



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:17 PM GMT

PDB ID : 1P80
Title : Crystal structure of the D181Q variant of catalase HP11 from E. coli
Authors : Chelikani, P.; Carpena, X.; Fita, I.; Loewen, P.C.
Deposited on : 2003-05-06
Resolution : 1.65 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>

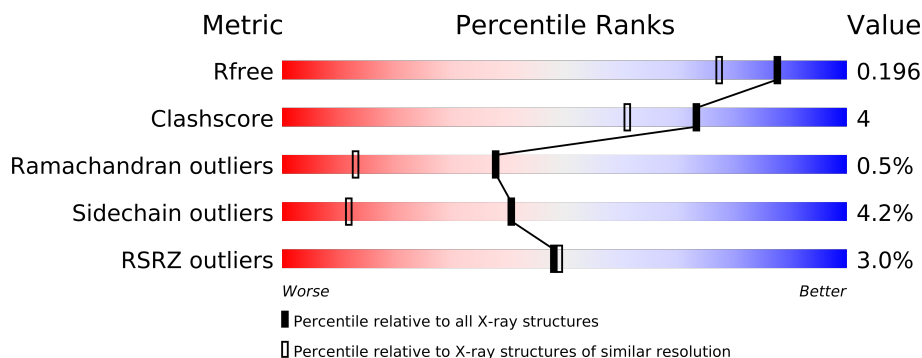
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.65 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	1404 (1.68-1.64)
Clashscore	79885	1001 (1.66-1.66)
Ramachandran outliers	78287	1581 (1.68-1.64)
Sidechain outliers	78261	1580 (1.68-1.64)
RSRZ outliers	66119	1404 (1.68-1.64)

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	753	
1	B	753	
1	C	753	
1	D	753	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26401 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 Catalase HPIL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	1	0
			5752	3651	1008	1081	12			
1	B	727	Total	C	N	O	S	0	1	0
			5752	3651	1008	1081	12			
1	C	727	Total	C	N	O	S	0	1	0
			5752	3651	1008	1081	12			
1	D	727	Total	C	N	O	S	0	1	0
			5752	3651	1008	1081	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	GLN	ASP	ENGINEERED	UNP P21179
B	181	GLN	ASP	ENGINEERED	UNP P21179
C	181	GLN	ASP	ENGINEERED	UNP P21179
D	181	GLN	ASP	ENGINEERED	UNP P21179

- 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 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is water.

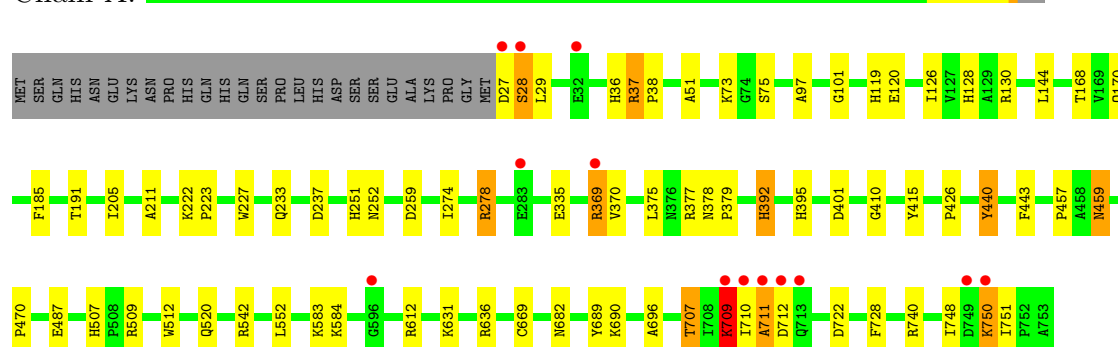
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	858	Total	O	0	0
			858	858		
3	B	740	Total	O	0	0
			740	740		
3	C	782	Total	O	0	0
			782	782		
3	D	841	Total	O	0	0
			841	841		

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.

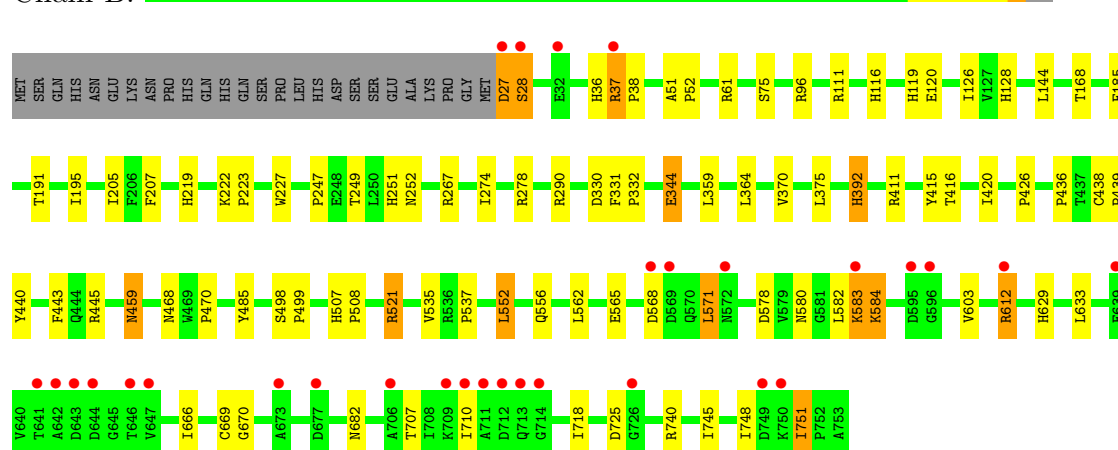
• Molecule 1: Catalase HP1I

Chain A:



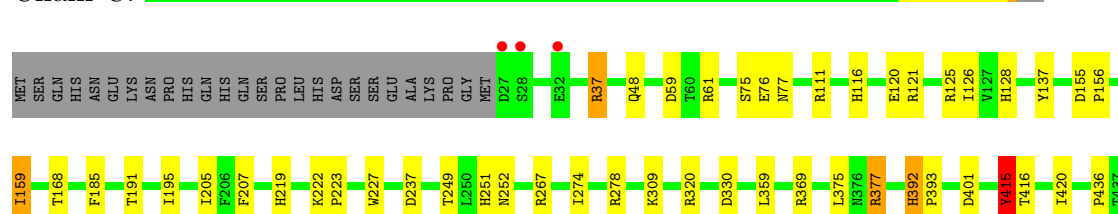
• Molecule 1: Catalase HP1I

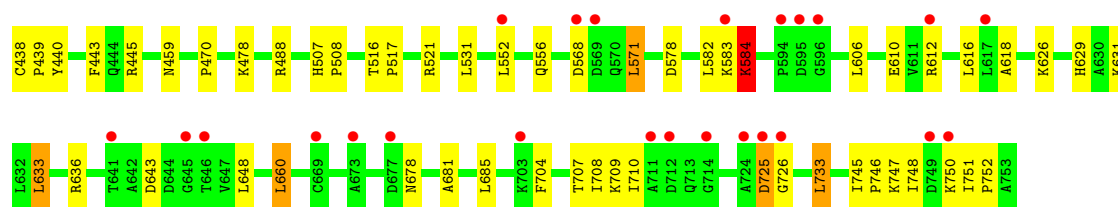
Chain B:



• Molecule 1: Catalase HP1I

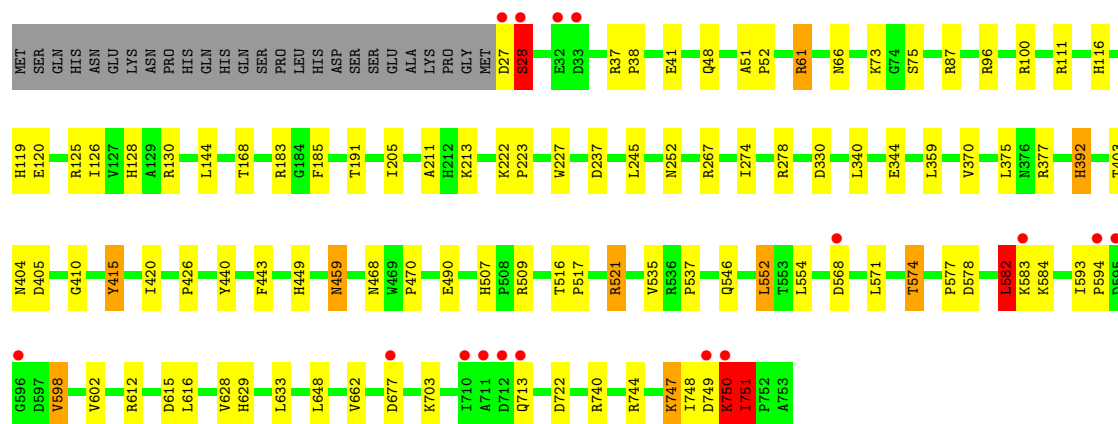
Chain C:





Molecule 1: Catalase HP11

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.76Å 133.13Å 122.50Å 90.00° 109.50° 90.00°	Depositor
Resolution (Å)	29.80 – 1.65 21.98 – 1.65	Depositor EDS
% Data completeness (in resolution range)	96.0 (29.80-1.65) 95.5 (21.98-1.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 1.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.168 , 0.202 0.166 , 0.196	Depositor DCC
R_{free} test set	16400 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	16.2	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.7	EDS
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 323591 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	26401	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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	0.45	0/5914	1.07	19/8041 (0.2%)
1	B	0.43	0/5914	1.05	13/8041 (0.2%)
1	C	0.44	0/5914	1.07	15/8041 (0.2%)
1	D	0.45	0/5914	1.12	25/8041 (0.3%)
All	All	0.44	0/23656	1.08	72/32164 (0.2%)

There are no bond length outliers.

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	377	ARG	NE-CZ-NH2	-10.95	114.82	120.30
1	C	415	TYR	CB-CG-CD1	-10.82	114.51	121.00
1	D	278	ARG	NE-CZ-NH1	-9.39	115.60	120.30
1	D	612	ARG	CD-NE-CZ	9.15	136.41	123.60
1	C	445	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	A	377	ARG	NE-CZ-NH2	-8.59	116.00	120.30
1	C	278	ARG	NE-CZ-NH1	-7.92	116.34	120.30
1	A	37	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	C	59	ASP	CB-CG-OD1	7.86	125.37	118.30
1	B	290	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	C	415	TYR	CB-CG-CD2	7.80	125.68	121.00
1	B	521	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	C	125	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	D	96	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	D	740	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	D	521	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	B	445	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	D	100	ARG	CD-NE-CZ	7.10	133.54	123.60
1	D	183	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	D	612	ARG	NE-CZ-NH2	6.93	123.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	726	GLY	N-CA-C	-6.88	95.89	113.10
1	D	130	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	509	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	A	130	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	B	111	ARG	NE-CZ-NH1	-6.59	117.00	120.30
1	A	37	ARG	CD-NE-CZ	6.56	132.78	123.60
1	A	278	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	A	369	ARG	NE-CZ-NH2	6.51	123.56	120.30
1	D	568	ASP	CB-CG-OD2	6.43	124.08	118.30
1	D	61	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	D	449	HIS	CA-CB-CG	6.19	124.12	113.60
1	D	96	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	B	278	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	A	233	GLN	CG-CD-OE1	6.01	133.61	121.60
1	C	320	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	B	28	SER	N-CA-CB	5.96	119.44	110.50
1	A	542	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	C	121	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	D	377	ARG	NH1-CZ-NH2	5.86	125.85	119.40
1	D	615	ASP	CB-CG-OD2	5.86	123.57	118.30
1	C	401	ASP	CB-CG-OD2	5.82	123.54	118.30
1	D	61	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	A	740	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	278	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	A	636	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	D	509	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	D	87	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	C	320	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	D	125	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	C	111	ARG	NE-CZ-NH1	-5.47	117.57	120.30
1	B	111	ARG	NH1-CZ-NH2	5.46	125.41	119.40
1	D	740	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	111	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	C	377	ARG	NE-CZ-NH1	-5.41	117.59	120.30
1	C	636	ARG	NE-CZ-NH2	5.39	122.99	120.30
1	B	96	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	61	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	B	485	TYR	CB-CG-CD1	-5.34	117.79	121.00
1	A	37	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	740	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	D	722	ASP	CB-CG-OD1	5.31	123.08	118.30
1	D	677	ASP	CB-CG-OD2	5.26	123.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	722	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	401	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	259	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	440	TYR	N-CA-CB	5.13	119.84	110.60
1	D	403	THR	N-CA-CB	5.13	120.04	110.30
1	A	631	LYS	N-CA-CB	5.08	119.75	110.60
1	B	445	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	170	GLN	CG-CD-NE2	5.05	128.83	116.70
1	C	725	ASP	N-CA-CB	5.05	119.70	110.60
1	D	582	LEU	CA-CB-CG	5.01	126.83	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	5752	0	5585	44	0
1	B	5752	0	5585	64	0
1	C	5752	0	5585	50	0
1	D	5752	0	5585	50	0
2	A	43	0	30	1	0
2	B	43	0	30	2	0
2	C	43	0	30	1	0
2	D	43	0	30	1	0
3	A	858	0	0	2	0
3	B	740	0	0	6	0
3	C	782	0	0	7	0
3	D	841	0	0	8	0
All	All	26401	0	22460	190	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 4.

All (190) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:392[B]:HIS:ND1	1:B:415:TYR:HB2	1.16	1.49
1:A:392[B]:HIS:ND1	1:A:415:TYR:HB2	1.30	1.41
1:D:392[B]:HIS:ND1	1:D:415:TYR:HB2	1.50	1.26
1:C:392[B]:HIS:ND1	1:C:415:TYR:HB2	1.47	1.25
1:B:392[B]:HIS:ND1	1:B:415:TYR:CB	2.00	1.22
1:B:392[B]:HIS:CE1	1:B:415:TYR:HB2	1.73	1.22
1:A:392[B]:HIS:ND1	1:A:415:TYR:CB	2.17	1.08
1:A:392[B]:HIS:CE1	1:A:415:TYR:HB2	2.01	0.96
1:D:750:LYS:HD3	1:D:751:ILE:H	1.42	0.85
1:B:552:LEU:HD22	1:B:556:GLN:HG3	1.70	0.74
1:D:392[B]:HIS:CE1	1:D:415:TYR:HB2	2.24	0.73
1:B:612:ARG:HD3	1:B:670:GLY:HA2	1.70	0.73
1:A:682:ASN:HB3	1:A:707:THR:HG21	1.71	0.72
1:D:744:ARG:HA	1:D:747:LYS:HD3	1.73	0.71
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.76	0.68
1:C:392[B]:HIS:CE1	1:C:415:TYR:HB2	2.27	0.68
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.76	0.67
1:C:552:LEU:HD21	1:C:571:LEU:HD12	1.78	0.66
1:A:748:ILE:O	1:A:751:ILE:HG13	1.96	0.65
1:C:583:LYS:O	1:C:584:LYS:HB3	1.96	0.65
1:C:267:ARG:HG3	3:C:3862:HOH:O	1.98	0.65
1:D:111:ARG:HB3	3:D:3414:HOH:O	1.95	0.64
1:D:267:ARG:HG3	3:D:2871:HOH:O	1.98	0.63
1:D:27:ASP:O	1:D:28:SER:HB2	1.97	0.63
1:D:552:LEU:HD11	1:D:571:LEU:HD23	1.82	0.62
1:A:28:SER:HB2	1:D:245:LEU:HD13	1.82	0.62
1:B:583:LYS:NZ	1:B:583:LYS:H	1.97	0.61
1:A:709:LYS:HA	1:A:709:LYS:HE3	1.83	0.61
1:C:392[B]:HIS:ND1	1:C:415:TYR:CB	2.43	0.61
1:C:704:PHE:O	1:C:707:THR:HG22	2.01	0.61
1:B:583:LYS:O	1:B:584:LYS:HB3	2.01	0.60
1:B:144:LEU:HD11	1:B:370:VAL:HG13	1.83	0.60
1:B:468:ASN:HD22	1:D:27:ASP:N	1.99	0.60
1:B:27:ASP:OD2	1:D:468:ASN:ND2	2.30	0.60
1:C:748:ILE:O	1:C:751:ILE:HG22	2.02	0.59
1:D:61:ARG:HH11	1:D:66:ASN:HA	1.69	0.58
1:A:144:LEU:HD11	1:A:370:VAL:HG13	1.86	0.57
1:A:27:ASP:O	1:A:28:SER:C	2.42	0.57
1:B:267:ARG:HG3	3:B:2872:HOH:O	2.03	0.57
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.34	0.57
1:C:274:ILE:HD12	2:C:760:HEM:HMB1	1.87	0.56
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.90	0.55
1:B:521:ARG:HH21	1:B:745:ILE:HG21	1.72	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:51:ALA:HB1	1:B:52:PRO:HD2	1.89	0.54
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.91	0.54
1:A:36:HIS:H	1:A:36:HIS:CD2	2.25	0.53
1:B:521:ARG:HH21	1:B:745:ILE:HD13	1.73	0.53
1:B:359:LEU:H	1:B:507:HIS:HD2	1.55	0.53
1:D:359:LEU:H	1:D:507:HIS:HD2	1.56	0.53
1:C:610:GLU:OE1	1:C:643:ASP:HA	2.08	0.53
1:C:416:THR:HA	3:C:4199:HOH:O	2.08	0.53
1:A:751:ILE:O	1:A:751:ILE:HD12	2.09	0.53
1:D:222:LYS:HB3	1:D:223:PRO:HD2	1.91	0.53
1:B:392[B]:HIS:CE1	1:B:415:TYR:CB	2.68	0.52
1:B:535:VAL:O	1:B:537:PRO:HD3	2.10	0.52
1:D:748:ILE:O	1:D:751:ILE:HG22	2.10	0.52
1:D:274:ILE:HD12	2:D:760:HEM:HMB1	1.91	0.52
1:D:535:VAL:O	1:D:537:PRO:HD3	2.09	0.52
1:C:578:ASP:HB2	1:C:582:LEU:O	2.09	0.51
1:A:689:TYR:OH	1:A:710:ILE:HG21	2.10	0.51
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.93	0.51
1:B:438:CYS:HB2	1:B:439:PRO:HD2	1.91	0.51
1:D:598:VAL:HG13	1:D:628:VAL:CG2	2.41	0.51
1:B:748:ILE:O	1:B:751:ILE:HG22	2.11	0.51
1:B:521:ARG:NH2	1:B:745:ILE:HG21	2.26	0.51
1:B:578:ASP:HB3	1:B:582:LEU:O	2.11	0.50
1:A:222:LYS:HB3	1:A:223:PRO:HD2	1.93	0.50
1:C:309:LYS:HB3	1:C:660:LEU:HD21	1.93	0.50
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.94	0.50
1:C:745:ILE:HD13	3:C:3866:HOH:O	2.10	0.50
1:C:222:LYS:HB3	1:C:223:PRO:HD2	1.93	0.49
1:B:416:THR:HG21	3:D:3414:HOH:O	2.11	0.49
1:B:37:ARG:HD2	3:B:3832:HOH:O	2.12	0.49
1:A:583:LYS:O	1:A:584:LYS:HB3	2.12	0.49
3:B:1589:HOH:O	1:D:73:LYS:HD2	2.11	0.49
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.47	0.49
1:A:29:LEU:HD22	3:C:3355:HOH:O	2.12	0.49
1:C:631:LYS:HG3	1:C:633:LEU:HD13	1.95	0.49
1:B:126:ILE:CD1	1:C:120:GLU:HB2	2.43	0.49
1:B:195:ILE:HD11	1:B:436:PRO:HA	1.95	0.49
1:A:37:ARG:HA	1:A:38:PRO:HD3	1.75	0.48
1:D:629:HIS:HD2	3:D:2510:HOH:O	1.96	0.48
1:D:51:ALA:HB1	1:D:52:PRO:HD2	1.96	0.48
1:A:612:ARG:HH11	1:A:669:CYS:CB	2.27	0.48
1:D:359:LEU:H	1:D:507:HIS:CD2	2.32	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:750:LYS:O	1:A:750:LYS:HE3	2.14	0.48
1:A:29:LEU:HD13	3:C:3355:HOH:O	2.13	0.48
1:A:128:HIS:HA	1:A:168:THR:O	2.14	0.48
1:A:443:PHE:CZ	1:A:470:PRO:HD2	2.48	0.48
1:C:137:TYR:HB2	1:C:159:ILE:HD13	1.96	0.48
1:D:546:GLN:HG3	3:D:3688:HOH:O	2.13	0.47
1:D:577:PRO:HG2	3:D:4041:HOH:O	2.14	0.47
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.30	0.47
1:A:274:ILE:HD12	2:A:760:HEM:HMB1	1.96	0.47
1:A:28:SER:CB	1:D:245:LEU:HD22	2.45	0.47
1:B:222:LYS:HB3	1:B:223:PRO:HD2	1.97	0.47
1:A:335:GLU:OE1	1:A:369:ARG:HD3	2.14	0.47
1:A:395:HIS:HE1	3:A:4187:HOH:O	1.98	0.46
1:B:745:ILE:O	1:B:748:ILE:HG12	2.14	0.46
1:C:626:LYS:HG3	1:C:733:LEU:HG	1.95	0.46
1:A:612:ARG:HE	1:A:669:CYS:HB3	1.80	0.46
1:D:583:LYS:O	1:D:584:LYS:HB3	2.16	0.46
1:C:751:ILE:HG13	1:C:752:PRO:HD2	1.98	0.46
1:B:36:HIS:HD1	1:B:36:HIS:H	1.63	0.45
1:A:711:ALA:HB3	3:A:4038:HOH:O	2.16	0.45
1:B:119:HIS:CE1	1:D:420:ILE:HG21	2.52	0.45
1:B:521:ARG:NH2	1:B:745:ILE:HD13	2.31	0.45
1:B:459:ASN:H	1:B:459:ASN:HD22	1.65	0.45
1:B:274:ILE:HD12	2:B:760:HEM:HMB1	1.98	0.45
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.52	0.45
1:A:120:GLU:HB2	1:D:126:ILE:CD1	2.46	0.45
1:D:128:HIS:HA	1:D:168:THR:O	2.17	0.45
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.52	0.45
1:D:578:ASP:HB3	1:D:582:LEU:O	2.16	0.45
1:B:507:HIS:N	1:B:508:PRO:CD	2.80	0.45
1:D:37:ARG:HA	1:D:38:PRO:HD3	1.85	0.44
1:A:126:ILE:CD1	1:D:120:GLU:HB2	2.47	0.44
1:B:128:HIS:HA	1:B:168:THR:O	2.17	0.44
1:D:574:THR:HG22	3:D:2568:HOH:O	2.16	0.44
1:B:521:ARG:HD3	3:B:3992:HOH:O	2.17	0.44
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.52	0.44
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.21	0.44
1:B:359:LEU:H	1:B:507:HIS:CD2	2.33	0.44
1:A:38:PRO:HG2	1:A:51:ALA:HB2	1.99	0.44
1:C:552:LEU:HD22	1:C:556:GLN:HG3	1.99	0.44
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.98	0.44
1:B:426:PRO:HB2	1:D:116:HIS:CD2	2.53	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:438:CYS:HB2	1:C:439:PRO:HD2	1.99	0.44
1:D:516:THR:HB	1:D:517:PRO:HD2	2.00	0.44
1:C:251:HIS:CE1	1:C:507:HIS:HB3	2.53	0.44
1:B:411:ARG:HG2	2:B:760:HEM:C2C	2.53	0.43
1:A:126:ILE:HD11	1:D:120:GLU:HB2	2.00	0.43
1:D:144:LEU:HD11	1:D:370:VAL:HG13	2.00	0.43
1:B:344:GLU:H	1:B:344:GLU:CD	2.20	0.43
1:A:426:PRO:HB2	1:C:116:HIS:CD2	2.53	0.43
1:B:603:VAL:HG11	1:B:666:ILE:HD12	2.00	0.43
1:D:703:LYS:HE2	3:D:3690:HOH:O	2.18	0.43
1:B:120:GLU:HB2	1:C:126:ILE:CD1	2.49	0.43
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.34	0.43
1:B:710:ILE:CD1	1:B:718:ILE:HG13	2.46	0.43
1:B:420:ILE:HG21	1:D:119:HIS:CE1	2.53	0.43
1:B:392[B]:HIS:ND1	1:B:415:TYR:HB3	2.16	0.43
1:C:392[A]:HIS:ND1	1:C:393:PRO:HD2	2.34	0.43
1:C:359:LEU:H	1:C:507:HIS:CD2	2.37	0.43
1:C:618:ALA:HB1	1:C:725:ASP:HB2	2.01	0.43
1:B:682:ASN:HB3	1:B:707:THR:HG21	2.00	0.43
1:C:359:LEU:H	1:C:507:HIS:HD2	1.67	0.42
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.49	0.42
1:C:195:ILE:HD11	1:C:436:PRO:HA	2.02	0.42
1:C:207:PHE:O	1:C:249:THR:HA	2.19	0.42
1:D:404:ASN:O	1:D:405:ASP:C	2.57	0.42
1:B:267:ARG:HG2	1:B:332:PRO:HB3	2.01	0.42
1:B:669:CYS:SG	1:B:670:GLY:N	2.93	0.42
1:B:331:PHE:HA	1:B:332:PRO:HD3	1.92	0.42
1:A:612:ARG:HH11	1:A:669:CYS:HB2	1.84	0.42
1:C:128:HIS:HA	1:C:168:THR:O	2.19	0.42
1:C:516:THR:HB	1:C:517:PRO:HD2	2.02	0.42
1:D:521:ARG:HH11	1:D:521:ARG:HD3	1.65	0.42
1:C:48:GLN:NE2	3:C:4048:HOH:O	2.53	0.42
1:B:498:SER:HA	1:B:499:PRO:HD3	1.93	0.42
1:B:207:PHE:O	1:B:249:THR:HA	2.20	0.42
1:B:552:LEU:CD2	1:B:556:GLN:HG3	2.45	0.41
1:C:610:GLU:O	1:C:610:GLU:HG3	2.20	0.41
1:D:602:VAL:HG13	1:D:662:VAL:HA	2.01	0.41
1:B:416:THR:HA	3:B:4196:HOH:O	2.19	0.41
1:B:27:ASP:HB3	3:B:3519:HOH:O	2.20	0.41
1:A:251:HIS:CE1	1:A:507:HIS:HB3	2.55	0.41
1:A:378:ASN:HB3	1:A:379:PRO:HD2	2.02	0.41
1:C:745:ILE:N	1:C:746:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:37:ARG:HA	1:B:38:PRO:HD3	1.88	0.41
1:A:119:HIS:CE1	1:C:420:ILE:HG21	2.56	0.41
1:B:443:PHE:CZ	1:B:470:PRO:HD2	2.55	0.41
1:D:61:ARG:NH1	1:D:66:ASN:HA	2.33	0.41
1:A:457:PRO:HG2	1:C:37:ARG:HH21	1.86	0.41
1:C:76:GLU:O	1:C:77:ASN:HB2	2.19	0.41
1:C:155:ASP:HA	1:C:156:PRO:HD2	1.93	0.41
1:D:750:LYS:HD3	1:D:751:ILE:N	2.22	0.40
1:C:507:HIS:N	1:C:508:PRO:CD	2.83	0.40
1:A:512:TRP:CH2	1:A:520:GLN:HB3	2.56	0.40
1:D:593:ILE:HA	1:D:594:PRO:HD2	1.94	0.40
1:B:144:LEU:HD11	1:B:370:VAL:CG1	2.50	0.40
1:A:97:ALA:O	1:A:101:GLY:HA3	2.22	0.40
1:B:364:LEU:HD11	1:B:580:ASN:HB2	2.04	0.40
1:C:678:ASN:HB3	1:C:681:ALA:HB3	2.03	0.40
1:C:222:LYS:HB3	1:C:223:PRO:CD	2.51	0.40
1:C:507:HIS:N	1:C:508:PRO:HD2	2.36	0.40
1:B:116:HIS:CD2	1:D:426:PRO:HB2	2.55	0.40
1:C:747:LYS:HE2	3:C:3968:HOH:O	2.21	0.40
1:B:507:HIS:N	1:B:508:PRO:HD2	2.36	0.40
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.52	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	726/753 (96%)	705 (97%)	17 (2%)	4 (1%)	33	10
1	B	726/753 (96%)	710 (98%)	12 (2%)	4 (1%)	33	10
1	C	726/753 (96%)	710 (98%)	14 (2%)	2 (0%)	50	24
1	D	726/753 (96%)	708 (98%)	14 (2%)	4 (1%)	33	10
All	All	2904/3012 (96%)	2833 (98%)	57 (2%)	14 (0%)	38	13

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	28	SER
1	B	725	ASP
1	D	28	SER
1	D	751	ILE
1	A	28	SER
1	A	709	LYS
1	D	750	LYS
1	A	711	ALA
1	B	584	LYS
1	A	75	SER
1	C	584	LYS
1	C	75	SER
1	B	75	SER
1	D	75	SER

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	613/636 (96%)	596 (97%)	17 (3%)	56	24
1	B	613/636 (96%)	590 (96%)	23 (4%)	44	14
1	C	613/636 (96%)	579 (94%)	34 (6%)	30	6
1	D	613/636 (96%)	581 (95%)	32 (5%)	32	7
All	All	2452/2544 (96%)	2346 (96%)	106 (4%)	40	11

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LYS
1	A	185	PHE
1	A	191	THR
1	A	205	ILE
1	A	227	TRP
1	A	237	ASP
1	A	252	ASN

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Mol	Chain	Res	Type
1	A	375	LEU
1	A	392[A]	HIS
1	A	392[B]	HIS
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	707	THR
1	A	709	LYS
1	A	712	ASP
1	A	750	LYS
1	B	27	ASP
1	B	37	ARG
1	B	185	PHE
1	B	191	THR
1	B	205	ILE
1	B	227	TRP
1	B	247	PRO
1	B	252	ASN
1	B	344	GLU
1	B	375	LEU
1	B	392[A]	HIS
1	B	392[B]	HIS
1	B	440	TYR
1	B	459	ASN
1	B	552	LEU
1	B	562	LEU
1	B	565	GLU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	612	ARG
1	B	633	LEU
1	B	751	ILE
1	C	37	ARG
1	C	61	ARG
1	C	159	ILE
1	C	185	PHE
1	C	191	THR
1	C	205	ILE
1	C	227	TRP
1	C	237	ASP
1	C	252	ASN

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Mol	Chain	Res	Type
1	C	369	ARG
1	C	375	LEU
1	C	377	ARG
1	C	392[A]	HIS
1	C	392[B]	HIS
1	C	415	TYR
1	C	440	TYR
1	C	459	ASN
1	C	478	LYS
1	C	488	ARG
1	C	521	ARG
1	C	531	LEU
1	C	568	ASP
1	C	571	LEU
1	C	584	LYS
1	C	606	LEU
1	C	612	ARG
1	C	616	LEU
1	C	633	LEU
1	C	648	LEU
1	C	660	LEU
1	C	685	LEU
1	C	709	LYS
1	C	733	LEU
1	C	750	LYS
1	D	28	SER
1	D	41	GLU
1	D	48	GLN
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	213	LYS
1	D	227	TRP
1	D	237	ASP
1	D	252	ASN
1	D	340	LEU
1	D	344	GLU
1	D	375	LEU
1	D	392[A]	HIS
1	D	392[B]	HIS
1	D	415	TYR
1	D	440	TYR

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Mol	Chain	Res	Type
1	D	459	ASN
1	D	490	GLU
1	D	552	LEU
1	D	554	LEU
1	D	574	THR
1	D	582	LEU
1	D	598	VAL
1	D	616	LEU
1	D	633	LEU
1	D	648	LEU
1	D	713	GLN
1	D	747	LYS
1	D	749	ASP
1	D	750	LYS
1	D	751	ILE

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

Mol	Chain	Res	Type
1	A	36	HIS
1	A	252	ASN
1	A	459	ASN
1	A	515	GLN
1	A	713	GLN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	C	252	ASN
1	C	459	ASN
1	C	507	HIS
1	C	556	GLN
1	C	572	ASN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	252	ASN
1	D	449	HIS
1	D	459	ASN
1	D	507	HIS
1	D	556	GLN
1	D	629	HIS

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Mol	Chain	Res	Type
1	D	671	ASN
1	D	713	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 ⓘ

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$
2	HEM	A	760	1	49,50,50	2.20	14 (28%)	46,82,82	1.66	9 (19%)
2	HEM	B	760	1	49,50,50	2.47	14 (28%)	46,82,82	1.78	12 (26%)
2	HEM	C	760	1	49,50,50	2.52	12 (24%)	46,82,82	1.61	8 (17%)
2	HEM	D	760	1	49,50,50	2.29	13 (26%)	46,82,82	1.70	8 (17%)

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	760	1	-	0/14/114/114	0/0/8/8
2	HEM	B	760	1	-	0/14/114/114	0/0/8/8
2	HEM	C	760	1	-	0/14/114/114	0/0/8/8
2	HEM	D	760	1	-	0/14/114/114	0/0/8/8

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	760	HEM	C2B-C1B	7.10	1.46	1.44
2	C	760	HEM	C2D-C1D	6.14	1.46	1.44
2	B	760	HEM	C3D-C2D	-6.03	1.33	1.43
2	C	760	HEM	C3D-C2D	-5.97	1.33	1.43
2	A	760	HEM	C3D-C2D	-5.95	1.33	1.43
2	B	760	HEM	C2B-C1B	5.82	1.46	1.44
2	B	760	HEM	C3B-C2B	-5.67	1.33	1.43
2	B	760	HEM	C3C-C2C	-5.67	1.33	1.43
2	D	760	HEM	C3D-C2D	-5.64	1.33	1.43
2	A	760	HEM	C3C-C2C	-5.63	1.33	1.43
2	D	760	HEM	C3C-C2C	-5.56	1.34	1.43
2	C	760	HEM	C3C-C2C	-5.54	1.34	1.43
2	D	760	HEM	C2D-C1D	5.51	1.45	1.44
2	C	760	HEM	C3B-C2B	-5.43	1.34	1.43
2	A	760	HEM	C3B-C2B	-5.37	1.34	1.43
2	D	760	HEM	C3B-C2B	-5.16	1.34	1.43
2	B	760	HEM	C4A-C3A	4.90	1.46	1.40
2	C	760	HEM	C4A-C3A	4.86	1.46	1.40
2	C	760	HEM	C3B-CAB	4.81	1.55	1.40
2	D	760	HEM	C4A-C3A	4.48	1.45	1.40
2	B	760	HEM	C3C-CAC	4.45	1.54	1.40
2	D	760	HEM	C3C-CAC	4.42	1.54	1.40
2	B	760	HEM	C3B-CAB	4.42	1.54	1.40
2	D	760	HEM	C3B-CAB	4.41	1.54	1.40
2	A	760	HEM	C3C-CAC	4.40	1.54	1.40
2	A	760	HEM	C3B-CAB	4.39	1.54	1.40
2	C	760	HEM	C3C-CAC	4.38	1.54	1.40
2	A	760	HEM	C4A-C3A	4.38	1.45	1.40
2	B	760	HEM	C2D-C1D	3.98	1.45	1.44
2	B	760	HEM	C3D-C4D	3.64	1.45	1.44
2	A	760	HEM	C2B-C1B	3.46	1.45	1.44
2	D	760	HEM	FE-NA	2.81	2.04	1.92
2	D	760	HEM	C2B-C1B	2.67	1.45	1.44
2	B	760	HEM	FE-NA	2.63	2.03	1.92
2	A	760	HEM	CMD-C2D	2.61	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	760	HEM	CMB-C2B	2.60	1.55	1.47
2	D	760	HEM	CMC-C2C	2.58	1.55	1.47
2	A	760	HEM	FE-NA	2.58	2.03	1.92
2	D	760	HEM	CMD-C2D	2.53	1.55	1.47
2	D	760	HEM	CMB-C2B	2.50	1.55	1.47
2	C	760	HEM	FE-NA	2.49	2.03	1.92
2	A	760	HEM	CMB-C2B	2.49	1.55	1.47
2	B	760	HEM	CMC-C2C	2.47	1.55	1.47
2	B	760	HEM	CMD-C2D	2.46	1.55	1.47
2	C	760	HEM	CMD-C2D	2.45	1.55	1.47
2	A	760	HEM	C2D-C1D	2.39	1.45	1.44
2	A	760	HEM	CMC-C2C	2.36	1.54	1.47
2	D	760	HEM	CHA-C4D	2.36	1.39	1.35
2	C	760	HEM	CMB-C2B	2.34	1.54	1.47
2	C	760	HEM	CMC-C2C	2.33	1.54	1.47
2	A	760	HEM	CHA-C4D	2.21	1.39	1.35
2	B	760	HEM	CHA-C4D	2.09	1.38	1.35
2	A	760	HEM	CHB-C1B	2.00	1.38	1.35

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	760	HEM	C3B-C4B-NB	-6.97	109.01	114.00
2	D	760	HEM	C3B-C4B-NB	-6.85	109.10	114.00
2	C	760	HEM	C3B-C4B-NB	-6.43	109.40	114.00
2	A	760	HEM	C3B-C4B-NB	-5.91	109.77	114.00
2	A	760	HEM	CMA-C3A-C4A	-3.90	122.62	128.62
2	B	760	HEM	CMA-C3A-C4A	-3.62	123.05	128.62
2	D	760	HEM	CMA-C3A-C4A	-3.37	123.44	128.62
2	B	760	HEM	O2D-CGD-O1D	3.16	131.34	123.30
2	C	760	HEM	C2D-C1D-ND	-2.90	109.50	112.93
2	B	760	HEM	O2A-CGA-O1A	2.88	130.63	123.30
2	D	760	HEM	C4A-CHB-C1B	-2.88	123.69	127.47
2	A	760	HEM	CMA-C3A-C2A	2.85	130.31	124.94
2	D	760	HEM	O2A-CGA-O1A	2.84	130.51	123.30
2	A	760	HEM	O1D-CGD-CBD	-2.83	113.30	123.03
2	A	760	HEM	C1A-CHA-C4D	-2.76	123.84	127.47
2	C	760	HEM	O1D-CGD-CBD	-2.67	113.84	123.03
2	D	760	HEM	C1A-CHA-C4D	-2.67	123.95	127.47
2	B	760	HEM	O1D-CGD-CBD	-2.66	113.89	123.03
2	B	760	HEM	CMA-C3A-C2A	2.61	129.87	124.94
2	B	760	HEM	O1A-CGA-CBA	-2.50	114.42	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	760	HEM	O2A-CGA-O1A	2.48	129.61	123.30
2	A	760	HEM	C2D-C1D-ND	-2.48	110.00	112.93
2	C	760	HEM	O1A-CGA-CBA	-2.42	114.70	123.03
2	D	760	HEM	CMA-C3A-C2A	2.41	129.48	124.94
2	C	760	HEM	O2A-CGA-O1A	2.39	129.37	123.30
2	B	760	HEM	C4A-CHB-C1B	-2.38	124.34	127.47
2	D	760	HEM	C2D-C1D-ND	-2.33	110.18	112.93
2	A	760	HEM	CMD-C2D-C3D	2.33	130.88	125.60
2	A	760	HEM	CHD-C1D-ND	2.33	126.52	124.58
2	C	760	HEM	CMD-C2D-C3D	2.28	130.76	125.60
2	C	760	HEM	C1A-CHA-C4D	-2.25	124.52	127.47
2	D	760	HEM	O1A-CGA-CBA	-2.24	115.32	123.03
2	B	760	HEM	CMD-C2D-C3D	2.23	130.65	125.60
2	B	760	HEM	C1A-CHA-C4D	-2.21	124.56	127.47
2	C	760	HEM	CMA-C3A-C4A	-2.17	125.28	128.62
2	B	760	HEM	C2D-C1D-ND	-2.16	110.38	112.93
2	B	760	HEM	CAA-CBA-CGA	-2.00	107.03	113.47

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	727/753 (96%)	-0.28	13 (1%) 65 67	10, 16, 31, 54	0
1	B	727/753 (96%)	-0.15	30 (4%) 35 35	10, 18, 38, 48	0
1	C	727/753 (96%)	-0.18	27 (3%) 39 40	10, 18, 38, 47	0
1	D	727/753 (96%)	-0.25	16 (2%) 59 60	9, 16, 31, 50	0
All	All	2908/3012 (96%)	-0.22	86 (2%) 48 49	9, 17, 36, 54	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	ASP	10.8
1	A	28	SER	8.5
1	A	711	ALA	7.5
1	D	27	ASP	7.0
1	D	28	SER	6.7
1	C	28	SER	5.6
1	A	710	ILE	5.1
1	C	27	ASP	5.0
1	A	712	ASP	5.0
1	B	27	ASP	4.7
1	C	726	GLY	4.5
1	B	713	GLN	4.4
1	D	749	ASP	4.3
1	D	750	LYS	4.2
1	B	726	GLY	4.0
1	B	596	GLY	3.9
1	A	713	GLN	3.8
1	D	712	ASP	3.8
1	C	594	PRO	3.8
1	B	712	ASP	3.7
1	B	749	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	713	GLN	3.7
1	B	32	GLU	3.5
1	B	750	LYS	3.5
1	B	28	SER	3.4
1	C	712	ASP	3.4
1	A	32	GLU	3.4
1	A	709	LYS	3.3
1	C	617	LEU	3.2
1	C	750	LYS	3.2
1	B	677	ASP	3.1
1	C	673	ALA	3.1
1	A	750	LYS	3.1
1	D	32	GLU	3.1
1	C	725	ASP	3.0
1	A	749	ASP	2.8
1	B	583	LYS	2.8
1	B	673	ALA	2.8
1	D	711	ALA	2.7
1	B	646	THR	2.7
1	B	644	ASP	2.7
1	B	642	ALA	2.7
1	C	703	LYS	2.6
1	D	568	ASP	2.6
1	C	32	GLU	2.6
1	B	569	ASP	2.6
1	B	709	LYS	2.6
1	D	596	GLY	2.5
1	C	569	ASP	2.5
1	C	595	ASP	2.5
1	C	724	ALA	2.5
1	B	710	ILE	2.5
1	D	710	ILE	2.5
1	C	677	ASP	2.5
1	A	369	ARG	2.4
1	A	596	GLY	2.4
1	C	645	GLY	2.4
1	C	641	THR	2.4
1	B	612	ARG	2.4
1	B	568	ASP	2.3
1	C	711	ALA	2.3
1	D	583	LYS	2.3
1	B	37	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	749	ASP	2.3
1	D	33	ASP	2.3
1	C	669	CYS	2.3
1	B	595	ASP	2.3
1	B	641	THR	2.3
1	C	596	GLY	2.3
1	C	714	GLY	2.3
1	D	594	PRO	2.2
1	B	714	GLY	2.2
1	C	552	LEU	2.1
1	A	283	GLU	2.1
1	B	711	ALA	2.1
1	D	595	ASP	2.1
1	D	677	ASP	2.1
1	C	646	THR	2.1
1	B	647	VAL	2.1
1	C	583	LYS	2.1
1	B	639	GLU	2.1
1	C	612	ARG	2.1
1	B	706	ALA	2.0
1	B	643	ASP	2.0
1	B	572	ASN	2.0
1	C	568	ASP	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(\AA^2)	Q<0.9
2	HEM	D	760	43/43	0.06	-0.14	9,11,12,13	0
2	HEM	A	760	43/43	0.06	-0.22	9,10,12,12	0
2	HEM	C	760	43/43	0.06	-0.27	10,11,13,14	0
2	HEM	B	760	43/43	0.06	-0.67	10,12,13,15	0

6.5 Other polymers ⓘ

There are no such residues in this entry.