Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:37 PM GMT

PDB ID	:	1GGK
Title	:	CRYSTAL STRUCTURE OF CATALASE HPII FROM ESCHERICHIA COLI, ASN201HIS VARIANT.
Authors	:	Melik-Adamyan, W.R.; Bravo, J.; Carpena, X.; Switala, J.; Mate, M.J.; Fita, I.; Loewen, P.C.
Deposited on	:	2000-08-21
Resolution	:	2.26 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:

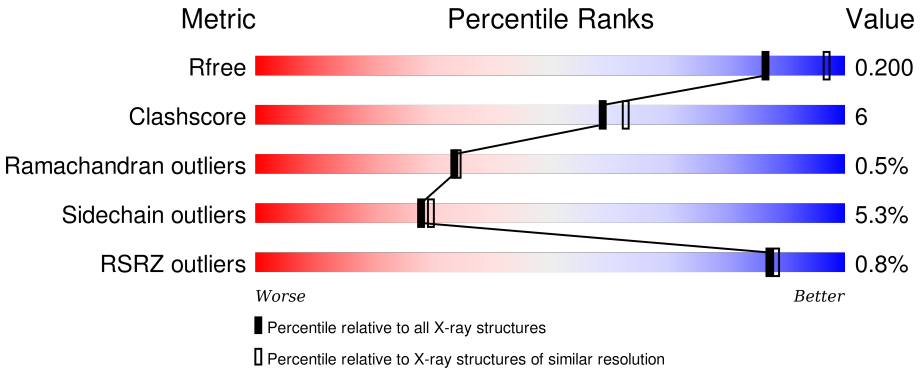
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.26 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	% 80% 16%
1	B	753	% 79% 15%
1	C	753	% 76% 17%
1	D	753	% 77% 16%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 24887 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.

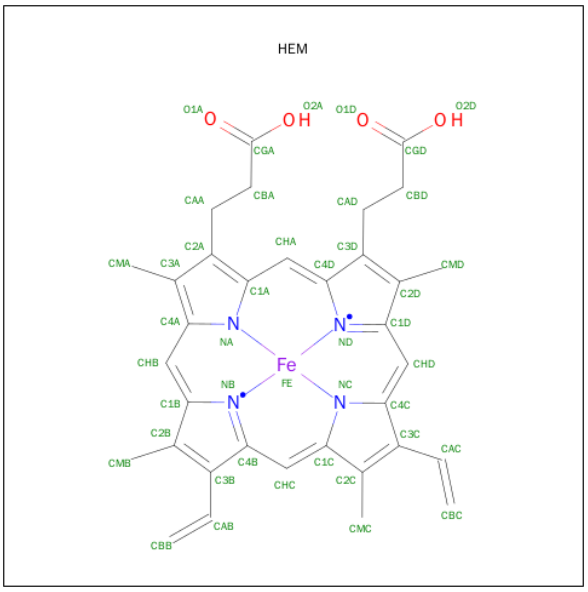
- Molecule 1 is a protein called CATALASE HPII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5748	3649	1006	1081	12			
1	B	727	Total	C	N	O	S	0	0	0
			5748	3649	1006	1081	12			
1	C	727	Total	C	N	O	S	0	0	0
			5748	3649	1006	1081	12			
1	D	727	Total	C	N	O	S	0	0	0
			5748	3649	1006	1081	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASN	ENGINEERED	UNP P21179
B	201	HIS	ASN	ENGINEERED	UNP P21179
C	201	HIS	ASN	ENGINEERED	UNP P21179
D	201	HIS	ASN	ENGINEERED	UNP P21179

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is water.

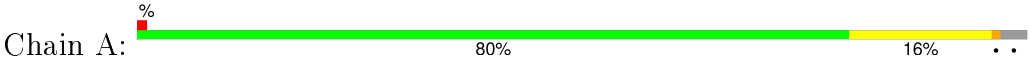
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	460	Total	O	0	0
			460	460		
3	B	409	Total	O	0	0
			409	409		
3	C	404	Total	O	0	0
			404	404		
3	D	450	Total	O	0	0
			450	450		

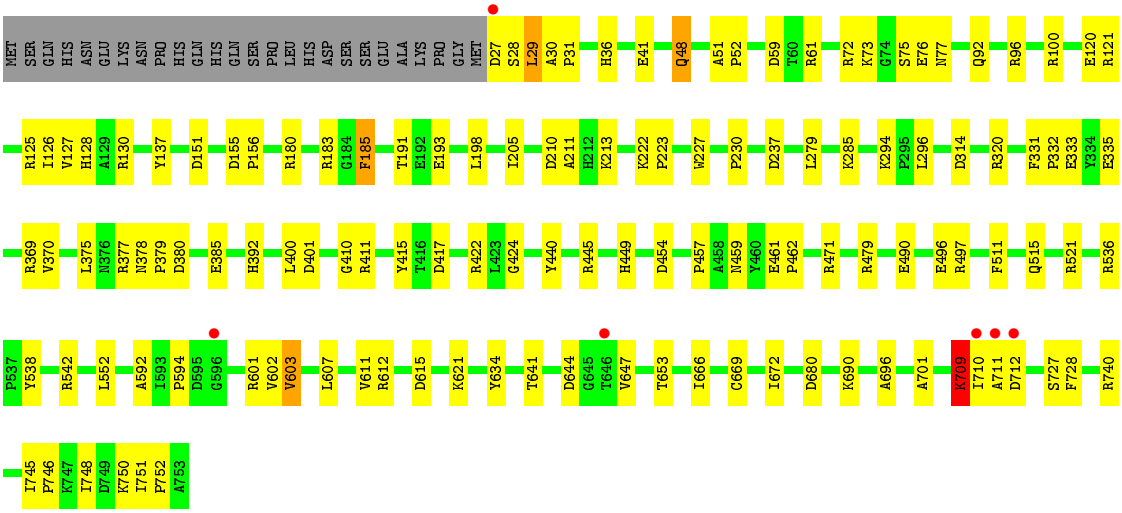
3 Residue-property plots (i)

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

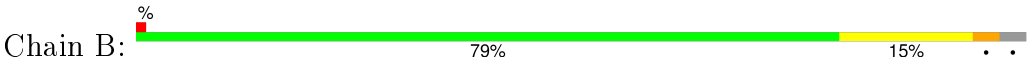
Chain A:

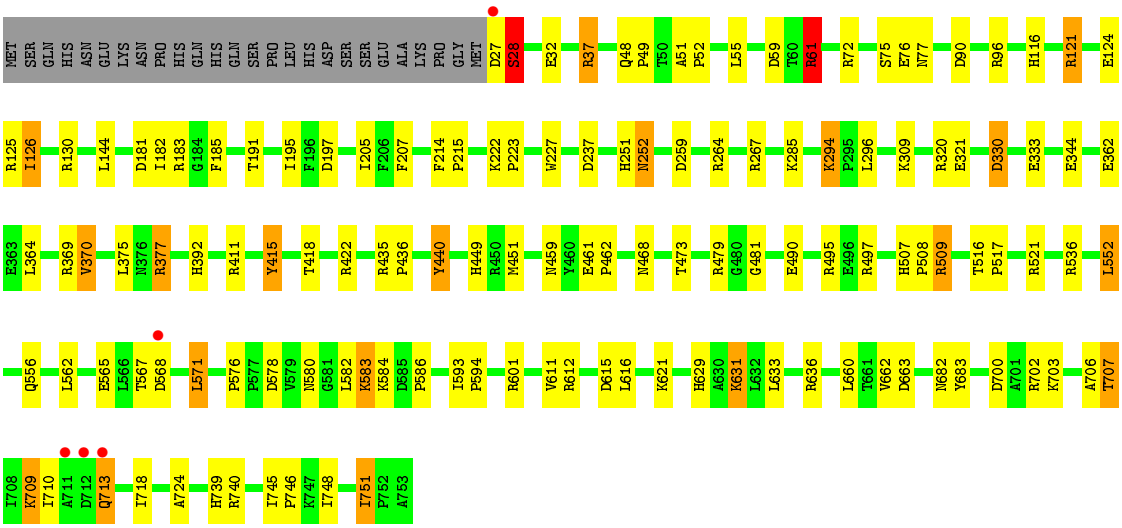




- Molecule 1: CATALASE HPII

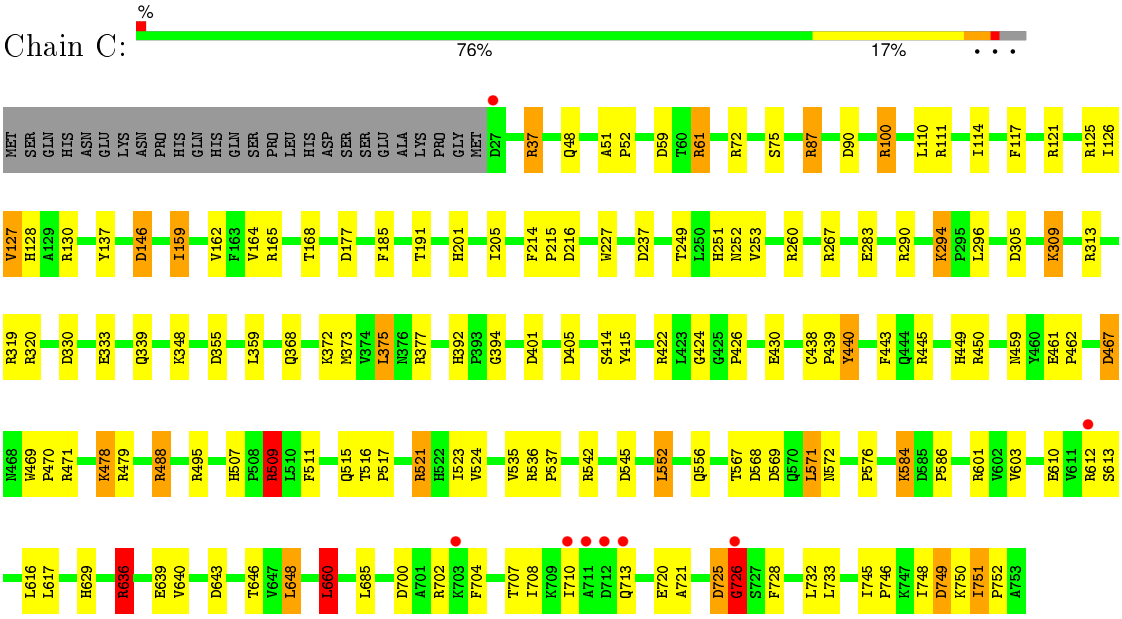
Chain B:





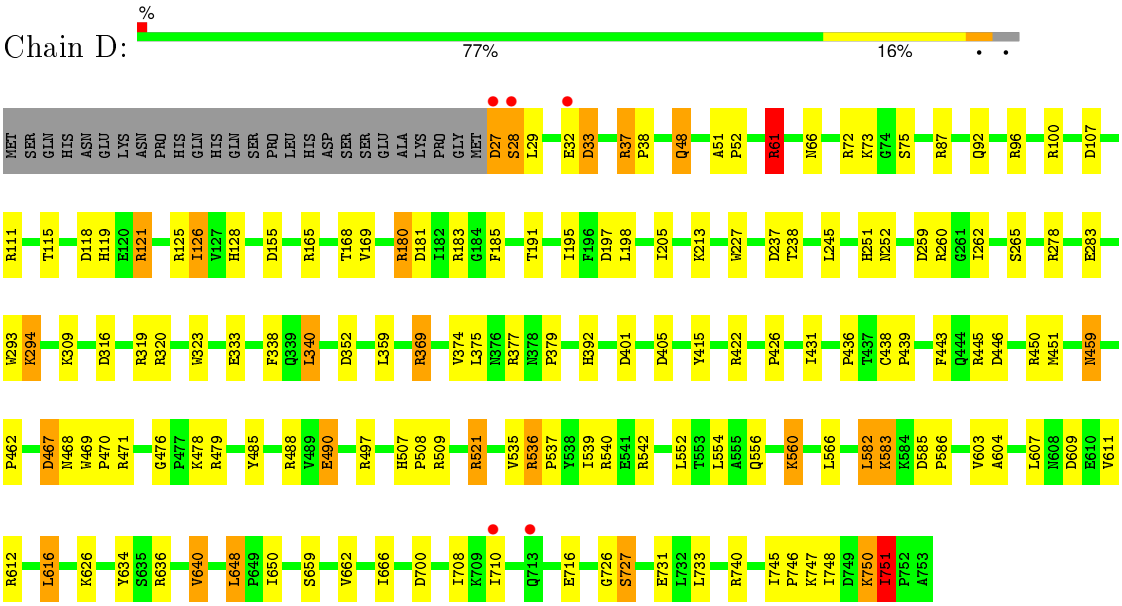
• Molecule 1: CATALASE HPII

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	95.23Å 134.70Å 124.45Å 90.00° 109.41° 90.00°	Depositor
Resolution (Å)	117.38 – 2.26 12.54 – 2.26	Depositor EDS
% Data completeness (in resolution range)	87.6 (117.38-2.26) 88.2 (12.54-2.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.95 (at 2.26Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.130 , 0.208 0.138 , 0.200	Depositor DCC
R_{free} test set	6111 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	14.0	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 67.9	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 120733 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	24887	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.50	0/5905	1.36	50/8028 (0.6%)
1	B	0.50	0/5905	1.42	53/8028 (0.7%)
1	C	0.50	0/5905	1.36	62/8028 (0.8%)
1	D	0.50	0/5905	1.42	69/8028 (0.9%)
All	All	0.50	0/23620	1.39	234/32112 (0.7%)

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	C	0	1

There are no bond length outliers.

All (234) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	521	ARG	CD-NE-CZ	26.25	160.35	123.60
1	A	61	ARG	NE-CZ-NH2	-21.24	109.68	120.30
1	B	377	ARG	NE-CZ-NH2	-19.13	110.73	120.30
1	B	125	ARG	NE-CZ-NH2	-15.75	112.42	120.30
1	D	369	ARG	CD-NE-CZ	14.02	143.23	123.60
1	C	313	ARG	NE-CZ-NH1	13.77	127.18	120.30
1	A	445	ARG	NE-CZ-NH2	-13.08	113.76	120.30
1	B	521	ARG	NE-CZ-NH1	12.20	126.40	120.30
1	D	61	ARG	CD-NE-CZ	12.13	140.59	123.60
1	D	72	ARG	NE-CZ-NH1	12.13	126.36	120.30
1	B	61	ARG	CD-NE-CZ	11.75	140.05	123.60
1	D	72	ARG	CD-NE-CZ	11.72	140.01	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	479	ARG	CD-NE-CZ	11.61	139.86	123.60
1	C	636	ARG	NE-CZ-NH2	-11.41	114.59	120.30
1	D	121	ARG	NE-CZ-NH1	11.36	125.98	120.30
1	C	495	ARG	NE-CZ-NH2	-11.31	114.64	120.30
1	C	636	ARG	CD-NE-CZ	11.11	139.15	123.60
1	D	121	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	D	165	ARG	NE-CZ-NH2	10.45	125.53	120.30
1	B	125	ARG	NH1-CZ-NH2	10.34	130.77	119.40
1	A	479	ARG	CD-NE-CZ	10.23	137.93	123.60
1	D	61	ARG	NE-CZ-NH1	10.15	125.38	120.30
1	B	130	ARG	NE-CZ-NH1	9.83	125.21	120.30
1	B	509	ARG	NE-CZ-NH2	9.81	125.20	120.30
1	D	401	ASP	CB-CG-OD2	9.72	127.05	118.30
1	D	405	ASP	CB-CG-OD1	9.66	126.99	118.30
1	B	320	ARG	NE-CZ-NH2	-9.65	115.47	120.30
1	D	183	ARG	NE-CZ-NH2	9.60	125.10	120.30
1	D	509	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	C	165	ARG	NE-CZ-NH1	9.47	125.03	120.30
1	D	612	ARG	CD-NE-CZ	9.33	136.66	123.60
1	D	509	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	B	509	ARG	NE-CZ-NH1	-9.11	115.75	120.30
1	C	121	ARG	NE-CZ-NH1	9.11	124.85	120.30
1	A	601	ARG	NE-CZ-NH2	-9.09	115.76	120.30
1	B	495	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	A	61	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	D	540	ARG	NE-CZ-NH1	8.99	124.80	120.30
1	B	422	ARG	NE-CZ-NH1	8.95	124.77	120.30
1	B	264	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	C	87	ARG	NE-CZ-NH2	-8.75	115.93	120.30
1	A	100	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	D	369	ARG	NE-CZ-NH2	8.44	124.52	120.30
1	D	278	ARG	NE-CZ-NH1	-8.42	116.09	120.30
1	C	479	ARG	NE-CZ-NH2	8.41	124.51	120.30
1	C	725	ASP	C-N-CA	8.39	139.92	122.30
1	D	37	ARG	N-CA-CB	-8.37	95.54	110.60
1	B	259	ASP	CB-CG-OD2	8.33	125.80	118.30
1	B	636	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	D	479	ARG	CD-NE-CZ	8.31	135.23	123.60
1	A	320	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	C	467	ASP	CB-CG-OD1	8.26	125.73	118.30
1	A	125	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	D	180	ARG	NE-CZ-NH1	8.22	124.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	612	ARG	NE-CZ-NH2	8.20	124.40	120.30
1	C	125	ARG	NE-CZ-NH2	8.19	124.40	120.30
1	D	180	ARG	NE-CZ-NH2	-8.17	116.21	120.30
1	C	111	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	C	509	ARG	NE-CZ-NH1	-8.09	116.25	120.30
1	D	540	ARG	CD-NE-CZ	8.09	134.92	123.60
1	D	100	ARG	CD-NE-CZ	7.99	134.79	123.60
1	A	740	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	B	377	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	A	180	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	479	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	B	264	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	B	435	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	A	479	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	A	125	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	A	314	ASP	CB-CG-OD1	7.67	125.20	118.30
1	B	740	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	B	37	ARG	CA-CB-CG	7.65	130.23	113.40
1	C	545	ASP	CB-CG-OD1	7.63	125.16	118.30
1	D	260	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	A	183	ARG	NE-CZ-NH1	-7.57	116.51	120.30
1	B	497	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	D	197	ASP	CB-CG-OD2	7.48	125.03	118.30
1	C	702	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	A	121	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	96	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	D	542	ARG	CD-NE-CZ	7.32	133.84	123.60
1	A	422	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	B	121	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	A	471	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	C	72	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	D	260	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	B	61	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	B	422	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	D	422	ARG	NE-CZ-NH2	7.13	123.86	120.30
1	D	319	ARG	CD-NE-CZ	7.11	133.56	123.60
1	B	125	ARG	NE-CZ-NH1	-7.02	116.79	120.30
1	B	536	ARG	CD-NE-CZ	7.01	133.41	123.60
1	B	497	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	C	61	ARG	NE-CZ-NH1	-6.99	116.80	120.30
1	B	96	ARG	NE-CZ-NH1	-6.96	116.82	120.30
1	C	536	ARG	NE-CZ-NH1	-6.93	116.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	536	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	C	305	ASP	CB-CG-OD1	6.93	124.53	118.30
1	A	411	ARG	NE-CZ-NH2	6.91	123.75	120.30
1	B	72	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	663	ASP	CB-CG-OD1	6.83	124.44	118.30
1	C	450	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	D	278	ARG	CD-NE-CZ	6.72	133.01	123.60
1	C	319	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	B	121	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	C	146	ASP	CB-CG-OD2	6.59	124.23	118.30
1	A	401	ASP	CB-CG-OD2	6.55	124.19	118.30
1	B	479	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	72	ARG	NE-CZ-NH1	-6.51	117.05	120.30
1	B	130	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	B	440	TYR	CB-CG-CD1	6.49	124.89	121.00
1	D	636	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	C	725	ASP	CA-C-O	6.40	133.54	120.10
1	D	155	ASP	CB-CG-OD2	6.34	124.00	118.30
1	B	418	THR	CA-CB-CG2	6.34	121.27	112.40
1	C	726	GLY	N-CA-C	-6.33	97.26	113.10
1	C	601	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	C	509	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	D	125	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	D	450	ARG	NE-CZ-NH2	6.29	123.44	120.30
1	A	155	ASP	CB-CG-OD2	6.25	123.92	118.30
1	D	27	ASP	CA-CB-CG	6.23	127.10	113.40
1	D	107	ASP	CB-CG-OD1	6.22	123.90	118.30
1	B	411	ARG	NE-CZ-NH1	-6.21	117.19	120.30
1	A	96	ARG	NE-CZ-NH1	-6.20	117.20	120.30
1	D	293	TRP	N-CA-CB	6.16	121.69	110.60
1	C	100	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	D	609	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	601	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	C	636	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	C	401	ASP	CB-CG-OD2	6.07	123.77	118.30
1	C	177	ASP	CB-CG-OD2	6.07	123.76	118.30
1	B	28	SER	N-CA-CB	6.06	119.60	110.50
1	D	320	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	D	96	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	B	683	TYR	CB-CG-CD2	-6.05	117.37	121.00
1	A	377	ARG	CD-NE-CZ	6.01	132.01	123.60
1	B	702	ARG	NE-CZ-NH2	-5.99	117.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	319	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	D	352	ASP	CB-CG-OD2	5.99	123.69	118.30
1	C	495	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	D	536	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	C	320	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	B	415	TYR	CB-CG-CD1	5.88	124.53	121.00
1	D	485	TYR	CB-CG-CD1	-5.87	117.47	121.00
1	A	185	PHE	CB-CG-CD1	5.87	124.91	120.80
1	D	446	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	615	ASP	CB-CG-OD2	5.85	123.57	118.30
1	C	440	TYR	CB-CG-CD1	5.83	124.50	121.00
1	B	181	ASP	CB-CG-OD1	5.83	123.55	118.30
1	C	440	TYR	CB-CG-CD2	-5.81	117.52	121.00
1	C	702	ARG	NH1-CZ-NH2	5.78	125.76	119.40
1	C	725	ASP	N-CA-C	5.77	126.57	111.00
1	D	582	LEU	CA-CB-CG	5.75	128.53	115.30
1	C	290	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	C	445	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	D	320	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	C	59	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	C	422	ARG	NE-CZ-NH2	5.69	123.14	120.30
1	C	445	ARG	CD-NE-CZ	5.68	131.55	123.60
1	B	197	ASP	CB-CG-OD1	-5.67	113.20	118.30
1	D	87	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	D	542	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	48	GLN	CB-CA-C	-5.65	99.11	110.40
1	D	401	ASP	CB-CG-OD1	-5.65	113.22	118.30
1	A	137	TYR	CB-CG-CD2	-5.64	117.61	121.00
1	C	216	ASP	CB-CG-OD2	5.59	123.33	118.30
1	D	72	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	D	377	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	C	749	ASP	CB-CA-C	-5.58	99.24	110.40
1	A	151	ASP	CB-CG-OD2	5.57	123.32	118.30
1	A	61	ARG	NH1-CZ-NH2	5.55	125.51	119.40
1	A	380	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	C	445	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	C	59	ASP	CB-CG-OD1	5.54	123.29	118.30
1	D	352	ASP	CB-CG-OD1	-5.53	113.32	118.30
1	C	377	ARG	NE-CZ-NH1	-5.51	117.54	120.30
1	D	740	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	479	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	B	294	LYS	N-CA-CB	-5.49	100.72	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	636	ARG	CD-NE-CZ	5.48	131.27	123.60
1	B	90	ASP	CB-CG-OD2	5.46	123.22	118.30
1	B	330	ASP	CB-CG-OD2	5.44	123.20	118.30
1	D	265	SER	N-CA-CB	-5.43	102.35	110.50
1	B	521	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	424	GLY	N-CA-C	5.43	126.67	113.10
1	C	542	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	A	497	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	D	198	LEU	CA-CB-CG	5.41	127.74	115.30
1	D	238	THR	CA-CB-CG2	-5.41	104.83	112.40
1	A	193	GLU	OE1-CD-OE2	-5.39	116.83	123.30
1	C	405	ASP	CB-CG-OD2	5.39	123.16	118.30
1	D	183	ARG	NH1-CZ-NH2	-5.38	113.48	119.40
1	A	680	ASP	CB-CG-OD2	5.37	123.14	118.30
1	A	479	ARG	CG-CD-NE	5.37	123.08	111.80
1	C	260	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	A	210	ASP	CB-CG-OD1	5.35	123.11	118.30
1	C	90	ASP	CB-CG-OD2	5.33	123.10	118.30
1	C	372	LYS	CA-CB-CG	5.31	125.08	113.40
1	D	37	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	C	660	LEU	CA-CB-CG	5.31	127.50	115.30
1	A	130	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	D	259	ASP	CB-CG-OD2	5.30	123.07	118.30
1	C	702	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	A	380	ASP	CB-CG-OD1	5.28	123.05	118.30
1	D	316	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	454	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	A	644	ASP	CB-CG-OD2	5.25	123.02	118.30
1	D	37	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	A	445	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	B	713	GLN	CA-CB-CG	5.19	124.81	113.40
1	C	355	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	41	GLU	CA-CB-CG	5.18	124.79	113.40
1	C	430	GLU	OE1-CD-OE2	-5.17	117.10	123.30
1	D	485	TYR	CB-CG-CD2	5.17	124.10	121.00
1	A	411	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	C	700	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	631	LYS	CB-CA-C	5.15	120.71	110.40
1	D	445	ARG	CD-NE-CZ	5.13	130.78	123.60
1	C	339	GLN	N-CA-CB	5.12	119.82	110.60
1	D	467	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	683	TYR	CB-CG-CD1	5.11	124.07	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	125	ARG	CD-NE-CZ	5.11	130.75	123.60
1	B	377	ARG	NH1-CZ-NH2	5.10	125.01	119.40
1	A	496	GLU	N-CA-CB	-5.09	101.43	110.60
1	C	414	SER	N-CA-CB	-5.09	102.86	110.50
1	A	385	GLU	OE1-CD-OE2	-5.08	117.21	123.30
1	C	267	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	B	267	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	C	424	GLY	N-CA-C	5.07	125.78	113.10
1	D	111	ARG	CD-NE-CZ	5.05	130.67	123.60
1	D	560	LYS	CB-CA-C	5.00	120.41	110.40
1	A	155	ASP	N-CA-CB	-5.00	101.60	110.60
1	C	130	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	726	GLY	Mainchain

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	5748	0	5579	57	0
1	B	5748	0	5579	74	0
1	C	5748	0	5579	68	0
1	D	5748	0	5579	75	0
2	A	43	0	30	2	0
2	B	43	0	30	0	0
2	C	43	0	30	2	0
2	D	43	0	30	0	0
3	A	460	0	0	10	0
3	B	409	0	0	10	0
3	C	404	0	0	10	0
3	D	450	0	0	7	0
All	All	24887	0	22436	260	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 6.

All (260) 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:A:392:HIS:ND1	1:A:415:TYR:HB2	1.13	1.45
1:B:392:HIS:ND1	1:B:415:TYR:HB2	1.20	1.40
1:D:392:HIS:ND1	1:D:415:TYR:HB2	1.11	1.40
1:C:392:HIS:ND1	1:C:415:TYR:HB2	1.10	1.39
1:C:552:LEU:HD11	1:C:571:LEU:HD12	1.43	1.00
1:B:392:HIS:CE1	1:B:415:TYR:HB2	2.03	0.93
1:B:583:LYS:HE2	1:B:583:LYS:H	1.34	0.92
1:D:392:HIS:CE1	1:D:415:TYR:HB2	2.08	0.86
1:A:641:THR:HA	3:A:1219:HOH:O	1.76	0.86
1:A:612:ARG:HE	1:A:669:CYS:HB3	1.43	0.84
1:A:392:HIS:CE1	1:A:415:TYR:HB2	2.10	0.84
3:B:1162:HOH:O	1:C:126:ILE:HB	1.78	0.83
1:C:392:HIS:CE1	1:C:415:TYR:HB2	2.11	0.83
1:B:451:MET:HG3	1:D:451:MET:HE1	1.62	0.80
1:D:611:VAL:HG11	1:D:616:LEU:HD12	1.65	0.78
1:C:438:CYS:HB2	1:C:439:PRO:HD2	1.67	0.77
1:D:640:VAL:HG23	1:D:648:LEU:HD23	1.68	0.76
1:B:51:ALA:HB1	1:B:52:PRO:HD2	1.69	0.74
1:C:751:ILE:HD12	1:C:752:PRO:HD2	1.73	0.71
1:B:682:ASN:OD1	1:B:707:THR:HG21	1.93	0.69
1:B:369:ARG:HB3	3:B:1149:HOH:O	1.92	0.69
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.75	0.69
1:D:27:ASP:O	1:D:28:SER:HB3	1.94	0.67
1:C:552:LEU:HD13	1:C:556:GLN:NE2	2.09	0.67
1:B:309:LYS:HG2	1:B:660:LEU:HD11	1.77	0.67
1:A:294:LYS:HB2	3:A:985:HOH:O	1.95	0.67
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.76	0.66
1:C:51:ALA:HB1	1:C:52:PRO:HD2	1.78	0.66
1:C:704:PHE:O	1:C:707:THR:HG22	1.96	0.65
1:A:51:ALA:HB1	1:A:52:PRO:HD2	1.78	0.65
1:B:611:VAL:HG11	1:B:616:LEU:HG	1.79	0.65
1:A:709:LYS:HA	1:A:709:LYS:HE3	1.79	0.64
1:C:469:TRP:CE3	1:C:471:ARG:HG3	2.33	0.64
1:D:603:VAL:HG11	1:D:666:ILE:HD12	1.79	0.63
2:A:760:HEM:HMC1	2:A:760:HEM:HBC2	1.79	0.63
1:B:567:THR:O	1:B:571:LEU:HD22	1.99	0.63
1:A:672:ILE:HG21	3:A:1216:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:GLU:HG2	1:B:490:GLU:HG2	1.81	0.62
1:B:709:LYS:NZ	1:B:709:LYS:HA	2.15	0.62
1:D:32:GLU:O	1:D:33:ASP:HB3	2.00	0.62
1:A:294:LYS:NZ	1:A:369:ARG:HH21	1.98	0.61
1:A:28:SER:HB2	1:D:245:LEU:HD13	1.82	0.61
1:C:478:LYS:N	1:C:478:LYS:HD3	2.16	0.61
1:B:294:LYS:HE2	3:B:1164:HOH:O	2.01	0.61
1:B:294:LYS:HB2	3:B:1006:HOH:O	2.00	0.61
2:A:760:HEM:HBC2	2:A:760:HEM:CMC	2.31	0.60
1:D:488:ARG:NH1	1:D:490:GLU:OE1	2.35	0.60
1:D:708:ILE:HG13	1:D:710:ILE:HG12	1.82	0.60
1:B:195:ILE:HD11	1:B:436:PRO:HA	1.85	0.59
1:D:648:LEU:HD21	3:D:1205:HOH:O	2.02	0.59
1:D:607:LEU:HD13	1:D:640:VAL:HG21	1.86	0.58
1:C:749:ASP:HB2	1:C:750:LYS:HD3	1.85	0.58
1:B:468:ASN:HD22	1:D:27:ASP:N	2.02	0.58
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.34	0.58
1:C:127:VAL:O	1:C:128:HIS:HB2	2.04	0.57
1:C:535:VAL:O	1:C:537:PRO:HD3	2.03	0.57
1:C:296:LEU:HD12	1:C:333:GLU:HB3	1.86	0.57
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.35	0.57
1:B:509:ARG:HD2	1:B:576:PRO:HD2	1.86	0.57
1:D:61:ARG:HG3	1:D:66:ASN:OD1	2.05	0.57
1:B:700:ASP:HA	1:B:703:LYS:HD3	1.87	0.57
1:B:583:LYS:CE	1:B:583:LYS:H	2.12	0.56
1:C:488:ARG:HD2	3:C:1158:HOH:O	2.04	0.56
1:A:701:ALA:HA	3:A:1216:HOH:O	2.05	0.56
1:D:583:LYS:HB2	1:D:583:LYS:NZ	2.19	0.56
1:C:567:THR:O	1:C:571:LEU:HD22	2.04	0.56
1:C:646:THR:O	1:C:648:LEU:HD13	2.06	0.56
1:C:110:LEU:O	1:C:114:ILE:HG12	2.06	0.56
1:A:294:LYS:HZ1	1:A:369:ARG:HH21	1.54	0.56
1:C:488:ARG:NH1	3:C:1137:HOH:O	2.38	0.56
1:B:706:ALA:HA	1:B:709:LYS:NZ	2.21	0.55
1:A:607:LEU:HD22	1:A:611:VAL:HG21	1.87	0.55
1:B:48:GLN:HB3	1:B:49:PRO:HD2	1.88	0.55
1:B:710:ILE:CD1	1:B:718:ILE:HG13	2.36	0.55
1:C:516:THR:HB	1:C:517:PRO:CD	2.37	0.54
1:A:213:LYS:HD3	1:D:92:GLN:HA	1.90	0.54
1:B:709:LYS:HZ2	1:B:709:LYS:HA	1.71	0.54
1:A:751:ILE:O	1:A:751:ILE:HD12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:725:ASP:HA	1:C:728:PHE:HB3	1.90	0.53
1:C:294:LYS:HB2	3:C:1034:HOH:O	2.08	0.53
1:A:369:ARG:HG2	3:A:1209:HOH:O	2.08	0.53
1:D:611:VAL:CG1	1:D:616:LEU:HD12	2.37	0.53
1:C:612:ARG:HA	1:C:643:ASP:OD2	2.08	0.53
1:A:369:ARG:HG3	3:A:1006:HOH:O	2.08	0.52
1:D:469:TRP:CE3	1:D:471:ARG:HG3	2.44	0.52
1:B:552:LEU:HD21	1:B:556:GLN:NE2	2.25	0.52
1:C:478:LYS:HD3	1:C:478:LYS:H	1.73	0.52
1:B:706:ALA:O	1:B:709:LYS:HD2	2.10	0.52
1:C:521:ARG:HB2	1:C:521:ARG:HH11	1.75	0.52
1:A:76:GLU:O	1:A:77:ASN:HB2	2.10	0.52
1:B:222:LYS:HB3	1:B:223:PRO:HD2	1.92	0.52
1:D:556:GLN:HG3	1:D:566:LEU:CD1	2.40	0.51
1:C:249:THR:O	1:C:253:VAL:HG23	2.11	0.51
1:B:516:THR:HB	1:B:517:PRO:CD	2.40	0.51
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.93	0.51
1:D:359:LEU:H	1:D:507:HIS:HD2	1.59	0.51
1:D:626:LYS:HG3	1:D:733:LEU:HD13	1.92	0.51
1:D:603:VAL:CG1	1:D:666:ILE:HD12	2.41	0.51
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.46	0.50
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.46	0.50
1:A:511:PHE:O	1:A:515:GLN:HG2	2.10	0.50
1:A:748:ILE:O	1:A:751:ILE:HG13	2.11	0.50
1:A:120:GLU:HB2	1:D:126:ILE:CD1	2.41	0.50
1:D:611:VAL:HB	3:D:1205:HOH:O	2.12	0.50
1:C:745:ILE:N	1:C:746:PRO:HD2	2.27	0.50
1:B:748:ILE:O	1:B:751:ILE:HG22	2.12	0.50
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.94	0.49
1:C:309:LYS:HD2	1:C:660:LEU:HD21	1.94	0.49
1:A:294:LYS:NZ	1:A:369:ARG:NH2	2.60	0.49
1:D:359:LEU:H	1:D:507:HIS:CD2	2.30	0.49
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.95	0.48
1:A:457:PRO:HG2	1:C:37:ARG:HH21	1.78	0.48
1:C:613:SER:O	1:C:617:LEU:HD13	2.13	0.48
1:C:636:ARG:HD3	3:C:1132:HOH:O	2.14	0.48
1:D:323:TRP:CZ3	1:D:379:PRO:HD2	2.48	0.48
1:D:27:ASP:HB2	1:D:29:LEU:HG	1.94	0.48
1:A:603:VAL:HG11	1:A:666:ILE:HD12	1.95	0.47
1:D:115:THR:O	1:D:119:HIS:HD2	1.97	0.47
1:A:222:LYS:HB3	1:A:223:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.48	0.47
1:C:392:HIS:CD2	1:C:394:GLY:H	2.31	0.47
1:B:631:LYS:HE3	1:B:662:VAL:CG1	2.44	0.47
1:C:720:GLU:O	1:C:721:ALA:HB2	2.15	0.47
1:D:536:ARG:HB2	1:D:539:ILE:HD12	1.97	0.47
1:B:586:PRO:HB2	1:B:593:ILE:HD12	1.96	0.47
1:B:615:ASP:HA	1:B:724:ALA:HB3	1.97	0.47
1:B:631:LYS:HD3	3:B:1150:HOH:O	2.13	0.47
1:A:461:GLU:HB2	1:A:462:PRO:HA	1.97	0.47
1:B:296:LEU:HD12	1:B:333:GLU:HB3	1.95	0.47
1:A:612:ARG:HE	1:A:669:CYS:CB	2.22	0.47
1:B:516:THR:HB	1:B:517:PRO:HD2	1.97	0.47
1:C:572:ASN:HB3	3:C:1139:HOH:O	2.14	0.47
1:B:364:LEU:HD11	1:B:580:ASN:HB2	1.96	0.47
1:D:521:ARG:HE	1:D:521:ARG:HA	1.80	0.47
1:B:745:ILE:N	1:B:746:PRO:HD2	2.30	0.47
1:A:745:ILE:N	1:A:746:PRO:HD2	2.30	0.46
1:A:92:GLN:HA	1:D:213:LYS:HD3	1.97	0.46
1:B:552:LEU:HD13	1:B:552:LEU:C	2.36	0.46
1:A:538:TYR:O	1:A:542:ARG:HG3	2.15	0.46
1:D:27:ASP:O	1:D:28:SER:CB	2.62	0.46
1:B:629:HIS:HD2	3:B:1100:HOH:O	1.97	0.46
1:A:369:ARG:HH21	1:A:369:ARG:HG2	1.79	0.46
1:B:126:ILE:HD13	1:C:117:PHE:O	2.15	0.46
1:D:438:CYS:HB2	1:D:439:PRO:HD2	1.97	0.46
1:A:127:VAL:O	1:A:128:HIS:HB2	2.16	0.46
1:D:51:ALA:HB1	1:D:52:PRO:HD2	1.98	0.46
1:D:459:ASN:HD22	1:D:459:ASN:H	1.63	0.46
1:D:333:GLU:HG2	1:D:374:VAL:HG22	1.98	0.46
1:D:32:GLU:O	1:D:33:ASP:CB	2.64	0.46
1:D:604:ALA:HB2	1:D:662:VAL:HG11	1.98	0.46
1:B:344:GLU:H	1:B:344:GLU:CD	2.19	0.45
1:D:521:ARG:CA	1:D:521:ARG:HE	2.28	0.45
1:B:28:SER:HA	1:D:467:ASP:OD1	2.17	0.45
1:B:207:PHE:CD2	1:B:252:ASN:HB3	2.51	0.45
1:D:556:GLN:HG3	1:D:566:LEU:HD12	1.98	0.45
1:A:30:ALA:HB1	1:A:36:HIS:CD2	2.52	0.45
1:D:128:HIS:CE1	1:D:169:VAL:HG22	2.52	0.45
1:A:294:LYS:HZ3	1:A:369:ARG:NH2	2.14	0.45
1:D:251:HIS:CE1	1:D:507:HIS:HB3	2.51	0.45
1:D:338:PHE:HB3	1:D:340:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:PHE:HA	1:A:332:PRO:HD3	1.77	0.45
1:A:51:ALA:HB1	1:A:52:PRO:CD	2.44	0.45
1:D:180:ARG:O	1:D:181:ASP:HB2	2.17	0.45
1:A:521:ARG:HG3	3:A:1211:HOH:O	2.16	0.45
1:A:296:LEU:HD21	1:A:335:GLU:HG3	1.98	0.45
1:D:27:ASP:HB2	1:D:29:LEU:CG	2.47	0.45
1:A:592:ALA:O	1:A:594:PRO:HD3	2.17	0.45
1:C:51:ALA:HB1	1:C:52:PRO:CD	2.46	0.44
1:D:61:ARG:NH1	1:D:66:ASN:OD1	2.45	0.44
1:B:59:ASP:HA	1:B:61:ARG:CZ	2.47	0.44
1:B:76:GLU:O	1:B:77:ASN:HB2	2.17	0.44
1:B:222:LYS:HB3	1:B:223:PRO:CD	2.47	0.44
1:C:201:HIS:CG	2:C:760:HEM:HMB2	2.52	0.44
1:C:509:ARG:HD3	1:C:576:PRO:HG2	2.00	0.44
1:B:706:ALA:HA	1:B:709:LYS:HZ2	1.82	0.44
1:C:521:ARG:CB	1:C:521:ARG:HH11	2.30	0.44
1:B:593:ILE:HA	1:B:594:PRO:HD2	1.77	0.44
1:B:461:GLU:HA	1:B:462:PRO:C	2.37	0.44
1:B:214:PHE:HB3	1:B:215:PRO:HD3	1.98	0.44
1:C:128:HIS:HA	1:C:168:THR:O	2.17	0.44
1:B:59:ASP:OD2	1:B:61:ARG:NH2	2.50	0.44
1:C:359:LEU:C	1:C:359:LEU:HD12	2.37	0.44
1:C:87:ARG:NH2	3:C:1130:HOH:O	2.49	0.44
1:C:251:HIS:CE1	1:C:507:HIS:HB3	2.52	0.44
1:B:507:HIS:N	1:B:508:PRO:CD	2.81	0.44
3:A:1218:HOH:O	1:C:449:HIS:CE1	2.70	0.44
1:D:294:LYS:NZ	3:D:1181:HOH:O	2.44	0.43
1:D:745:ILE:HB	1:D:746:PRO:HD3	1.99	0.43
1:B:27:ASP:HB3	1:B:28:SER:H	1.61	0.43
1:B:601:ARG:HH12	1:B:739:HIS:CE1	2.36	0.43
1:D:727:SER:O	1:D:731:GLU:HG3	2.18	0.43
1:A:156:PRO:HG2	3:A:1194:HOH:O	2.18	0.43
1:D:748:ILE:O	1:D:751:ILE:HG22	2.18	0.43
1:C:751:ILE:HD12	1:C:752:PRO:CD	2.45	0.43
1:D:507:HIS:N	1:D:508:PRO:HD2	2.34	0.43
1:B:37:ARG:HD3	3:B:1073:HOH:O	2.19	0.43
1:B:369:ARG:HG2	3:B:768:HOH:O	2.19	0.43
1:B:182:ILE:HG22	1:B:183:ARG:N	2.34	0.43
1:D:634:TYR:HB3	1:D:650:ILE:HD13	2.00	0.43
1:C:146:ASP:HB2	3:C:1163:HOH:O	2.18	0.43
1:A:461:GLU:HA	1:A:462:PRO:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ASN:HB3	1:A:379:PRO:HD2	2.01	0.43
1:B:362:GLU:HG3	3:B:988:HOH:O	2.18	0.43
1:B:449:HIS:CE1	1:D:431:ILE:HG13	2.53	0.43
1:D:535:VAL:O	1:D:537:PRO:HD3	2.18	0.43
1:C:552:LEU:HG	3:C:1142:HOH:O	2.19	0.43
1:C:201:HIS:CD2	2:C:760:HEM:HMB2	2.54	0.43
1:C:214:PHE:HB3	1:C:215:PRO:HD3	2.01	0.43
1:C:461:GLU:HA	1:C:462:PRO:C	2.39	0.43
1:B:631:LYS:HE3	1:B:662:VAL:HG12	2.00	0.42
1:A:279:LEU:HD23	1:A:400:LEU:HD23	2.01	0.42
1:C:162:VAL:HG21	1:C:373:MET:SD	2.59	0.42
1:B:583:LYS:O	1:B:584:LYS:HB3	2.18	0.42
1:D:700:ASP:HB2	3:D:1209:HOH:O	2.19	0.42
1:C:748:ILE:O	1:C:751:ILE:HG23	2.19	0.42
1:D:38:PRO:HA	1:D:48:GLN:NE2	2.35	0.42
1:D:488:ARG:NH2	1:D:490:GLU:OE1	2.52	0.42
1:A:285:LYS:HE2	3:A:1106:HOH:O	2.19	0.42
1:C:523:ILE:O	1:C:524:VAL:C	2.58	0.42
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.54	0.42
1:B:124:GLU:HG2	3:C:803:HOH:O	2.20	0.42
1:B:121:ARG:CZ	1:C:126:ILE:HD12	2.49	0.42
1:A:31:PRO:HD2	1:A:36:HIS:CD2	2.54	0.42
1:A:449:HIS:CE1	3:C:1152:HOH:O	2.72	0.42
1:B:473:THR:O	1:B:481:GLY:HA3	2.20	0.41
1:C:610:GLU:O	1:C:610:GLU:HG3	2.20	0.41
1:C:584:LYS:HZ2	1:C:586:PRO:HD3	1.85	0.41
1:C:725:ASP:HA	1:C:728:PHE:CB	2.50	0.41
1:D:128:HIS:HA	1:D:168:THR:O	2.20	0.41
1:B:55:LEU:HD13	3:B:1073:HOH:O	2.20	0.41
1:B:116:HIS:CD2	1:D:426:PRO:HB2	2.55	0.41
1:B:285:LYS:HB3	1:B:285:LYS:NZ	2.35	0.41
1:B:615:ASP:O	1:B:616:LEU:C	2.59	0.41
1:A:36:HIS:CD2	1:A:36:HIS:H	2.38	0.41
1:D:262:ILE:O	1:D:262:ILE:HG13	2.20	0.41
1:D:392:HIS:ND1	1:D:415:TYR:CG	2.83	0.41
1:B:59:ASP:HA	1:B:61:ARG:NE	2.35	0.41
1:D:195:ILE:HD11	1:D:436:PRO:HA	2.02	0.41
1:A:612:ARG:HH11	1:A:669:CYS:CB	2.33	0.41
1:D:27:ASP:HB2	1:D:29:LEU:HD21	2.02	0.41
1:A:751:ILE:HA	1:A:752:PRO:HD3	1.94	0.41
1:D:462:PRO:HA	1:D:468:ASN:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:GLU:HG3	3:D:1136:HOH:O	2.21	0.41
1:A:417:ASP:OD2	1:D:118:ASP:OD1	2.38	0.41
1:B:507:HIS:N	1:B:508:PRO:HD2	2.36	0.41
1:B:144:LEU:HD11	1:B:370:VAL:HG22	2.01	0.41
1:D:648:LEU:HD22	1:D:648:LEU:N	2.36	0.41
1:D:585:ASP:HA	1:D:586:PRO:HD2	1.92	0.41
1:A:126:ILE:HD12	1:D:121:ARG:CZ	2.51	0.41
1:D:640:VAL:HG23	1:D:648:LEU:HB2	2.02	0.41
1:C:164:VAL:HG21	1:C:375:LEU:HD11	2.03	0.41
1:D:476:GLY:HA3	3:D:1097:HOH:O	2.21	0.41
1:D:478:LYS:HE2	3:D:1167:HOH:O	2.20	0.41
1:C:745:ILE:O	1:C:748:ILE:HG12	2.21	0.40
1:A:29:LEU:HB2	1:C:467:ASP:OD1	2.21	0.40
1:B:578:ASP:HB3	1:B:582:LEU:O	2.22	0.40
1:C:137:TYR:CD1	1:C:159:ILE:HD13	2.55	0.40
1:C:488:ARG:HB2	1:C:488:ARG:HE	1.58	0.40
1:C:511:PHE:O	1:C:515:GLN:HG2	2.21	0.40
1:A:634:TYR:O	1:A:653:THR:HA	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	725/753 (96%)	701 (97%)	20 (3%)	4 (1%)	30	30
1	B	725/753 (96%)	703 (97%)	20 (3%)	2 (0%)	46	52
1	C	725/753 (96%)	699 (96%)	24 (3%)	2 (0%)	46	52
1	D	725/753 (96%)	700 (97%)	19 (3%)	6 (1%)	24	21
All	All	2900/3012 (96%)	2803 (97%)	83 (3%)	14 (0%)	34	34

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	711	ALA
1	B	28	SER
1	D	28	SER
1	D	33	ASP
1	A	709	LYS
1	C	75	SER
1	D	726	GLY
1	D	750	LYS
1	D	751	ILE
1	A	75	SER
1	D	75	SER
1	A	647	VAL
1	B	75	SER
1	C	726	GLY

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	612/636 (96%)	586 (96%)	26 (4%)	36	42
1	B	612/636 (96%)	584 (95%)	28 (5%)	33	37
1	C	612/636 (96%)	570 (93%)	42 (7%)	19	18
1	D	612/636 (96%)	578 (94%)	34 (6%)	26	27
All	All	2448/2544 (96%)	2318 (95%)	130 (5%)	28	30

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASP
1	A	29	LEU
1	A	48	GLN
1	A	59	ASP
1	A	73	LYS
1	A	185	PHE
1	A	191	THR
1	A	198	LEU

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Mol	Chain	Res	Type
1	A	205	ILE
1	A	227	TRP
1	A	230	PRO
1	A	237	ASP
1	A	333	GLU
1	A	370	VAL
1	A	375	LEU
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	602	VAL
1	A	603	VAL
1	A	621	LYS
1	A	709	LYS
1	A	710	ILE
1	A	712	ASP
1	A	727	SER
1	A	750	LYS
1	B	32	GLU
1	B	61	ARG
1	B	126	ILE
1	B	185	PHE
1	B	191	THR
1	B	205	ILE
1	B	227	TRP
1	B	237	ASP
1	B	252	ASN
1	B	321	GLU
1	B	370	VAL
1	B	375	LEU
1	B	377	ARG
1	B	440	TYR
1	B	459	ASN
1	B	552	LEU
1	B	562	LEU
1	B	565	GLU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	612	ARG
1	B	621	LYS
1	B	633	LEU

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Mol	Chain	Res	Type
1	B	707	THR
1	B	709	LYS
1	B	713	GLN
1	B	751	ILE
1	C	37	ARG
1	C	48	GLN
1	C	61	ARG
1	C	100	ARG
1	C	127	VAL
1	C	159	ILE
1	C	185	PHE
1	C	191	THR
1	C	205	ILE
1	C	227	TRP
1	C	237	ASP
1	C	252	ASN
1	C	283	GLU
1	C	294	LYS
1	C	309	LYS
1	C	348	LYS
1	C	368	GLN
1	C	375	LEU
1	C	426	PRO
1	C	440	TYR
1	C	459	ASN
1	C	478	LYS
1	C	488	ARG
1	C	509	ARG
1	C	521	ARG
1	C	552	LEU
1	C	568	ASP
1	C	569	ASP
1	C	571	LEU
1	C	584	LYS
1	C	603	VAL
1	C	616	LEU
1	C	636	ARG
1	C	639	GLU
1	C	640	VAL
1	C	648	LEU
1	C	660	LEU
1	C	685	LEU

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Mol	Chain	Res	Type
1	C	713	GLN
1	C	732	LEU
1	C	733	LEU
1	C	751	ILE
1	D	37	ARG
1	D	48	GLN
1	D	61	ARG
1	D	73	LYS
1	D	126	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	294	LYS
1	D	309	LYS
1	D	340	LEU
1	D	369	ARG
1	D	375	LEU
1	D	459	ASN
1	D	490	GLU
1	D	497	ARG
1	D	521	ARG
1	D	552	LEU
1	D	554	LEU
1	D	560	LYS
1	D	582	LEU
1	D	583	LYS
1	D	616	LEU
1	D	640	VAL
1	D	648	LEU
1	D	659	SER
1	D	716	GLU
1	D	727	SER
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 (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	48	GLN
1	A	252	ASN
1	A	459	ASN
1	A	515	GLN
1	A	713	GLN
1	B	157	ASN
1	B	252	ASN
1	B	459	ASN
1	B	492	ASN
1	B	507	HIS
1	B	556	GLN
1	B	629	HIS
1	C	252	ASN
1	C	449	HIS
1	C	459	ASN
1	C	507	HIS
1	C	556	GLN
1	C	572	ASN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	252	ASN
1	D	368	GLN
1	D	449	HIS
1	D	459	ASN
1	D	507	HIS
1	D	546	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

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	A	760	1,3	30,50,50	2.51	8 (26%)	24,82,82	2.72	11 (45%)
2	HEM	B	760	1	30,50,50	2.41	5 (16%)	24,82,82	2.63	12 (50%)
2	HEM	C	760	1	30,50,50	2.44	6 (20%)	24,82,82	2.65	9 (37%)
2	HEM	D	760	1	30,50,50	2.52	9 (30%)	24,82,82	2.52	10 (41%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	760	1,3	-	0/10/54/54	0/0/8/8
2	HEM	B	760	1	-	0/10/54/54	0/0/8/8
2	HEM	C	760	1	-	0/10/54/54	0/0/8/8
2	HEM	D	760	1	-	0/10/54/54	0/0/8/8

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	760	HEM	C2D-C3D	-7.33	1.32	1.54
2	D	760	HEM	C2D-C3D	-7.11	1.33	1.54
2	C	760	HEM	C3B-C4B	-7.09	1.45	1.51
2	A	760	HEM	C3B-C4B	-7.06	1.45	1.51
2	B	760	HEM	C3B-C4B	-7.02	1.45	1.51
2	B	760	HEM	C2D-C3D	-6.95	1.33	1.54
2	D	760	HEM	C3B-C4B	-6.84	1.45	1.51
2	A	760	HEM	C2D-C3D	-6.71	1.34	1.54
2	A	760	HEM	C3D-C4D	-5.67	1.44	1.51
2	D	760	HEM	C3D-C4D	-5.48	1.44	1.51
2	C	760	HEM	C3D-C4D	-4.79	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	760	HEM	C3D-C4D	-4.37	1.46	1.51
2	B	760	HEM	C2C-C1C	-3.95	1.45	1.52
2	A	760	HEM	C2C-C1C	-3.65	1.45	1.52
2	C	760	HEM	C2C-C1C	-3.65	1.45	1.52
2	D	760	HEM	C2C-C1C	-3.52	1.45	1.52
2	B	760	HEM	C2D-C1D	-2.25	1.44	1.51
2	A	760	HEM	C2D-C1D	-2.17	1.44	1.51
2	D	760	HEM	C3B-CAB	2.08	1.55	1.51
2	D	760	HEM	CMA-C3A	2.11	1.56	1.51
2	A	760	HEM	FE-NC	2.13	2.04	1.95
2	C	760	HEM	C3C-CAC	2.15	1.55	1.51
2	A	760	HEM	C3C-CAC	2.23	1.55	1.51
2	D	760	HEM	C3C-CAC	2.34	1.55	1.51
2	D	760	HEM	FE-NC	2.62	2.06	1.95
2	C	760	HEM	C4C-NC	2.63	1.39	1.36
2	A	760	HEM	C4C-NC	2.89	1.39	1.36
2	D	760	HEM	C4C-NC	2.93	1.39	1.36

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	760	HEM	C3C-CAC-CBC	-4.89	116.96	124.46
2	A	760	HEM	C3C-CAC-CBC	-4.77	117.13	124.46
2	A	760	HEM	CMA-C3A-C4A	-3.75	122.15	128.36
2	C	760	HEM	CMA-C3A-C4A	-3.01	123.38	128.36
2	B	760	HEM	C3C-CAC-CBC	-2.98	119.89	124.46
2	B	760	HEM	CAA-C2A-C1A	-2.89	123.87	127.01
2	B	760	HEM	CMA-C3A-C4A	-2.84	123.67	128.36
2	B	760	HEM	CAA-CBA-CGA	-2.73	107.75	112.75
2	A	760	HEM	CAA-C2A-C1A	-2.66	124.11	127.01
2	B	760	HEM	CBD-CAD-C3D	-2.37	106.67	113.55
2	D	760	HEM	C1D-CHD-C4C	-2.06	122.37	125.82
2	D	760	HEM	CAA-C2A-C1A	-2.02	124.82	127.01
2	B	760	HEM	CBA-CAA-C2A	2.09	116.28	112.53
2	D	760	HEM	CBA-CAA-C2A	2.10	116.30	112.53
2	A	760	HEM	CMA-C3A-C2A	2.18	129.78	125.24
2	D	760	HEM	C2C-C1C-CHC	2.42	127.36	123.68
2	D	760	HEM	CAD-C3D-C4D	2.55	121.47	112.47
2	C	760	HEM	CAD-C3D-C4D	2.84	122.50	112.47
2	A	760	HEM	CAD-C3D-C4D	3.03	123.14	112.47
2	C	760	HEM	CBA-CAA-C2A	3.15	118.18	112.53
2	B	760	HEM	CAD-C3D-C4D	3.17	123.64	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	760	HEM	CMD-C2D-C3D	3.21	128.53	114.35
2	A	760	HEM	CBA-CAA-C2A	3.21	118.28	112.53
2	B	760	HEM	CMD-C2D-C3D	3.31	128.99	114.35
2	C	760	HEM	CMD-C2D-C3D	3.33	129.09	114.35
2	D	760	HEM	CMD-C2D-C3D	3.44	129.57	114.35
2	A	760	HEM	C2D-C3D-C4D	3.73	107.83	101.50
2	B	760	HEM	C2D-C3D-C4D	4.01	108.30	101.50
2	C	760	HEM	C2D-C3D-C4D	4.07	108.40	101.50
2	D	760	HEM	CMC-C2C-C3C	4.26	127.16	116.53
2	D	760	HEM	C2D-C3D-C4D	4.38	108.93	101.50
2	C	760	HEM	CMB-C2B-C3B	4.42	127.56	116.53
2	A	760	HEM	CMB-C2B-C3B	4.65	128.13	116.53
2	B	760	HEM	CMB-C2B-C3B	4.90	128.76	116.53
2	A	760	HEM	CMC-C2C-C3C	4.94	128.86	116.53
2	D	760	HEM	CMB-C2B-C3B	5.10	129.26	116.53
2	B	760	HEM	CAD-C3D-C2D	5.15	128.03	113.22
2	B	760	HEM	CMC-C2C-C3C	5.22	129.56	116.53
2	C	760	HEM	CMC-C2C-C3C	5.24	129.62	116.53
2	A	760	HEM	CAD-C3D-C2D	5.50	129.03	113.22
2	C	760	HEM	CAD-C3D-C2D	5.53	129.10	113.22
2	D	760	HEM	CAD-C3D-C2D	5.70	129.60	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	760	HEM	2	0
2	C	760	HEM	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	727/753 (96%)	-0.82	6 (0%)	87	88	5, 14, 42, 82	1 (0%)
1	B	727/753 (96%)	-0.77	5 (0%)	89	90	5, 16, 44, 84	1 (0%)
1	C	727/753 (96%)	-0.76	8 (1%)	82	84	6, 17, 44, 82	1 (0%)
1	D	727/753 (96%)	-0.83	5 (0%)	89	90	5, 15, 42, 82	1 (0%)
All	All	2908/3012 (96%)	-0.80	24 (0%)	87	88	5, 15, 44, 84	4 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	ASP	6.0
1	A	711	ALA	5.3
1	B	713	GLN	4.5
1	B	27	ASP	4.4
1	C	27	ASP	4.1
1	B	712	ASP	3.8
1	D	713	GLN	3.7
1	A	710	ILE	3.4
1	D	27	ASP	3.3
1	D	32	GLU	3.2
1	C	711	ALA	3.1
1	D	28	SER	2.9
1	C	710	ILE	2.8
1	A	646	THR	2.7
1	C	712	ASP	2.7
1	A	712	ASP	2.6
1	D	710	ILE	2.5
1	B	568	ASP	2.3
1	B	711	ALA	2.3
1	A	596	GLY	2.3
1	C	726	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	612	ARG	2.1
1	C	703	LYS	2.0
1	C	713	GLN	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	HEM	B	760	43/43	0.98	0.08	0.94	6,8,10,11	0
2	HEM	A	760	43/43	0.98	0.08	0.90	5,9,12,14	0
2	HEM	C	760	43/43	0.98	0.08	0.71	10,11,15,17	0
2	HEM	D	760	43/43	0.99	0.07	-0.01	5,9,12,15	0

6.5 Other polymers (i)

There are no such residues in this entry.