



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:32 PM UTC

PDB ID : 3VLK / pdb_00003vlk
Title : Crystal Structure Analysis of the Ser305Ala variant of KatG from *Haloarcula marismortui*
Authors : Sato, T.; Higuchi, W.; Yoshimatsu, K.; Fujiwara, T.
Deposited on : 2011-12-01
Resolution : 2.00 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

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>.

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

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

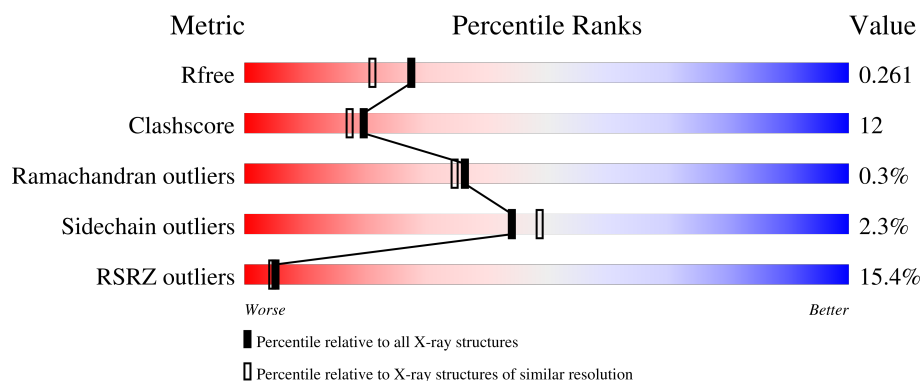
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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	17% 74% 21% ..
1	B	737	13% 79% 18% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11488 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.

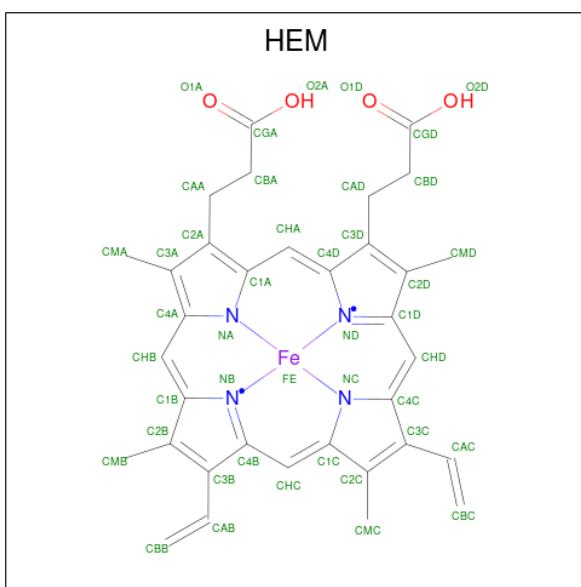
- Molecule 1 is a protein called Catalase-peroxidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	714	Total	C	N	O	S	0	0	0
			5619	3512	945	1143	19			
1	B	714	Total	C	N	O	S	0	0	0
			5619	3512	945	1143	19			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	305	ALA	SER	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	305	ALA	SER	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 (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

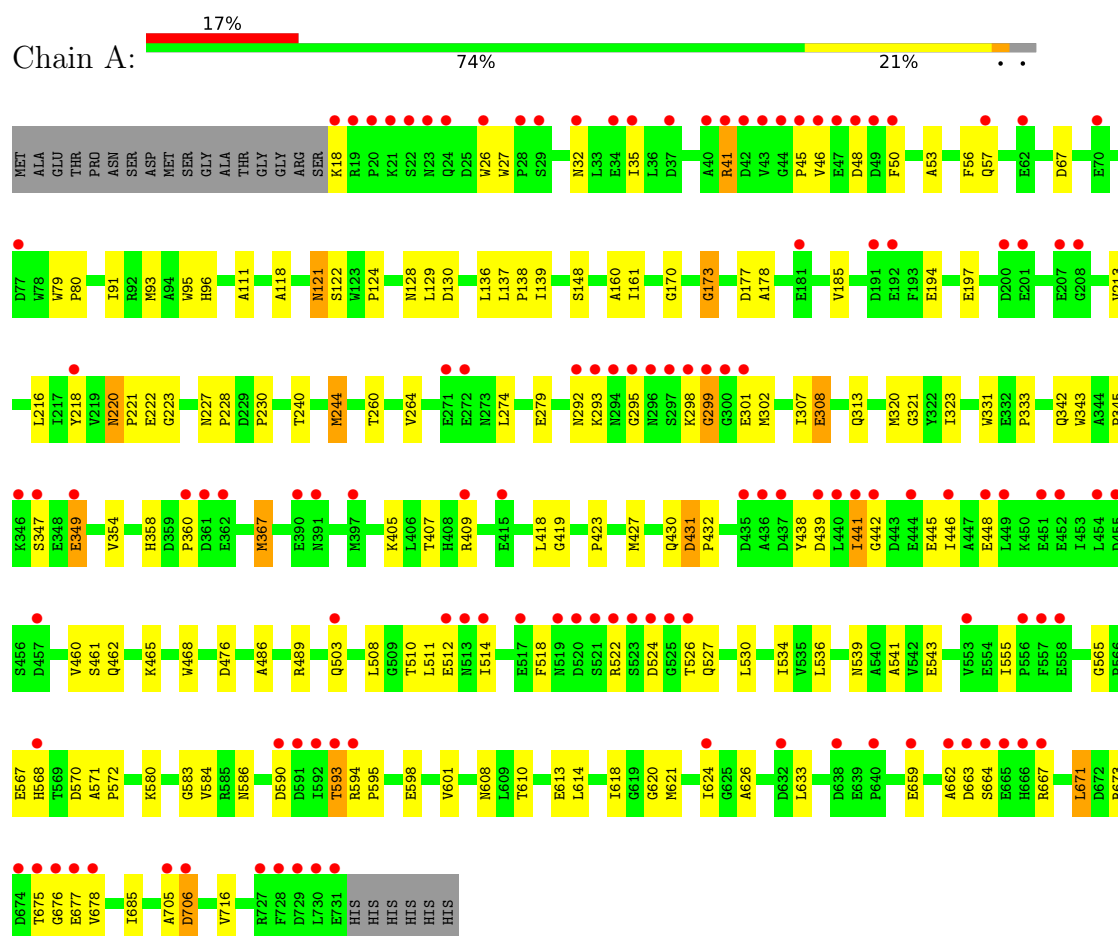
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	162	Total O 162 162	0	0
3	B	2	Total O 2 2	0	0

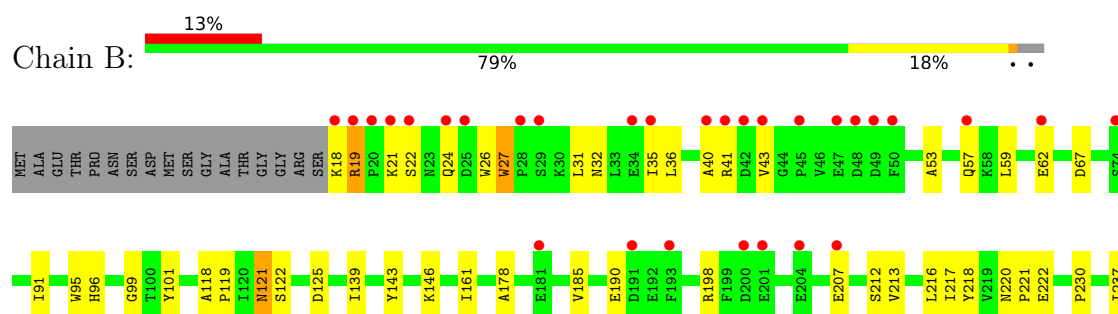
3 Residue-property plots [i](#)

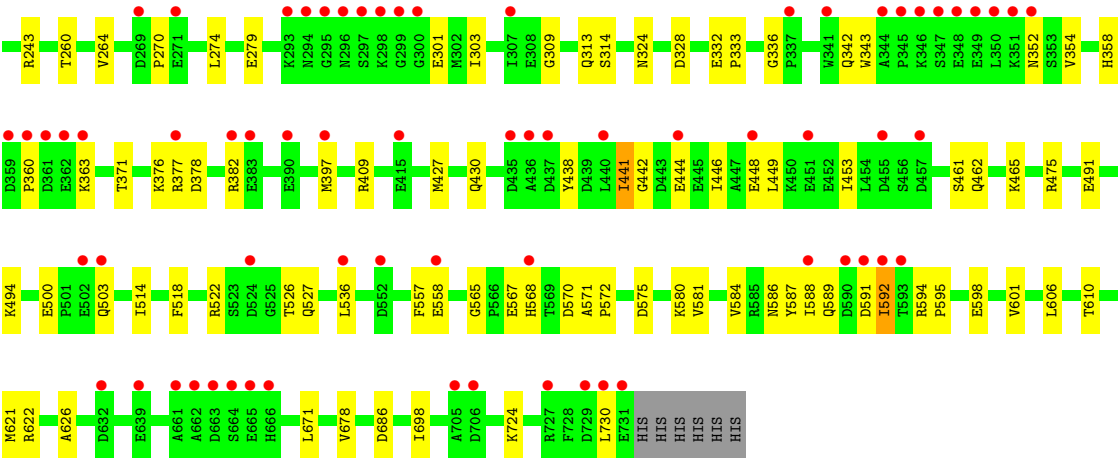
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 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, α , β , γ	321.24Å 76.67Å 74.71Å 90.00° 99.54° 90.00°	Depositor
Resolution (Å)	49.97 – 2.00 49.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.97-2.00) 99.4 (49.97-2.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.54 (at 1.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.242 , 0.270 0.233 , 0.261	Depositor DCC
R_{free} test set	8123 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.807	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11488	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.42	1/5755 (0.0%)	0.90	15/7819 (0.2%)
1	B	0.38	0/5755	0.87	13/7819 (0.2%)
All	All	0.40	1/11510 (0.0%)	0.88	28/15638 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	367	MET	SD-CE	-6.39	1.63	1.79

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	THR	N-CA-C	-7.54	103.35	112.54
1	B	260	THR	N-CA-C	-7.34	103.78	112.89
1	A	129	LEU	N-CA-C	-7.05	104.65	113.18
1	A	308	GLU	N-CA-C	6.40	119.57	108.76
1	B	99	GLY	N-CA-C	6.12	121.40	114.67
1	B	27	TRP	CA-C-N	5.85	126.25	119.47
1	B	27	TRP	C-N-CA	5.85	126.25	119.47
1	B	314	SER	CA-C-N	5.81	125.48	119.56
1	B	314	SER	C-N-CA	5.81	125.48	119.56
1	A	178	ALA	N-CA-C	-5.81	102.17	110.59
1	A	580	LYS	N-CA-C	-5.70	106.49	113.50
1	A	407	THR	N-CA-C	5.59	119.94	113.18
1	A	79	TRP	CA-C-N	5.56	125.88	119.93
1	A	79	TRP	C-N-CA	5.56	125.88	119.93
1	A	185	VAL	N-CA-C	5.54	116.23	109.30
1	B	378	ASP	CA-C-N	5.51	124.97	119.24
1	B	378	ASP	C-N-CA	5.51	124.97	119.24
1	B	580	LYS	N-CA-C	-5.51	106.72	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	ALA	N-CA-C	5.49	118.77	111.75
1	A	173	GLY	N-CA-C	-5.28	104.24	112.58
1	B	185	VAL	N-CA-C	5.15	115.69	108.89
1	A	431	ASP	CA-C-N	5.15	125.14	119.89
1	A	431	ASP	C-N-CA	5.15	125.14	119.89
1	A	321	GLY	N-CA-C	5.12	119.08	112.83
1	B	178	ALA	N-CA-C	-5.11	102.90	110.46
1	B	500	GLU	CA-C-N	5.06	126.16	119.84
1	B	500	GLU	C-N-CA	5.06	126.16	119.84
1	A	197	GLU	N-CA-C	-5.01	104.35	110.61

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	5619	0	5265	145	0
1	B	5619	0	5265	119	0
2	A	43	0	30	1	0
2	B	43	0	30	0	0
3	A	162	0	0	2	0
3	B	2	0	0	0	0
All	All	11488	0	10590	252	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 12.

All (252) 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	1.03	1.65
1:B:95:TRP:CH2	1:B:218:TYR:HE1	1.11	1.65
1:B:95:TRP:HH2	1:B:218:TYR:CE1	1.13	1.62
1:A:95:TRP:HH2	1:A:218:TYR:CE1	0.99	1.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:TYR:CE2	1:A:244:MET:SD	2.16	1.38
1:A:218:TYR:HE2	1:A:244:MET:SD	1.50	1.33
1:A:95:TRP:CH2	1:A:218:TYR:CE1	1.88	1.29
1:B:95:TRP:CH2	1:B:218:TYR:CE1	1.98	1.15
1:A:584:VAL:HG13	1:A:621:MET:HG2	1.44	1.00
1:B:584:VAL:HG13	1:B:621:MET:HG2	1.46	0.95
1:A:218:TYR:HE2	1:A:244:MET:CG	1.82	0.93
1:A:95:TRP:HH2	1:A:218:TYR:CD1	1.86	0.90
1:A:35:ILE:HD11	1:A:601:VAL:HG12	1.54	0.89
1:A:95:TRP:CZ3	1:A:218:TYR:HE1	1.89	0.89
1:A:298:LYS:CE	1:A:301:GLU:HB2	2.06	0.85
1:A:298:LYS:HE3	1:A:301:GLU:HB2	1.61	0.82
1:A:441:ILE:HD13	1:A:441:ILE:H	1.43	0.82
1:B:427:MET:H	1:B:430:GLN:HE21	1.25	0.82
1:A:95:TRP:CH2	1:A:218:TYR:CD1	2.64	0.81
1:B:35:ILE:HD11	1:B:601:VAL:HG12	1.62	0.81
1:B:567:GLU:HG2	1:B:568:HIS:ND1	1.99	0.78
1:A:427:MET:H	1:A:430:GLN:HE21	1.31	0.78
1:A:313:GLN:HA	1:A:354:VAL:HG22	1.64	0.77
1:A:45:PRO:HD3	1:B:698:ILE:HD12	1.68	0.75
1:A:218:TYR:CZ	1:A:244:MET:SD	2.80	0.74
1:A:298:LYS:CD	1:A:301:GLU:HB2	2.19	0.72
1:B:462:GLN:HE21	1:B:503:GLN:NE2	1.88	0.72
1:A:121:ASN:HD22	1:A:122:SER:N	1.87	0.71
1:B:95:TRP:CH2	1:B:218:TYR:CD1	2.76	0.70
1:B:441:ILE:HD13	1:B:441:ILE:H	1.56	0.69
1:B:427:MET:H	1:B:430:GLN:NE2	1.90	0.69
1:B:121:ASN:HD22	1:B:122:SER:N	1.91	0.69
1:B:270:PRO:HA	1:B:274:LEU:HD13	1.73	0.69
1:A:67:ASP:HB3	1:A:139:ILE:HD11	1.75	0.69
1:A:80:PRO:HD2	1:A:298:LYS:O	1.92	0.68
1:B:313:GLN:HA	1:B:354:VAL:HG22	1.76	0.68
1:A:671:LEU:HD22	1:A:678:VAL:HG12	1.75	0.68
1:B:274:LEU:HD11	1:B:303:ILE:HB	1.76	0.67
1:B:444:GLU:O	1:B:448:GLU:HG3	1.94	0.67
1:A:298:LYS:HG3	1:A:299:GLY:H	1.59	0.67
1:A:91:ILE:HD11	1:A:160:ALA:HB3	1.77	0.67
1:A:220:ASN:HD22	1:A:220:ASN:C	2.03	0.67
1:A:427:MET:H	1:A:430:GLN:NE2	1.92	0.66
1:A:53:ALA:O	1:A:57:GLN:HG2	1.96	0.66
1:A:18:LYS:HB2	1:B:594:ARG:HD3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:PRO:HG2	1:A:194:GLU:HG3	1.77	0.66
1:A:664:SER:HB3	1:A:667:ARG:HB3	1.78	0.65
1:B:91:ILE:CD1	1:B:161:ILE:HG12	2.27	0.65
1:A:442:GLY:O	1:A:446:ILE:HG12	1.98	0.64
1:A:220:ASN:ND2	1:A:222:GLU:H	1.95	0.64
1:A:567:GLU:HG2	1:A:568:HIS:ND1	2.12	0.64
1:B:462:GLN:NE2	1:B:503:GLN:HE22	1.96	0.64
1:B:143:TYR:O	1:B:146:LYS:HE3	1.98	0.63
1:B:462:GLN:HE21	1:B:503:GLN:HE22	1.43	0.63
1:A:118:ALA:HB2	1:A:279:GLU:CD	2.23	0.63
1:A:431:ASP:N	1:A:432:PRO:HD3	2.13	0.63
1:A:308:GLU:H	1:A:342:GLN:HE22	1.46	0.63
1:A:530:LEU:O	1:A:534:ILE:HG12	2.00	0.62
1:B:41:ARG:HG3	1:B:41:ARG:HH11	1.65	0.62
1:A:445:GLU:OE2	1:A:526:THR:HG21	2.00	0.61
1:A:298:LYS:HG3	1:A:299:GLY:N	2.15	0.61
1:A:298:LYS:HD2	1:A:301:GLU:HB2	1.82	0.61
1:A:595:PRO:HD2	1:A:598:GLU:OE1	2.00	0.61
1:A:441:ILE:HB	1:A:445:GLU:HB2	1.83	0.61
1:A:539:ASN:O	1:A:543:GLU:HG3	2.02	0.60
1:B:589:GLN:HG2	1:B:591:ASP:OD1	2.01	0.59
1:B:19:ARG:HD3	1:B:19:ARG:N	2.16	0.59
1:B:333:PRO:HG3	1:B:343:TRP:CH2	2.38	0.59
1:A:583:GLY:HA2	1:A:685:ILE:HD13	1.84	0.59
1:A:41:ARG:HH21	1:B:41:ARG:HE	1.49	0.58
1:A:595:PRO:HB2	1:A:598:GLU:HG3	1.85	0.58
1:B:475:ARG:HB2	1:B:606:LEU:HD22	1.84	0.58
1:B:35:ILE:CD1	1:B:601:VAL:HG12	2.32	0.58
1:A:565:GLY:H	1:A:568:HIS:CE1	2.22	0.57
1:B:536:LEU:HG	1:B:557:PHE:CE1	2.39	0.57
1:A:95:TRP:CZ3	1:A:218:TYR:CE1	2.76	0.57
1:B:565:GLY:H	1:B:568:HIS:CE1	2.23	0.57
1:A:503:GLN:HB2	3:A:889:HOH:O	2.05	0.57
1:A:518:PHE:O	1:A:522:ARG:HG2	2.05	0.56
1:A:45:PRO:HD3	1:B:698:ILE:CD1	2.35	0.56
1:B:571:ALA:HB3	1:B:572:PRO:HD3	1.87	0.56
1:B:31:LEU:HG	1:B:601:VAL:HG21	1.86	0.56
1:A:218:TYR:CE2	1:A:244:MET:CG	2.74	0.56
1:A:41:ARG:HE	1:B:41:ARG:HD3	1.71	0.56
1:A:570:ASP:OD1	1:A:572:PRO:HD2	2.04	0.56
1:A:594:ARG:HD3	1:B:18:LYS:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ASN:C	1:B:220:ASN:HD22	2.12	0.56
1:A:218:TYR:HE2	1:A:244:MET:HG3	1.68	0.56
1:A:462:GLN:HE21	1:A:503:GLN:HE22	1.54	0.56
1:B:91:ILE:HD11	1:B:161:ILE:HG12	1.88	0.56
1:A:128:ASN:HA	1:A:130:ASP:OD2	2.06	0.56
1:B:198:ARG:HD2	1:B:212:SER:C	2.32	0.55
1:A:41:ARG:HG3	1:B:41:ARG:HB3	1.87	0.55
1:A:593:THR:HG23	1:A:594:ARG:H	1.71	0.55
1:A:91:ILE:CD1	1:A:161:ILE:HG13	2.37	0.55
1:A:41:ARG:HG2	1:B:40:ALA:O	2.07	0.55
1:B:453:ILE:HD13	1:B:514:ILE:HD13	1.89	0.54
1:A:298:LYS:HE3	1:A:301:GLU:CB	2.34	0.54
1:A:298:LYS:CG	1:A:299:GLY:H	2.19	0.54
1:B:95:TRP:CZ2	1:B:218:TYR:CE1	2.86	0.53
1:A:441:ILE:HD13	1:A:441:ILE:N	2.20	0.53
1:A:445:GLU:HG2	1:A:518:PHE:HZ	1.74	0.53
1:A:91:ILE:CD1	1:A:160:ALA:HB3	2.38	0.53
1:A:170:GLY:HA3	1:A:423:PRO:HG3	1.89	0.53
1:A:220:ASN:HD22	1:A:221:PRO:N	2.07	0.53
1:B:220:ASN:ND2	1:B:222:GLU:H	2.06	0.53
1:A:610:THR:OG1	1:A:613:GLU:HG3	2.09	0.53
1:A:333:PRO:HD3	1:A:343:TRP:CZ3	2.44	0.53
1:B:220:ASN:HD22	1:B:221:PRO:N	2.07	0.53
1:A:571:ALA:HB3	1:A:572:PRO:HD3	1.90	0.52
1:B:53:ALA:O	1:B:57:GLN:HG2	2.10	0.52
1:B:352:ASN:HD22	1:B:363:LYS:HB2	1.74	0.52
1:B:592:ILE:HD13	1:B:592:ILE:N	2.24	0.52
1:A:633:LEU:HD21	1:A:667:ARG:NH2	2.25	0.52
1:A:409:ARG:HD3	1:A:409:ARG:O	2.09	0.52
1:B:438:TYR:CG	1:B:527:GLN:HB2	2.44	0.52
1:B:449:LEU:O	1:B:453:ILE:HG12	2.09	0.52
1:A:218:TYR:CE2	1:A:244:MET:HG3	2.44	0.52
1:A:41:ARG:CG	1:B:41:ARG:HB3	2.40	0.52
1:A:67:ASP:HB3	1:A:139:ILE:CD1	2.40	0.52
1:A:93:MET:HE1	1:A:136:LEU:HD11	1.92	0.52
1:B:35:ILE:HG13	1:B:36:LEU:N	2.25	0.52
1:B:125:ASP:OD2	1:B:217:ILE:HG12	2.10	0.51
1:B:91:ILE:HD12	1:B:161:ILE:HG12	1.92	0.51
1:A:220:ASN:HD22	1:A:222:GLU:H	1.57	0.51
1:B:592:ILE:HD13	1:B:592:ILE:H	1.75	0.51
1:A:298:LYS:O	1:A:302:MET:HE3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:LYS:HG2	1:B:626:ALA:HB1	1.93	0.51
1:A:320:MET:HE1	1:A:323:ILE:HD12	1.92	0.51
1:A:292:ASN:HB3	1:A:295:GLY:CA	2.40	0.51
1:A:41:ARG:HH21	1:B:41:ARG:NE	2.08	0.50
1:A:358:HIS:O	1:A:360:PRO:HD3	2.11	0.50
1:B:522:ARG:HD2	1:B:522:ARG:N	2.25	0.50
1:A:95:TRP:CD1	1:A:96:HIS:HD2	2.31	0.49
1:A:405:LYS:O	1:A:409:ARG:HB2	2.13	0.49
1:B:491:GLU:HG2	1:B:494:LYS:HE2	1.94	0.49
1:A:26:TRP:HB2	1:A:27:TRP:CE3	2.48	0.49
1:A:299:GLY:CA	1:A:358:HIS:CD2	2.95	0.49
1:A:32:ASN:ND2	1:A:35:ILE:HG23	2.28	0.49
1:B:21:LYS:HD3	1:B:26:TRP:CE2	2.48	0.49
1:B:237:ILE:HD11	1:B:371:THR:HG22	1.95	0.49
1:A:438:TYR:CG	1:A:527:GLN:HB2	2.48	0.48
1:A:705:ALA:O	1:A:706:ASP:HB3	2.13	0.48
1:B:446:ILE:HD12	1:B:536:LEU:HD11	1.94	0.48
1:B:558:GLU:HG2	1:B:724:LYS:HE3	1.95	0.48
1:A:121:ASN:C	1:A:121:ASN:ND2	2.71	0.48
1:A:508:LEU:O	1:A:512:GLU:HG3	2.14	0.48
1:B:121:ASN:HD22	1:B:121:ASN:C	2.21	0.48
1:B:336:GLY:HA3	1:B:342:GLN:NE2	2.29	0.48
1:A:46:VAL:HG11	1:A:50:PHE:CD2	2.48	0.48
1:A:441:ILE:H	1:A:441:ILE:CD1	2.17	0.48
1:A:91:ILE:HD11	1:A:161:ILE:HG13	1.95	0.48
1:A:121:ASN:ND2	1:A:122:SER:N	2.59	0.48
1:B:441:ILE:H	1:B:441:ILE:CD1	2.25	0.48
1:B:587:TYR:O	1:B:588:ILE:HD13	2.14	0.48
1:A:213:VAL:HB	1:A:216:LEU:HD12	1.95	0.47
1:B:324:ASN:O	1:B:328:ASP:HB2	2.15	0.47
1:B:382:ARG:HG2	1:B:382:ARG:HH11	1.79	0.47
1:A:331:TRP:CZ3	1:A:345:PRO:HD3	2.50	0.47
1:A:486:ALA:O	1:A:489:ARG:HG2	2.13	0.47
1:A:95:TRP:CZ2	1:A:218:TYR:CD1	3.03	0.47
1:A:298:LYS:HG2	1:A:301:GLU:C	2.40	0.47
1:A:510:THR:O	1:A:514:ILE:HG12	2.15	0.47
1:B:230:PRO:HB2	1:B:377:ARG:HG3	1.96	0.47
1:B:121:ASN:C	1:B:121:ASN:ND2	2.73	0.47
1:A:462:GLN:HE21	1:A:503:GLN:NE2	2.12	0.47
1:A:460:VAL:HG13	1:A:541:ALA:HB1	1.97	0.46
1:A:419:GLY:HA3	3:A:750:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:LYS:HG2	1:A:626:ALA:HB1	1.98	0.46
1:B:62:GLU:OE2	1:B:62:GLU:HA	2.14	0.46
1:B:22:SER:HB3	1:B:24:GLN:HG2	1.98	0.46
1:A:461:SER:O	1:A:465:LYS:HG3	2.15	0.46
1:A:80:PRO:HB2	1:A:358:HIS:CE1	2.51	0.46
1:B:101:TYR:CE2	1:B:409:ARG:HD2	2.51	0.46
1:A:445:GLU:HA	1:A:448:GLU:HB2	1.98	0.46
1:A:121:ASN:HD22	1:A:121:ASN:C	2.21	0.45
1:A:56:PHE:CZ	1:A:173:GLY:HA3	2.51	0.45
1:A:555:ILE:HG12	1:A:716:VAL:HG13	1.96	0.45
1:A:511:LEU:HD13	1:A:534:ILE:HD13	1.97	0.45
1:B:301:GLU:O	1:B:303:ILE:HG13	2.17	0.45
1:B:453:ILE:HD13	1:B:514:ILE:CD1	2.46	0.45
1:A:18:LYS:HD2	1:B:594:ARG:HD3	1.98	0.45
1:A:673:ARG:C	1:A:675:THR:H	2.25	0.45
1:B:536:LEU:HG	1:B:557:PHE:CD1	2.52	0.45
1:B:376:LYS:O	1:B:382:ARG:HD3	2.16	0.45
1:A:347:SER:HB2	1:A:349:GLU:OE1	2.16	0.45
1:B:67:ASP:HB3	1:B:139:ILE:HD12	1.98	0.45
1:B:518:PHE:O	1:B:522:ARG:CD	2.65	0.45
1:B:442:GLY:O	1:B:446:ILE:HG12	2.17	0.44
1:A:223:GLY:HA3	1:A:227:ASN:O	2.17	0.44
1:B:95:TRP:CZ2	1:B:218:TYR:CD1	3.05	0.44
1:B:352:ASN:ND2	1:B:363:LYS:HB2	2.32	0.44
1:B:441:ILE:HD13	1:B:441:ILE:N	2.26	0.44
1:B:190:GLU:H	1:B:190:GLU:CD	2.24	0.44
1:B:592:ILE:H	1:B:592:ILE:CD1	2.31	0.44
1:A:148:SER:HB2	1:A:177:ASP:CG	2.43	0.44
1:B:41:ARG:HG3	1:B:41:ARG:NH1	2.27	0.44
1:A:292:ASN:HB3	1:A:295:GLY:HA3	2.00	0.44
1:A:299:GLY:C	1:A:301:GLU:H	2.25	0.44
1:B:40:ALA:HB2	1:B:610:THR:CG2	2.48	0.44
1:B:264:VAL:HG22	1:B:309:GLY:O	2.17	0.44
1:B:518:PHE:O	1:B:522:ARG:HD3	2.18	0.44
1:B:526:THR:HG22	1:B:527:GLN:N	2.32	0.44
1:B:567:GLU:HG2	1:B:568:HIS:N	2.33	0.43
1:A:664:SER:CB	1:A:667:ARG:HB3	2.48	0.43
1:B:438:TYR:CD1	1:B:527:GLN:HB2	2.53	0.43
1:A:220:ASN:C	1:A:220:ASN:ND2	2.75	0.43
1:A:476:ASP:CG	1:A:608:ASN:HD21	2.27	0.43
1:B:461:SER:O	1:B:465:LYS:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:GLU:HA	1:B:243:ARG:NH2	2.34	0.43
1:B:570:ASP:OD1	1:B:572:PRO:HD2	2.18	0.43
1:A:264:VAL:HG12	2:A:800:HEM:CAA	2.48	0.42
1:A:41:ARG:NE	1:B:41:ARG:HD3	2.33	0.42
1:A:614:LEU:O	1:A:618:ILE:HG12	2.19	0.42
1:A:299:GLY:HA3	1:A:358:HIS:CD2	2.54	0.42
1:A:468:TRP:CZ2	1:A:584:VAL:HG21	2.54	0.42
1:B:26:TRP:HB2	1:B:27:TRP:CE3	2.54	0.42
1:B:121:ASN:ND2	1:B:122:SER:N	2.64	0.42
1:B:581:VAL:HG13	1:B:588:ILE:CD1	2.49	0.42
1:B:595:PRO:HD2	1:B:598:GLU:CD	2.44	0.42
1:B:213:VAL:HB	1:B:216:LEU:HD12	2.02	0.42
1:B:382:ARG:HG2	1:B:382:ARG:NH1	2.34	0.42
1:B:589:GLN:O	1:B:592:ILE:HD12	2.20	0.42
1:B:671:LEU:HD22	1:B:678:VAL:HG22	2.00	0.42
1:A:228:PRO:O	1:A:230:PRO:HD3	2.20	0.42
1:A:240:THR:O	1:A:244:MET:HG3	2.19	0.42
1:A:620:GLY:O	1:A:624:ILE:HG12	2.20	0.42
1:B:118:ALA:HB2	1:B:279:GLU:HG3	2.00	0.42
1:B:220:ASN:HD22	1:B:221:PRO:CD	2.33	0.42
1:B:358:HIS:O	1:B:360:PRO:HD3	2.19	0.42
1:A:567:GLU:HG2	1:A:568:HIS:N	2.34	0.41
1:B:41:ARG:NH1	1:B:43:VAL:HG13	2.35	0.41
1:B:332:GLU:HA	1:B:333:PRO:HD3	1.90	0.41
1:B:95:TRP:CD1	1:B:96:HIS:HD2	2.38	0.41
1:B:59:LEU:HD13	1:B:146:LYS:HB3	2.01	0.41
1:A:307:ILE:HG23	1:A:342:GLN:HB3	2.02	0.41
1:A:439:ASP:HB2	1:A:526:THR:HA	2.02	0.41
1:B:32:ASN:O	1:B:35:ILE:HG23	2.21	0.41
1:B:125:ASP:HB2	1:B:216:LEU:HA	2.03	0.41
1:A:673:ARG:C	1:A:675:THR:N	2.78	0.41
1:A:137:LEU:HB3	1:A:138:PRO:HD3	2.03	0.41
1:A:593:THR:HG23	1:A:594:ARG:N	2.36	0.41
1:A:662:ALA:O	1:A:663:ASP:HB2	2.20	0.41
1:A:41:ARG:HD2	1:A:41:ARG:C	2.47	0.40
1:A:343:TRP:CD1	1:A:343:TRP:N	2.88	0.40
1:A:91:ILE:HD12	1:A:161:ILE:HG13	2.02	0.40
1:A:298:LYS:CG	1:A:301:GLU:C	2.95	0.40
1:B:622:ARG:NE	1:B:686:ASP:OD1	2.46	0.40
1:B:67:ASP:HB3	1:B:139:ILE:CD1	2.51	0.40
1:B:671:LEU:CD2	1:B:678:VAL:HG22	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ASN:HD22	1:A:122:SER:H	1.67	0.40
1:B:220:ASN:C	1:B:220:ASN:ND2	2.80	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	712/737 (97%)	677 (95%)	31 (4%)	4 (1%)	21	17
1	B	712/737 (97%)	683 (96%)	29 (4%)	0	100	100
All	All	1424/1474 (97%)	1360 (96%)	60 (4%)	4 (0%)	36	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	706	ASP
1	A	524	ASP
1	A	299	GLY
1	A	676	GLY

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	589/607 (97%)	571 (97%)	18 (3%)	35	37
1	B	589/607 (97%)	580 (98%)	9 (2%)	57	64
All	All	1178/1214 (97%)	1151 (98%)	27 (2%)	44	49

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	48	ASP
1	A	121	ASN
1	A	220	ASN
1	A	244	MET
1	A	274	LEU
1	A	293	LYS
1	A	349	GLU
1	A	367	MET
1	A	418	LEU
1	A	441	ILE
1	A	536	LEU
1	A	586	ASN
1	A	590	ASP
1	A	593	THR
1	A	659	GLU
1	A	671	LEU
1	A	677	GLU
1	B	19	ARG
1	B	119	PRO
1	B	121	ASN
1	B	397	MET
1	B	441	ILE
1	B	575	ASP
1	B	586	ASN
1	B	592	ILE
1	B	730	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	121	ASN
1	A	206	GLN
1	A	220	ASN
1	A	285	GLN
1	A	286	GLN
1	A	324	ASN
1	A	342	GLN
1	A	352	ASN
1	A	389	GLN
1	A	430	GLN
1	A	493	GLN
1	A	503	GLN
1	A	515	GLN
1	A	527	GLN
1	A	586	ASN
1	A	589	GLN
1	A	608	ASN
1	A	666	HIS
1	B	24	GLN
1	B	32	ASN
1	B	121	ASN
1	B	145	GLN
1	B	220	ASN
1	B	286	GLN
1	B	324	ASN
1	B	342	GLN
1	B	352	ASN
1	B	389	GLN
1	B	398	ASN
1	B	430	GLN
1	B	495	ASN
1	B	503	GLN
1	B	515	GLN
1	B	586	ASN
1	B	608	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	800	1	50,50,50	2.63	13 (26%)	67,82,82	5.66	46 (68%)
2	HEM	B	800	1	50,50,50	2.89	11 (22%)	67,82,82	7.29	49 (73%)

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	-	4/14/54/54	-
2	HEM	B	800	1	-	3/14/54/54	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	HEM	FE-NB	9.61	2.24	1.94
2	A	800	HEM	FE-NC	9.43	2.26	1.95
2	B	800	HEM	FE-NC	9.31	2.25	1.95
2	B	800	HEM	FE-NA	7.41	2.19	1.95
2	B	800	HEM	FE-ND	7.15	2.16	1.94
2	A	800	HEM	FE-NA	6.92	2.18	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	HEM	FE-ND	5.96	2.13	1.94
2	A	800	HEM	CBC-CAC	5.44	1.56	1.30
2	B	800	HEM	CBC-CAC	5.20	1.55	1.30
2	B	800	HEM	CBB-CAB	5.18	1.55	1.30
2	A	800	HEM	CBB-CAB	4.84	1.53	1.30
2	A	800	HEM	FE-NB	4.42	2.08	1.94
2	A	800	HEM	CBD-CGD	-4.24	1.40	1.50
2	B	800	HEM	CBA-CGA	-3.86	1.41	1.50
2	B	800	HEM	CBD-CGD	-3.84	1.41	1.50
2	A	800	HEM	CBA-CGA	-3.83	1.41	1.50
2	A	800	HEM	CAC-C3C	2.75	1.54	1.47
2	A	800	HEM	O1A-CGA	2.71	1.31	1.22
2	B	800	HEM	C4D-ND	-2.53	1.35	1.40
2	B	800	HEM	O1A-CGA	2.53	1.30	1.22
2	A	800	HEM	C4D-ND	-2.52	1.35	1.40
2	B	800	HEM	CBD-CAD	2.28	1.59	1.51
2	A	800	HEM	CHC-C1C	-2.15	1.34	1.38
2	A	800	HEM	C4C-NC	-2.05	1.35	1.39

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	HEM	CHD-C1D-ND	-19.49	103.45	124.42
2	B	800	HEM	CHD-C4C-NC	-15.51	107.57	124.45
2	B	800	HEM	CHC-C4B-NB	-15.07	108.20	124.42
2	B	800	HEM	CHD-C4C-C3C	14.35	149.40	125.21
2	B	800	HEM	C4C-CHD-C1D	13.78	155.31	126.02
2	B	800	HEM	CHA-C4D-ND	-13.56	107.60	124.37
2	A	800	HEM	CHC-C4B-NB	-13.29	110.12	124.42
2	A	800	HEM	CHD-C4C-NC	-11.78	111.62	124.45
2	B	800	HEM	CHC-C4B-C3B	11.42	147.86	125.07
2	A	800	HEM	C4C-CHD-C1D	11.26	149.94	126.02
2	B	800	HEM	C1C-CHC-C4B	10.90	149.19	126.02
2	B	800	HEM	C3B-C2B-C1B	-10.75	98.34	106.41
2	A	800	HEM	CHD-C1D-ND	-10.66	112.95	124.42
2	B	800	HEM	C1D-C2D-C3D	-10.54	95.90	106.98
2	B	800	HEM	C4A-CHB-C1B	10.53	151.02	126.25
2	A	800	HEM	C1C-CHC-C4B	10.45	148.23	126.02
2	B	800	HEM	CHB-C1B-NB	-10.37	111.54	124.37
2	A	800	HEM	C1D-C2D-C3D	-9.94	96.52	106.98
2	A	800	HEM	CMD-C2D-C1D	9.90	140.50	125.03
2	B	800	HEM	C4C-C3C-C2C	9.84	115.35	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	HEM	C1A-CHA-C4D	9.76	149.20	126.25
2	A	800	HEM	CHD-C4C-C3C	9.64	141.46	125.21
2	B	800	HEM	C4B-C3B-C2B	9.63	116.13	107.28
2	B	800	HEM	CHB-C4A-NA	-9.49	106.65	123.86
2	B	800	HEM	CHA-C4D-C3D	8.92	141.68	125.23
2	A	800	HEM	CHB-C1B-NB	-8.87	113.40	124.37
2	B	800	HEM	CHA-C1A-C2A	8.61	144.15	125.30
2	A	800	HEM	C4A-CHB-C1B	8.50	146.24	126.25
2	B	800	HEM	C2D-C1D-ND	8.44	119.66	109.90
2	B	800	HEM	CAD-C3D-C4D	-8.37	110.11	124.70
2	A	800	HEM	CHC-C1C-NC	-8.16	115.57	124.45
2	B	800	HEM	C4A-C3A-C2A	-8.14	97.49	106.82
2	B	800	HEM	C3B-C4B-NB	-8.00	103.72	109.47
2	A	800	HEM	CAD-C3D-C4D	-7.90	110.93	124.70
2	A	800	HEM	C4A-C3A-C2A	-7.80	97.89	106.82
2	A	800	HEM	C2A-C1A-NA	-7.68	101.64	110.15
2	B	800	HEM	CHC-C1C-NC	-7.45	116.34	124.45
2	A	800	HEM	C1A-C2A-C3A	7.31	118.17	106.87
2	B	800	HEM	CHD-C1D-C2D	7.17	136.35	125.03
2	A	800	HEM	CHA-C4D-ND	-7.01	115.69	124.37
2	B	800	HEM	CHA-C1A-NA	-7.00	111.17	123.86
2	A	800	HEM	C2D-C1D-ND	6.94	117.93	109.90
2	A	800	HEM	CHA-C1A-C2A	6.69	139.94	125.30
2	B	800	HEM	O2A-CGA-O1A	-6.31	107.10	123.33
2	A	800	HEM	C3B-C4B-NB	6.26	113.96	109.47
2	A	800	HEM	CHA-C4D-C3D	6.23	136.72	125.23
2	B	800	HEM	C1A-C2A-C3A	6.17	116.41	106.87
2	B	800	HEM	O2A-CGA-CBA	5.98	132.89	114.00
2	B	800	HEM	CAA-C2A-C1A	-5.92	113.38	124.94
2	A	800	HEM	CHB-C4A-NA	-5.88	113.20	123.86
2	A	800	HEM	C4D-C3D-C2D	5.87	115.44	106.89
2	A	800	HEM	C2B-C1B-NB	5.87	116.58	109.84
2	A	800	HEM	CHC-C1C-C2C	5.78	137.51	125.49
2	B	800	HEM	CAC-C3C-C4C	-5.63	111.37	124.82
2	B	800	HEM	CHC-C1C-C2C	5.59	137.12	125.49
2	B	800	HEM	C4D-C3D-C2D	5.45	114.83	106.89
2	A	800	HEM	CHC-C4B-C3B	5.42	135.90	125.07
2	A	800	HEM	O2A-CGA-O1A	-5.37	109.51	123.33
2	A	800	HEM	C1B-NB-C4B	-5.31	98.92	105.21
2	A	800	HEM	C1A-CHA-C4D	5.31	138.72	126.25
2	B	800	HEM	C2A-C1A-NA	-5.15	104.44	110.15
2	A	800	HEM	CMC-C2C-C1C	-5.08	115.78	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	HEM	CAA-CBA-CGA	-5.07	100.23	113.67
2	A	800	HEM	C4C-C3C-C2C	4.91	111.07	106.81
2	A	800	HEM	CMA-C3A-C2A	4.72	135.63	125.62
2	B	800	HEM	C4C-NC-C1C	4.57	113.28	105.82
2	A	800	HEM	CAC-C3C-C4C	-4.53	114.00	124.82
2	B	800	HEM	CMD-C2D-C1D	4.49	132.05	125.03
2	B	800	HEM	C2B-C1B-NB	4.46	114.97	109.84
2	B	800	HEM	CAA-CBA-CGA	-4.28	102.31	113.67
2	A	800	HEM	CMC-C2C-C3C	4.17	138.53	128.43
2	B	800	HEM	CMA-C3A-C2A	4.16	134.44	125.62
2	A	800	HEM	O2A-CGA-CBA	4.08	126.90	114.00
2	B	800	HEM	CAD-C3D-C2D	3.84	135.06	127.87
2	A	800	HEM	CAA-C2A-C1A	-3.81	117.50	124.94
2	A	800	HEM	C3D-C4D-ND	-3.54	106.28	110.17
2	B	800	HEM	CHB-C4A-C3A	3.44	137.41	127.43
2	B	800	HEM	C3A-C4A-NA	3.21	115.28	110.14
2	A	800	HEM	CHA-C1A-NA	-3.19	118.07	123.86
2	B	800	HEM	C4D-ND-C1D	-3.05	101.60	105.21
2	A	800	HEM	O2D-CGD-O1D	-2.96	115.73	123.33
2	B	800	HEM	CBD-CAD-C3D	2.82	120.32	112.53
2	A	800	HEM	CBC-CAC-C3C	-2.75	113.76	127.53
2	A	800	HEM	C4C-NC-C1C	2.61	110.08	105.82
2	A	800	HEM	CHD-C1D-C2D	2.58	129.10	125.03
2	A	800	HEM	C3B-C2B-C1B	-2.57	104.48	106.41
2	B	800	HEM	C3C-C2C-C1C	-2.56	104.62	107.05
2	B	800	HEM	CAB-C3B-C4B	-2.54	113.16	124.39
2	B	800	HEM	CMC-C2C-C3C	2.50	134.48	128.43
2	A	800	HEM	C4A-NA-C1A	2.45	109.82	105.82
2	A	800	HEM	CAD-C3D-C2D	2.40	132.35	127.87
2	B	800	HEM	C2C-C1C-NC	-2.30	105.38	109.64
2	A	800	HEM	CHB-C4A-C3A	2.26	133.99	127.43
2	B	800	HEM	CMC-C2C-C1C	-2.18	120.90	124.73
2	B	800	HEM	CMD-C2D-C3D	2.17	132.01	126.15

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	800	HEM	C2C-C3C-CAC-CBC
2	A	800	HEM	C2B-C3B-CAB-CBB
2	A	800	HEM	C2C-C3C-CAC-CBC
2	B	800	HEM	CAA-CBA-CGA-O1A

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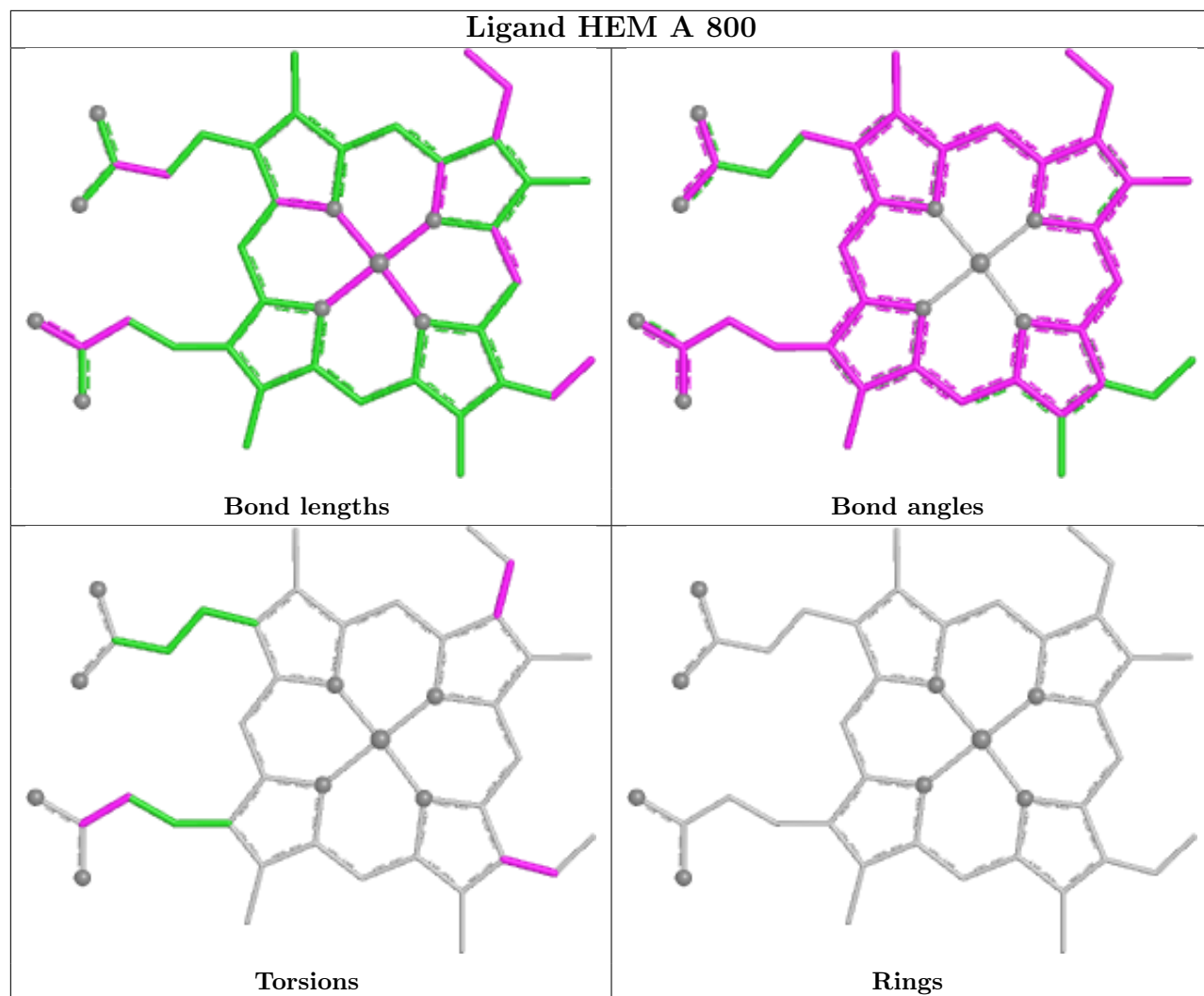
Mol	Chain	Res	Type	Atoms
2	A	800	HEM	CAA-CBA-CGA-O2A
2	A	800	HEM	CAA-CBA-CGA-O1A
2	B	800	HEM	CAA-CBA-CGA-O2A

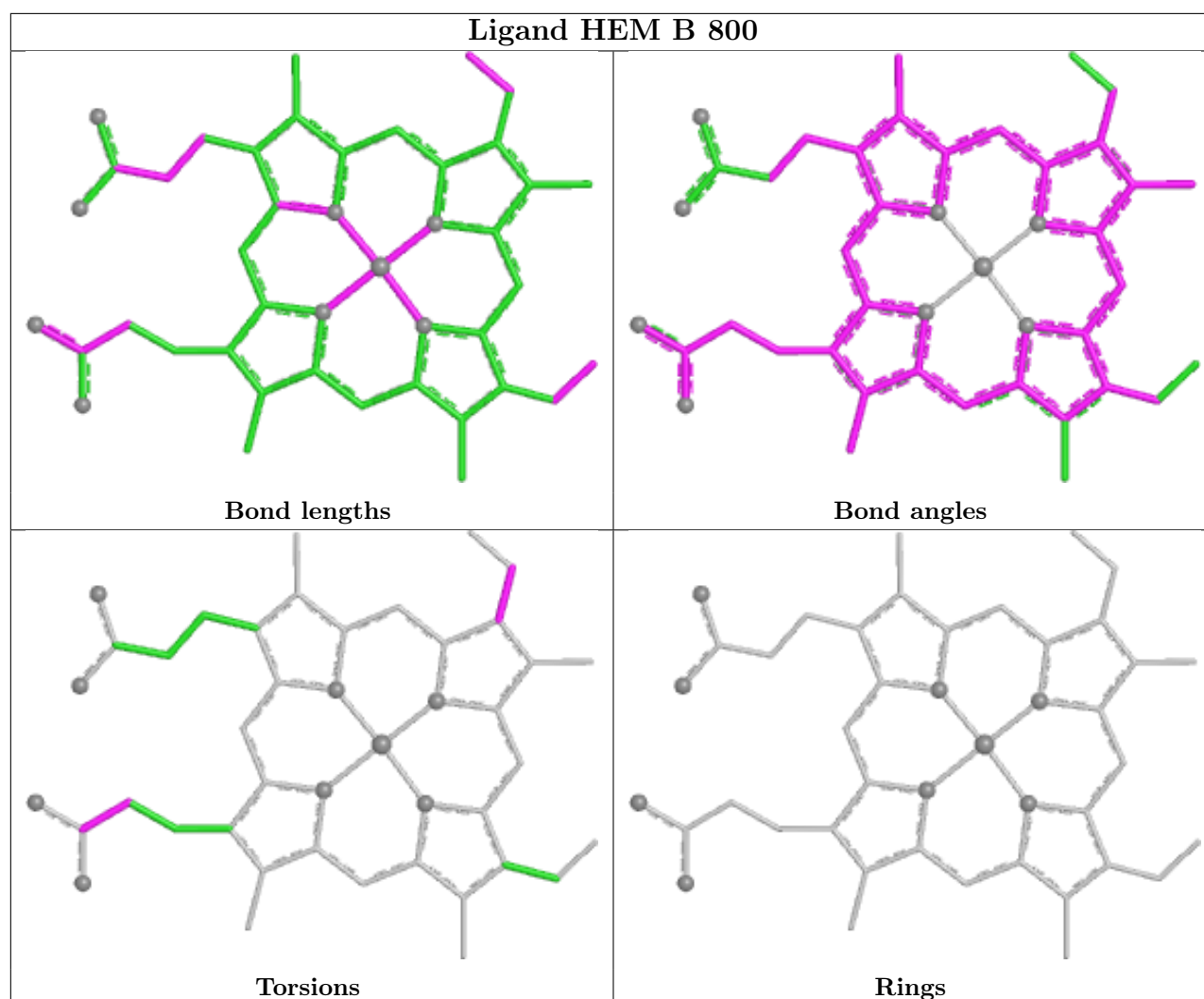
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	HEM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	714/737 (96%)	0.88	122 (17%) 4 4	7, 19, 43, 56	2 (0%)
1	B	714/737 (96%)	0.79	98 (13%) 6 6	10, 21, 39, 54	0
All	All	1428/1474 (96%)	0.84	220 (15%) 5 4	7, 20, 41, 56	2 (0%)

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	295	GLY	18.5
1	A	298	LYS	11.0
1	A	296	ASN	10.6
1	A	299	GLY	10.1
1	A	300	GLY	9.4
1	A	297	SER	9.0
1	A	294	ASN	8.9
1	B	730	LEU	8.6
1	A	20	PRO	8.0
1	A	675	THR	7.9
1	B	48	ASP	7.8
1	B	20	PRO	7.7
1	A	409	ARG	7.5
1	A	730	LEU	7.3
1	B	729	ASP	6.5
1	A	24	GLN	6.5
1	B	663	ASP	6.4
1	A	181	GLU	6.3
1	A	638	ASP	6.3
1	B	18	LYS	6.2
1	A	19	ARG	6.1
1	A	18	LYS	6.1
1	A	665	GLU	6.0
1	A	667	ARG	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	674	ASP	5.8
1	A	727	ARG	5.6
1	A	513	ASN	5.5
1	B	19	ARG	5.3
1	A	525	GLY	5.3
1	A	677	GLU	5.2
1	A	729	ASP	5.2
1	A	663	ASP	5.1
1	A	731	GLU	5.1
1	B	662	ALA	5.0
1	A	48	ASP	4.9
1	A	568	HIS	4.9
1	A	49	ASP	4.9
1	A	705	ALA	4.8
1	B	731	GLU	4.8
1	B	592	ILE	4.8
1	A	293	LYS	4.7
1	B	593	THR	4.7
1	B	40	ALA	4.7
1	A	22	SER	4.7
1	B	361	ASP	4.7
1	B	347	SER	4.6
1	A	590	ASP	4.5
1	B	191	ASP	4.5
1	B	34	GLU	4.4
1	B	348	GLU	4.3
1	A	666	HIS	4.2
1	B	293	LYS	4.2
1	B	437	ASP	4.1
1	A	437	ASP	4.1
1	A	593	THR	4.1
1	A	41	ARG	4.0
1	A	446	ILE	4.0
1	B	558	GLU	4.0
1	A	29	SER	3.9
1	B	727	ARG	3.9
1	A	43	VAL	3.9
1	A	520	ASP	3.9
1	B	49	ASP	3.9
1	A	591	ASP	3.8
1	B	200	ASP	3.8
1	B	568	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	34	GLU	3.7
1	A	517	GLU	3.7
1	B	271	GLU	3.7
1	A	523	SER	3.7
1	A	28	PRO	3.7
1	A	35	ILE	3.7
1	B	21	LYS	3.7
1	B	502	GLU	3.7
1	B	42	ASP	3.7
1	B	24	GLN	3.6
1	B	352	ASN	3.6
1	B	47	GLU	3.6
1	A	678	VAL	3.5
1	B	346	LYS	3.5
1	A	272	GLU	3.5
1	A	522	ARG	3.5
1	A	208	GLY	3.4
1	A	706	ASP	3.4
1	B	590	ASP	3.4
1	B	383	GLU	3.4
1	A	271	GLU	3.4
1	B	299	GLY	3.4
1	B	41	ARG	3.3
1	B	632	ASP	3.3
1	A	664	SER	3.3
1	B	664	SER	3.3
1	A	451	GLU	3.3
1	B	591	ASP	3.2
1	B	706	ASP	3.2
1	A	640	PRO	3.2
1	A	662	ALA	3.2
1	A	77	ASP	3.2
1	A	191	ASP	3.1
1	A	524	ASP	3.1
1	B	294	ASN	3.1
1	B	360	PRO	3.1
1	B	350	LEU	3.1
1	B	351	LYS	3.1
1	A	659	GLU	3.1
1	A	514	ILE	3.1
1	B	297	SER	3.1
1	B	298	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	43	VAL	3.0
1	B	503	GLN	3.0
1	A	440	LEU	3.0
1	A	50	PHE	3.0
1	A	558	GLU	2.9
1	A	556	PRO	2.9
1	A	448	GLU	2.9
1	B	22	SER	2.9
1	A	40	ALA	2.9
1	A	21	LYS	2.9
1	A	201	GLU	2.9
1	B	50	PHE	2.9
1	A	519	ASN	2.9
1	B	363	LYS	2.9
1	B	295	GLY	2.9
1	A	200	ASP	2.8
1	B	359	ASP	2.8
1	A	415	GLU	2.8
1	A	301	GLU	2.8
1	A	361	ASP	2.8
1	A	436	ALA	2.8
1	A	346	LYS	2.8
1	A	592	ILE	2.8
1	A	57	GLN	2.8
1	A	42	ASP	2.8
1	A	449	LEU	2.8
1	B	345	PRO	2.8
1	A	455	ASP	2.7
1	B	435	ASP	2.7
1	A	676	GLY	2.7
1	A	349	GLU	2.7
1	B	455	ASP	2.7
1	A	390	GLU	2.7
1	B	207	GLU	2.7
1	B	349	GLU	2.7
1	B	451	GLU	2.7
1	B	25	ASP	2.7
1	A	46	VAL	2.6
1	A	442	GLY	2.6
1	B	377	ARG	2.6
1	B	415	GLU	2.6
1	B	436	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	435	ASP	2.6
1	A	444	GLU	2.6
1	A	23	ASN	2.6
1	A	26	TRP	2.6
1	B	181	GLU	2.5
1	B	440	LEU	2.5
1	B	35	ILE	2.5
1	B	382	ARG	2.5
1	A	632	ASP	2.5
1	B	74	SER	2.5
1	B	269	ASP	2.5
1	B	457	ASP	2.5
1	B	204	GLU	2.5
1	B	397	MET	2.5
1	A	441	ILE	2.5
1	B	29	SER	2.4
1	A	362	GLU	2.4
1	B	28	PRO	2.4
1	A	503	GLN	2.4
1	B	665	GLU	2.4
1	A	37	ASP	2.4
1	A	553	VAL	2.4
1	A	360	PRO	2.4
1	A	207	GLU	2.3
1	B	524	ASP	2.3
1	A	347	SER	2.3
1	A	526	THR	2.3
1	B	362	GLU	2.3
1	A	44	GLY	2.3
1	A	454	LEU	2.3
1	B	300	GLY	2.3
1	B	588	ILE	2.3
1	B	201	GLU	2.3
1	B	705	ALA	2.3
1	A	218	TYR	2.3
1	A	292	ASN	2.3
1	B	344	ALA	2.3
1	B	552	ASP	2.3
1	B	341	TRP	2.3
1	A	192	GLU	2.2
1	A	728	PHE	2.2
1	A	457	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	47	GLU	2.2
1	B	666	HIS	2.2
1	A	521	SER	2.2
1	A	557	PHE	2.2
1	B	193	PHE	2.2
1	B	307	ILE	2.2
1	A	439	ASP	2.2
1	B	57	GLN	2.2
1	B	296	ASN	2.2
1	B	448	GLU	2.2
1	A	32	ASN	2.2
1	A	391	ASN	2.2
1	A	62	GLU	2.1
1	B	444	GLU	2.1
1	A	397	MET	2.1
1	B	390	GLU	2.1
1	A	624	ILE	2.1
1	A	594	ARG	2.1
1	A	452	GLU	2.1
1	B	337	PRO	2.1
1	B	536	LEU	2.1
1	B	62	GLU	2.1
1	A	512	GLU	2.0
1	B	661	ALA	2.1
1	A	70	GLU	2.0
1	B	639	GLU	2.0
1	A	45	PRO	2.0
1	B	45	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

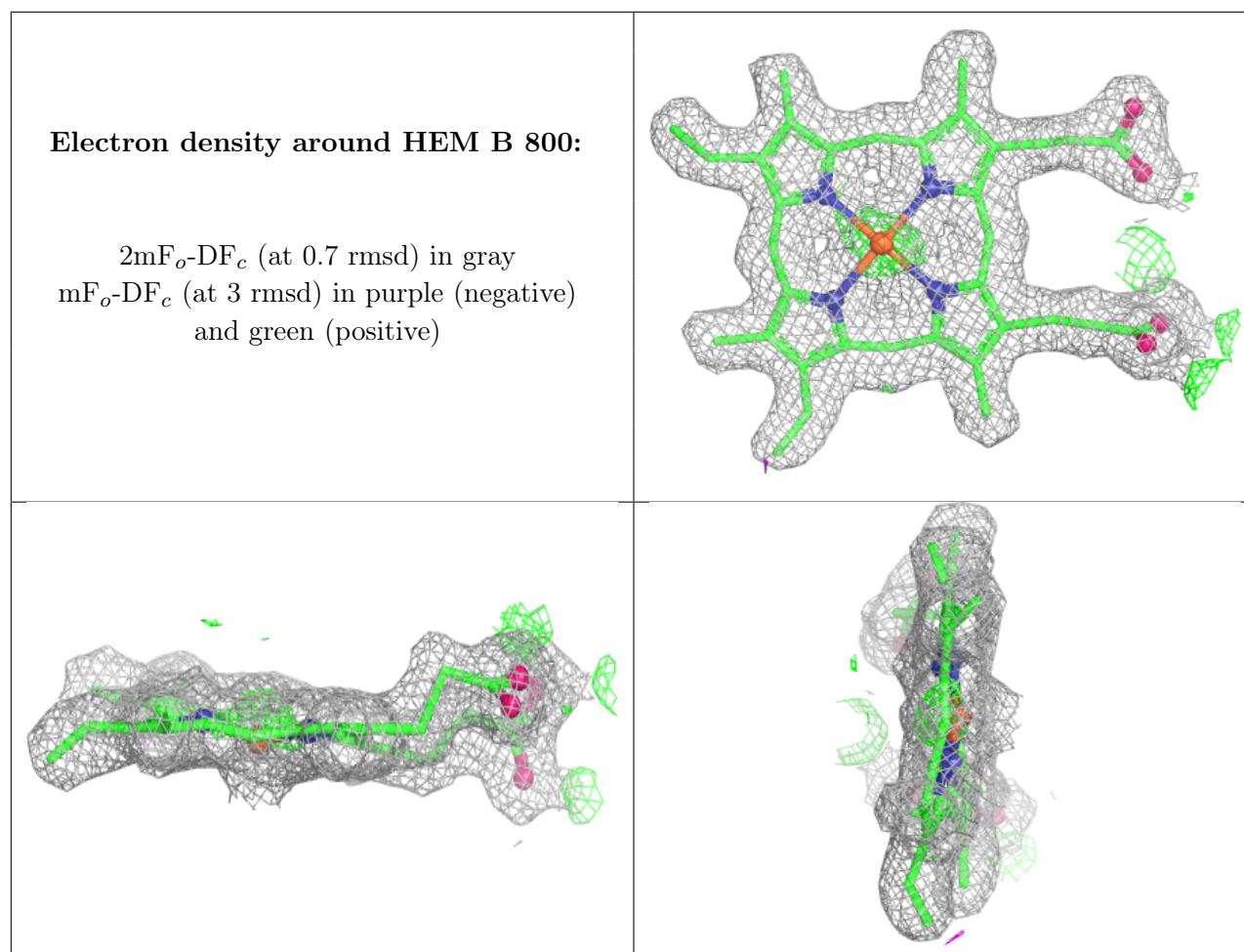
6.4 Ligands [i](#)

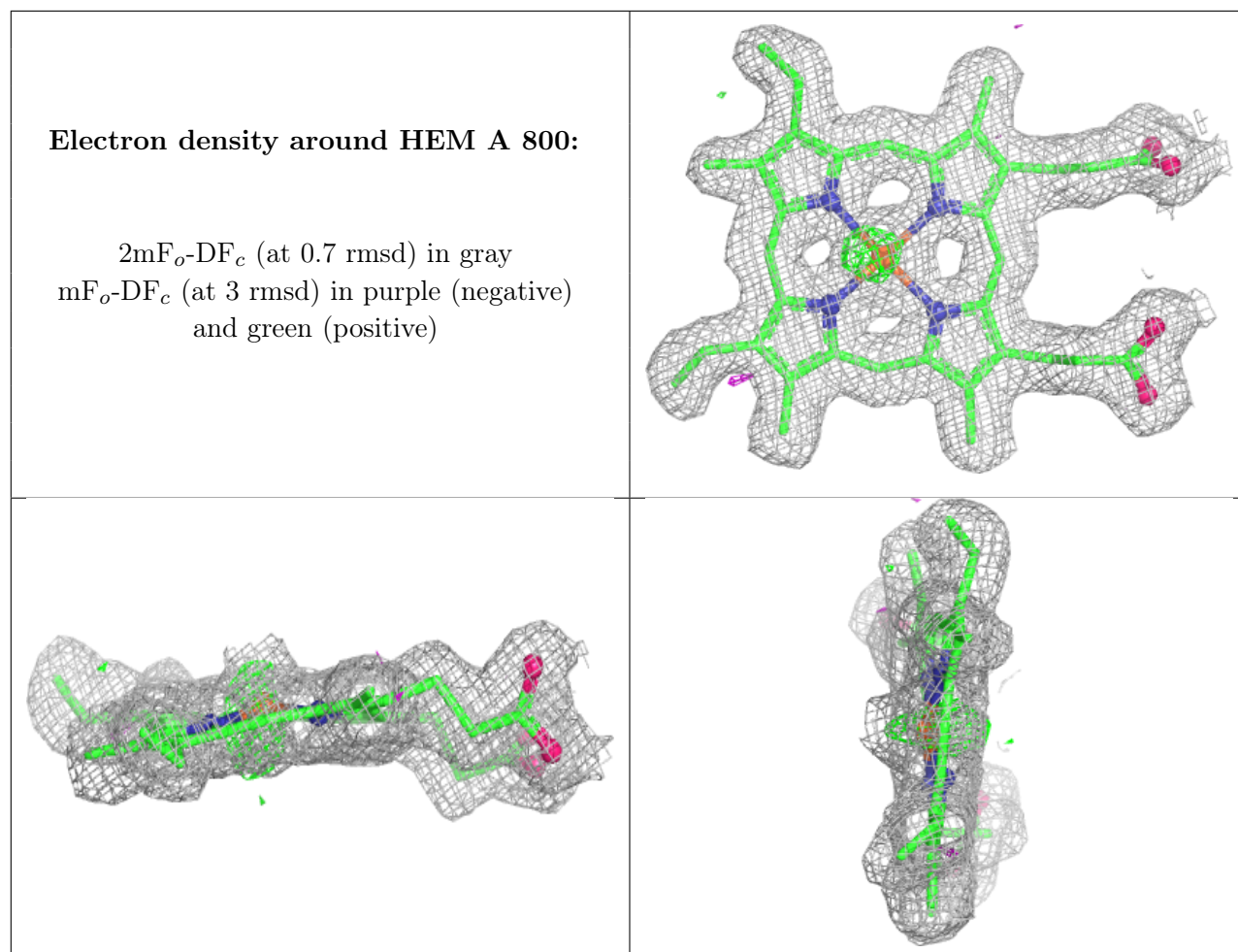
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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($\text{\AA}^2$)	Q<0.9
2	HEM	B	800	43/43	0.97	0.08	10,14,17,18	0
2	HEM	A	800	43/43	0.98	0.07	3,9,12,13	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.