



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:30 PM GMT

PDB ID : 4IJ2  
Title : Human methemoglobin in complex with the second and third NEAT domains of IsdH from Staphylococcus aureus  
Authors : Dickson, C.F.; Jacques, D.A.; Guss, J.M.; Gell, D.A.  
Deposited on : 2012-12-21  
Resolution : 4.24 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

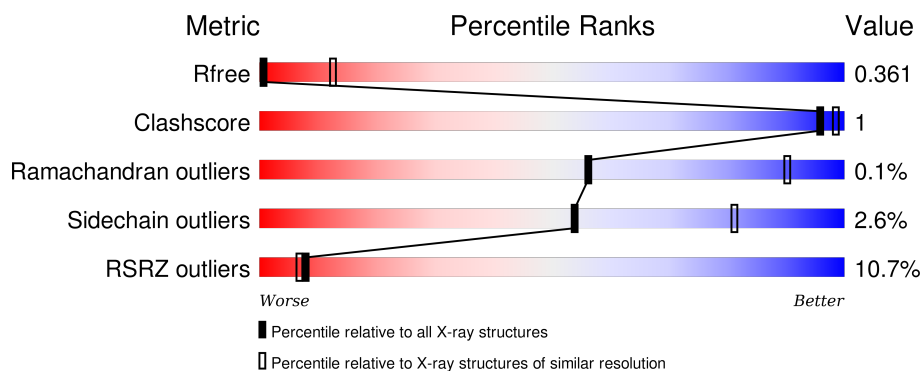
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.24 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))
$R_{free}$	91344	1041 (4.84-3.60)
Clashscore	102246	1143 (4.84-3.60)
Ramachandran outliers	100387	1086 (4.84-3.60)
Sidechain outliers	100360	1070 (4.84-3.60)
RSRZ outliers	91569	1045 (4.84-3.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	141	<div> <div>7%</div> <div>92%</div> <div>6%</div> </div>
1	C	141	<div> <div>%</div> <div>92%</div> <div>6%</div> </div>
2	B	146	<div> <div>5%</div> <div>94%</div> <div>6%</div> </div>
2	D	146	<div> <div>5%</div> <div>94%</div> <div>6%</div> </div>
3	E	336	<div> <div>9%</div> <div>83%</div> <div>7%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	336	
3	G	336	
3	H	336	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	HEM	A	201	-	-	-	X
4	HEM	B	201	-	-	-	X
4	HEM	C	201	-	-	-	X
4	HEM	D	201	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13547 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 Hemoglobin subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	0	0	0
			1044	670	181	190	3			
1	C	139	Total	C	N	O	S	0	0	0
			1044	670	181	190	3			

- Molecule 2 is a protein called Hemoglobin subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			
2	D	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			

- Molecule 3 is a protein called Iron-regulated surface determinant protein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	300	Total	C	N	O	S	0	0	0
			2456	1577	401	474	4			
3	F	309	Total	C	N	O	S	0	0	0
			2515	1612	412	487	4			
3	G	300	Total	C	N	O	S	0	0	0
			2456	1577	401	474	4			
3	H	197	Total	C	N	O	S	0	0	0
			1614	1035	264	313	2			

There are 8 discrepancies between the modelled and reference sequences:

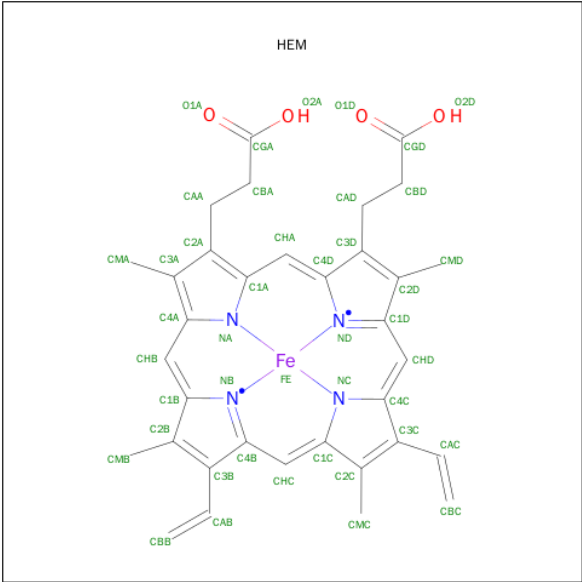
Chain	Residue	Modelled	Actual	Comment	Reference
E	325	SER	-	EXPRESSION TAG	UNP Q2FG07
E	642	ALA	TYR	ENGINEERED MUTATION	UNP Q2FG07
F	325	SER	-	EXPRESSION TAG	UNP Q2FG07
F	642	ALA	TYR	ENGINEERED MUTATION	UNP Q2FG07

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Chain	Residue	Modelled	Actual	Comment	Reference
G	325	SER	-	EXPRESSION TAG	UNP Q2FG07
G	642	ALA	TYR	ENGINEERED MUTATION	UNP Q2FG07
H	325	SER	-	EXPRESSION TAG	UNP Q2FG07
H	642	ALA	TYR	ENGINEERED MUTATION	UNP Q2FG07

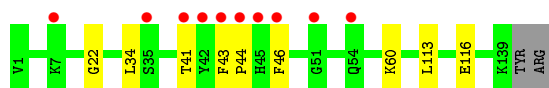
- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



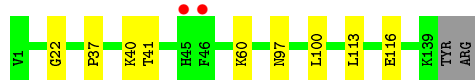
### 3 Residue-property plots [i](#)

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.

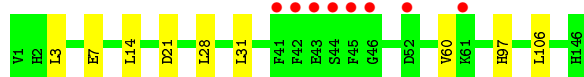
- Molecule 1: Hemoglobin subunit alpha



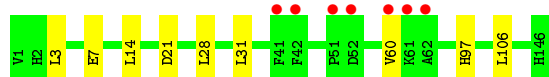
- Molecule 1: Hemoglobin subunit alpha



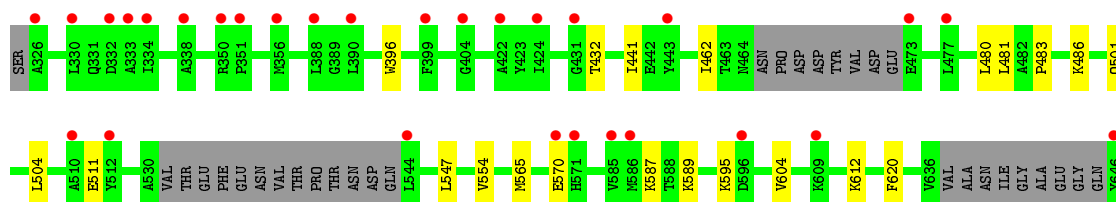
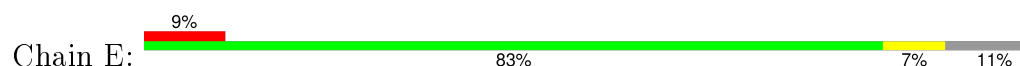
- Molecule 2: Hemoglobin subunit beta



- Molecule 2: Hemoglobin subunit beta



- Molecule 3: Iron-regulated surface determinant protein H





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.90 Å   185.30 Å   103.20 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	29.15 – 4.24 49.71 – 4.24	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.15-4.24) 98.2 (49.71-4.24)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 4.29 Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.299   ,   0.310 0.352   ,   0.361	Depositor DCC
$R_{free}$ test set	945 reflections (5.43%)	DCC
Wilson B-factor (Å <sup>2</sup> )	206.8	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30   ,   106.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 18574 reflections	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	13547	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.38	0/1071	0.50	0/1457
1	C	0.38	0/1071	0.50	0/1457
2	B	0.40	0/1153	0.50	0/1566
2	D	0.40	0/1153	0.50	0/1566
3	E	0.38	0/2509	0.51	0/3395
3	F	0.38	0/2569	0.51	0/3478
3	G	0.38	0/2509	0.51	0/3395
3	H	0.37	0/1649	0.50	0/2229
All	All	0.38	0/13684	0.50	0/18543

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1044	0	1047	5	0
1	C	1044	0	1047	5	0
2	B	1123	0	1118	5	0
2	D	1123	0	1118	6	0
3	E	2456	0	2425	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	2515	0	2482	8	0
3	G	2456	0	2425	5	0
3	H	1614	0	1595	3	0
4	A	43	0	30	0	0
4	B	43	0	30	1	0
4	C	43	0	30	0	0
4	D	43	0	30	1	0
All	All	13547	0	13377	40	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 1.

All (40) 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)
2:B:97:HIS:HB3	1:C:41:THR:HG22	1.73	0.70
2:B:3:LEU:HD23	2:B:7:GLU:HB3	1.77	0.67
2:D:3:LEU:HD23	2:D:7:GLU:HB3	1.77	0.66
2:B:106:LEU:HD23	4:B:201:HEM:HBB2	1.82	0.61
3:F:570:GLU:HG2	3:F:589:LYS:HE3	1.86	0.58
3:E:570:GLU:HG2	3:E:589:LYS:HE3	1.86	0.58
3:G:570:GLU:HG2	3:G:589:LYS:HE3	1.86	0.57
3:F:604:VAL:HG12	3:F:620:PHE:HB3	1.92	0.52
3:E:604:VAL:HG12	3:E:620:PHE:HB3	1.92	0.51
3:G:604:VAL:HG12	3:G:620:PHE:HB3	1.92	0.51
3:H:432:THR:HB	3:H:462:ILE:HD12	1.94	0.49
3:E:432:THR:HB	3:E:462:ILE:HD12	1.95	0.49
3:G:432:THR:HB	3:G:462:ILE:HD12	1.95	0.49
2:D:106:LEU:HD23	4:D:201:HEM:HBB2	1.96	0.48
3:F:432:THR:HB	3:F:462:ILE:HD12	1.95	0.48
3:F:490:LEU:HA	3:F:493:GLN:HE21	1.79	0.47
1:A:41:THR:HB	2:D:97:HIS:HB2	1.96	0.47
1:A:43:PHE:HB3	1:A:46:PHE:HB2	1.95	0.47
3:H:490:LEU:HD13	3:H:526:GLN:HE22	1.80	0.46
1:C:113:LEU:HB3	1:C:116:GLU:HB2	1.98	0.46
1:A:113:LEU:HB3	1:A:116:GLU:HB2	1.98	0.46
1:C:37:PRO:HA	1:C:40:LYS:HG3	1.98	0.45
1:C:97:ASN:HA	1:C:100:LEU:HD12	1.98	0.45
3:E:483:PRO:HA	3:E:486:LYS:HG2	1.97	0.45
3:F:483:PRO:HA	3:F:486:LYS:HG2	1.99	0.45
3:F:487:ALA:HB1	3:F:492:ARG:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:THR:HB	2:D:97:HIS:CB	2.47	0.44
3:E:554:VAL:HG11	3:E:565:MET:HB3	2.00	0.43
3:F:554:VAL:HG11	3:F:565:MET:HB3	2.00	0.43
2:D:31:LEU:HD22	2:D:106:LEU:HD13	2.00	0.43
1:A:22:GLY:HA3	1:A:60:LYS:HD2	2.01	0.42
3:G:554:VAL:HG11	3:G:565:MET:HB3	2.00	0.42
1:C:22:GLY:HA3	1:C:60:LYS:HD2	2.02	0.42
3:E:396:TRP:HA	3:E:441:ILE:HG22	2.02	0.41
3:H:396:TRP:HA	3:H:441:ILE:HG22	2.02	0.41
2:B:28:LEU:HD23	2:B:60:VAL:HG13	2.02	0.41
3:G:396:TRP:HA	3:G:441:ILE:HG22	2.02	0.41
2:D:28:LEU:HD23	2:D:60:VAL:HG13	2.02	0.41
2:B:31:LEU:HD22	2:B:106:LEU:HD13	2.02	0.40
3:F:396:TRP:HA	3:F:441:ILE:HG22	2.02	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	137/141 (97%)	131 (96%)	5 (4%)	1 (1%)	26	71
1	C	137/141 (97%)	131 (96%)	6 (4%)	0	100	100
2	B	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
2	D	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
3	E	292/336 (87%)	281 (96%)	11 (4%)	0	100	100
3	F	303/336 (90%)	291 (96%)	12 (4%)	0	100	100
3	G	292/336 (87%)	281 (96%)	11 (4%)	0	100	100
3	H	193/336 (57%)	186 (96%)	7 (4%)	0	100	100
All	All	1642/1918 (86%)	1579 (96%)	62 (4%)	1 (0%)	56	90

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	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	110/113 (97%)	109 (99%)	1 (1%)	84	93
1	C	110/113 (97%)	110 (100%)	0	100	100
2	B	118/118 (100%)	116 (98%)	2 (2%)	68	88
2	D	118/118 (100%)	116 (98%)	2 (2%)	68	88
3	E	271/305 (89%)	261 (96%)	10 (4%)	41	75
3	F	276/305 (90%)	266 (96%)	10 (4%)	42	76
3	G	271/305 (89%)	262 (97%)	9 (3%)	45	78
3	H	175/305 (57%)	171 (98%)	4 (2%)	58	83
All	All	1449/1682 (86%)	1411 (97%)	38 (3%)	54	81

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
2	B	14	LEU
2	B	21	ASP
2	D	14	LEU
2	D	21	ASP
3	E	480	LEU
3	E	481	LEU
3	E	501	GLN
3	E	504	LEU
3	E	511	GLU
3	E	547	LEU
3	E	587	LYS
3	E	595	LYS

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Mol	Chain	Res	Type
3	E	612	LYS
3	E	652	ASN
3	F	480	LEU
3	F	492	ARG
3	F	501	GLN
3	F	504	LEU
3	F	511	GLU
3	F	547	LEU
3	F	587	LYS
3	F	595	LYS
3	F	612	LYS
3	F	652	ASN
3	G	480	LEU
3	G	493	GLN
3	G	504	LEU
3	G	511	GLU
3	G	547	LEU
3	G	587	LYS
3	G	595	LYS
3	G	612	LYS
3	G	652	ASN
3	H	480	LEU
3	H	501	GLN
3	H	504	LEU
3	H	511	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	97	ASN
2	B	39	GLN
2	B	63	HIS
1	C	58	HIS
2	D	39	GLN
2	D	63	HIS
3	F	493	GLN
3	G	478	GLN
3	H	493	GLN
3	H	526	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 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	$\# Z  > 2$
4	HEM	A	201	1	30,50,50	2.19	11 (36%)	24,82,82	2.26	8 (33%)
4	HEM	B	201	2	30,50,50	2.17	11 (36%)	24,82,82	2.19	8 (33%)
4	HEM	C	201	1	30,50,50	2.20	10 (33%)	24,82,82	2.31	9 (37%)
4	HEM	D	201	2	30,50,50	2.21	12 (40%)	24,82,82	2.25	8 (33%)

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
4	HEM	A	201	1	-	0/10/54/54	0/0/8/8
4	HEM	B	201	2	-	0/10/54/54	0/0/8/8
4	HEM	C	201	1	-	0/10/54/54	0/0/8/8
4	HEM	D	201	2	-	0/10/54/54	0/0/8/8

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	201	HEM	C3B-C4B	-6.83	1.45	1.51
4	A	201	HEM	C3B-C4B	-6.74	1.45	1.51
4	B	201	HEM	C3B-C4B	-6.69	1.45	1.51
4	C	201	HEM	C3B-C4B	-6.59	1.46	1.51
4	A	201	HEM	C3D-C4D	-4.98	1.45	1.51
4	C	201	HEM	C3D-C4D	-4.80	1.45	1.51
4	D	201	HEM	C3D-C4D	-4.59	1.45	1.51
4	B	201	HEM	C3D-C4D	-4.48	1.45	1.51
4	D	201	HEM	C2C-C1C	-3.61	1.45	1.52
4	B	201	HEM	C2C-C1C	-3.58	1.45	1.52
4	C	201	HEM	C2C-C1C	-3.51	1.45	1.52
4	A	201	HEM	C2C-C1C	-3.51	1.45	1.52
4	D	201	HEM	C2D-C1D	-2.03	1.45	1.51
4	B	201	HEM	C1C-NC	2.06	1.38	1.36
4	A	201	HEM	C4C-NC	2.07	1.38	1.36
4	B	201	HEM	C4C-NC	2.08	1.38	1.36
4	B	201	HEM	FE-NB	2.09	2.08	1.97
4	A	201	HEM	FE-ND	2.09	2.08	1.97
4	C	201	HEM	C3C-CAC	2.12	1.55	1.51
4	D	201	HEM	C1C-NC	2.16	1.38	1.36
4	C	201	HEM	C4C-NC	2.17	1.38	1.36
4	A	201	HEM	C3C-CAC	2.18	1.55	1.51
4	B	201	HEM	C3C-CAC	2.21	1.55	1.51
4	B	201	HEM	CAA-C2A	2.21	1.55	1.52
4	C	201	HEM	CAA-C2A	2.21	1.55	1.52
4	D	201	HEM	CAA-C2A	2.21	1.55	1.52
4	A	201	HEM	C1C-NC	2.21	1.38	1.36
4	A	201	HEM	CAA-C2A	2.24	1.55	1.52
4	D	201	HEM	C3C-CAC	2.25	1.55	1.51
4	A	201	HEM	FE-NB	2.26	2.09	1.97
4	D	201	HEM	C4C-NC	2.27	1.38	1.36
4	D	201	HEM	FE-NB	2.28	2.09	1.97
4	D	201	HEM	C3B-CAB	2.38	1.55	1.51
4	C	201	HEM	C1C-NC	2.38	1.38	1.36
4	B	201	HEM	FE-ND	2.41	2.10	1.97
4	A	201	HEM	C3B-CAB	2.46	1.55	1.51
4	C	201	HEM	C3B-CAB	2.51	1.56	1.51
4	B	201	HEM	C3B-CAB	2.53	1.56	1.51
4	D	201	HEM	FE-ND	2.66	2.11	1.97
4	C	201	HEM	FE-NB	2.81	2.12	1.97
4	A	201	HEM	FE-NC	2.93	2.07	1.95
4	B	201	HEM	FE-NC	3.23	2.08	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	201	HEM	FE-NC	3.27	2.08	1.95
4	C	201	HEM	FE-NC	3.28	2.08	1.95

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	201	HEM	C3C-CAC-CBC	-2.86	120.07	124.46
4	C	201	HEM	C3C-CAC-CBC	-2.75	120.24	124.46
4	C	201	HEM	CBA-CAA-C2A	-2.21	108.56	112.53
4	D	201	HEM	C3C-CAC-CBC	-2.19	121.10	124.46
4	B	201	HEM	C3C-CAC-CBC	-2.15	121.16	124.46
4	A	201	HEM	C2D-C3D-C4D	2.05	104.97	101.50
4	C	201	HEM	C2D-C3D-C4D	2.08	105.02	101.50
4	A	201	HEM	C3B-C4B-CHC	2.10	126.11	123.16
4	B	201	HEM	C3B-C4B-CHC	2.21	126.27	123.16
4	D	201	HEM	C3B-C4B-CHC	2.29	126.39	123.16
4	C	201	HEM	C3B-C4B-CHC	2.32	126.43	123.16
4	B	201	HEM	C2D-C3D-C4D	2.36	105.49	101.50
4	D	201	HEM	C2D-C3D-C4D	2.41	105.58	101.50
4	A	201	HEM	CMD-C2D-C3D	2.83	126.89	114.35
4	C	201	HEM	CMD-C2D-C3D	2.89	127.12	114.35
4	D	201	HEM	CMD-C2D-C3D	2.93	127.29	114.35
4	B	201	HEM	CMD-C2D-C3D	2.93	127.32	114.35
4	B	201	HEM	CMB-C2B-C3B	3.56	125.42	116.53
4	D	201	HEM	CMB-C2B-C3B	3.64	125.62	116.53
4	A	201	HEM	CMB-C2B-C3B	3.91	126.30	116.53
4	C	201	HEM	CMB-C2B-C3B	3.95	126.39	116.53
4	A	201	HEM	CMC-C2C-C3C	3.99	126.48	116.53
4	C	201	HEM	CMC-C2C-C3C	4.00	126.51	116.53
4	B	201	HEM	CMC-C2C-C3C	4.12	126.82	116.53
4	D	201	HEM	CMC-C2C-C3C	4.12	126.83	116.53
4	C	201	HEM	CAD-C3D-C4D	4.17	127.18	112.47
4	A	201	HEM	CAD-C3D-C4D	4.20	127.30	112.47
4	D	201	HEM	CAD-C3D-C4D	4.33	127.73	112.47
4	B	201	HEM	CAD-C3D-C4D	4.43	128.09	112.47
4	B	201	HEM	CAD-C3D-C2D	4.57	126.36	113.22
4	D	201	HEM	CAD-C3D-C2D	4.68	126.67	113.22
4	A	201	HEM	CAD-C3D-C2D	5.04	127.72	113.22
4	C	201	HEM	CAD-C3D-C2D	5.07	127.79	113.22

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	201	HEM	1	0
4	D	201	HEM	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	139/141 (98%)	0.57	10 (7%)	18 13	14, 57, 197, 278	0
1	C	139/141 (98%)	0.07	2 (1%)	78 69	3, 47, 121, 147	0
2	B	146/146 (100%)	0.37	8 (5%)	29 22	4, 66, 153, 195	0
2	D	146/146 (100%)	0.31	7 (4%)	34 26	21, 73, 198, 273	0
3	E	300/336 (89%)	0.46	29 (9%)	10 8	39, 81, 185, 285	0
3	F	309/336 (91%)	0.79	55 (17%)	2 3	23, 80, 154, 272	0
3	G	300/336 (89%)	0.84	46 (15%)	3 4	41, 92, 184, 280	0
3	H	197/336 (58%)	0.62	23 (11%)	6 6	39, 91, 176, 286	0
All	All	1676/1918 (87%)	0.56	180 (10%)	8 7	3, 79, 172, 286	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	326	ALA	12.5
3	G	326	ALA	10.1
3	H	326	ALA	8.0
1	A	46	PHE	7.9
3	G	609	LYS	7.4
3	E	326	ALA	7.3
1	A	43	PHE	7.2
1	A	45	HIS	7.1
1	A	44	PRO	6.9
3	F	327	ASP	6.3
1	C	46	PHE	6.0
3	F	443	TYR	6.0
3	E	586	MET	6.0
3	G	616	ARG	5.9
1	C	45	HIS	5.7
3	G	544	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	42	TYR	5.6
3	G	343	GLU	5.5
3	G	345	THR	5.4
2	B	42	PHE	5.4
3	E	333	ALA	5.3
3	F	442	GLU	5.3
3	H	422	ALA	5.3
3	G	399	PHE	5.2
2	B	44	SER	5.1
2	B	45	PHE	5.1
3	G	344	HIS	4.8
3	G	608	SER	4.5
3	E	477	LEU	4.5
3	F	414	SER	4.5
3	G	330	LEU	4.5
3	E	544	LEU	4.5
3	G	587	LYS	4.4
3	H	327	ASP	4.4
2	B	43	GLU	4.4
3	H	452	ASP	4.2
3	G	351	PRO	4.2
3	H	413	VAL	4.1
3	G	422	ALA	4.1
3	G	327	ASP	4.1
3	H	455	LEU	4.0
3	G	586	MET	4.0
3	G	352	ILE	4.0
3	F	399	PHE	4.0
2	D	60	VAL	4.0
3	G	617	THR	4.0
3	G	433	ARG	3.9
3	G	549	GLU	3.8
3	F	445	GLU	3.8
3	G	462	ILE	3.8
3	E	646	TYR	3.8
3	H	444	GLY	3.7
3	F	627	ALA	3.7
3	F	582	LYS	3.7
3	G	512	TYR	3.7
3	F	581	GLN	3.7
3	G	396	TRP	3.6
1	A	41	THR	3.6

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Mol	Chain	Res	Type	RSRZ
3	E	351	PRO	3.5
3	F	377	VAL	3.5
3	F	421	TYR	3.5
3	F	441	ILE	3.5
3	F	608	SER	3.5
3	G	430	ASN	3.5
2	D	41	PHE	3.4
3	E	350	ARG	3.4
3	E	473	GLU	3.4
3	H	414	SER	3.4
3	H	489	THR	3.4
3	E	596	ASP	3.4
3	F	348	ASN	3.4
2	D	61	LYS	3.4
3	F	437	ILE	3.3
3	F	609	LYS	3.3
3	E	570	GLU	3.3
3	E	332	ASP	3.3
3	F	439	SER	3.2
3	H	412	LEU	3.2
3	H	446	ASN	3.2
3	E	388	LEU	3.2
3	H	528	LYS	3.2
3	E	424	ILE	3.2
3	E	356	MET	3.1
3	G	391	LYS	3.1
3	F	373	GLU	3.1
3	G	431	GLY	3.1
3	G	578	LEU	3.0
3	F	501	GLN	3.0
3	H	504	LEU	3.0
3	G	390	LEU	3.0
2	D	42	PHE	3.0
3	E	431	GLY	3.0
3	F	580	GLY	3.0
3	F	372	VAL	2.9
3	F	651	ILE	2.9
3	G	397	LYS	2.9
3	F	596	ASP	2.9
3	E	404	GLY	2.9
3	F	401	VAL	2.9
3	E	510	ALA	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	F	551	HIS	2.8
3	F	378	ILE	2.8
3	F	344	HIS	2.8
3	H	421	TYR	2.8
3	F	444	GLY	2.8
3	E	585	VAL	2.8
3	H	498	GLU	2.7
3	F	577	THR	2.7
3	G	497	LEU	2.7
3	G	441	ILE	2.6
3	E	390	LEU	2.6
3	E	422	ALA	2.6
3	E	399	PHE	2.6
3	H	527	VAL	2.6
3	G	612	LYS	2.6
3	E	330	LEU	2.6
3	F	451	TYR	2.6
3	E	571	HIS	2.5
3	E	443	TYR	2.5
2	D	52	ASP	2.5
2	B	52	ASP	2.5
3	G	366	TYR	2.5
3	F	548	GLN	2.5
3	F	423	TYR	2.5
3	H	503	LYS	2.5
3	H	399	PHE	2.5
3	F	438	VAL	2.5
3	F	652	ASN	2.4
3	G	346	ALA	2.4
3	F	330	LEU	2.4
3	G	473	GLU	2.4
3	E	338	ALA	2.4
3	F	617	THR	2.4
3	F	400	GLU	2.4
3	G	508	TYR	2.4
2	D	51	PRO	2.4
3	F	328	GLU	2.4
3	G	442	GLU	2.4
2	B	61	LYS	2.4
3	F	586	MET	2.4
3	G	504	LEU	2.4
2	B	41	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
3	G	588	THR	2.3
3	G	655	ILE	2.3
3	G	618	LEU	2.3
3	F	407	LYS	2.3
3	F	654	ASP	2.3
3	F	607	VAL	2.3
3	F	594	TRP	2.3
2	D	62	ALA	2.2
3	G	378	ILE	2.2
3	F	436	LYS	2.2
3	F	449	GLU	2.2
3	G	610	ASP	2.2
3	E	512	TYR	2.2
3	F	342	LYS	2.2
3	H	530	ALA	2.2
3	G	331	GLN	2.2
2	B	46	GLY	2.1
3	E	609	LYS	2.1
3	F	350	ARG	2.1
3	G	594	TRP	2.1
3	E	334	ILE	2.1
3	F	386	ILE	2.1
3	F	618	LEU	2.1
1	A	7	LYS	2.1
1	A	54	GLN	2.1
3	G	425	ARG	2.1
3	G	494	VAL	2.1
3	H	390	LEU	2.1
1	A	51	GLY	2.1
3	H	445	GLU	2.1
3	H	454	THR	2.1
1	A	35	SER	2.1
3	H	499	LYS	2.0
3	F	367	HIS	2.0
3	F	550	ALA	2.0
3	F	553	VAL	2.0
3	F	446	ASN	2.0
3	F	391	LYS	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 carbohydrates 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. 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, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	HEM	D	201	43/43	0.91	0.47	0.10	40,74,127,153	0
4	HEM	C	201	43/43	0.86	0.44	0.04	3,26,79,88	0
4	HEM	B	201	43/43	0.91	0.52	0.01	44,74,123,149	0
4	HEM	A	201	43/43	0.92	0.52	-0.18	16,55,122,146	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.