Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 05:31 PM EST

PDB ID	:	3VLH
Title	:	Crystal Structure Analysis of the Arg409Leu Variants of KatG from HALOAR-CULA MARISMORTUI
Authors	:	Sato, T.; Higuchi, W.; Yoshimatsu, K.; Fujiwara, T.
Deposited on	:	2011-12-01
Resolution	:	1.73 Å(reported)

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

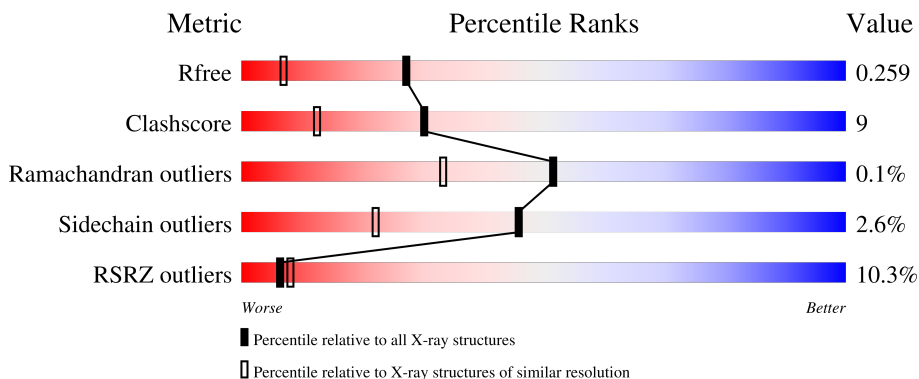|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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:
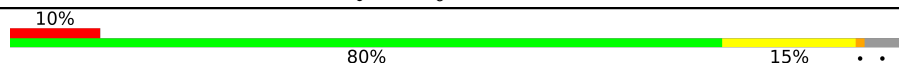*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.73 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	Percentile Ranks	Value
Rfree		0.259
Clashscore		9
Ramachandran outliers		0.1%
Sidechain outliers		2.6%
RSRZ outliers		10.3%

Worse .... *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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 >=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 <=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	10% / 80% 15% · ·
1	B	737	10% / 80% 15% · ·

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 11601 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.
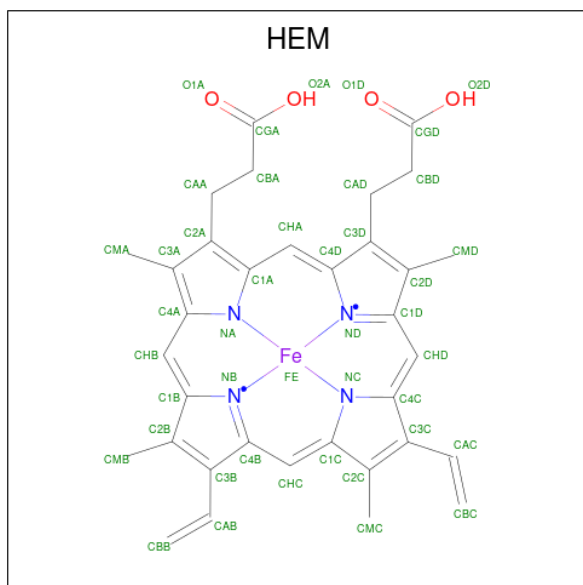
- Molecule 1 is a protein called Catalase-peroxidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	710	Total 5590	C 3497	N 936	O 1138	S 19	0	0	0
1	B	714	Total 5617	C 3512	N 942	O 1144	S 19	0	0	0

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: $C_{34}H_{32}FeN_4O_4$).

HEM

O1A O O2A OH O1D O O2D OH
CGA CGD
CAA CBA CAD CBD
C2A CHA C3D
CMA C3A C4D CMD
C1A C2D
C4A N N C1D
NA ND
CHB CHD
Fe
NB FE NC
C1B N· N C4C
C2B C3C
CMB CAC
C4B C1C
C3B CHC C2C CBC
CAB
CBB CMC

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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	112	Total O		0	0
			112 112			
3	B	196	Total O		0	0
			196 196			

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for whi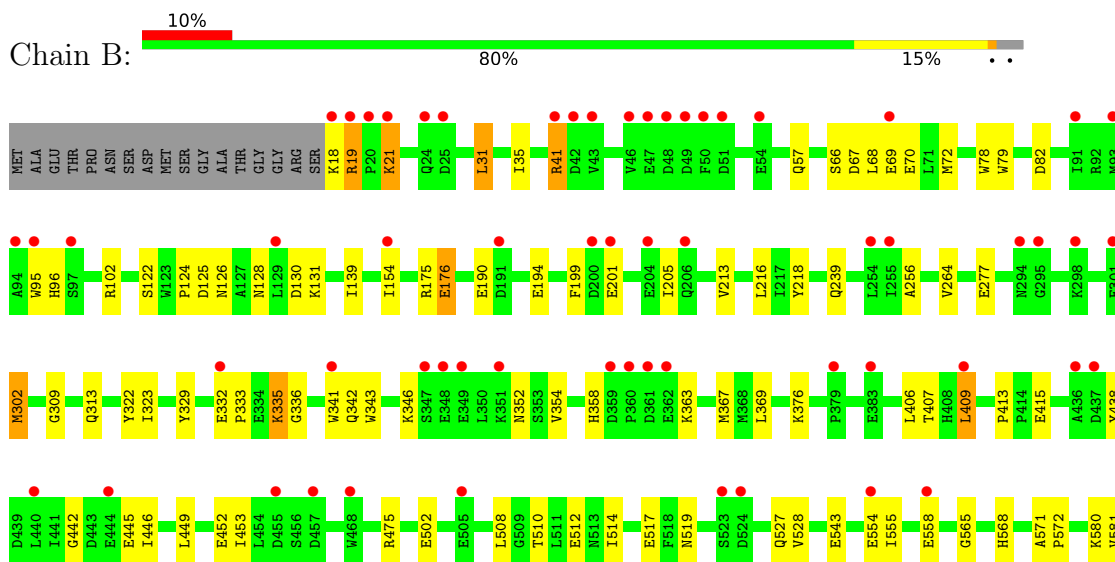ch they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Catalase-peroxidase 2

• Molecule 1: Catalase-peroxidase 2

V584 R585 N586 Y587 I588 Q589 D590 D591 I592 T593 R594 L600 V601 L606 T610 E613 M621 D638 E639 T644 A662 D663 S664 E665 H666 R667 L671 V678 I685 I688 N692 L695 R696 E700 D706 A707 E708 V716 R727 F728 D729

L730 E731 HIS HIS HIS HIS HIS HIS
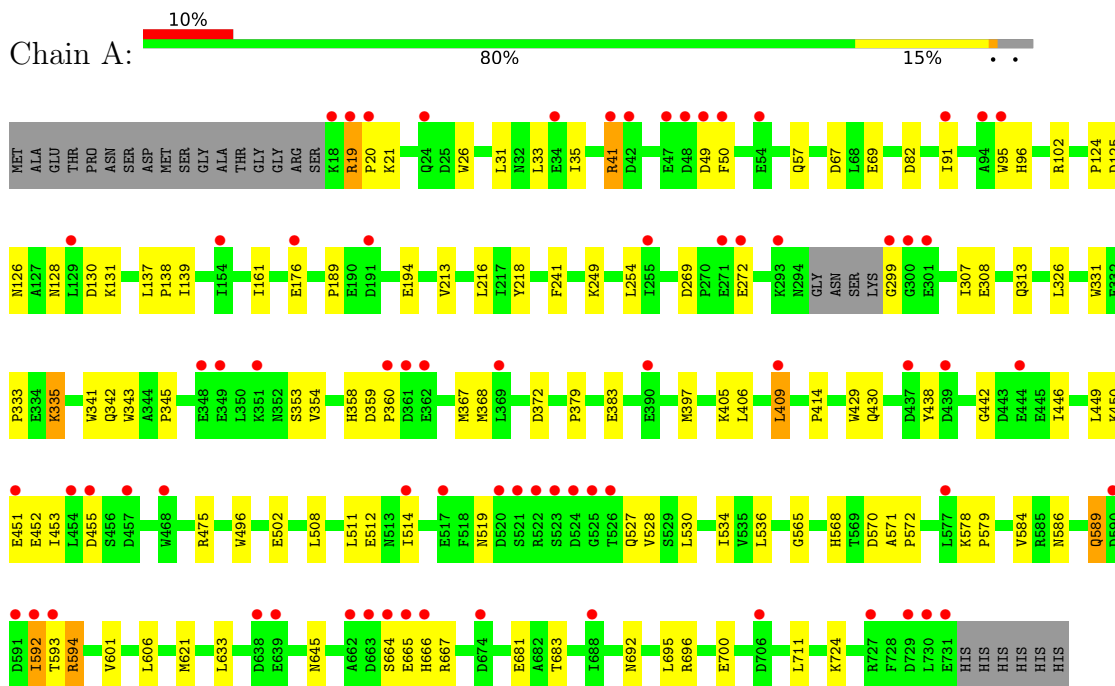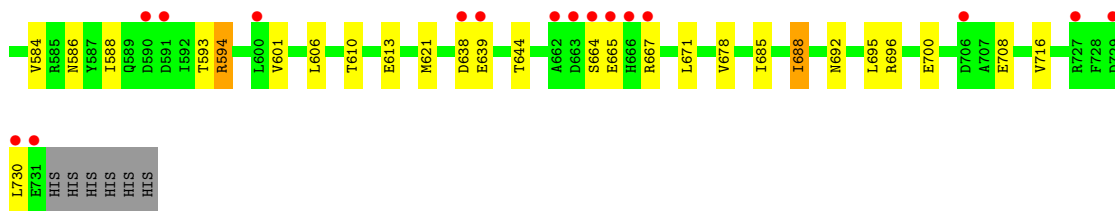
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	317.15Å 81.86Å 75.56Å 90.00° 99.98° 90.00°	Depositor
Resolution (Å)	37.07 – 1.73 37.07 – 1.73	Depositor EDS
% Data completeness (in resolution range)	98.5 (37.07-1.73) 98.7 (37.07-1.73)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 1.73Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.268 0.240 , 0.259	Depositor DCC
R_{free} test set	9624 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 41.5	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11601	wwPDB-VP
Average B, all atoms (Å^2)	31.0	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.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.32	0/5725	0.57	0/7779
1	B	0.29	0/5753	0.54	0/7817
All	All	0.30	0/11478	0.56	0/15596

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 (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	A	5590	0	5235	106	0
1	B	5617	0	5263	100	0
2	A	43	0	30	2	0
2	B	43	0	30	0	0
3	A	112	0	0	0	0
3	B	196	0	0	0	0
All	All	11601	0	10558	204	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 (204) 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:A:95:TRP:CH2	1:A:218:TYR:HE1	1.06	1.68
1:A:95:TRP:HH2	1:A:218:TYR:CE1	1.10	1.65
1:B:95:TRP:HH2	1:B:218:TYR:CE2	1.15	1.64
1:B:95:TRP:CH2	1:B:218:TYR:HE2	1.16	1.60
1:A:95:TRP:CH2	1:A:218:TYR:CE1	1.91	1.29
1:B:95:TRP:CH2	1:B:218:TYR:CE2	1.98	1.26
1:B:35:ILE:HD11	1:B:601:VAL:HG12	1.36	1.04
1:A:95:TRP:HH2	1:A:218:TYR:CD1	1.89	0.89
1:A:95:TRP:CZ3	1:A:218:TYR:HE1	1.89	0.89
1:B:565:GLY:H	1:B:568:HIS:HD2	1.20	0.86
1:A:565:GLY:H	1:A:568:HIS:HD2	1.22	0.86
1:A:95:TRP:CH2	1:A:218:TYR:CD1	2.64	0.85
1:B:594:ARG:HE	1:B:594:ARG:H	1.23	0.85
1:B:692:ASN:HD22	1:B:695:LEU:H	1.22	0.84
1:B:593:THR:H	1:B:594:ARG:HH21	1.26	0.82
1:A:692:ASN:HD22	1:A:695:LEU:H	1.28	0.81
1:B:588:ILE:HD11	1:B:685:ILE:HD11	1.60	0.81
1:B:688:ILE:HD12	1:B:695:LEU:HD12	1.61	0.80
1:B:313:GLN:HA	1:B:354:VAL:HG22	1.62	0.80
1:A:91:ILE:HD11	1:A:161:ILE:HG13	1.65	0.79
1:B:555:ILE:HD12	1:B:716:VAL:HG13	1.64	0.79
1:A:35:ILE:HD11	1:A:601:VAL:HG12	1.62	0.78
1:A:326:LEU:HB2	1:A:368:MET:HE2	1.64	0.78
1:A:397:MET:HA	1:A:397:MET:HE2	1.66	0.77
1:B:610:THR:HG23	1:B:613:GLU:H	1.52	0.75
1:A:665:GLU:H	1:A:667:ARG:HH21	1.33	0.74
1:A:326:LEU:HD13	1:A:368:MET:CE	2.18	0.74
1:A:124:PRO:HG3	1:A:194:GLU:HG3	1.71	0.73
1:B:323:ILE:H	1:B:323:ILE:HD12	1.54	0.73
1:A:41:ARG:HD3	1:A:41:ARG:H	1.54	0.72
1:A:326:LEU:HD13	1:A:368:MET:HE2	1.72	0.72
1:B:519:ASN:HD21	1:B:528:VAL:H	1.37	0.71
1:B:558:GLU:HG3	1:B:730:LEU:HD11	1.73	0.70
1:B:78:TRP:HZ3	1:B:131:LYS:HG3	1.57	0.70
1:B:452:GLU:HG3	1:B:514:ILE:HD12	1.74	0.69
1:A:19:ARG:N	1:A:19:ARG:HD3	2.07	0.69
1:A:594:ARG:HE	1:A:594:ARG:H	1.38	0.69
1:A:519:ASN:HD21	1:A:528:VAL:H	1.41	0.68
1:B:154:ILE:HD12	1:B:175:ARG:NE	2.09	0.68
1:A:91:ILE:CD1	1:A:161:ILE:HG13	2.23	0.67
1:A:589:GLN:O	1:A:592:ILE:HD12	1.94	0.67

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:TRP:CZ2	1:B:218:TYR:CE2	2.77	0.66
1:B:688:ILE:HD13	1:B:688:ILE:O	1.95	0.66
1:B:154:ILE:HD12	1:B:175:ARG:CZ	2.26	0.65
1:B:199:PHE:HB3	1:B:205:ILE:HD13	1.78	0.65
1:B:19:ARG:HD2	1:B:19:ARG:H	1.62	0.64
1:B:571:ALA:HB3	1:B:572:PRO:HD3	1.79	0.64
1:A:593:THR:H	1:A:594:ARG:HH21	1.44	0.64
1:A:397:MET:HA	1:A:397:MET:CE	2.27	0.64
1:B:665:GLU:H	1:B:667:ARG:NH2	1.95	0.64
1:A:313:GLN:HA	1:A:354:VAL:HG22	1.80	0.64
1:A:502:GLU:H	1:A:502:GLU:CD	2.01	0.64
1:A:299:GLY:N	1:A:359:ASP:HB2	2.13	0.63
1:B:588:ILE:HD11	1:B:685:ILE:CD1	2.29	0.63
1:A:189:PRO:HB3	1:B:18:LYS:HG3	1.82	0.62
1:A:308:GLU:H	1:A:342:GLN:HE22	1.47	0.62
1:B:124:PRO:HG3	1:B:194:GLU:HG3	1.81	0.62
1:B:95:TRP:CH2	1:B:218:TYR:CD2	2.81	0.61
1:A:664:SER:HB2	1:A:667:ARG:HB2	1.82	0.61
1:B:688:ILE:CD1	1:B:695:LEU:HD12	2.29	0.61
1:B:332:GLU:HG2	1:B:346:LYS:HE2	1.83	0.61
1:A:594:ARG:H	1:A:594:ARG:NE	1.98	0.60
1:B:406:LEU:O	1:B:409:LEU:HD22	2.01	0.60
1:B:502:GLU:H	1:B:502:GLU:CD	2.04	0.60
1:B:610:THR:HG22	1:B:613:GLU:CG	2.32	0.59
1:B:323:ILE:HD12	1:B:323:ILE:N	2.17	0.59
1:A:584:VAL:HG13	1:A:621:MET:HG2	1.84	0.59
1:A:333:PRO:HD3	1:A:343:TRP:CZ3	2.36	0.59
1:B:584:VAL:HG13	1:B:621:MET:HG2	1.85	0.59
1:A:326:LEU:CB	1:A:368:MET:HE2	2.33	0.58
1:A:19:ARG:HD3	1:A:19:ARG:H	1.68	0.58
1:A:511:LEU:CD1	1:A:534:ILE:HD13	2.34	0.58
1:B:332:GLU:CG	1:B:346:LYS:HE2	2.34	0.57
1:B:610:THR:HG22	1:B:613:GLU:HG3	1.85	0.57
1:A:368:MET:CE	1:A:372:ASP:HB3	2.34	0.57
1:B:352:ASN:O	1:B:363:LYS:HE3	2.05	0.56
1:A:49:ASP:CG	1:A:50:PHE:H	2.09	0.56
1:A:593:THR:H	1:A:594:ARG:NH2	2.03	0.56
1:A:565:GLY:H	1:A:568:HIS:CD2	2.12	0.56
1:A:452:GLU:HG3	1:A:514:ILE:HD12	1.88	0.56
1:A:307:ILE:HG22	1:A:367:MET:HE3	1.87	0.55
1:A:307:ILE:CG2	1:A:367:MET:HE3	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ASP:HB3	1:B:139:ILE:HD11	1.88	0.55
1:B:336:GLY:HA3	1:B:342:GLN:NE2	2.21	0.55
1:A:406:LEU:O	1:A:409:LEU:HD22	2.07	0.55
1:B:332:GLU:HG3	1:B:346:LYS:HG2	1.87	0.55
1:B:696:ARG:O	1:B:700:GLU:HG3	2.06	0.55
1:A:41:ARG:HD3	1:A:41:ARG:N	2.22	0.54
1:A:449:LEU:O	1:A:453:ILE:HG12	2.07	0.54
1:A:508:LEU:O	1:A:512:GLU:HG3	2.07	0.54
1:B:508:LEU:O	1:B:512:GLU:HG3	2.08	0.54
1:B:67:ASP:HB3	1:B:139:ILE:CD1	2.38	0.54
1:A:496:TRP:CD1	1:A:578:LYS:HE2	2.42	0.53
1:A:31:LEU:HB3	1:A:33:LEU:CD1	2.37	0.53
1:A:342:GLN:HB2	1:A:367:MET:HE1	1.90	0.53
1:B:19:ARG:HD2	1:B:19:ARG:N	2.22	0.53
1:B:41:ARG:N	1:B:41:ARG:HD3	2.24	0.53
1:A:326:LEU:HD13	1:A:368:MET:HE3	1.91	0.52
1:A:666:HIS:O	1:A:683:THR:HA	2.10	0.52
1:A:368:MET:HE3	1:A:372:ASP:HB3	1.90	0.52
1:B:581:VAL:HG13	1:B:588:ILE:CD1	2.40	0.52
1:A:530:LEU:O	1:A:534:ILE:HG12	2.10	0.52
1:A:665:GLU:H	1:A:667:ARG:NH2	2.04	0.52
1:B:199:PHE:CB	1:B:205:ILE:HD13	2.40	0.52
1:B:442:GLY:O	1:B:446:ILE:HG13	2.10	0.51
1:B:565:GLY:H	1:B:568:HIS:CD2	2.12	0.51
1:A:313:GLN:HG3	1:A:353:SER:O	2.09	0.51
1:A:724:LYS:NZ	1:A:724:LYS:HB2	2.25	0.51
1:B:692:ASN:ND2	1:B:695:LEU:H	2.02	0.51
1:B:95:TRP:CZ2	1:B:218:TYR:CD2	2.98	0.51
1:B:610:THR:CG2	1:B:613:GLU:HG3	2.41	0.51
1:A:633:LEU:HD23	1:A:681:GLU:HG3	1.93	0.50
1:B:580:LYS:HE3	1:B:594:ARG:HH12	1.76	0.50
1:B:323:ILE:H	1:B:323:ILE:CD1	2.22	0.50
1:B:78:TRP:CZ3	1:B:131:LYS:HG3	2.44	0.50
1:B:688:ILE:HD12	1:B:695:LEU:CD1	2.36	0.50
1:A:82:ASP:OD2	1:A:358:HIS:HE1	1.95	0.49
1:B:449:LEU:O	1:B:453:ILE:HG13	2.12	0.49
1:B:176:GLU:H	1:B:176:GLU:CD	2.15	0.49
1:A:95:TRP:CZ2	1:A:218:TYR:CE1	2.85	0.49
1:A:326:LEU:HB2	1:A:368:MET:CE	2.37	0.49
1:A:442:GLY:O	1:A:446:ILE:HG13	2.13	0.49
1:B:154:ILE:HD13	1:B:407:THR:HB	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:581:VAL:HG13	1:B:588:ILE:HD13	1.94	0.49
1:B:610:THR:CG2	1:B:613:GLU:H	2.22	0.49
1:A:96:HIS:HD2	1:A:126:ASN:OD1	1.96	0.49
1:A:213:VAL:HB	1:A:216:LEU:HD12	1.95	0.49
1:A:33:LEU:HD12	1:A:33:LEU:N	2.28	0.48
1:A:95:TRP:CZ2	1:A:218:TYR:CD1	3.00	0.48
1:A:645:ASN:HA	1:A:711:LEU:HD23	1.94	0.48
1:B:213:VAL:HB	1:B:216:LEU:HD12	1.95	0.48
1:B:82:ASP:OD2	1:B:358:HIS:HE1	1.97	0.48
1:B:329:TYR:O	1:B:376:LYS:NZ	2.47	0.48
1:B:333:PRO:HD3	1:B:343:TRP:CZ3	2.49	0.48
1:B:31:LEU:HD12	1:B:688:ILE:HD11	1.96	0.48
1:B:413:PRO:HB2	1:B:415:GLU:OE1	2.13	0.48
1:B:594:ARG:H	1:B:594:ARG:NE	2.01	0.48
1:B:128:ASN:HA	1:B:130:ASP:OD2	2.14	0.48
1:B:671:LEU:HD23	1:B:678:VAL:HA	1.96	0.48
1:B:96:HIS:HD2	1:B:126:ASN:OD1	1.97	0.47
1:A:571:ALA:HB3	1:A:572:PRO:HD3	1.96	0.47
1:A:645:ASN:CB	1:A:711:LEU:HD23	2.45	0.47
1:A:21:LYS:HD3	1:A:26:TRP:CE2	2.49	0.47
1:A:95:TRP:CZ3	1:A:218:TYR:CE1	2.79	0.47
1:B:475:ARG:HB2	1:B:606:LEU:HD22	1.97	0.47
1:A:82:ASP:OD2	1:A:358:HIS:CE1	2.68	0.46
1:B:205:ILE:HG12	1:B:239:GLN:OE1	2.16	0.46
1:B:332:GLU:HG3	1:B:346:LYS:CG	2.45	0.46
1:A:326:LEU:CD1	1:A:368:MET:HE2	2.43	0.46
1:B:79:TRP:CZ2	1:B:302:MET:HE3	2.51	0.46
1:A:342:GLN:HB2	1:A:367:MET:CE	2.45	0.45
1:A:67:ASP:HB3	1:A:139:ILE:CD1	2.47	0.45
1:B:671:LEU:CD2	1:B:678:VAL:HG22	2.47	0.45
1:B:664:SER:HB3	1:B:667:ARG:HB2	1.99	0.45
1:A:335:LYS:HE3	1:A:341:TRP:CE2	2.52	0.44
1:A:41:ARG:HD2	1:B:41:ARG:HD2	2.00	0.44
1:A:49:ASP:CG	1:A:50:PHE:N	2.70	0.44
1:A:592:ILE:N	1:A:592:ILE:HD13	2.33	0.44
1:A:450:LYS:HG2	1:A:536:LEU:HG	2.00	0.44
1:A:594:ARG:HE	1:A:594:ARG:N	2.13	0.44
1:A:696:ARG:O	1:A:700:GLU:HG3	2.18	0.44
1:B:68:LEU:O	1:B:72:MET:HG2	2.17	0.44
1:B:264:VAL:HG11	1:B:369:LEU:HD21	2.00	0.44
1:B:367:MET:HE3	1:B:369:LEU:HD23	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:HIS:O	1:A:360:PRO:HD3	2.18	0.43
1:B:335:LYS:HE3	1:B:341:TRP:CE2	2.52	0.43
1:A:578:LYS:HA	1:A:579:PRO:HD3	1.87	0.43
1:B:438:TYR:CG	1:B:527:GLN:HB2	2.52	0.43
1:B:644:THR:HB	1:B:708:GLU:OE1	2.18	0.43
1:A:331:TRP:CZ3	1:A:345:PRO:HD3	2.52	0.43
1:B:124:PRO:HG3	1:B:194:GLU:CG	2.46	0.43
1:A:269:ASP:HB3	1:A:272:GLU:OE1	2.19	0.43
1:A:405:LYS:HA	1:A:429:TRP:CZ2	2.54	0.43
1:B:510:THR:O	1:B:514:ILE:HG12	2.19	0.43
1:B:638:ASP:OD2	1:B:639:GLU:HG3	2.18	0.43
1:A:128:ASN:HA	1:A:130:ASP:OD2	2.19	0.42
1:A:241:PHE:HE1	2:A:800:HEM:HBB1	1.83	0.42
1:A:379:PRO:O	1:A:383:GLU:HG3	2.18	0.42
1:A:475:ARG:HB2	1:A:606:LEU:HD22	1.99	0.42
1:A:645:ASN:CA	1:A:711:LEU:HD23	2.49	0.42
1:B:256:ALA:HA	1:B:322:TYR:CE2	2.54	0.42
1:A:665:GLU:N	1:A:667:ARG:HH21	2.09	0.42
1:A:570:ASP:OD1	1:A:572:PRO:HD2	2.19	0.42
1:A:645:ASN:HA	1:A:711:LEU:CD2	2.50	0.42
1:B:555:ILE:CD1	1:B:716:VAL:HG13	2.41	0.42
1:B:264:VAL:HG22	1:B:309:GLY:O	2.20	0.42
1:A:249:LYS:NZ	1:A:249:LYS:HB3	2.35	0.41
1:B:122:SER:HB3	1:B:277:GLU:HG3	2.02	0.41
1:A:438:TYR:CG	1:A:527:GLN:HB2	2.55	0.41
1:B:19:ARG:C	1:B:21:LYS:H	2.24	0.41
1:B:201:GLU:HA	1:B:201:GLU:OE1	2.21	0.41
1:A:452:GLU:CG	1:A:514:ILE:HD12	2.51	0.41
1:B:664:SER:CB	1:B:667:ARG:HB2	2.50	0.41
1:A:19:ARG:HB2	1:A:20:PRO:HD2	2.03	0.41
1:A:137:LEU:HB3	1:A:138:PRO:HD3	2.02	0.41
1:A:414:PRO:HD3	1:A:430:GLN:HB3	2.01	0.41
1:A:511:LEU:HD12	1:A:534:ILE:HD13	2.01	0.41
1:A:593:THR:N	1:A:594:ARG:HH21	2.16	0.41
1:B:190:GLU:H	1:B:190:GLU:CD	2.25	0.41
1:A:409:LEU:H	1:A:409:LEU:CD2	2.34	0.40
1:A:451:GLU:HG2	1:A:455:ASP:OD2	2.21	0.40
1:A:254:LEU:O	2:A:800:HEM:HBC2	2.22	0.40
1:B:66:SER:O	1:B:70:GLU:HG3	2.22	0.40
1:B:543:GLU:HG3	1:B:555:ILE:HG12	2.03	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	A	706/737 (96%)	688 (98%)	18 (2%)	0	100	100
1	B	712/737 (97%)	690 (97%)	21 (3%)	1 (0%)	51	33
All	All	1418/1474 (96%)	1378 (97%)	39 (3%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	21	LYS

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	587/608 (96%)	573 (98%)	14 (2%)	49	26
1	B	590/608 (97%)	573 (97%)	17 (3%)	42	18
All	All	1177/1216 (97%)	1146 (97%)	31 (3%)	46	22

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	41	ARG
1	A	57	GLN
1	A	69	GLU
1	A	102	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	125	ASP
1	A	131	LYS
1	A	176	GLU
1	A	335	LYS
1	A	409	LEU
1	A	586	ASN
1	A	589	GLN
1	A	592	ILE
1	A	594	ARG
1	B	19	ARG
1	B	31	LEU
1	B	41	ARG
1	B	57	GLN
1	B	69	GLU
1	B	102	ARG
1	B	125	ASP
1	B	176	GLU
1	B	302	MET
1	B	335	LYS
1	B	409	LEU
1	B	445	GLU
1	B	517	GLU
1	B	554	GLU
1	B	586	ASN
1	B	594	ARG
1	B	688	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	96	HIS
1	A	206	GLN
1	A	285	GLN
1	A	286	GLN
1	A	294	ASN
1	A	313	GLN
1	A	342	GLN
1	A	358	HIS
1	A	515	GLN
1	A	519	ASN
1	A	568	HIS

Continued from previous page...

Mol	Chain	Res	Type
1	A	586	ASN
1	A	608	ASN
1	A	692	ASN
1	B	24	GLN
1	B	96	HIS
1	B	206	GLN
1	B	285	GLN
1	B	286	GLN
1	B	342	GLN
1	B	358	HIS
1	B	513	ASN
1	B	515	GLN
1	B	519	ASN
1	B	544	GLN
1	B	568	HIS
1	B	586	ASN
1	B	608	ASN
1	B	692	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	#$|Z| > 2$
2	HEM	B	800	1	41,50,50	1.88	10 (24%)	45,82,82	8.64	33 (73%)
2	HEM	A	800	1	41,50,50	1.89	11 (26%)	45,82,82	5.75	29 (64%)

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	B	800	1	-	3/12/54/54	-
2	HEM	A	800	1	-	4/12/54/54	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	HEM	CBB-CAB	5.12	1.55	1.30
2	B	800	HEM	CBB-CAB	5.01	1.55	1.30
2	A	800	HEM	C3C-C2C	-4.19	1.34	1.40
2	B	800	HEM	C3C-C2C	-4.16	1.34	1.40
2	B	800	HEM	CBD-CGD	-4.00	1.41	1.50
2	B	800	HEM	CBC-CAC	3.99	1.55	1.29
2	B	800	HEM	CBA-CGA	-3.96	1.41	1.50
2	A	800	HEM	CBD-CGD	-3.91	1.41	1.50
2	A	800	HEM	CBC-CAC	3.89	1.55	1.29
2	A	800	HEM	CBA-CGA	-3.58	1.42	1.50
2	B	800	HEM	FE-NB	2.82	2.10	1.96
2	A	800	HEM	FE-NB	2.59	2.09	1.96
2	A	800	HEM	O1A-CGA	2.56	1.30	1.22
2	A	800	HEM	C3C-CAC	2.49	1.52	1.47
2	B	800	HEM	O1A-CGA	2.43	1.30	1.22
2	B	800	HEM	C3C-CAC	2.37	1.52	1.47
2	A	800	HEM	CBD-CAD	2.36	1.59	1.52
2	B	800	HEM	CBD-CAD	2.27	1.59	1.52
2	A	800	HEM	C4D-ND	-2.26	1.36	1.40
2	A	800	HEM	CHA-C4D	2.22	1.40	1.35
2	B	800	HEM	CHA-C4D	2.15	1.40	1.35

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	800	HEM	C4B-CHC-C1C	24.17	154.46	122.56
2	B	800	HEM	C3B-C2B-C1B	-18.03	93.11	106.49
2	B	800	HEM	C4C-CHD-C1D	17.68	145.89	122.56
2	B	800	HEM	CHC-C4B-NB	-15.13	108.00	124.43
2	A	800	HEM	C4C-CHD-C1D	15.06	142.43	122.56
2	B	800	HEM	CHA-C4D-ND	-13.84	107.28	124.38
2	B	800	HEM	CHC-C4B-C3B	13.35	145.01	124.57
2	B	800	HEM	C2C-C3C-C4C	13.28	116.17	106.90
2	B	800	HEM	C4B-C3B-C2B	13.15	117.56	107.11
2	B	800	HEM	CHB-C1B-NB	-12.60	108.81	124.38
2	A	800	HEM	C4B-CHC-C1C	12.53	139.09	122.56
2	B	800	HEM	CHD-C1D-ND	-11.48	111.96	124.43
2	A	800	HEM	CHC-C4B-NB	-11.35	112.10	124.43
2	B	800	HEM	C2D-C1D-ND	11.32	123.44	109.88
2	B	800	HEM	C2B-C1B-NB	11.10	122.99	109.84
2	A	800	HEM	CHD-C1D-ND	-10.97	112.51	124.43
2	A	800	HEM	C2C-C3C-C4C	10.78	114.43	106.90
2	A	800	HEM	CHB-C1B-NB	-10.47	111.45	124.38
2	B	800	HEM	C4D-ND-C1D	-10.35	94.38	105.07
2	B	800	HEM	C1D-C2D-C3D	-9.23	97.25	106.96
2	A	800	HEM	C1D-C2D-C3D	-9.06	97.44	106.96
2	A	800	HEM	C2D-C1D-ND	8.25	119.76	109.88
2	B	800	HEM	CMD-C2D-C1D	8.25	137.60	125.04
2	B	800	HEM	O2A-CGA-O1A	-8.24	102.77	123.30
2	A	800	HEM	C1B-NB-C4B	-8.10	96.71	105.07
2	A	800	HEM	CHA-C4D-ND	-8.04	114.44	124.38
2	A	800	HEM	CMA-C3A-C4A	-7.02	117.68	128.46
2	B	800	HEM	CMC-C2C-C3C	6.32	136.50	124.68
2	A	800	HEM	C4B-C3B-C2B	-6.27	102.14	107.11
2	A	800	HEM	C2B-C1B-NB	5.76	116.67	109.84
2	B	800	HEM	CHA-C4D-C3D	5.54	135.72	125.33
2	A	800	HEM	CMA-C3A-C2A	5.23	134.80	124.94
2	A	800	HEM	C4D-ND-C1D	-5.11	99.79	105.07
2	B	800	HEM	C1B-NB-C4B	-5.10	99.80	105.07
2	B	800	HEM	C3D-C4D-ND	5.07	115.81	110.17
2	B	800	HEM	O2A-CGA-CBA	5.01	130.14	114.03
2	B	800	HEM	CAD-C3D-C4D	-4.66	116.52	124.66
2	B	800	HEM	O2D-CGD-CBD	4.50	128.48	114.03
2	A	800	HEM	CHA-C4D-C3D	4.49	133.76	125.33
2	B	800	HEM	CMB-C2B-C1B	4.34	131.65	125.04
2	B	800	HEM	CAA-CBA-CGA	-4.32	101.65	113.76
2	A	800	HEM	CAA-CBA-CGA	-4.28	101.77	113.76
2	B	800	HEM	C3C-C4C-NC	-4.18	103.04	110.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	800	HEM	CMC-C2C-C3C	4.11	132.36	124.68
2	A	800	HEM	C3C-C4C-NC	-4.10	103.20	110.94
2	A	800	HEM	C4D-C3D-C2D	3.74	112.35	106.90
2	B	800	HEM	CMA-C3A-C4A	-3.65	122.86	128.46
2	B	800	HEM	O1D-CGD-CBD	-3.64	111.38	123.08
2	A	800	HEM	CMD-C2D-C1D	3.61	130.53	125.04
2	B	800	HEM	CAD-C3D-C2D	3.41	134.23	127.88
2	A	800	HEM	O2A-CGA-CBA	3.32	124.68	114.03
2	B	800	HEM	CAA-C2A-C3A	3.00	135.85	127.25
2	A	800	HEM	O2A-CGA-O1A	-2.98	115.88	123.30
2	A	800	HEM	CAD-C3D-C4D	-2.95	119.51	124.66
2	B	800	HEM	CMA-C3A-C2A	2.84	130.30	124.94
2	B	800	HEM	CMB-C2B-C3B	2.83	135.23	128.30
2	A	800	HEM	CBA-CAA-C2A	2.31	116.56	112.62
2	A	800	HEM	CBB-CAB-C3B	-2.29	116.21	127.62
2	A	800	HEM	CAD-CBD-CGD	2.27	118.50	113.60
2	A	800	HEM	CHC-C4B-C3B	2.26	128.03	124.57
2	B	800	HEM	CAB-C3B-C4B	-2.14	114.49	124.47
2	A	800	HEM	O2D-CGD-CBD	2.05	120.61	114.03

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	800	HEM	C4B-C3B-CAB-CBB
2	A	800	HEM	C2B-C3B-CAB-CBB
2	B	800	HEM	CAA-CBA-CGA-O1A
2	A	800	HEM	CAA-CBA-CGA-O1A
2	B	800	HEM	CAA-CBA-CGA-O2A
2	A	800	HEM	CAA-CBA-CGA-O2A
2	B	800	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	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 then 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 HEM B 800

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 800

Bond lengths

Bond angles

Torsions

Rings
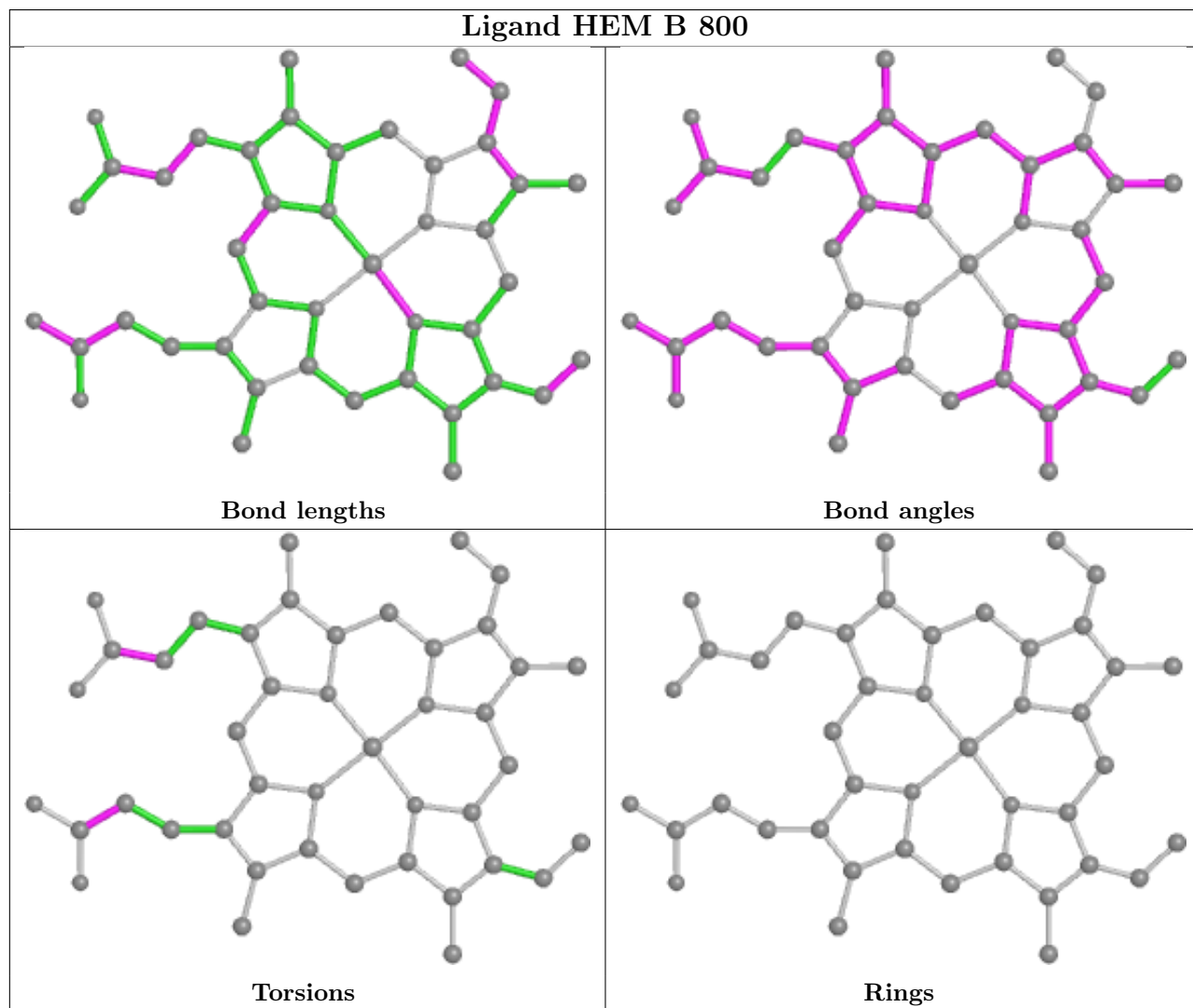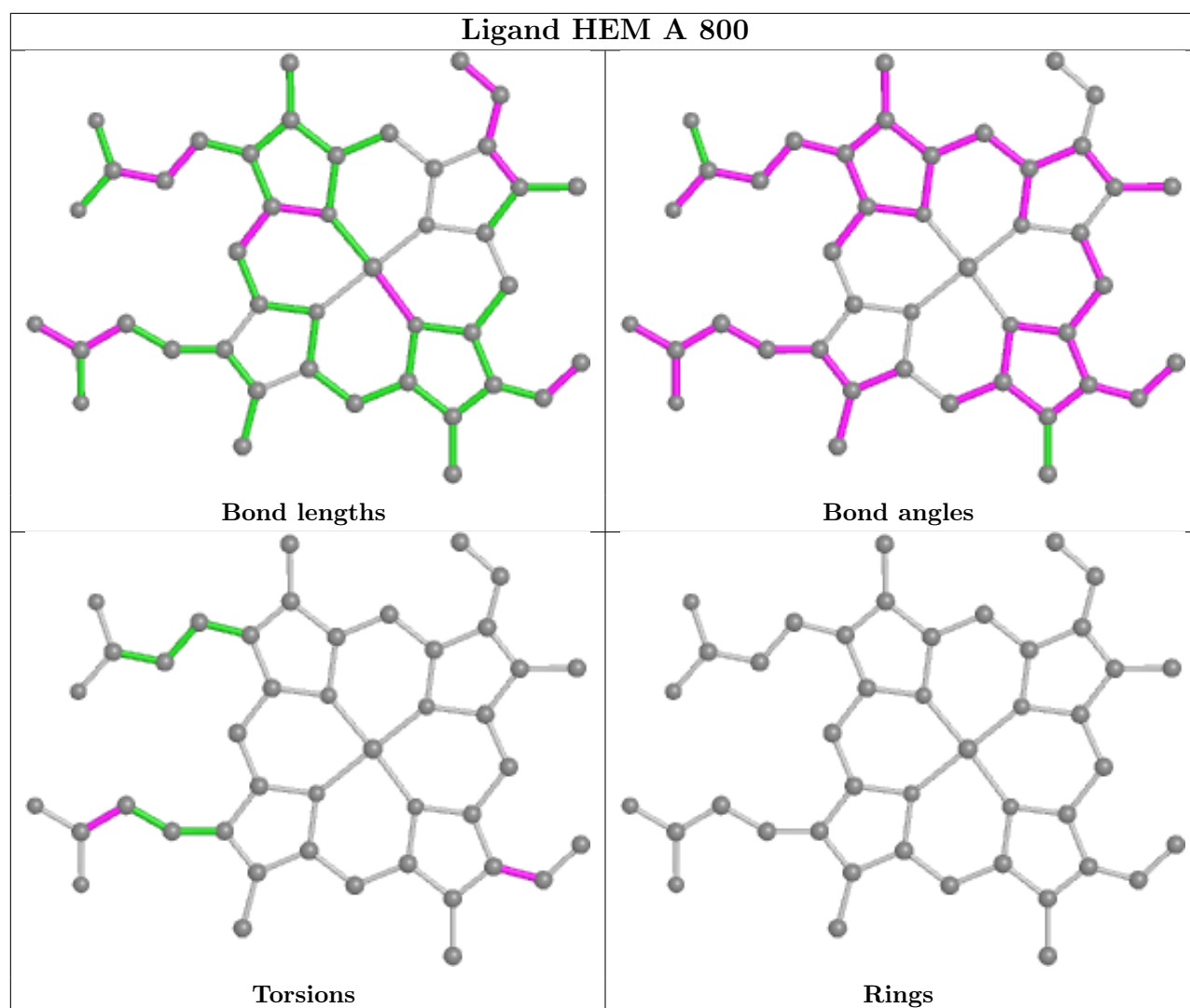
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6　Fit of model and data ⓘ

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, 95th 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^2)	Q<0.9
1	A	710/737 (96%)	0.72	71 (10%)	7	9	16, 25, 50, 72	0
1	B	714/737 (96%)	0.81	76 (10%)	6	7	21, 31, 49, 71	0
All	All	1424/1474 (96%)	0.77	147 (10%)	6	8	16, 29, 49, 72	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	50	PHE	15.5
1	A	300	GLY	15.4
1	A	730	LEU	14.3
1	B	50	PHE	12.7
1	B	20	PRO	8.5
1	B	730	LEU	8.0
1	A	18	LYS	7.9
1	B	48	ASP	7.3
1	B	49	ASP	7.2
1	A	19	ARG	7.2
1	A	729	ASP	7.2
1	B	19	ARG	7.0
1	B	18	LYS	7.0
1	B	729	ASP	7.0
1	A	49	ASP	6.8
1	A	523	SER	6.7
1	A	299	GLY	6.4
1	A	663	ASP	6.0
1	A	525	GLY	5.9
1	A	591	ASP	5.9
1	A	524	ASP	5.9
1	A	48	ASP	5.6
1	B	200	ASP	5.5
1	A	348	GLU	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	731	GLU	5.2
1	A	20	PRO	5.2
1	B	437	ASP	5.1
1	B	191	ASP	5.0
1	B	591	ASP	4.7
1	B	590	ASP	4.6
1	B	43	VAL	4.5
1	B	361	ASP	4.4
1	A	590	ASP	4.3
1	A	522	ARG	4.3
1	A	664	SER	4.2
1	B	731	GLU	4.1
1	A	360	PRO	4.1
1	B	349	GLU	4.0
1	B	663	ASP	4.0
1	B	409	LEU	3.9
1	A	191	ASP	3.9
1	A	526	THR	3.8
1	B	47	GLU	3.8
1	A	47	GLU	3.8
1	B	295	GLY	3.7
1	A	349	GLU	3.6
1	A	455	ASP	3.6
1	A	706	ASP	3.6
1	B	204	GLU	3.5
1	A	521	SER	3.5
1	B	638	ASP	3.5
1	B	665	GLU	3.5
1	B	254	LEU	3.4
1	A	91	ILE	3.4
1	B	54	GLU	3.4
1	A	361	ASP	3.4
1	B	383	GLU	3.3
1	B	95	TRP	3.3
1	B	294	ASN	3.3
1	B	298	LYS	3.3
1	A	437	ASP	3.3
1	B	359	ASP	3.3
1	B	662	ALA	3.1
1	A	444	GLU	3.1
1	B	301	GLU	3.1
1	B	91	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	517	GLU	3.1
1	B	348	GLU	3.1
1	A	593	THR	3.0
1	B	360	PRO	3.0
1	A	665	GLU	3.0
1	A	457	ASP	3.0
1	A	362	GLU	3.0
1	B	69	GLU	3.0
1	A	41	ARG	2.9
1	A	390	GLU	2.9
1	A	514	ILE	2.9
1	B	727	ARG	2.9
1	A	42	ASP	2.9
1	B	440	LEU	2.8
1	B	379	PRO	2.8
1	A	662	ALA	2.8
1	A	129	LEU	2.8
1	A	95	TRP	2.8
1	B	347	SER	2.8
1	B	94	ALA	2.8
1	B	332	GLU	2.7
1	B	42	ASP	2.7
1	B	706	ASP	2.7
1	A	688	ILE	2.7
1	B	558	GLU	2.7
1	B	351	LYS	2.7
1	A	272	GLU	2.7
1	B	362	GLU	2.6
1	A	369	LEU	2.6
1	B	523	SER	2.6
1	A	520	ASP	2.5
1	B	341	TRP	2.5
1	B	457	ASP	2.5
1	B	436	ALA	2.5
1	B	21	LYS	2.5
1	B	41	ARG	2.5
1	A	451	GLU	2.5
1	B	255	ILE	2.5
1	A	674	ASP	2.5
1	A	24	GLN	2.5
1	A	94	ALA	2.4
1	B	455	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	154	ILE	2.4
1	B	129	LEU	2.4
1	A	727	ARG	2.4
1	B	444	GLU	2.4
1	A	592	ILE	2.3
1	A	54	GLU	2.3
1	A	271	GLU	2.3
1	B	97	SER	2.3
1	B	51	ASP	2.3
1	A	468	TRP	2.3
1	B	505	GLU	2.3
1	B	93	MET	2.3
1	A	439	ASP	2.3
1	B	524	ASP	2.3
1	A	293	LYS	2.3
1	B	201	GLU	2.3
1	B	25	ASP	2.3
1	B	664	SER	2.2
1	A	255	ILE	2.2
1	A	577	LEU	2.2
1	A	176	GLU	2.2
1	A	301	GLU	2.2
1	A	454	LEU	2.2
1	A	34	GLU	2.2
1	B	24	GLN	2.1
1	A	409	LEU	2.1
1	B	667	ARG	2.1
1	B	639	GLU	2.1
1	A	639	GLU	2.1
1	B	206	GLN	2.1
1	B	554	GLU	2.1
1	B	600	LEU	2.1
1	B	666	HIS	2.1
1	B	468	TRP	2.1
1	B	154	ILE	2.1
1	A	666	HIS	2.0
1	A	351	LYS	2.0
1	B	46	VAL	2.0
1	A	638	ASP	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 monosaccharides in this entry.
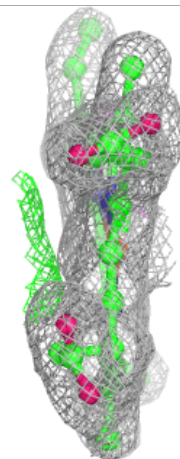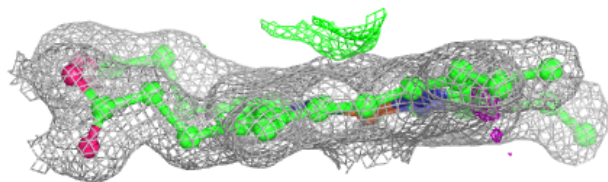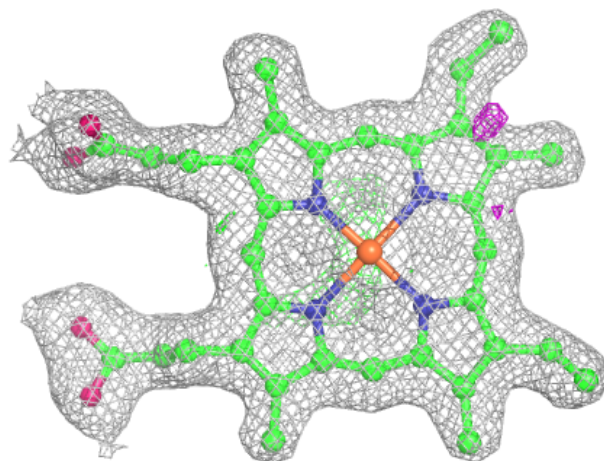
6.4 Ligands ⓘ

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, 95th 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.
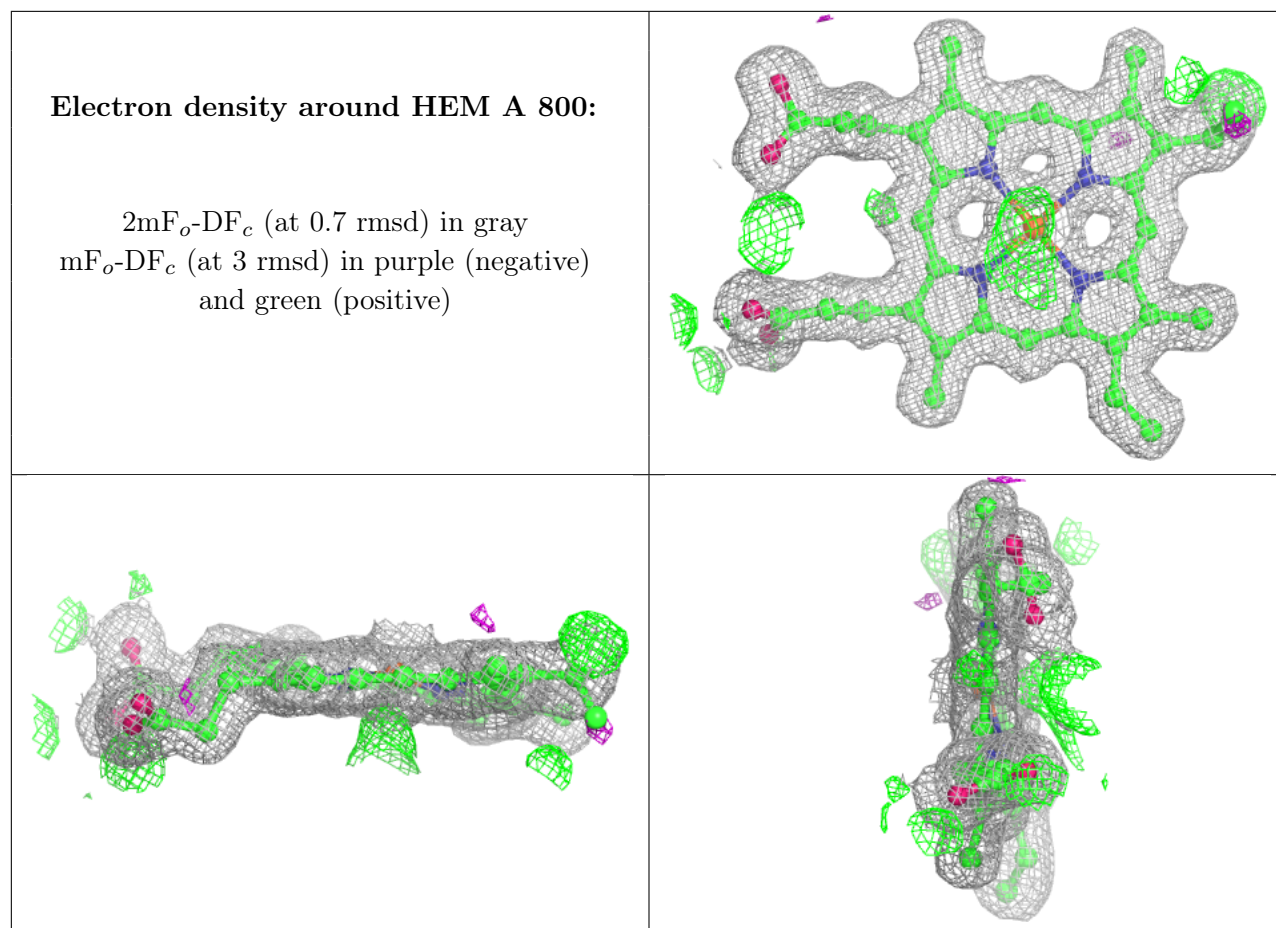
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	B	800	43/43	0.97	0.16	23,27,29,30	0
2	HEM	A	800	43/43	0.98	0.13	15,19,23,32	0

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 B 800:

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

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 ⓘ

There are no such residues in this entry.