



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 06:34 am BST

PDB ID : 3VLI  
Title : Crystal Structure Analysis of the Cyanide Arg409Leu Variant KatG from HALOARCULA MARISMORTUI  
Authors : Sato, T.; Higuchi, W.; Yoshimatsu, K.; Fujiwara, T.  
Deposited on : 2011-12-01  
Resolution : 1.70 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

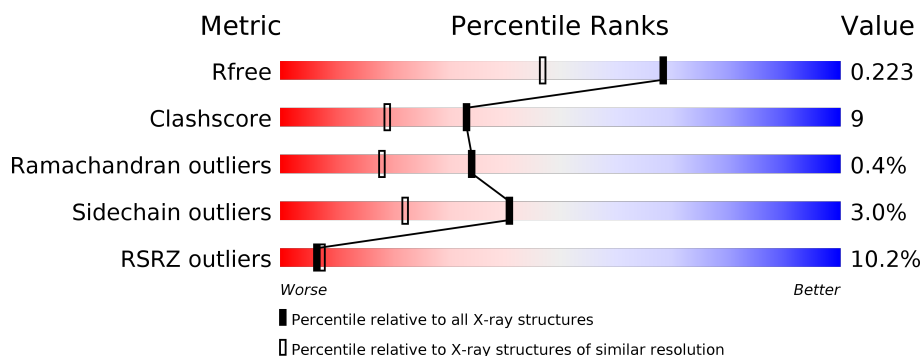
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	A	737	<div> <div>8%</div> <div>82%</div> <div>13%</div> <div>••</div> </div>
1	B	737	<div> <div>11%</div> <div>82%</div> <div>14%</div> <div>••</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CYN	A	802	-	-	X	X
3	CYN	B	802	-	-	X	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11870 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 Catalase-peroxidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	711	Total	C	N	O	S	0	0	0
			5599	3503	938	1139	19			
1	B	714	Total	C	N	O	S	0	0	0
			5617	3512	942	1144	19			

There are 14 discrepancies between the modelled and reference sequences:

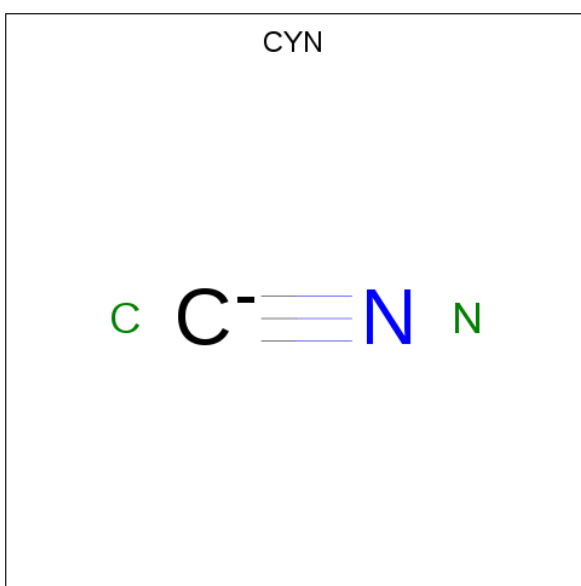
Chain	Residue	Modelled	Actual	Comment	Reference
A	409	LEU	ARG	ENGINEERED MUTATION	UNP O59651
A	732	HIS	-	EXPRESSION TAG	UNP O59651
A	733	HIS	-	EXPRESSION TAG	UNP O59651
A	734	HIS	-	EXPRESSION TAG	UNP O59651
A	735	HIS	-	EXPRESSION TAG	UNP O59651
A	736	HIS	-	EXPRESSION TAG	UNP O59651
A	737	HIS	-	EXPRESSION TAG	UNP O59651
B	409	LEU	ARG	ENGINEERED MUTATION	UNP O59651
B	732	HIS	-	EXPRESSION TAG	UNP O59651
B	733	HIS	-	EXPRESSION TAG	UNP O59651
B	734	HIS	-	EXPRESSION TAG	UNP O59651
B	735	HIS	-	EXPRESSION TAG	UNP O59651
B	736	HIS	-	EXPRESSION TAG	UNP O59651
B	737	HIS	-	EXPRESSION TAG	UNP O59651

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 3 is CYANIDE ION (three-letter code: CYN) (formula: CN).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	352	Total 352	O 352	0	0
4	B	212	Total 212	O 212	0	0

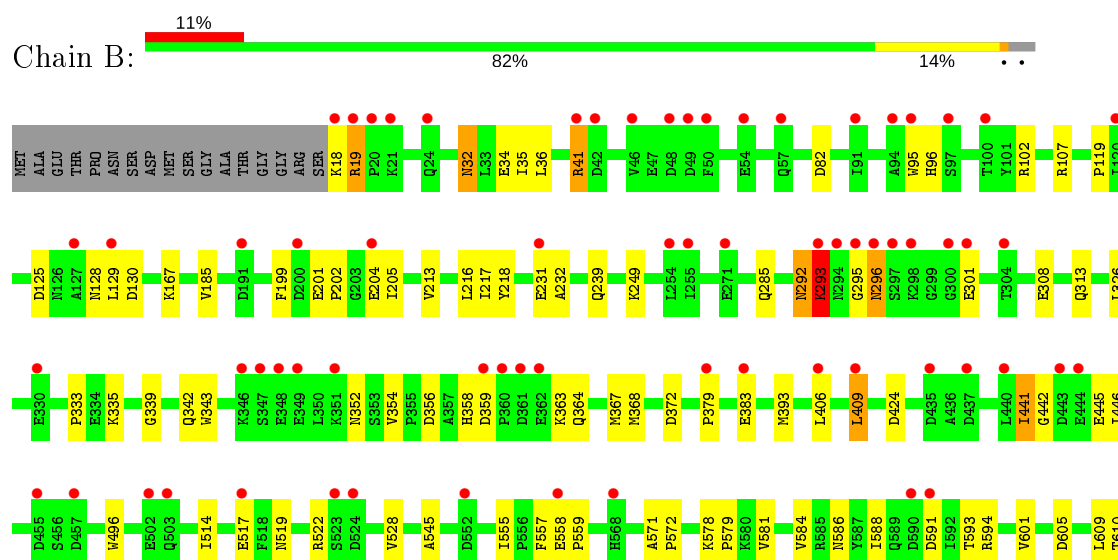
### 3 Residue-property plots [i](#)

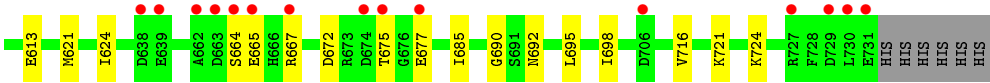
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Catalase-peroxidase 2



#### • Molecule 1: Catalase-peroxidase 2







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	315.88Å 81.43Å 75.58Å 90.00° 99.72° 90.00°	Depositor
Resolution (Å)	39.39 – 1.70 39.39 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.1 (39.39-1.70) 97.3 (39.39-1.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.92 (at 1.70Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.218 , 0.234 0.209 , 0.223	Depositor DCC
$R_{free}$ test set	9892 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.7	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 50.8	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	11870	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.54	0/5734	0.69	0/7790
1	B	0.43	0/5753	0.60	0/7817
All	All	0.49	0/11487	0.64	0/15607

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	5599	0	5248	95	0
1	B	5617	0	5263	98	0
2	A	43	0	30	3	0
2	B	43	0	30	0	0
3	A	2	0	0	4	0
3	B	2	0	0	2	0
4	A	352	0	0	6	0
4	B	212	0	0	3	0
All	All	11870	0	10571	187	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 (187) 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:B:95:TRP:CH2	1:B:218:TYR:HE1	1.16	1.58
1:B:95:TRP:HH2	1:B:218:TYR:CE1	0.97	1.57
1:B:95:TRP:CH2	1:B:218:TYR:CE1	1.86	1.57
1:A:199:PHE:HB3	1:A:205:ILE:HD13	1.40	1.00
1:A:298:LYS:HD2	1:A:301:GLU:HB3	1.41	0.98
1:A:95:TRP:CD1	3:A:802:CYN:N	2.36	0.94
1:B:95:TRP:HH2	1:B:218:TYR:CD1	1.86	0.93
1:A:565:GLY:H	1:A:568:HIS:HD2	1.16	0.91
1:B:326:LEU:HD13	1:B:368:MET:HE2	1.54	0.90
1:A:632:ASP:HB2	1:A:681:GLU:OE1	1.72	0.89
1:A:95:TRP:HD1	3:A:802:CYN:N	1.69	0.88
1:A:675:THR:HG22	1:A:677:GLU:H	1.39	0.87
1:A:45:PRO:HD3	1:B:698:ILE:HD12	1.56	0.85
1:B:95:TRP:CH2	1:B:218:TYR:CD1	2.64	0.83
1:A:588:ILE:HD11	1:A:685:ILE:HD11	1.59	0.83
1:B:32:ASN:ND2	1:B:34:GLU:HG2	1.93	0.82
1:B:95:TRP:CZ3	1:B:218:TYR:HE1	1.96	0.82
1:B:35:ILE:HD11	1:B:601:VAL:HG12	1.62	0.82
1:B:692:ASN:HD22	1:B:695:LEU:H	1.28	0.79
1:A:519:ASN:HD21	1:A:528:VAL:H	1.30	0.79
1:A:362:GLU:HG2	1:A:363:LYS:N	1.99	0.77
1:B:35:ILE:HD12	1:B:605:ASP:HB2	1.67	0.77
1:A:692:ASN:HD22	1:A:695:LEU:H	1.34	0.75
1:B:326:LEU:HD13	1:B:368:MET:CE	2.17	0.73
1:B:514:ILE:O	1:B:517:GLU:HG2	1.88	0.73
1:A:154:ILE:HD12	1:A:175:ARG:CZ	2.19	0.72
1:B:584:VAL:HG13	1:B:621:MET:HG2	1.71	0.71
1:B:588:ILE:HD11	1:B:685:ILE:HD11	1.72	0.70
1:A:675:THR:HG21	4:A:808:HOH:O	1.91	0.69
1:B:441:ILE:HD11	1:B:559:PRO:HB3	1.74	0.69
1:B:19:ARG:H	1:B:19:ARG:HD3	1.58	0.68
1:B:95:TRP:CZ3	1:B:218:TYR:CE1	2.76	0.68
1:A:154:ILE:HD12	1:A:175:ARG:NE	2.10	0.67
1:B:519:ASN:HD21	1:B:528:VAL:H	1.43	0.67
1:B:368:MET:CE	1:B:372:ASP:HB3	2.25	0.66
1:B:581:VAL:HG13	1:B:588:ILE:HD13	1.78	0.66
1:B:199:PHE:HB3	1:B:205:ILE:HD13	1.77	0.66
1:A:35:ILE:HD11	1:A:601:VAL:HG12	1.77	0.66
1:A:362:GLU:HG2	1:A:363:LYS:H	1.62	0.65
1:A:354:VAL:HB	1:A:364:GLN:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:ALA:HB3	1:B:572:PRO:HD3	1.80	0.63
1:B:32:ASN:HD21	1:B:34:GLU:HG2	1.61	0.63
1:A:199:PHE:CB	1:A:205:ILE:HD13	2.23	0.63
1:A:452:GLU:HG3	1:A:514:ILE:HD12	1.81	0.63
1:A:368:MET:HG3	1:A:372:ASP:HB2	1.81	0.63
1:A:565:GLY:H	1:A:568:HIS:CD2	2.07	0.62
1:A:675:THR:HG22	1:A:677:GLU:N	2.13	0.62
1:B:313:GLN:HA	1:B:354:VAL:HG22	1.81	0.62
1:A:441:ILE:HD11	1:A:559:PRO:HB3	1.82	0.62
1:A:22:SER:HB3	1:A:25:ASP:OD1	2.01	0.61
1:A:633:LEU:HD23	1:A:681:GLU:HG3	1.83	0.60
1:B:368:MET:HE3	1:B:372:ASP:HB3	1.83	0.60
1:A:31:LEU:HD21	1:A:597:GLU:HG3	1.83	0.60
1:B:308:GLU:H	1:B:342:GLN:HE22	1.48	0.60
1:A:308:GLU:H	1:A:342:GLN:HE22	1.50	0.60
1:B:558:GLU:HG2	1:B:724:LYS:HE3	1.85	0.58
1:A:584:VAL:HG13	1:A:621:MET:HG2	1.84	0.58
1:A:364:GLN:NE2	4:A:743:HOH:O	2.36	0.57
1:B:333:PRO:HD3	1:B:343:TRP:CZ3	2.40	0.57
1:B:441:ILE:HD13	1:B:441:ILE:H	1.70	0.56
1:B:557:PHE:CE2	1:B:559:PRO:HG3	2.41	0.56
1:A:514:ILE:O	1:A:517:GLU:HG3	2.06	0.55
1:B:249:LYS:HB2	1:B:249:LYS:NZ	2.21	0.55
1:B:326:LEU:CD1	1:B:368:MET:HE2	2.33	0.55
1:A:444:GLU:O	1:A:448:GLU:HG3	2.07	0.55
1:A:305:SER:HB3	1:A:307:ILE:HD12	1.89	0.54
1:A:299:GLY:O	1:A:302:MET:HG3	2.07	0.54
1:A:441:ILE:H	1:A:441:ILE:HD13	1.73	0.54
1:B:441:ILE:HD13	1:B:441:ILE:N	2.23	0.53
1:A:292:ASN:HD21	1:A:294:ASN:ND2	2.06	0.53
1:B:301:GLU:HB3	4:B:924:HOH:O	2.08	0.53
1:A:124:PRO:HG3	1:A:194:GLU:HG3	1.91	0.53
1:B:514:ILE:HA	1:B:517:GLU:OE1	2.09	0.53
1:A:441:ILE:HB	1:A:445:GLU:HB2	1.92	0.52
1:B:96:HIS:CD2	1:B:217:ILE:HG13	2.44	0.52
1:A:452:GLU:CG	1:A:514:ILE:HD12	2.39	0.52
1:A:581:VAL:HG13	1:A:588:ILE:HD13	1.92	0.51
1:B:293:LYS:NZ	1:B:293:LYS:HB3	2.25	0.51
1:A:101:TYR:O	1:A:244:MET:CE	2.58	0.51
1:A:450:LYS:HD2	1:A:540:ALA:HB2	1.91	0.51
1:A:23:ASN:HD21	1:B:119:PRO:HD3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:PRO:HG2	1:B:232:ALA:HB1	1.92	0.51
1:B:588:ILE:HD11	1:B:685:ILE:CD1	2.41	0.51
1:B:292:ASN:HD22	1:B:293:LYS:N	2.09	0.50
1:B:352:ASN:HD22	1:B:363:LYS:HB2	1.76	0.50
1:A:154:ILE:HD13	1:A:407:THR:HB	1.93	0.50
1:A:503:GLN:HG2	4:A:1085:HOH:O	2.12	0.50
1:B:128:ASN:HA	1:B:130:ASP:OD2	2.12	0.50
1:B:199:PHE:CB	1:B:205:ILE:HD13	2.42	0.50
1:B:95:TRP:CD1	3:B:802:CYN:N	2.79	0.50
1:A:181:GLU:CD	1:A:181:GLU:H	2.14	0.50
1:B:356:ASP:HB3	1:B:359:ASP:O	2.12	0.50
1:B:35:ILE:CD1	1:B:605:ASP:HB2	2.40	0.50
1:B:609:LEU:HD23	1:B:721:LYS:HE3	1.92	0.50
1:B:545:ALA:HB1	1:B:624:ILE:HD12	1.93	0.50
1:A:305:SER:OG	2:A:800:HEM:HBA1	2.12	0.49
1:B:326:LEU:HB2	1:B:368:MET:HE2	1.94	0.49
1:B:96:HIS:CE1	1:B:125:ASP:O	2.64	0.49
1:B:393:MET:HB2	4:B:896:HOH:O	2.12	0.49
1:B:95:TRP:HD1	3:B:802:CYN:N	2.10	0.49
1:A:593:THR:HG23	1:A:594:ARG:N	2.27	0.49
1:B:35:ILE:HG13	1:B:36:LEU:N	2.28	0.49
1:B:406:LEU:O	1:B:409:LEU:HD22	2.12	0.49
1:A:505:GLU:HG2	4:A:976:HOH:O	2.12	0.49
1:B:19:ARG:N	1:B:19:ARG:HD3	2.25	0.49
1:B:675:THR:HG23	1:B:677:GLU:H	1.77	0.48
1:B:368:MET:HE1	1:B:372:ASP:HB3	1.94	0.48
1:A:633:LEU:HA	1:A:681:GLU:HG3	1.95	0.48
1:A:397:MET:HA	1:A:397:MET:HE2	1.95	0.48
1:A:588:ILE:HD11	1:A:685:ILE:CD1	2.39	0.48
1:B:107:ARG:HD3	1:B:185:VAL:HG22	1.96	0.48
1:B:593:THR:HG23	1:B:594:ARG:N	2.28	0.48
1:A:632:ASP:CB	1:A:681:GLU:OE1	2.55	0.48
1:B:201:GLU:HB2	1:B:204:GLU:HG3	1.96	0.47
1:A:633:LEU:HD23	1:A:681:GLU:CG	2.44	0.47
1:B:213:VAL:HB	1:B:216:LEU:HD12	1.96	0.47
1:B:96:HIS:HE1	1:B:125:ASP:O	1.97	0.47
1:B:82:ASP:OD2	1:B:358:HIS:HE1	1.98	0.47
1:B:41:ARG:NH1	4:B:856:HOH:O	2.47	0.47
1:A:292:ASN:CG	1:A:298:LYS:HE3	2.34	0.47
1:A:415:GLU:H	1:A:415:GLU:CD	2.17	0.47
1:A:661:ALA:HB1	1:A:669:LYS:NZ	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ASN:C	1:B:292:ASN:HD22	2.17	0.47
1:B:95:TRP:CZ2	1:B:218:TYR:CD1	3.03	0.47
1:A:441:ILE:N	1:A:441:ILE:HD13	2.29	0.46
1:B:496:TRP:CD1	1:B:578:LYS:HE2	2.50	0.46
1:B:354:VAL:HB	1:B:364:GLN:HG3	1.98	0.46
1:A:264:VAL:HG12	2:A:800:HEM:CAA	2.46	0.46
1:A:450:LYS:CD	1:A:540:ALA:HB2	2.45	0.46
1:A:595:PRO:HD2	1:A:598:GLU:CD	2.36	0.46
1:B:441:ILE:H	1:B:441:ILE:CD1	2.29	0.46
1:A:545:ALA:HB1	1:A:624:ILE:HD12	1.97	0.46
1:B:593:THR:HG23	1:B:594:ARG:H	1.81	0.45
1:B:442:GLY:O	1:B:446:ILE:HG13	2.16	0.45
1:B:555:ILE:HG12	1:B:716:VAL:HG13	1.99	0.45
1:A:305:SER:CB	1:A:307:ILE:HD12	2.47	0.45
1:B:205:ILE:HG12	1:B:239:GLN:OE1	2.17	0.45
1:B:35:ILE:CD1	1:B:601:VAL:HG12	2.41	0.45
1:A:96:HIS:CE1	1:A:125:ASP:O	2.70	0.45
1:B:18:LYS:HB3	1:B:19:ARG:HD3	1.99	0.44
1:A:313:GLN:HA	1:A:354:VAL:HG22	1.98	0.44
1:A:570:ASP:OD1	1:A:572:PRO:HD2	2.17	0.44
1:B:664:SER:HG	1:B:667:ARG:H	1.65	0.44
1:A:286:GLN:HE22	1:B:690:GLY:HA3	1.82	0.44
1:B:32:ASN:HD21	1:B:34:GLU:CG	2.30	0.44
1:A:308:GLU:H	1:A:342:GLN:NE2	2.14	0.43
1:A:335:LYS:HE2	1:A:341:TRP:CE2	2.53	0.43
1:A:364:GLN:NE2	4:A:833:HOH:O	2.48	0.43
1:A:292:ASN:HD21	1:A:294:ASN:HD22	1.66	0.43
1:B:665:GLU:H	1:B:667:ARG:NH2	2.15	0.43
1:B:335:LYS:HE3	1:B:339:GLY:O	2.17	0.43
1:A:124:PRO:HG3	1:A:194:GLU:CG	2.49	0.43
1:A:441:ILE:CD1	1:A:441:ILE:H	2.32	0.43
1:A:665:GLU:H	1:A:665:GLU:CD	2.22	0.43
1:A:41:ARG:HB3	1:B:41:ARG:HB3	2.00	0.43
1:B:672:ASP:HB3	1:B:675:THR:HG23	2.00	0.43
1:A:95:TRP:HE1	3:A:802:CYN:C	2.32	0.43
1:A:264:VAL:HG12	2:A:800:HEM:HAA1	2.00	0.43
1:B:445:GLU:HG3	1:B:522:ARG:HH21	1.83	0.42
1:A:249:LYS:HB3	1:A:249:LYS:NZ	2.34	0.42
1:B:514:ILE:HD13	1:B:517:GLU:OE1	2.19	0.42
1:A:240:THR:O	1:A:244:MET:HG3	2.19	0.42
1:A:294:ASN:N	1:A:294:ASN:ND2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:HIS:NE2	3:A:802:CYN:C	2.83	0.42
1:B:610:THR:OG1	1:B:613:GLU:HG3	2.20	0.42
1:B:129:LEU:HA	1:B:129:LEU:HD23	1.88	0.42
1:B:368:MET:HE3	1:B:372:ASP:CB	2.49	0.42
1:B:578:LYS:HA	1:B:579:PRO:HD3	1.87	0.42
1:A:96:HIS:HE1	1:A:125:ASP:O	2.03	0.41
1:A:128:ASN:HA	1:A:130:ASP:OD2	2.19	0.41
1:B:167:LYS:HE3	1:B:167:LYS:HB3	1.95	0.41
1:A:545:ALA:HB1	1:A:624:ILE:CD1	2.50	0.41
1:A:557:PHE:CE2	1:A:559:PRO:HG3	2.56	0.41
1:B:231:GLU:CD	1:B:231:GLU:H	2.23	0.41
1:B:296:ASN:HA	1:B:296:ASN:HD22	1.65	0.41
1:A:451:GLU:HG2	1:A:455:ASP:OD2	2.21	0.41
1:A:20:PRO:HB3	1:B:185:VAL:O	2.21	0.41
1:A:154:ILE:HD12	1:A:175:ARG:NH2	2.34	0.41
1:B:379:PRO:O	1:B:383:GLU:HG3	2.21	0.41
1:A:545:ALA:CB	1:A:624:ILE:HD12	2.50	0.41
1:A:581:VAL:HG13	1:A:588:ILE:CD1	2.51	0.41
1:A:249:LYS:HG3	4:A:921:HOH:O	2.19	0.40
1:A:31:LEU:HD21	1:A:597:GLU:CG	2.48	0.40
1:A:405:LYS:HA	1:A:429:TRP:CZ2	2.57	0.40
1:A:286:GLN:NE2	1:B:690:GLY:HA3	2.37	0.40
1:A:442:GLY:O	1:A:446:ILE:HG13	2.20	0.40
1:B:496:TRP:NE1	1:B:578:LYS:HE2	2.37	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	707/737 (96%)	687 (97%)	17 (2%)	3 (0%)	34 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	712/737 (97%)	691 (97%)	18 (2%)	3 (0%)	34	18
All	All	1419/1474 (96%)	1378 (97%)	35 (2%)	6 (0%)	34	18

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	729	ASP
1	B	591	ASP
1	A	591	ASP
1	A	675	THR
1	B	293	LYS
1	B	295	GLY

### 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	A	588/608 (97%)	566 (96%)	22 (4%)	34	15
1	B	590/608 (97%)	577 (98%)	13 (2%)	52	34
All	All	1178/1216 (97%)	1143 (97%)	35 (3%)	41	22

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	41	ARG
1	A	45	PRO
1	A	57	GLN
1	A	102	ARG
1	A	119	PRO
1	A	125	ASP
1	A	131	LYS
1	A	181	GLU
1	A	246	MET

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Mol	Chain	Res	Type
1	A	285	GLN
1	A	292	ASN
1	A	294	ASN
1	A	335	LYS
1	A	367	MET
1	A	441	ILE
1	A	522	ARG
1	A	586	ASN
1	A	665	GLU
1	A	677	GLU
1	A	696	ARG
1	A	706	ASP
1	B	19	ARG
1	B	32	ASN
1	B	41	ARG
1	B	102	ARG
1	B	285	GLN
1	B	292	ASN
1	B	293	LYS
1	B	296	ASN
1	B	367	MET
1	B	409	LEU
1	B	424	ASP
1	B	441	ILE
1	B	586	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	24	GLN
1	A	286	GLN
1	A	292	ASN
1	A	294	ASN
1	A	342	GLN
1	A	352	ASN
1	A	364	GLN
1	A	513	ASN
1	A	515	GLN
1	A	519	ASN
1	A	568	HIS
1	A	586	ASN

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Mol	Chain	Res	Type
1	A	608	ASN
1	A	692	ASN
1	B	32	ASN
1	B	286	GLN
1	B	292	ASN
1	B	294	ASN
1	B	296	ASN
1	B	342	GLN
1	B	358	HIS
1	B	364	GLN
1	B	513	ASN
1	B	515	GLN
1	B	519	ASN
1	B	568	HIS
1	B	586	ASN
1	B	692	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	CYN	A	802	-	0,1,1	0.00	-	-		
3	CYN	B	802	-	0,1,1	0.00	-	-		
2	HEM	A	800	1	27,50,50	1.95	7 (25%)	17,82,82	5.23	13 (76%)
2	HEM	B	800	1	27,50,50	1.92	7 (25%)	17,82,82	5.05	8 (47%)

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	A	800	1	-	0/6/54/54	-
2	HEM	B	800	1	-	0/6/54/54	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	HEM	C3C-C2C	-4.94	1.33	1.40
2	B	800	HEM	C3C-C2C	-4.89	1.33	1.40
2	B	800	HEM	CBC-CAC	3.97	1.55	1.29
2	B	800	HEM	CBB-CAB	3.89	1.55	1.29
2	A	800	HEM	CBB-CAB	3.79	1.54	1.29
2	A	800	HEM	CBC-CAC	3.57	1.53	1.29
2	A	800	HEM	C3C-CAC	3.35	1.54	1.47
2	B	800	HEM	C3C-CAC	3.12	1.54	1.47
2	A	800	HEM	C3B-C2B	-3.04	1.36	1.40
2	B	800	HEM	C1D-ND	2.64	1.41	1.36
2	B	800	HEM	C3B-C2B	-2.56	1.36	1.40
2	A	800	HEM	C3B-CAB	2.41	1.52	1.47
2	A	800	HEM	C4B-NB	2.37	1.41	1.36
2	B	800	HEM	C4D-C3D	2.16	1.47	1.42

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	HEM	C1D-C2D-C3D	-13.64	97.51	107.00
2	A	800	HEM	C4A-C3A-C2A	-11.51	98.99	107.00
2	A	800	HEM	C4C-C3C-C2C	9.13	113.27	106.90
2	B	800	HEM	C4A-C3A-C2A	-9.00	100.74	107.00
2	A	800	HEM	CMA-C3A-C2A	7.40	138.89	124.94
2	B	800	HEM	C3B-C4B-NB	7.36	118.72	109.21
2	B	800	HEM	CAA-CBA-CGA	-6.46	101.83	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	HEM	C1D-C2D-C3D	-6.43	102.52	107.00
2	A	800	HEM	CMB-C2B-C3B	6.35	136.55	124.68
2	A	800	HEM	C3C-C4C-NC	-4.63	102.21	110.94
2	B	800	HEM	CMA-C3A-C2A	4.51	133.45	124.94
2	A	800	HEM	CMA-C3A-C4A	-4.45	121.62	128.46
2	A	800	HEM	CAD-CBD-CGD	4.38	120.03	112.67
2	B	800	HEM	CMC-C2C-C3C	4.25	132.64	124.68
2	A	800	HEM	CBA-CAA-C2A	4.24	120.31	112.49
2	A	800	HEM	CMD-C2D-C3D	3.77	132.04	124.94
2	A	800	HEM	CAA-CBA-CGA	-2.64	108.23	112.67
2	B	800	HEM	CMD-C2D-C1D	2.64	132.52	128.46
2	B	800	HEM	CMD-C2D-C3D	2.61	129.87	124.94
2	A	800	HEM	CAA-C2A-C3A	-2.15	121.08	127.25
2	A	800	HEM	CMD-C2D-C1D	-2.12	125.21	128.46

There are no chirality outliers.

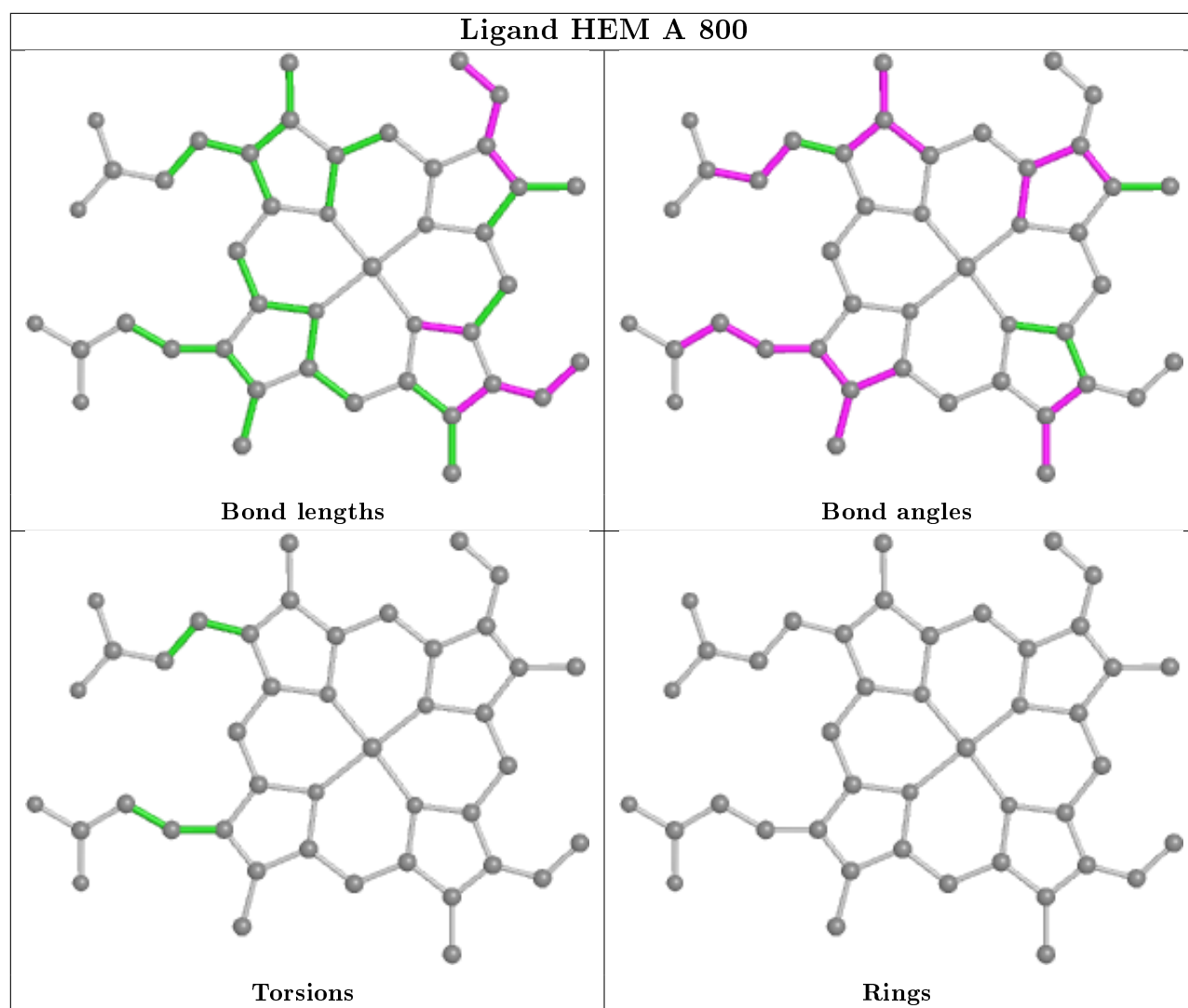
There are no torsion outliers.

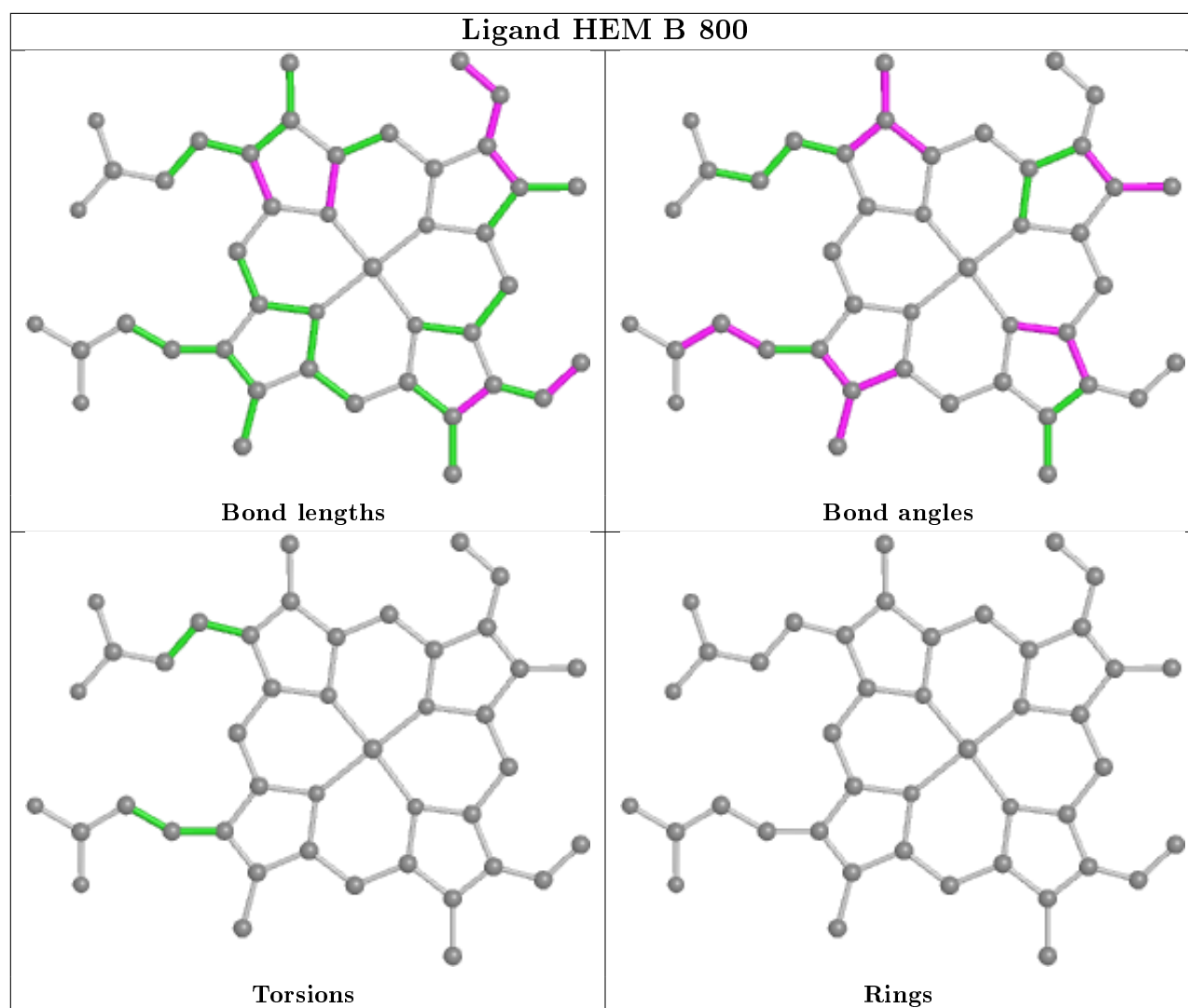
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	CYN	4	0
3	B	802	CYN	2	0
2	A	800	HEM	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.





## 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

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	A	711/737 (96%)	0.45	62 (8%) <b>10</b> <b>11</b>	13, 21, 41, 60	0
1	B	714/737 (96%)	0.73	83 (11%) <b>4</b> <b>5</b>	18, 29, 44, 60	0
All	All	1425/1474 (96%)	0.59	145 (10%) <b>6</b> <b>7</b>	13, 26, 43, 60	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	730	LEU	16.9
1	A	50	PHE	13.8
1	A	300	GLY	13.3
1	B	730	LEU	12.9
1	A	299	GLY	10.3
1	B	50	PHE	9.5
1	B	729	ASP	8.5
1	B	19	ARG	8.2
1	B	294	ASN	7.9
1	A	298	LYS	7.7
1	A	729	ASP	7.3
1	A	18	LYS	7.2
1	B	49	ASP	7.1
1	A	731	GLU	6.9
1	B	731	GLU	6.7
1	B	48	ASP	6.7
1	B	663	ASP	6.5
1	B	18	LYS	6.4
1	B	590	ASP	6.4
1	A	523	SER	6.1
1	A	19	ARG	6.1
1	B	591	ASP	5.9
1	A	590	ASP	5.5
1	B	298	LYS	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	200	ASP	5.2
1	A	524	ASP	5.1
1	A	663	ASP	5.0
1	A	593	THR	5.0
1	B	361	ASP	4.9
1	B	295	GLY	4.9
1	A	49	ASP	4.8
1	B	349	GLU	4.8
1	A	525	GLY	4.8
1	A	591	ASP	4.7
1	B	437	ASP	4.6
1	B	20	PRO	4.6
1	A	437	ASP	4.6
1	B	348	GLU	4.6
1	B	296	ASN	4.6
1	B	21	LYS	4.4
1	B	662	ALA	4.3
1	B	362	GLU	4.3
1	A	347	SER	4.2
1	B	54	GLU	4.1
1	B	665	GLU	4.0
1	B	523	SER	4.0
1	A	48	ASP	4.0
1	A	522	ARG	3.9
1	B	675	THR	3.8
1	A	349	GLU	3.8
1	B	359	ASP	3.8
1	A	526	THR	3.6
1	A	674	ASP	3.6
1	A	455	ASP	3.6
1	A	348	GLU	3.5
1	B	360	PRO	3.4
1	A	47	GLU	3.4
1	B	293	LYS	3.4
1	B	444	GLU	3.3
1	A	521	SER	3.2
1	A	517	GLU	3.2
1	A	440	LEU	3.2
1	B	457	ASP	3.1
1	B	347	SER	3.1
1	B	677	GLU	3.1
1	A	361	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	191	ASP	3.0
1	B	346	LYS	3.0
1	A	191	ASP	3.0
1	B	455	ASP	3.0
1	B	638	ASP	3.0
1	B	330	GLU	2.9
1	B	297	SER	2.9
1	B	674	ASP	2.9
1	B	129	LEU	2.9
1	A	457	ASP	2.9
1	B	517	GLU	2.9
1	B	46	VAL	2.9
1	A	727	ARG	2.9
1	B	351	LYS	2.9
1	B	664	SER	2.9
1	A	294	ASN	2.9
1	B	568	HIS	2.9
1	A	665	GLU	2.9
1	A	272	GLU	2.8
1	B	639	GLU	2.8
1	B	204	GLU	2.8
1	B	502	GLU	2.7
1	A	293	LYS	2.7
1	B	255	ILE	2.7
1	B	91	ILE	2.6
1	B	524	ASP	2.6
1	A	728	PHE	2.6
1	A	445	GLU	2.6
1	A	390	GLU	2.6
1	B	94	ALA	2.5
1	A	520	ASP	2.5
1	B	95	TRP	2.5
1	A	154	ILE	2.5
1	A	554	GLU	2.5
1	A	301	GLU	2.4
1	A	706	ASP	2.4
1	A	271	GLU	2.4
1	A	95	TRP	2.4
1	B	57	GLN	2.4
1	B	558	GLU	2.4
1	B	42	ASP	2.4
1	A	54	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	451	GLU	2.3
1	A	132	ALA	2.3
1	B	301	GLU	2.3
1	B	409	LEU	2.3
1	B	435	ASP	2.3
1	B	127	ALA	2.3
1	A	129	LEU	2.3
1	B	727	ARG	2.3
1	B	24	GLN	2.2
1	A	675	THR	2.2
1	B	254	LEU	2.2
1	B	706	ASP	2.2
1	A	21	LYS	2.2
1	B	406	LEU	2.2
1	A	435	ASP	2.2
1	A	558	GLU	2.2
1	B	440	LEU	2.2
1	B	443	ASP	2.2
1	B	552	ASP	2.2
1	B	97	SER	2.1
1	B	503	GLN	2.1
1	A	364	GLN	2.1
1	A	22	SER	2.1
1	B	379	PRO	2.1
1	B	120	ILE	2.1
1	B	383	GLU	2.1
1	B	300	GLY	2.1
1	A	502	GLU	2.1
1	B	271	GLU	2.1
1	B	41	ARG	2.0
1	B	231	GLU	2.0
1	B	667	ARG	2.0
1	B	304	THR	2.0
1	A	94	ALA	2.0
1	A	254	LEU	2.0
1	A	443	ASP	2.0
1	B	100	THR	2.0

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

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

## 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 Ligands

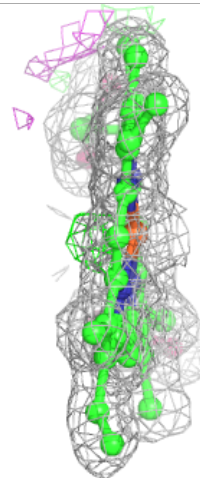
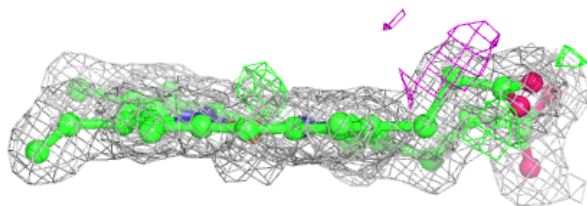
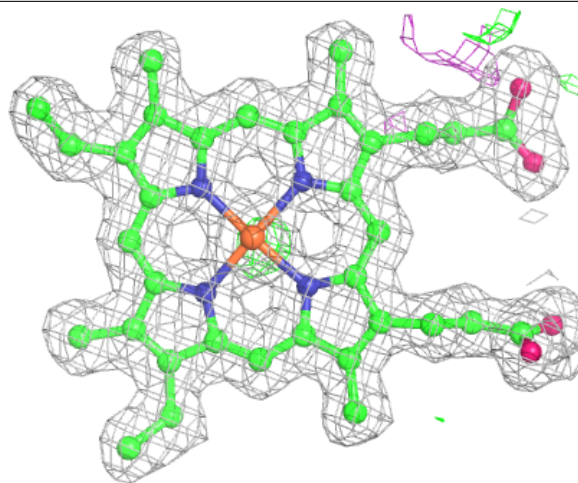
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

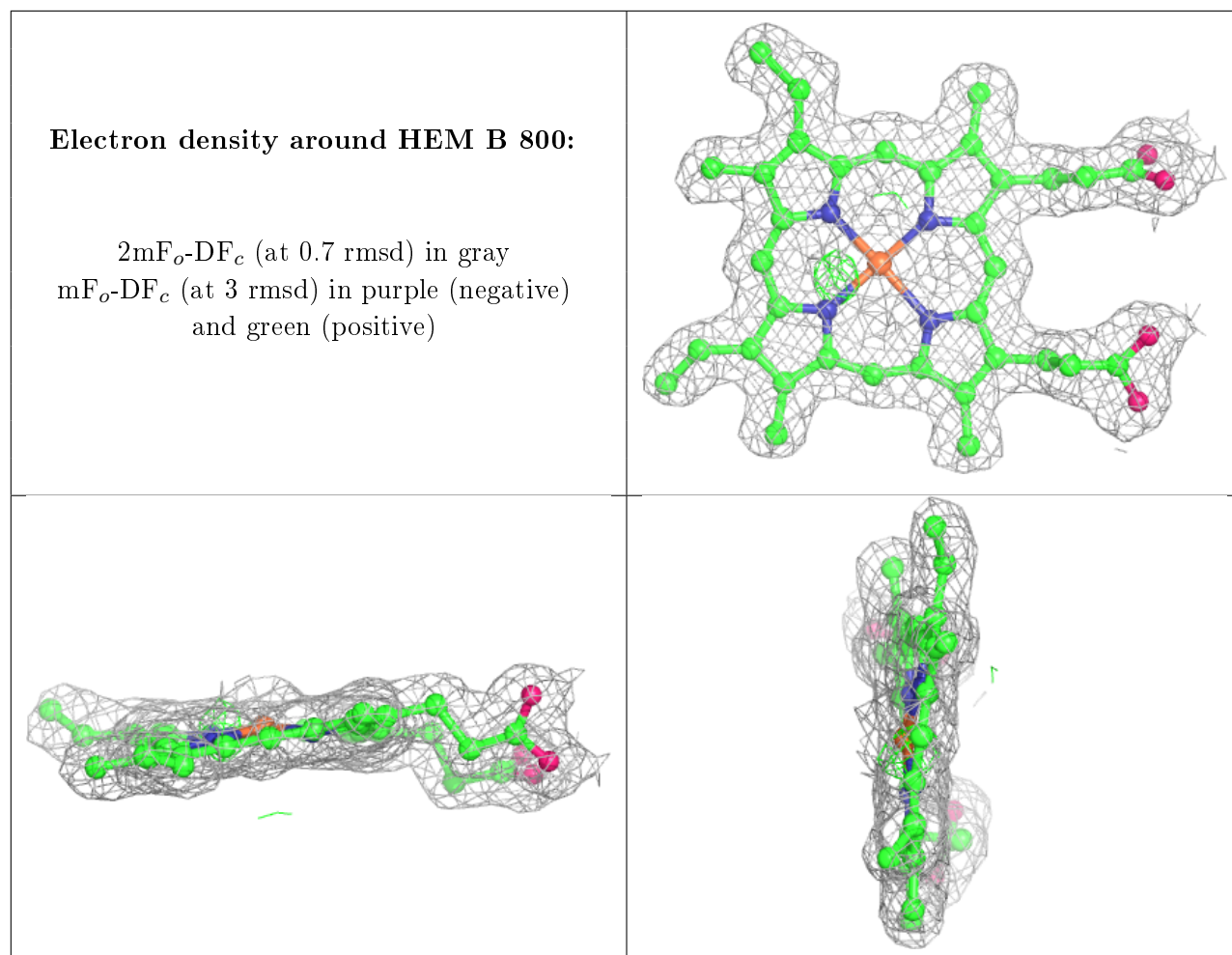
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CYN	B	802	2/2	0.44	0.62	47,47,47,48	0
3	CYN	A	802	2/2	0.55	0.42	34,34,34,36	0
2	HEM	A	800	43/43	0.98	0.12	12,14,17,22	0
2	HEM	B	800	43/43	0.98	0.17	19,22,25,28	0

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 HEM A 800:**

$2mF_o-DF_c$  (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.