HEC:HMC1	1.80	0.63
3:L:182:VAL:HG22	8:L:1278:BCB:C1	2.28	0.63
1:C:163:VAL:HG23	14:C:2061:HOH:O	1.98	0.63
1:C:278:ASN:HB3	1:C:302:GLN:NE2	2.15	0.61
4:M:160:CYS:C	4:M:163:PRO:HD2	2.20	0.61
4:M:155:VAL:CG2	8:M:1324:BCB:H71	2.30	0.61
8:L:1275:BCB:HBB2	8:L:1275:BCB:HMB1	1.82	0.61
9:M:1325:BPB:HHC	9:M:1325:BPB:HBBB	1.83	0.61
3:L:182:VAL:HG22	8:L:1278:BCB:H12	1.83	0.60
4:M:59:PHE:HA	9:M:1325:BPB:H5	1.83	0.60
1:C:148:LEU:O	1:C:191:THR:HG21	2.01	0.59
2:H:152:PRO:HA	2:H:155:LEU:HD12	1.85	0.59
3:L:79:PRO:HG2	3:L:82:GLU:HB2	1.85	0.59
4:M:198:PRO:HG3	6:M:1330:LDA:H81	1.85	0.58
9:L:1276:BPB:HHC	9:L:1276:BPB:CBB	2.31	0.58
4:M:107:LEU:HA	4:M:111:GLY:HA3	1.86	0.58
2:H:235:GLU:CD	4:M:231:ARG:HH22	2.08	0.57
2:H:161:ASP:HB3	2:H:214:LEU:HD22	1.84	0.57
8:M:1324:BCB:HMB1	8:M:1324:BCB:CBB	2.34	0.57
4:M:299:HIS:HB3	6:M:1330:LDA:HM21	1.87	0.57
1:C:122:THR:HG22	1:C:123[B]:GLN:NE2	2.19	0.56
1:C:108:ARG:NH1	5:C:1333:HEC:O2D	2.37	0.56
1:C:145:VAL:O	1:C:146[A]:ARG:HD2	2.05	0.56
2:H:20:GLN:HG2	4:M:202:PHE:CE2	2.41	0.56
1:C:281:TYR:O	1:C:285:LEU:HG	2.06	0.56
2:H:200:PHE:CZ	4:M:226:ARG:HD3	2.41	0.56
1:C:26:ALA:O	1:C:29:LYS:HG3	2.05	0.55
3:L:135:ARG:HB3	3:L:136:PRO:HD3	1.87	0.55
1:C:60:LYS:HB2	1:C:108:ARG:NH1	2.21	0.55
9:L:1276:BPB:HBB	4:M:208:TYR:CD2	2.42	0.55
1:C:15:ARG:HG2	14:L:2020:HOH:O	2.07	0.54
1:C:52:VAL:HB	1:C:56:TYR:HD2	1.71	0.54
3:L:214:GLN:NE2	4:M:19:VAL:H	2.06	0.54
2:H:235:GLU:OE1	4:M:231:ARG:NH2	2.41	0.53
8:L:1275:BCB:HMD2	8:M:1324:BCB:HBB3	1.90	0.53
4:M:136:ARG:HA	4:M:136:ARG:NE	2.20	0.53
1:C:181:ALA:O	1:C:182:TYR:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:1275:BCB:CBB	8:L:1275:BCB:HMB1	2.38	0.53
8:M:1324:BCB:HAA2	8:M:1324:BCB:HBD	1.90	0.53
1:C:123[B]:GLN:CD	1:C:123[B]:GLN:H	2.13	0.52
1:C:278:ASN:HB3	1:C:302:GLN:HE21	1.74	0.52
4:M:2:ASP:OD1	4:M:4:GLN:HB2	2.09	0.52
8:L:1274:BCB:HBB3	8:L:1274:BCB:HMB1	1.91	0.52
2:H:231:THR:OG1	2:H:234:GLU:HG3	2.09	0.52
1:C:283:ALA:HB3	1:C:284:PRO:HD3	1.91	0.52
1:C:85:GLU:HG2	1:C:89:TYR:CD1	2.45	0.52
2:H:142:ASP:OD1	2:H:142:ASP:N	2.40	0.52
8:L:1274:BCB:HHC	8:L:1274:BCB:OB	2.10	0.52
3:L:182:VAL:HG13	8:L:1278:BCB:C4	2.39	0.52
3:L:197:VAL:HG13	3:L:207:LYS:HB2	1.91	0.51
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.45	0.51
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.46	0.51
3:L:181:PHE:HB3	9:M:1325:BPB:HBBA	1.91	0.51
2:H:133:LYS:HE2	2:H:176:SER:OG	2.11	0.51
8:L:1274:BCB:CBB	8:L:1274:BCB:HMB1	2.41	0.51
3:L:182:VAL:HG22	8:L:1278:BCB:H11	1.93	0.51
6:M:1330:LDA:HM21	6:M:1330:LDA:H32	1.92	0.50
1:C:182:TYR:CE1	3:L:261:GLU:HG3	2.47	0.50
2:H:134:ILE:N	2:H:134:ILE:HD12	2.27	0.50
3:L:167:TRP:HE1	3:L:173:HIS:CD2	2.30	0.49
1:C:161:THR:OG1	1:C:164:GLU:HG3	2.12	0.49
3:L:29:TYR:OH	6:M:1332:LDA:H32	2.13	0.49
3:L:230:HIS:CD2	4:M:221:ILE:HG13	2.48	0.49
4:M:29:VAL:HG12	4:M:30:GLY:N	2.27	0.49
2:H:138:ARG:NH2	2:H:184:GLU:OE1	2.41	0.49
1:C:182:TYR:CD1	3:L:261:GLU:HG3	2.48	0.49
3:L:79:PRO:HG2	3:L:82:GLU:CB	2.43	0.49
4:M:120:MET:CE	13:M:1328:NS5:H273	2.43	0.49
8:M:1324:BCB:H203	9:M:1325:BPB:H4B	1.95	0.49
8:L:1278:BCB:HBB3	8:M:1324:BCB:H62	1.95	0.49
3:L:214:GLN:HE21	4:M:19:VAL:H	1.60	0.49
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.49	0.48
2:H:184:GLU:HG3	2:H:195:LEU:HD23	1.95	0.48
8:M:1324:BCB:HBB3	8:M:1324:BCB:HMB1	1.96	0.48
4:M:132:TYR:CE1	4:M:142:THR:HG21	2.48	0.48
4:M:34:TYR:CD1	4:M:34:TYR:N	2.81	0.48
8:L:1278:BCB:H91	8:L:1278:BCB:C12	2.35	0.48
4:M:155:VAL:HG21	8:M:1324:BCB:H71	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:2:ASP:OD2	4:M:226:ARG:HG3	2.14	0.47
2:H:258:LEU:HB2	3:L:17:ILE:HG22	1.96	0.47
2:H:134:ILE:HG22	2:H:172:TRP:HE3	1.78	0.47
1:C:146[B]:ARG:HB3	1:C:146[B]:ARG:NH1	2.26	0.47
4:M:160:CYS:SG	13:M:1328:NS5:H322	2.55	0.46
2:H:90:LEU:HD23	2:H:103:PRO:HA	1.96	0.46
4:M:241:THR:O	4:M:245:ARG:HG3	2.15	0.46
2:H:96:PHE:HD1	2:H:96:PHE:H	1.62	0.46
4:M:231:ARG:HD2	14:M:2050:HOH:O	2.16	0.46
4:M:147:ASN:HD22	9:M:1325:BPB:HMDA	1.81	0.46
4:M:38:LEU:HD22	4:M:46:ILE:HD11	1.97	0.45
10:L:1277:SMA:H19	8:L:1278:BCB:H92	1.98	0.45
4:M:98:ALA:HB3	4:M:100:TYR:CZ	2.51	0.45
2:H:86:ARG:HH22	2:H:111:ALA:HB3	1.82	0.45
2:H:34:ARG:HG2	2:H:61:GLU:O	2.17	0.45
8:L:1274:BCB:H11	8:L:1275:BCB:H2C	1.99	0.45
4:M:155:VAL:HG23	8:M:1324:BCB:H71	1.97	0.45
3:L:35:GLY:O	3:L:39:ILE:HG12	2.17	0.45
2:H:56:ASP:HB3	2:H:60:TYR:CE2	2.52	0.44
3:L:168:HIS:CE1	8:L:1274:BCB:HMC2	2.53	0.44
8:L:1275:BCB:OBB	8:L:1275:BCB:HHC	2.16	0.44
8:L:1278:BCB:H141	8:L:1278:BCB:C17	2.40	0.44
1:C:96:LEU:O	5:C:1333:HEC:HBA1	2.17	0.44
1:C:216:ARG:O	1:C:219:GLU:HG3	2.18	0.44
4:M:73:MET:HE3	4:M:91:LEU:HB2	1.99	0.44
8:M:1324:BCB:OBB	8:M:1324:BCB:HHC	2.17	0.44
2:H:117:TYR:HB2	2:H:236:ASP:HB3	2.00	0.43
5:C:1334:HEC:HBC3	5:C:1334:HEC:HMC1	2.00	0.43
14:H:2032:HOH:O	4:M:231:ARG:HD2	2.18	0.43
2:H:138:ARG:HH22	2:H:184:GLU:CD	2.19	0.43
3:L:244:GLY:O	8:L:1274:BCB:HED3	2.18	0.43
2:H:121:ALA:HB1	2:H:123:VAL:HG13	2.00	0.43
1:C:146[A]:ARG:NH2	1:C:150:PRO:HA	2.34	0.43
1:C:18:SER:HB2	3:L:156:TRP:CD1	2.54	0.43
4:M:258:ALA:HB1	4:M:262:SER:OG	2.19	0.43
4:M:162:HIS:HB3	4:M:163:PRO:HD3	2.01	0.42
3:L:208:THR:OG1	3:L:211:HIS:HD2	2.02	0.42
2:H:173:VAL:HG22	2:H:174:ASP:N	2.33	0.42
1:C:144:TYR:CD2	1:C:310:GLN:HG2	2.54	0.42
1:C:146[A]:ARG:HH21	1:C:150:PRO:HA	1.85	0.42
2:H:204:LYS:HB2	2:H:207:LYS:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:1276:BPB:H44	9:L:1276:BPB:HBAA	1.92	0.42
1:C:159:THR:HA	1:C:160:PRO:HD3	1.87	0.42
1:C:290:PRO:HG2	1:C:293:ARG:HG2	2.01	0.42
1:C:65:LEU:CD1	1:C:327:GLU:HG2	2.46	0.42
1:C:163:VAL:HB	3:L:273:SER:O	2.20	0.42
13:M:1328:NS5:H29	13:M:1328:NS5:H271	1.81	0.42
3:L:239:ASN:HD22	3:L:242:LEU:HB2	1.85	0.41
4:M:192:GLY:O	4:M:193:ASN:HB3	2.19	0.41
4:M:11:GLN:HB3	4:M:13:ARG:HH12	1.85	0.41
1:C:217:GLY:HA2	4:M:167:GLY:O	2.19	0.41
1:C:146[A]:ARG:NH2	1:C:151:THR:H	2.19	0.41
1:C:304:ASP:OD1	1:C:304:ASP:C	2.59	0.41
2:H:14:GLN:HE21	6:M:1330:LDA:CM1	2.29	0.41
3:L:239:ASN:HD22	3:L:239:ASN:HA	1.76	0.41
3:L:259:TRP:N	3:L:260:PRO:CD	2.84	0.41
4:M:95:PRO:HB2	4:M:96:PRO:HD2	2.02	0.41
1:C:133:TYR:CE1	1:C:137:ARG:HA	2.55	0.41
3:L:60:ASP:HA	3:L:61:PRO:HD3	1.88	0.41
2:H:30:LEU:O	2:H:34:ARG:HD2	2.21	0.41
10:L:1277:SMA:C15	8:L:1278:BCB:H92	2.50	0.41
4:M:157:CYS:HA	4:M:161:ILE:HB	2.02	0.41
4:M:162:HIS:N	4:M:163:PRO:CD	2.84	0.41
4:M:200:HIS:CE1	4:M:204:ILE:HD11	2.56	0.41
2:H:25:TRP:CE3	2:H:25:TRP:HA	2.56	0.40
3:L:115:TRP:O	3:L:118:PRO:HG2	2.21	0.40
3:L:249:ILE:HA	3:L:249:ILE:HD13	1.98	0.40
4:M:178:TRP:N	4:M:179:PRO:CD	2.85	0.40
1:C:52:VAL:HG23	1:C:63:GLY:HA2	2.02	0.40
3:L:7:ARG:HH11	3:L:7:ARG:HG3	1.87	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	332/356 (93%)	317 (96%)	15 (4%)	0	100	100
2	H	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
3	L	271/273 (99%)	262 (97%)	9 (3%)	0	100	100
4	M	321/323 (99%)	310 (97%)	10 (3%)	1 (0%)	41	55
All	All	1180/1210 (98%)	1131 (96%)	48 (4%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	M	177	ILE

### 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	282/297 (95%)	279 (99%)	3 (1%)	73	87
2	H	212/212 (100%)	209 (99%)	3 (1%)	67	82
3	L	218/218 (100%)	215 (99%)	3 (1%)	67	82
4	M	249/249 (100%)	242 (97%)	7 (3%)	43	63
All	All	961/976 (98%)	945 (98%)	16 (2%)	60	78

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	15	ARG
1	C	38	TYR
1	C	152	LEU
2	H	22	LEU
2	H	236	ASP
2	H	257	LEU
3	L	82	GLU
3	L	160	PHE
3	L	272	TRP
4	M	37	TRP

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Mol	Chain	Res	Type
4	M	71	PHE
4	M	114	LEU
4	M	136	ARG
4	M	194	PHE
4	M	214	PHE
4	M	290	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	302	GLN
2	H	58	GLN
2	H	220	ASN
3	L	211	HIS
3	L	214	GLN
3	L	239	ASN
4	M	147	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FME	H	1	2	8,9,10	0.61	0	7,9,11	3.11	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
2	FME	H	1	2	-	2/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	FME	CA-N-CN	-5.79	113.91	122.82
2	H	1	FME	O1-CN-N	-5.47	110.88	125.27

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	FME	CB-CA-N-CN
2	H	1	FME	O1-CN-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	$\# Z  > 2$
8	BCB	L	1275	3	60,74,74	3.61	22 (36%)	48,115,115	2.41	13 (27%)
6	LDA	M	1330	-	12,15,15	2.36	1 (8%)	14,17,17	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	SO4	M	1336	-	4,4,4	0.58	0	6,6,6	0.45	0
7	SO4	M	1335	-	4,4,4	0.61	0	6,6,6	0.07	0
6	LDA	H	1259	-	12,15,15	2.38	1 (8%)	14,17,17	0.53	0
6	LDA	M	1329	-	12,15,15	2.22	1 (8%)	14,17,17	0.57	0
7	SO4	M	1334	-	4,4,4	0.84	0	6,6,6	0.38	0
10	SMA	L	1277	-	35,38,38	1.63	8 (22%)	46,52,52	1.52	5 (10%)
9	BPB	M	1325	-	64,70,70	1.23	8 (12%)	64,101,101	1.72	11 (17%)
8	BCB	L	1274	3	60,74,74	3.63	23 (38%)	48,115,115	2.45	16 (33%)
5	HEC	C	1333	1	26,50,50	1.60	2 (7%)	18,82,82	0.67	0
8	BCB	M	1324	4	60,74,74	3.61	23 (38%)	48,115,115	2.62	18 (37%)
12	MQ7	M	1327	-	49,49,49	1.48	9 (18%)	60,63,63	1.22	8 (13%)
6	LDA	M	1332	-	12,15,15	2.42	1 (8%)	14,17,17	0.54	0
8	BCB	L	1278	4	60,74,74	3.64	22 (36%)	48,115,115	2.68	18 (37%)
5	HEC	C	1334	1	26,50,50	1.59	2 (7%)	18,82,82	1.09	1 (5%)
6	LDA	M	1333	-	12,15,15	2.42	1 (8%)	14,17,17	0.52	0
5	HEC	C	1335	1	26,50,50	1.57	2 (7%)	18,82,82	0.86	1 (5%)
7	SO4	H	1260	-	4,4,4	0.52	0	6,6,6	0.18	0
5	HEC	C	1336	1	26,50,50	1.51	2 (7%)	18,82,82	0.66	0
6	LDA	M	1331	-	12,15,15	2.26	1 (8%)	14,17,17	0.46	0
9	BPB	L	1276	-	64,70,70	1.29	6 (9%)	64,101,101	1.69	10 (15%)
13	NS5	M	1328	-	39,39,39	0.67	0	44,46,46	1.10	4 (9%)

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	LDA	M	1332	-	-	0/13/13/13	-
6	LDA	H	1259	-	-	0/13/13/13	-
12	MQ7	M	1327	-	-	1/41/61/61	0/2/2/2
6	LDA	M	1329	-	-	0/13/13/13	-
8	BCB	L	1278	4	-	1/41/177/177	-
8	BCB	L	1275	3	-	4/41/177/177	-
10	SMA	L	1277	-	-	5/33/34/34	0/2/2/2
6	LDA	M	1331	-	-	2/13/13/13	-
5	HEC	C	1336	1	-	0/6/54/54	-
6	LDA	M	1330	-	-	0/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BPB	M	1325	-	-	7/47/105/105	0/5/6/6
9	BPB	L	1276	-	-	4/47/105/105	0/5/6/6
8	BCB	L	1274	3	-	6/41/177/177	-
5	HEC	C	1334	1	-	0/6/54/54	-
5	HEC	C	1333	1	-	0/6/54/54	-
6	LDA	M	1333	-	-	0/13/13/13	-
13	NS5	M	1328	-	-	8/43/43/43	-
8	BCB	M	1324	4	1/1/31/36	7/41/177/177	-
5	HEC	C	1335	1	-	0/6/54/54	-

All (135) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	1324	BCB	CHD-C1D	-8.65	1.39	1.53
8	L	1274	BCB	CHD-C1D	-8.61	1.40	1.53
8	L	1278	BCB	CHC-C4B	-8.57	1.40	1.53
8	L	1275	BCB	CHB-C1B	-8.55	1.40	1.53
8	L	1274	BCB	CHB-C1B	-8.55	1.40	1.53
8	M	1324	BCB	C1A-CHA	-8.55	1.40	1.54
8	L	1278	BCB	CHD-C1D	-8.51	1.40	1.53
6	M	1332	LDA	O1-N1	-8.37	1.22	1.42
6	M	1333	LDA	O1-N1	-8.36	1.22	1.42
8	L	1278	BCB	CHB-C1B	-8.30	1.40	1.53
6	H	1259	LDA	O1-N1	-8.24	1.22	1.42
6	M	1330	LDA	O1-N1	-8.15	1.23	1.42
8	L	1275	BCB	C1A-CHA	-8.10	1.41	1.54
8	M	1324	BCB	CHB-C1B	-8.02	1.40	1.53
8	L	1274	BCB	CHD-C4C	-7.94	1.40	1.53
8	L	1274	BCB	C1A-CHA	-7.92	1.41	1.54
8	L	1275	BCB	CHC-C4B	-7.92	1.41	1.53
8	L	1278	BCB	C1A-CHA	-7.91	1.41	1.54
8	L	1275	BCB	CHD-C1D	-7.90	1.41	1.53
8	L	1274	BCB	CHC-C4B	-7.87	1.41	1.53
8	M	1324	BCB	CHC-C4B	-7.84	1.41	1.53
6	M	1331	LDA	O1-N1	-7.79	1.23	1.42
6	M	1329	LDA	O1-N1	-7.68	1.24	1.42
8	L	1278	BCB	CHD-C4C	-7.58	1.40	1.53
8	M	1324	BCB	CHD-C4C	-7.58	1.40	1.53
8	L	1275	BCB	CHD-C4C	-7.28	1.41	1.53
8	L	1275	BCB	C3B-C2B	-7.24	1.36	1.55
8	M	1324	BCB	C3B-C2B	-7.13	1.36	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	1278	BCB	C3B-C2B	-6.95	1.37	1.55
8	L	1275	BCB	C3D-C2D	-6.90	1.37	1.55
8	L	1274	BCB	C3B-C2B	-6.87	1.37	1.55
8	M	1324	BCB	C3D-C2D	-6.86	1.37	1.55
8	L	1278	BCB	C3D-C2D	-6.84	1.37	1.55
8	L	1274	BCB	C3D-C2D	-6.83	1.37	1.55
8	M	1324	BCB	C4D-ND	-6.62	1.36	1.50
8	L	1275	BCB	C4D-ND	-6.49	1.36	1.50
8	L	1274	BCB	C4D-ND	-6.46	1.36	1.50
8	L	1278	BCB	C4D-ND	-6.42	1.36	1.50
8	M	1324	BCB	C1D-ND	-6.10	1.37	1.50
8	L	1278	BCB	C1D-ND	-6.03	1.37	1.50
8	L	1274	BCB	C1D-ND	-5.99	1.37	1.50
8	L	1275	BCB	C1D-ND	-5.95	1.37	1.50
8	M	1324	BCB	C4B-NB	-5.94	1.37	1.50
8	L	1278	BCB	CHC-C1C	-5.85	1.39	1.52
8	L	1275	BCB	CHB-C4A	-5.83	1.39	1.52
8	L	1275	BCB	C4B-NB	-5.82	1.38	1.50
8	L	1275	BCB	CHC-C1C	-5.76	1.39	1.52
8	L	1274	BCB	C4B-NB	-5.76	1.38	1.50
8	L	1278	BCB	C4B-NB	-5.74	1.38	1.50
8	M	1324	BCB	C1B-NB	-5.67	1.38	1.50
8	L	1274	BCB	CHB-C4A	-5.66	1.39	1.52
8	L	1275	BCB	C1B-NB	-5.65	1.38	1.50
8	L	1278	BCB	C1B-NB	-5.53	1.38	1.50
8	L	1274	BCB	C1B-NB	-5.51	1.38	1.50
8	M	1324	BCB	CHC-C1C	-5.44	1.40	1.52
8	L	1275	BCB	C3B-CAB	-5.44	1.46	1.52
8	L	1274	BCB	C3B-CAB	-5.44	1.46	1.52
8	L	1274	BCB	CHC-C1C	-5.43	1.40	1.52
8	L	1278	BCB	CHB-C4A	-5.42	1.40	1.52
8	M	1324	BCB	CHB-C4A	-5.41	1.40	1.52
5	C	1333	HEC	C3B-C2B	-5.14	1.35	1.40
5	C	1335	HEC	C3C-C2C	-5.02	1.35	1.40
8	L	1274	BCB	C2B-C1B	-4.90	1.44	1.53
8	M	1324	BCB	C3B-CAB	-4.85	1.46	1.52
8	L	1278	BCB	C3B-CAB	-4.77	1.46	1.52
8	L	1278	BCB	O2A-CGA	4.75	1.47	1.33
8	L	1275	BCB	C2B-C1B	-4.74	1.44	1.53
5	C	1333	HEC	C3C-C2C	-4.73	1.35	1.40
5	C	1336	HEC	C3C-C2C	-4.73	1.35	1.40
5	C	1334	HEC	C3C-C2C	-4.64	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1336	HEC	C3B-C2B	-4.57	1.36	1.40
8	M	1324	BCB	C2B-C1B	-4.57	1.45	1.53
5	C	1334	HEC	C3B-C2B	-4.55	1.36	1.40
8	L	1278	BCB	C2B-C1B	-4.52	1.45	1.53
5	C	1335	HEC	C3B-C2B	-4.48	1.36	1.40
9	L	1276	BPB	C3B-C4B	4.29	1.46	1.41
8	L	1275	BCB	O2D-CED	-4.28	1.35	1.45
10	L	1277	SMA	O1-C2	4.28	1.41	1.35
8	L	1278	BCB	C2D-C1D	-4.20	1.45	1.53
8	L	1274	BCB	C2D-C1D	-4.15	1.45	1.53
10	L	1277	SMA	C20-C19	4.10	1.36	1.33
8	M	1324	BCB	C2D-C1D	-4.06	1.45	1.53
8	M	1324	BCB	O2D-CED	-4.05	1.35	1.45
9	L	1276	BPB	O2D-CED	-4.05	1.35	1.45
9	M	1325	BPB	O2D-CED	-4.01	1.35	1.45
8	L	1278	BCB	O2D-CED	-3.98	1.35	1.45
8	L	1275	BCB	C2D-C1D	-3.96	1.46	1.53
9	L	1276	BPB	O2D-CGD	3.95	1.42	1.33
8	L	1274	BCB	O2D-CED	-3.81	1.36	1.45
9	M	1325	BPB	C3B-C4B	3.78	1.46	1.41
8	L	1274	BCB	O2D-CGD	3.63	1.42	1.33
8	L	1278	BCB	C3D-CAD	-3.63	1.44	1.51
8	L	1274	BCB	C3D-CAD	-3.57	1.44	1.51
8	L	1275	BCB	C3D-CAD	-3.56	1.44	1.51
8	M	1324	BCB	C3D-CAD	-3.51	1.44	1.51
10	L	1277	SMA	C4-C3	3.38	1.51	1.41
8	M	1324	BCB	C4C-C3C	-3.30	1.40	1.50
12	M	1327	MQ7	C11-C12	-3.26	1.45	1.50
9	M	1325	BPB	O2D-CGD	3.25	1.41	1.33
8	L	1274	BCB	C1-C2	-3.19	1.39	1.49
8	L	1275	BCB	O2D-CGD	3.12	1.40	1.33
8	L	1278	BCB	C4C-C3C	-3.06	1.41	1.50
8	M	1324	BCB	O2A-CGA	3.04	1.42	1.33
8	L	1274	BCB	C4C-C3C	-3.03	1.41	1.50
8	L	1278	BCB	O2D-CGD	2.98	1.40	1.33
8	L	1275	BCB	O2A-CGA	2.96	1.42	1.33
8	L	1275	BCB	C4C-C3C	-2.94	1.42	1.50
8	L	1278	BCB	C2-C3	2.93	1.40	1.33
9	M	1325	BPB	C2-C3	2.86	1.39	1.33
9	L	1276	BPB	C2-C3	2.75	1.39	1.33
9	L	1276	BPB	O2A-CGA	2.75	1.41	1.33
12	M	1327	MQ7	C37-C38	2.71	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	1275	BCB	C2-C3	2.71	1.39	1.33
12	M	1327	MQ7	C42-C43	2.70	1.40	1.32
9	M	1325	BPB	CAC-C3C	2.70	1.40	1.33
12	M	1327	MQ7	C32-C33	2.67	1.39	1.33
8	M	1324	BCB	C2-C3	2.66	1.39	1.33
9	M	1325	BPB	O2A-CGA	2.60	1.40	1.33
8	L	1274	BCB	C2A-C3A	-2.55	1.50	1.54
12	M	1327	MQ7	C27-C28	2.53	1.39	1.33
8	M	1324	BCB	O2D-CGD	2.52	1.39	1.33
12	M	1327	MQ7	C12-C13	2.47	1.38	1.33
12	M	1327	MQ7	C17-C18	2.45	1.38	1.33
12	M	1327	MQ7	C22-C23	2.45	1.38	1.33
10	L	1277	SMA	O7-C7	2.34	1.40	1.37
8	L	1274	BCB	C2-C3	2.33	1.38	1.33
9	L	1276	BPB	CAC-C3C	2.33	1.39	1.33
10	L	1277	SMA	O1-C8A	2.28	1.40	1.36
9	M	1325	BPB	C4C-C3C	-2.25	1.40	1.45
10	L	1277	SMA	C4A-C8A	2.23	1.44	1.41
8	M	1324	BCB	C1A-C2A	-2.22	1.51	1.53
10	L	1277	SMA	C7-C8	2.18	1.43	1.40
9	M	1325	BPB	C3B-C2B	-2.14	1.35	1.39
10	L	1277	SMA	C6-C7	2.07	1.42	1.38
12	M	1327	MQ7	C10-C5	-2.03	1.37	1.40

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	1278	BCB	C1D-CHD-C4C	7.36	128.05	112.37
8	L	1275	BCB	C1D-CHD-C4C	7.30	127.93	112.37
8	M	1324	BCB	C1D-CHD-C4C	7.26	127.83	112.37
8	L	1274	BCB	C1D-CHD-C4C	7.17	127.65	112.37
9	M	1325	BPB	O2D-CGD-CBD	6.95	123.61	111.27
8	L	1278	BCB	CBB-CAB-C3B	6.69	123.63	116.80
9	L	1276	BPB	O2D-CGD-CBD	6.44	122.71	111.27
8	L	1274	BCB	CMB-C2B-C3B	6.20	129.69	114.29
8	L	1274	BCB	CMD-C2D-C3D	6.08	129.39	114.29
8	L	1275	BCB	CMB-C2B-C3B	5.93	129.01	114.29
8	M	1324	BCB	CMD-C2D-C3D	5.93	129.01	114.29
8	L	1278	BCB	CMD-C2D-C3D	5.91	128.96	114.29
8	M	1324	BCB	CMB-C2B-C3B	5.90	128.95	114.29
8	L	1275	BCB	O2D-CGD-CBD	5.69	124.47	111.11
8	L	1275	BCB	CMD-C2D-C3D	5.66	128.35	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	1275	BCB	O1D-CGD-CBD	-5.35	113.94	124.54
8	L	1278	BCB	CMB-C2B-C3B	5.18	127.15	114.29
8	L	1278	BCB	O2D-CGD-CBD	5.08	123.04	111.11
8	M	1324	BCB	O2D-CGD-CBD	4.99	122.82	111.11
9	M	1325	BPB	O1D-CGD-CBD	-4.95	114.35	124.48
10	L	1277	SMA	C9-C2-C3	4.94	127.39	120.39
8	L	1278	BCB	O1D-CGD-CBD	-4.88	114.87	124.54
8	L	1274	BCB	O2D-CGD-CBD	4.84	122.47	111.11
10	L	1277	SMA	C3-C4-C4A	-4.82	115.73	120.58
9	L	1276	BPB	O1D-CGD-CBD	-4.74	114.78	124.48
8	L	1274	BCB	O1D-CGD-CBD	-4.67	115.29	124.54
9	L	1276	BPB	C1-C2-C3	4.67	134.12	126.04
8	M	1324	BCB	CHA-CBD-CGD	-4.62	104.56	115.02
8	L	1274	BCB	CHA-CBD-CGD	-4.59	104.64	115.02
8	M	1324	BCB	O1D-CGD-CBD	-4.57	115.49	124.54
8	M	1324	BCB	O2A-CGA-CBA	4.55	126.20	111.91
8	L	1278	BCB	CHA-CBD-CGD	-4.29	105.30	115.02
9	M	1325	BPB	C6-C5-C3	4.26	124.64	113.45
9	M	1325	BPB	C1-C2-C3	4.13	133.19	126.04
8	L	1275	BCB	CHA-CBD-CGD	-4.13	105.68	115.02
8	M	1324	BCB	OBB-CAB-C3B	4.03	125.76	121.52
8	L	1278	BCB	C1-C2-C3	4.02	133.00	126.04
8	L	1278	BCB	C4-C3-C5	-4.01	108.52	115.27
12	M	1327	MQ7	C11-C12-C13	4.01	133.47	126.79
13	M	1328	NS5	C19-C18-C17	3.65	130.96	123.47
9	L	1276	BPB	C3C-C2C-C1C	3.58	105.59	100.72
8	M	1324	BCB	CHC-C4B-C3B	3.57	126.92	118.17
8	L	1278	BCB	O2A-CGA-CBA	3.47	122.80	111.91
8	L	1274	BCB	CHC-C4B-C3B	3.46	126.66	118.17
8	M	1324	BCB	O2A-CGA-O1A	-3.43	114.94	123.59
8	L	1275	BCB	CHC-C4B-C3B	3.37	126.44	118.17
10	L	1277	SMA	C4-C3-C2	3.36	120.32	116.63
8	L	1274	BCB	O2A-CGA-CBA	3.36	122.44	111.91
8	L	1278	BCB	CHC-C4B-C3B	3.29	126.24	118.17
9	M	1325	BPB	C4B-C3B-CAB	-3.29	120.06	127.19
12	M	1327	MQ7	C41-C42-C43	3.28	138.95	127.75
9	M	1325	BPB	C3C-C2C-C1C	3.23	105.11	100.72
8	M	1324	BCB	C15-C13-C12	-3.21	95.25	112.13
5	C	1334	HEC	CBD-CAD-C3D	3.19	118.37	112.49
8	M	1324	BCB	CHC-C1C-C2C	3.10	126.56	117.19
13	M	1328	NS5	C16-C15-C14	-3.05	113.27	118.08
8	L	1278	BCB	OBB-CAB-C3B	-3.05	118.30	121.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	1274	BCB	OBB-CAB-C3B	2.94	124.62	121.52
8	L	1275	BCB	OBB-CAB-C3B	2.94	124.61	121.52
8	L	1274	BCB	CHC-C1C-C2C	2.88	125.90	117.19
8	L	1275	BCB	CHC-C1C-C2C	2.87	125.87	117.19
8	L	1278	BCB	CHC-C1C-C2C	2.79	125.62	117.19
8	L	1278	BCB	OBD-CAD-CBD	-2.72	120.96	127.49
8	M	1324	BCB	OBD-CAD-CBD	-2.70	121.01	127.49
8	L	1274	BCB	OBD-CAD-CBD	-2.69	121.05	127.49
8	L	1275	BCB	OBD-CAD-CBD	-2.68	121.06	127.49
8	L	1274	BCB	O2A-CGA-O1A	-2.65	116.90	123.59
8	L	1274	BCB	C15-C13-C12	-2.64	98.22	112.13
9	L	1276	BPB	O2A-CGA-CBA	2.62	120.13	111.91
8	M	1324	BCB	C5-C3-C2	2.59	126.35	121.12
8	M	1324	BCB	OBD-CAD-C3D	2.58	131.27	126.73
13	M	1328	NS5	C18-C19-C20	2.54	128.68	123.47
8	L	1275	BCB	OBD-CAD-C3D	2.53	131.20	126.73
8	L	1278	BCB	C3B-C4B-NB	2.53	108.36	103.75
8	L	1275	BCB	C3B-C4B-NB	2.51	108.34	103.75
8	L	1278	BCB	OBD-CAD-C3D	2.51	131.16	126.73
10	L	1277	SMA	O12-C12-C13	-2.51	104.27	107.97
8	L	1278	BCB	O2A-CGA-O1A	-2.51	117.26	123.59
8	L	1274	BCB	OBD-CAD-C3D	2.50	131.14	126.73
9	M	1325	BPB	CBD-CHA-C4D	-2.48	105.75	108.54
8	M	1324	BCB	C3B-C4B-NB	2.45	108.23	103.75
8	L	1274	BCB	C3B-C4B-NB	2.44	108.19	103.75
8	M	1324	BCB	C4-C3-C5	-2.42	111.19	115.27
8	L	1275	BCB	C4-C3-C5	-2.42	111.21	115.27
9	L	1276	BPB	C4B-C3B-CAB	-2.40	121.98	127.19
9	L	1276	BPB	CBD-CHA-C4D	-2.33	105.92	108.54
12	M	1327	MQ7	C40-C38-C37	2.30	125.77	121.12
9	L	1276	BPB	CED-O2D-CGD	2.27	121.08	115.94
12	M	1327	MQ7	C36-C37-C38	2.27	133.12	127.66
9	M	1325	BPB	O2A-CGA-CBA	2.23	118.92	111.91
13	M	1328	NS5	C14-C15-C17	2.22	122.35	118.94
8	M	1324	BCB	C1-C2-C3	2.21	129.87	126.04
12	M	1327	MQ7	C39-C38-C40	-2.19	111.58	115.27
9	L	1276	BPB	C3A-C2A-C1A	2.15	104.56	101.34
12	M	1327	MQ7	C45-C43-C42	2.14	128.84	122.65
10	L	1277	SMA	O1-C2-C9	-2.14	109.37	111.91
9	M	1325	BPB	CBD-CHA-C1A	2.13	130.24	126.84
12	M	1327	MQ7	C45-C43-C44	-2.11	109.94	114.60
8	L	1274	BCB	C4-C3-C5	2.10	118.80	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	1325	BPB	C10-C8-C7	2.10	123.15	112.13
9	L	1276	BPB	C4-C3-C5	-2.08	111.78	115.27
8	L	1278	BCB	C5-C3-C2	2.07	125.31	121.12
12	M	1327	MQ7	C34-C33-C35	-2.06	111.81	115.27
5	C	1335	HEC	CMC-C2C-C3C	-2.04	123.42	125.82
9	M	1325	BPB	C3C-C4C-NC	2.02	112.81	109.58

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	M	1324	BCB	C8

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	L	1275	BCB	C2B-C3B-CAB-OBB
8	L	1275	BCB	C2B-C3B-CAB-CBB
8	L	1274	BCB	C2B-C3B-CAB-OBB
8	L	1274	BCB	C2B-C3B-CAB-CBB
8	M	1324	BCB	C2B-C3B-CAB-OBB
8	M	1324	BCB	C2B-C3B-CAB-CBB
8	M	1324	BCB	CAD-CBD-CGD-O1D
8	M	1324	BCB	CAD-CBD-CGD-O2D
13	M	1328	NS5	C11-C10-C12-C13
13	M	1328	NS5	C10-C12-C13-C14
13	M	1328	NS5	C13-C14-C15-C16
13	M	1328	NS5	C13-C14-C15-C17
9	M	1325	BPB	C4-C3-C5-C6
8	L	1274	BCB	C4-C3-C5-C6
9	M	1325	BPB	C2-C3-C5-C6
8	L	1274	BCB	C2-C3-C5-C6
8	M	1324	BCB	C2A-CAA-CBA-CGA
9	L	1276	BPB	O2A-C1-C2-C3
9	L	1276	BPB	C2-C3-C5-C6
9	L	1276	BPB	C4-C3-C5-C6
9	M	1325	BPB	CBA-CGA-O2A-C1
8	L	1275	BCB	C12-C13-C15-C16
9	M	1325	BPB	O1A-CGA-O2A-C1
9	L	1276	BPB	CAD-CBD-CGD-O2D
8	L	1274	BCB	CAD-CBD-CGD-O1D
10	L	1277	SMA	C22-C11-C12-C13
10	L	1277	SMA	C15-C14-O14-C25

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Mol	Chain	Res	Type	Atoms
9	M	1325	BPB	O2A-C1-C2-C3
13	M	1328	NS5	C17-C18-C19-C20
10	L	1277	SMA	C9-C10-C11-C22
13	M	1328	NS5	C7-C8-C9-C10
12	M	1327	MQ7	C39-C38-C40-C41
13	M	1328	NS5	C23-C24-C25-C26
8	M	1324	BCB	C11-C12-C13-C14
8	L	1275	BCB	C3A-C2A-CAA-CBA
6	M	1331	LDA	C5-C6-C7-C8
8	L	1274	BCB	CAD-CBD-CGD-O2D
8	M	1324	BCB	CAA-CBA-CGA-O2A
8	L	1278	BCB	C4B-C3B-CAB-OB
10	L	1277	SMA	C10-C11-C12-O12
10	L	1277	SMA	C13-C14-O14-C25
9	M	1325	BPB	C6-C7-C8-C10
13	M	1328	NS5	C29-C30-C31-C33
6	M	1331	LDA	C3-C4-C5-C6
9	M	1325	BPB	C5-C6-C7-C8

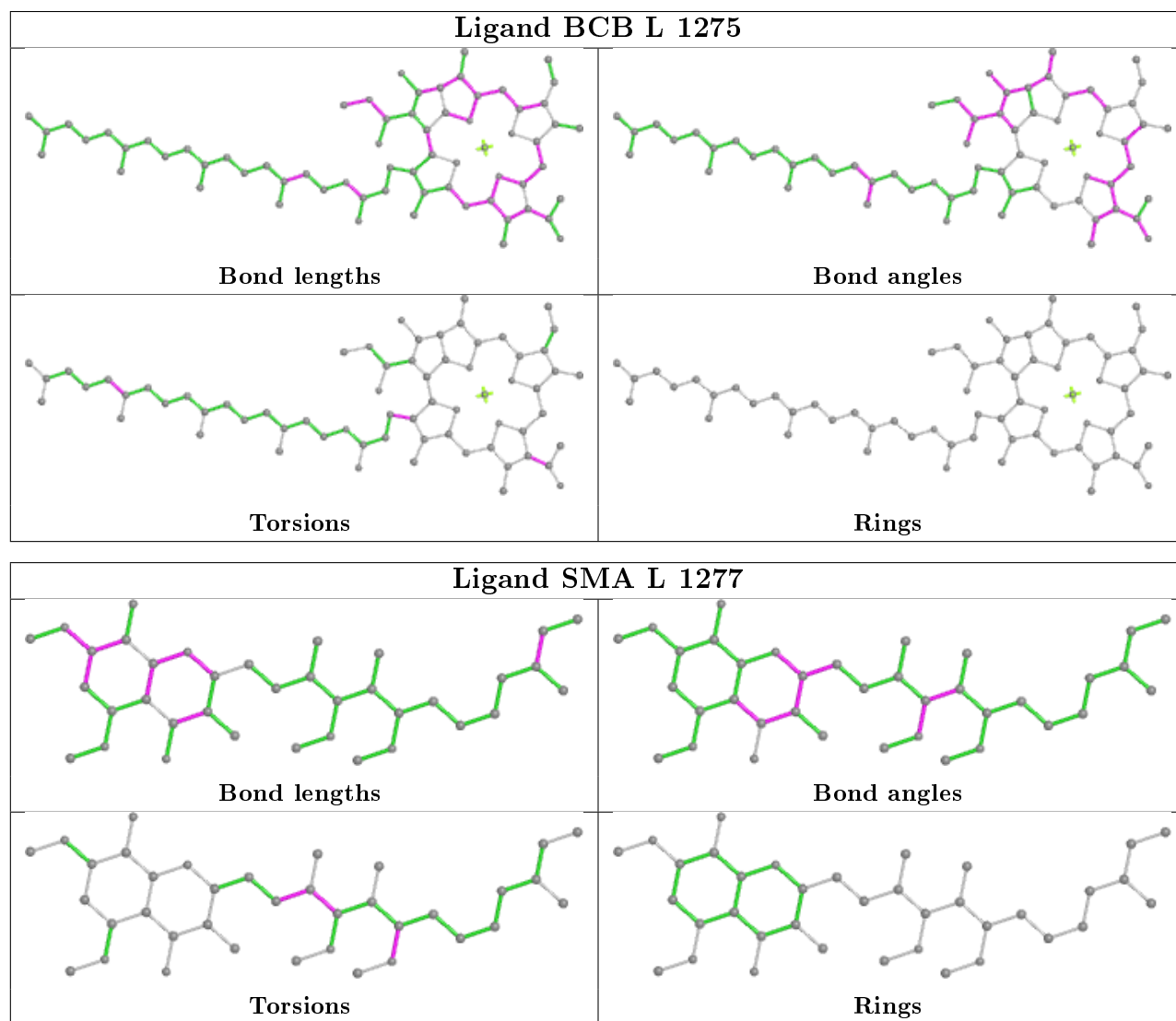
There are no ring outliers.

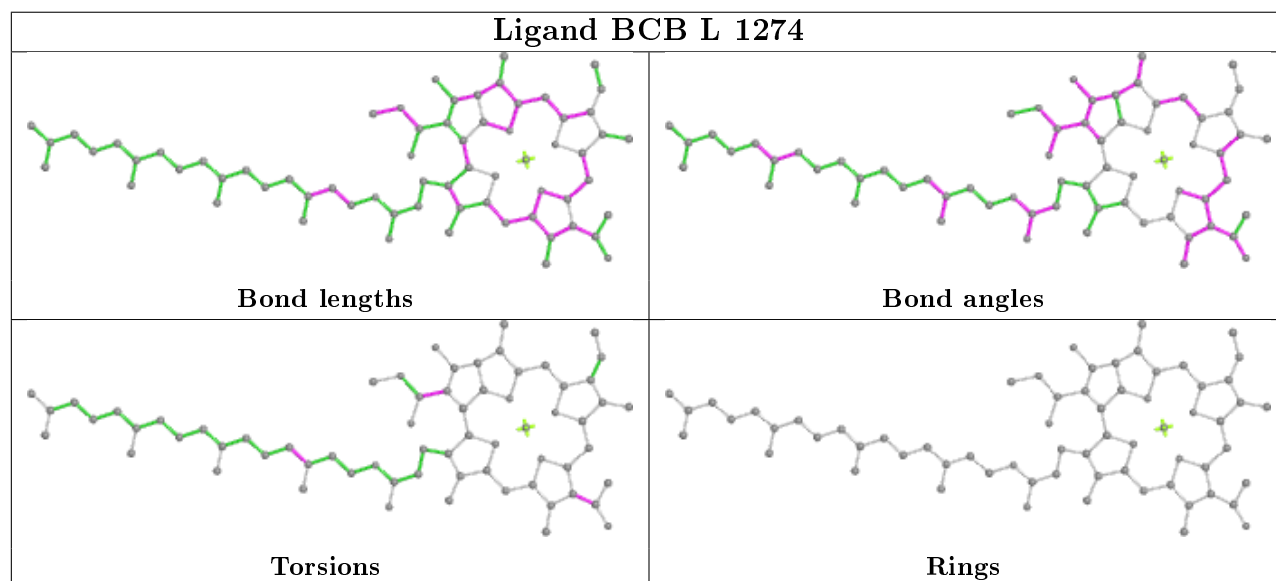
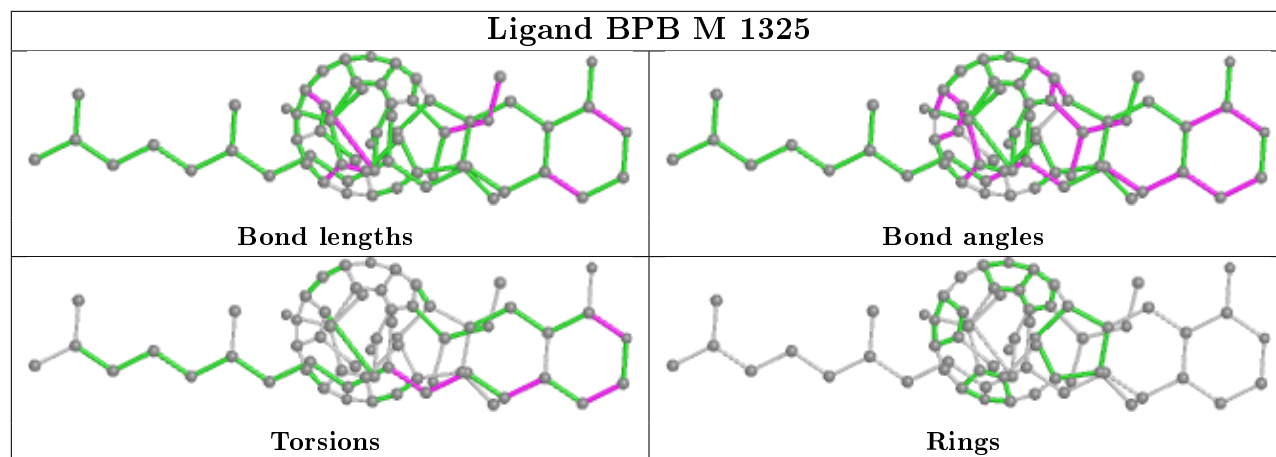
15 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	1275	BCB	5	0
6	M	1330	LDA	5	0
6	H	1259	LDA	1	0
10	L	1277	SMA	2	0
9	M	1325	BPB	7	0
8	L	1274	BCB	6	0
5	C	1333	HEC	2	0
8	M	1324	BCB	10	0
6	M	1332	LDA	1	0
8	L	1278	BCB	13	0
5	C	1334	HEC	1	0
5	C	1335	HEC	1	0
6	M	1331	LDA	1	0
9	L	1276	BPB	5	0
13	M	1328	NS5	3	0

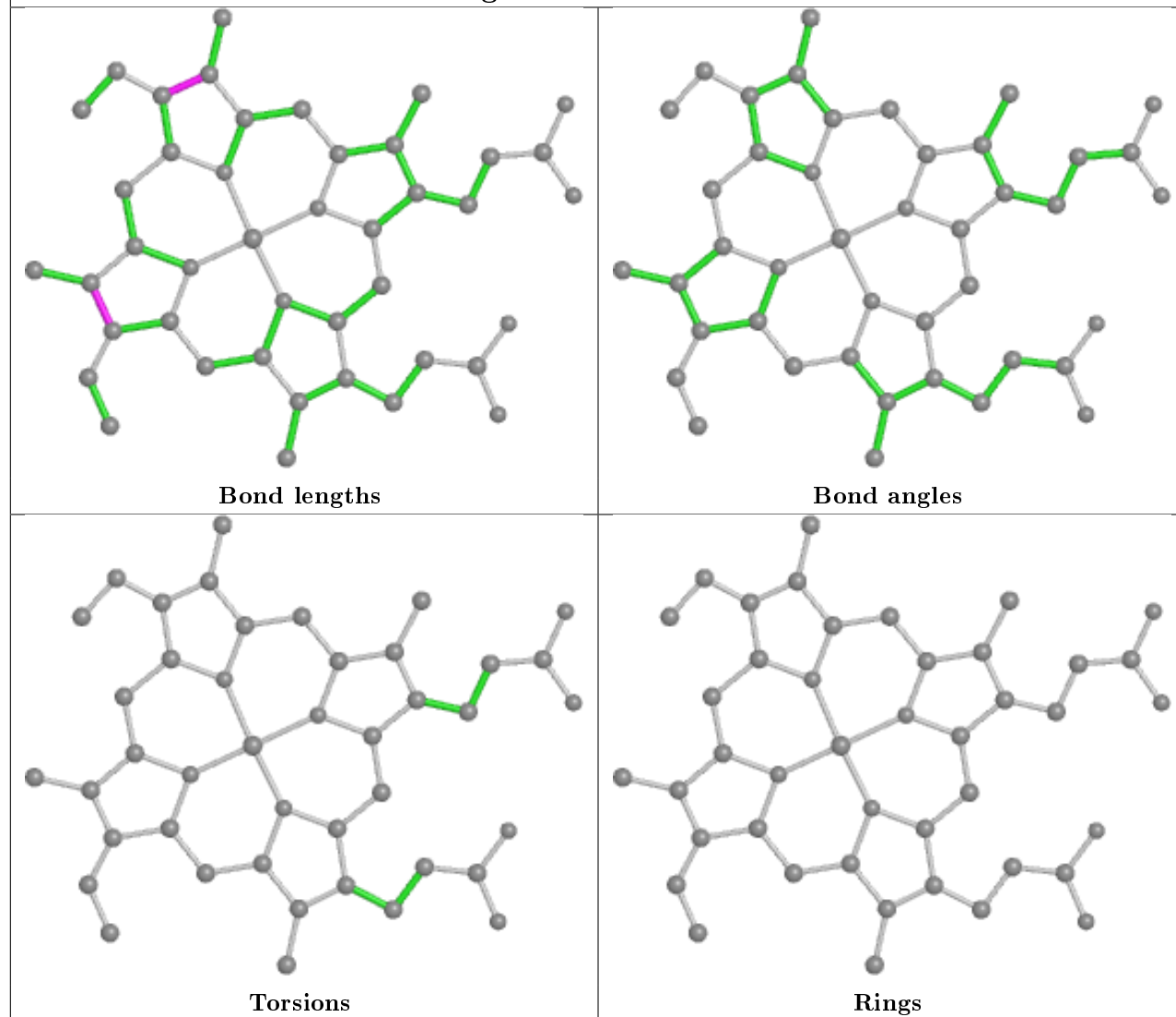
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

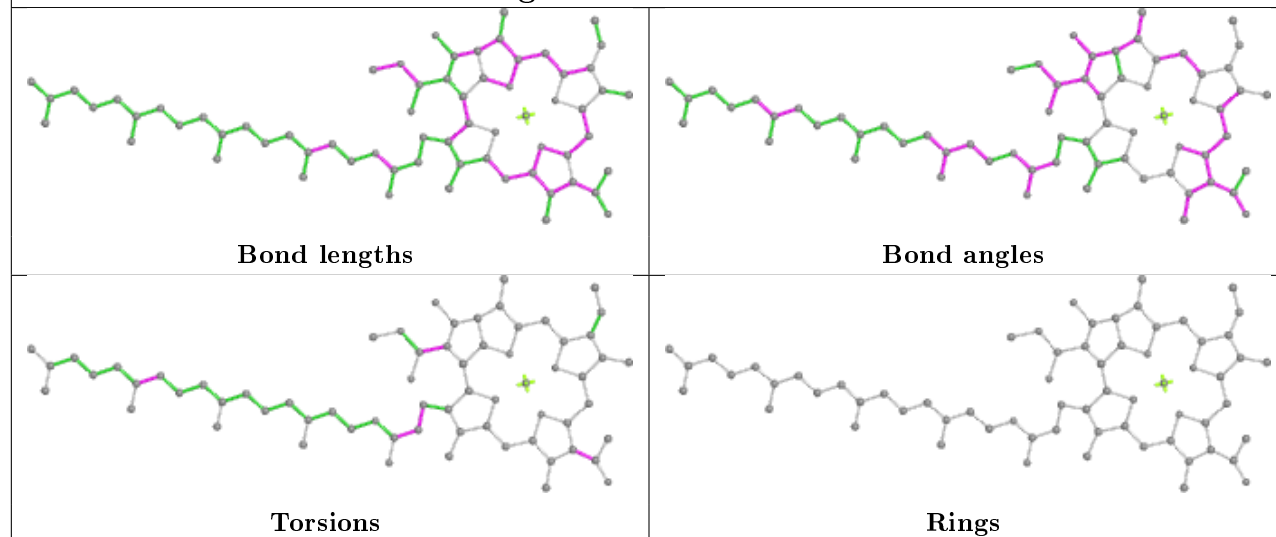


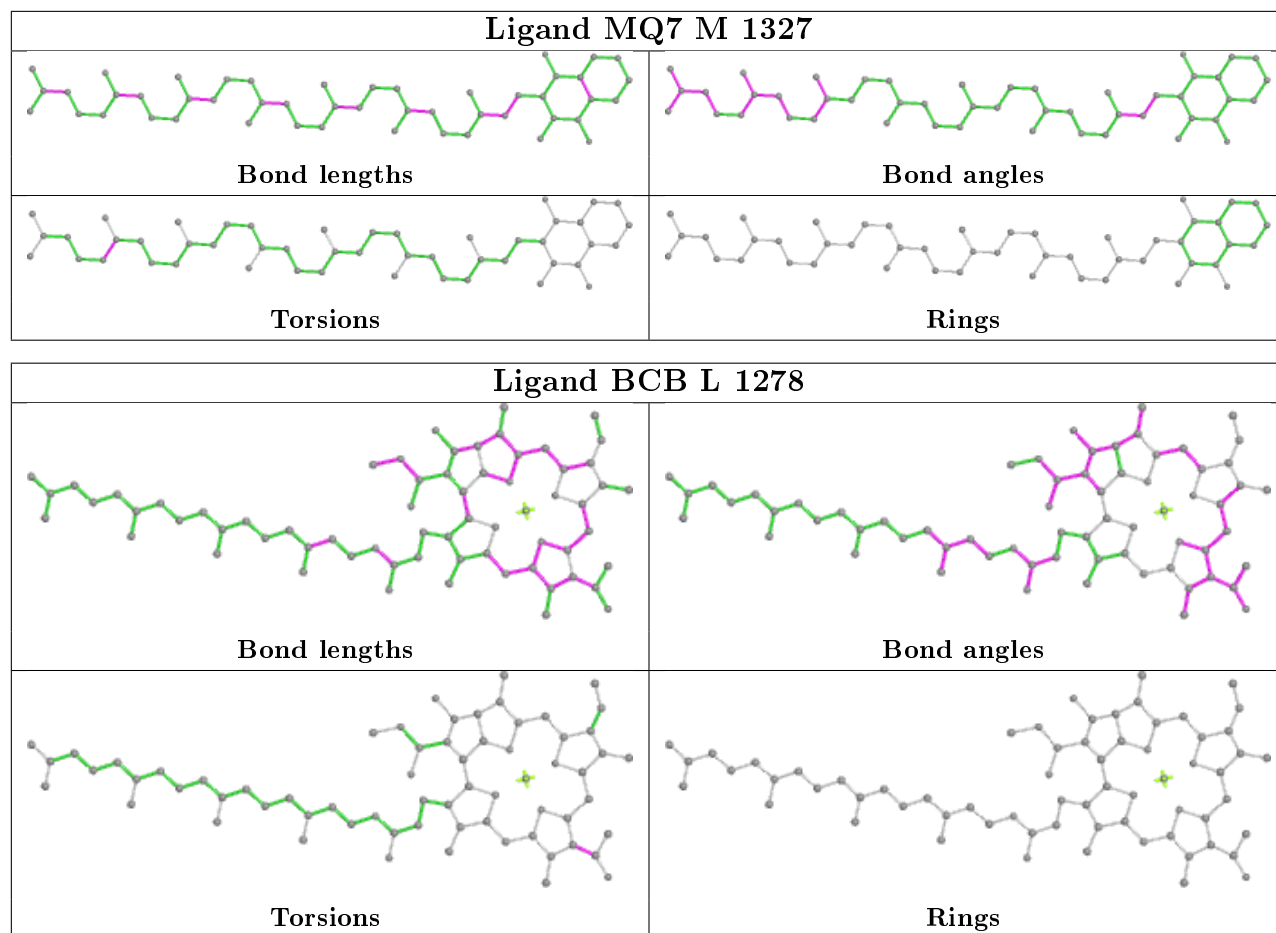


## Ligand HEC C 1333

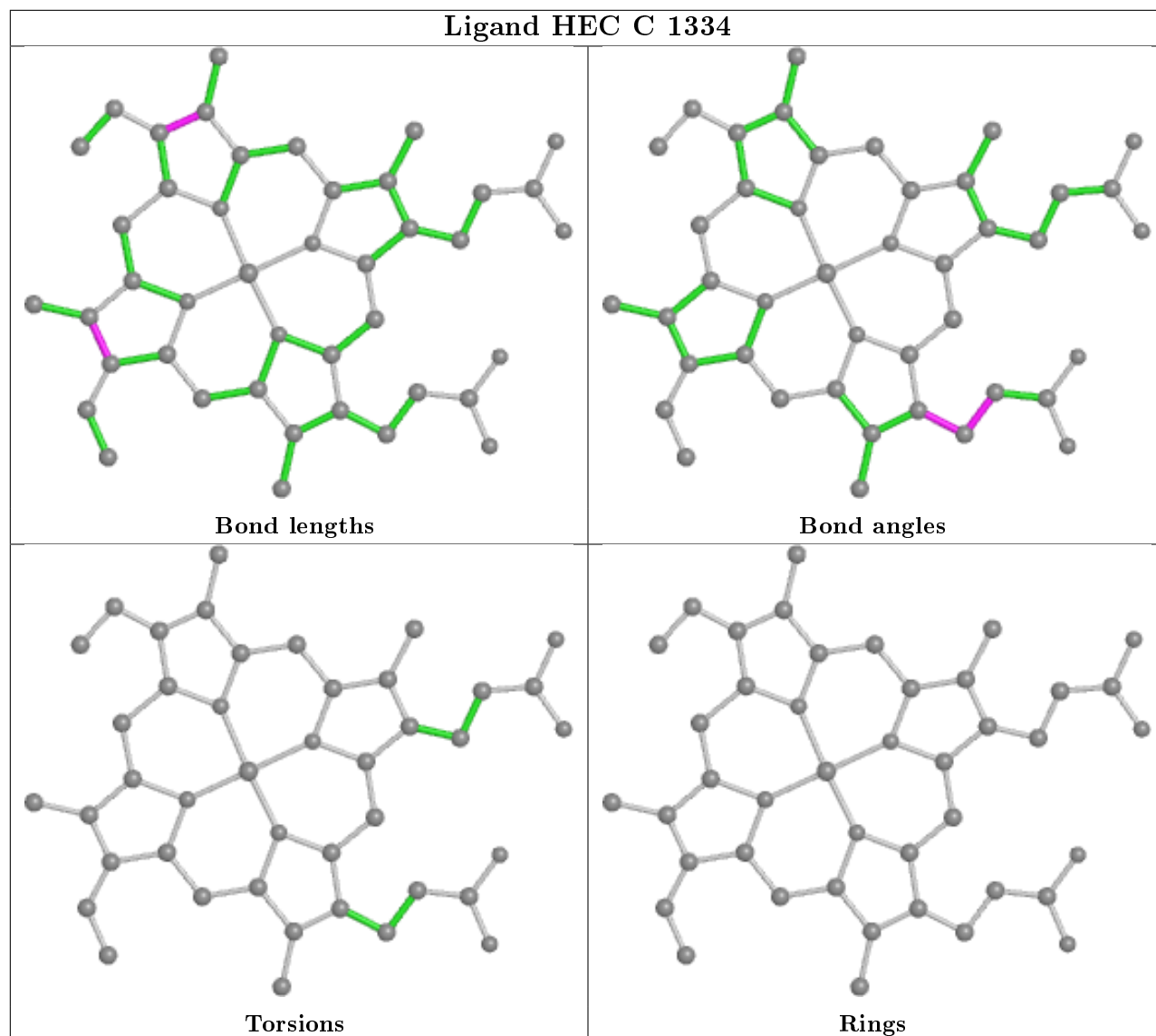


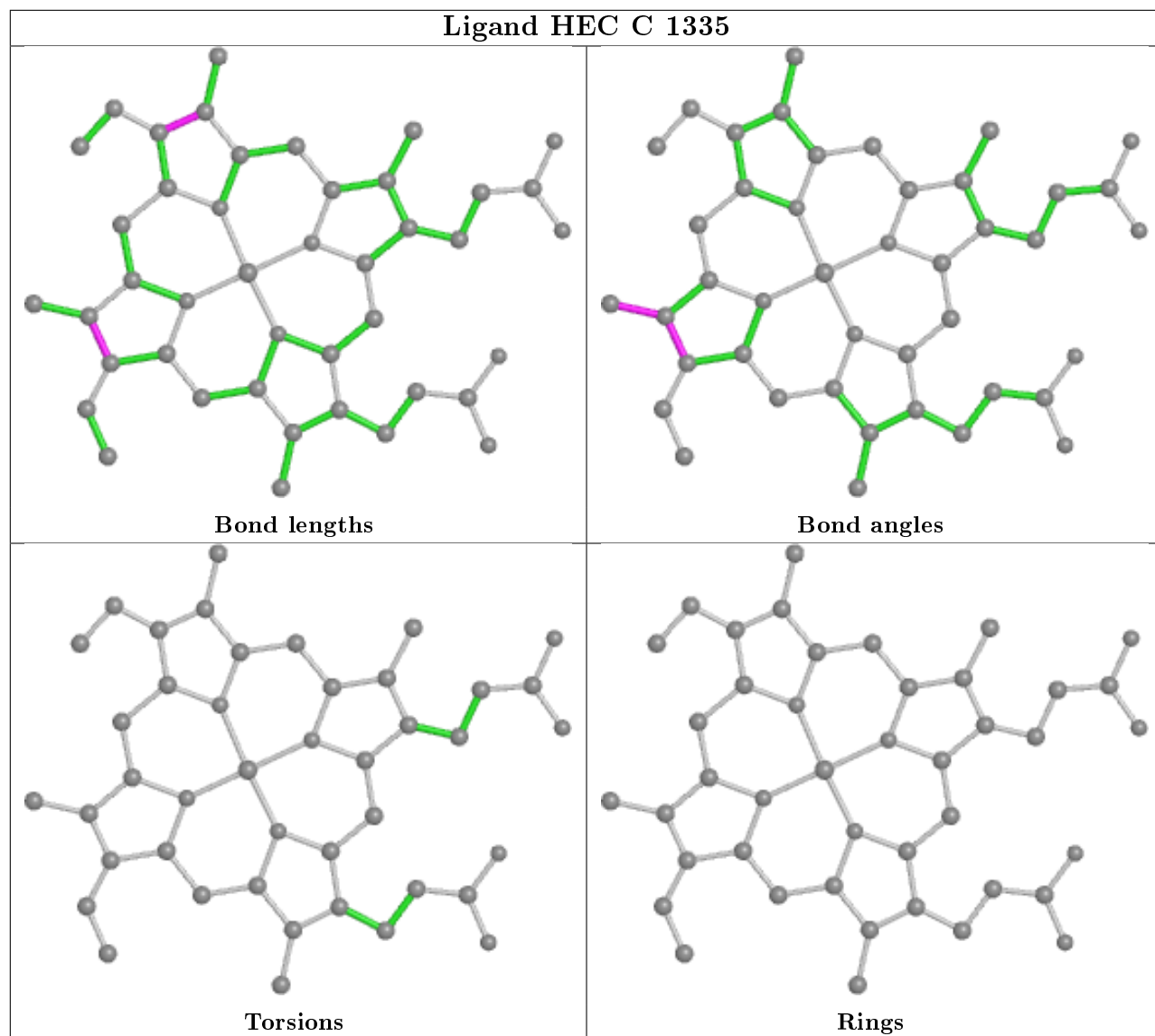
## Ligand BCB M 1324



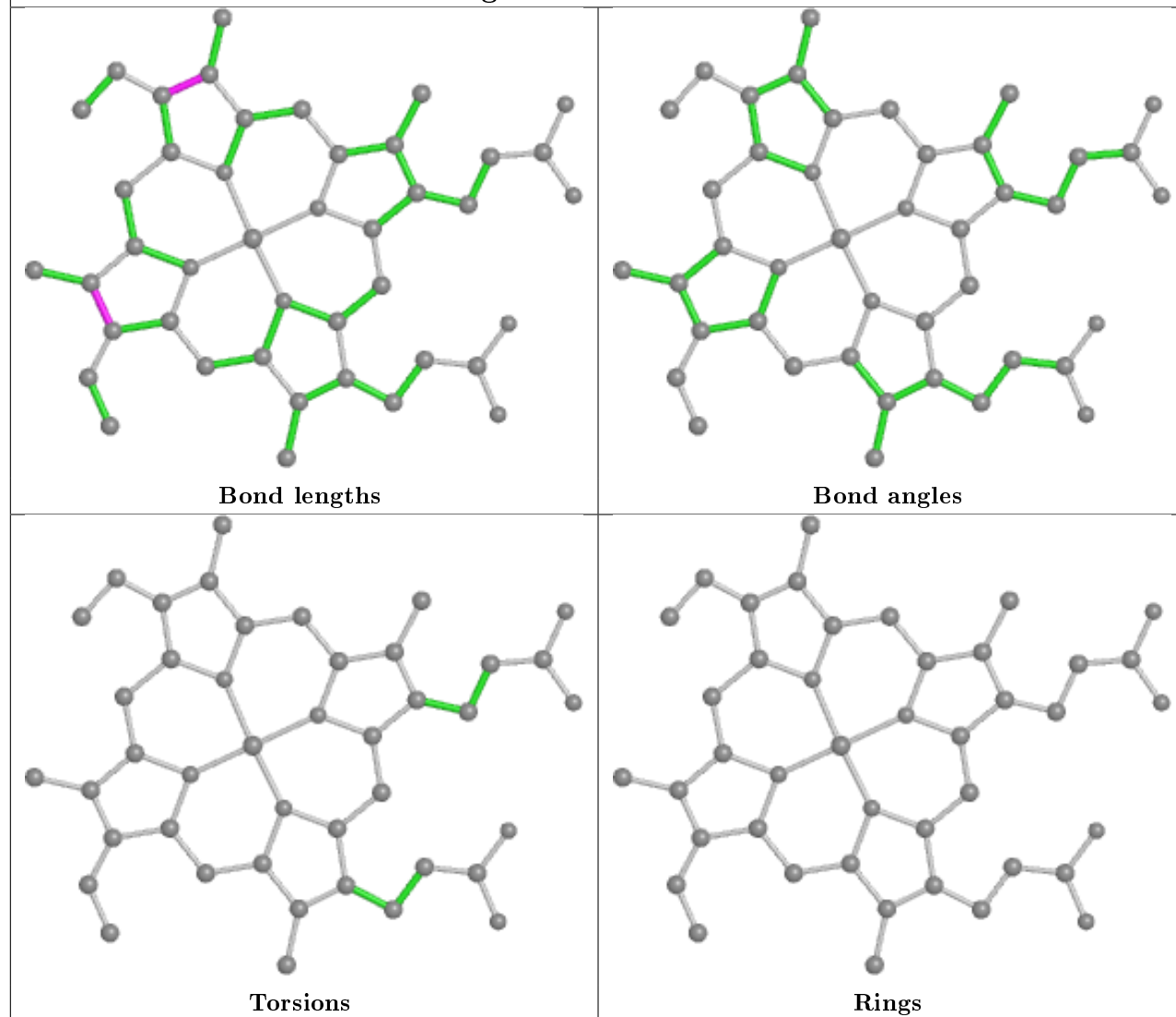


## Ligand HEC C 1334

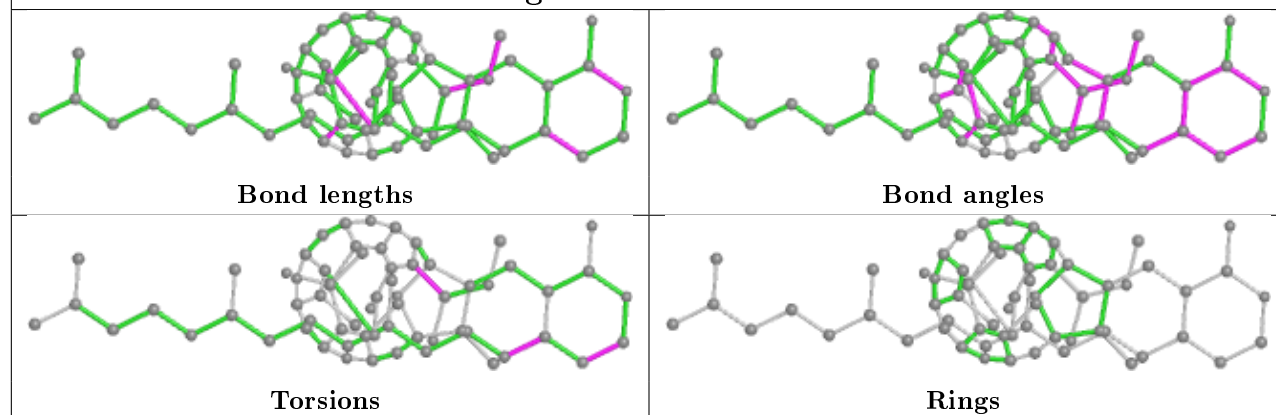


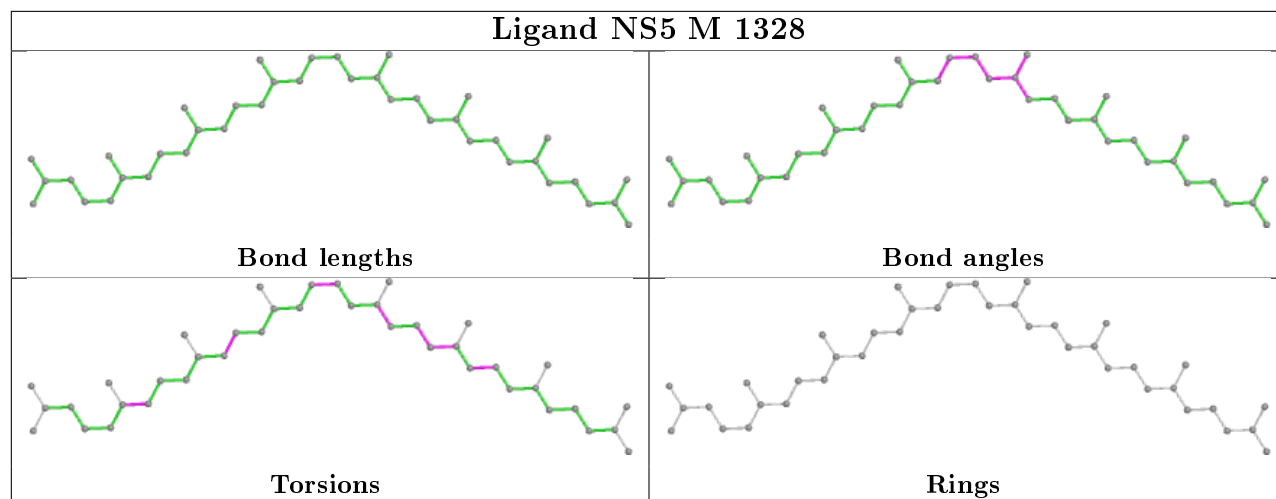


## Ligand HEC C 1336



## Ligand BPB L 1276





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	C	332/356 (93%)	-0.52	4 (1%) 79 77	21, 36, 58, 76	19 (5%)
2	H	249/258 (96%)	-0.62	1 (0%) 92 91	24, 41, 66, 81	20 (8%)
3	L	273/273 (100%)	-0.66	0 100 100	21, 30, 51, 62	7 (2%)
4	M	323/323 (100%)	-0.55	3 (0%) 84 82	20, 34, 58, 64	12 (3%)
All	All	1177/1210 (97%)	-0.58	8 (0%) 87 86	20, 35, 59, 81	58 (4%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	M	85	PHE	3.2
1	C	1	CYS	3.1
1	C	65	LEU	2.2
4	M	319	PRO	2.2
1	C	291	ALA	2.1
2	H	8	GLN	2.1
4	M	37	TRP	2.1
1	C	63	GLY	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FME	H	1	10/11	0.96	0.12	41,44,53,61	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

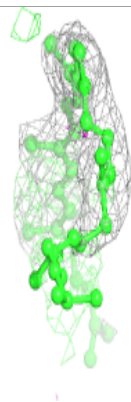
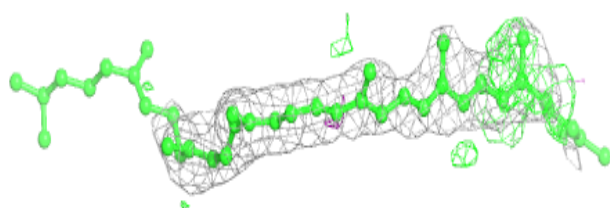
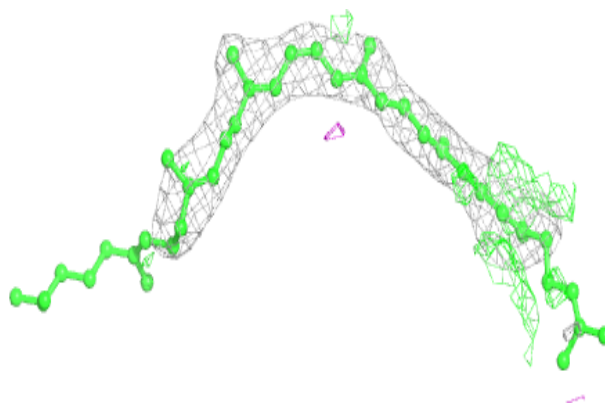
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	LDA	M	1330	16/16	0.60	0.33	52,71,83,83	0
6	LDA	M	1331	16/16	0.71	0.41	83,84,93,93	0
6	LDA	M	1332	16/16	0.72	0.36	86,88,90,90	5
6	LDA	M	1333	16/16	0.81	0.25	86,90,90,90	4
13	NS5	M	1328	40/40	0.92	0.18	50,58,79,80	14
6	LDA	H	1259	16/16	0.93	0.22	52,60,66,67	0
9	BPB	M	1325	65/65	0.94	0.13	25,35,61,62	7
8	BCB	L	1278	66/66	0.95	0.18	20,29,49,50	20
12	MQ7	M	1327	48/48	0.96	0.13	24,27,54,58	0
10	SMA	L	1277	37/37	0.96	0.15	28,36,66,69	0
8	BCB	L	1275	66/66	0.97	0.14	15,22,46,50	0
8	BCB	M	1324	66/66	0.97	0.17	17,24,47,49	0
6	LDA	M	1329	16/16	0.97	0.16	41,44,46,47	0
7	SO4	M	1335	5/5	0.97	0.11	85,86,87,87	0
8	BCB	L	1274	66/66	0.98	0.17	16,21,34,39	0
7	SO4	H	1260	5/5	0.98	0.11	75,76,76,77	0
5	HEC	C	1336	43/43	0.98	0.10	24,29,42,49	0
5	HEC	C	1333	43/43	0.98	0.10	34,39,49,53	0
9	BPB	L	1276	65/65	0.98	0.14	19,27,32,34	0
5	HEC	C	1334	43/43	0.98	0.10	29,35,40,42	0
5	HEC	C	1335	43/43	0.99	0.11	21,25,29,34	0
7	SO4	M	1336	5/5	0.99	0.13	57,57,58,59	0
7	SO4	M	1334	5/5	0.99	0.10	39,41,42,44	0
11	FE	M	1326	1/1	1.00	0.08	25,25,25,25	0

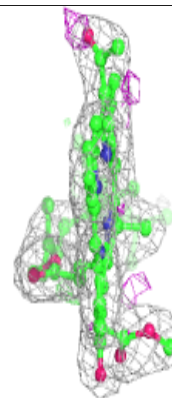
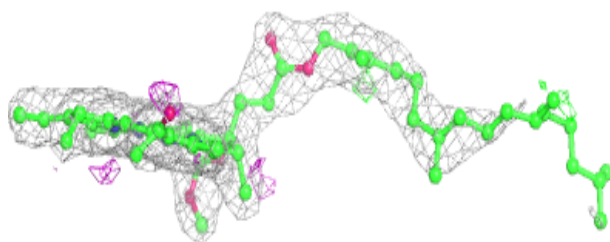
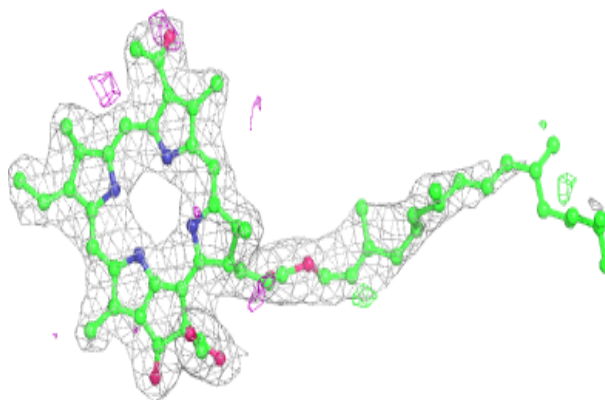
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NS5 M 1328:**

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

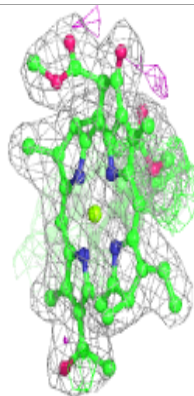
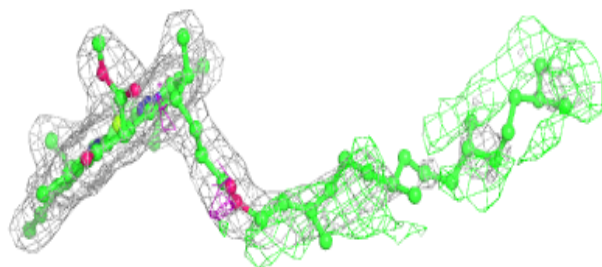
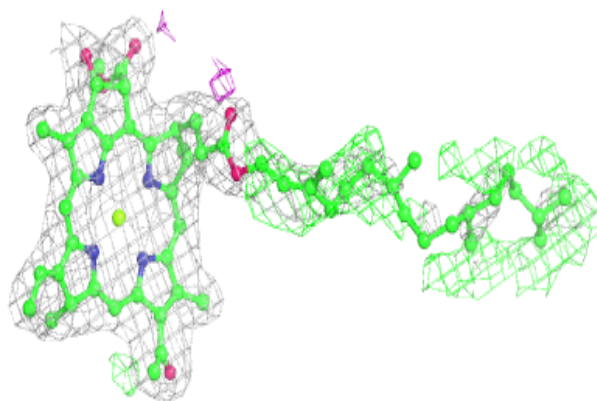
**Electron density around BPB M 1325:**

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

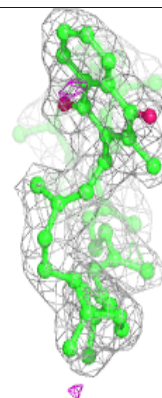
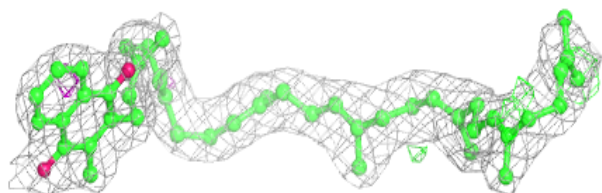
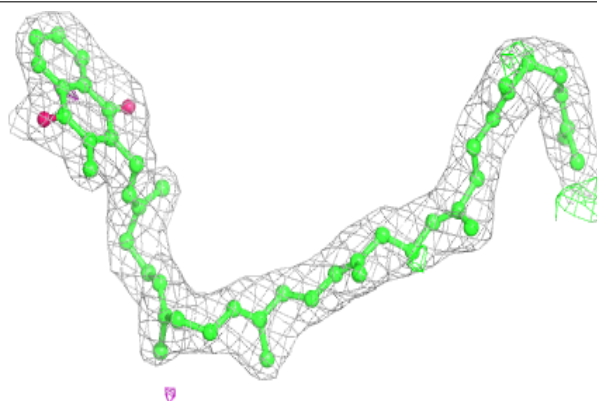


**Electron density around BCB L 1278:**

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

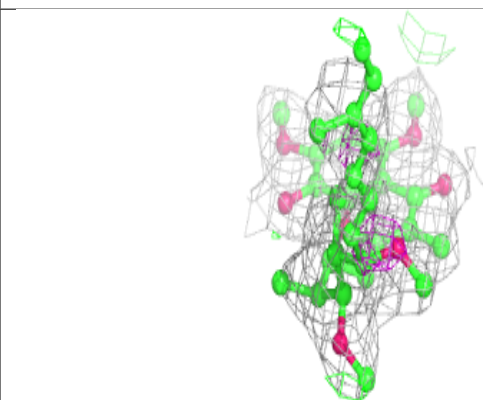
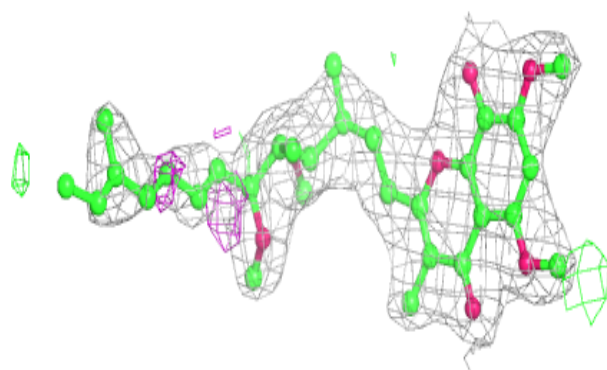
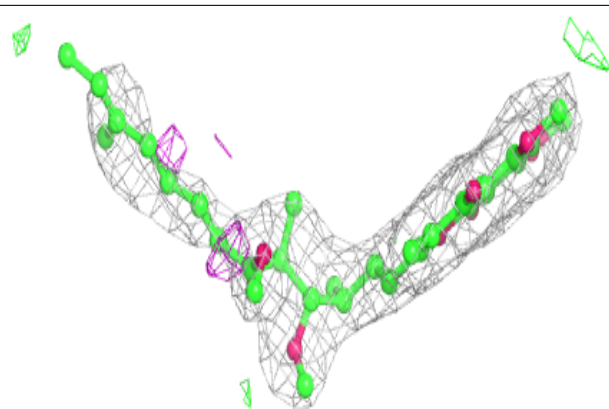
**Electron density around MQ7 M 1327:**

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

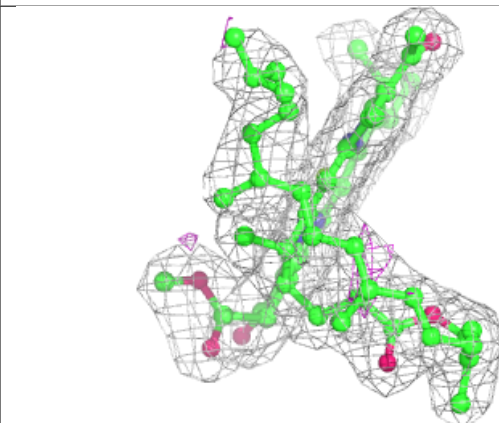
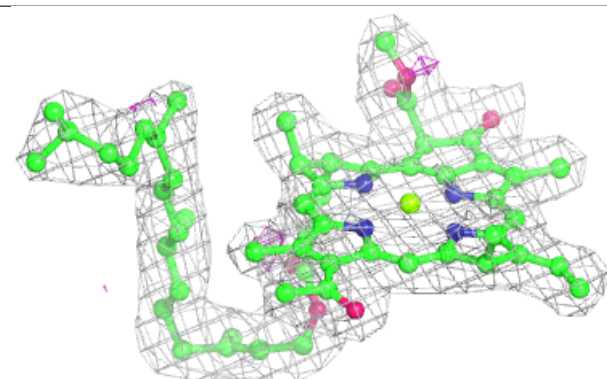
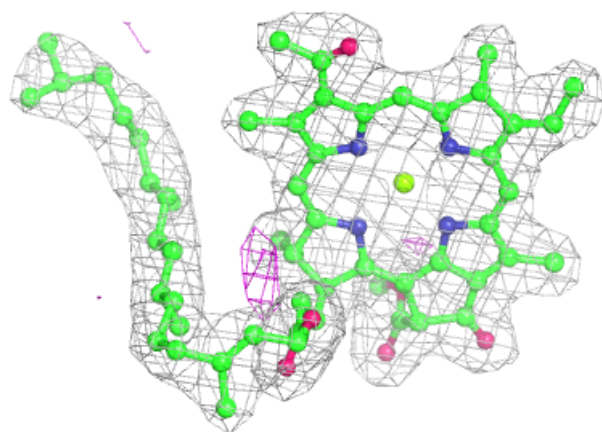


**Electron density around SMA L 1277:**

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

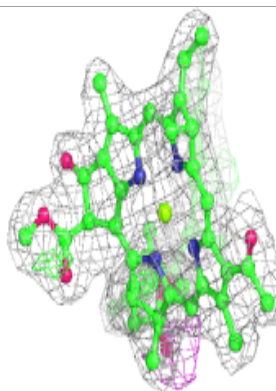
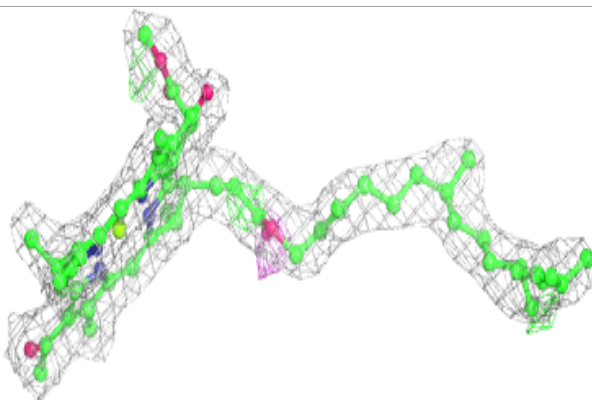
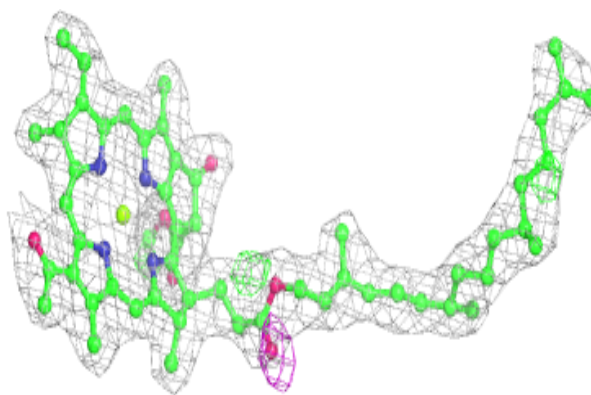
**Electron density around BCB L 1275:**

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

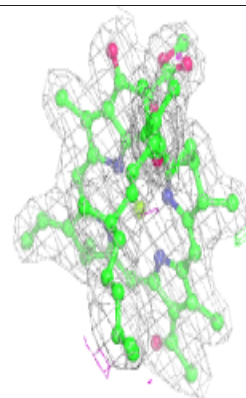
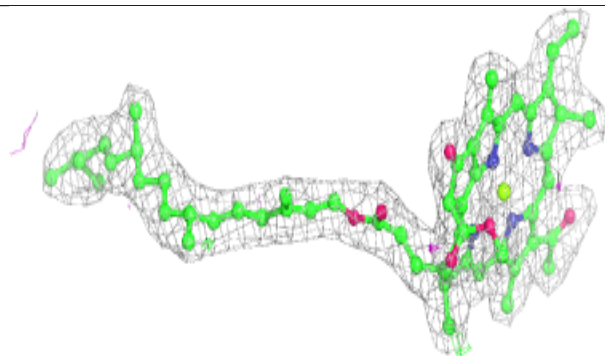
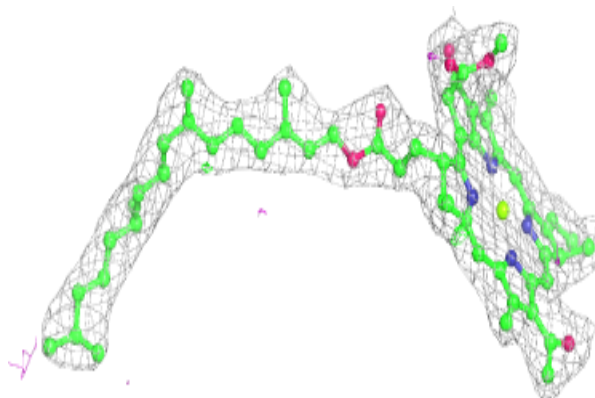


**Electron density around BCB M 1324:**

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

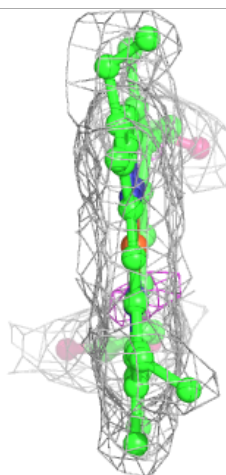
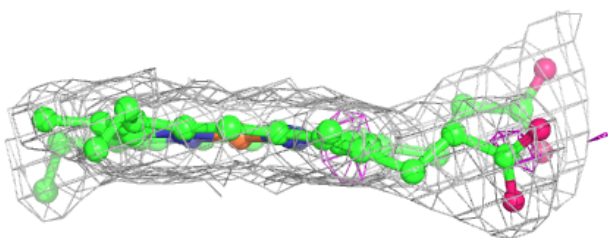
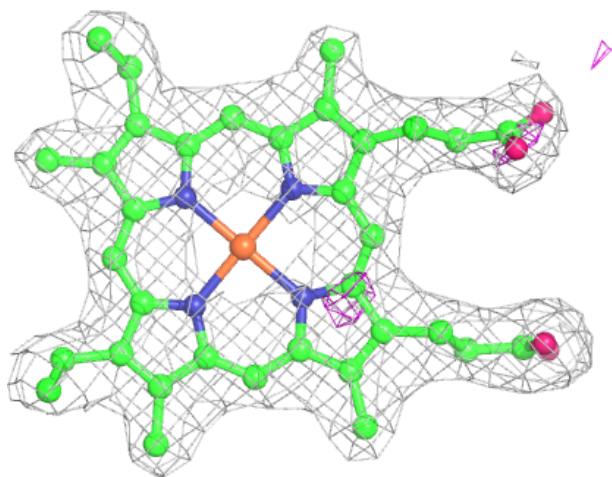
**Electron density around BCB L 1274:**

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



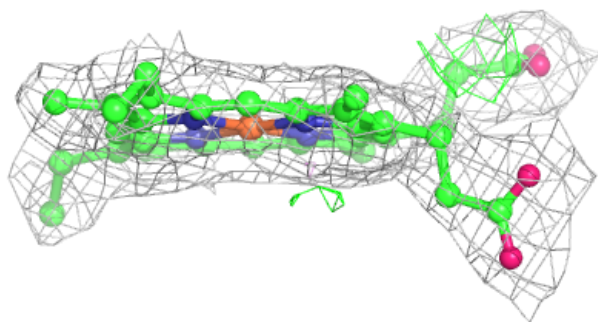
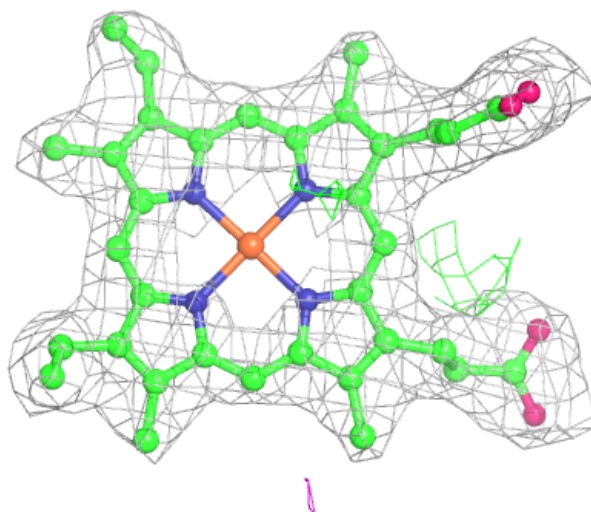
**Electron density around HEC C 1336:**

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



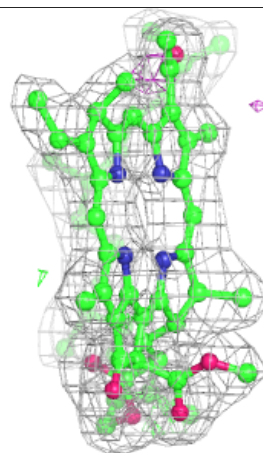
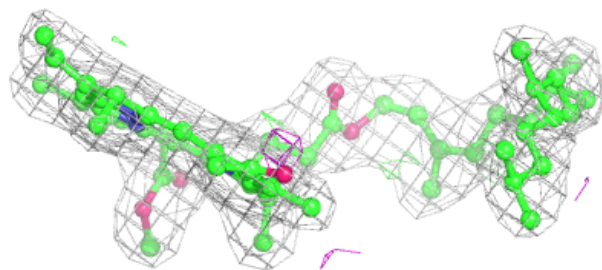
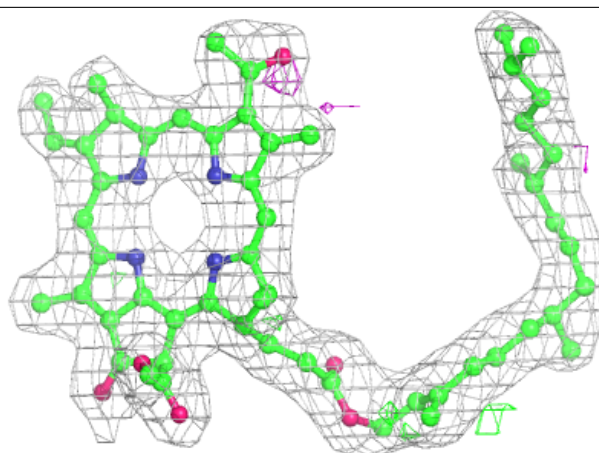
**Electron density around HEC C 1333:**

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



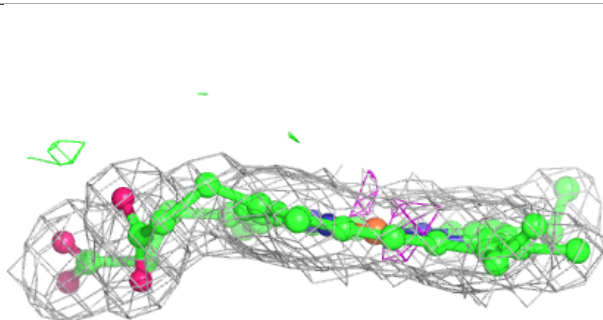
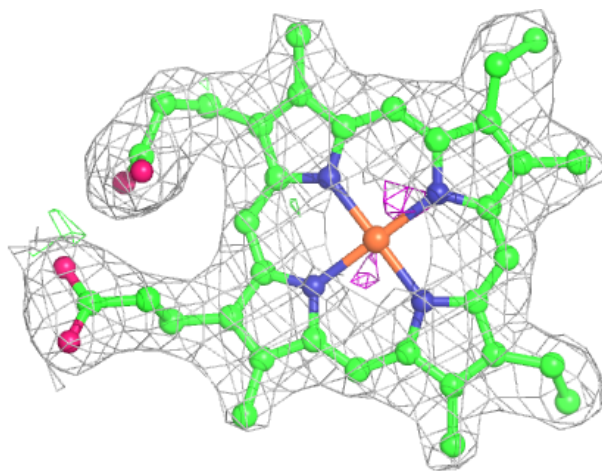
**Electron density around BPB L 1276:**

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



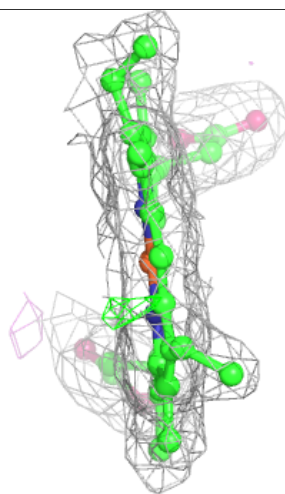
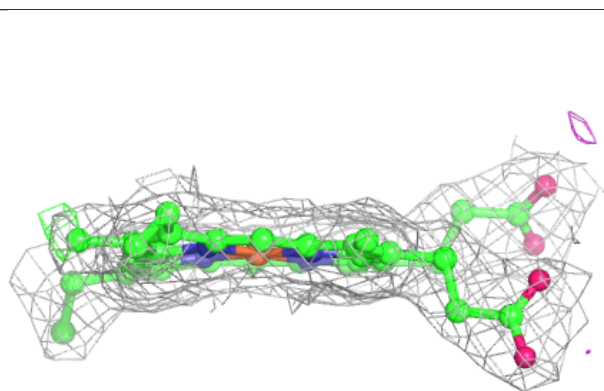
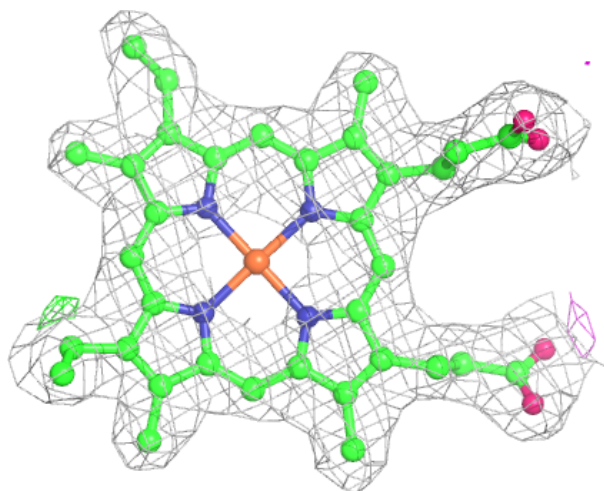
**Electron density around HEC C 1334:**

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



**Electron density around HEC C 1335:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.