



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 05:14 AM GMT

PDB ID : 4FVC
Title : HmoB structure with heme
Authors : Park, S.
Deposited on : 2012-06-29
Resolution : 1.75 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

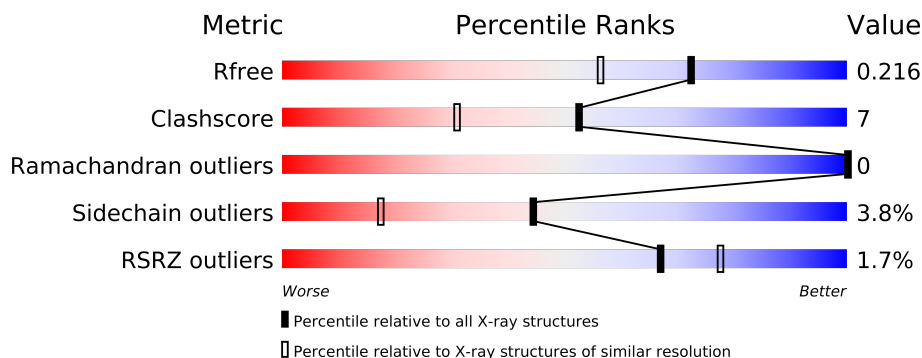
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance




The reported resolution of this entry is 1.75 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}	66092	1134 (1.76-1.76)
Clashscore	79885	1304 (1.76-1.76)
Ramachandran outliers	78287	1288 (1.76-1.76)
Sidechain outliers	78261	1288 (1.76-1.76)
RSRZ outliers	66119	1135 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	166	
1	B	166	
1	C	166	
1	D	166	
1	E	166	
1	F	166	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8378 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Putative uncharacterized protein yhgC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1202	774	199	227	2			
1	B	149	Total	C	N	O	S	0	0	0
			1202	774	199	227	2			
1	C	149	Total	C	N	O	S	0	0	0
			1202	774	199	227	2			
1	D	149	Total	C	N	O	S	0	0	0
			1202	774	199	227	2			
1	E	151	Total	C	N	O	S	0	0	0
			1218	783	201	232	2			
1	F	154	Total	C	N	O	S	0	0	0
			1236	794	204	236	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	ALA	ASN	CONFLICT	UNP E0TXX3
A	163	PHE	SER	CONFLICT	UNP E0TXX3
B	70	ALA	ASN	CONFLICT	UNP E0TXX3
B	163	PHE	SER	CONFLICT	UNP E0TXX3
C	70	ALA	ASN	CONFLICT	UNP E0TXX3
C	163	PHE	SER	CONFLICT	UNP E0TXX3
D	70	ALA	ASN	CONFLICT	UNP E0TXX3
D	163	PHE	SER	CONFLICT	UNP E0TXX3
E	70	ALA	ASN	CONFLICT	UNP E0TXX3
E	163	PHE	SER	CONFLICT	UNP E0TXX3
F	70	ALA	ASN	CONFLICT	UNP E0TXX3
F	163	PHE	SER	CONFLICT	UNP E0TXX3

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 3 is water.

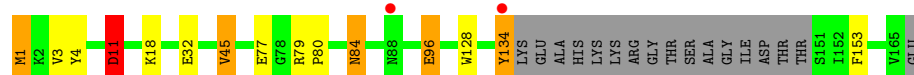
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	156	Total	O	0	0
			156	156		
3	B	136	Total	O	0	0
			136	136		
3	C	139	Total	O	0	0
			139	139		
3	D	132	Total	O	0	0
			132	132		
3	E	142	Total	O	0	0
			142	142		
3	F	153	Total	O	0	0
			153	153		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

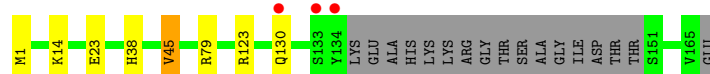
- Molecule 1: Putative uncharacterized protein yhgC

Chain A: 



- Molecule 1: Putative uncharacterized protein yhgC

Chain B: 



- Molecule 1: Putative uncharacterized protein yhgC

Chain C: 



- Molecule 1: Putative uncharacterized protein yhgC

Chain D: 



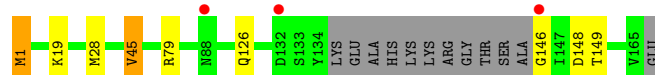
- Molecule 1: Putative uncharacterized protein yhgC

Chain E: 



- Molecule 1: Putative uncharacterized protein yhgC

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.82Å 117.52Å 70.85Å 90.00° 91.22° 90.00°	Depositor
Resolution (Å)	19.58 – 1.75 19.58 – 1.75	Depositor EDS
% Data completeness (in resolution range)	95.3 (19.58-1.75) 95.3 (19.58-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.98 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.199 , 0.233 0.201 , 0.216	Depositor DCC
R_{free} test set	5581 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 29.3	EDS
Estimated twinning fraction	0.014 for l,k,-h 0.021 for h,-k,-l 0.479 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 111527 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8378	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.87	1/1231 (0.1%)	1.14	6/1671 (0.4%)
1	B	0.77	0/1231	0.84	3/1671 (0.2%)
1	C	0.83	0/1231	1.05	5/1671 (0.3%)
1	D	0.85	0/1231	1.09	5/1671 (0.3%)
1	E	0.82	2/1247 (0.2%)	1.00	5/1693 (0.3%)
1	F	0.83	0/1265	1.02	4/1718 (0.2%)
All	All	0.83	3/7436 (0.0%)	1.03	28/10095 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	ASP	CB-CG	5.53	1.63	1.51
1	E	155	ARG	CD-NE	-5.27	1.37	1.46
1	E	155	ARG	CG-CD	5.21	1.65	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ARG	NE-CZ-NH2	-21.44	109.58	120.30
1	D	79	ARG	NE-CZ-NH1	21.23	130.91	120.30
1	A	79	ARG	NE-CZ-NH1	20.87	130.74	120.30
1	E	155	ARG	NE-CZ-NH2	-20.46	110.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	79	ARG	NE-CZ-NH1	19.94	130.27	120.30
1	D	79	ARG	NE-CZ-NH2	-19.89	110.35	120.30
1	C	79	ARG	NE-CZ-NH2	-18.80	110.90	120.30
1	F	79	ARG	NE-CZ-NH1	18.54	129.57	120.30
1	F	79	ARG	NE-CZ-NH2	-16.77	111.92	120.30
1	E	155	ARG	NE-CZ-NH1	11.39	126.00	120.30
1	B	79	ARG	NE-CZ-NH1	10.54	125.57	120.30
1	A	11	ASP	CB-CG-OD1	9.57	126.92	118.30
1	E	155	ARG	CG-CD-NE	-8.49	93.97	111.80
1	D	79	ARG	CD-NE-CZ	8.28	135.19	123.60
1	A	79	ARG	CD-NE-CZ	8.02	134.83	123.60
1	B	79	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	E	45	VAL	CG1-CB-CG2	7.67	123.17	110.90
1	C	79	ARG	CD-NE-CZ	7.49	134.08	123.60
1	F	79	ARG	CD-NE-CZ	7.01	133.41	123.60
1	D	45	VAL	CG1-CB-CG2	6.94	122.00	110.90
1	B	45	VAL	CG1-CB-CG2	6.62	121.50	110.90
1	F	45	VAL	CG1-CB-CG2	6.61	121.47	110.90
1	E	155	ARG	CD-NE-CZ	5.86	131.81	123.60
1	A	45	VAL	CG1-CB-CG2	5.70	120.02	110.90
1	C	45	VAL	CG1-CB-CG2	5.67	119.97	110.90
1	D	79	ARG	CB-CG-CD	5.35	125.51	111.60
1	A	84	ASN	CB-CA-C	5.18	120.76	110.40
1	C	79	ARG	CB-CG-CD	5.10	124.86	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	155	ARG	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1202	0	0	14	0
1	B	1202	0	0	6	0
1	C	1202	0	0	6	0
1	D	1202	0	0	10	1
1	E	1218	0	0	8	0
1	F	1236	0	0	6	0
2	A	43	0	0	2	0
2	B	43	0	0	0	0
2	C	43	0	0	1	0
2	D	43	0	0	0	0
2	E	43	0	0	2	0
2	F	43	0	0	0	0
3	A	156	0	0	11	0
3	B	136	0	0	4	0
3	C	139	0	0	4	0
3	D	132	0	0	8	0
3	E	142	0	0	4	1
3	F	153	0	0	7	0
All	All	8378	0	0	53	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (53) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:96:GLU:OE2	1:A:128:TRP:CD1	1.72	1.42
1:D:151:SER:N	3:D:368:HOH:O	1.99	0.93
1:A:1:MET:N	3:A:454:HOH:O	2.05	0.90
1:A:134:TYR:O	3:A:379:HOH:O	1.98	0.81
1:B:14:LYS:NZ	3:B:378:HOH:O	2.13	0.81
1:A:11:ASP:OD2	3:A:384:HOH:O	1.96	0.81
1:D:126:GLN:NE2	3:D:393:HOH:O	2.14	0.80
1:E:1:MET:N	3:E:366:HOH:O	2.17	0.78
1:E:26:LEU:CD1	1:E:28:MET:CE	2.63	0.77
1:D:39:GLU:OE2	3:D:344:HOH:O	2.08	0.70
1:D:1:MET:CG	3:F:338:HOH:O	2.38	0.70
1:C:96:GLU:OE2	1:C:133:SER:OG	2.11	0.69
1:F:1:MET:CB	3:F:317:HOH:O	2.41	0.68
1:C:1:MET:N	3:C:301:HOH:O	2.27	0.68
1:D:1:MET:N	3:D:309:HOH:O	2.28	0.66
1:A:84:ASN:CB	3:A:315:HOH:O	2.45	0.64
1:A:153:PHE:CZ	2:A:201:HEM:CB	2.83	0.61
1:D:98:GLY:N	3:D:423:HOH:O	2.32	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:77:GLU:CG	3:E:416:HOH:O	2.49	0.60
1:C:1:MET:N	3:C:431:HOH:O	2.33	0.60
1:C:151:SER:N	3:C:429:HOH:O	2.34	0.59
1:B:123:ARG:CD	3:B:429:HOH:O	2.50	0.59
1:A:1:MET:CE	3:A:399:HOH:O	2.51	0.58
1:F:146:GLY:N	3:F:437:HOH:O	2.36	0.58
1:A:3:VAL:CG1	3:A:434:HOH:O	2.53	0.57
1:D:84:ASN:OD1	3:D:395:HOH:O	2.18	0.54
1:B:123:ARG:NH1	3:B:341:HOH:O	2.41	0.54
1:C:92:LYS:CB	3:C:390:HOH:O	2.57	0.53
1:F:148:ASP:CG	1:F:149:THR:N	2.63	0.52
1:D:39:GLU:CG	3:D:344:HOH:O	2.58	0.51
1:F:1:MET:N	3:F:306:HOH:O	2.44	0.50
1:A:1:MET:N	3:A:302:HOH:O	2.44	0.50
1:A:11:ASP:CG	3:A:384:HOH:O	2.47	0.50
1:E:111:ASP:OD1	1:E:155:ARG:NH2	2.46	0.48
1:F:148:ASP:CB	3:F:396:HOH:O	2.61	0.48
1:A:128:TRP:CZ2	1:A:134:TYR:CB	2.98	0.47
1:D:130:GLN:NE2	3:D:393:HOH:O	2.47	0.47
3:A:455:HOH:O	1:B:1:MET:N	2.48	0.47
1:D:1:MET:CB	3:F:317:HOH:O	2.63	0.46
1:B:123:ARG:NE	3:B:429:HOH:O	2.50	0.45
1:A:4:TYR:O	3:A:434:HOH:O	2.21	0.44
1:A:80:PRO:O	1:A:84:ASN:ND2	2.51	0.44
2:C:201:HEM:CBC	2:C:201:HEM:CMC	2.96	0.43
1:C:128:TRP:CZ2	1:C:134:TYR:CB	3.01	0.43
1:E:28:MET:CE	3:E:344:HOH:O	2.67	0.42
1:A:11:ASP:CB	3:A:350:HOH:O	2.68	0.42
1:F:19:LYS:NZ	3:F:440:HOH:O	2.53	0.42
1:E:128:TRP:CD1	1:E:133:SER:OG	2.72	0.42
1:E:153:PHE:CZ	2:E:201:HEM:CBC	3.03	0.41
2:A:201:HEM:CBC	2:A:201:HEM:CHD	2.99	0.41
2:E:201:HEM:CBB	2:E:201:HEM:CHC	2.98	0.41
1:E:3:VAL:CG2	3:E:402:HOH:O	2.69	0.41
1:B:23:GLU:OE1	1:B:38:HIS:CE1	2.73	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:123:ARG:NH2	3:E:408:HOH:O[1_454]	2.09	0.11

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	145/166 (87%)	144 (99%)	1 (1%)	0	100	100
1	B	145/166 (87%)	143 (99%)	2 (1%)	0	100	100
1	C	145/166 (87%)	143 (99%)	2 (1%)	0	100	100
1	D	145/166 (87%)	144 (99%)	1 (1%)	0	100	100
1	E	147/166 (89%)	146 (99%)	1 (1%)	0	100	100
1	F	150/166 (90%)	148 (99%)	2 (1%)	0	100	100
All	All	877/996 (88%)	868 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	130/143 (91%)	122 (94%)	8 (6%)	26	6
1	B	130/143 (91%)	128 (98%)	2 (2%)	76	59
1	C	130/143 (91%)	125 (96%)	5 (4%)	44	17
1	D	130/143 (91%)	124 (95%)	6 (5%)	37	12
1	E	132/143 (92%)	127 (96%)	5 (4%)	44	17
1	F	134/143 (94%)	130 (97%)	4 (3%)	53	25
All	All	786/858 (92%)	756 (96%)	30 (4%)	44	17

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	11	ASP
1	A	18	LYS
1	A	32	GLU
1	A	45	VAL
1	A	77	GLU
1	A	96	GLU
1	A	134	TYR
1	B	45	VAL
1	B	130	GLN
1	C	32	GLU
1	C	45	VAL
1	C	47	GLN
1	C	87	LYS
1	C	88	ASN
1	D	1	MET
1	D	45	VAL
1	D	60	GLU
1	D	81	LEU
1	D	85	LYS
1	D	92	LYS
1	E	19	LYS
1	E	45	VAL
1	E	62	LYS
1	E	155	ARG
1	E	166	GLU
1	F	1	MET
1	F	28	MET
1	F	45	VAL
1	F	126	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry

6 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	201	1	49,50,50	2.36	13 (26%)	46,82,82	1.85	8 (17%)
2	HEM	B	201	1	49,50,50	2.32	13 (26%)	46,82,82	1.85	7 (15%)
2	HEM	C	201	1	49,50,50	2.26	15 (30%)	46,82,82	2.07	9 (19%)
2	HEM	D	201	1	49,50,50	2.28	13 (26%)	46,82,82	2.23	12 (26%)
2	HEM	E	201	1	49,50,50	2.38	14 (28%)	46,82,82	1.96	9 (19%)
2	HEM	F	201	1	49,50,50	2.33	14 (28%)	46,82,82	2.43	13 (28%)

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	201	1	-	0/14/114/114	0/0/8/8
2	HEM	B	201	1	-	0/14/114/114	0/0/8/8
2	HEM	C	201	1	-	0/14/114/114	0/0/8/8
2	HEM	D	201	1	-	0/14/114/114	0/0/8/8
2	HEM	E	201	1	-	0/14/114/114	0/0/8/8
2	HEM	F	201	1	-	0/14/114/114	0/0/8/8

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	HEM	C3C-C2C	-7.01	1.31	1.43
2	F	201	HEM	C3C-C2C	-6.54	1.32	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201	HEM	C3B-C2B	-6.49	1.32	1.43
2	A	201	HEM	C3C-C2C	-6.43	1.32	1.43
2	E	201	HEM	C2B-C1B	6.43	1.46	1.44
2	A	201	HEM	C3B-C2B	-6.20	1.32	1.43
2	B	201	HEM	C2B-C1B	5.94	1.46	1.44
2	B	201	HEM	C3B-C2B	-5.90	1.33	1.43
2	B	201	HEM	C3C-C2C	-5.83	1.33	1.43
2	C	201	HEM	C3C-C2C	-5.78	1.33	1.43
2	E	201	HEM	C3B-C2B	-5.75	1.33	1.43
2	E	201	HEM	C3C-C2C	-5.71	1.33	1.43
2	E	201	HEM	C3D-C2D	5.46	1.53	1.43
2	C	201	HEM	C3D-C2D	5.42	1.53	1.43
2	A	201	HEM	C3D-C2D	5.41	1.53	1.43
2	B	201	HEM	C3D-C2D	5.29	1.53	1.43
2	F	201	HEM	C3B-C2B	-5.21	1.34	1.43
2	F	201	HEM	C3D-C2D	5.21	1.52	1.43
2	D	201	HEM	C3B-C2B	-5.17	1.34	1.43
2	D	201	HEM	C3D-C2D	5.12	1.52	1.43
2	A	201	HEM	C2B-C1B	4.99	1.45	1.44
2	A	201	HEM	C3B-CAB	4.98	1.56	1.40
2	E	201	HEM	C3B-CAB	4.79	1.55	1.40
2	B	201	HEM	C3B-CAB	4.72	1.55	1.40
2	B	201	HEM	C4A-C3A	4.70	1.46	1.40
2	D	201	HEM	C2D-C1D	-4.53	1.43	1.44
2	F	201	HEM	C2D-C1D	-4.51	1.43	1.44
2	A	201	HEM	C4A-C3A	4.50	1.45	1.40
2	D	201	HEM	C3C-CAC	4.27	1.53	1.40
2	E	201	HEM	C3C-CAC	4.26	1.53	1.40
2	C	201	HEM	C3B-CAB	4.16	1.53	1.40
2	F	201	HEM	C3C-CAC	4.15	1.53	1.40
2	F	201	HEM	C3B-CAB	4.14	1.53	1.40
2	B	201	HEM	C3C-CAC	4.02	1.53	1.40
2	D	201	HEM	C3B-CAB	3.97	1.52	1.40
2	C	201	HEM	C3C-CAC	3.96	1.52	1.40
2	C	201	HEM	C4A-C3A	3.92	1.45	1.40
2	F	201	HEM	FE-NA	3.85	2.09	1.92
2	E	201	HEM	C4A-C3A	3.84	1.45	1.40
2	F	201	HEM	FE-NC	3.79	2.12	1.97
2	E	201	HEM	C3D-C4D	3.77	1.45	1.44
2	A	201	HEM	C3C-CAC	3.70	1.52	1.40
2	F	201	HEM	C4A-C3A	3.64	1.44	1.40
2	D	201	HEM	C4A-C3A	3.56	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	HEM	FE-NA	3.48	2.07	1.92
2	C	201	HEM	C3D-C4D	3.17	1.45	1.44
2	F	201	HEM	C2B-C1B	-3.12	1.43	1.44
2	F	201	HEM	CMB-C2B	3.09	1.57	1.47
2	A	201	HEM	CAA-C2A	3.07	1.57	1.52
2	B	201	HEM	FE-NC	3.06	2.09	1.97
2	D	201	HEM	CMD-C2D	3.04	1.56	1.47
2	C	201	HEM	FE-NA	2.98	2.05	1.92
2	E	201	HEM	FE-NC	2.92	2.08	1.97
2	D	201	HEM	CMB-C2B	2.90	1.56	1.47
2	C	201	HEM	C2B-C1B	2.90	1.45	1.44
2	D	201	HEM	C2B-C1B	-2.84	1.43	1.44
2	B	201	HEM	CMC-C2C	2.72	1.55	1.47
2	D	201	HEM	CMC-C2C	2.69	1.55	1.47
2	F	201	HEM	CMC-C2C	2.69	1.55	1.47
2	E	201	HEM	CMD-C2D	2.68	1.55	1.47
2	C	201	HEM	FE-ND	2.68	2.07	1.97
2	E	201	HEM	CMC-C2C	2.65	1.55	1.47
2	B	201	HEM	CMD-C2D	2.63	1.55	1.47
2	D	201	HEM	FE-NC	2.58	2.07	1.97
2	C	201	HEM	CMD-C2D	2.56	1.55	1.47
2	A	201	HEM	CMB-C2B	2.56	1.55	1.47
2	A	201	HEM	CMD-C2D	2.55	1.55	1.47
2	C	201	HEM	CMB-C2B	2.54	1.55	1.47
2	C	201	HEM	CMC-C2C	2.54	1.55	1.47
2	E	201	HEM	CMB-C2B	2.47	1.55	1.47
2	F	201	HEM	CMD-C2D	2.41	1.54	1.47
2	C	201	HEM	CAA-C2A	2.31	1.56	1.52
2	E	201	HEM	FE-NA	2.31	2.02	1.92
2	F	201	HEM	FE-ND	2.30	2.06	1.97
2	A	201	HEM	FE-NC	2.27	2.06	1.97
2	A	201	HEM	CMC-C2C	2.26	1.54	1.47
2	A	201	HEM	FE-ND	2.24	2.06	1.97
2	B	201	HEM	CAA-C2A	2.19	1.55	1.52
2	E	201	HEM	FE-NB	2.14	2.05	1.97
2	B	201	HEM	CMB-C2B	2.13	1.54	1.47
2	C	201	HEM	CHB-C1B	2.13	1.38	1.35
2	B	201	HEM	FE-NA	2.07	2.01	1.92

All (58) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	201	HEM	C3B-C4B-NB	-8.98	107.58	114.00
2	C	201	HEM	C3B-C4B-NB	-8.14	108.18	114.00
2	D	201	HEM	C3B-C4B-NB	-7.70	108.49	114.00
2	E	201	HEM	C3B-C4B-NB	-7.52	108.62	114.00
2	B	201	HEM	C3B-C4B-NB	-7.40	108.70	114.00
2	F	201	HEM	C4D-ND-C1D	6.61	111.93	105.16
2	A	201	HEM	C3B-C4B-NB	-6.06	109.66	114.00
2	C	201	HEM	C4D-ND-C1D	5.90	111.20	105.16
2	A	201	HEM	C4D-ND-C1D	5.79	111.08	105.16
2	D	201	HEM	C4D-ND-C1D	5.70	111.00	105.16
2	D	201	HEM	CHD-C1D-ND	5.21	128.91	124.58
2	E	201	HEM	C4D-ND-C1D	4.83	110.11	105.16
2	B	201	HEM	C4D-ND-C1D	4.80	110.08	105.16
2	C	201	HEM	CBA-CAA-C2A	-4.64	104.51	112.69
2	F	201	HEM	CHD-C1D-ND	4.64	128.44	124.58
2	F	201	HEM	CBA-CAA-C2A	-4.57	104.64	112.69
2	D	201	HEM	CBA-CAA-C2A	-4.45	104.86	112.69
2	B	201	HEM	CBA-CAA-C2A	-4.41	104.92	112.69
2	E	201	HEM	CBA-CAA-C2A	-4.40	104.94	112.69
2	F	201	HEM	C2D-C1D-ND	-3.92	108.31	112.93
2	A	201	HEM	CBA-CAA-C2A	-3.91	105.80	112.69
2	A	201	HEM	C2D-C1D-ND	-3.84	108.39	112.93
2	F	201	HEM	CHC-C4B-NB	3.64	127.61	124.58
2	C	201	HEM	C2D-C1D-ND	-3.34	108.98	112.93
2	D	201	HEM	C2D-C1D-ND	-3.27	109.07	112.93
2	A	201	HEM	C1A-CHA-C4D	-3.27	123.17	127.47
2	C	201	HEM	C4A-CHB-C1B	-3.13	123.36	127.47
2	F	201	HEM	CMA-C3A-C4A	-3.04	123.94	128.62
2	E	201	HEM	CMA-C3A-C4A	-2.94	124.10	128.62
2	E	201	HEM	CHD-C1D-ND	2.93	127.02	124.58
2	E	201	HEM	C4A-CHB-C1B	-2.90	123.66	127.47
2	D	201	HEM	CMA-C3A-C4A	-2.82	124.28	128.62
2	A	201	HEM	CBD-CAD-C3D	-2.78	108.31	114.37
2	C	201	HEM	C4C-NC-C1C	2.75	108.39	105.53
2	F	201	HEM	C4C-NC-C1C	2.72	108.37	105.53
2	F	201	HEM	C4A-NA-C1A	2.70	110.32	106.76
2	C	201	HEM	CMA-C3A-C4A	-2.69	124.49	128.62
2	B	201	HEM	CHD-C1D-ND	2.66	126.79	124.58
2	D	201	HEM	C4A-CHB-C1B	-2.62	124.02	127.47
2	E	201	HEM	C2D-C1D-ND	-2.62	109.84	112.93
2	E	201	HEM	CAD-C3D-C4D	2.53	129.07	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	201	HEM	C3A-C4A-NA	-2.53	107.50	109.41
2	C	201	HEM	CAD-C3D-C4D	2.51	129.04	124.53
2	B	201	HEM	C2D-C1D-ND	-2.50	109.98	112.93
2	D	201	HEM	CHC-C4B-NB	2.47	126.64	124.58
2	F	201	HEM	C4A-CHB-C1B	-2.39	124.33	127.47
2	F	201	HEM	CHA-C4D-ND	2.38	127.58	124.31
2	A	201	HEM	C4C-NC-C1C	2.38	108.01	105.53
2	B	201	HEM	CMA-C3A-C4A	-2.37	124.97	128.62
2	F	201	HEM	C2A-C1A-NA	-2.29	106.55	109.73
2	B	201	HEM	C4A-CHB-C1B	-2.27	124.48	127.47
2	A	201	HEM	CHD-C1D-ND	2.21	126.42	124.58
2	D	201	HEM	C1A-CHA-C4D	-2.15	124.65	127.47
2	D	201	HEM	CMA-C3A-C2A	2.14	128.98	124.94
2	D	201	HEM	CHA-C4D-ND	2.12	127.21	124.31
2	D	201	HEM	O2A-CGA-CBA	2.07	121.54	114.22
2	E	201	HEM	C4C-NC-C1C	2.06	107.67	105.53
2	C	201	HEM	C1A-CHA-C4D	-2.06	124.77	127.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	149/166 (89%)	0.12	2 (1%) 74 84	14, 22, 38, 47	0
1	B	149/166 (89%)	0.12	3 (2%) 62 73	14, 24, 40, 66	0
1	C	149/166 (89%)	0.12	4 (2%) 52 62	13, 22, 38, 48	0
1	D	149/166 (89%)	0.05	2 (1%) 74 84	13, 22, 36, 47	0
1	E	151/166 (90%)	0.14	1 (0%) 84 91	13, 23, 46, 61	0
1	F	154/166 (92%)	0.13	3 (1%) 64 74	13, 23, 44, 48	0
All	All	901/996 (90%)	0.11	15 (1%) 67 77	13, 23, 39, 66	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	146	GLY	3.4
1	C	134	TYR	3.2
1	B	134	TYR	2.9
1	B	133	SER	2.9
1	A	88	ASN	2.8
1	F	132	ASP	2.6
1	C	88	ASN	2.5
1	D	88	ASN	2.5
1	C	90	ALA	2.4
1	A	134	TYR	2.4
1	D	132	ASP	2.2
1	C	87	LYS	2.2
1	E	87	LYS	2.1
1	F	88	ASN	2.0
1	B	130	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	HEM	F	201	43/43	0.13	0.47	20,23,39,48	0
2	HEM	B	201	43/43	0.12	0.42	24,29,45,50	0
2	HEM	D	201	43/43	0.12	0.31	20,23,37,46	0
2	HEM	E	201	43/43	0.12	0.20	26,30,46,52	0
2	HEM	C	201	43/43	0.13	0.19	21,29,47,53	0
2	HEM	A	201	43/43	0.12	0.16	19,27,44,50	0

6.5 Other polymers ⓘ

There are no such residues in this entry.