Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:25 PM GMT

PDB ID	:	4ENS
Title	:	Structure of E530Q variant of E. coli KatE
Authors	:	Loewen, P.C.; Jha, V.
Deposited on	:	2012-04-13
Resolution	:	1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

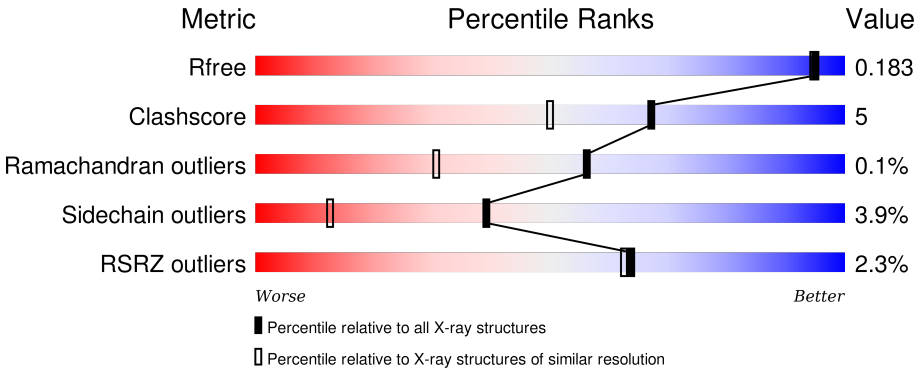
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.60 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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. 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	86% 10%
1	B	753	3% 84% 11%
1	C	753	3% 83% 11%
1	D	753	2% 82% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26323 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.

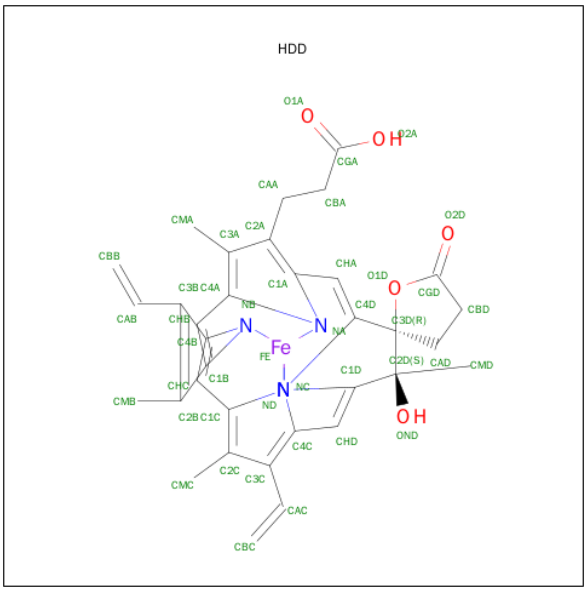
- Molecule 1 is a protein called Catalase HPII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	4	0
			5755	3655	1007	1081	12			
1	B	726	Total	C	N	O	S	0	4	0
			5758	3658	1008	1080	12			
1	C	726	Total	C	N	O	S	0	3	0
			5756	3658	1008	1078	12			
1	D	726	Total	C	N	O	S	0	4	0
			5758	3657	1008	1081	12			

There are 4 discrepancies between the modelled and reference sequences:

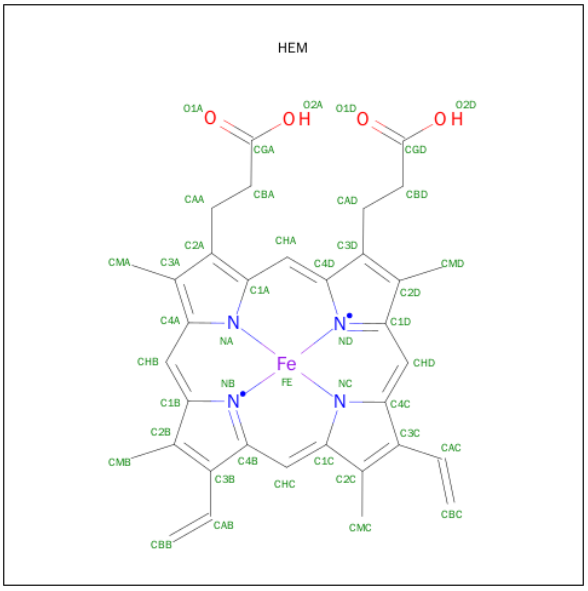
Chain	Residue	Modelled	Actual	Comment	Reference
A	530	GLN	GLU	ENGINEERED MUTATION	UNP P21179
B	530	GLN	GLU	ENGINEERED MUTATION	UNP P21179
C	530	GLN	GLU	ENGINEERED MUTATION	UNP P21179
D	530	GLN	GLU	ENGINEERED MUTATION	UNP P21179

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

- Molecule 4 is water.

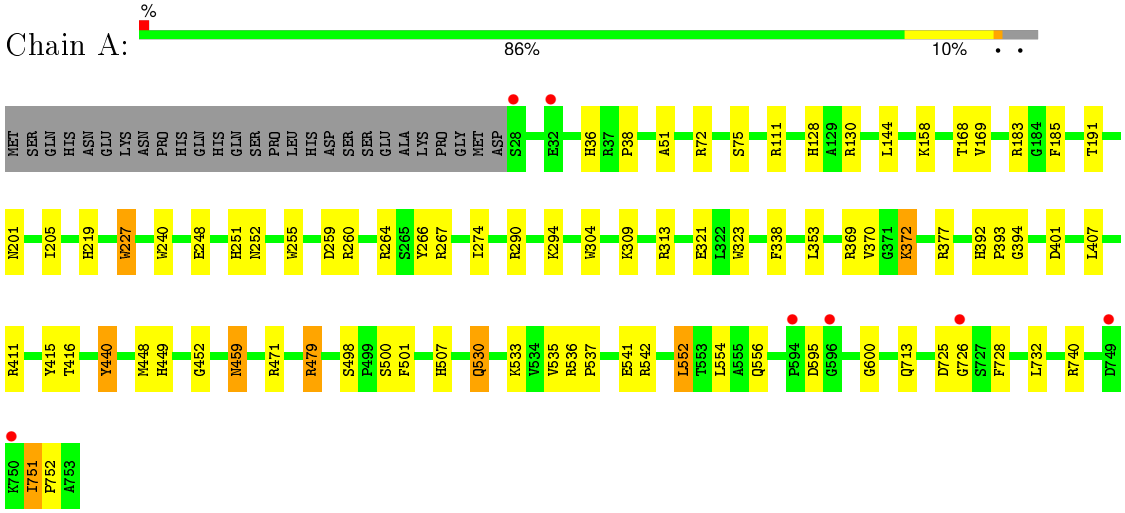
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	769	Total	O	0	0
			769	769		
4	B	696	Total	O	0	0
			696	696		
4	C	709	Total	O	0	0
			709	709		
4	D	774	Total	O	0	0
			774	774		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

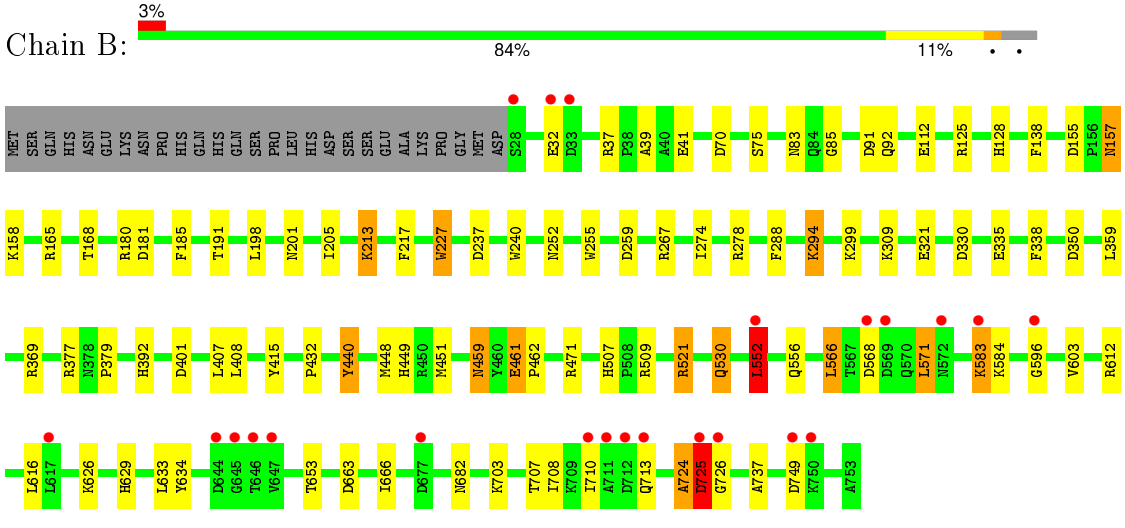
- Molecule 1: Catalase HPII

Chain A:



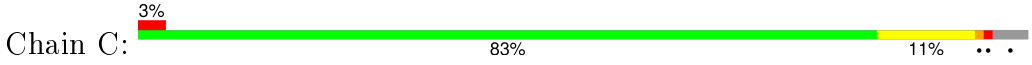
- Molecule 1: Catalase HPII

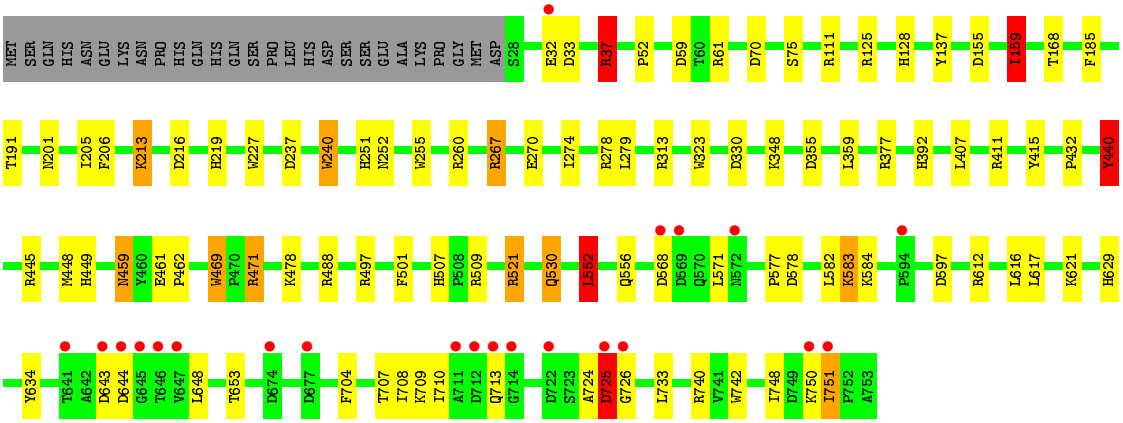
Chain B:



- Molecule 1: Catalase HPII

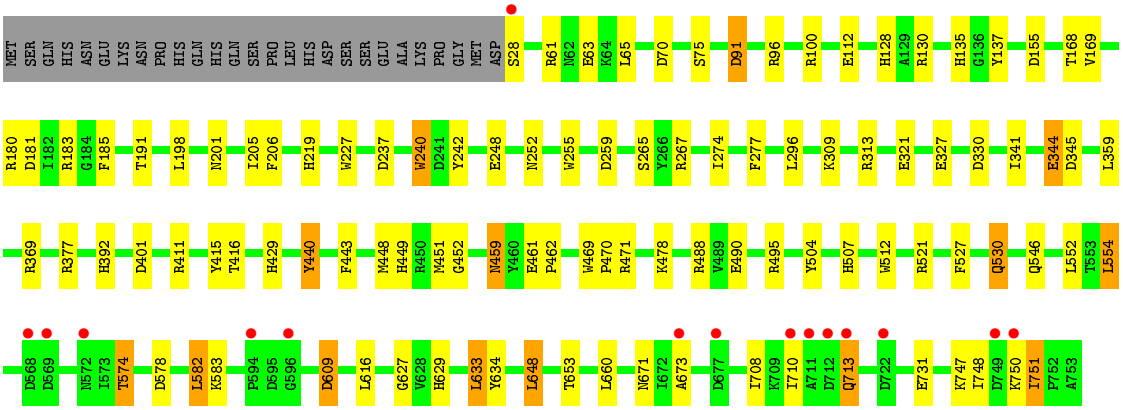
Chain C:





• 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	93.45Å 133.40Å 123.24Å 90.00° 109.18° 90.00°	Depositor
Resolution (Å)	32.19 – 1.60 32.19 – 1.60	Depositor EDS
% Data completeness (in resolution range)	91.8 (32.19-1.60) 91.8 (32.19-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.151 , 0.184 0.149 , 0.183	Depositor DCC
R_{free} test set	17269 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	13.1	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 343592 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	26323	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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	1.31	14/5924 (0.2%)	1.22	37/8054 (0.5%)
1	B	1.26	12/5927 (0.2%)	1.18	29/8058 (0.4%)
1	C	1.22	10/5922 (0.2%)	1.19	32/8050 (0.4%)
1	D	1.30	18/5927 (0.3%)	1.20	35/8058 (0.4%)
All	All	1.27	54/23700 (0.2%)	1.20	133/32220 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	2
All	All	0	3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	440	TYR	CE1-CZ	9.24	1.50	1.38
1	D	112	GLU	CD-OE2	7.79	1.34	1.25
1	D	440	TYR	CE1-CZ	7.66	1.48	1.38
1	A	255	TRP	CD2-CE2	7.65	1.50	1.41
1	A	440	TYR	CE1-CZ	7.51	1.48	1.38
1	A	227	TRP	CD2-CE2	7.29	1.50	1.41
1	A	321	GLU	CD-OE1	7.13	1.33	1.25
1	A	323	TRP	CD2-CE2	6.86	1.49	1.41
1	B	112	GLU	CD-OE2	6.79	1.33	1.25
1	B	85	GLY	N-CA	6.79	1.56	1.46
1	D	28	SER	CB-OG	6.74	1.51	1.42
1	C	323	TRP	CG-CD1	6.74	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	321	GLU	CD-OE1	6.37	1.32	1.25
1	A	304	TRP	CD2-CE2	6.19	1.48	1.41
1	C	255	TRP	CD2-CE2	6.17	1.48	1.41
1	D	344	GLU	CD-OE2	6.09	1.32	1.25
1	B	227	TRP	CD2-CE2	6.06	1.48	1.41
1	A	377	ARG	CZ-NH1	6.00	1.40	1.33
1	D	469	TRP	CD2-CE2	5.91	1.48	1.41
1	D	240	TRP	CG-CD1	5.88	1.45	1.36
1	D	327	GLU	CD-OE1	5.88	1.32	1.25
1	C	240	TRP	CD2-CE2	5.82	1.48	1.41
1	C	742	TRP	CD2-CE2	5.75	1.48	1.41
1	B	165	ARG	CZ-NH1	5.74	1.40	1.33
1	B	112	GLU	CB-CG	5.71	1.63	1.52
1	D	255	TRP	CD2-CE2	5.63	1.48	1.41
1	D	265	SER	CA-CB	5.61	1.61	1.52
1	A	227	TRP	CG-CD1	5.61	1.44	1.36
1	D	63	GLU	CD-OE2	5.51	1.31	1.25
1	C	323	TRP	CD2-CE2	5.46	1.48	1.41
1	C	469	TRP	CD2-CE2	5.44	1.47	1.41
1	D	242	TYR	CB-CG	5.43	1.59	1.51
1	B	255	TRP	CD2-CE2	5.34	1.47	1.41
1	A	498	SER	CB-OG	5.33	1.49	1.42
1	B	157	ASN	CB-CG	5.33	1.63	1.51
1	D	452	GLY	C-O	5.32	1.32	1.23
1	A	500	SER	CB-OG	5.27	1.49	1.42
1	B	217	PHE	CE1-CZ	5.24	1.47	1.37
1	B	181	ASP	CB-CG	5.22	1.62	1.51
1	C	270	GLU	CD-OE2	5.21	1.31	1.25
1	A	452	GLY	C-O	5.20	1.31	1.23
1	D	377	ARG	CZ-NH1	5.19	1.39	1.33
1	D	377	ARG	CZ-NH2	5.18	1.39	1.33
1	A	394	GLY	N-CA	5.18	1.53	1.46
1	C	440	TYR	CE1-CZ	5.17	1.45	1.38
1	C	255	TRP	CZ2-CH2	5.12	1.47	1.37
1	A	600	GLY	N-CA	5.08	1.53	1.46
1	D	627	GLY	N-CA	5.07	1.53	1.46
1	D	504	TYR	CG-CD1	5.07	1.45	1.39
1	B	461	GLU	CD-OE1	5.05	1.31	1.25
1	D	512	TRP	CG-CD1	5.05	1.43	1.36
1	C	59	ASP	CB-CG	5.02	1.62	1.51
1	B	335	GLU	CD-OE1	5.01	1.31	1.25
1	A	266	TYR	CE1-CZ	5.01	1.45	1.38

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	471	ARG	NE-CZ-NH2	-12.26	114.17	120.30
1	B	521	ARG	NE-CZ-NH2	12.21	126.41	120.30
1	D	61	ARG	NE-CZ-NH2	9.51	125.06	120.30
1	B	401	ASP	CB-CG-OD2	9.36	126.72	118.30
1	A	377	ARG	NE-CZ-NH2	-9.35	115.62	120.30
1	C	377	ARG	NE-CZ-NH1	-9.12	115.74	120.30
1	C	37	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	C	111	ARG	NE-CZ-NH1	-9.04	115.78	120.30
1	D	377	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	B	521	ARG	NE-CZ-NH1	-8.75	115.92	120.30
1	A	183	ARG	NE-CZ-NH2	-8.43	116.08	120.30
1	D	648	LEU	CB-CG-CD2	8.42	125.32	111.00
1	A	501	PHE	CB-CG-CD2	-8.37	114.94	120.80
1	D	633	LEU	CB-CG-CD1	8.24	125.01	111.00
1	B	259	ASP	CB-CG-OD2	8.11	125.59	118.30
1	A	740	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	A	372	LYS	CD-CE-NZ	-7.97	93.36	111.70
1	B	338	PHE	CB-CG-CD1	-7.82	115.33	120.80
1	B	377	ARG	NE-CZ-NH1	-7.72	116.44	120.30
1	A	130	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	C	313	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	C	267	ARG	NE-CZ-NH1	-7.60	116.50	120.30
1	A	479	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	D	377	ARG	NE-CZ-NH1	-7.55	116.53	120.30
1	C	445	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	D	554	LEU	CB-CG-CD2	7.42	123.62	111.00
1	C	37	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	D	377	ARG	NH1-CZ-NH2	7.40	127.54	119.40
1	C	159	ILE	CB-CG1-CD1	-7.39	93.20	113.90
1	A	552	LEU	CB-CG-CD1	7.38	123.54	111.00
1	A	595	ASP	CB-CG-OD2	7.33	124.89	118.30
1	B	663	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	D	91	ASP	CB-CG-OD1	-7.18	111.83	118.30
1	A	130	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	D	582	LEU	CB-CG-CD1	7.16	123.18	111.00
1	C	740	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	D	180	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	D	180	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	D	471	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	A	183	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	501	PHE	CB-CG-CD1	7.06	125.74	120.80
1	D	401	ASP	CB-CG-OD2	7.04	124.64	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	198	LEU	CB-CG-CD1	6.98	122.86	111.00
1	C	125	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	B	259	ASP	CB-CG-OD1	-6.76	112.22	118.30
1	A	471	ARG	NE-CZ-NH1	-6.73	116.94	120.30
1	B	552	LEU	CA-CB-CG	6.66	130.62	115.30
1	C	278	ARG	NE-CZ-NH1	-6.65	116.97	120.30
1	A	72	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	D	96	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	D	183	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	A	294	LYS	CD-CE-NZ	-6.57	96.58	111.70
1	C	471	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	D	521	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	C	740	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	542	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	C	552	LEU	CA-CB-CG	6.41	130.04	115.30
1	C	70	ASP	CB-CG-OD2	6.38	124.04	118.30
1	A	536	ARG	NE-CZ-NH2	6.35	123.47	120.30
1	B	70	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	260	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	B	509	ARG	NE-CZ-NH2	6.23	123.41	120.30
1	B	471	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	D	61	ARG	NE-CZ-NH1	-6.14	117.23	120.30
1	D	277	PHE	CB-CG-CD2	6.11	125.07	120.80
1	D	155	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	377	ARG	CG-CD-NE	-6.09	99.02	111.80
1	C	59	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	A	740	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	C	33	ASP	CB-CG-OD1	5.90	123.61	118.30
1	C	377	ARG	CG-CD-NE	-5.89	99.44	111.80
1	A	309	LYS	CD-CE-NZ	-5.88	98.18	111.70
1	D	259	ASP	CB-CG-OD2	5.86	123.57	118.30
1	D	70	ASP	CB-CG-OD1	5.85	123.57	118.30
1	B	278	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	C	155	ASP	CB-CG-OD1	-5.81	113.07	118.30
1	D	96	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	536	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	A	401	ASP	CB-CG-OD2	5.77	123.50	118.30
1	B	309	LYS	CD-CE-NZ	-5.71	98.56	111.70
1	A	533	LYS	CG-CD-CE	-5.70	94.81	111.90
1	C	501	PHE	CB-CG-CD2	-5.70	116.81	120.80
1	A	248	GLU	OE1-CD-OE2	-5.69	116.47	123.30
1	D	198	LEU	CB-CG-CD2	-5.69	101.33	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	521	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	C	348	LYS	CA-CB-CG	-5.67	100.92	113.40
1	C	155	ASP	CB-CG-OD2	5.67	123.40	118.30
1	B	180	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	264	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	554	LEU	CB-CG-CD2	-5.64	101.41	111.00
1	D	137	TYR	CB-CG-CD1	-5.63	117.62	121.00
1	B	288	PHE	CB-CG-CD2	-5.63	116.86	120.80
1	D	248	GLU	OE1-CD-OE2	-5.61	116.56	123.30
1	B	37	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	B	125	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	C	497	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	D	181	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	338	PHE	CB-CG-CD2	5.50	124.65	120.80
1	D	495	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	C	260	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	D	552	LEU	CB-CG-CD2	5.48	120.31	111.00
1	A	111	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	C	59	ASP	CB-CG-OD1	5.45	123.21	118.30
1	B	138	PHE	CB-CG-CD2	-5.45	116.99	120.80
1	B	377	ARG	CG-CD-NE	-5.43	100.39	111.80
1	D	527	PHE	CB-CG-CD1	-5.42	117.01	120.80
1	D	277	PHE	CB-CG-CD1	-5.41	117.01	120.80
1	D	345	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	B	350	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	D	130	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	313	ARG	NE-CZ-NH1	-5.23	117.68	120.30
1	C	725	ASP	N-CA-C	5.21	125.08	111.00
1	A	377	ARG	NH1-CZ-NH2	5.20	125.12	119.40
1	C	159	ILE	CB-CA-C	5.18	121.96	111.60
1	B	294	LYS	CD-CE-NZ	-5.18	99.80	111.70
1	B	408	LEU	CB-CG-CD2	-5.16	102.22	111.00
1	A	267	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	A	290	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	A	479	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	181	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	259	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	369	ARG	NE-CZ-NH2	5.11	122.85	120.30
1	A	353	LEU	CB-CG-CD1	-5.10	102.33	111.00
1	B	267	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	725	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	D	609	ASP	CB-CG-OD2	5.09	122.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	299	LYS	CD-CE-NZ	-5.07	100.03	111.70
1	C	355	ASP	CB-CG-OD2	5.05	122.85	118.30
1	C	216	ASP	CB-CG-OD1	-5.04	113.76	118.30
1	C	509	ARG	NE-CZ-NH1	-5.03	117.78	120.30
1	D	183	ARG	NE-CZ-NH2	5.03	122.82	120.30
1	C	279	LEU	CB-CG-CD2	-5.03	102.45	111.00
1	A	338	PHE	CB-CG-CD1	-5.00	117.30	120.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	724	ALA	Peptide
1	C	724	ALA	Peptide
1	C	725	ASP	Peptide

5.2 Too-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 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	5755	0	5599	34	0
1	B	5758	0	5605	59	0
1	C	5756	0	5606	58	0
1	D	5758	0	5602	59	0
2	A	44	0	31	2	0
2	B	44	0	31	3	0
2	C	44	0	31	2	0
2	D	44	0	31	6	0
3	A	43	0	30	13	0
3	B	43	0	30	12	0
3	C	43	0	30	13	0
3	D	43	0	30	8	0
4	A	769	0	0	9	0
4	B	696	0	0	11	0
4	C	709	0	0	9	0
4	D	774	0	0	16	0
All	All	26323	0	22656	222	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (222) 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:D:392:HIS:ND1	1:D:415:TYR:CB	1.69	1.52
1:C:392:HIS:ND1	1:C:415:TYR:CB	1.72	1.51
1:A:392:HIS:ND1	1:A:415:TYR:CB	1.75	1.50
1:B:392:HIS:ND1	1:B:415:TYR:CB	1.70	1.49
1:B:157:ASN:HB2	4:B:1578:HOH:O	1.28	1.30
1:C:521:ARG:CG	1:C:521:ARG:HH11	1.46	1.27
1:D:392:HIS:CE1	1:D:415:TYR:HB2	1.71	1.24
1:D:449[B]:HIS:NE2	4:D:1534:HOH:O	1.66	1.21
1:B:392:HIS:CE1	1:B:415:TYR:HB2	1.76	1.19
1:A:392:HIS:CE1	1:A:415:TYR:HB2	1.80	1.17
1:C:392:HIS:CE1	1:C:415:TYR:HB2	1.84	1.13
1:C:440:TYR:CD1	4:C:1370:HOH:O	2.00	1.13
1:A:392:HIS:ND1	1:A:415:TYR:HB2	0.80	1.13
3:A:802[B]:HEM:HBC2	3:A:802[B]:HEM:HMC2	1.22	1.13
1:D:546:GLN:HG3	4:D:1590:HOH:O	1.50	1.11
1:D:392:HIS:ND1	1:D:415:TYR:HB2	0.78	1.11
1:C:392:HIS:ND1	1:C:415:TYR:HB2	0.77	1.09
1:B:392:HIS:ND1	1:B:415:TYR:HB2	0.76	1.09
1:C:583[A]:LYS:H	1:C:583[A]:LYS:HE2	1.06	1.06
1:C:440:TYR:HD1	4:C:1370:HOH:O	1.35	1.04
1:A:541:GLU:OE2	4:A:1540:HOH:O	1.76	1.01
1:C:521:ARG:NH1	1:C:521:ARG:HG2	1.27	0.97
1:B:369:ARG:HG2	4:B:1302:HOH:O	1.64	0.96
1:C:392:HIS:CG	1:C:415:TYR:HB2	2.04	0.93
3:C:802[B]:HEM:HBC2	3:C:802[B]:HEM:HMC2	1.52	0.89
1:C:521:ARG:CG	1:C:521:ARG:NH1	2.16	0.87
1:D:449[B]:HIS:CE1	4:D:1534:HOH:O	2.18	0.84
1:D:267:ARG:HG3	4:D:1384:HOH:O	1.79	0.83
1:C:578:ASP:HB2	1:C:582:LEU:O	1.77	0.83
1:A:392:HIS:CG	1:A:415:TYR:HB2	2.07	0.82
1:B:407:LEU:CD2	3:B:802[B]:HEM:HBB1	2.11	0.81
1:C:521:ARG:HG2	1:C:521:ARG:HH11	0.67	0.80
1:B:708:ILE:HD12	1:B:710:ILE:HD11	1.63	0.80
1:C:583[A]:LYS:H	1:C:583[A]:LYS:CE	1.91	0.80
1:C:201:ASN:CG	3:C:802[B]:HEM:HMB2	2.04	0.78
2:C:801[A]:HDD:HBB1	2:C:801[A]:HDD:HMB1	1.66	0.77
3:A:802[B]:HEM:CMC	3:A:802[B]:HEM:HBC2	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:490:GLU:OE1	4:D:1482:HOH:O	2.02	0.75
1:C:748:ILE:O	1:C:751:ILE:HG22	1.86	0.75
1:C:440:TYR:CE1	4:C:1370:HOH:O	2.33	0.74
1:D:731:GLU:OE2	4:D:1653:HOH:O	2.06	0.74
1:D:546:GLN:CG	4:D:1590:HOH:O	2.19	0.73
1:D:341:ILE:HG13	4:D:1651:HOH:O	1.87	0.73
2:D:801[A]:HDD:HMB1	2:D:801[A]:HDD:HBB1	1.71	0.72
1:D:392:HIS:ND1	1:D:415:TYR:CG	2.58	0.70
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.74	0.70
1:C:201:ASN:ND2	3:C:802[B]:HEM:CMB	2.55	0.70
1:C:206:PHE:CG	3:C:802[B]:HEM:HAB	2.27	0.69
1:C:392:HIS:ND1	1:C:415:TYR:CG	2.59	0.69
1:A:392:HIS:ND1	1:A:415:TYR:CG	2.60	0.68
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.75	0.68
2:A:801[A]:HDD:HMB1	2:A:801[A]:HDD:HBB1	1.75	0.68
1:B:407:LEU:HD21	3:B:802[B]:HEM:HBB1	1.74	0.68
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.78	0.67
2:B:801[A]:HDD:HMB1	2:B:801[A]:HDD:HBB1	1.78	0.66
1:B:157:ASN:CB	4:B:1578:HOH:O	2.07	0.66
1:B:407:LEU:HD23	3:B:802[B]:HEM:HBB1	1.76	0.66
1:B:392:HIS:ND1	1:B:415:TYR:CG	2.61	0.64
1:B:556:GLN:HG2	1:B:566:LEU:HD23	1.78	0.64
1:A:416[B]:THR:HG22	4:A:1016:HOH:O	1.97	0.64
1:B:521:ARG:HD3	4:B:1566:HOH:O	1.97	0.64
1:D:629:HIS:HD2	4:D:1267:HOH:O	1.81	0.64
1:A:201:ASN:CG	3:A:802[B]:HEM:HMB2	2.16	0.64
2:D:801[A]:HDD:HMC1	2:D:801[A]:HDD:HBC1	1.79	0.64
1:D:206:PHE:HB2	3:D:802[B]:HEM:HBB1	1.79	0.64
1:D:201:ASN:CG	3:D:802[B]:HEM:HMB2	2.19	0.63
1:D:546:GLN:CD	4:D:1590:HOH:O	2.33	0.63
1:C:206:PHE:CD2	3:C:802[B]:HEM:HAB	2.33	0.63
1:A:36:HIS:CD2	1:A:36:HIS:H	2.17	0.62
1:D:574:THR:HG22	4:D:1313:HOH:O	2.00	0.61
4:C:1452:HOH:O	1:D:488:ARG:HD2	2.01	0.60
1:C:201:ASN:ND2	3:C:802[B]:HEM:HMB1	2.16	0.60
1:D:392:HIS:ND1	1:D:415:TYR:HB3	2.02	0.60
1:C:629:HIS:HD2	4:C:1210:HOH:O	1.84	0.59
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.85	0.59
1:B:294:LYS:HB2	4:B:1189:HOH:O	2.01	0.59
1:B:359:LEU:H	1:B:507:HIS:HD2	1.50	0.59
1:A:240:TRP:HE1	1:A:530:GLN:HE21	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:448:MET:O	1:D:449[A]:HIS:HB2	2.03	0.58
1:B:552:LEU:HD22	1:B:556:GLN:HG3	1.83	0.58
1:D:206:PHE:CG	3:D:802[B]:HEM:HAB	2.37	0.57
1:B:201:ASN:CG	3:B:802[B]:HEM:HMB2	2.25	0.57
1:B:708:ILE:CD1	1:B:710:ILE:HD11	2.34	0.57
1:B:521:ARG:CD	4:B:1566:HOH:O	2.52	0.57
1:D:274:ILE:HD12	3:D:802[B]:HEM:HMB1	1.88	0.56
1:D:359:LEU:H	1:D:507:HIS:HD2	1.53	0.56
1:A:448:MET:O	1:A:449[B]:HIS:HB2	2.06	0.56
1:B:583:LYS:NZ	1:B:583:LYS:H	2.04	0.56
1:A:479:ARG:NH2	4:A:1549:HOH:O	2.04	0.56
1:C:201:ASN:ND2	3:C:802[B]:HEM:HMB2	2.19	0.55
1:A:274:ILE:HD12	3:A:802[B]:HEM:HMB1	1.88	0.55
1:D:713:GLN:O	1:D:713:GLN:HG2	2.07	0.55
1:B:407:LEU:HD21	3:B:802[B]:HEM:CBB	2.36	0.55
1:C:521:ARG:CB	1:C:521:ARG:HH11	2.17	0.54
2:D:801[A]:HDD:CBC	2:D:801[A]:HDD:HMC1	2.36	0.54
1:B:629:HIS:HD2	4:B:1157:HOH:O	1.89	0.54
1:D:708:ILE:HG13	1:D:710:ILE:HG12	1.89	0.54
1:C:201:ASN:CG	3:C:802[B]:HEM:CMB	2.76	0.54
1:D:206:PHE:HB2	3:D:802[B]:HEM:CBB	2.38	0.54
1:D:416[B]:THR:CG2	4:D:1169:HOH:O	2.56	0.53
1:B:725:ASP:OD1	1:B:725:ASP:C	2.46	0.53
1:B:240:TRP:HE1	1:B:530:GLN:HE21	1.57	0.53
4:A:1169:HOH:O	1:D:100:ARG:HG3	2.08	0.53
1:D:609:ASP:O	4:D:1345:HOH:O	2.18	0.53
1:B:201:ASN:ND2	3:B:802[B]:HEM:HMB1	2.25	0.52
1:D:411:ARG:HG2	3:D:802[B]:HEM:C2C	2.44	0.52
1:D:478:LYS:NZ	4:D:1005:HOH:O	2.42	0.52
1:A:407:LEU:CD2	3:A:802[B]:HEM:HBB1	2.39	0.52
1:B:634:TYR:O	1:B:653:THR:HA	2.08	0.52
4:B:1339:HOH:O	1:D:449[A]:HIS:HE1	1.92	0.52
1:B:392:HIS:ND1	1:B:415:TYR:HB3	2.06	0.52
1:A:407:LEU:HD23	3:A:802[B]:HEM:HBB1	1.92	0.52
1:C:621:LYS:HE3	4:C:1595:HOH:O	2.09	0.52
4:B:1139:HOH:O	1:D:449[B]:HIS:HD2	1.93	0.52
1:B:407:LEU:CD2	3:B:802[B]:HEM:CBB	2.86	0.52
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.92	0.52
1:C:411:ARG:HG2	3:C:802[B]:HEM:C2C	2.45	0.52
1:B:201:ASN:CG	3:B:802[B]:HEM:CMB	2.79	0.52
4:A:1344:HOH:O	1:C:449[B]:HIS:HE1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:LYS:O	1:B:584:LYS:HB3	2.10	0.51
4:A:1047:HOH:O	1:C:52:PRO:HG3	2.09	0.51
1:D:748:ILE:O	1:D:751:ILE:HG22	2.10	0.51
1:B:521:ARG:NE	4:B:1566:HOH:O	2.43	0.51
1:D:671:ASN:HD21	1:D:673:ALA:HB3	1.76	0.50
1:D:416[B]:THR:HG22	4:D:1169:HOH:O	2.11	0.50
1:C:240:TRP:HE1	1:C:530:GLN:HE21	1.60	0.50
1:C:359:LEU:H	1:C:507:HIS:HD2	1.60	0.50
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.28	0.49
1:A:372:LYS:NZ	4:A:1629:HOH:O	2.44	0.49
1:B:359:LEU:H	1:B:507:HIS:CD2	2.29	0.49
3:A:802[B]:HEM:CBC	3:A:802[B]:HEM:HMC2	2.15	0.49
2:C:801[A]:HDD:CBB	2:C:801[A]:HDD:HMB1	2.41	0.49
3:B:802[B]:HEM:HMC2	3:B:802[B]:HEM:HBC2	1.96	0.48
3:A:802[B]:HEM:CBC	3:A:802[B]:HEM:CMC	2.80	0.48
1:C:704:PHE:O	1:C:707:THR:HG22	2.12	0.48
1:C:577:PRO:HG2	4:C:1495:HOH:O	2.13	0.48
1:D:240:TRP:HE1	1:D:530:GLN:HE21	1.61	0.48
1:A:411:ARG:HD2	3:A:802[B]:HEM:HBB2	1.96	0.48
3:B:802[B]:HEM:CMC	3:B:802[B]:HEM:HBC2	2.44	0.47
1:C:597:ASP:OD2	4:C:1417:HOH:O	2.20	0.47
2:D:801[A]:HDD:CMC	2:D:801[A]:HDD:HBC1	2.44	0.47
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.30	0.47
1:B:461:GLU:HA	1:B:462:PRO:C	2.34	0.46
3:A:802[B]:HEM:CBB	3:A:802[B]:HEM:HHC	2.44	0.46
1:B:461:GLU:OE1	1:D:91:ASP:OD1	2.34	0.46
1:B:724:ALA:O	1:B:726:GLY:N	2.45	0.46
1:B:448:MET:O	1:B:449[B]:HIS:HB2	2.15	0.46
1:C:359:LEU:H	1:C:507:HIS:CD2	2.34	0.46
3:C:802[B]:HEM:HMC2	3:C:802[B]:HEM:CBC	2.35	0.46
1:A:36:HIS:HD2	1:A:36:HIS:H	1.62	0.46
1:B:201:ASN:OD1	3:B:802[B]:HEM:HMB2	2.16	0.45
1:B:274:ILE:HD12	2:B:801[A]:HDD:HMB1	1.99	0.45
1:D:634:TYR:O	1:D:653:THR:HA	2.15	0.45
1:A:726:GLY:HA2	4:A:1492:HOH:O	2.16	0.45
1:C:37:ARG:HD3	4:C:1509:HOH:O	2.16	0.45
1:D:128:HIS:HA	1:D:168:THR:O	2.17	0.45
1:B:201:ASN:ND2	3:B:802[B]:HEM:CMB	2.80	0.45
1:D:359:LEU:H	1:D:507:HIS:CD2	2.31	0.45
1:B:39:ALA:HB1	1:B:41:GLU:HG2	1.98	0.45
1:A:144:LEU:HD11	1:A:370:VAL:HG13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.47	0.45
1:B:92:GLN:HA	1:C:213:LYS:HD2	1.99	0.44
3:A:802[B]:HEM:CBB	3:A:802[B]:HEM:CHC	2.94	0.44
1:A:128:HIS:HA	1:A:168:THR:O	2.18	0.44
1:B:128:HIS:HA	1:B:168:THR:O	2.17	0.44
1:B:530:GLN:HE21	1:B:530:GLN:HB3	1.63	0.44
1:A:128:HIS:CE1	1:A:169:VAL:HG22	2.53	0.44
1:B:157:ASN:CA	4:B:1578:HOH:O	2.58	0.43
1:A:201:ASN:ND2	3:A:802[B]:HEM:CMB	2.81	0.43
1:C:201:ASN:OD1	3:C:802[B]:HEM:HMB2	2.16	0.43
2:D:801[A]:HDD:CMB	2:D:801[A]:HDD:HBB1	2.44	0.43
1:D:128:HIS:CE1	1:D:169:VAL:HG22	2.53	0.43
1:B:603:VAL:HG11	1:B:666:ILE:HD12	2.00	0.43
1:D:359:LEU:HD21	4:D:1643:HOH:O	2.19	0.43
1:C:461:GLU:HB2	1:C:462:PRO:HA	2.01	0.43
1:B:451:MET:HE2	1:D:451:MET:HE1	2.01	0.43
1:A:393:PRO:HD2	1:A:415:TYR:CD2	2.54	0.43
1:D:201:ASN:ND2	3:D:802[B]:HEM:CMB	2.82	0.43
1:B:556:GLN:HG2	1:B:566:LEU:CD2	2.47	0.43
1:C:448:MET:O	1:C:449[B]:HIS:HB2	2.19	0.43
1:B:213:LYS:HE3	1:B:213:LYS:HB3	1.82	0.43
1:C:274:ILE:HD12	3:C:802[B]:HEM:HMB1	2.01	0.43
1:A:201:ASN:CG	3:A:802[B]:HEM:CMB	2.85	0.42
1:A:449[B]:HIS:CG	1:C:449[B]:HIS:CG	2.36	0.42
1:B:83:ASN:HB3	1:D:429:HIS:CD2	2.54	0.42
1:A:459:ASN:H	1:A:459:ASN:HD22	1.66	0.42
1:D:206:PHE:CG	3:D:802[B]:HEM:CAB	3.02	0.42
1:C:643:ASP:OD1	1:C:644:ASP:N	2.52	0.42
1:A:535:VAL:O	1:A:537:PRO:HD3	2.20	0.42
1:B:459:ASN:H	1:B:459:ASN:HD22	1.66	0.42
2:D:801[A]:HDD:HMB1	2:D:801[A]:HDD:CBB	2.46	0.42
1:C:251:HIS:CE1	1:C:507:HIS:HB3	2.54	0.42
1:D:65:LEU:HD21	1:D:135:HIS:CG	2.54	0.42
1:D:448:MET:O	1:D:449[A]:HIS:CB	2.67	0.42
1:D:461:GLU:HA	1:D:462:PRO:C	2.41	0.42
1:D:578:ASP:OD1	1:D:583:LYS:HE3	2.20	0.42
1:B:91:ASP:OD1	1:D:461:GLU:OE1	2.38	0.41
1:B:583:LYS:HZ2	1:B:583:LYS:H	1.68	0.41
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.35	0.41
1:A:251:HIS:CE1	1:A:507:HIS:HB3	2.55	0.41
1:C:407:LEU:HD23	3:C:802[B]:HEM:HBB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:725:ASP:HB3	1:C:726:GLY:H	1.65	0.41
1:A:751:ILE:HA	1:A:752:PRO:HD3	1.73	0.41
1:A:725:ASP:H	1:A:728:PHE:HB3	1.85	0.41
1:D:313:ARG:HG3	1:D:660:LEU:HD12	2.03	0.41
2:A:801[A]:HDD:HMB1	2:A:801[A]:HDD:CBB	2.47	0.41
1:B:552:LEU:HD21	1:B:571:LEU:HD12	2.03	0.41
1:A:38:PRO:HG2	1:A:51:ALA:HB2	2.03	0.41
2:B:801[A]:HDD:HMB1	2:B:801[A]:HDD:CBB	2.49	0.41
1:C:128:HIS:HA	1:C:168:THR:O	2.20	0.41
1:C:469:TRP:CE3	1:C:471:ARG:HG3	2.56	0.41
1:C:634:TYR:O	1:C:653:THR:HA	2.21	0.40
1:B:596:GLY:HA3	1:B:737:ALA:O	2.22	0.40
1:D:296:LEU:HA	1:D:296:LEU:HD23	1.93	0.40
1:C:552:LEU:HD22	1:C:556:GLN:HG3	2.03	0.40
1:C:267:ARG:HD2	1:C:267:ARG:HH11	1.63	0.40
1:A:449[B]:HIS:HE1	4:A:1344:HOH:O	2.03	0.40
1:B:83:ASN:HB3	1:D:429:HIS:CG	2.56	0.40
1:B:626:LYS:HA	1:B:626:LYS:HD3	1.69	0.40
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	728/753 (97%)	710 (98%)	17 (2%)	1 (0%)	56	31
1	B	728/753 (97%)	714 (98%)	13 (2%)	1 (0%)	56	31
1	C	727/753 (96%)	709 (98%)	17 (2%)	1 (0%)	56	31
1	D	728/753 (97%)	715 (98%)	12 (2%)	1 (0%)	56	31
All	All	2911/3012 (97%)	2848 (98%)	59 (2%)	4 (0%)	56	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	SER
1	B	75	SER
1	C	75	SER
1	D	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	615/636 (97%)	601 (98%)	14 (2%)	58 29
1	B	615/636 (97%)	587 (95%)	28 (5%)	33 9
1	C	614/636 (96%)	581 (95%)	33 (5%)	27 6
1	D	615/636 (97%)	593 (96%)	22 (4%)	42 15
All	All	2459/2544 (97%)	2362 (96%)	97 (4%)	39 13

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	LYS
1	A	185	PHE
1	A	191	THR
1	A	205	ILE
1	A	227	TRP
1	A	252	ASN
1	A	440	TYR
1	A	459	ASN
1	A	530	GLN
1	A	552	LEU
1	A	556	GLN
1	A	713	GLN
1	A	732	LEU
1	A	751	ILE
1	B	32	GLU
1	B	155	ASP

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Mol	Chain	Res	Type
1	B	158	LYS
1	B	185	PHE
1	B	191	THR
1	B	205	ILE
1	B	213	LYS
1	B	227	TRP
1	B	237	ASP
1	B	252	ASN
1	B	321	GLU
1	B	379	PRO
1	B	432	PRO
1	B	440	TYR
1	B	459	ASN
1	B	530	GLN
1	B	552	LEU
1	B	566	LEU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	612	ARG
1	B	616	LEU
1	B	633	LEU
1	B	703	LYS
1	B	713	GLN
1	B	725	ASP
1	B	749	ASP
1	C	32	GLU
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	213	LYS
1	C	227	TRP
1	C	237	ASP
1	C	252	ASN
1	C	432	PRO
1	C	440	TYR
1	C	459	ASN
1	C	478	LYS
1	C	488	ARG

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Mol	Chain	Res	Type
1	C	521	ARG
1	C	530	GLN
1	C	552	LEU
1	C	568	ASP
1	C	571	LEU
1	C	583[A]	LYS
1	C	583[B]	LYS
1	C	612	ARG
1	C	616	LEU
1	C	617	LEU
1	C	648	LEU
1	C	709	LYS
1	C	713	GLN
1	C	725	ASP
1	C	733	LEU
1	C	750	LYS
1	C	751	ILE
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	344	GLU
1	D	369	ARG
1	D	440	TYR
1	D	459	ASN
1	D	530	GLN
1	D	554	LEU
1	D	574	THR
1	D	582	LEU
1	D	616	LEU
1	D	633	LEU
1	D	648	LEU
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 (32) 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	530	GLN
1	A	556	GLN
1	A	713	GLN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	530	GLN
1	B	629	HIS
1	B	713	GLN
1	C	252	ASN
1	C	368	GLN
1	C	419	GLN
1	C	459	ASN
1	C	507	HIS
1	C	530	GLN
1	C	572	ASN
1	C	629	HIS
1	C	671	ASN
1	C	713	GLN
1	D	48	GLN
1	D	252	ASN
1	D	419	GLN
1	D	459	ASN
1	D	507	HIS
1	D	530	GLN
1	D	556	GLN
1	D	629	HIS
1	D	671	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates (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	1.55	6 (20%)	20,89,89	3.88	11 (55%)
3	HEM	A	802[B]	1,4	30,50,50	3.56	14 (46%)	24,82,82	3.45	14 (58%)
2	HDD	B	801[A]	1,4	30,52,52	1.58	5 (16%)	20,89,89	4.46	12 (60%)
3	HEM	B	802[B]	4	30,50,50	3.23	14 (46%)	24,82,82	3.20	15 (62%)
2	HDD	C	801[A]	1,4	30,52,52	1.57	7 (23%)	20,89,89	3.43	12 (60%)
3	HEM	C	802[B]	-	30,50,50	3.71	14 (46%)	24,82,82	3.53	14 (58%)
2	HDD	D	801[A]	1,4	30,52,52	1.53	6 (20%)	20,89,89	4.02	15 (75%)
3	HEM	D	802[B]	1,4	30,50,50	3.43	14 (46%)	24,82,82	3.10	13 (54%)

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

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802[B]	HEM	C3B-C4B	-8.17	1.44	1.51
3	C	802[B]	HEM	C3B-C4B	-8.11	1.44	1.51
3	C	802[B]	HEM	C3D-C4D	-4.93	1.45	1.51
3	B	802[B]	HEM	C3B-C4B	-4.70	1.47	1.51
3	A	802[B]	HEM	C3D-C4D	-4.69	1.45	1.51
3	D	802[B]	HEM	C3D-C4D	-4.60	1.45	1.51
3	D	802[B]	HEM	C3B-C4B	-4.34	1.48	1.51
3	A	802[B]	HEM	C3B-CAB	-3.96	1.43	1.51
3	B	802[B]	HEM	C2D-C3D	-3.81	1.43	1.54
3	C	802[B]	HEM	C2C-C1C	-3.45	1.46	1.52
3	A	802[B]	HEM	C2D-C3D	-3.20	1.45	1.54
3	C	802[B]	HEM	C2D-C3D	-3.13	1.45	1.54
3	B	802[B]	HEM	C3D-C4D	-3.12	1.47	1.51
3	D	802[B]	HEM	C2D-C3D	-2.94	1.45	1.54
2	A	801[A]	HDD	CAD-C3D	-2.90	1.48	1.53
3	B	802[B]	HEM	C2B-C1B	-2.73	1.42	1.51
2	C	801[A]	HDD	CAA-C2A	-2.59	1.47	1.52
3	C	802[B]	HEM	C3B-CAB	-2.19	1.47	1.51
3	C	802[B]	HEM	C3C-CAC	-2.12	1.47	1.51
3	B	802[B]	HEM	CAD-C3D	-2.10	1.49	1.54
3	A	802[B]	HEM	C2C-C1C	-2.07	1.48	1.52
3	A	802[B]	HEM	CAD-C3D	-2.06	1.50	1.54
3	D	802[B]	HEM	CAA-C2A	2.11	1.55	1.52
2	D	801[A]	HDD	CMA-C3A	2.15	1.56	1.51
2	A	801[A]	HDD	C2A-C3A	2.20	1.44	1.37
2	B	801[A]	HDD	C1A-CHA	2.21	1.45	1.39
2	C	801[A]	HDD	C2A-C3A	2.22	1.44	1.37
2	B	801[A]	HDD	C4A-CHB	2.23	1.46	1.39
3	A	802[B]	HEM	CHC-C4B	2.24	1.45	1.38
3	B	802[B]	HEM	FE-NB	2.29	2.09	1.97
2	C	801[A]	HDD	O1D-C3D	2.29	1.50	1.46
2	D	801[A]	HDD	CMD-C2D	2.34	1.56	1.53
2	A	801[A]	HDD	C4A-CHB	2.34	1.46	1.39
2	D	801[A]	HDD	CMC-C2C	2.40	1.56	1.51
2	C	801[A]	HDD	O1D-CGD	2.41	1.39	1.35
3	D	802[B]	HEM	FE-NB	2.53	2.10	1.97
3	B	802[B]	HEM	FE-ND	2.56	2.11	1.97
3	C	802[B]	HEM	FE-NB	2.57	2.11	1.97
3	C	802[B]	HEM	FE-ND	2.64	2.11	1.97
3	D	802[B]	HEM	FE-ND	2.71	2.11	1.97
3	D	802[B]	HEM	C1A-CHA	2.76	1.47	1.39
3	B	802[B]	HEM	CHD-C1D	2.77	1.46	1.38
2	D	801[A]	HDD	C1A-CHA	2.77	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801[A]	HDD	O1D-C3D	2.79	1.51	1.46
3	D	802[B]	HEM	CHC-C4B	2.81	1.46	1.38
2	B	801[A]	HDD	O1D-CGD	2.82	1.40	1.35
3	D	802[B]	HEM	C2A-C3A	2.84	1.46	1.37
3	A	802[B]	HEM	CHD-C4C	2.86	1.43	1.36
3	C	802[B]	HEM	C2A-C3A	2.88	1.46	1.37
2	D	801[A]	HDD	OND-C2D	2.91	1.48	1.42
3	A	802[B]	HEM	C2A-C3A	2.92	1.46	1.37
2	A	801[A]	HDD	C4B-NB	2.92	1.40	1.36
3	B	802[B]	HEM	C2A-C3A	2.93	1.46	1.37
2	B	801[A]	HDD	O1D-C3D	2.96	1.51	1.46
3	A	802[B]	HEM	FE-ND	2.97	2.13	1.97
3	B	802[B]	HEM	CHC-C4B	3.01	1.47	1.38
3	D	802[B]	HEM	CHC-C1C	3.13	1.43	1.36
2	C	801[A]	HDD	C3C-C2C	3.13	1.44	1.40
2	C	801[A]	HDD	C1C-CHC	3.17	1.48	1.39
3	A	802[B]	HEM	CHD-C1D	3.24	1.47	1.38
2	C	801[A]	HDD	C4A-CHB	3.28	1.48	1.39
3	C	802[B]	HEM	CHD-C1D	3.42	1.48	1.38
3	D	802[B]	HEM	CHD-C1D	3.42	1.48	1.38
3	D	802[B]	HEM	CHD-C4C	3.50	1.44	1.36
3	B	802[B]	HEM	CHD-C4C	3.58	1.44	1.36
2	A	801[A]	HDD	OND-C2D	3.67	1.50	1.42
3	C	802[B]	HEM	CHC-C1C	3.84	1.45	1.36
3	A	802[B]	HEM	CHC-C1C	4.11	1.46	1.36
2	D	801[A]	HDD	O1D-CGD	4.18	1.42	1.35
3	C	802[B]	HEM	CHD-C4C	4.26	1.46	1.36
3	B	802[B]	HEM	CHC-C1C	4.29	1.46	1.36
2	B	801[A]	HDD	C4D-ND	5.08	1.45	1.38
3	B	802[B]	HEM	C4C-NC	7.66	1.45	1.36
3	A	802[B]	HEM	C4C-NC	8.58	1.46	1.36
3	C	802[B]	HEM	C4C-NC	9.45	1.47	1.36
3	A	802[B]	HEM	C1C-NC	9.96	1.48	1.36
3	D	802[B]	HEM	C4C-NC	10.37	1.48	1.36
3	D	802[B]	HEM	C1C-NC	10.39	1.48	1.36
3	B	802[B]	HEM	C1C-NC	10.39	1.48	1.36
3	C	802[B]	HEM	C1C-NC	10.65	1.49	1.36

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801[A]	HDD	OND-C2D-CMD	-9.79	91.74	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	802[B]	HEM	C3B-CAB-CBB	-8.30	111.73	124.46
2	A	801[A]	HDD	O1D-CGD-CBD	-8.07	100.74	110.20
2	B	801[A]	HDD	C4D-ND-C1D	-8.06	102.16	107.36
2	D	801[A]	HDD	C4D-ND-C1D	-7.61	102.45	107.36
3	C	802[B]	HEM	C3B-CAB-CBB	-7.59	112.81	124.46
2	C	801[A]	HDD	C4D-ND-C1D	-7.09	102.79	107.36
2	A	801[A]	HDD	C4D-ND-C1D	-6.75	103.01	107.36
2	D	801[A]	HDD	CAA-CBA-CGA	-6.31	101.17	112.75
2	B	801[A]	HDD	CAA-CBA-CGA	-6.22	101.35	112.75
2	C	801[A]	HDD	OND-C2D-CMD	-6.02	98.54	109.41
2	B	801[A]	HDD	O1D-CGD-CBD	-5.98	103.20	110.20
2	C	801[A]	HDD	CAA-CBA-CGA	-5.37	102.90	112.75
3	A	802[B]	HEM	CAA-CBA-CGA	-5.12	103.36	112.75
3	C	802[B]	HEM	C2C-C1C-CHC	-5.00	116.08	123.68
2	D	801[A]	HDD	O1D-CGD-CBD	-4.84	104.53	110.20
3	B	802[B]	HEM	C3B-CAB-CBB	-4.79	117.11	124.46
2	B	801[A]	HDD	C3C-CAC-CBC	-4.75	116.60	126.32
2	A	801[A]	HDD	OND-C2D-CMD	-4.62	101.07	109.41
3	C	802[B]	HEM	C4B-CHC-C1C	-4.58	118.17	125.82
2	A	801[A]	HDD	CAA-CBA-CGA	-4.50	104.50	112.75
2	A	801[A]	HDD	C3C-CAC-CBC	-4.20	117.72	126.32
2	B	801[A]	HDD	CBA-CAA-C2A	-4.18	105.04	112.53
2	D	801[A]	HDD	OND-C2D-CMD	-4.14	101.93	109.41
3	A	802[B]	HEM	C3C-CAC-CBC	-4.10	118.17	124.46
2	D	801[A]	HDD	C3B-CAB-CBB	-4.09	117.96	126.32
2	C	801[A]	HDD	C2D-C1D-CHD	-3.94	117.34	123.48
2	D	801[A]	HDD	C3C-CAC-CBC	-3.75	118.64	126.32
3	B	802[B]	HEM	CBD-CAD-C3D	-3.64	102.97	113.55
2	C	801[A]	HDD	CBA-CAA-C2A	-3.55	106.16	112.53
3	C	802[B]	HEM	C3B-C4B-CHC	-3.51	118.22	123.16
2	D	801[A]	HDD	CBA-CAA-C2A	-3.43	106.38	112.53
3	C	802[B]	HEM	CBD-CAD-C3D	-3.42	103.60	113.55
3	A	802[B]	HEM	C2C-C1C-CHC	-3.41	118.49	123.68
3	D	802[B]	HEM	C1D-CHD-C4C	-3.40	120.14	125.82
3	C	802[B]	HEM	C1D-CHD-C4C	-3.26	120.37	125.82
3	D	802[B]	HEM	C4B-CHC-C1C	-3.15	120.56	125.82
2	C	801[A]	HDD	C3C-CAC-CBC	-3.06	120.05	126.32
3	D	802[B]	HEM	CAA-CBA-CGA	-3.02	107.21	112.75
3	A	802[B]	HEM	C1D-CHD-C4C	-2.87	121.02	125.82
3	D	802[B]	HEM	CBD-CAD-C3D	-2.81	105.38	113.55
2	D	801[A]	HDD	CMA-C3A-C4A	-2.78	123.77	128.36
3	A	802[B]	HEM	C4B-CHC-C1C	-2.71	121.29	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	802[B]	HEM	C2C-C1C-CHC	-2.67	119.61	123.68
3	A	802[B]	HEM	CMA-C3A-C4A	-2.38	124.42	128.36
2	A	801[A]	HDD	CBA-CAA-C2A	-2.36	108.30	112.53
2	D	801[A]	HDD	C2D-C1D-CHD	-2.28	119.93	123.48
3	B	802[B]	HEM	C1D-CHD-C4C	-2.24	122.07	125.82
3	B	802[B]	HEM	CAA-CBA-CGA	-2.20	108.72	112.75
3	B	802[B]	HEM	C3C-CAC-CBC	-2.14	121.18	124.46
3	B	802[B]	HEM	CMA-C3A-C4A	-2.03	125.01	128.36
3	C	802[B]	HEM	CBA-CAA-C2A	2.00	116.11	112.53
2	C	801[A]	HDD	CMC-C2C-C3C	2.05	129.09	125.09
2	B	801[A]	HDD	CMC-C2C-C1C	2.16	131.94	128.36
3	B	802[B]	HEM	CMA-C3A-C2A	2.23	129.89	125.24
3	B	802[B]	HEM	CBA-CAA-C2A	2.26	116.58	112.53
2	C	801[A]	HDD	CMA-C3A-C2A	2.27	129.99	125.24
3	C	802[B]	HEM	CAA-C2A-C1A	2.31	129.51	127.01
2	B	801[A]	HDD	CAD-CBD-CGD	2.46	108.91	104.64
2	C	801[A]	HDD	CAA-C2A-C1A	2.47	129.69	127.01
2	B	801[A]	HDD	CMC-C2C-C3C	2.48	129.93	125.09
2	D	801[A]	HDD	CMA-C3A-C2A	2.51	130.48	125.24
2	B	801[A]	HDD	CMB-C2B-C3B	2.61	130.18	125.09
2	A	801[A]	HDD	CMC-C2C-C3C	2.64	130.25	125.09
3	D	802[B]	HEM	CBA-CAA-C2A	2.65	117.27	112.53
3	A	802[B]	HEM	CAA-C2A-C1A	2.78	130.03	127.01
3	D	802[B]	HEM	CMC-C2C-C3C	2.95	123.90	116.53
2	B	801[A]	HDD	CMA-C3A-C2A	3.04	131.60	125.24
3	D	802[B]	HEM	CAD-C3D-C4D	3.07	123.29	112.47
3	B	802[B]	HEM	CMD-C2D-C3D	3.17	128.37	114.35
3	A	802[B]	HEM	C2C-C1C-NC	3.17	115.56	110.21
2	A	801[A]	HDD	C3C-C4C-NC	3.23	113.38	109.21
3	D	802[B]	HEM	C3C-CAC-CBC	3.29	129.51	124.46
3	B	802[B]	HEM	CAD-C3D-C4D	3.30	124.11	112.47
3	B	802[B]	HEM	CAA-C2A-C1A	3.38	130.68	127.01
3	C	802[B]	HEM	CAD-C3D-C4D	3.39	124.44	112.47
3	B	802[B]	HEM	C2C-C1C-NC	3.40	115.93	110.21
3	A	802[B]	HEM	CMD-C2D-C3D	3.57	130.13	114.35
2	A	801[A]	HDD	CMB-C2B-C3B	3.59	132.11	125.09
2	D	801[A]	HDD	C3C-C4C-NC	3.60	113.86	109.21
2	D	801[A]	HDD	CMB-C2B-C3B	3.65	132.23	125.09
2	D	801[A]	HDD	CMC-C2C-C1C	3.66	134.42	128.36
3	A	802[B]	HEM	CAD-C3D-C4D	3.71	125.57	112.47
2	C	801[A]	HDD	C3C-C4C-NC	3.80	114.12	109.21
3	B	802[B]	HEM	CMC-C2C-C3C	3.91	126.30	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	802[B]	HEM	CMD-C2D-C3D	4.00	132.03	114.35
3	C	802[B]	HEM	C2C-C1C-NC	4.02	116.99	110.21
3	C	802[B]	HEM	CMD-C2D-C3D	4.06	132.31	114.35
2	C	801[A]	HDD	CMB-C2B-C3B	4.23	133.37	125.09
2	D	801[A]	HDD	CAA-C2A-C1A	4.38	131.76	127.01
3	A	802[B]	HEM	CMC-C2C-C3C	4.44	127.61	116.53
3	D	802[B]	HEM	C2C-C1C-NC	4.51	117.82	110.21
3	C	802[B]	HEM	CMC-C2C-C3C	4.61	128.04	116.53
2	A	801[A]	HDD	CAA-C2A-C1A	4.76	132.17	127.01
3	A	802[B]	HEM	CMB-C2B-C3B	5.01	129.03	116.53
2	C	801[A]	HDD	O1D-CGD-O2D	5.05	125.60	120.80
3	C	802[B]	HEM	CMB-C2B-C3B	5.78	130.97	116.53
3	A	802[B]	HEM	CAD-C3D-C2D	6.16	130.93	113.22
3	C	802[B]	HEM	CAD-C3D-C2D	6.39	131.59	113.22
3	B	802[B]	HEM	CAD-C3D-C2D	6.65	132.32	113.22
3	D	802[B]	HEM	CAD-C3D-C2D	7.09	133.60	113.22
3	D	802[B]	HEM	CMB-C2B-C3B	7.45	135.13	116.53
2	D	801[A]	HDD	O1D-CGD-O2D	7.71	128.13	120.80
2	A	801[A]	HDD	O1D-CGD-O2D	7.76	128.18	120.80
3	B	802[B]	HEM	CMB-C2B-C3B	8.22	137.05	116.53
2	B	801[A]	HDD	O1D-CGD-O2D	8.91	129.27	120.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801[A]	HDD	2	0
3	A	802[B]	HEM	13	0
2	B	801[A]	HDD	3	0
3	B	802[B]	HEM	12	0
2	C	801[A]	HDD	2	0
3	C	802[B]	HEM	13	0
2	D	801[A]	HDD	6	0
3	D	802[B]	HEM	8	0

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, 95^{th} 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	726/753 (96%)	-0.36	7 (0%)	84	84	6, 12, 26, 58	1 (0%)
1	B	726/753 (96%)	-0.23	23 (3%)	51	48	6, 13, 36, 65	1 (0%)
1	C	726/753 (96%)	-0.26	22 (3%)	54	51	6, 13, 36, 62	1 (0%)
1	D	726/753 (96%)	-0.29	15 (2%)	67	65	6, 12, 32, 62	1 (0%)
All	All	2904/3012 (96%)	-0.29	67 (2%)	64	62	6, 13, 33, 65	4 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	726	GLY	5.1
1	B	726	GLY	5.0
1	C	711	ALA	4.3
1	A	726	GLY	4.0
1	B	28	SER	4.0
1	B	713	GLN	4.0
1	D	713	GLN	3.9
1	D	750	LYS	3.9
1	D	28	SER	3.7
1	B	32	GLU	3.7
1	B	725	ASP	3.5
1	B	712	ASP	3.5
1	C	712	ASP	3.4
1	C	750	LYS	3.4
1	B	750	LYS	3.3
1	B	677	ASP	3.3
1	C	751	ILE	3.3
1	D	673	ALA	3.2
1	C	641	THR	3.1
1	D	712	ASP	3.1
1	D	749	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	714	GLY	3.0
1	B	645	GLY	3.0
1	B	568	ASP	2.9
1	B	596	GLY	2.8
1	B	647	VAL	2.8
1	A	750	LYS	2.7
1	B	646	THR	2.7
1	B	569	ASP	2.6
1	C	646	THR	2.6
1	A	28	SER	2.6
1	B	572	ASN	2.6
1	D	569	ASP	2.5
1	C	594	PRO	2.5
1	B	644	ASP	2.5
1	C	568	ASP	2.5
1	D	594	PRO	2.5
1	B	583	LYS	2.4
1	B	749	ASP	2.4
1	C	725	ASP	2.4
1	A	596	GLY	2.4
1	D	596	GLY	2.4
1	C	713	GLN	2.4
1	B	33	ASP	2.4
1	C	677	ASP	2.4
1	A	32	GLU	2.3
1	B	710	ILE	2.3
1	B	711	ALA	2.3
1	D	572	ASN	2.3
1	D	722	ASP	2.3
1	D	710	ILE	2.3
1	C	569	ASP	2.3
1	C	647	VAL	2.3
1	C	644	ASP	2.2
1	D	568	ASP	2.2
1	C	32	GLU	2.2
1	C	643	ASP	2.2
1	A	594	PRO	2.2
1	D	711	ALA	2.2
1	C	572	ASN	2.2
1	A	749	ASP	2.1
1	D	677	ASP	2.1
1	B	552	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	645	GLY	2.1
1	C	722	ASP	2.1
1	B	617	LEU	2.0
1	C	674	ASP	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, 95^{th} 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	0.99	0.09	0.79	5,6,12,15	44
3	HEM	A	802[B]	43/43	0.99	0.08	0.66	3,5,6,7	43
3	HEM	C	802[B]	43/43	0.99	0.09	0.57	4,6,8,9	43
2	HDD	D	801[A]	44/44	0.98	0.08	0.41	5,7,12,16	44
3	HEM	D	802[B]	43/43	0.99	0.08	0.34	4,6,8,9	43
2	HDD	C	801[A]	44/44	0.99	0.08	0.30	6,7,14,18	44
3	HEM	B	802[B]	43/43	0.99	0.08	0.30	4,7,8,8	43
2	HDD	B	801[A]	44/44	0.98	0.08	0.20	6,7,14,18	44

6.5 Other polymers (i)

There are no such residues in this entry.