W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:23 PM GMT

PDB ID	:	4ENV
Title	:	Structure of the S234I variant of E. coli KatE
Authors	:	Loewen, P.C.; Jha, V.
Deposited on	:	2012-04-13
Resolution	:	1.70 Å(reported)

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

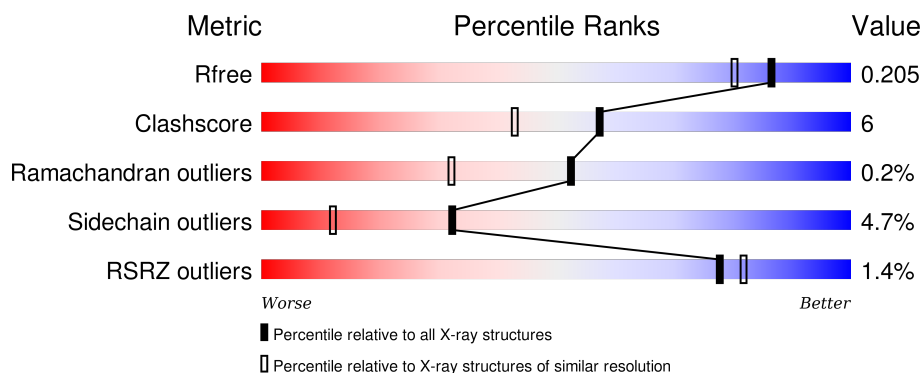|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1　Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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		0.205
Clashscore		6
Ramachandran outliers		0.2%
Sidechain outliers		4.7%
RSRZ outliers		1.4%

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}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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. 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	753	% 84% 11% • •
1	B	753	2% 83% 11% • •
1	C	753	2% 83% 11% • • •
1	D	753	% 84% 10% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26342 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.
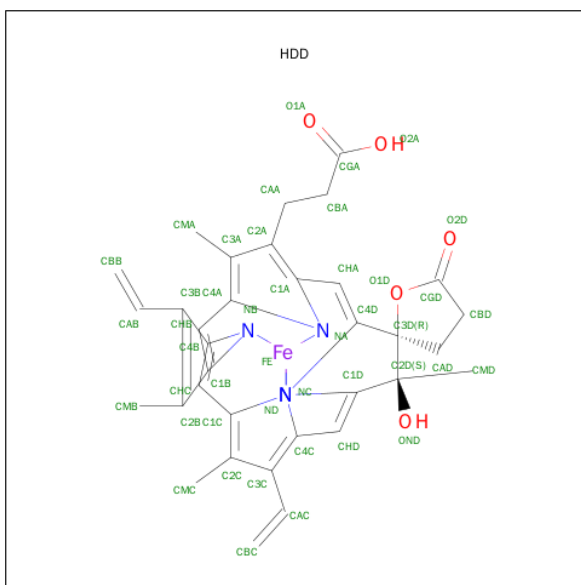
- Molecule 1 is a protein called Catalase HPII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	2	0
			5752	3654	1007	1079	12			
1	B	726	Total	C	N	O	S	0	1	0
			5745	3649	1005	1079	12			
1	C	726	Total	C	N	O	S	0	2	0
			5752	3654	1007	1079	12			
1	D	726	Total	C	N	O	S	0	1	0
			5744	3648	1005	1079	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	234	ILE	SER	ENGINEERED MUTATION	UNP P21179
B	234	ILE	SER	ENGINEERED MUTATION	UNP P21179
C	234	ILE	SER	ENGINEERED MUTATION	UNP P21179
D	234	ILE	SER	ENGINEERED MUTATION	UNP P21179

- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (three-letter code: HDD) (formula: $C_{34}H_{32}FeN_4O_5$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	B	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	C	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	D	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
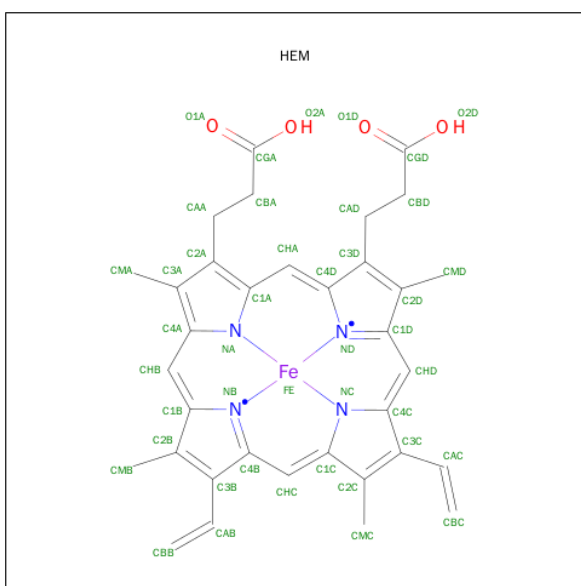
| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	1
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	1
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	1
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	1

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	772	Total 772	O 772	0	0
4	B	695	Total 695	O 695	0	0
4	C	735	Total 735	O 735	0	0
4	D	799	Total 799	O 799	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.
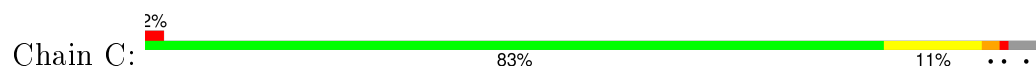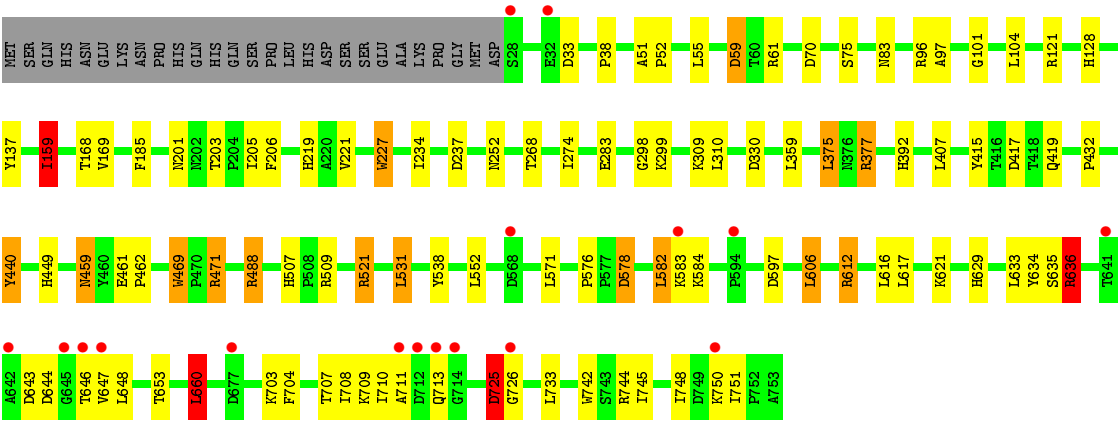
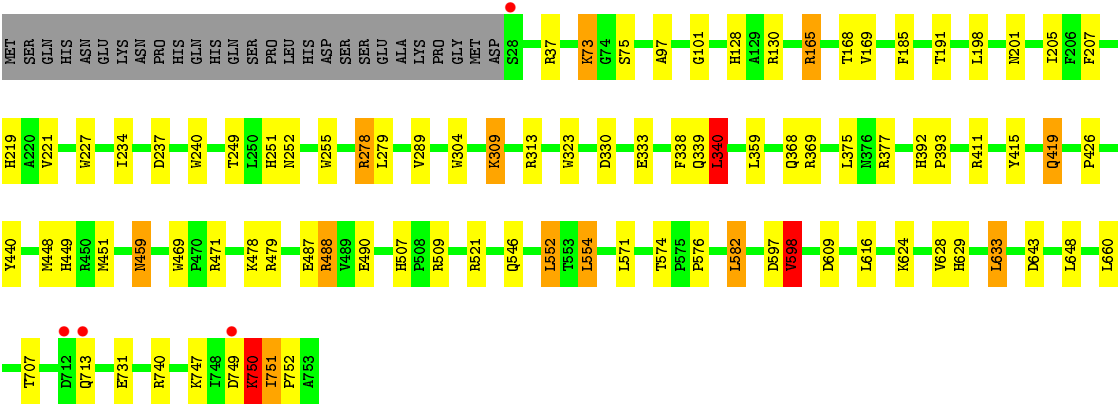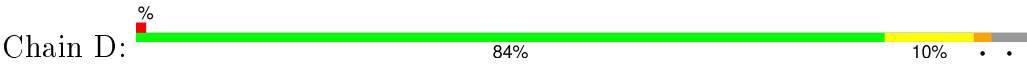- Molecule 1: Catalase HPII
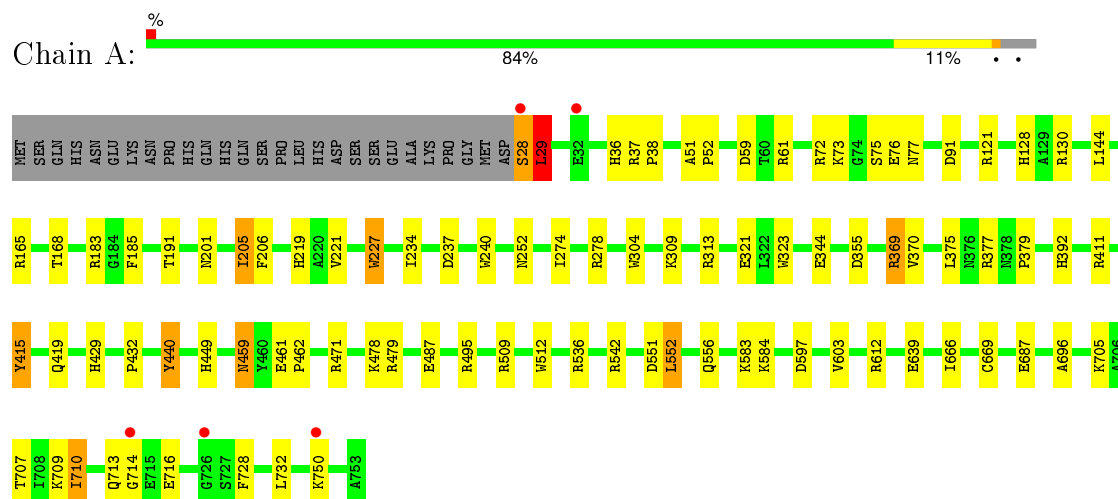
Chain A:

- Molecule 1: Catalase HPII

Chain B:

- Molecule 1: Catalase HPII

Chain C:

• Molecule 1: Catalase HPII

Chain D:
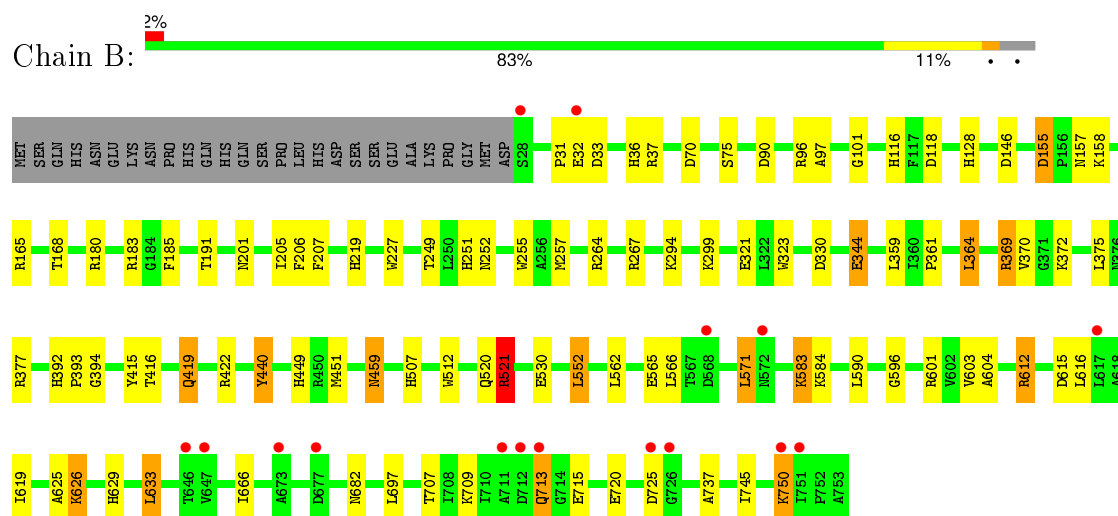
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.23Å 133.13Å 122.71Å 90.00° 109.39° 90.00°	Depositor
Resolution (Å)	32.12 – 1.70 32.12 – 1.70	Depositor EDS
% Data completeness (in resolution range)	79.5 (32.12-1.70) 79.5 (32.12-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.167 , 0.207 0.165 , 0.205	Depositor DCC
R_{free} test set	12422 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	12.6	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.2	EDS
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
L-test for twinning [2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 245687 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	26342	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, HDD

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	1.13	10/5916 (0.2%)	1.08	19/8043 (0.2%)
1	B	1.06	5/5905 (0.1%)	1.05	22/8028 (0.3%)
1	C	1.07	7/5916 (0.1%)	1.02	16/8043 (0.2%)
1	D	1.14	7/5905 (0.1%)	1.08	21/8028 (0.3%)
All	All	1.10	29/23642 (0.1%)	1.06	78/32142 (0.2%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	59	ASP	CB-CG	7.65	1.67	1.51
1	B	255	TRP	CD2-CE2	6.95	1.49	1.41
1	D	333	GLU	CD-OE2	-6.92	1.18	1.25
1	D	469	TRP	CD2-CE2	6.15	1.48	1.41
1	B	165	ARG	CZ-NH1	6.13	1.41	1.33
1	C	742	TRP	CD2-CE2	5.98	1.48	1.41
1	A	512	TRP	CG-CD1	5.90	1.45	1.36
1	A	227	TRP	CD2-CE2	5.73	1.48	1.41
1	C	377	ARG	CZ-NH1	5.72	1.40	1.33
1	D	304	TRP	CD2-CE2	5.71	1.48	1.41
1	A	121	ARG	CZ-NH2	5.69	1.40	1.33
1	A	323	TRP	CD2-CE2	5.63	1.48	1.41
1	D	255	TRP	CD2-CE2	5.54	1.48	1.41
1	C	227	TRP	CD2-CE2	5.50	1.48	1.41
1	A	321	GLU	CD-OE1	5.43	1.31	1.25
1	A	415	TYR	CG-CD1	5.40	1.46	1.39
1	C	538	TYR	CG-CD2	5.37	1.46	1.39
1	B	440	TYR	CE2-CZ	5.36	1.45	1.38
1	A	227	TRP	CG-CD1	5.31	1.44	1.36
1	A	240	TRP	CD2-CE2	5.28	1.47	1.41
1	D	240	TRP	CD2-CE2	5.28	1.47	1.41
1	B	323	TRP	CD2-CE2	5.27	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	449	HIS	CG-CD2	5.25	1.44	1.35
1	D	323	TRP	CD2-CE2	5.23	1.47	1.41
1	C	203	THR	C-O	5.20	1.33	1.23
1	A	440	TYR	CE2-CZ	5.10	1.45	1.38
1	C	469	TRP	CD2-CE2	5.07	1.47	1.41
1	D	165	ARG	CZ-NH2	5.06	1.39	1.33
1	A	304	TRP	CD2-CE2	5.05	1.47	1.41

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	471	ARG	NE-CZ-NH2	-10.49	115.05	120.30
1	A	377	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	D	471	ARG	NE-CZ-NH2	-9.49	115.55	120.30
1	C	59	ASP	CB-CG-OD1	9.34	126.70	118.30
1	A	479	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	D	377	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	B	422	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	A	536	ARG	NE-CZ-NH2	7.55	124.08	120.30
1	D	554	LEU	CB-CG-CD2	7.45	123.66	111.00
1	B	294	LYS	CD-CE-NZ	-7.42	94.62	111.70
1	D	278	ARG	NE-CZ-NH1	-7.32	116.64	120.30
1	A	542	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	A	130	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	A	29	LEU	CA-CB-CG	7.09	131.61	115.30
1	D	582	LEU	CB-CG-CD1	6.95	122.82	111.00
1	B	369	ARG	NE-CZ-NH1	-6.85	116.88	120.30
1	A	495	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	B	180	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	C	636	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	C	636	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	A	471	ARG	NE-CZ-NH1	-6.61	116.99	120.30
1	D	609	ASP	CB-CG-OD1	6.54	124.19	118.30
1	D	749	ASP	C-N-CA	6.45	137.81	121.70
1	D	643	ASP	CB-CG-OD1	6.41	124.06	118.30
1	B	90	ASP	CB-CG-OD1	6.24	123.91	118.30
1	C	96	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	D	471	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	A	183	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	C	617	LEU	CA-CB-CG	6.15	129.44	115.30
1	D	340	LEU	CB-CG-CD1	6.10	121.37	111.00
1	C	33	ASP	CB-CG-OD1	6.08	123.78	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	509	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	590	LEU	CB-CG-CD2	-6.07	100.68	111.00
1	A	551	ASP	CB-CG-OD2	6.03	123.73	118.30
1	B	96	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	B	369	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	B	267	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	D	598	VAL	CG1-CB-CG2	5.95	120.42	110.90
1	B	521	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	D	279	LEU	CB-CG-CD2	-5.87	101.03	111.00
1	D	597	ASP	CB-CG-OD1	5.84	123.56	118.30
1	B	364	LEU	CB-CG-CD1	-5.84	101.07	111.00
1	C	606	LEU	CB-CG-CD1	5.81	120.88	111.00
1	B	70	ASP	CB-CG-OD2	5.75	123.48	118.30
1	B	33	ASP	CB-CG-OD1	5.67	123.41	118.30
1	D	130	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	479	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	D	633	LEU	CB-CG-CD1	5.52	120.38	111.00
1	B	521	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	D	377	ARG	NH1-CZ-NH2	5.48	125.42	119.40
1	B	264	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	377	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	C	531	LEU	CB-CG-CD1	5.39	120.16	111.00
1	D	198	LEU	CB-CG-CD2	-5.37	101.87	111.00
1	D	740	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	A	355	ASP	CB-CG-OD1	5.35	123.11	118.30
1	D	377	ARG	CG-CD-NE	-5.34	100.58	111.80
1	C	375	LEU	CB-CG-CD1	5.32	120.05	111.00
1	C	725	ASP	CA-C-N	5.32	126.85	116.20
1	B	180	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	660	LEU	CB-CG-CD1	5.29	120.00	111.00
1	A	419[A]	GLN	CB-CA-C	5.29	120.97	110.40
1	A	419[B]	GLN	CB-CA-C	5.29	120.97	110.40
1	C	70	ASP	CB-CG-OD1	5.27	123.05	118.30
1	A	72	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	419[A]	GLN	CB-CA-C	5.22	120.85	110.40
1	B	419[B]	GLN	CB-CA-C	5.22	120.85	110.40
1	B	146	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	597	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	61	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	552	LEU	CB-CG-CD1	5.16	119.78	111.00
1	B	601	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	B	183	ARG	NE-CZ-NH1	-5.13	117.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	749	ASP	CA-C-N	5.13	128.48	117.20
1	D	479	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	C	121	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	C	582	LEU	CB-CG-CD1	-5.05	102.42	111.00
1	C	159	ILE	CB-CG1-CD1	-5.04	99.78	113.90

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	5752	0	5591	59	1
1	B	5745	0	5584	66	1
1	C	5752	0	5591	77	1
1	D	5744	0	5584	66	0
2	A	44	0	31	4	0
2	B	44	0	31	3	0
2	C	44	0	31	2	0
2	D	44	0	31	3	0
3	A	43	0	30	15	0
3	B	43	0	30	7	0
3	C	43	0	30	12	0
3	D	43	0	30	10	0
4	A	772	0	0	11	0
4	B	695	0	0	12	1
4	C	735	0	0	18	0
4	D	799	0	0	15	0
All	All	26342	0	22594	274	2

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 6.

All (274) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:HIS:ND1	1:C:415:TYR:CB	1.67	1.54
1:B:392:HIS:ND1	1:B:415:TYR:CB	1.68	1.51
1:D:392:HIS:ND1	1:D:415:TYR:CB	1.73	1.50
1:A:392:HIS:ND1	1:A:415:TYR:CB	1.76	1.48
1:C:392:HIS:CE1	1:C:415:TYR:HB2	1.64	1.30
1:D:521:ARG:HD2	4:D:1642:HOH:O	1.36	1.25
1:D:546:GLN:HG3	4:D:1601:HOH:O	1.05	1.22
1:B:392:HIS:CE1	1:B:415:TYR:HB2	1.73	1.21
1:D:392:HIS:CE1	1:D:415:TYR:HB2	1.76	1.20
1:C:521:ARG:CG	1:C:521:ARG:HH11	1.52	1.20
1:A:392:HIS:CE1	1:A:415:TYR:HB2	1.80	1.17
1:A:392:HIS:ND1	1:A:415:TYR:HB2	0.81	1.13
3:C:802[B]:HEM:HBC2	3:C:802[B]:HEM:HMC2	1.17	1.13
1:C:521:ARG:NH1	1:C:521:ARG:HG2	1.33	1.13
1:D:392:HIS:ND1	1:D:415:TYR:HB2	0.80	1.12
1:C:392:HIS:ND1	1:C:415:TYR:HB2	0.79	1.11
1:B:392:HIS:ND1	1:B:415:TYR:HB2	0.76	1.08
3:D:802[B]:HEM:HBC2	3:D:802[B]:HEM:HMC2	1.43	0.98
1:C:612:ARG:HG3	1:C:612:ARG:HH11	1.27	0.96
4:B:1503:HOH:O	1:D:73:LYS:HD3	1.67	0.95
1:B:416:THR:HG21	4:D:1528:HOH:O	1.64	0.95
1:A:344:GLU:OE1	4:A:1588:HOH:O	1.84	0.95
1:A:369:ARG:HH21	1:A:369:ARG:HG3	1.28	0.94
1:A:201:ASN:CG	3:A:802[B]:HEM:HMB2	1.89	0.92
1:D:731:GLU:OE2	4:D:1670:HOH:O	1.86	0.92
3:A:802[B]:HEM:CMC	3:A:802[B]:HEM:HBC2	1.98	0.92
1:A:392:HIS:CG	1:A:415:TYR:HB2	2.04	0.92
1:D:392:HIS:CG	1:D:415:TYR:HB2	2.04	0.89
1:C:725:ASP:HB2	1:C:726:GLY:C	1.93	0.89
1:C:725:ASP:HB2	1:C:726:GLY:O	1.72	0.89
1:C:521:ARG:HG2	1:C:521:ARG:HH11	0.74	0.89
1:C:521:ARG:CG	1:C:521:ARG:NH1	2.20	0.88
1:A:716:GLU:HG2	4:A:1647:HOH:O	1.74	0.88
1:B:392:HIS:CG	1:B:415:TYR:HB2	2.04	0.87
3:D:802[B]:HEM:CMC	3:D:802[B]:HEM:HBC2	2.03	0.87
1:A:29:LEU:HD22	4:C:1476:HOH:O	1.75	0.85
1:D:201:ASN:CG	3:D:802[B]:HEM:HMB2	1.99	0.83
1:B:157:ASN:HB2	4:B:1581:HOH:O	1.78	0.82
1:A:369:ARG:HH21	1:A:369:ARG:CG	1.94	0.80
3:A:802[B]:HEM:HMC1	3:A:802[B]:HEM:HBC2	1.62	0.80
1:C:59:ASP:OD2	4:C:1498:HOH:O	1.99	0.80
1:C:629:HIS:HD2	4:C:1209:HOH:O	1.65	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:802[B]:HEM:CMC	3:C:802[B]:HEM:HBC2	1.94	0.80
4:B:1503:HOH:O	1:D:73:LYS:CD	2.25	0.77
1:C:612:ARG:HH11	1:C:612:ARG:CG	1.96	0.77
1:C:621:LYS:HG2	4:C:1618:HOH:O	1.85	0.77
1:C:636:ARG:HD3	4:C:1540:HOH:O	1.85	0.77
1:D:221:VAL:CG2	1:D:234:ILE:HG22	2.15	0.77
1:C:201:ASN:CG	3:C:802[B]:HEM:HMB2	2.06	0.76
1:C:392:HIS:ND1	1:C:415:TYR:HB3	1.96	0.75
1:C:597:ASP:OD1	4:C:1425:HOH:O	2.04	0.75
1:C:206:PHE:CG	3:C:802[B]:HEM:HAB	2.22	0.74
1:B:369:ARG:HG2	4:B:1306:HOH:O	1.87	0.73
1:D:751:ILE:HG12	1:D:752:PRO:HD2	1.69	0.72
1:D:488:ARG:NE	4:D:1586:HOH:O	2.03	0.72
1:D:488:ARG:NH2	4:D:1586:HOH:O	2.21	0.72
1:D:392:HIS:ND1	1:D:415:TYR:CG	2.57	0.71
1:C:612:ARG:HG3	1:C:612:ARG:NH1	2.05	0.71
1:A:369:ARG:HD3	4:A:1495:HOH:O	1.91	0.70
1:A:639:GLU:HG3	4:A:1498:HOH:O	1.92	0.69
1:C:392:HIS:ND1	1:C:415:TYR:CG	2.58	0.69
1:B:330:ASP:OD2	1:B:629:HIS:HE1	1.75	0.69
1:D:629:HIS:HD2	4:D:1260:HOH:O	1.74	0.69
1:C:578:ASP:HB2	1:C:582:LEU:O	1.93	0.69
1:A:392:HIS:ND1	1:A:415:TYR:CG	2.60	0.68
3:A:802[B]:HEM:CBC	3:A:802[B]:HEM:HMC1	2.24	0.68
1:A:710:ILE:HD11	1:A:714:GLY:HA2	1.76	0.68
1:D:368:GLN:OE1	4:D:1587:HOH:O	2.12	0.67
1:C:221:VAL:CG2	1:C:234:ILE:HG22	2.25	0.67
1:C:440:TYR:HD2	4:C:1375:HOH:O	1.78	0.66
2:B:801[A]:HDD:HMB1	2:B:801[A]:HDD:HBB1	1.78	0.66
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.77	0.66
1:D:598:VAL:HG13	1:D:628:VAL:CG2	2.26	0.66
1:C:521:ARG:CD	4:C:1440:HOH:O	2.44	0.65
1:C:330:ASP:OD2	1:C:629:HIS:HE1	1.80	0.65
1:A:369:ARG:NH2	1:A:369:ARG:HG3	2.04	0.64
1:B:392:HIS:ND1	1:B:415:TYR:CG	2.63	0.64
1:C:488:ARG:HD3	4:C:1472:HOH:O	1.98	0.64
1:C:201:ASN:ND2	3:C:802[B]:HEM:HMB2	2.12	0.64
1:A:206:PHE:CG	3:A:802[B]:HEM:HAB	2.33	0.63
1:A:28:SER:OG	1:A:28:SER:O	2.15	0.63
1:C:407:LEU:HD23	3:C:802[B]:HEM:HBB1	1.81	0.62
1:A:344:GLU:HB3	4:A:1588:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ASN:ND2	3:A:802[B]:HEM:CMB	2.63	0.61
1:A:144:LEU:HD11	1:A:370:VAL:HG13	1.82	0.61
3:D:802[B]:HEM:HMC2	3:D:802[B]:HEM:CBC	2.24	0.61
1:A:201:ASN:CG	3:A:802[B]:HEM:CMB	2.67	0.61
1:B:201:ASN:CG	3:B:802[B]:HEM:HMB2	2.21	0.60
1:C:274:ILE:HD12	3:C:802[B]:HEM:HMB1	1.83	0.60
1:D:330:ASP:OD2	1:D:629:HIS:HE1	1.83	0.60
1:B:625:ALA:O	1:B:626:LYS:HE3	2.01	0.60
1:C:201:ASN:ND2	3:C:802[B]:HEM:CMB	2.65	0.60
1:D:415:TYR:O	1:D:419[B]:GLN:HG2	2.01	0.60
1:D:488:ARG:HH12	1:D:490:GLU:CD	2.06	0.59
1:C:521:ARG:HD2	4:C:1440:HOH:O	2.02	0.59
1:B:583:LYS:O	1:B:584:LYS:HB3	2.02	0.59
2:A:801[A]:HDD:HMB1	2:A:801[A]:HDD:HBB1	1.85	0.59
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.18	0.58
2:C:801[A]:HDD:HBD2	4:C:1091:HOH:O	2.02	0.58
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.34	0.58
1:C:745:ILE:HD13	4:C:1570:HOH:O	2.03	0.58
2:A:801[A]:HDD:HBD2	4:A:995:HOH:O	2.03	0.58
1:C:725:ASP:HB2	1:C:726:GLY:CA	2.34	0.57
1:D:201:ASN:ND2	3:D:802[B]:HEM:CMB	2.68	0.57
1:C:52:PRO:HG2	1:C:55:LEU:HD12	1.87	0.57
1:B:392:HIS:CG	1:B:415:TYR:CB	2.78	0.57
1:B:392:HIS:ND1	1:B:415:TYR:HB3	2.02	0.57
1:D:490:GLU:OE2	4:D:1485:HOH:O	2.18	0.57
1:C:221:VAL:HG22	1:C:234:ILE:HG22	1.87	0.56
1:D:411:ARG:HG2	3:D:802[B]:HEM:C2C	2.40	0.56
1:D:201:ASN:CG	3:D:802[B]:HEM:CMB	2.74	0.56
1:A:369:ARG:NH2	1:A:369:ARG:CG	2.63	0.56
2:D:801[A]:HDD:HBD2	4:D:1141:HOH:O	2.05	0.56
1:D:478:LYS:NZ	4:D:999:HOH:O	2.26	0.56
1:A:612:ARG:HE	1:A:669:CYS:HB3	1.71	0.55
1:C:206:PHE:CD1	3:C:802[B]:HEM:HAB	2.41	0.55
1:A:274:ILE:HD12	3:A:802[B]:HEM:HMB1	1.89	0.55
1:D:359:LEU:H	1:D:507:HIS:HD2	1.55	0.55
1:C:359:LEU:H	1:C:507:HIS:HD2	1.55	0.55
1:B:359:LEU:H	1:B:507:HIS:HD2	1.54	0.55
1:D:750:LYS:C	1:D:750:LYS:HD2	2.27	0.55
1:A:449[B]:HIS:HD2	4:C:1192:HOH:O	1.88	0.55
1:B:629:HIS:HD2	4:B:1162:HOH:O	1.89	0.54
1:A:710:ILE:CD1	1:A:714:GLY:HA2	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ASN:CG	3:B:802[B]:HEM:CMB	2.76	0.54
1:C:704:PHE:O	1:C:707:THR:HG22	2.07	0.54
3:A:802[B]:HEM:HMC3	3:A:802[B]:HEM:HBC2	1.87	0.54
1:A:201:ASN:ND2	3:A:802[B]:HEM:HMB2	2.23	0.54
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.90	0.54
1:A:478:LYS:HG2	4:A:1370:HOH:O	2.08	0.54
3:C:802[B]:HEM:CMC	3:C:802[B]:HEM:CBC	2.76	0.54
1:C:359:LEU:H	1:C:507:HIS:CD2	2.26	0.54
1:B:583:LYS:NZ	1:B:583:LYS:H	2.05	0.53
1:B:451:MET:HE2	1:D:451:MET:HE1	1.90	0.53
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.12	0.53
1:C:469:TRP:CE3	1:C:471:ARG:HG3	2.43	0.53
1:D:165:ARG:HD3	2:D:801[A]:HDD:O2A	2.09	0.53
1:C:521:ARG:HG2	4:C:1570:HOH:O	2.09	0.53
1:B:257:MET:SD	1:B:530:GLU:HG3	2.49	0.53
1:B:361:PRO:HD2	1:B:364:LEU:HD12	1.90	0.52
1:C:38:PRO:HG2	1:C:51:ALA:HB2	1.90	0.52
1:B:206:PHE:CG	3:B:802[B]:HEM:HAB	2.45	0.52
1:B:626:LYS:HA	1:B:626:LYS:HE3	1.90	0.52
1:D:338:PHE:HB3	1:D:340:LEU:HD13	1.91	0.52
1:C:392:HIS:CE1	1:C:415:TYR:CB	2.57	0.52
1:D:449:HIS:CE1	4:D:1348:HOH:O	2.62	0.52
1:A:201:ASN:OD1	3:A:802[B]:HEM:HMB2	2.10	0.51
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.25	0.51
1:B:97:ALA:O	1:B:101:GLY:HA3	2.10	0.51
1:B:615:ASP:O	1:B:619:ILE:HG13	2.10	0.51
2:B:801[A]:HDD:HBD2	4:B:1042:HOH:O	2.10	0.51
1:B:713:GLN:H	1:B:713:GLN:NE2	2.10	0.50
1:D:207:PHE:O	1:D:249:THR:HA	2.11	0.50
1:B:521:ARG:NH2	1:B:745:ILE:HD13	2.27	0.50
1:B:201:ASN:ND2	3:B:802[B]:HEM:HMB1	2.27	0.49
1:B:451:MET:CE	1:D:451:MET:CE	2.90	0.49
1:B:521:ARG:HH22	1:B:745:ILE:HD13	1.77	0.49
1:D:449:HIS:HE1	4:D:1348:HOH:O	1.94	0.49
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.27	0.49
1:B:359:LEU:H	1:B:507:HIS:CD2	2.30	0.49
1:C:521:ARG:CB	1:C:521:ARG:HH11	2.21	0.49
1:A:429:HIS:CD2	1:C:83:ASN:HB3	2.48	0.49
1:B:612:ARG:CZ	1:B:612:ARG:HB2	2.42	0.49
1:A:76:GLU:O	1:A:77:ASN:HB2	2.13	0.48
1:A:274:ILE:HD12	2:A:801[A]:HDD:HMB1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:HIS:HA	1:B:168:THR:O	2.14	0.48
1:A:603:VAL:HG11	1:A:666:ILE:HD12	1.95	0.48
1:D:221:VAL:HG22	1:D:234:ILE:HG22	1.94	0.47
1:A:705:LYS:HE3	1:A:710:ILE:CG1	2.44	0.47
1:A:128:HIS:HA	1:A:168:THR:O	2.14	0.47
1:C:634:TYR:CG	1:C:635:SER:N	2.81	0.47
1:D:37:ARG:HD2	4:D:1444:HOH:O	2.14	0.47
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.17	0.47
1:A:583:LYS:O	1:A:584:LYS:HB3	2.14	0.47
1:C:745:ILE:O	1:C:748:ILE:HG12	2.15	0.47
1:D:201:ASN:ND2	3:D:802[B]:HEM:HMB2	2.30	0.47
1:A:313:ARG:NH1	1:D:309:LYS:HD2	2.30	0.47
1:C:509:ARG:HD3	1:C:576:PRO:HG2	1.97	0.47
1:B:451:MET:HE1	1:D:451:MET:HE2	1.97	0.47
1:C:407:LEU:CD2	3:C:802[B]:HEM:HBB1	2.45	0.47
1:B:201:ASN:ND2	3:B:802[B]:HEM:CMB	2.78	0.47
1:C:583:LYS:HB2	4:C:1373:HOH:O	2.14	0.47
1:B:521:ARG:NH2	1:B:521:ARG:HB3	2.30	0.46
1:B:155:ASP:OD2	4:B:1581:HOH:O	2.21	0.46
1:A:205:ILE:H	1:A:205:ILE:HD13	1.80	0.46
1:D:392:HIS:CG	1:D:415:TYR:CB	2.82	0.46
1:A:36:HIS:CD2	1:A:36:HIS:H	2.33	0.46
1:A:36:HIS:HE1	4:A:1352:HOH:O	1.99	0.46
1:B:393:PRO:HD2	1:B:415:TYR:CG	2.51	0.46
1:B:451:MET:HE2	1:D:451:MET:CE	2.45	0.46
1:C:274:ILE:HD12	3:C:802[B]:HEM:CMB	2.47	0.46
1:D:201:ASN:ND2	3:D:802[B]:HEM:HMB1	2.31	0.46
4:B:1503:HOH:O	1:D:73:LYS:HG3	2.16	0.45
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.32	0.45
1:D:201:ASN:OD1	3:D:802[B]:HEM:HMB2	2.15	0.45
1:B:201:ASN:OD1	3:B:802[B]:HEM:HMB2	2.17	0.45
1:C:711:ALA:HB1	4:C:1575:HOH:O	2.16	0.45
1:D:509:ARG:HD2	1:D:576:PRO:HD2	1.98	0.45
1:B:604:ALA:HB1	1:B:633:LEU:HD22	1.98	0.45
1:B:713:GLN:CD	1:B:713:GLN:H	2.21	0.45
1:A:201:ASN:ND2	3:A:802[B]:HEM:HMB1	2.32	0.45
1:C:128:HIS:CE1	1:C:169:VAL:HG22	2.52	0.45
1:D:598:VAL:HG13	1:D:628:VAL:HG22	1.98	0.44
1:C:309:LYS:HB3	1:C:660:LEU:HD21	2.00	0.44
1:B:566:LEU:HD23	4:B:1216:HOH:O	2.17	0.44
1:D:128:HIS:HA	1:D:168:THR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:647:VAL:O	4:C:1488:HOH:O	2.20	0.44
1:C:725:ASP:CB	1:C:726:GLY:C	2.77	0.44
1:D:552:LEU:HD11	1:D:571:LEU:HA	2.00	0.44
1:B:393:PRO:HD2	1:B:415:TYR:CD1	2.52	0.44
1:D:251:HIS:CE1	1:D:507:HIS:HB3	2.53	0.44
1:B:521:ARG:HH21	1:B:521:ARG:CG	2.31	0.44
2:C:801[A]:HDD:HBB1	2:C:801[A]:HDD:HMB1	2.00	0.44
1:D:128:HIS:CE1	1:D:169:VAL:HG22	2.53	0.44
1:A:221:VAL:CG2	1:A:234:ILE:HG22	2.48	0.44
1:B:596:GLY:HA3	1:B:737:ALA:O	2.18	0.44
1:D:313:ARG:HG3	1:D:660:LEU:HD12	1.99	0.44
1:B:207:PHE:O	1:B:249:THR:HA	2.18	0.43
2:B:801[A]:HDD:HMB1	2:B:801[A]:HDD:CBB	2.46	0.43
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.53	0.43
1:A:392:HIS:CE1	1:A:415:TYR:CB	2.68	0.43
1:D:221:VAL:HG23	1:D:234:ILE:HG22	1.97	0.43
1:D:359:LEU:H	1:D:507:HIS:CD2	2.34	0.43
1:A:411:ARG:HG2	3:A:802[B]:HEM:C2C	2.53	0.43
1:D:488:ARG:NH1	1:D:490:GLU:CD	2.72	0.43
1:B:566:LEU:HD22	1:B:566:LEU:N	2.34	0.43
4:B:1503:HOH:O	1:D:73:LYS:CG	2.60	0.43
1:A:309:LYS:NZ	1:A:687:GLU:OE2	2.37	0.43
1:B:709:LYS:HG3	1:B:750:LYS:HE3	2.00	0.43
1:B:299:LYS:HE2	4:B:991:HOH:O	2.18	0.43
1:B:31:PRO:HD2	1:B:36:HIS:HB3	2.01	0.43
1:A:91:ASP:OD2	1:C:461:GLU:OE1	2.37	0.43
1:A:461:GLU:HA	1:A:462:PRO:C	2.38	0.42
1:D:448:MET:O	1:D:449:HIS:HB2	2.20	0.42
1:C:612:ARG:NH1	1:C:612:ARG:CG	2.67	0.42
1:B:419[B]:GLN:HE22	3:B:802[B]:HEM:CGD	2.31	0.42
1:A:38:PRO:HG2	1:A:51:ALA:HB2	2.01	0.42
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.54	0.42
1:B:116:HIS:CD2	1:D:426:PRO:HB2	2.54	0.42
1:B:451:MET:CE	1:D:451:MET:HE2	2.48	0.42
1:A:29:LEU:HB2	4:C:1476:HOH:O	2.20	0.42
1:C:128:HIS:HA	1:C:168:THR:O	2.19	0.42
1:A:165:ARG:HD3	2:A:801[A]:HDD:O2A	2.20	0.41
1:C:643:ASP:OD1	1:C:644:ASP:N	2.53	0.41
1:D:507:HIS:HE1	4:D:1112:HOH:O	2.03	0.41
1:A:51:ALA:HB1	1:A:52:PRO:HD2	2.02	0.41
4:A:1096:HOH:O	1:C:449[B]:HIS:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1237:HOH:O	1:C:104:LEU:HB3	2.21	0.41
1:C:634:TYR:O	1:C:653:THR:HA	2.20	0.41
1:D:289:VAL:HA	1:D:339:GLN:O	2.20	0.41
1:C:97:ALA:O	1:C:101:GLY:HA3	2.21	0.41
1:B:37:ARG:HD3	4:B:1542:HOH:O	2.21	0.41
1:C:461:GLU:HA	1:C:462:PRO:C	2.40	0.41
1:D:97:ALA:O	1:D:101:GLY:HA3	2.21	0.41
1:B:552:LEU:HD21	1:B:571:LEU:HD12	2.02	0.41
3:A:802[B]:HEM:HHA	3:A:802[B]:HEM:HAA2	1.94	0.41
1:B:118:ASP:OD2	1:C:417:ASP:OD2	2.38	0.41
1:B:512:TRP:CH2	1:B:520:GLN:HB3	2.56	0.41
1:B:697:LEU:O	1:B:720:GLU:HA	2.21	0.41
1:D:393:PRO:HD2	1:D:415:TYR:CD1	2.56	0.41
1:A:392:HIS:CG	1:A:415:TYR:CB	2.85	0.41
1:C:310:LEU:HD13	1:C:660:LEU:HB3	2.02	0.41
1:C:744:ARG:HG2	1:C:744:ARG:O	2.21	0.41
1:A:205:ILE:HD13	1:A:205:ILE:N	2.35	0.41
1:A:556:GLN:NE2	4:A:1482:HOH:O	2.54	0.40
1:A:206:PHE:CD1	3:A:802[B]:HEM:HAB	2.56	0.40
1:C:725:ASP:CB	1:C:726:GLY:O	2.58	0.40
2:D:801[A]:HDD:HAD2	2:D:801[A]:HDD:HMD2	1.94	0.40
1:C:299:LYS:HE3	1:C:299:LYS:HB2	1.91	0.40
1:B:344:GLU:CD	1:B:344:GLU:H	2.25	0.40
1:B:603:VAL:HG11	1:B:666:ILE:HD12	2.03	0.40
1:B:392:HIS:CD2	1:B:394:GLY:H	2.40	0.40
1:C:268:THR:HA	1:C:298:GLY:O	2.21	0.40

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:ASP:CB	4:B:1591:HOH:O[2_545]	2.07	0.13
1:A:59:ASP:OD1	1:B:369:ARG:NH1[2_545]	2.19	0.01

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%)	20 (3%)	1 (0%)	56	35
1	B	725/753 (96%)	702 (97%)	21 (3%)	2 (0%)	46	26
1	C	726/753 (96%)	708 (98%)	17 (2%)	1 (0%)	56	35
1	D	725/753 (96%)	708 (98%)	15 (2%)	2 (0%)	46	26
All	All	2902/3012 (96%)	2823 (97%)	73 (2%)	6 (0%)	52	32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	725	ASP
1	D	750	LYS
1	C	75	SER
1	D	75	SER
1	A	75	SER
1	B	75	SER

5.3.2 Protein sidechains (i)

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%)	590 (96%)	23 (4%)	40	17
1	B	612/636 (96%)	584 (95%)	28 (5%)	33	12
1	C	613/636 (96%)	578 (94%)	35 (6%)	25	8
1	D	612/636 (96%)	582 (95%)	30 (5%)	31	11
All	All	2450/2544 (96%)	2334 (95%)	116 (5%)	32	12

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	29	LEU
1	A	37	ARG
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
1	A	369	ARG
1	A	375	LEU
1	A	379	PRO
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	707	THR
1	A	709	LYS
1	A	710	ILE
1	A	713	GLN
1	A	732	LEU
1	A	750	LYS
1	B	32	GLU
1	B	155	ASP
1	B	158	LYS
1	B	185	PHE
1	B	191	THR
1	B	205	ILE
1	B	227	TRP
1	B	252	ASN
1	B	321	GLU
1	B	344	GLU
1	B	370	VAL
1	B	372	LYS
1	B	375	LEU
1	B	440	TYR
1	B	459	ASN
1	B	521	ARG
1	B	552	LEU
1	B	562	LEU
1	B	565	GLU
1	B	571	LEU

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Mol	Chain	Res	Type
1	B	583	LYS
1	B	612	ARG
1	B	616	LEU
1	B	626	LYS
1	B	633	LEU
1	B	713	GLN
1	B	715	GLU
1	B	750	LYS
1	C	61	ARG
1	C	159	ILE
1	C	185	PHE
1	C	205	ILE
1	C	227	TRP
1	C	237	ASP
1	C	252	ASN
1	C	283	GLU
1	C	375	LEU
1	C	377	ARG
1	C	432	PRO
1	C	440	TYR
1	C	459	ASN
1	C	488	ARG
1	C	521	ARG
1	C	531	LEU
1	C	552	LEU
1	C	571	LEU
1	C	578	ASP
1	C	584	LYS
1	C	606	LEU
1	C	612	ARG
1	C	616	LEU
1	C	633	LEU
1	C	636	ARG
1	C	646	THR
1	C	648	LEU
1	C	660	LEU
1	C	703	LYS
1	C	709	LYS
1	C	713	GLN
1	C	725	ASP
1	C	733	LEU
1	C	750	LYS

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Mol	Chain	Res	Type
1	C	751	ILE
1	D	73	LYS
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	227	TRP
1	D	237	ASP
1	D	252	ASN
1	D	309	LYS
1	D	340	LEU
1	D	369	ARG
1	D	375	LEU
1	D	419[A]	GLN
1	D	419[B]	GLN
1	D	440	TYR
1	D	459	ASN
1	D	488	ARG
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	624	LYS
1	D	633	LEU
1	D	648	LEU
1	D	707	THR
1	D	713	GLN
1	D	747	LYS
1	D	750	LYS
1	D	751	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) 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	556	GLN
1	B	252	ASN
1	B	368	GLN

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Mol	Chain	Res	Type
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	B	713	GLN
1	C	252	ASN
1	C	368	GLN
1	C	459	ASN
1	C	507	HIS
1	C	556	GLN
1	C	629	HIS
1	C	671	ASN
1	C	713	GLN
1	D	48	GLN
1	D	252	ASN
1	D	449	HIS
1	D	459	ASN
1	D	507	HIS
1	D	546	GLN
1	D	556	GLN
1	D	629	HIS
1	D	671	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

8 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	HDD	A	801[A]	1,4	30,52,52	1.65	7 (23%)	20,89,89	3.11	13 (65%)
3	HEM	A	802[B]	1,4	30,50,50	3.43	12 (40%)	24,82,82	3.30	13 (54%)
2	HDD	B	801[A]	1,4	30,52,52	1.84	8 (26%)	20,89,89	3.30	12 (60%)
3	HEM	B	802[B]	1,4	30,50,50	3.29	16 (53%)	24,82,82	3.67	14 (58%)
2	HDD	C	801[A]	1,4	30,52,52	1.94	10 (33%)	20,89,89	2.89	11 (55%)
3	HEM	C	802[B]	1	30,50,50	3.80	16 (53%)	24,82,82	4.02	15 (62%)
2	HDD	D	801[A]	1	30,52,52	1.82	6 (20%)	20,89,89	2.78	11 (55%)
3	HEM	D	802[B]	1	30,50,50	3.48	16 (53%)	24,82,82	3.55	14 (58%)

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	HDD	A	801[A]	1,4	-	0/3/89/89	0/1/9/9
3	HEM	A	802[B]	1,4	-	0/10/54/54	0/0/8/8
2	HDD	B	801[A]	1,4	-	0/3/89/89	0/1/9/9
3	HEM	B	802[B]	1,4	-	0/10/54/54	0/0/8/8
2	HDD	C	801[A]	1,4	-	0/3/89/89	0/1/9/9
3	HEM	C	802[B]	1	-	0/10/54/54	0/0/8/8
2	HDD	D	801[A]	1	-	0/3/89/89	0/1/9/9
3	HEM	D	802[B]	1	-	0/10/54/54	0/0/8/8

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	802[B]	HEM	C3B-C4B	-8.50	1.44	1.51
3	B	802[B]	HEM	C3B-C4B	-6.44	1.46	1.51
3	D	802[B]	HEM	C3B-C4B	-6.09	1.46	1.51
3	A	802[B]	HEM	C3B-C4B	-5.36	1.47	1.51
3	D	802[B]	HEM	C3D-C4D	-4.36	1.46	1.51
3	A	802[B]	HEM	C3D-C4D	-4.19	1.46	1.51
3	C	802[B]	HEM	C2C-C1C	-3.69	1.45	1.52
3	B	802[B]	HEM	C2D-C3D	-3.68	1.43	1.54
3	A	802[B]	HEM	C3B-CAB	-3.57	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	802[B]	HEM	C3D-C4D	-3.55	1.47	1.51
3	B	802[B]	HEM	C3D-C4D	-3.48	1.47	1.51
3	A	802[B]	HEM	C2D-C3D	-3.19	1.45	1.54
3	B	802[B]	HEM	C2C-C1C	-3.05	1.46	1.52
3	D	802[B]	HEM	C2D-C3D	-3.02	1.45	1.54
3	B	802[B]	HEM	C3B-CAB	-2.76	1.46	1.51
3	B	802[B]	HEM	CMB-C2B	-2.75	1.46	1.53
3	B	802[B]	HEM	C2B-C1B	-2.73	1.42	1.51
3	D	802[B]	HEM	CMB-C2B	-2.59	1.47	1.53
3	C	802[B]	HEM	C2D-C3D	-2.53	1.47	1.54
3	C	802[B]	HEM	C3C-CAC	-2.51	1.46	1.51
3	D	802[B]	HEM	C3C-CAC	-2.31	1.47	1.51
3	C	802[B]	HEM	C3B-CAB	-2.31	1.47	1.51
2	C	801[A]	HDD	CMB-C2B	-2.30	1.46	1.51
3	D	802[B]	HEM	C2B-C1B	-2.28	1.44	1.51
3	D	802[B]	HEM	CAD-C3D	-2.26	1.49	1.54
2	C	801[A]	HDD	CAA-C2A	-2.13	1.48	1.52
2	A	801[A]	HDD	C2A-C3A	2.14	1.44	1.37
2	B	801[A]	HDD	C1C-CHC	2.15	1.45	1.39
2	A	801[A]	HDD	C1C-CHC	2.24	1.46	1.39
2	C	801[A]	HDD	C4C-CHD	2.29	1.46	1.39
3	B	802[B]	HEM	FE-NB	2.30	2.09	1.97
3	C	802[B]	HEM	CHC-C4B	2.32	1.45	1.38
3	D	802[B]	HEM	CHC-C4B	2.36	1.45	1.38
3	B	802[B]	HEM	FE-ND	2.46	2.10	1.97
3	D	802[B]	HEM	FE-NB	2.47	2.10	1.97
2	A	801[A]	HDD	C4A-CHB	2.47	1.46	1.39
3	D	802[B]	HEM	C2A-C3A	2.48	1.45	1.37
3	D	802[B]	HEM	FE-ND	2.50	2.10	1.97
2	C	801[A]	HDD	C3B-C2B	2.53	1.43	1.40
2	B	801[A]	HDD	C1A-CHA	2.55	1.46	1.39
2	C	801[A]	HDD	C1A-CHA	2.62	1.47	1.39
2	B	801[A]	HDD	C4C-CHD	2.63	1.47	1.39
2	D	801[A]	HDD	C2A-C3A	2.67	1.45	1.37
3	A	802[B]	HEM	C2A-C3A	2.68	1.45	1.37
3	C	802[B]	HEM	C4A-CHB	2.68	1.47	1.39
3	B	802[B]	HEM	CHD-C1D	2.75	1.46	1.38
3	C	802[B]	HEM	FE-ND	2.80	2.12	1.97
3	B	802[B]	HEM	CHC-C4B	2.81	1.46	1.38
2	D	801[A]	HDD	C4C-CHD	2.90	1.47	1.39
3	A	802[B]	HEM	CHC-C4B	2.90	1.46	1.38
2	C	801[A]	HDD	C2A-C3A	2.92	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801[A]	HDD	C3C-C2C	2.92	1.44	1.40
3	C	802[B]	HEM	FE-NB	2.93	2.13	1.97
2	A	801[A]	HDD	C3B-C2B	2.94	1.44	1.40
3	C	802[B]	HEM	CHD-C1D	2.98	1.47	1.38
3	A	802[B]	HEM	FE-ND	3.03	2.13	1.97
3	A	802[B]	HEM	CHD-C1D	3.06	1.47	1.38
3	C	802[B]	HEM	C2A-C3A	3.06	1.46	1.37
3	B	802[B]	HEM	C2A-C3A	3.09	1.46	1.37
3	D	802[B]	HEM	CHD-C1D	3.10	1.47	1.38
3	A	802[B]	HEM	CHD-C4C	3.10	1.43	1.36
2	B	801[A]	HDD	C2A-C3A	3.21	1.47	1.37
2	D	801[A]	HDD	C4A-CHB	3.21	1.48	1.39
2	A	801[A]	HDD	C1A-CHA	3.25	1.48	1.39
2	B	801[A]	HDD	C4A-CHB	3.30	1.48	1.39
2	C	801[A]	HDD	C4A-CHB	3.31	1.49	1.39
3	B	802[B]	HEM	CHC-C1C	3.34	1.44	1.36
3	D	802[B]	HEM	CHC-C1C	3.39	1.44	1.36
2	B	801[A]	HDD	C3C-C2C	3.40	1.44	1.40
2	C	801[A]	HDD	C1C-CHC	3.47	1.49	1.39
2	B	801[A]	HDD	O1D-CGD	3.54	1.41	1.35
3	C	802[B]	HEM	CHC-C1C	3.61	1.44	1.36
2	A	801[A]	HDD	C3C-C2C	3.68	1.45	1.40
2	A	801[A]	HDD	O1D-CGD	3.86	1.42	1.35
3	C	802[B]	HEM	CHD-C4C	3.93	1.45	1.36
2	C	801[A]	HDD	O1D-CGD	3.94	1.42	1.35
3	B	802[B]	HEM	CHD-C4C	4.21	1.46	1.36
3	D	802[B]	HEM	CHD-C4C	4.31	1.46	1.36
2	D	801[A]	HDD	O1D-CGD	4.34	1.43	1.35
3	A	802[B]	HEM	CHC-C1C	4.37	1.46	1.36
2	D	801[A]	HDD	C3B-C2B	4.47	1.46	1.40
2	B	801[A]	HDD	C3B-C2B	4.84	1.46	1.40
2	C	801[A]	HDD	C3C-C2C	4.90	1.46	1.40
3	B	802[B]	HEM	C4C-NC	8.22	1.46	1.36
3	B	802[B]	HEM	C1C-NC	8.77	1.46	1.36
3	A	802[B]	HEM	C4C-NC	9.04	1.47	1.36
3	D	802[B]	HEM	C4C-NC	9.82	1.48	1.36
3	D	802[B]	HEM	C1C-NC	10.03	1.48	1.36
3	C	802[B]	HEM	C4C-NC	10.25	1.48	1.36
3	A	802[B]	HEM	C1C-NC	10.80	1.49	1.36
3	C	802[B]	HEM	C1C-NC	11.03	1.49	1.36

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	802[B]	HEM	C3B-CAB-CBB	-8.94	110.74	124.46
3	D	802[B]	HEM	CAA-CBA-CGA	-8.16	97.80	112.75
3	A	802[B]	HEM	C3B-CAB-CBB	-7.74	112.59	124.46
2	B	801[A]	HDD	C4D-ND-C1D	-6.65	103.07	107.36
3	B	802[B]	HEM	CAA-CBA-CGA	-6.63	100.59	112.75
2	C	801[A]	HDD	C4D-ND-C1D	-6.18	103.37	107.36
2	D	801[A]	HDD	C4D-ND-C1D	-6.09	103.44	107.36
3	C	802[B]	HEM	C4B-CHC-C1C	-5.88	115.99	125.82
2	B	801[A]	HDD	OND-C2D-CMD	-5.80	98.94	109.41
3	C	802[B]	HEM	C3C-CAC-CBC	-5.59	115.88	124.46
3	A	802[B]	HEM	CAA-CBA-CGA	-5.26	103.10	112.75
3	A	802[B]	HEM	C3C-CAC-CBC	-5.19	116.50	124.46
3	C	802[B]	HEM	C2C-C1C-CHC	-5.09	115.94	123.68
3	C	802[B]	HEM	C3B-C4B-CHC	-5.08	116.02	123.16
2	A	801[A]	HDD	CAA-CBA-CGA	-5.03	103.52	112.75
3	B	802[B]	HEM	C2C-C1C-CHC	-4.99	116.09	123.68
3	B	802[B]	HEM	C3B-CAB-CBB	-4.96	116.85	124.46
3	D	802[B]	HEM	C2C-C1C-CHC	-4.87	116.27	123.68
2	C	801[A]	HDD	OND-C2D-CMD	-4.85	100.66	109.41
2	A	801[A]	HDD	OND-C2D-CMD	-4.78	100.79	109.41
2	C	801[A]	HDD	CAA-CBA-CGA	-4.59	104.34	112.75
3	C	802[B]	HEM	CAA-CBA-CGA	-4.56	104.39	112.75
3	D	802[B]	HEM	C4B-CHC-C1C	-4.42	118.43	125.82
3	D	802[B]	HEM	C3C-CAC-CBC	-4.28	117.89	124.46
2	B	801[A]	HDD	CAA-CBA-CGA	-4.19	105.08	112.75
2	B	801[A]	HDD	C2D-C1D-CHD	-4.12	117.07	123.48
2	A	801[A]	HDD	C4D-ND-C1D	-4.10	104.72	107.36
2	D	801[A]	HDD	OND-C2D-CMD	-4.02	102.16	109.41
3	D	802[B]	HEM	C1D-CHD-C4C	-3.97	119.18	125.82
3	B	802[B]	HEM	C4B-CHC-C1C	-3.95	119.22	125.82
3	A	802[B]	HEM	C1D-CHD-C4C	-3.67	119.68	125.82
2	B	801[A]	HDD	C3C-CAC-CBC	-3.52	119.11	126.32
3	D	802[B]	HEM	CBD-CAD-C3D	-3.46	103.47	113.55
2	C	801[A]	HDD	C2D-C1D-CHD	-3.32	118.31	123.48
2	C	801[A]	HDD	CBA-CAA-C2A	-3.27	106.66	112.53
2	D	801[A]	HDD	C2D-C1D-CHD	-3.25	118.41	123.48
2	A	801[A]	HDD	C2D-C1D-CHD	-3.11	118.64	123.48
2	D	801[A]	HDD	C3B-CAB-CBB	-3.01	120.16	126.32
3	B	802[B]	HEM	CBD-CAD-C3D	-3.00	104.83	113.55
3	D	802[B]	HEM	C3B-CAB-CBB	-2.92	119.98	124.46
2	A	801[A]	HDD	C3C-CAC-CBC	-2.91	120.37	126.32
3	C	802[B]	HEM	CBD-CAD-C3D	-2.90	105.13	113.55
2	B	801[A]	HDD	O1D-CGD-CBD	-2.86	106.85	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802[B]	HEM	C1D-CHD-C4C	-2.81	121.12	125.82
3	D	802[B]	HEM	C3B-C4B-CHC	-2.71	119.36	123.16
3	C	802[B]	HEM	C1D-CHD-C4C	-2.65	121.39	125.82
2	A	801[A]	HDD	CAD-CBD-CGD	-2.53	100.27	104.64
3	A	802[B]	HEM	CBD-CAD-C3D	-2.46	106.39	113.55
2	B	801[A]	HDD	CMA-C3A-C4A	-2.42	124.35	128.36
3	A	802[B]	HEM	C4B-CHC-C1C	-2.40	121.81	125.82
2	B	801[A]	HDD	CBA-CAA-C2A	-2.38	108.26	112.53
2	A	801[A]	HDD	CMA-C3A-C4A	-2.32	124.53	128.36
2	A	801[A]	HDD	O1D-CGD-CBD	-2.24	107.58	110.20
3	A	802[B]	HEM	CAA-C2A-C1A	-2.21	124.60	127.01
2	C	801[A]	HDD	C3C-CAC-CBC	-2.18	121.87	126.32
2	D	801[A]	HDD	CAA-CBA-CGA	-2.17	108.77	112.75
3	B	802[B]	HEM	CMA-C3A-C4A	-2.15	124.80	128.36
2	D	801[A]	HDD	C3C-CAC-CBC	-2.08	122.06	126.32
2	D	801[A]	HDD	O1D-CGD-O2D	2.23	122.92	120.80
2	A	801[A]	HDD	CMA-C3A-C2A	2.30	130.04	125.24
2	B	801[A]	HDD	C3C-C4C-NC	2.46	112.39	109.21
2	B	801[A]	HDD	CMC-C2C-C1C	2.54	132.56	128.36
2	C	801[A]	HDD	C3C-C4C-NC	2.60	112.57	109.21
2	C	801[A]	HDD	O1D-CGD-O2D	2.60	123.28	120.80
3	C	802[B]	HEM	CAA-C2A-C1A	2.74	129.99	127.01
3	B	802[B]	HEM	CMA-C3A-C2A	2.75	130.98	125.24
2	C	801[A]	HDD	CAA-C2A-C1A	2.82	130.07	127.01
3	A	802[B]	HEM	C2C-C1C-NC	2.82	114.96	110.21
2	D	801[A]	HDD	CMC-C2C-C1C	3.00	133.33	128.36
3	A	802[B]	HEM	CMC-C2C-C3C	3.15	124.38	116.53
2	D	801[A]	HDD	CMB-C2B-C3B	3.21	131.36	125.09
2	C	801[A]	HDD	CMA-C3A-C2A	3.23	131.99	125.24
3	A	802[B]	HEM	CMD-C2D-C3D	3.40	129.40	114.35
3	B	802[B]	HEM	CAD-C3D-C4D	3.41	124.51	112.47
2	A	801[A]	HDD	CMB-C2B-C3B	3.44	131.82	125.09
3	C	802[B]	HEM	CMB-C2B-C3B	3.49	125.25	116.53
2	A	801[A]	HDD	C3C-C4C-NC	3.53	113.78	109.21
3	C	802[B]	HEM	CAD-C3D-C4D	3.58	125.08	112.47
3	D	802[B]	HEM	CAD-C3D-C4D	3.65	125.36	112.47
2	B	801[A]	HDD	CMA-C3A-C2A	3.66	132.88	125.24
2	C	801[A]	HDD	CMB-C2B-C3B	3.66	132.24	125.09
3	B	802[B]	HEM	C2C-C1C-NC	3.76	116.54	110.21
3	D	802[B]	HEM	CMC-C2C-C3C	3.81	126.03	116.53
2	D	801[A]	HDD	CAA-C2A-C1A	3.81	131.15	127.01
3	A	802[B]	HEM	CAD-C3D-C4D	3.84	126.00	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	802[B]	HEM	C2C-C1C-NC	3.89	116.77	110.21
3	D	802[B]	HEM	CMD-C2D-C3D	3.92	131.68	114.35
3	C	802[B]	HEM	CMD-C2D-C3D	4.22	133.00	114.35
3	B	802[B]	HEM	CMD-C2D-C3D	4.39	133.79	114.35
3	A	802[B]	HEM	CMB-C2B-C3B	4.64	128.12	116.53
3	C	802[B]	HEM	C2C-C1C-NC	4.64	118.04	110.21
3	D	802[B]	HEM	CMB-C2B-C3B	4.76	128.43	116.53
2	A	801[A]	HDD	CAA-C2A-C1A	4.97	132.41	127.01
3	C	802[B]	HEM	CMC-C2C-C3C	5.00	129.01	116.53
2	A	801[A]	HDD	O1D-CGD-O2D	5.13	125.68	120.80
2	D	801[A]	HDD	C3C-C4C-NC	5.34	116.12	109.21
3	B	802[B]	HEM	CMC-C2C-C3C	6.14	131.86	116.53
3	D	802[B]	HEM	CAD-C3D-C2D	6.15	130.91	113.22
3	A	802[B]	HEM	CAD-C3D-C2D	6.16	130.93	113.22
2	B	801[A]	HDD	O1D-CGD-O2D	6.28	126.78	120.80
3	B	802[B]	HEM	CAD-C3D-C2D	6.46	131.78	113.22
3	C	802[B]	HEM	CAD-C3D-C2D	6.54	132.03	113.22
3	B	802[B]	HEM	CMB-C2B-C3B	7.25	134.62	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801[A]	HDD	4	0
3	A	802[B]	HEM	15	0
2	B	801[A]	HDD	3	0
3	B	802[B]	HEM	7	0
2	C	801[A]	HDD	2	0
3	C	802[B]	HEM	12	0
2	D	801[A]	HDD	3	0
3	D	802[B]	HEM	10	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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	726/753 (96%)	-0.51	5 (0%)	89	91	6, 12, 28, 57	1 (0%)
1	B	726/753 (96%)	-0.37	16 (2%)	65	70	6, 14, 35, 56	1 (0%)
1	C	726/753 (96%)	-0.40	17 (2%)	64	68	7, 14, 35, 60	1 (0%)
1	D	726/753 (96%)	-0.51	4 (0%)	90	92	5, 12, 28, 50	1 (0%)
All	All	2904/3012 (96%)	-0.45	42 (1%)	78	82	5, 13, 32, 60	4 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	726	GLY	6.0
1	B	713	GLN	4.2
1	B	28	SER	3.7
1	B	32	GLU	3.6
1	A	750	LYS	3.5
1	C	726	GLY	3.4
1	C	750	LYS	3.3
1	D	713	GLN	3.2
1	D	28	SER	3.1
1	C	711	ALA	3.0
1	C	712	ASP	2.9
1	A	28	SER	2.9
1	C	646	THR	2.7
1	B	647	VAL	2.7
1	A	32	GLU	2.6
1	C	594	PRO	2.6
1	B	711	ALA	2.6
1	C	677	ASP	2.5
1	B	751	ILE	2.5
1	B	617	LEU	2.5
1	B	572	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	568	ASP	2.4
1	D	749	ASP	2.4
1	A	714	GLY	2.4
1	B	677	ASP	2.4
1	A	726	GLY	2.4
1	C	583	LYS	2.4
1	B	725	ASP	2.4
1	B	712	ASP	2.4
1	B	673	ALA	2.3
1	C	714	GLY	2.3
1	C	641	THR	2.3
1	D	712	ASP	2.3
1	C	28	SER	2.2
1	C	645	GLY	2.2
1	C	713	GLN	2.1
1	C	647	VAL	2.1
1	C	32	GLU	2.1
1	C	568	ASP	2.1
1	B	646	THR	2.0
1	C	642	ALA	2.0
1	B	750	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no 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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	HDD	A	801[A]	44/44	0.98	0.07	0.41	6,8,11,12	44

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	HDD	B	801[A]	44/44	0.98	0.08	0.21	7,9,11,12	44
3	HEM	A	802[B]	43/43	0.99	0.07	0.16	6,6,7,8	43
2	HDD	C	801[A]	44/44	0.98	0.07	0.15	7,8,12,14	44
3	HEM	C	802[B]	43/43	0.99	0.07	0.13	6,7,8,9	43
3	HEM	B	802[B]	43/43	0.98	0.07	0.08	5,7,8,8	43
2	HDD	D	801[A]	44/44	0.98	0.06	-0.11	6,7,11,12	44
3	HEM	D	802[B]	43/43	0.99	0.06	-0.21	4,5,6,7	43

6.5 Other polymers (i)

There are no such residues in this entry.