Full wwPDB X-ray Structure Validation Report (i)

May 6, 2014 – 10:20 AM EDT

PDB ID	:	4KMM
Title	:	M76H variant of human ferrochelatase
Authors	:	Lanzilotta, W.N.; Medlock, A.E.
Deposited on	:	2013-05-08
Resolution	:	2.60 Å(reported)
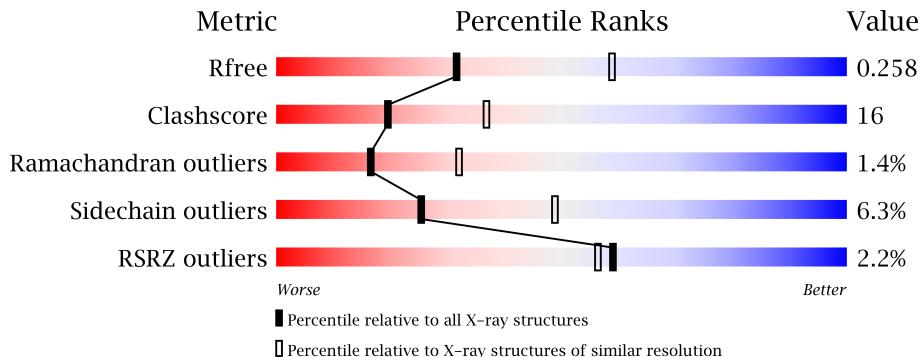
The following versions of software and data (see references) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable22978
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)	:	stable22978

1 Overall quality at a glance ⓘ
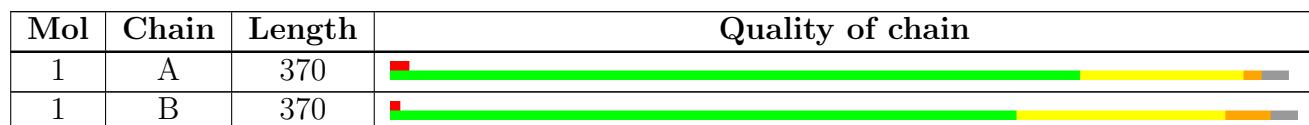
The reported resolution of this entry is 2.60 Å.

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	Percentile Ranks	Value
Rfree		0.258
Clashscore		16
Ramachandran outliers		1.4%
Sidechain outliers		6.3%
RSRZ outliers		2.2%

Worse | | Better

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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 >=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	370	
1	B	370	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	HEM	A	501	-	X
2	HEM	B	501	-	X
4	CHD	B	503	-	X
4	CHD	B	504	-	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 6127 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.
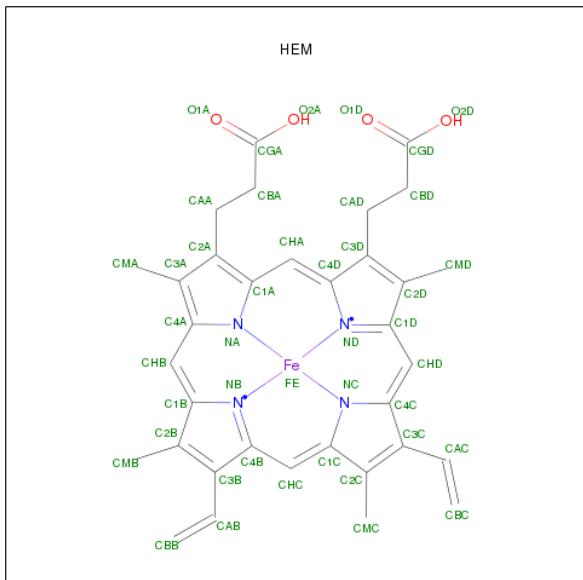
- Molecule 1 is a protein called Ferrochelatase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total 2903	C 1848	N 508	O 530	S 17	0	1	0
1	B	359	Total 2903	C 1848	N 508	O 530	S 17	0	1	0

There are 24 discrepancies between the modelled and reference sequences:
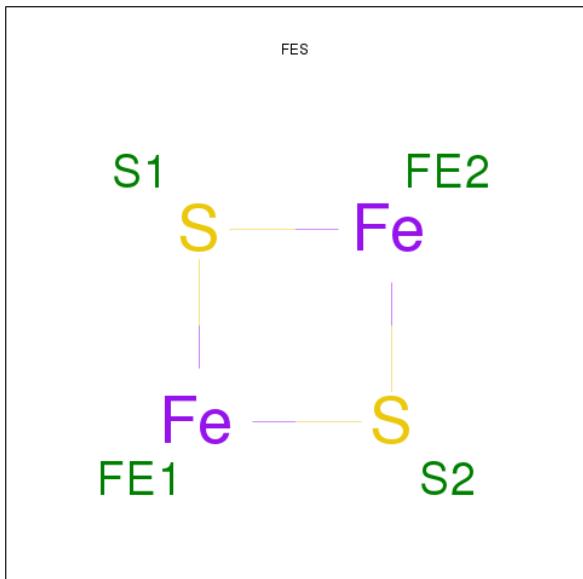
Chain	Residue	Modelled	Actual	Comment	Reference
A	54	MET	-	EXPRESSION TAG	UNP P22830
A	55	GLY	-	EXPRESSION TAG	UNP P22830
A	56	GLY	-	EXPRESSION TAG	UNP P22830
A	57	SER	-	EXPRESSION TAG	UNP P22830
A	58	HIS	-	EXPRESSION TAG	UNP P22830
A	59	HIS	-	EXPRESSION TAG	UNP P22830
A	60	HIS	-	EXPRESSION TAG	UNP P22830
A	61	HIS	-	EXPRESSION TAG	UNP P22830
A	62	HIS	-	EXPRESSION TAG	UNP P22830
A	63	HIS	-	EXPRESSION TAG	UNP P22830
A	64	GLY	-	EXPRESSION TAG	UNP P22830
A	76	HIS	MET	ENGINEERED MUTATION	UNP P22830
B	54	MET	-	EXPRESSION TAG	UNP P22830
B	55	GLY	-	EXPRESSION TAG	UNP P22830
B	56	GLY	-	EXPRESSION TAG	UNP P22830
B	57	SER	-	EXPRESSION TAG	UNP P22830
B	58	HIS	-	EXPRESSION TAG	UNP P22830
B	59	HIS	-	EXPRESSION TAG	UNP P22830
B	60	HIS	-	EXPRESSION TAG	UNP P22830
B	61	HIS	-	EXPRESSION TAG	UNP P22830
B	62	HIS	-	EXPRESSION TAG	UNP P22830
B	63	HIS	-	EXPRESSION TAG	UNP P22830
B	64	GLY	-	EXPRESSION TAG	UNP P22830
B	76	HIS	MET	ENGINEERED MUTATION	UNP P22830

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
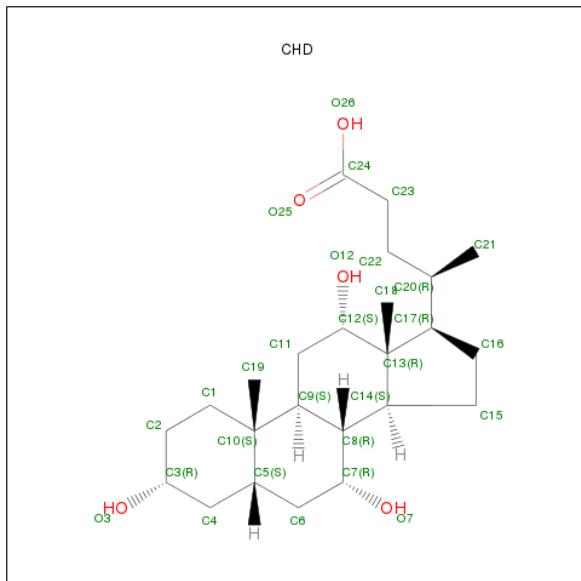
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	Fe 2	S 2	0	0
3	B	1	Total 4	Fe 2	S 2	0	0

- Molecule 4 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 29	C 24	O 5	0	0
4	A	1	Total 29	C 24	O 5	0	0
4	B	1	Total 29	C 24	O 5	0	0
4	B	1	Total 29	C 24	O 5	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Cl 1	0	0
5	A	1	Total 1	Cl 1	0	0

- Molecule 6 is water.
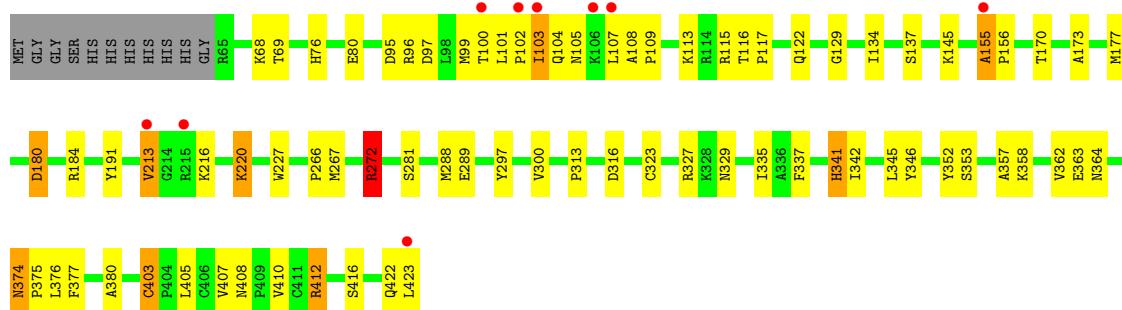
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	59	Total O 59 59		0	0
6	B	50	Total O 50 50		0	0

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.
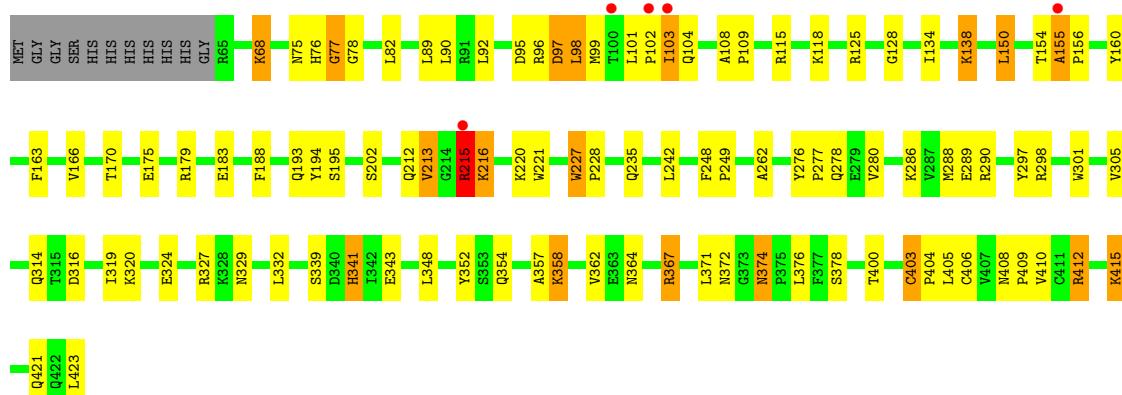
- Molecule 1: Ferrochelatase, mitochondrial

Chain A:

- Molecule 1: Ferrochelatase, mitochondrial

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.14Å 93.42Å 110.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.26 – 2.60 47.47 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.3 (71.26-2.60) 93.8 (47.47-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.205 , 0.259 0.210 , 0.258	Depositor DCC
R_{free} test set	1510 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	32.6	Xtriage
Anisotropy	0.894	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 17.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	4 of 30008 reflections (0.013%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6127	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.78 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.4764e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities 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, CHD, FES, CL

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	0.84	1/2975 (0.0%)	0.86	3/4031 (0.1%)
1	B	0.83	0/2975	0.86	2/4031 (0.0%)
All	All	0.83	1/5950 (0.0%)	0.86	5/8062 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	403	CYS	CB-SG	-5.27	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	ARG	NE-CZ-NH1	7.85	124.23	120.30
1	A	272	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	B	150	LEU	CA-CB-CG	6.14	129.42	115.30
1	B	406	CYS	N-CA-CB	5.49	120.49	110.60
1	A	345	LEU	CA-CB-CG	5.38	127.68	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2903	0	2903	73	0
1	B	2903	0	2903	93	0
2	A	43	0	30	17	0
2	B	43	0	30	20	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	58	0	78	13	0
4	B	58	0	78	10	0
5	A	1	0	0	1	0
5	B	1	0	0	1	0
6	A	59	0	0	1	0
6	B	50	0	0	2	0
All	All	6127	0	6022	195	0

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 16.

All (195) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:501:HEM:HHA	2:B:501:HEM:HBD2	1.36	1.08
2:A:501:HEM:CMB	2:A:501:HEM:HBB2	1.84	1.07
2:A:501:HEM:CMB	4:A:503:CHD:H192	1.88	1.02
2:A:501:HEM:HMB2	4:A:503:CHD:H192	1.40	1.01
2:A:501:HEM:CBB	2:A:501:HEM:HMB1	1.90	1.00
1:B:155:ALA:HB1	1:B:156:PRO:CD	1.92	0.98
2:A:501:HEM:HBB2	2:A:501:HEM:HMB1	1.00	0.97
2:A:501:HEM:HBC2	2:A:501:HEM:HMC2	1.45	0.96
1:A:155:ALA:HB1	1:A:156:PRO:CD	1.96	0.95
1:B:76[A]:HIS:NE2	2:B:501:HEM:HMD3	1.83	0.94
1:B:77:GLY:HA2	1:B:166:VAL:HG22	1.52	0.92
2:B:501:HEM:CBD	2:B:501:HEM:HHA	2.04	0.88
1:A:155:ALA:HB1	1:A:156:PRO:HD2	1.56	0.86
2:B:501:HEM:CBD	2:B:501:HEM:CHA	2.53	0.85
2:A:501:HEM:HMB2	4:A:503:CHD:C19	2.07	0.84
1:A:68:LYS:HD3	1:A:155:ALA:CB	2.10	0.81
1:B:155:ALA:HB1	1:B:156:PRO:HD2	1.63	0.81
1:A:323:CYS:SG	1:A:362:VAL:HG12	2.21	0.81
1:A:68:LYS:HD3	1:A:155:ALA:HB3	1.65	0.79
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.13	0.78
1:B:374:ASN:HD22	1:B:376:LEU:H	1.33	0.76
1:A:337:PHE:HB2	6:A:629:HOH:O	1.85	0.75
1:B:77:GLY:CA	1:B:166:VAL:HG22	2.16	0.75
4:A:503:CHD:H183	4:A:503:CHD:H212	1.68	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:68:LYS:HB2	1:B:155:ALA:HB3	1.71	0.73
1:B:155:ALA:CB	1:B:156:PRO:CD	2.64	0.73
1:B:68:LYS:CB	1:B:155:ALA:HB3	2.19	0.73
1:A:113:LYS:NZ	1:A:113:LYS:HB3	2.04	0.72
1:A:422:GLN:HG2	1:A:423:LEU:H	1.54	0.72
1:B:102:PRO:C	1:B:103:ILE:HG13	2.10	0.72
2:B:501:HEM:HBC2	2:B:501:HEM:HHD	1.72	0.72
1:A:115:ARG:HE	4:A:503:CHD:H232	1.53	0.71
1:A:68:LYS:CB	1:A:155:ALA:HB3	2.21	0.71
1:A:374:ASN:ND2	1:A:376:LEU:H	1.89	0.71
1:B:403:CYS:O	1:B:405:LEU:N	2.24	0.70
1:B:115:ARG:HD2	4:B:503:CHD:H232	1.74	0.70
1:B:357:ALA:HB1	1:B:362:VAL:HG21	1.72	0.70
1:B:374:ASN:ND2	1:B:376:LEU:H	1.89	0.70
1:B:76[A]:HIS:HD2	1:B:77:GLY:O	1.75	0.69
1:B:341:HIS:HB2	5:B:505:CL:CL	2.30	0.69
1:A:374:ASN:HD22	1:A:376:LEU:H	1.39	0.69
2:A:501:HEM:HBD2	2:A:501:HEM:CHA	2.22	0.69
1:A:353:SER:O	1:A:357:ALA:HB3	1.93	0.69
2:B:501:HEM:HBB2	2:B:501:HEM:CMB	2.24	0.68
2:B:501:HEM:CMB	4:B:503:CHD:H193	2.22	0.68
1:B:115:ARG:NH1	4:B:503:CHD:H211	2.08	0.68
1:A:220:LYS:O	1:A:220:LYS:HG3	1.93	0.68
1:A:155:ALA:CB	1:A:156:PRO:CD	2.70	0.67
1:A:173:ALA:O	1:A:177:MET:HG3	1.95	0.67
1:B:155:ALA:HB1	1:B:156:PRO:HD3	1.75	0.66
1:B:400:THR:HA	1:B:415:LYS:HD3	1.77	0.66
1:B:289:GLU:OE2	6:B:644:HOH:O	2.14	0.66
1:B:314:GLN:HG2	6:B:636:HOH:O	1.95	0.65
1:B:76[A]:HIS:CE1	2:B:501:HEM:HMD3	2.32	0.65
1:A:102:PRO:C	1:A:103:ILE:HD13	2.16	0.65
1:A:115:ARG:NE	4:A:503:CHD:H232	2.11	0.65
2:B:501:HEM:HBD1	2:B:501:HEM:CHA	2.26	0.65
1:A:329:ASN:HD22	1:A:364:ASN:HB2	1.63	0.64
1:B:348:LEU:HD12	1:B:367:ARG:HD3	1.78	0.64
1:A:155:ALA:CB	1:A:156:PRO:HD2	2.28	0.64
1:A:300:VAL:HG12	1:A:313:PRO:HG2	1.78	0.64
1:A:341:HIS:HB2	5:A:505:CL:CL	2.35	0.64
1:B:76[A]:HIS:CE1	2:B:501:HEM:CMD	2.80	0.64
1:B:77:GLY:HA2	1:B:166:VAL:CG2	2.28	0.62
1:B:235:GLN:HG3	1:B:290:ARG:NH2	2.15	0.62
1:A:288:MET:HG3	1:A:297:TYR:CE2	2.33	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:408:ASN:OD1	1:A:410:VAL:HG12	2.01	0.61
2:A:501:HEM:CMB	4:A:503:CHD:C19	2.71	0.61
1:A:68:LYS:HB2	1:A:155:ALA:HB3	1.82	0.61
2:B:501:HEM:CHD	2:B:501:HEM:HBC2	2.30	0.61
2:A:501:HEM:HMB3	4:A:503:CHD:H192	1.76	0.61
1:A:103:ILE:HD13	1:A:103:ILE:N	2.16	0.61
1:A:102:PRO:HB2	1:A:103:ILE:HD13	1.84	0.60
1:B:276:TYR:HB3	1:B:277:PRO:HD3	1.83	0.59
1:A:412:ARG:HH22	1:B:327:ARG:HD3	1.67	0.59
1:A:113:LYS:HZ3	1:A:113:LYS:HB3	1.68	0.59
1:A:281:SER:HB3	1:B:278:GLN:HG2	1.85	0.59
1:A:403:CYS:HB3	1:B:298:ARG:HH21	1.68	0.59
1:A:101:LEU:HB3	1:A:107:LEU:HD12	1.85	0.58
1:A:422:GLN:HG2	1:A:423:LEU:N	2.17	0.58
1:B:76[A]:HIS:CE1	2:B:501:HEM:HHD	2.39	0.58
1:A:68:LYS:HD3	1:A:155:ALA:HB2	1.84	0.58
1:A:76[A]:HIS:CD2	1:A:191:TYR:OH	2.57	0.57
1:B:155:ALA:CB	1:B:156:PRO:HD2	2.33	0.57
1:B:134:ILE:O	1:B:138:LYS:HG3	2.05	0.56
2:B:501:HEM:CMB	2:B:501:HEM:CBB	2.83	0.56
1:B:175:GLU:O	1:B:179:ARG:HG3	2.05	0.56
1:A:289:GLU:OE2	1:B:286:LYS:NZ	2.31	0.56
1:B:319:ILE:HD11	1:B:332:LEU:HD21	1.87	0.56
1:A:115:ARG:HH12	2:A:501:HEM:CGA	2.18	0.56
1:A:357:ALA:HB1	1:A:362:VAL:HG21	1.86	0.56
1:B:115:ARG:HD2	4:B:503:CHD:C23	2.36	0.56
1:B:358:LYS:HE3	1:B:358:LYS:HA	1.88	0.55
1:B:138:LYS:HB3	1:B:138:LYS:NZ	2.22	0.55
1:B:221:TRP:O	1:B:421:GLN:HG2	2.07	0.55
2:B:501:HEM:HMB2	2:B:501:HEM:CBB	2.36	0.55
1:B:320:LYS:O	1:B:324:GLU:HG3	2.06	0.54
1:A:272:ARG:HH11	1:A:272:ARG:CG	2.21	0.54
1:A:374:ASN:HD22	1:A:375:PRO:N	2.05	0.53
1:A:122:GLN:HG2	1:A:346:TYR:CE2	2.44	0.53
1:B:134:ILE:O	1:B:138:LYS:CG	2.56	0.52
1:B:288:MET:HG3	1:B:297:TYR:CD2	2.43	0.52
1:A:266:PRO:O	1:A:267:MET:C	2.46	0.52
1:B:288:MET:HG3	1:B:297:TYR:CE2	2.45	0.52
1:A:316:ASP:HB3	1:A:352:TYR:CE1	2.46	0.51
1:A:327:ARG:HH11	1:B:412:ARG:HH22	1.57	0.51
1:A:288:MET:HG3	1:A:297:TYR:CD2	2.46	0.51
1:A:341:HIS:N	1:A:341:HIS:CD2	2.79	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:501:HEM:CMB	2:A:501:HEM:CBB	2.61	0.50
1:B:227:TRP:N	1:B:228:PRO:HD3	2.26	0.50
1:A:374:ASN:HD22	1:A:374:ASN:C	2.15	0.50
1:A:408:ASN:CG	1:A:410:VAL:HG12	2.32	0.50
1:B:101:LEU:HD12	1:B:104:GLN:HG2	1.94	0.50
1:A:134:ILE:O	1:A:137:SER:HB2	2.12	0.49
1:A:357:ALA:HB1	1:A:362:VAL:CG2	2.42	0.49
1:B:99:MET:HB3	4:B:503:CHD:H191	1.95	0.49
1:A:76[A]:HIS:NE2	2:A:501:HEM:HMD2	2.27	0.49
2:A:501:HEM:HMC2	2:A:501:HEM:CBC	2.27	0.49
1:A:76[A]:HIS:HD2	1:A:191:TYR:OH	1.95	0.48
1:A:99:MET:HB3	1:A:104:GLN:HE22	1.77	0.48
1:A:155:ALA:HB1	1:A:156:PRO:HD3	1.88	0.48
2:B:501:HEM:HBA1	2:B:501:HEM:O1D	2.13	0.48
1:B:68:LYS:HE2	1:B:154:THR:C	2.34	0.48
1:B:195:SER:HB2	1:B:276:TYR:HB2	1.95	0.47
1:B:403:CYS:C	1:B:405:LEU:H	2.17	0.47
1:B:101:LEU:HB2	1:B:104:GLN:HG3	1.96	0.47
1:B:68:LYS:HZ3	1:B:155:ALA:HB2	1.79	0.47
1:B:374:ASN:HD22	1:B:376:LEU:N	2.08	0.47
1:A:80:GLU:O	1:A:129:GLY:HA3	2.15	0.47
2:B:501:HEM:HMB1	4:B:503:CHD:H193	1.97	0.47
1:A:69:THR:HG23	1:A:184:ARG:HG3	1.96	0.46
1:A:377:PHE:O	1:A:380:ALA:HB3	2.15	0.46
1:B:371:LEU:O	1:B:372:ASN:C	2.54	0.46
1:B:341:HIS:CD2	1:B:341:HIS:N	2.82	0.46
1:B:329:ASN:HD22	1:B:364:ASN:HB2	1.80	0.46
1:B:301:TRP:CD1	1:B:301:TRP:N	2.84	0.46
1:B:90:LEU:HD13	1:B:109:PRO:HA	1.96	0.46
1:A:403:CYS:O	1:A:405:LEU:N	2.48	0.46
4:B:503:CHD:H151	4:B:504:CHD:H152	1.97	0.46
1:B:108:ALA:HB3	1:B:109:PRO:HD3	1.98	0.46
1:B:194:TYR:C	1:B:194:TYR:CD2	2.89	0.45
1:A:95:ASP:C	1:A:97:ASP:H	2.20	0.45
1:B:213:VAL:HG22	1:B:215:ARG:HH11	1.80	0.45
2:B:501:HEM:HBB2	2:B:501:HEM:HMB2	1.96	0.45
1:B:76[A]:HIS:HE2	2:B:501:HEM:HMD3	1.74	0.45
1:A:68:LYS:CD	1:A:155:ALA:HB3	2.42	0.45
1:B:78:GLY:H	1:B:166:VAL:HG21	1.81	0.45
1:B:227:TRP:N	1:B:228:PRO:CD	2.80	0.44
1:B:160:TYR:CD1	1:B:160:TYR:N	2.84	0.44
2:A:501:HEM:HBD2	2:A:501:HEM:HHA	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:504:CHD:H162	4:A:504:CHD:H222	1.51	0.44
1:B:408:ASN:HA	1:B:409:PRO:HD3	1.84	0.44
1:B:357:ALA:HB1	1:B:362:VAL:CG2	2.43	0.44
1:A:363:GLU:O	1:A:364:ASN:ND2	2.51	0.43
1:A:99:MET:HB3	1:A:104:GLN:NE2	2.32	0.43
1:A:122:GLN:HG2	1:A:346:TYR:CZ	2.53	0.43
1:B:216:LYS:HB2	1:B:216:LYS:HE3	1.83	0.43
1:A:102:PRO:O	1:A:103:ILE:C	2.57	0.43
1:B:193:GLN:HG2	1:B:280:VAL:HA	2.01	0.43
1:B:316:ASP:HB3	1:B:352:TYR:CE1	2.52	0.43
4:B:503:CHD:H151	4:B:504:CHD:C15	2.49	0.43
1:A:95:ASP:O	1:A:97:ASP:N	2.52	0.43
1:B:262:ALA:O	1:B:301:TRP:HA	2.19	0.43
1:B:115:ARG:HH12	4:B:503:CHD:H211	1.81	0.42
1:B:75:ASN:O	1:B:163:PHE:HA	2.19	0.42
1:B:354:GLN:O	1:B:358:LYS:HB2	2.20	0.42
1:B:89:LEU:HD23	1:B:89:LEU:HA	1.88	0.42
4:A:503:CHD:H193	4:A:503:CHD:H111	1.72	0.42
1:B:76[A]:HIS:CE1	2:B:501:HEM:HMD1	2.54	0.42
1:B:125:ARG:HD2	1:B:125:ARG:HA	1.90	0.42
1:A:115:ARG:CZ	4:A:503:CHD:H211	2.49	0.42
1:B:96:ARG:CD	1:B:96:ARG:H	2.33	0.42
1:B:357:ALA:O	1:B:362:VAL:HG22	2.19	0.42
4:A:503:CHD:C18	4:A:503:CHD:H212	2.45	0.41
4:A:504:CHD:H183	4:A:504:CHD:H20	1.98	0.41
1:B:68:LYS:HB2	1:B:155:ALA:CB	2.46	0.41
1:B:82:LEU:HD21	1:B:128:GLY:HA2	2.01	0.41
1:B:235:GLN:HG3	1:B:290:ARG:CZ	2.50	0.41
1:B:95:ASP:OD2	1:B:97:ASP:HB2	2.21	0.41
1:B:99:MET:CE	4:B:503:CHD:H182	2.51	0.41
1:B:68:LYS:HD3	1:B:183:GLU:OE1	2.20	0.41
1:B:408:ASN:OD1	1:B:410:VAL:HG12	2.21	0.41
1:A:335:ILE:HG13	1:A:335:ILE:O	2.21	0.41
1:A:342:ILE:HA	1:A:342:ILE:HD12	1.90	0.41
1:B:98:LEU:O	1:B:98:LEU:HG	2.21	0.41
1:A:116:THR:N	1:A:117:PRO:HD2	2.35	0.41
1:B:242:LEU:HA	1:B:242:LEU:HD23	1.95	0.41
1:A:180:ASP:OD1	1:A:180:ASP:N	2.54	0.41
1:B:248:PHE:O	1:B:249:PRO:C	2.58	0.41
1:B:76[A]:HIS:ND1	2:B:501:HEM:HHD	2.36	0.41
1:A:115:ARG:NH1	2:A:501:HEM:CGA	2.83	0.40
1:B:341:HIS:NE2	1:B:343:GLU:HB2	2.36	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:108:ALA:HB3	1:A:109:PRO:HD3	2.03	0.40
1:B:115:ARG:HH21	1:B:118:LYS:HE2	1.86	0.40
1:A:102:PRO:HB2	1:A:103:ILE:CD1	2.49	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	358/370 (97%)	328 (92%)	26 (7%)	4 (1%)	21	42
1	B	358/370 (97%)	331 (92%)	21 (6%)	6 (2%)	14	26
All	All	716/740 (97%)	659 (92%)	47 (7%)	10 (1%)	16	32

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	ARG
1	A	155	ALA
1	B	97	ASP
1	B	155	ALA
1	B	404	PRO
1	A	213	VAL
1	B	215	ARG
1	A	227	TRP
1	B	77	GLY
1	B	227	TRP

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	325/332 (98%)	309 (95%)	16 (5%)	35	62
1	B	325/332 (98%)	300 (92%)	25 (8%)	18	35
All	All	650/664 (98%)	609 (94%)	41 (6%)	25	49

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	THR
1	A	103	ILE
1	A	105	ASN
1	A	145	LYS
1	A	170	THR
1	A	180	ASP
1	A	213	VAL
1	A	216	LYS
1	A	220	LYS
1	A	272	ARG
1	A	341	HIS
1	A	358	LYS
1	A	374	ASN
1	A	407	VAL
1	A	412	ARG
1	A	416	SER
1	B	68	LYS
1	B	92	LEU
1	B	98	LEU
1	B	103	ILE
1	B	138	LYS
1	B	150	LEU
1	B	170	THR
1	B	188	PHE
1	B	202	SER
1	B	212	GLN
1	B	213	VAL
1	B	215	ARG
1	B	216	LYS
1	B	220	LYS
1	B	305	VAL
1	B	339	SER
1	B	341	HIS
1	B	358	LYS
1	B	367	ARG

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Mol	Chain	Res	Type
1	B	374	ASN
1	B	378	SER
1	B	403	CYS
1	B	412	ARG
1	B	415	LYS
1	B	423	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	235	GLN
1	A	247	HIS
1	A	314	GLN
1	A	329	ASN
1	A	341	HIS
1	A	354	GLN
1	A	364	ASN
1	A	374	ASN
1	A	392	ASN
1	A	421	GLN
1	B	104	GLN
1	B	329	ASN
1	B	374	ASN
1	B	421	GLN

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 (i)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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	501	-	42,50,50	3.96	13 (30%)	27,82,82	1.59	4 (14%)
3	FES	A	502	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CHD	A	503	-	32,32,32	0.70	0	51,51,51	2.22	18 (35%)
4	CHD	A	504	-	32,32,32	0.59	0	51,51,51	1.70	11 (21%)
2	HEM	B	501	-	42,50,50	3.79	15 (35%)	27,82,82	1.89	6 (22%)
3	FES	B	502	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CHD	B	503	-	32,32,32	0.65	0	51,51,51	1.88	10 (19%)
4	CHD	B	504	-	32,32,32	0.62	0	51,51,51	1.91	11 (21%)

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	501	-	-	0/14/114/114	0/0/8/8
3	FES	A	502	1	-	0/0/4/4	0/1/1/1
4	CHD	A	503	-	-	0/9/74/74	0/4/4/4
4	CHD	A	504	-	-	0/9/74/74	0/4/4/4
2	HEM	B	501	-	-	1/14/114/114	0/0/8/8
3	FES	B	502	1	-	0/0/4/4	0/1/1/1
4	CHD	B	503	-	-	0/9/74/74	0/4/4/4
4	CHD	B	504	-	-	0/9/74/74	0/4/4/4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3C-C2C	-13.50	1.34	1.45
2	A	501	HEM	C3B-C2B	-13.33	1.32	1.45
2	B	501	HEM	C3C-C2C	-13.05	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3B-C2B	-12.97	1.33	1.45
2	A	501	HEM	FE-NC	7.41	2.25	1.95
2	A	501	HEM	CMD-C2D	6.01	1.55	1.45
2	A	501	HEM	CMC-C2C	5.97	1.55	1.45
2	B	501	HEM	CMC-C2C	5.93	1.55	1.45
2	A	501	HEM	FE-ND	5.83	2.18	1.95
2	B	501	HEM	CMD-C2D	5.77	1.54	1.45
2	B	501	HEM	FE-NC	5.36	2.17	1.95
2	B	501	HEM	CMB-C2B	5.13	1.53	1.45
2	B	501	HEM	FE-NB	5.06	2.13	1.95
2	A	501	HEM	CMB-C2B	5.00	1.53	1.45
2	A	501	HEM	C3C-CAC	4.72	1.55	1.40
2	B	501	HEM	C3C-CAC	4.59	1.55	1.40
2	A	501	HEM	C3B-CAB	4.42	1.54	1.40
2	B	501	HEM	C3B-CAB	4.38	1.54	1.40
2	A	501	HEM	C3D-C2D	3.93	1.53	1.43
2	A	501	HEM	FE-NB	3.77	2.09	1.95
2	B	501	HEM	C3D-C2D	3.75	1.53	1.43
2	B	501	HEM	FE-ND	3.30	2.08	1.95
2	B	501	HEM	C1D-ND	2.75	1.40	1.33
2	A	501	HEM	C1D-ND	2.70	1.40	1.33
2	B	501	HEM	FE-NA	2.21	2.11	1.94
2	B	501	HEM	C4C-NC	2.11	1.39	1.33
2	B	501	HEM	C1C-NC	2.06	1.38	1.33
2	A	501	HEM	C4C-NC	2.04	1.38	1.33

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	503	CHD	C4-C5-C10	5.77	118.91	112.68
4	B	503	CHD	C9-C10-C5	5.68	116.59	108.69
4	B	503	CHD	C4-C5-C10	5.39	118.50	112.68
4	A	503	CHD	C9-C10-C5	5.27	116.01	108.69
4	B	504	CHD	C9-C10-C5	5.01	115.66	108.69
2	B	501	HEM	CBD-CAD-C3D	-4.98	103.71	114.51
4	A	503	CHD	C6-C5-C4	-4.93	105.34	111.08
4	B	504	CHD	C4-C5-C10	4.50	117.54	112.68
2	A	501	HEM	CBD-CAD-C3D	-4.44	104.87	114.51
2	B	501	HEM	CBA-CAA-C2A	-4.29	105.50	112.63
4	A	504	CHD	C10-C9-C8	4.19	116.31	111.88
4	B	504	CHD	C1-C10-C9	-4.10	104.91	111.46
4	A	504	CHD	C9-C10-C5	3.96	114.19	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	503	CHD	C1-C10-C5	3.85	112.03	107.78
4	A	503	CHD	C5-C4-C3	3.82	118.56	112.94
4	B	504	CHD	C10-C9-C8	3.81	115.92	111.88
4	B	503	CHD	C19-C10-C5	-3.80	103.70	110.25
4	B	504	CHD	C1-C10-C5	3.76	111.93	107.78
4	B	503	CHD	C10-C9-C8	3.76	115.86	111.88
4	B	503	CHD	C1-C10-C5	3.72	111.89	107.78
4	B	504	CHD	C6-C5-C4	-3.69	106.78	111.08
4	A	504	CHD	C4-C5-C10	3.68	116.66	112.68
4	A	504	CHD	C14-C8-C9	-3.55	104.78	109.63
4	A	503	CHD	C6-C5-C10	3.53	116.49	112.68
4	A	504	CHD	C14-C8-C7	3.35	115.89	111.77
4	B	503	CHD	C6-C5-C4	-3.31	107.22	111.08
2	A	501	HEM	C3A-C4A-NA	-3.31	107.28	109.50
4	A	503	CHD	C1-C10-C9	-3.27	106.23	111.46
4	A	503	CHD	C5-C6-C7	3.26	117.91	114.46
2	B	501	HEM	CAD-CBD-CGD	-3.19	107.50	113.53
4	A	503	CHD	C19-C10-C9	-3.09	107.19	111.19
4	B	504	CHD	C14-C8-C7	3.09	115.56	111.77
4	A	503	CHD	C9-C8-C7	-2.99	108.57	111.97
2	B	501	HEM	C3A-C4A-NA	-2.92	107.55	109.50
2	A	501	HEM	CAA-CBA-CGA	-2.88	104.27	113.66
4	B	504	CHD	C14-C8-C9	-2.88	105.71	109.63
4	A	503	CHD	C14-C8-C7	2.86	115.29	111.77
4	B	504	CHD	C22-C20-C17	2.84	116.37	110.25
4	A	503	CHD	C23-C22-C20	-2.72	109.61	114.48
4	A	504	CHD	C6-C7-C8	2.64	114.23	111.47
4	A	504	CHD	C16-C17-C13	2.62	106.18	103.60
4	A	503	CHD	C9-C11-C12	2.61	117.74	114.36
2	A	501	HEM	CBA-CAA-C2A	-2.58	108.34	112.63
4	A	503	CHD	C11-C9-C8	2.51	114.46	110.80
4	A	503	CHD	C11-C9-C10	-2.45	111.17	113.75
4	A	503	CHD	C17-C13-C12	-2.41	115.55	117.67
4	A	503	CHD	C14-C13-C12	2.37	109.56	107.40
2	B	501	HEM	CAA-CBA-CGA	-2.32	106.12	113.66
2	B	501	HEM	C2A-C1A-NA	-2.25	106.61	109.73
4	A	504	CHD	C19-C10-C5	-2.25	106.37	110.25
4	A	504	CHD	C1-C10-C5	2.25	110.26	107.78
4	A	504	CHD	C5-C4-C3	2.24	116.23	112.94
4	B	503	CHD	C5-C4-C3	2.24	116.23	112.94
4	A	503	CHD	C13-C17-C20	2.21	122.13	119.50
4	B	503	CHD	C9-C8-C7	-2.21	109.46	111.97

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	504	CHD	C17-C13-C14	2.18	102.25	100.07
4	B	503	CHD	C13-C14-C8	2.16	117.22	114.80
4	A	504	CHD	C6-C5-C4	-2.13	108.60	111.08
4	B	504	CHD	C18-C13-C12	-2.12	107.02	109.09
4	B	503	CHD	C19-C10-C1	-2.07	104.69	108.18

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	HEM	C2D-C3D-CAD-CBD

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	359/370 (97%)	-0.28	9 (2%) 54	52	13, 31, 58, 67	0
1	B	359/370 (97%)	-0.25	5 (1%) 72	72	13, 31, 58, 73	0
All	All	718/740 (97%)	-0.26	14 (1%) 59	61	13, 31, 58, 73	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	ILE	3.9
1	A	155	ALA	3.1
1	B	100	THR	2.9
1	A	423	LEU	2.7
1	A	102	PRO	2.7
1	B	103	ILE	2.7
1	A	100	THR	2.6
1	B	155	ALA	2.4
1	A	107	LEU	2.2
1	B	102	PRO	2.2
1	B	215	ARG	2.1
1	A	106	LYS	2.1
1	A	215	ARG	2.0
1	A	213	VAL	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 (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, 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	A	501	43/43	0.42	5.58	46,58,60,62	39
2	HEM	B	501	43/43	0.38	3.80	47,54,55,57	39
4	CHD	B	504	29/29	0.46	3.08	103,105,112,113	0
4	CHD	B	503	29/29	0.42	2.50	115,118,119,119	0
4	CHD	A	503	29/29	0.34	1.93	80,82,89,89	0
4	CHD	A	504	29/29	0.39	1.80	93,95,98,98	0
5	CL	B	505	1/1	0.18	0.51	49,49,49,49	0
5	CL	A	505	1/1	0.10	-1.13	36,36,36,36	0
3	FES	B	502	4/4	0.07	-2.71	31,37,38,40	0
3	FES	A	502	4/4	0.07	-2.88	25,30,34,35	0

6.5 Other polymers (i)

There are no such residues in this entry.