



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 09:44 PM EDT

PDB ID : 3VU3
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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

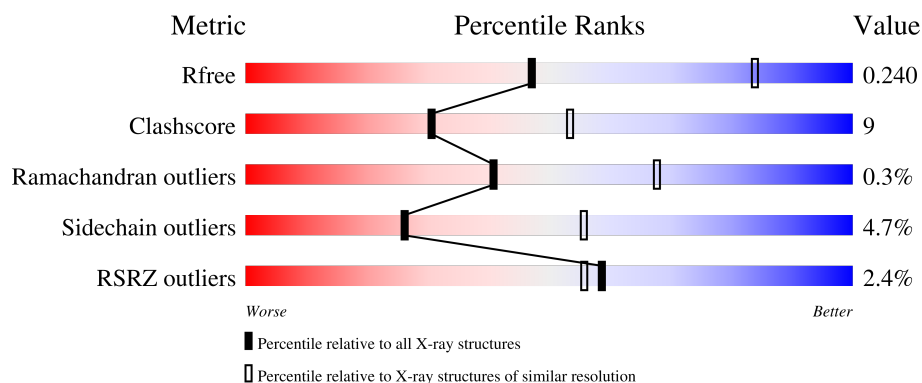
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	
2	C	102	
2	D	102	
2	E	102	
2	F	102	

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Mol	Chain	Length	Quality of chain
2	G	102	<div><div><div>6%</div><div>41%</div><div>20%</div><div>38%</div></div></div>
2	H	102	<div><div><div>%</div><div>48%</div><div>13%</div><div>38%</div></div></div>

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.

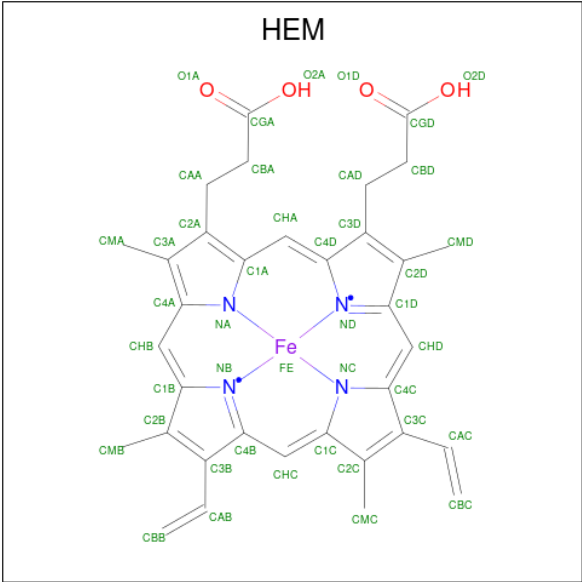
- Molecule 1 is a protein called Catalase HPIL.

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 (three-letter code: 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		

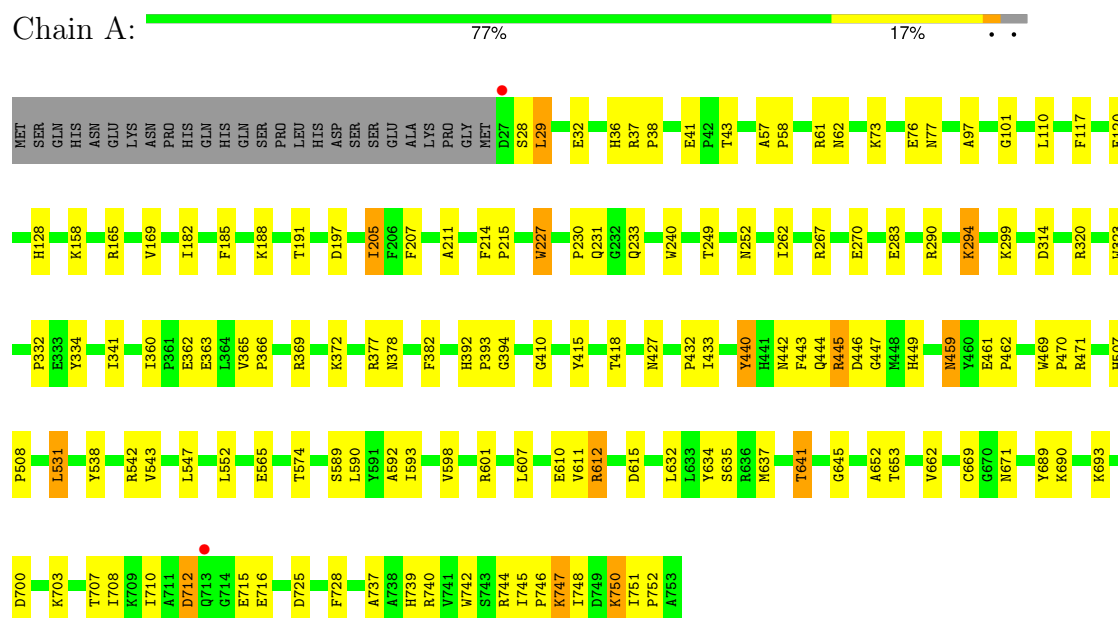
- Molecule 4 is water.

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

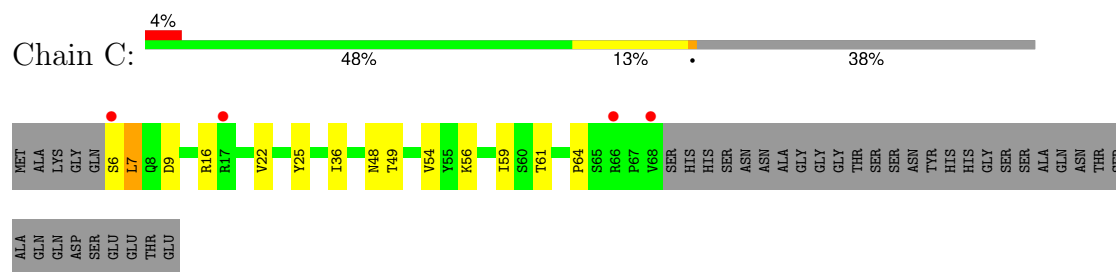
3 Residue-property plots

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.

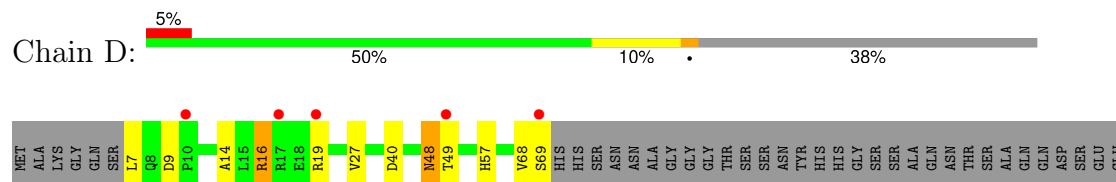
• Molecule 1: Catalase HPII



• Molecule 2: Protein hfq



• Molecule 2: Protein hfq



THR
GLU

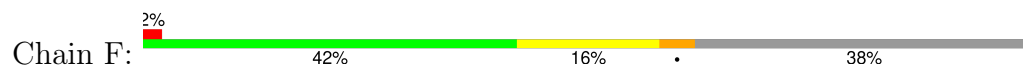
● Molecule 2: Protein hfq



MET ALA LYS SER GLY GLN ASP D9 N13 A14 L15 R16 R17 R18 E19 R19 L26 V27 V28 N28 G29 I30 I36 E37 E38 F39 D40 V43 I44 L45 T49 R66 PRO VAL SER HIS HIS SER SER ASN ASN ALA GLY GLY THR SER SER ASN TYR HIS HIS SER SER ALA GLN

ASN
THR
SER
ALA
GLN
ASP
SER
GLU
THR
GLU

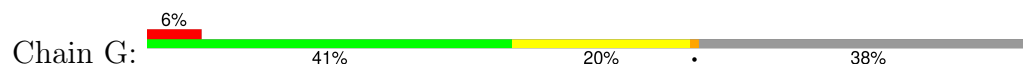
● Molecule 2: Protein hfq



MET ALA LYS SER GLY GLN ASP D9 N13 A14 L15 R16 R17 R18 E19 R19 L26 V27 V28 N28 G29 I30 I36 E37 E38 F39 D40 V43 I44 L45 T49 R66 PRO VAL SER HIS HIS SER SER ASN ASN ALA GLY GLY THR SER SER ASN TYR HIS HIS SER SER ALA GLN

ASN
THR
SER
ALA
GLN
ASP
SER
GLU
THR
GLU

● Molecule 2: Protein hfq



MET ALA LYS SER GLY GLN ASP D9 N13 A14 L15 R16 R17 R18 E19 R19 L26 V27 V28 N28 G29 I30 I36 E37 E38 F39 D40 V43 I44 L45 T49 R66 PRO VAL SER HIS HIS SER SER ASN ASN ALA GLY GLY THR SER SER ASN TYR HIS HIS SER SER ALA GLN

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

● Molecule 2: Protein hfq



MET ALA LYS SER GLY GLN ASP D9 N13 A14 L15 R16 R17 R18 E19 R19 L26 V27 V28 N28 G29 I30 I36 E37 E38 F39 D40 V43 I44 L45 T49 R66 PRO VAL SER HIS HIS SER SER ASN ASN ALA GLY GLY THR SER SER ASN TYR HIS HIS SER SER ALA GLN

GLN
ASP
SER
GLU
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 19.98 – 2.86	Depositor EDS
% Data completeness (in resolution range)	94.8 (20.00-2.85) 95.0 (19.98-2.86)	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 , 0.240	Depositor DCC
R_{free} test set	2032 reflections (5.05%)	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 , 33.4	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	0.80	3/5902 (0.1%)	0.90	7/8024 (0.1%)
2	C	0.51	0/513	0.78	1/696 (0.1%)
2	D	0.51	0/513	0.76	0/696
2	E	0.45	0/507	0.64	0/686
2	F	0.51	0/515	0.73	0/698
2	G	0.59	0/515	0.78	0/698
2	H	0.57	0/513	0.79	0/696
All	All	0.72	3/8978 (0.0%)	0.85	8/12194 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	440	TYR	CE1-CZ	8.64	1.49	1.38
1	A	240	TRP	CD2-CE2	5.88	1.48	1.41
1	A	227	TRP	CD2-CE2	5.86	1.48	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	446	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	A	110	LEU	CB-CG-CD2	-6.50	99.96	111.00
1	A	290	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	A	314	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	377	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	531	LEU	CA-CB-CG	-5.24	103.26	115.30
1	A	433	ILE	CG1-CB-CG2	-5.17	100.02	111.40
2	C	7	LEU	CB-CG-CD1	-5.09	102.34	111.00

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	96	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	13	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
All	All	8841	0	8778	160	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 (160) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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
1:A:461:GLU:HA	1:A:462:PRO:C	2.29	0.53
2:H:7:LEU:O	2:H:10:PRO:HD2	2.08	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:7:LEU:H	2:D:40:ASP:CG	2.15	0.50
1:A:689:TYR:CZ	1:A:710:ILE:HD11	2.47	0.50
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
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:D:48:ASN:CG	2:D:49:THR:H	2.18	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:593:ILE:HD13	2:H:33:GLN:CD	2.34	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
1:A:62:ASN:OD1	1:A:62:ASN:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:207:PHE:O	1:A:249:THR:HA	2.18	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
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
2:C:48:ASN:CG	2:C:49:THR:H	2.22	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:382:PHE:CD2	1:A:382:PHE:C	2.92	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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 ⓘ

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	725/753 (96%)	688 (95%)	35 (5%)	2 (0%)	41	68
2	C	61/102 (60%)	55 (90%)	6 (10%)	0	100	100
2	D	61/102 (60%)	58 (95%)	2 (3%)	1 (2%)	9	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	41	68

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%)	584 (95%)	28 (5%)	27	56
2	C	59/89 (66%)	58 (98%)	1 (2%)	60	83
2	D	59/89 (66%)	57 (97%)	2 (3%)	37	67
2	E	58/89 (65%)	56 (97%)	2 (3%)	37	67
2	F	59/89 (66%)	52 (88%)	7 (12%)	5	13
2	G	59/89 (66%)	56 (95%)	3 (5%)	24	52
2	H	59/89 (66%)	57 (97%)	2 (3%)	37	67
All	All	965/1170 (82%)	920 (95%)	45 (5%)	26	56

All (45) 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

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Mol	Chain	Res	Type
1	A	73	LYS
1	A	158	LYS
1	A	185	PHE
1	A	191	THR
1	A	205	ILE
1	A	227	TRP
1	A	252	ASN
1	A	283	GLU
1	A	294	LYS
1	A	369	ARG
1	A	440	TYR
1	A	445	ARG
1	A	449	HIS
1	A	459	ASN
1	A	552	LEU
1	A	565	GLU
1	A	574	THR
1	A	612	ARG
1	A	632	LEU
1	A	641	THR
1	A	707	THR
1	A	712	ASP
1	A	716	GLU
1	A	747	LYS
1	A	750	LYS
2	C	9	ASP
2	D	9	ASP
2	D	16	ARG
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	66	ARG
2	G	31	LYS
2	G	40	ASP
2	G	51	SER
2	H	38	SER
2	H	49	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	233	GLN
1	A	252	ASN
1	A	368	GLN
1	A	427	ASN
1	A	459	ASN
1	A	515	GLN
1	A	556	GLN
1	A	713	GLN
2	C	35	GLN
2	D	8	GLN
2	E	5	GLN
2	E	8	GLN
2	E	35	GLN
2	F	8	GLN
2	F	33	GLN
2	F	57	HIS
2	G	35	GLN
2	G	48	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	42,50,50	2.50	17 (40%)	46,82,82	4.00	26 (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	-	7/12/54/54	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	HEM	C3C-C2C	5.79	1.48	1.40
3	A	801	HEM	C3D-C2D	5.31	1.48	1.36
3	A	801	HEM	C1A-NA	4.85	1.46	1.36
3	A	801	HEM	C4A-NA	4.73	1.46	1.36
3	A	801	HEM	C4D-ND	-4.27	1.32	1.40
3	A	801	HEM	CHA-C4D	3.72	1.43	1.34
3	A	801	HEM	CHB-C1B	3.64	1.43	1.34
3	A	801	HEM	C2C-C1C	3.55	1.50	1.42
3	A	801	HEM	C3B-C2B	3.53	1.44	1.37
3	A	801	HEM	C4B-NB	-3.29	1.32	1.38
3	A	801	HEM	C3C-C4C	3.25	1.46	1.41
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	C2A-C3A	2.23	1.44	1.37
3	A	801	HEM	C3B-C4B	2.13	1.49	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

All (26) 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	HEM	C3B-C4B-NB	6.75	114.31	109.47
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	CBA-CAA-C2A	-5.32	103.59	112.54
3	A	801	HEM	C1D-C2D-C3D	-5.29	101.42	106.98
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	C4A-C3A-C2A	-4.35	103.97	107.00
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-C1B-C2B	-3.07	118.24	126.94
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	CHA-C4D-ND	-2.51	121.26	124.37
3	A	801	HEM	CBB-CAB-C3B	-2.42	115.43	127.53
3	A	801	HEM	CHD-C1D-ND	-2.23	122.03	124.44
3	A	801	HEM	C2C-C3C-C4C	2.14	108.40	106.90
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:

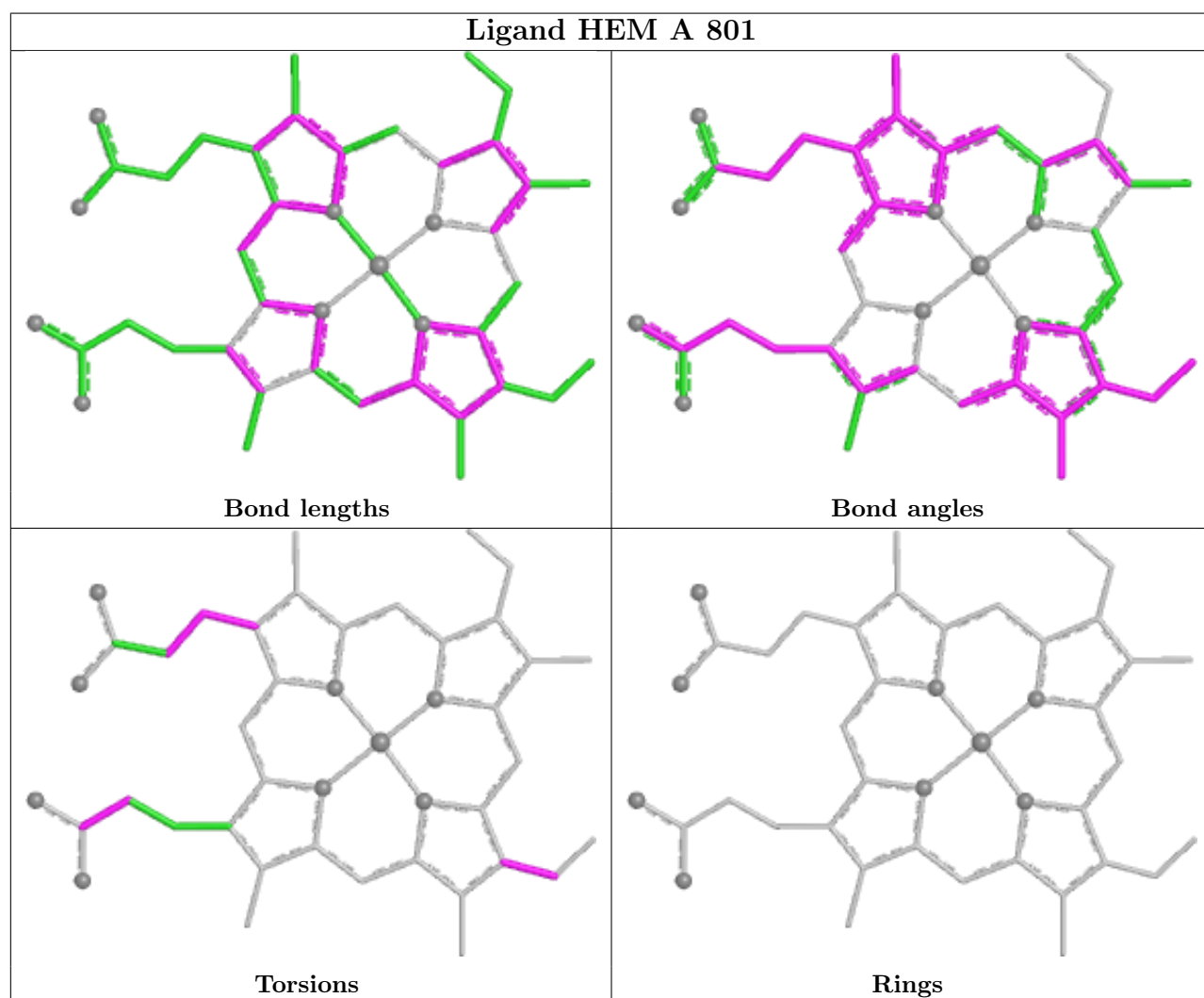
Mol	Chain	Res	Type	Atoms
3	A	801	HEM	C2B-C3B-CAB-CBB
3	A	801	HEM	C4B-C3B-CAB-CBB
3	A	801	HEM	C4D-C3D-CAD-CBD
3	A	801	HEM	C2D-C3D-CAD-CBD
3	A	801	HEM	C3D-CAD-CBD-CGD
3	A	801	HEM	CAA-CBA-CGA-O1A
3	A	801	HEM	CAA-CBA-CGA-O2A

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 ⓘ

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	727/753 (96%)	-0.82	2 (0%) 94 94	13, 31, 60, 91	1 (0%)
2	C	63/102 (61%)	0.02	4 (6%) 20 15	45, 69, 98, 110	0
2	D	63/102 (61%)	0.36	5 (7%) 12 9	39, 83, 110, 113	0
2	E	62/102 (60%)	0.59	6 (9%) 7 5	54, 94, 119, 128	0
2	F	63/102 (61%)	0.26	2 (3%) 47 42	51, 75, 109, 119	0
2	G	63/102 (61%)	0.10	6 (9%) 8 5	42, 65, 95, 103	0
2	H	63/102 (61%)	-0.19	1 (1%) 72 70	35, 59, 81, 95	0
All	All	1104/1365 (80%)	-0.48	26 (2%) 59 56	13, 39, 99, 128	1 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	67	PRO	3.9
2	E	66	ARG	3.8
2	E	17	ARG	3.7
2	D	69	SER	3.5
2	F	67	PRO	3.4
2	C	6	SER	3.3
2	D	17	ARG	3.1
2	E	6	SER	3.0
2	C	66	ARG	3.0
2	G	17	ARG	2.9
2	G	5	GLN	2.9
2	D	10	PRO	2.8
2	D	19	ARG	2.7
2	C	17	ARG	2.7
2	D	49	THR	2.7
1	A	27	ASP	2.5
2	G	48	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	19	ARG	2.4
2	E	49	THR	2.3
1	A	713	GLN	2.3
2	H	48	ASN	2.3
2	G	19	ARG	2.2
2	C	68	VAL	2.1
2	F	19	ARG	2.0
2	G	66	ARG	2.0
2	E	37	GLU	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](#)

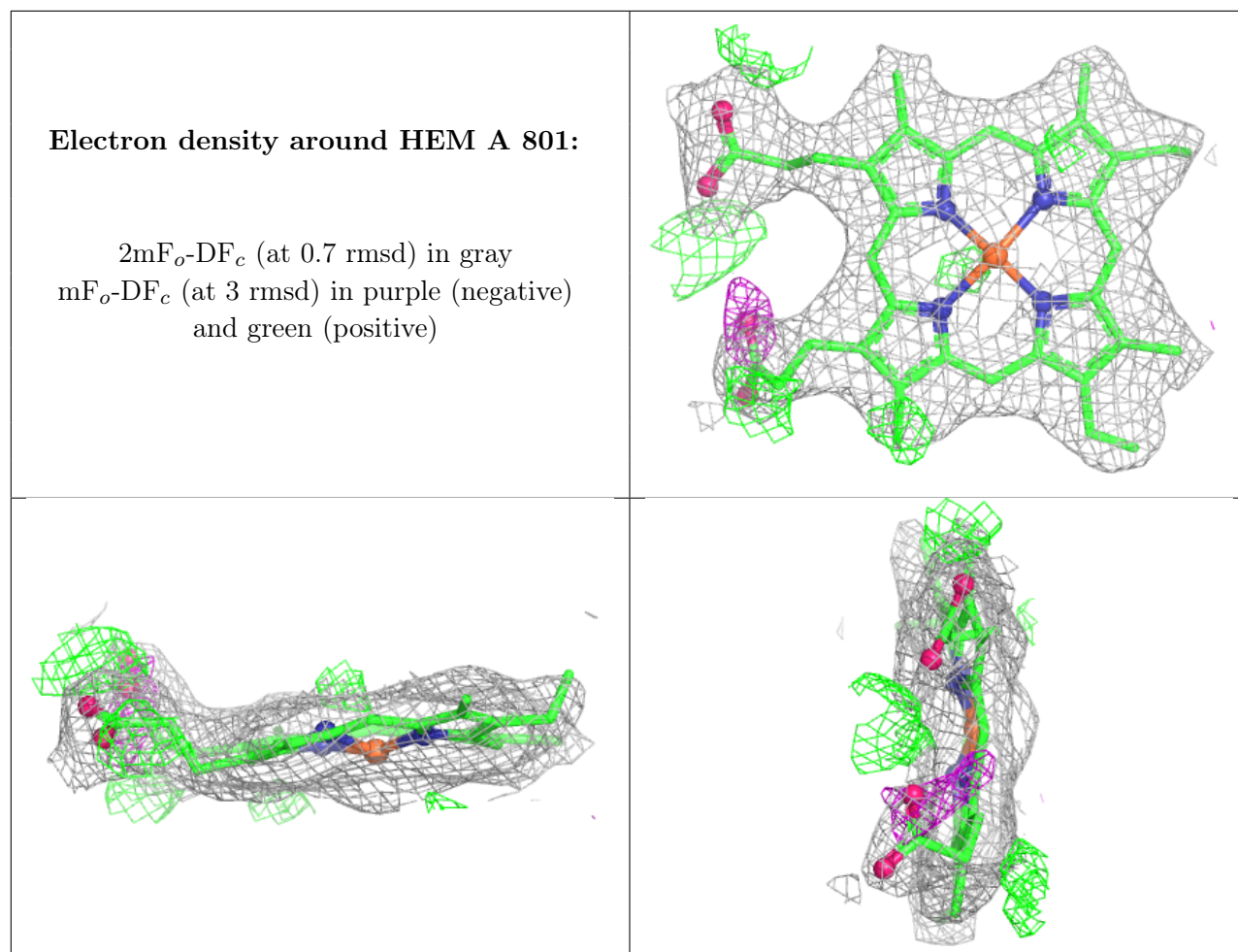
There are no monosaccharides in this entry.

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(\AA^2)	Q<0.9
3	HEM	A	801	43/43	0.98	0.13	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.