



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2023 – 03:16 am GMT

PDB ID : 2VV8  
Title : Co-bound structure of bjFixLH  
Authors : Ayers, R.A.; Moffat, K.  
Deposited on : 2008-06-04  
Resolution : 1.61 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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

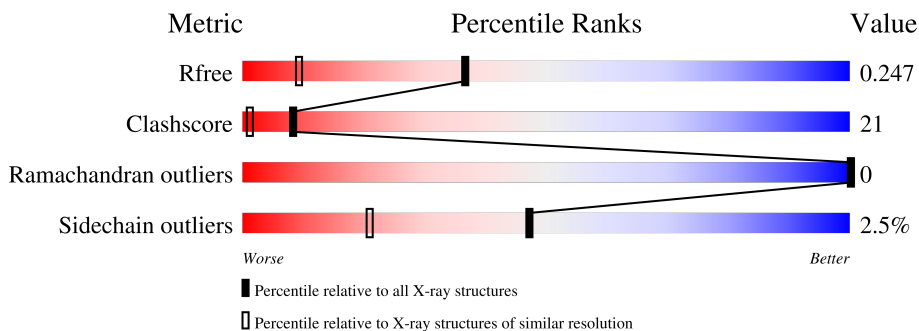
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.61 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	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)

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  $\leq 5\%$ .

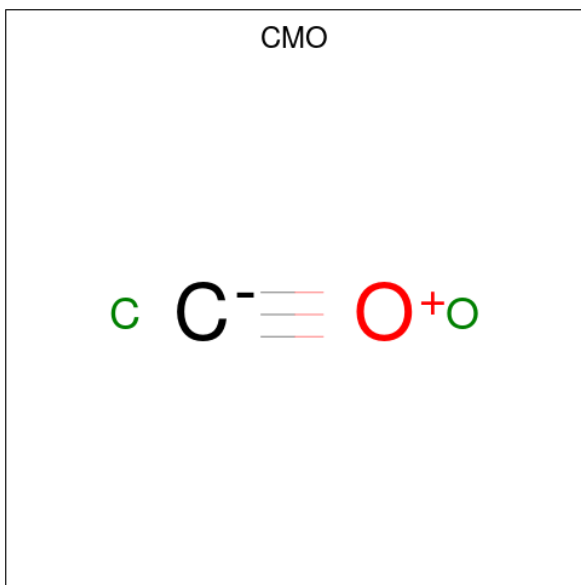
Mol	Chain	Length	Quality of chain
1	A	119	
1	B	119	
1	C	119	
1	D	119	



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

- Molecule 3 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	0
			2	1 1		
3	B	1	Total	C O	0	0
			2	1 1		
3	C	1	Total	C O	0	0
			2	1 1		
3	D	1	Total	C O	0	0
			2	1 1		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Na	0	0
			1 1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	2	Total Cl 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	126	Total O 126 126	0	0
6	B	120	Total O 120 120	0	0
6	C	125	Total O 125 125	0	0
6	D	97	Total O 97 97	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.92Å 50.30Å 58.99Å 73.37° 70.26° 72.13°	Depositor
Resolution (Å)	46.88 – 1.61 46.87 – 1.61	Depositor EDS
% Data completeness (in resolution range)	91.6 (46.88-1.61) 81.1 (46.87-1.61)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.55 (at 1.61Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.206 , 0.249 0.205 , 0.247	Depositor DCC
$R_{free}$ test set	2619 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.1	Xtrriage
Anisotropy	0.031	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 24.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4190	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.79% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CMO, CL, NA

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	A	0.64	0/998	0.84	2/1345 (0.1%)
1	B	0.65	0/928	0.79	0/1253
1	C	0.67	0/896	0.85	1/1209 (0.1%)
1	D	0.67	0/910	0.80	1/1232 (0.1%)
All	All	0.66	0/3732	0.82	4/5039 (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	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	162	HIS	N-CA-C	6.37	128.20	111.00
1	D	236	LEU	CB-CG-CD2	-5.87	101.03	111.00
1	A	174[A]	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	A	174[B]	ARG	NE-CZ-NH2	-5.19	117.71	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	159	ILE	Peptide
1	C	161	GLY	Peptide



## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	925	0	979	66	0
1	B	882	0	899	51	0
1	C	859	0	866	32	0
1	D	873	0	878	31	0
2	A	43	0	30	5	0
2	B	43	0	30	3	0
2	C	43	0	30	2	0
2	D	43	0	30	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	C	1	0	0	0	0
5	C	2	0	0	0	0
6	A	126	0	0	13	0
6	B	120	0	0	3	0
6	C	125	0	0	5	0
6	D	97	0	0	3	0
All	All	4190	0	3742	157	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159[B]:ILE:CD1	1:D:188:VAL:HB	1.74	1.17
1:D:159[B]:ILE:HD11	1:D:188:VAL:HB	1.23	1.13
1:A:158[B]:VAL:CG2	1:A:167[B]:LEU:HB3	1.78	1.12
1:A:170:THR:O	1:A:173[B]:GLU:HG2	1.50	1.12
1:A:174[A]:ARG:HD3	6:A:2029:HOH:O	1.53	1.07
1:C:175:LEU:HD11	1:C:232:PHE:CZ	1.90	1.06
1:A:158[B]:VAL:HG22	1:A:167[B]:LEU:HB3	1.06	1.05
1:A:252:PHE:HE1	1:B:241[A]:MET:SD	1.84	1.01
1:C:156:MET:HE3	1:D:167:LEU:HD13	1.42	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:PRO:HG3	1:B:254[B]:ARG:HE	1.29	0.94
1:B:152:ILE:HA	6:B:2001:HOH:O	1.68	0.92
1:A:239:GLY:HA3	1:B:241[B]:MET:HG3	1.51	0.91
1:A:156[C]:MET:SD	1:B:156:MET:HE1	2.11	0.90
1:B:187:ASN:HD22	1:B:189:ASN:H	1.18	0.88
1:A:239:GLY:CA	1:B:241[B]:MET:HG3	2.02	0.87
1:A:170:THR:HG22	6:A:2022:HOH:O	1.74	0.85
1:A:254[A]:ARG:HG2	1:A:254[A]:ARG:HH21	1.42	0.84
1:D:187:ASN:HD22	1:D:189:ASN:H	1.25	0.84
1:D:154:ASP:HB3	6:D:2007:HOH:O	1.78	0.84
1:D:159[B]:ILE:HD11	1:D:188:VAL:CB	2.05	0.84
1:B:241[A]:MET:HE3	1:B:250[A]:THR:HG23	1.59	0.84
1:A:156[A]:MET:CE	1:B:156:MET:HE3	2.07	0.83
1:D:153:PRO:HG3	1:D:254[B]:ARG:HG3	1.60	0.83
1:A:252:PHE:CE1	1:B:241[A]:MET:SD	2.72	0.82
1:B:241[A]:MET:CE	1:B:250[A]:THR:CG2	2.57	0.82
1:B:241[A]:MET:CE	1:B:250[A]:THR:HG21	2.10	0.81
1:A:156[B]:MET:HG3	1:A:252:PHE:CE2	2.16	0.81
1:D:159[B]:ILE:HG21	1:D:163:GLY:HA2	1.62	0.81
1:C:156:MET:HE1	1:D:158:VAL:HG21	1.64	0.80
1:C:156:MET:CE	1:D:158:VAL:HG21	2.13	0.78
1:A:156[A]:MET:HE1	1:B:156:MET:HE3	1.65	0.77
1:B:213:PRO:HB3	1:B:216[B]:ILE:HB	1.65	0.77
1:A:156[A]:MET:CE	1:B:156:MET:CE	2.63	0.77
1:A:250[B]:THR:HG23	6:A:2122:HOH:O	1.84	0.75
1:A:174[A]:ARG:CD	6:A:2029:HOH:O	2.22	0.74
1:D:156:MET:C	1:D:157[A]:ILE:HD12	2.08	0.73
1:B:241[A]:MET:HE1	1:B:250[A]:THR:HG21	1.71	0.72
1:A:156[A]:MET:HE3	1:B:156:MET:CE	2.18	0.72
1:A:216:ILE:HG13	1:A:238[B]:ILE:HD12	1.70	0.72
1:A:254[A]:ARG:HH21	1:A:254[A]:ARG:CG	2.03	0.71
1:B:237[B]:SER:OG	1:B:252:PHE:HB2	1.91	0.70
1:A:254[A]:ARG:HG2	1:A:254[A]:ARG:NH2	2.05	0.70
1:A:167[A]:LEU:HD13	1:B:156:MET:HE2	1.74	0.70
1:C:175:LEU:CD1	1:C:232:PHE:CZ	2.73	0.69
1:A:173[B]:GLU:CD	1:A:174[B]:ARG:NH2	2.47	0.68
1:A:216:ILE:HA	1:A:238[B]:ILE:HG13	1.74	0.68
1:A:254[A]:ARG:HD2	6:A:2003:HOH:O	1.93	0.68
1:D:159[B]:ILE:CD1	1:D:188:VAL:CB	2.64	0.66
1:C:175:LEU:HD11	1:C:232:PHE:CE1	2.30	0.66
1:A:173[B]:GLU:OE2	1:A:174[B]:ARG:NH2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ASP:OD2	1:A:254[A]:ARG:HG3	1.95	0.66
1:A:156[A]:MET:HE3	1:B:156:MET:HE1	1.77	0.66
1:A:167[A]:LEU:CD1	1:B:156:MET:HE2	2.26	0.65
1:A:241[B]:MET:HB3	1:B:239:GLY:HA3	1.77	0.65
1:C:156:MET:CE	1:D:167:LEU:HD13	2.24	0.65
1:A:167[B]:LEU:HG	1:B:156:MET:HE2	1.79	0.64
1:A:158[B]:VAL:HG12	1:A:250[B]:THR:HG22	1.78	0.63
1:D:199:ARG:NH1	6:D:2043:HOH:O	2.29	0.63
1:C:250:THR:HG23	6:C:2117:HOH:O	1.98	0.63
1:B:154:ASP:HB2	6:B:2007:HOH:O	2.00	0.62
1:B:152:ILE:N	1:B:153:PRO:HD3	2.15	0.61
1:A:206[A]:ARG:HH22	1:A:214:HIS:CE1	2.18	0.61
1:A:250[B]:THR:HG21	1:B:250[B]:THR:HG21	1.81	0.61
1:D:159[B]:ILE:CG2	1:D:163:GLY:HA2	2.31	0.61
1:A:170:THR:HG21	6:A:2016:HOH:O	2.01	0.60
1:A:241[A]:MET:HE3	6:A:2115:HOH:O	1.99	0.60
1:B:192[B]:MET:HE2	1:B:196:ASP:HB3	1.83	0.60
1:B:246:GLU:HG3	6:B:2113:HOH:O	2.02	0.59
1:C:156:MET:HE1	1:C:252:PHE:CE1	2.38	0.59
1:D:159[B]:ILE:HG22	1:D:160:ASP:O	2.03	0.58
1:C:200:HIS:CE1	1:C:204[B]:ILE:HD11	2.39	0.58
1:A:221[B]:ILE:HD12	1:A:256:LEU:HD11	1.84	0.58
1:C:156:MET:SD	1:D:156:MET:HE3	2.44	0.57
1:C:175:LEU:C	1:C:175:LEU:HD13	2.25	0.57
1:B:241[A]:MET:CE	1:B:250[A]:THR:HG23	2.23	0.57
1:A:158[B]:VAL:CG2	1:A:167[B]:LEU:CB	2.71	0.57
1:A:167[A]:LEU:HD22	1:B:156:MET:HE1	1.86	0.57
1:A:166:GLN:NE2	6:A:2011:HOH:O	2.37	0.57
1:B:192[B]:MET:CE	1:B:196:ASP:HB3	2.35	0.57
1:B:187:ASN:ND2	1:B:189:ASN:H	1.96	0.56
1:A:167[A]:LEU:HD22	1:B:156:MET:CE	2.35	0.56
1:A:156[B]:MET:HE2	1:B:167:LEU:HD13	1.87	0.56
1:C:159:ILE:HD12	1:C:163:GLY:HA2	1.87	0.56
1:C:171:ALA:HA	1:C:174[B]:ARG:HG2	1.87	0.56
1:C:241[B]:MET:SD	1:D:252:PHE:CE1	2.98	0.56
1:A:156[B]:MET:HG3	1:A:252:PHE:CD2	2.40	0.56
1:B:152:ILE:N	1:B:153:PRO:CD	2.69	0.56
1:A:215[A]:ILE:CD1	2:A:1258:HEM:HBA1	2.36	0.55
2:A:1258:HEM:HBC2	2:A:1258:HEM:HMC2	1.88	0.55
1:A:200:HIS:HA	1:A:203:TYR:CD2	2.41	0.55
1:C:156:MET:CE	1:C:252:PHE:CE1	2.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:PRO:HB3	1:B:216[A]:ILE:HB	1.88	0.54
1:B:189:ASN:HA	1:B:192[B]:MET:SD	2.48	0.54
1:B:194:GLU:OE2	1:B:197[B]:ARG:HD2	2.08	0.54
1:A:206[A]:ARG:NH2	1:A:214:HIS:CE1	2.76	0.53
1:A:216:ILE:HG13	1:A:238[B]:ILE:CD1	2.36	0.53
1:C:175:LEU:HD11	1:C:232:PHE:HZ	1.65	0.53
1:A:190:ILE:HA	1:A:197:ARG:NH2	2.24	0.53
1:A:156[B]:MET:HB3	1:A:169[B]:SER:OG	2.09	0.53
1:A:170:THR:O	1:A:173[B]:GLU:CG	2.41	0.53
1:B:241[A]:MET:HE1	1:B:250[A]:THR:CG2	2.33	0.52
1:C:241[A]:MET:HG2	6:C:2117:HOH:O	2.08	0.52
1:B:241[A]:MET:HE3	1:B:250[A]:THR:CG2	2.26	0.52
1:B:241[B]:MET:HG2	1:B:242:GLN:H	1.75	0.52
6:A:2108:HOH:O	1:B:241[B]:MET:HG2	2.09	0.52
1:D:187:ASN:ND2	1:D:189:ASN:H	2.03	0.51
1:B:241[B]:MET:HG2	1:B:242:GLN:N	2.26	0.51
1:A:156[A]:MET:CE	1:B:156:MET:HE1	2.37	0.51
1:C:225:LYS:HD3	6:C:2039:HOH:O	2.10	0.50
1:A:250[B]:THR:CG2	6:A:2122:HOH:O	2.52	0.50
1:C:241[A]:MET:SD	1:D:252:PHE:HE1	2.35	0.49
1:C:234:MET:CE	1:C:236[B]:LEU:HD13	2.43	0.49
1:C:234:MET:HE2	1:C:236[B]:LEU:HD13	1.95	0.49
1:D:159[B]:ILE:CG2	1:D:163:GLY:CA	2.90	0.49
1:C:200:HIS:O	1:C:204[B]:ILE:HG12	2.13	0.48
1:D:242:GLN:HG2	6:D:2089:HOH:O	2.13	0.48
1:C:240:GLU:HG3	1:C:249:PHE:CE2	2.49	0.47
2:B:1259:HEM:HBB2	2:B:1259:HEM:HHC	1.96	0.47
1:A:241[B]:MET:SD	1:A:248:TYR:HB2	2.54	0.47
1:C:156:MET:HE1	1:C:252:PHE:HE1	1.80	0.47
1:B:182:GLU:OE1	1:B:227:ARG:NH2	2.48	0.47
1:D:159[B]:ILE:HD11	1:D:188:VAL:CG2	2.44	0.46
1:D:159[B]:ILE:HG23	1:D:163:GLY:C	2.35	0.46
1:B:154:ASP:OD1	1:B:154:ASP:N	2.46	0.46
1:A:215[A]:ILE:CD1	2:A:1258:HEM:CBA	2.94	0.46
1:C:167:LEU:HG	6:C:2010:HOH:O	2.16	0.45
1:D:250[B]:THR:HG22	1:D:252:PHE:CE1	2.51	0.45
1:A:158[B]:VAL:CG1	1:A:250[B]:THR:HG22	2.47	0.45
2:A:1258:HEM:HBC2	2:A:1258:HEM:CMC	2.47	0.45
1:B:200:HIS:HA	1:B:203:TYR:CD1	2.52	0.44
2:B:1259:HEM:HBC2	2:B:1259:HEM:HMC2	2.00	0.44
1:C:200:HIS:HA	1:C:203:TYR:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241[A]:MET:SD	1:D:252:PHE:CE1	3.11	0.43
1:A:156[B]:MET:SD	1:B:156:MET:HE1	2.59	0.43
1:C:234:MET:CE	1:C:236[A]:LEU:HG	2.49	0.43
1:B:153:PRO:HG3	1:B:254[B]:ARG:NE	2.14	0.43
1:D:158:VAL:HG22	1:D:250[A]:THR:HG22	2.01	0.43
1:A:215[A]:ILE:HD11	1:A:220:ARG:CZ	2.49	0.43
1:A:254[A]:ARG:HD3	6:A:2123:HOH:O	2.18	0.42
1:B:159:ILE:HD12	1:B:163:GLY:HA2	1.99	0.42
1:A:206[C]:ARG:HD2	1:A:206[C]:ARG:HA	1.77	0.42
1:A:199:ARG:HD3	6:A:2062:HOH:O	2.20	0.42
1:C:203:TYR:CD2	2:C:1259:HEM:C2A	3.07	0.42
1:A:189:ASN:HA	1:A:192:MET:HE3	2.02	0.41
1:A:241[B]:MET:HG3	6:A:2122:HOH:O	2.21	0.41
1:C:236[A]:LEU:HD11	2:C:1259:HEM:C4B	2.55	0.41
1:D:159[B]:ILE:HD12	1:D:188:VAL:HB	1.88	0.41
1:D:200:HIS:HA	1:D:203:TYR:CD1	2.55	0.41
1:A:219:GLY:HA2	1:A:236:LEU:O	2.20	0.41
2:A:1258:HEM:HHC	2:A:1258:HEM:HBB2	2.03	0.41
1:B:220:ARG:NH1	2:B:1259:HEM:HBA2	2.36	0.41
1:D:219:GLY:HA2	1:D:236:LEU:O	2.21	0.41
1:C:241[B]:MET:HG2	6:C:2117:HOH:O	2.22	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	A	122/119 (102%)	120 (98%)	2 (2%)	0	100	100
1	B	114/119 (96%)	111 (97%)	3 (3%)	0	100	100
1	C	110/119 (92%)	108 (98%)	2 (2%)	0	100	100
1	D	112/119 (94%)	112 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	458/476 (96%)	451 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	A	108/102 (106%)	105 (97%)	3 (3%)	43	17
1	B	99/102 (97%)	96 (97%)	3 (3%)	41	15
1	C	95/102 (93%)	93 (98%)	2 (2%)	53	27
1	D	97/102 (95%)	95 (98%)	2 (2%)	53	27
All	All	399/408 (98%)	389 (98%)	10 (2%)	47	21

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	ILE
1	A	254[A]	ARG
1	A	254[B]	ARG
1	B	152	ILE
1	B	187	ASN
1	B	212	ASP
1	C	160	ASP
1	C	211	SER
1	D	154	ASP
1	D	187	ASN

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

Mol	Chain	Res	Type
1	A	166	GLN
1	A	214	HIS

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Mol	Chain	Res	Type
1	B	187	ASN
1	C	166	GLN
1	C	186	GLN
1	C	214	HIS
1	D	186	GLN
1	D	187	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	$\# Z  > 2$
3	CMO	C	1260	-	0,1,1	-	-	-		
3	CMO	A	1259	-	0,1,1	-	-	-		
3	CMO	D	1260	-	0,1,1	-	-	-		
2	HEM	D	1259	1	41,50,50	1.98	9 (21%)	45,82,82	1.74	12 (26%)
2	HEM	A	1258	1	41,50,50	2.02	8 (19%)	45,82,82	2.58	19 (42%)
3	CMO	B	1260	-	0,1,1	-	-	-		
2	HEM	B	1259	1	41,50,50	1.82	7 (17%)	45,82,82	2.07	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	C	1259	1	41,50,50	1.75	5 (12%)	45,82,82	2.01	13 (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	HEM	D	1259	1	-	1/12/54/54	-
2	HEM	B	1259	1	-	6/12/54/54	-
2	HEM	C	1259	1	-	4/12/54/54	-
2	HEM	A	1258	1	-	3/12/54/54	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1258	HEM	C3D-C2D	7.86	1.53	1.36
2	D	1259	HEM	C3D-C2D	7.77	1.53	1.36
2	B	1259	HEM	C3D-C2D	6.75	1.51	1.36
2	C	1259	HEM	C3D-C2D	6.20	1.49	1.36
2	D	1259	HEM	C3C-CAC	4.24	1.56	1.47
2	C	1259	HEM	C3C-C2C	-3.75	1.35	1.40
2	A	1258	HEM	C3C-C2C	-3.70	1.35	1.40
2	B	1259	HEM	C3C-C2C	-3.59	1.35	1.40
2	C	1259	HEM	C3C-CAC	3.56	1.55	1.47
2	A	1258	HEM	CAA-C2A	3.39	1.57	1.52
2	A	1258	HEM	CAB-C3B	3.38	1.56	1.47
2	C	1259	HEM	CAB-C3B	3.26	1.56	1.47
2	A	1258	HEM	C3C-CAC	3.20	1.54	1.47
2	B	1259	HEM	CAB-C3B	3.09	1.55	1.47
2	D	1259	HEM	C3C-C2C	-3.07	1.36	1.40
2	B	1259	HEM	C3C-CAC	3.06	1.54	1.47
2	D	1259	HEM	CMB-C2B	2.84	1.56	1.50
2	D	1259	HEM	CAA-C2A	2.81	1.56	1.52
2	D	1259	HEM	CAB-C3B	2.77	1.55	1.47
2	C	1259	HEM	CAA-C2A	2.72	1.56	1.52
2	D	1259	HEM	CMD-C2D	2.35	1.55	1.50
2	B	1259	HEM	FE-ND	2.27	2.08	1.96
2	A	1258	HEM	C1A-NA	2.23	1.40	1.36
2	B	1259	HEM	CAA-C2A	2.19	1.55	1.52
2	B	1259	HEM	C3B-C2B	-2.18	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1258	HEM	C1D-ND	2.15	1.43	1.38
2	A	1258	HEM	CMA-C3A	2.09	1.56	1.51
2	D	1259	HEM	FE-ND	2.08	2.07	1.96
2	D	1259	HEM	CMA-C3A	2.05	1.55	1.51

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1258	HEM	C4A-C3A-C2A	5.68	110.95	107.00
2	A	1258	HEM	CHC-C4B-NB	-5.34	118.63	124.43
2	A	1258	HEM	CMA-C3A-C4A	-5.34	120.26	128.46
2	B	1259	HEM	CMA-C3A-C4A	-4.87	120.98	128.46
2	D	1259	HEM	C4D-ND-C1D	4.87	110.10	105.07
2	B	1259	HEM	C3B-C2B-C1B	4.85	110.08	106.49
2	A	1258	HEM	CAD-C3D-C4D	4.72	132.90	124.66
2	A	1258	HEM	CHD-C1D-ND	4.69	129.52	124.43
2	A	1258	HEM	C4B-C3B-C2B	-4.62	103.45	107.11
2	A	1258	HEM	C3B-C2B-C1B	4.46	109.80	106.49
2	B	1259	HEM	C2C-C3C-C4C	4.27	109.88	106.90
2	B	1259	HEM	C4D-ND-C1D	4.17	109.38	105.07
2	C	1259	HEM	C3B-C2B-C1B	3.93	109.40	106.49
2	B	1259	HEM	CHA-C4D-ND	3.86	129.15	124.38
2	C	1259	HEM	C4D-ND-C1D	3.77	108.97	105.07
2	D	1259	HEM	CMA-C3A-C4A	-3.75	122.70	128.46
2	B	1259	HEM	C3C-C4C-NC	-3.63	104.08	110.94
2	C	1259	HEM	CMA-C3A-C4A	-3.48	123.12	128.46
2	A	1258	HEM	C4B-CHC-C1C	3.47	127.14	122.56
2	C	1259	HEM	CAD-C3D-C4D	3.46	130.71	124.66
2	A	1258	HEM	C4C-CHD-C1D	3.46	127.13	122.56
2	C	1259	HEM	C4B-CHC-C1C	3.42	127.07	122.56
2	C	1259	HEM	CMC-C2C-C3C	3.39	131.02	124.68
2	C	1259	HEM	C4C-CHD-C1D	3.35	126.98	122.56
2	B	1259	HEM	C4A-C3A-C2A	3.33	109.31	107.00
2	A	1258	HEM	CHD-C1D-C2D	-3.23	119.93	124.98
2	C	1259	HEM	C2C-C3C-C4C	3.23	109.16	106.90
2	A	1258	HEM	CAD-C3D-C2D	-3.23	121.86	127.88
2	B	1259	HEM	CAA-CBA-CGA	-3.23	104.71	113.76
2	C	1259	HEM	C4A-C3A-C2A	2.94	109.04	107.00
2	A	1258	HEM	C4D-ND-C1D	2.91	108.08	105.07
2	A	1258	HEM	C2C-C3C-C4C	2.91	108.93	106.90
2	D	1259	HEM	CBA-CAA-C2A	-2.90	107.67	112.62
2	A	1258	HEM	CHA-C4D-ND	-2.81	120.91	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1259	HEM	C4B-CHC-C1C	2.76	126.20	122.56
2	D	1259	HEM	C3B-C2B-C1B	2.73	108.51	106.49
2	C	1259	HEM	C4B-C3B-C2B	-2.62	105.03	107.11
2	A	1258	HEM	CMD-C2D-C1D	2.55	128.93	125.04
2	C	1259	HEM	CAA-CBA-CGA	-2.53	106.66	113.76
2	B	1259	HEM	CMA-C3A-C2A	2.53	129.71	124.94
2	D	1259	HEM	CHA-C4D-ND	2.43	127.38	124.38
2	D	1259	HEM	CBD-CAD-C3D	-2.40	105.95	112.63
2	A	1258	HEM	C1B-NB-C4B	-2.36	102.63	105.07
2	A	1258	HEM	CMC-C2C-C3C	2.36	129.09	124.68
2	B	1259	HEM	O2A-CGA-CBA	2.33	121.53	114.03
2	C	1259	HEM	CHD-C1D-ND	2.32	126.95	124.43
2	C	1259	HEM	CBD-CAD-C3D	-2.32	106.19	112.63
2	D	1259	HEM	O2D-CGD-CBD	2.31	121.46	114.03
2	B	1259	HEM	CAD-C3D-C4D	2.31	128.69	124.66
2	D	1259	HEM	CMA-C3A-C2A	2.30	129.27	124.94
2	A	1258	HEM	O1D-CGD-CBD	-2.23	115.91	123.08
2	D	1259	HEM	O1D-CGD-CBD	-2.18	116.06	123.08
2	B	1259	HEM	CMC-C2C-C3C	2.18	128.75	124.68
2	D	1259	HEM	C4B-CHC-C1C	2.11	125.34	122.56
2	D	1259	HEM	CMC-C2C-C3C	2.10	128.62	124.68
2	A	1258	HEM	CMA-C3A-C2A	2.02	128.75	124.94
2	D	1259	HEM	CHD-C1D-ND	2.01	126.62	124.43

There are no chirality outliers.

All (14) torsion outliers are listed below:

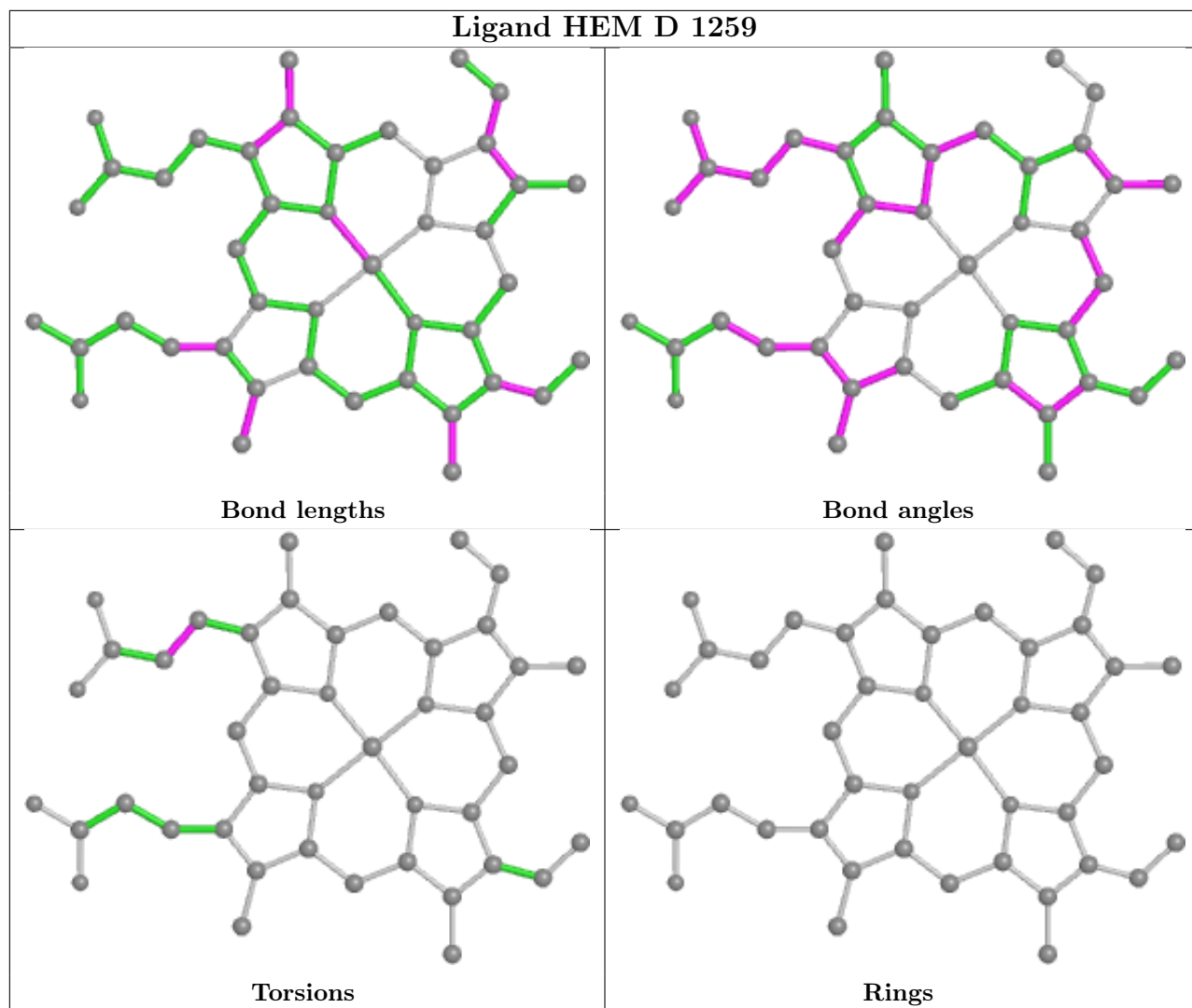
Mol	Chain	Res	Type	Atoms
2	B	1259	HEM	C2A-CAA-CBA-CGA
2	B	1259	HEM	C3D-CAD-CBD-CGD
2	A	1258	HEM	C3D-CAD-CBD-CGD
2	C	1259	HEM	C3D-CAD-CBD-CGD
2	D	1259	HEM	C3D-CAD-CBD-CGD
2	C	1259	HEM	C2A-CAA-CBA-CGA
2	C	1259	HEM	CAA-CBA-CGA-O1A
2	B	1259	HEM	CAD-CBD-CGD-O2D
2	A	1258	HEM	CAD-CBD-CGD-O2D
2	A	1258	HEM	CAD-CBD-CGD-O1D
2	B	1259	HEM	CAA-CBA-CGA-O2A
2	C	1259	HEM	CAA-CBA-CGA-O2A
2	B	1259	HEM	CAD-CBD-CGD-O1D
2	B	1259	HEM	CAA-CBA-CGA-O1A

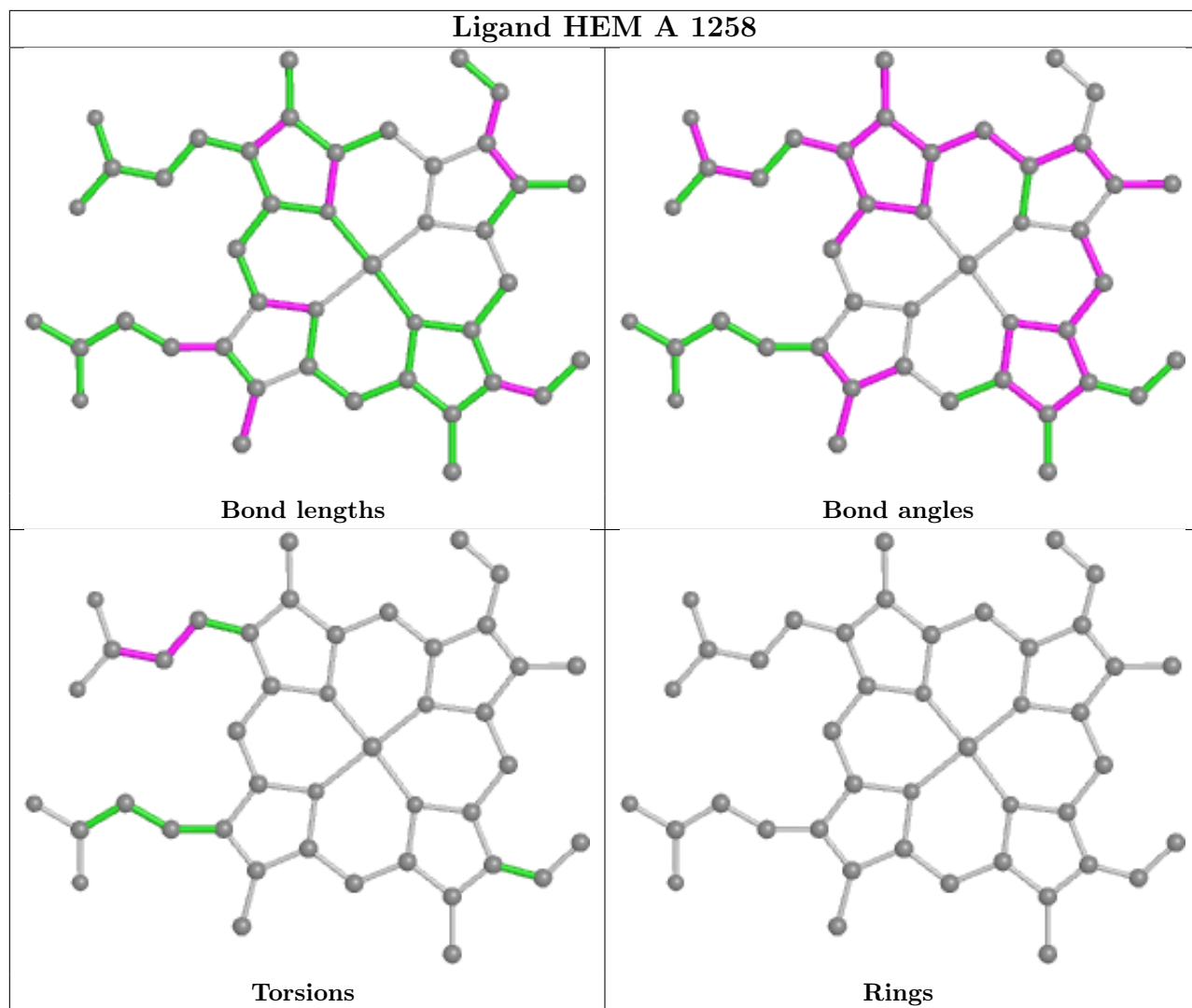
There are no ring outliers.

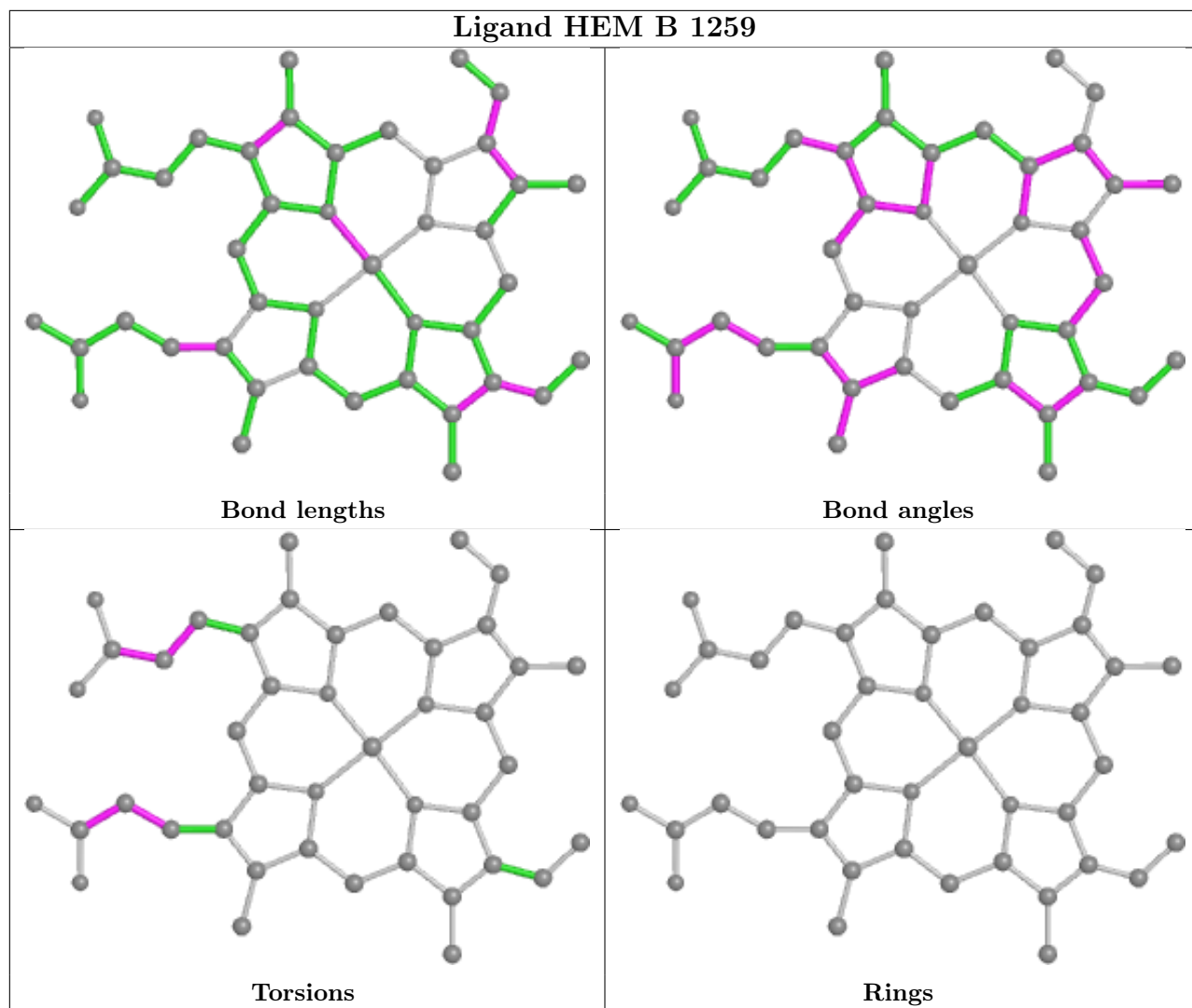
3 monomers are involved in 10 short contacts:

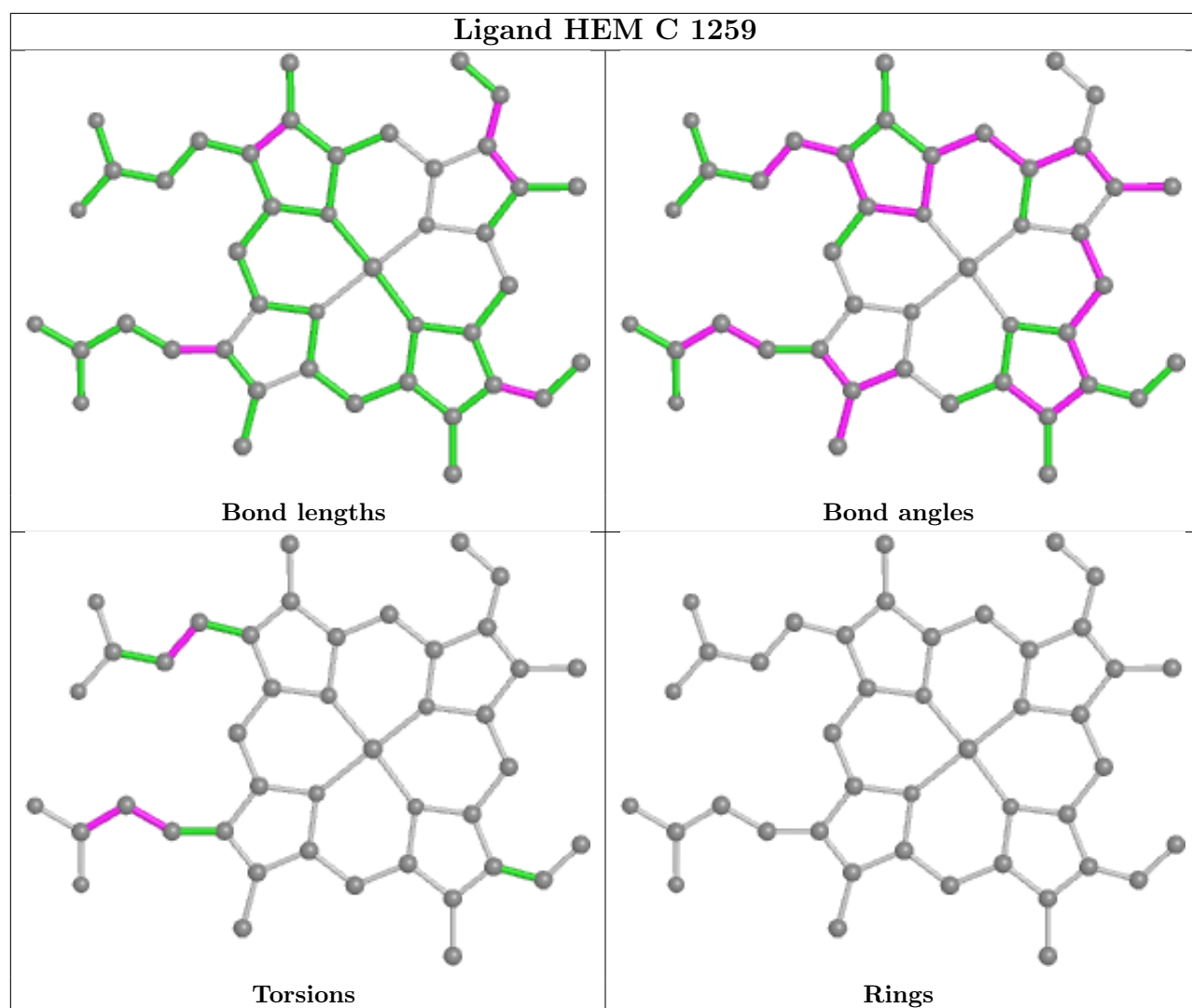
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1258	HEM	5	0
2	B	1259	HEM	3	0
2	C	1259	HEM	2	0

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](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

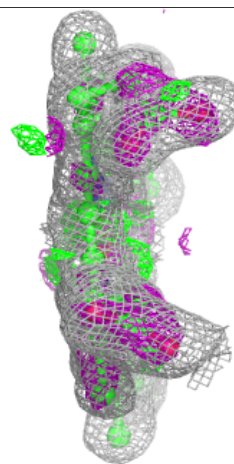
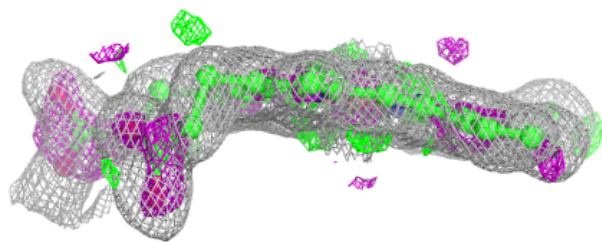
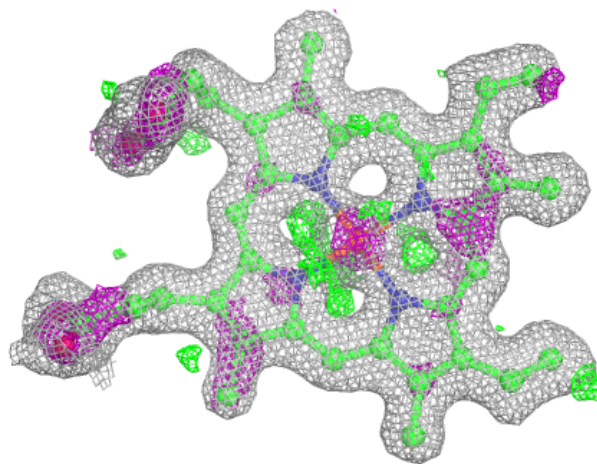
Unable to reproduce the depositors R factor - this section is therefore empty.

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.



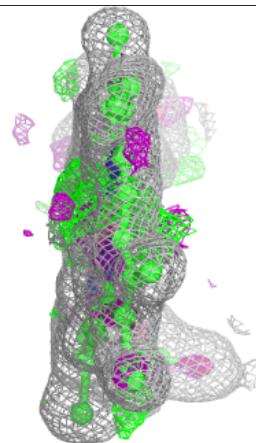
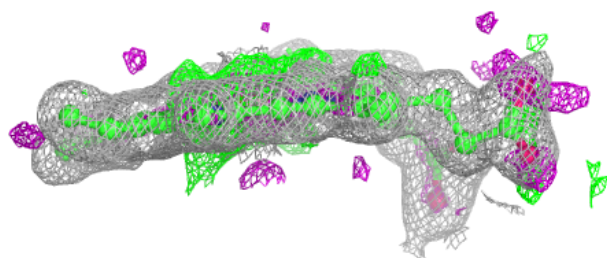
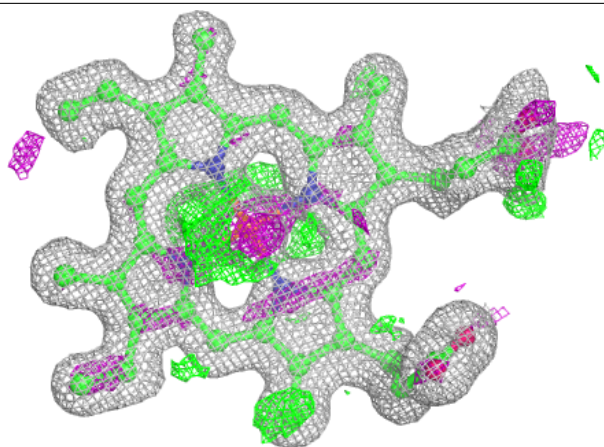
**Electron density around HEM A 1258:**

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



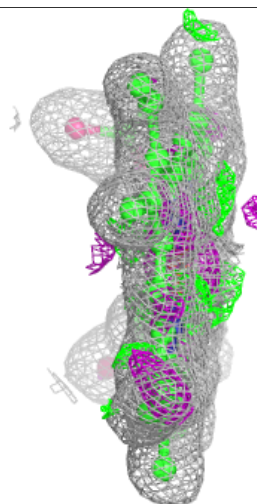
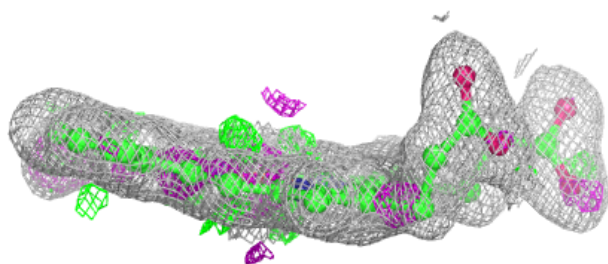
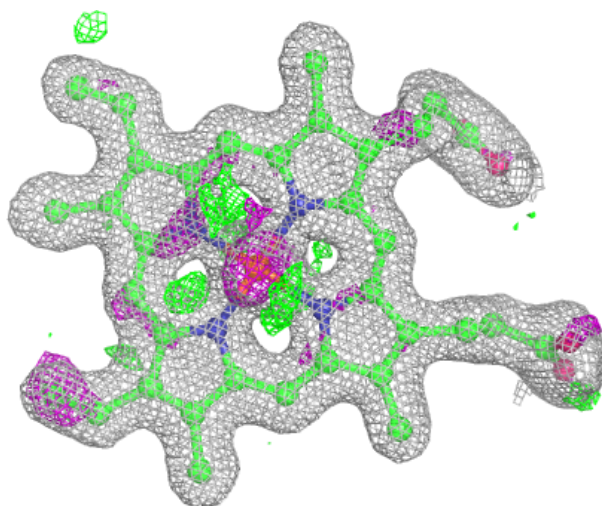
**Electron density around HEM B 1259:**

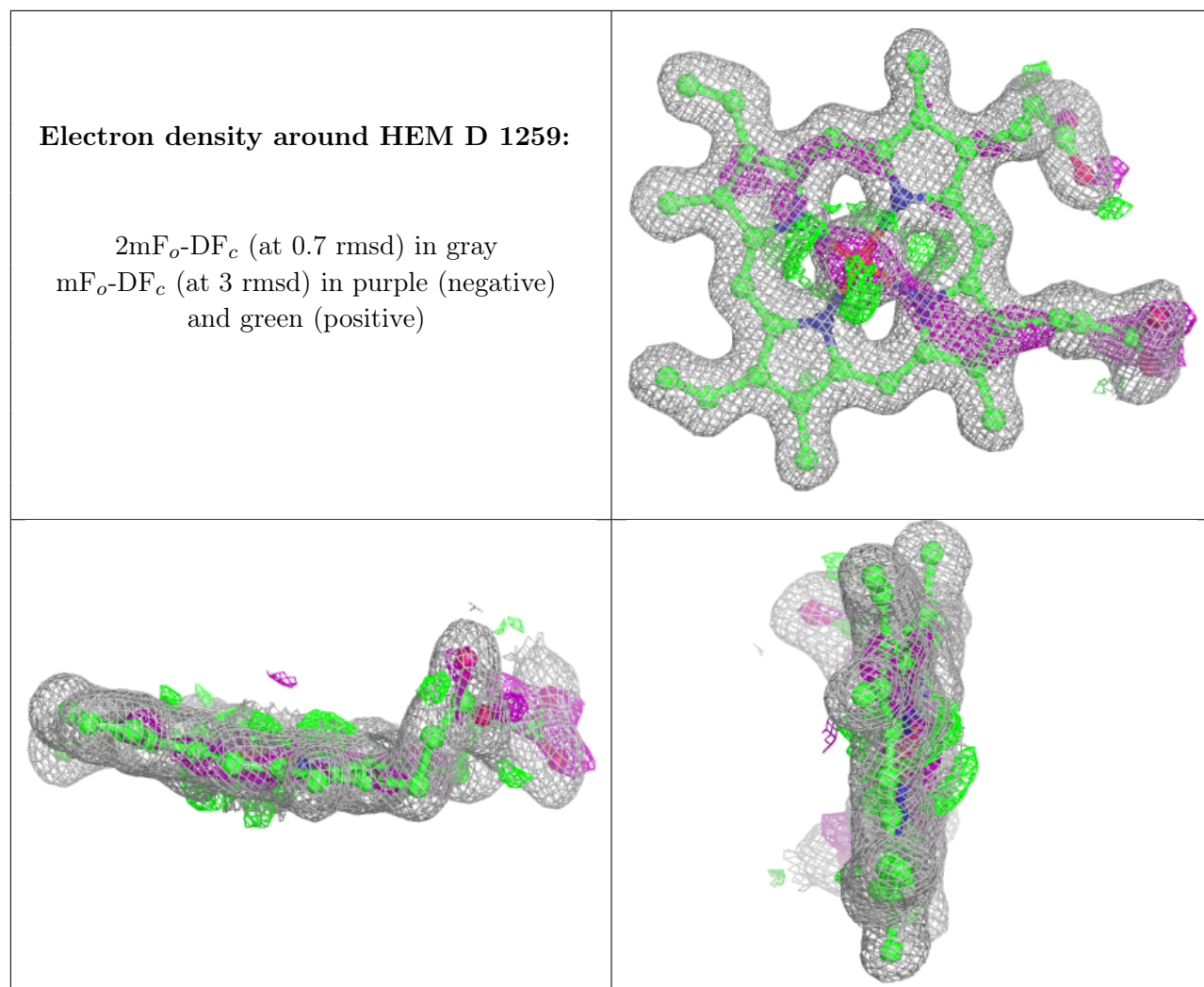
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM C 1259:**

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





## 6.5 Other polymers [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.