



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:33 AM UTC

PDB ID : 3VU3 / pdb_00003vu3
Title : Crystal structure of the Hfq and catalase HP11 complex
Authors : Watanabe, M.; Yonekura, K.
Deposited on : 2012-06-15
Resolution : 2.85 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:

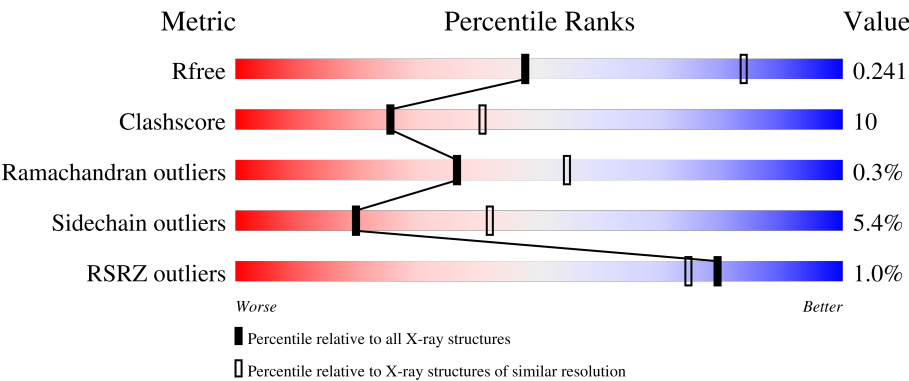
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	753	75%20%..
2	C	102	3% 48%14%38%
2	D	102	2% 50%10%38%
2	E	102	3% 44%16%39%
2	F	102	% 40%17%5%38%

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Mol	Chain	Length	Quality of chain
2	G	102	% 35%24%38%
2	H	102	% 46%15%38%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8841 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.

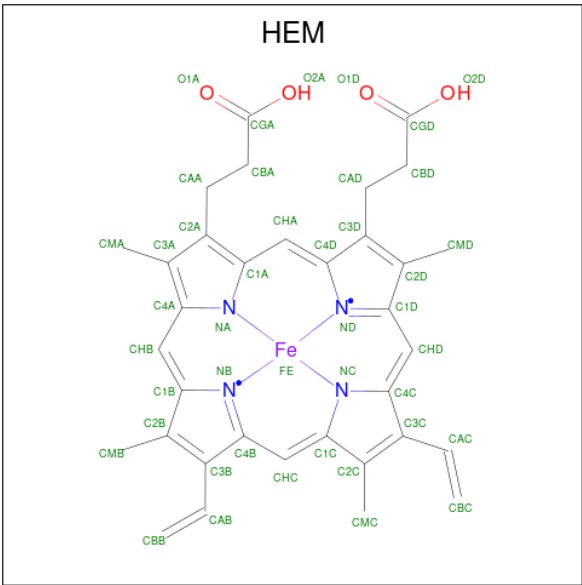
- Molecule 1 is a protein called Catalase HP11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5746	3647	1005	1082	12			

- Molecule 2 is a protein called Protein hfq.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	63	Total	C	N	O	S	0	0	0
			504	326	88	89	1			
2	D	63	Total	C	N	O	S	0	0	0
			504	326	88	89	1			
2	E	62	Total	C	N	O	S	0	0	0
			499	321	88	89	1			
2	F	63	Total	C	N	O	S	0	0	0
			506	326	89	90	1			
2	G	63	Total	C	N	O	S	0	0	0
			506	326	89	90	1			
2	H	63	Total	C	N	O	S	0	0	0
			504	326	88	89	1			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

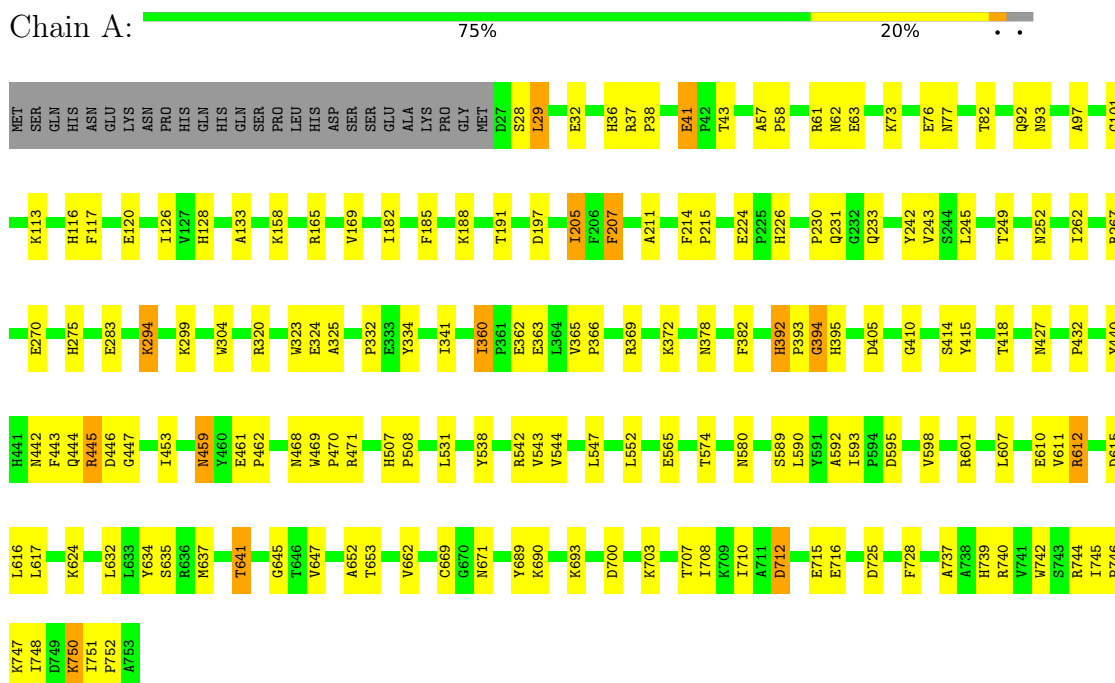
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		
4	D	1	Total	O	0	0
			1	1		
4	G	1	Total	O	0	0
			1	1		
4	H	1	Total	O	0	0
			1	1		

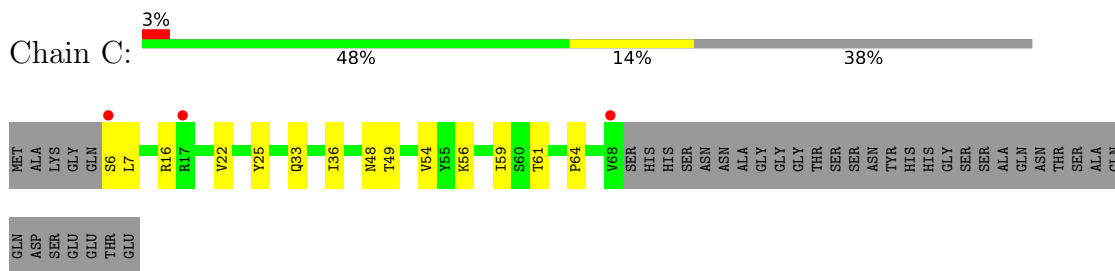
3 Residue-property plots

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 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.

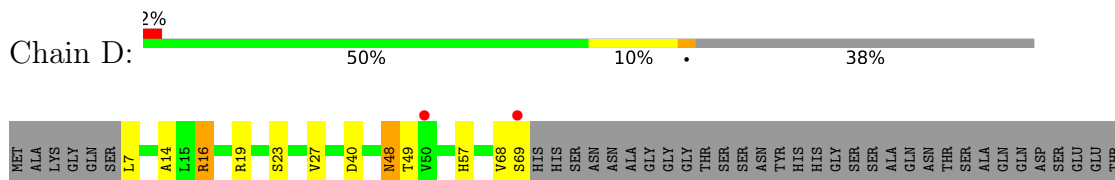
• Molecule 1: Catalase HP11



• Molecule 2: Protein hfq



• Molecule 2: Protein hfq



GLU

• Molecule 2: Protein hfq



MET ALA ALA LYS LYS GLY SER GLY Q5 S6 L7 Q8 D9 N13 L15 A14 R16 L15 R16 R17 E18 L26 V27 N28 G29 I30 I36 E37 S38 F39 D40 V43 I44 L45 T49 V50 R66 PRD VAL SER HIS HIS SER ASN ASN ALA GLY GLY THR SER SER ASN TYR HIS HIS GLY SER SER ALA

GLN ASN THR SER GLY ALA GLN ASP SER SER GLU THR GLU

• Molecule 2: Protein hfq



MET ALA ALA LYS LYS GLY SER GLY Q5 S6 L7 Q8 A14 L15 R16 R17 E18 R19 V20 P21 V22 Y25 I36 F39 D40 Q41 F42 V43 K56 H57 S60 T61 P64 S65 R66 P67 VAL SER HIS HIS SER ASN ASN ALA GLY GLY THR SER SER ASN TYR HIS HIS GLY SER SER

ALA GLN ASN THR SER GLY ALA GLN ASP SER SER GLU THR GLU

• Molecule 2: Protein hfq



MET ALA ALA LYS LYS GLY SER GLY Q5 S6 L7 P10 F11 A14 L15 R16 R17 E18 Y25 L26 I30 K31 I36 E37 S38 F39 D40 Q41 F42 V43 I44 K47 M48 T49 V50 S51 V54 H57 T61 V62 V63 P64 S65 R66 P67 VAL SER HIS HIS SER ASN ASN ALA GLY GLY THR SER SER ASN TYR HIS HIS GLY SER SER

GLY THR SER SER TYR HIS HIS SER SER ALA GLN ASN THR SER ALA GLN ASP SER SER GLU THR GLU

• Molecule 2: Protein hfq



MET ALA ALA LYS LYS GLY SER GLY S6 L7 Q8 D9 P10 N13 V20 I30 Q33 S38 F39 D40 Q41 F42 V43 M48 T49 M53 Y54 Y55 R56 H57 V68 SER HIS HIS SER SER ASN ASN ALA GLY GLY THR SER SER ASN TYR HIS HIS GLY SER SER ALA GLN ASN THR

SER ALA GLN ASP SER GLU THR GLU

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	136.43Å 159.01Å 167.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.85 20.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	94.8 (20.00-2.85) 94.6 (20.00-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.83Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.196 , 0.246 0.192 , 0.241	Depositor DCC
R_{free} test set	2145 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.034 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8841	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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	1.08	6/5902 (0.1%)	1.20	17/8024 (0.2%)
2	C	0.72	0/513	1.03	1/696 (0.1%)
2	D	0.74	0/513	1.04	0/696
2	E	0.64	0/507	0.96	1/686 (0.1%)
2	F	0.76	0/515	1.01	2/698 (0.3%)
2	G	0.83	0/515	1.09	4/698 (0.6%)
2	H	0.79	0/513	1.08	0/696
All	All	0.98	6/8978 (0.1%)	1.15	25/12194 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	92	GLN	CA-C	5.63	1.59	1.52
1	A	116	HIS	CG-CD2	5.63	1.42	1.35
1	A	207	PHE	N-CA	-5.42	1.39	1.46
1	A	395	HIS	CG-CD2	5.29	1.41	1.35
1	A	113	LYS	C-O	5.23	1.30	1.24
1	A	392	HIS	CG-CD2	5.17	1.41	1.35

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	49	THR	N-CA-C	-8.04	103.99	113.88
2	F	39	PHE	N-CA-C	7.91	119.66	108.74
1	A	126	ILE	N-CA-C	-7.28	103.43	110.42
1	A	93	ASN	N-CA-C	7.03	120.77	108.75
1	A	446	ASP	CA-C-N	-6.68	112.74	121.96
1	A	446	ASP	C-N-CA	-6.68	112.74	121.96
2	G	39	PHE	N-CA-C	6.41	117.59	108.74
2	E	49	THR	N-CA-C	-6.17	104.81	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	468	ASN	N-CA-C	6.17	120.04	111.90
1	A	41	GLU	CB-CA-C	-6.15	100.58	109.63
1	A	394	GLY	N-CA-C	-5.79	106.02	115.46
2	G	30	ILE	N-CA-C	5.73	116.47	109.30
1	A	304	TRP	N-CA-C	5.71	117.98	111.02
1	A	82	THR	N-CA-C	-5.59	103.32	110.53
2	G	54	VAL	N-CA-C	5.56	115.86	107.80
1	A	226	HIS	N-CA-C	-5.47	104.96	111.69
2	C	33	GLN	N-CA-C	5.43	117.65	109.23
1	A	133	ALA	N-CA-C	5.41	117.63	109.41
1	A	595	ASP	N-CA-C	-5.37	105.00	112.30
2	F	41	GLN	N-CA-C	-5.34	106.93	113.50
1	A	224	GLU	CB-CA-C	5.24	117.65	109.42
1	A	414	SER	N-CA-C	5.15	116.98	111.36
1	A	360	ILE	CB-CA-C	-5.14	104.99	110.95
1	A	446	ASP	N-CA-C	5.11	121.68	110.80
1	A	245	LEU	N-CA-C	5.10	119.14	113.02

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	5746	0	5578	102	0
2	C	504	0	530	13	0
2	D	504	0	530	11	0
2	E	499	0	522	12	0
2	F	506	0	529	14	0
2	G	506	0	529	14	0
2	H	504	0	530	11	0
3	A	43	0	30	11	0
4	A	26	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8841	0	8778	167	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 10.

All (167) 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:392:HIS:CE1	1:A:415:TYR:HB2	1.70	1.24
1:A:392:HIS:ND1	1:A:415:TYR:HB2	0.79	1.10
2:F:17:ARG:HH11	2:F:17:ARG:HG2	1.17	1.07
2:E:5:GLN:HG3	2:E:6:SER:H	1.10	1.06
2:E:5:GLN:CG	2:E:6:SER:H	1.68	1.05
1:A:708:ILE:HG13	1:A:710:ILE:HG12	1.33	1.04
2:E:5:GLN:HG3	2:E:6:SER:N	1.88	0.89
1:A:708:ILE:HG13	1:A:710:ILE:CG1	2.05	0.86
2:G:40:ASP:HB3	2:G:42:PHE:H	1.40	0.85
2:F:17:ARG:HG2	2:F:17:ARG:NH1	1.89	0.83
2:E:5:GLN:CG	2:E:6:SER:N	2.43	0.80
1:A:459:ASN:HD22	1:A:459:ASN:H	1.30	0.79
2:D:16:ARG:HH11	2:D:16:ARG:HB3	1.52	0.75
2:H:40:ASP:HB3	2:H:43:VAL:H	1.53	0.73
1:A:29:LEU:HD12	1:A:29:LEU:N	2.03	0.73
1:A:742:TRP:O	1:A:745:ILE:HG13	1.89	0.72
3:A:801:HEM:CMC	3:A:801:HEM:HBC2	2.24	0.67
1:A:270:GLU:OE2	1:A:294:LYS:HE2	1.94	0.66
1:A:128:HIS:HB2	3:A:801:HEM:HAA2	1.78	0.66
1:A:392:HIS:ND1	1:A:415:TYR:HB3	1.99	0.65
1:A:363:GLU:OE2	2:H:48:ASN:ND2	2.31	0.64
2:C:25:TYR:HB2	2:C:61:THR:CG2	2.29	0.63
2:F:15:LEU:HB3	2:F:36:ILE:HD12	1.82	0.61
1:A:689:TYR:CE1	1:A:710:ILE:HD11	2.35	0.61
2:D:7:LEU:HD13	2:E:45:LEU:HD12	1.82	0.60
2:H:9:ASP:O	2:H:13:ASN:HB2	2.03	0.59
2:G:37:GLU:OE1	2:G:47:LYS:HB2	2.02	0.59
1:A:700:ASP:O	1:A:703:LYS:HG2	2.03	0.58
1:A:214:PHE:CD2	3:A:801:HEM:CMC	2.86	0.58
2:C:25:TYR:HB2	2:C:61:THR:HG22	1.85	0.58
1:A:461:GLU:HA	1:A:462:PRO:C	2.29	0.58
1:A:612:ARG:HH11	1:A:669:CYS:CB	2.17	0.57
2:E:40:ASP:HB3	2:E:43:VAL:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:26:LEU:HD12	2:G:30:ILE:HB	1.86	0.57
2:F:14:ALA:O	2:F:18:GLU:HG2	2.05	0.56
1:A:459:ASN:HD22	1:A:459:ASN:N	1.97	0.56
2:D:14:ALA:HB1	2:D:68:VAL:HG11	1.88	0.55
1:A:29:LEU:N	1:A:29:LEU:CD1	2.69	0.55
3:A:801:HEM:HBC2	3:A:801:HEM:HMC1	1.85	0.55
2:C:22:VAL:HG12	2:C:64:PRO:HA	1.88	0.55
2:C:7:LEU:H	2:D:40:ASP:CG	2.15	0.55
2:E:26:LEU:HD12	2:E:30:ILE:HB	1.88	0.54
2:F:15:LEU:HD12	2:F:20:VAL:CG1	2.37	0.54
1:A:712:ASP:OD2	1:A:712:ASP:N	2.41	0.54
1:A:188:LYS:HG3	1:A:197:ASP:OD2	2.09	0.53
2:D:16:ARG:O	2:D:19:ARG:HG3	2.08	0.53
2:H:7:LEU:O	2:H:10:PRO:HD2	2.08	0.53
2:D:48:ASN:CG	2:D:49:THR:H	2.18	0.53
1:A:392:HIS:ND1	1:A:415:TYR:CG	2.67	0.52
2:G:14:ALA:O	2:G:18:GLU:HG2	2.10	0.52
1:A:366:PRO:HG2	2:H:30:ILE:HD13	1.90	0.52
2:C:54:VAL:HG12	2:C:59:ILE:HD11	1.91	0.52
1:A:593:ILE:HD13	2:H:33:GLN:CD	2.34	0.52
1:A:641:THR:HG22	1:A:645:GLY:HA2	1.92	0.52
2:C:16:ARG:HG3	2:C:36:ILE:O	2.10	0.52
2:F:40:ASP:HB3	2:F:43:VAL:H	1.75	0.51
1:A:690:LYS:HB2	1:A:751:ILE:HD11	1.92	0.51
1:A:662:VAL:O	1:A:693:LYS:HE2	2.10	0.51
1:A:538:TYR:O	1:A:542:ARG:HG3	2.11	0.51
1:A:739:HIS:CD2	1:A:740:ARG:HG2	2.46	0.51
2:D:27:VAL:O	2:E:28:ASN:HB3	2.11	0.50
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.42	0.50
1:A:689:TYR:CZ	1:A:710:ILE:HD11	2.47	0.50
1:A:62:ASN:OD1	1:A:62:ASN:C	2.54	0.49
1:A:607:LEU:HD22	1:A:611:VAL:HG21	1.93	0.49
2:F:15:LEU:HD12	2:F:20:VAL:HG11	1.92	0.49
1:A:689:TYR:CE1	1:A:744:ARG:HD3	2.47	0.49
1:A:165:ARG:HD3	3:A:801:HEM:O2A	2.12	0.49
1:A:262:ILE:HG13	1:A:262:ILE:O	2.12	0.49
2:E:36:ILE:H	2:E:36:ILE:HD12	1.78	0.49
1:A:612:ARG:HH11	1:A:669:CYS:HB2	1.78	0.49
1:A:418:THR:HG21	3:A:801:HEM:HBD2	1.94	0.49
1:A:443:PHE:CZ	1:A:470:PRO:HD2	2.48	0.49
1:A:97:ALA:O	1:A:101:GLY:HA3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:ILE:O	1:A:751:ILE:HG13	2.13	0.48
2:C:54:VAL:CG1	2:C:59:ILE:HD11	2.43	0.48
1:A:57:ALA:N	1:A:58:PRO:HD3	2.28	0.48
1:A:128:HIS:CE1	1:A:169:VAL:HG22	2.49	0.48
1:A:214:PHE:HB3	1:A:215:PRO:HD3	1.94	0.48
1:A:612:ARG:O	1:A:615:ASP:HB2	2.13	0.48
2:C:48:ASN:CG	2:C:49:THR:H	2.22	0.48
2:C:56:LYS:O	2:D:57:HIS:CE1	2.66	0.48
2:C:7:LEU:HB2	2:D:40:ASP:HB2	1.94	0.47
1:A:392:HIS:CG	1:A:415:TYR:CB	2.77	0.47
1:A:531:LEU:HA	1:A:531:LEU:HD23	1.78	0.47
1:A:382:PHE:CD2	1:A:382:PHE:C	2.92	0.47
2:G:40:ASP:HB3	2:G:42:PHE:N	2.19	0.47
1:A:444:GLN:O	1:A:445:ARG:HD3	2.15	0.47
1:A:589:SER:HB3	1:A:592:ALA:HB2	1.97	0.47
1:A:593:ILE:HD13	2:H:33:GLN:NE2	2.30	0.47
2:C:25:TYR:HB2	2:C:61:THR:HG23	1.96	0.47
2:C:6:SER:HA	2:D:40:ASP:OD1	2.15	0.46
1:A:598:VAL:HA	1:A:601:ARG:HG3	1.96	0.46
1:A:459:ASN:H	1:A:459:ASN:ND2	2.08	0.46
1:A:637:MET:SD	1:A:652:ALA:HA	2.56	0.46
1:A:737:ALA:HB2	2:C:49:THR:HG21	1.98	0.46
2:E:14:ALA:O	2:E:18:GLU:HG2	2.15	0.46
2:G:11:PHE:CE2	2:H:53:MET:HB2	2.50	0.46
1:A:710:ILE:HD12	1:A:715:GLU:OE2	2.16	0.46
2:F:25:TYR:HB2	2:F:61:THR:HG22	1.99	0.45
2:H:48:ASN:HB3	2:H:49:THR:H	1.49	0.45
1:A:205:ILE:HD13	1:A:205:ILE:H	1.82	0.45
1:A:612:ARG:HE	1:A:669:CYS:HB3	1.81	0.45
1:A:543:VAL:O	1:A:547:LEU:HG	2.16	0.45
2:D:68:VAL:HG12	2:D:69:SER:H	1.81	0.45
1:A:36:HIS:CD2	1:A:36:HIS:H	2.33	0.45
1:A:29:LEU:HD12	1:A:29:LEU:H	1.82	0.44
1:A:117:PHE:HA	1:A:120:GLU:OE2	2.18	0.44
2:G:66:ARG:HB2	2:G:67:PRO:CD	2.47	0.44
1:A:320:ARG:HH11	1:A:320:ARG:HG3	1.81	0.44
1:A:710:ILE:HD12	1:A:715:GLU:CD	2.43	0.44
1:A:207:PHE:O	1:A:249:THR:HA	2.18	0.44
1:A:275:HIS:HD1	1:A:405:ASP:CG	2.26	0.44
1:A:392:HIS:CD2	1:A:394:GLY:H	2.36	0.44
2:F:57:HIS:HA	2:G:57:HIS:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:16:ARG:HG3	2:G:36:ILE:O	2.17	0.44
1:A:427:ASN:ND2	1:A:447:GLY:HA3	2.33	0.44
1:A:507:HIS:N	1:A:508:PRO:HD2	2.32	0.44
1:A:267:ARG:HA	1:A:334:TYR:OH	2.18	0.43
1:A:418:THR:HG21	3:A:801:HEM:CMD	2.48	0.43
2:F:17:ARG:HH11	2:F:17:ARG:CG	2.03	0.43
1:A:341:ILE:HD11	1:A:360:ILE:HD13	2.00	0.43
2:G:25:TYR:HB2	2:G:61:THR:CG2	2.49	0.43
1:A:299:LYS:HB3	1:A:590:LEU:HD22	2.01	0.43
2:H:9:ASP:HB2	2:H:10:PRO:HD3	2.01	0.43
1:A:267:ARG:HG2	1:A:332:PRO:HB3	2.01	0.43
1:A:459:ASN:N	1:A:459:ASN:ND2	2.66	0.42
1:A:616:LEU:O	1:A:617:LEU:C	2.61	0.42
2:H:55:TYR:HB3	2:H:57:HIS:CE1	2.54	0.42
1:A:76:GLU:O	1:A:77:ASN:HB2	2.18	0.42
1:A:214:PHE:CD2	3:A:801:HEM:HMC2	2.54	0.42
1:A:231:GLN:O	1:A:233:GLN:HG3	2.20	0.42
1:A:362:GLU:HA	1:A:365:VAL:O	2.20	0.42
3:A:801:HEM:HMC1	3:A:801:HEM:CBC	2.49	0.42
1:A:324:GLU:O	1:A:325:ALA:C	2.62	0.42
2:F:8:GLN:NE2	2:F:56:LYS:NZ	2.67	0.42
2:F:16:ARG:CG	2:F:17:ARG:N	2.82	0.42
2:F:60:SER:HB2	2:G:26:LEU:HD22	2.00	0.42
1:A:214:PHE:CD2	3:A:801:HEM:HMC1	2.54	0.42
1:A:393:PRO:HD2	1:A:415:TYR:CG	2.54	0.42
1:A:747:LYS:O	1:A:750:LYS:HE2	2.19	0.42
1:A:61:ARG:O	1:A:62:ASN:HB3	2.20	0.42
1:A:169:VAL:HG21	1:A:182:ILE:HB	2.01	0.41
1:A:427:ASN:HD21	1:A:447:GLY:H	1.66	0.41
2:E:16:ARG:HD2	2:E:37:GLU:O	2.20	0.41
2:F:22:VAL:HG12	2:F:64:PRO:HA	2.03	0.41
1:A:610:GLU:HB3	1:A:671:ASN:HB2	2.02	0.41
1:A:690:LYS:HB2	1:A:751:ILE:CD1	2.51	0.41
1:A:41:GLU:O	1:A:43:THR:HG23	2.20	0.41
1:A:442:ASN:HB2	1:A:443:PHE:H	1.65	0.41
1:A:230:PRO:HB2	1:A:233:GLN:NE2	2.36	0.41
1:A:725:ASP:H	1:A:728:PHE:HB3	1.86	0.41
3:A:801:HEM:CMC	3:A:801:HEM:CBC	2.97	0.41
2:G:7:LEU:C	2:G:10:PRO:HD2	2.46	0.41
1:A:37:ARG:HA	1:A:38:PRO:HD3	1.82	0.41
1:A:323:TRP:CH2	1:A:378:ASN:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:LYS:HE2	1:A:372:LYS:HB3	1.54	0.41
1:A:634:TYR:O	1:A:653:THR:HA	2.20	0.41
1:A:745:ILE:N	1:A:746:PRO:HD2	2.35	0.41
1:A:469:TRP:CE3	1:A:471:ARG:HG3	2.56	0.40
1:A:242:TYR:O	1:A:243:VAL:C	2.63	0.40
1:A:744:ARG:O	1:A:745:ILE:C	2.65	0.40
1:A:751:ILE:O	1:A:751:ILE:HD12	2.22	0.40
2:G:63:VAL:HA	2:G:64:PRO:HD2	1.87	0.40
1:A:634:TYR:CG	1:A:635:SER:N	2.90	0.40
2:E:9:ASP:O	2:E:13:ASN:HB2	2.21	0.40
2:G:40:ASP:HB3	2:G:43:VAL:H	1.87	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	725/753 (96%)	688 (95%)	35 (5%)	2 (0%)	36	54
2	C	61/102 (60%)	55 (90%)	6 (10%)	0	100	100
2	D	61/102 (60%)	58 (95%)	2 (3%)	1 (2%)	7	17
2	E	60/102 (59%)	59 (98%)	1 (2%)	0	100	100
2	F	61/102 (60%)	58 (95%)	3 (5%)	0	100	100
2	G	61/102 (60%)	58 (95%)	3 (5%)	0	100	100
2	H	61/102 (60%)	57 (93%)	4 (7%)	0	100	100
All	All	1090/1365 (80%)	1033 (95%)	54 (5%)	3 (0%)	36	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	752	PRO
2	D	48	ASN
1	A	432	PRO

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	612/636 (96%)	581 (95%)	31 (5%)	21	43
2	C	59/89 (66%)	59 (100%)	0	100	100
2	D	59/89 (66%)	57 (97%)	2 (3%)	32	58
2	E	58/89 (65%)	56 (97%)	2 (3%)	32	58
2	F	59/89 (66%)	51 (86%)	8 (14%)	3	7
2	G	59/89 (66%)	54 (92%)	5 (8%)	10	22
2	H	59/89 (66%)	55 (93%)	4 (7%)	14	30
All	All	965/1170 (82%)	913 (95%)	52 (5%)	20	42

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	29	LEU
1	A	32	GLU
1	A	63	GLU
1	A	73	LYS
1	A	158	LYS
1	A	185	PHE
1	A	191	THR
1	A	205	ILE
1	A	252	ASN
1	A	283	GLU
1	A	294	LYS
1	A	369	ARG
1	A	440	TYR
1	A	445	ARG

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Mol	Chain	Res	Type
1	A	453	ILE
1	A	459	ASN
1	A	544	VAL
1	A	552	LEU
1	A	565	GLU
1	A	574	THR
1	A	580	ASN
1	A	612	ARG
1	A	624	LYS
1	A	632	LEU
1	A	641	THR
1	A	647	VAL
1	A	707	THR
1	A	712	ASP
1	A	716	GLU
1	A	750	LYS
2	D	16	ARG
2	D	23	SER
2	E	5	GLN
2	E	38	SER
2	F	6	SER
2	F	7	LEU
2	F	15	LEU
2	F	16	ARG
2	F	17	ARG
2	F	18	GLU
2	F	20	VAL
2	F	66	ARG
2	G	31	LYS
2	G	40	ASP
2	G	44	ILE
2	G	51	SER
2	G	63	VAL
2	H	20	VAL
2	H	38	SER
2	H	41	GLN
2	H	49	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	ASN

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Mol	Chain	Res	Type
1	A	233	GLN
1	A	252	ASN
1	A	368	GLN
1	A	427	ASN
1	A	459	ASN
1	A	556	GLN
1	A	713	GLN
2	C	35	GLN
2	C	52	GLN
2	D	8	GLN
2	E	5	GLN
2	E	8	GLN
2	E	35	GLN
2	E	52	GLN
2	F	8	GLN
2	F	33	GLN
2	F	41	GLN
2	F	52	GLN
2	F	57	HIS
2	G	35	GLN
2	G	48	ASN
2	G	52	GLN
2	G	57	HIS
2	H	33	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	HEM	A	801	1	50,50,50	2.45	26 (52%)	67,82,82	3.69	38 (56%)

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
3	HEM	A	801	1	-	7/14/54/54	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	HEM	C3C-C2C	5.44	1.48	1.37
3	A	801	HEM	C3D-C2D	5.31	1.48	1.36
3	A	801	HEM	FE-NB	4.49	2.08	1.94
3	A	801	HEM	FE-ND	4.42	2.08	1.94
3	A	801	HEM	C4D-ND	-4.27	1.32	1.40
3	A	801	HEM	C3B-C2B	3.53	1.44	1.37
3	A	801	HEM	C1A-NA	3.51	1.46	1.39
3	A	801	HEM	C1C-NC	3.38	1.46	1.39
3	A	801	HEM	C4A-NA	3.38	1.46	1.39
3	A	801	HEM	CHC-C1C	3.31	1.44	1.38
3	A	801	HEM	C4B-NB	-3.29	1.32	1.38
3	A	801	HEM	C4C-NC	2.90	1.45	1.39
3	A	801	HEM	CHC-C4B	2.81	1.45	1.39
3	A	801	HEM	CHD-C1D	2.71	1.45	1.39
3	A	801	HEM	CHA-C4D	2.61	1.43	1.38
3	A	801	HEM	C1C-C2C	2.59	1.50	1.45
3	A	801	HEM	CHA-C1A	2.58	1.45	1.39
3	A	801	HEM	CHD-C4C	2.55	1.43	1.38
3	A	801	HEM	C1B-NB	-2.53	1.35	1.40
3	A	801	HEM	C1D-C2D	2.53	1.49	1.44
3	A	801	HEM	CHB-C1B	2.51	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	HEM	C3B-C4B	2.13	1.49	1.44
3	A	801	HEM	C1A-C2A	2.12	1.48	1.44
3	A	801	HEM	C1B-C2B	2.11	1.48	1.44
3	A	801	HEM	C1D-ND	-2.07	1.34	1.38
3	A	801	HEM	C2A-C3A	2.06	1.44	1.38

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	HEM	C3B-C2B-C1B	-12.83	96.78	106.41
3	A	801	HEM	C2B-C1B-NB	9.34	120.58	109.84
3	A	801	HEM	C3D-C4D-ND	8.87	119.90	110.17
3	A	801	HEM	C3B-C4B-NB	6.75	114.31	109.47
3	A	801	HEM	C4A-NA-C1A	-6.60	95.07	105.82
3	A	801	HEM	C2A-C1A-NA	6.53	117.40	110.15
3	A	801	HEM	C2D-C1D-ND	6.51	117.43	109.90
3	A	801	HEM	CAD-C3D-C2D	6.21	139.49	127.87
3	A	801	HEM	C1D-C2D-C3D	-5.29	101.42	106.98
3	A	801	HEM	C3A-C4A-NA	5.15	118.39	110.14
3	A	801	HEM	C3C-C2C-C1C	-4.87	102.44	107.05
3	A	801	HEM	CAD-CBD-CGD	-4.81	100.90	113.67
3	A	801	HEM	CMB-C2B-C1B	4.71	132.40	125.03
3	A	801	HEM	C4D-C3D-C2D	-4.17	100.82	106.89
3	A	801	HEM	C4D-ND-C1D	-4.10	100.35	105.21
3	A	801	HEM	C1B-NB-C4B	-3.75	100.77	105.21
3	A	801	HEM	CHA-C4D-C3D	-3.47	118.83	125.23
3	A	801	HEM	CHB-C4A-C3A	-3.44	117.45	127.43
3	A	801	HEM	CBA-CAA-C2A	-3.24	103.59	112.53
3	A	801	HEM	CHB-C1B-C2B	-3.06	118.24	126.95
3	A	801	HEM	CHD-C1D-C2D	-2.99	120.30	125.03
3	A	801	HEM	CAD-C3D-C4D	-2.96	119.55	124.70
3	A	801	HEM	O1A-CGA-CBA	-2.78	114.29	123.09
3	A	801	HEM	CHB-C1B-NB	-2.76	120.96	124.37
3	A	801	HEM	CMD-C2D-C3D	2.73	133.54	126.15
3	A	801	HEM	CMC-C2C-C1C	2.68	129.44	124.73
3	A	801	HEM	C4A-CHB-C1B	-2.66	120.00	126.25
3	A	801	HEM	CHA-C1A-C2A	-2.62	119.57	125.30
3	A	801	HEM	CBC-CAC-C3C	-2.55	114.80	127.53
3	A	801	HEM	CHA-C4D-ND	-2.51	121.26	124.37
3	A	801	HEM	C4A-C3A-C2A	-2.49	103.97	106.82
3	A	801	HEM	CBB-CAB-C3B	-2.42	115.43	127.53
3	A	801	HEM	CAA-C2A-C1A	2.31	129.44	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	HEM	CHD-C1D-ND	-2.22	122.03	124.42
3	A	801	HEM	CHC-C1C-NC	-2.09	122.18	124.45
3	A	801	HEM	C2C-C1C-NC	2.09	113.49	109.64
3	A	801	HEM	C4C-NC-C1C	-2.07	102.44	105.82
3	A	801	HEM	CBD-CAD-C3D	2.06	118.22	112.53

There are no chirality outliers.

All (7) torsion outliers are listed below:

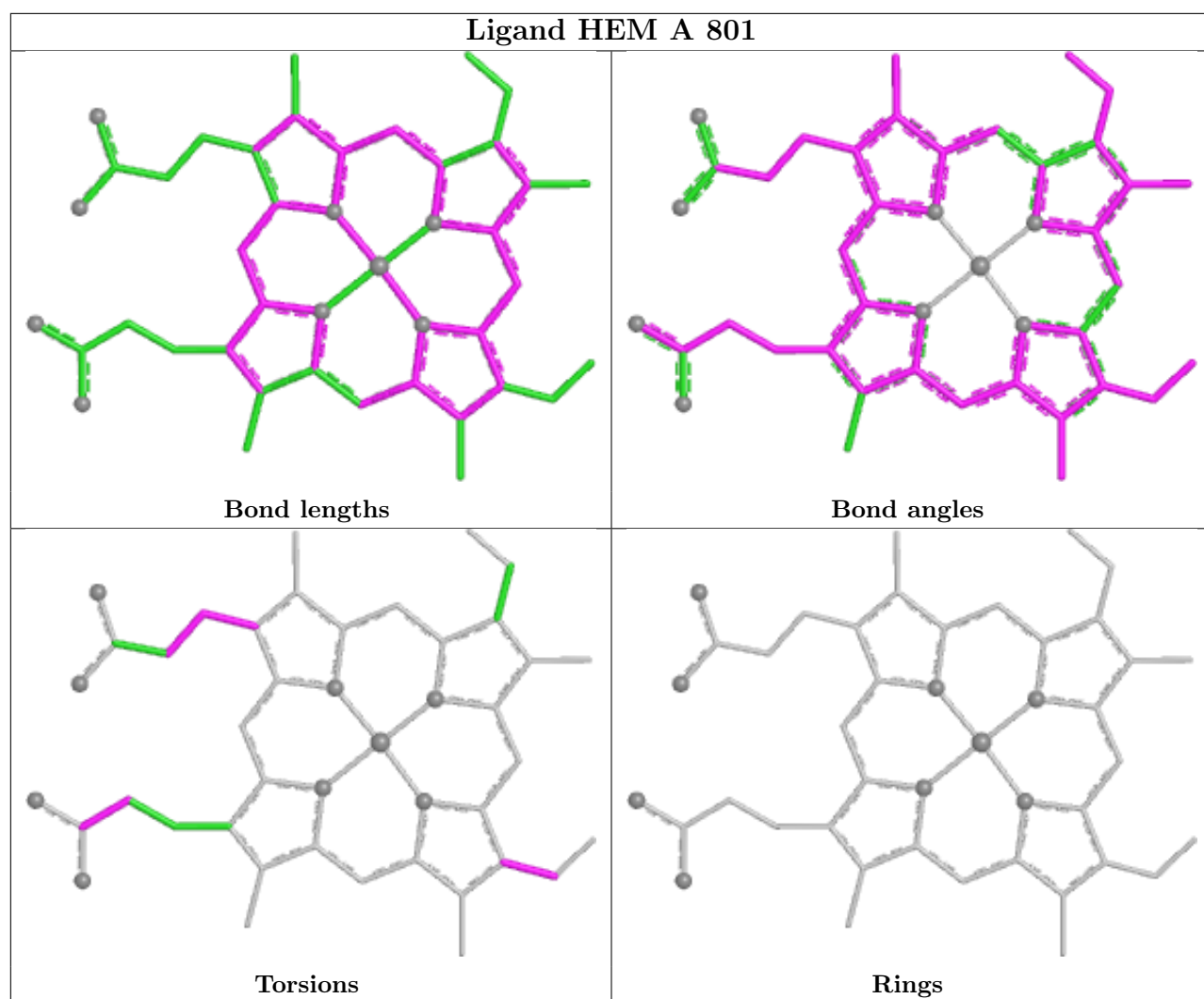
Mol	Chain	Res	Type	Atoms
3	A	801	HEM	C2B-C3B-CAB-CBB
3	A	801	HEM	C4B-C3B-CAB-CBB
3	A	801	HEM	C4D-C3D-CAD-CBD
3	A	801	HEM	C2D-C3D-CAD-CBD
3	A	801	HEM	C3D-CAD-CBD-CGD
3	A	801	HEM	CAA-CBA-CGA-O1A
3	A	801	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	HEM	11	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	727/753 (96%)	-0.81	0 100 100	13, 30, 60, 91	1 (0%)
2	C	63/102 (61%)	0.23	3 (4%) 35 28	45, 69, 98, 110	0
2	D	63/102 (61%)	0.35	2 (3%) 50 41	39, 83, 110, 113	0
2	E	62/102 (60%)	0.55	3 (4%) 35 28	54, 94, 119, 128	0
2	F	63/102 (61%)	0.28	1 (1%) 70 64	51, 75, 109, 119	0
2	G	63/102 (61%)	0.04	1 (1%) 70 64	42, 65, 95, 103	0
2	H	63/102 (61%)	-0.16	1 (1%) 70 64	35, 59, 81, 95	0
All	All	1104/1365 (80%)	-0.46	11 (0%) 79 74	13, 39, 99, 128	1 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	6	SER	3.1
2	H	68	VAL	2.7
2	D	50	VAL	2.6
2	C	68	VAL	2.5
2	G	5	GLN	2.5
2	C	17	ARG	2.3
2	E	66	ARG	2.3
2	F	67	PRO	2.2
2	E	50	VAL	2.1
2	E	7	LEU	2.1
2	D	69	SER	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 [i](#)

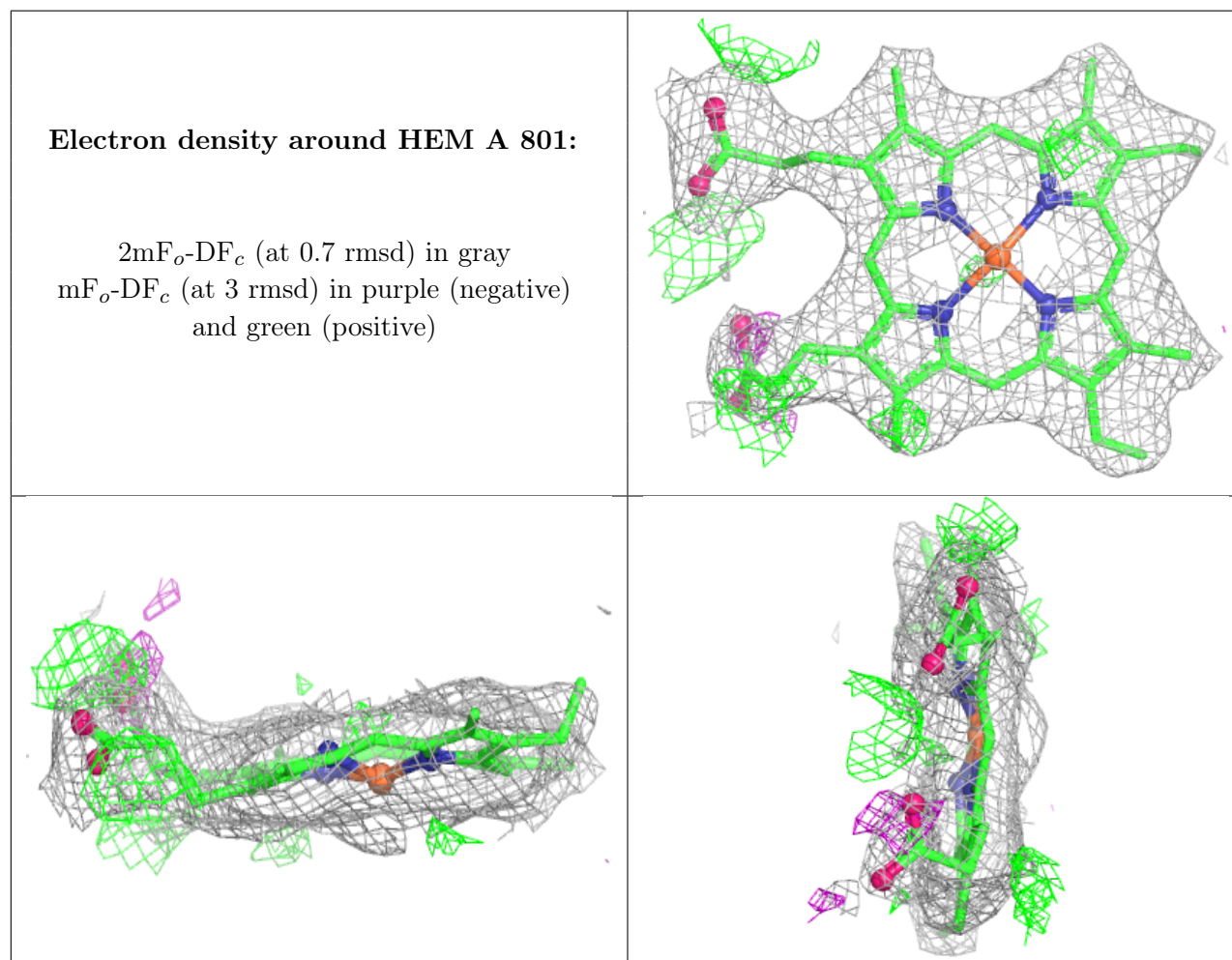
There are no oligosaccharides in this entry.

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
3	HEM	A	801	43/43	0.98	0.07	17,19,25,37	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.