W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:24 PM GMT

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PDB ID	:	3TTT
Title	:	Structure of F413Y variant of E. coli KatE
Authors	:	Loewen, P.C.; Jha, V.
Deposited on	:	2011-09-15
Resolution	:	1.58 Å(reported)

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 1.58 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.
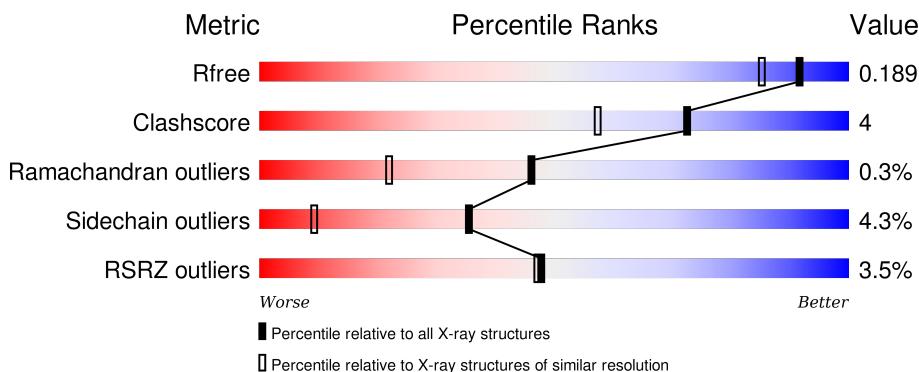
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3815 (1.60-1.56)
Clashscore	102246	4131 (1.60-1.56)
Ramachandran outliers	100387	4021 (1.60-1.56)
Sidechain outliers	100360	4018 (1.60-1.56)
RSRZ outliers	91569	3823 (1.60-1.56)

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	3% / 84% / 10% / · ·
1	B	753	5% / 84% / 11% / · ·
1	C	753	4% / 82% / 12% / · ·
1	D	753	2% / 81% / 13% / · ·

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26162 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	1	0
			5745	3647	1006	1080	12			
1	B	726	Total	C	N	O	S	0	1	0
			5746	3648	1006	1080	12			
1	C	726	Total	C	N	O	S	0	1	0
			5745	3647	1006	1080	12			
1	D	726	Total	C	N	O	S	0	1	0
			5746	3648	1006	1080	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	413	TYR	PHE	ENGINEERED MUTATION	UNP P21179
B	413	TYR	PHE	ENGINEERED MUTATION	UNP P21179
C	413	TYR	PHE	ENGINEERED MUTATION	UNP P21179
D	413	TYR	PHE	ENGINEERED MUTATION	UNP P21179

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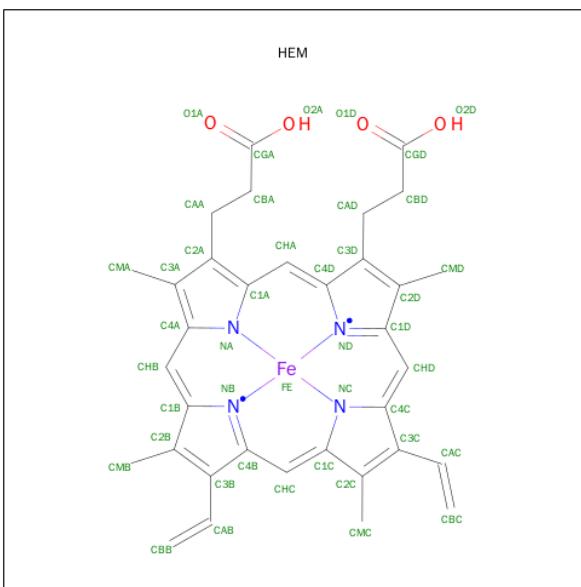
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	815	Total	O	0	0
			815	815		
3	B	673	Total	O	0	0
			673	673		
3	C	737	Total	O	0	0
			737	737		
3	D	783	Total	O	0	0
			783	783		

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
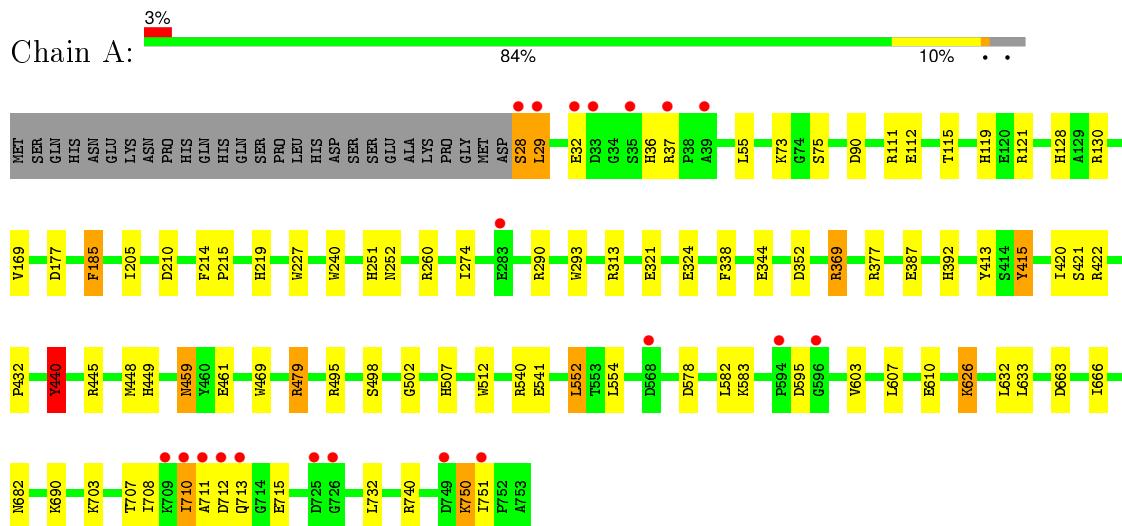
- Molecule 1: Catalase HPII

- Molecule 1: Catalase HPII

Chain C:

• Molecule 1: Catalase HPII

Chain D:
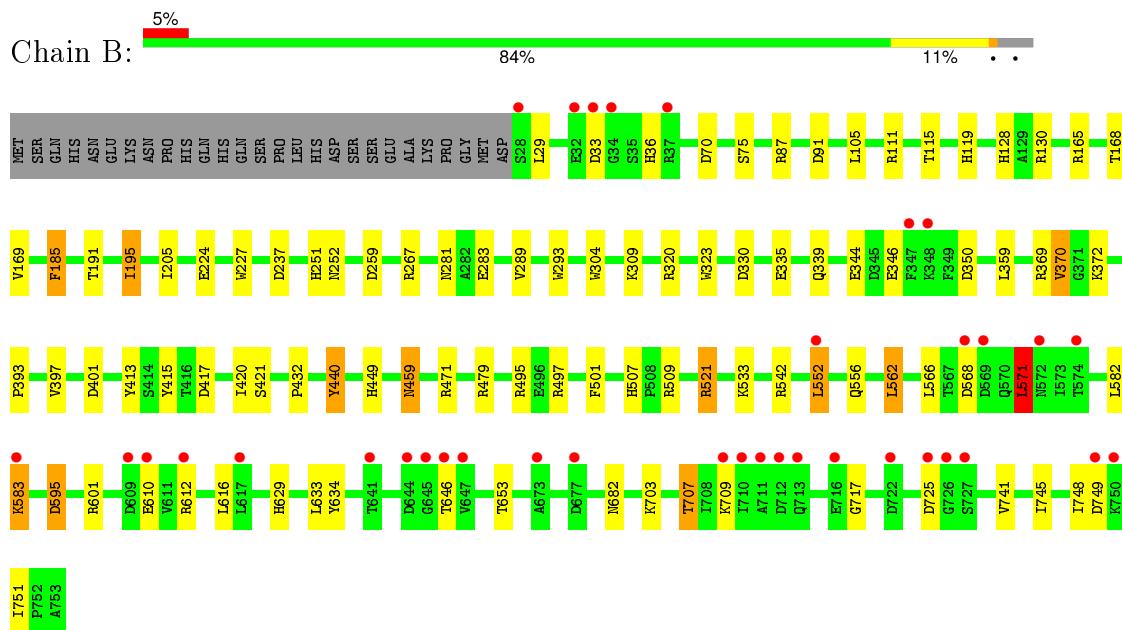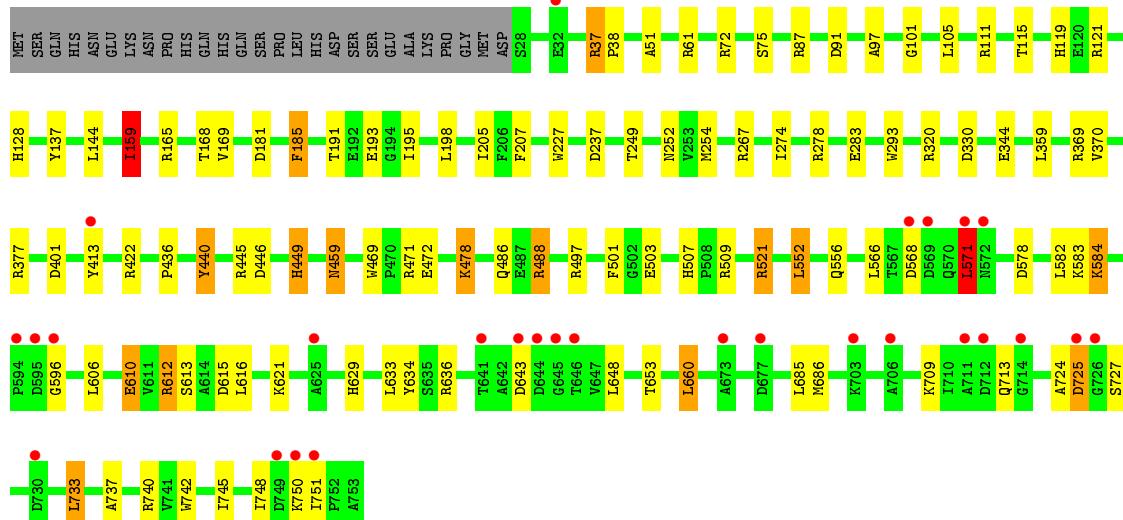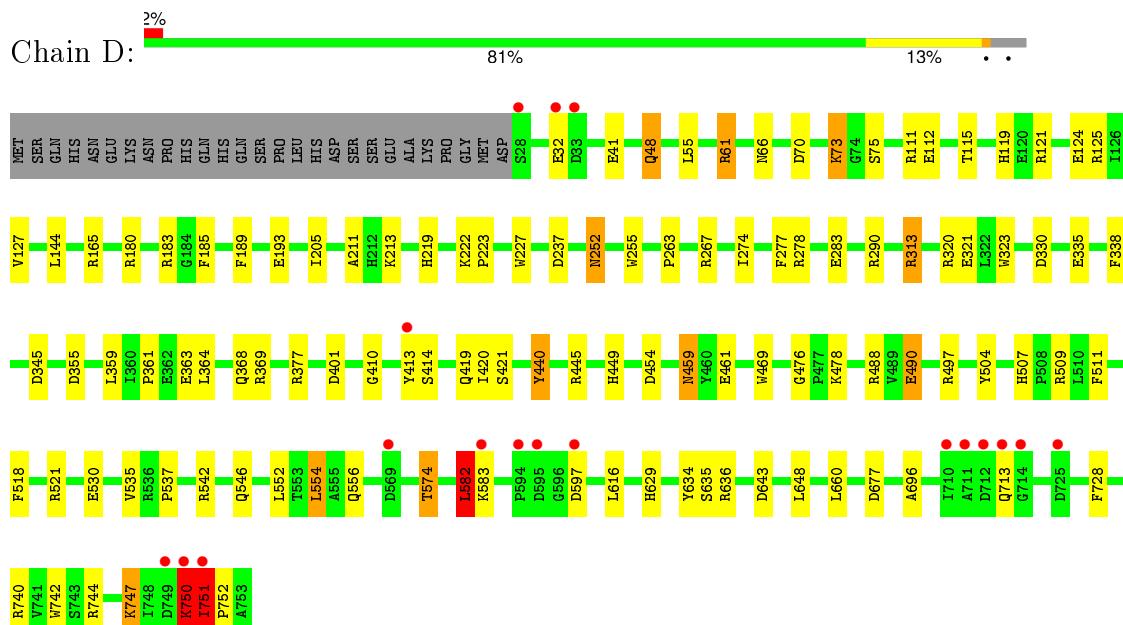
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.56Å 133.33Å 122.16Å 90.00° 109.58° 90.00°	Depositor
Resolution (Å)	29.23 – 1.58 29.23 – 1.58	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.23-1.58) 98.8 (29.23-1.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.157 , 0.189 0.157 , 0.189	Depositor DCC
R_{free} test set	18949 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	11.8	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.4	EDS
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	0 of 376838 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	26162	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 4.08% 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

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	1.27	16/5906 (0.3%)	1.20	29/8030 (0.4%)
1	B	1.20	12/5906 (0.2%)	1.17	27/8030 (0.3%)
1	C	1.18	9/5906 (0.2%)	1.18	29/8030 (0.4%)
1	D	1.27	18/5906 (0.3%)	1.21	40/8030 (0.5%)
All	All	1.23	55/23624 (0.2%)	1.19	125/32120 (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	A	0	2
1	C	0	3
All	All	0	5

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	440	TYR	CE1-CZ	9.49	1.50	1.38
1	A	415	TYR	CG-CD2	8.14	1.49	1.39
1	D	440	TYR	CE1-CZ	7.82	1.48	1.38
1	A	440	TYR	CE1-CZ	7.79	1.48	1.38
1	D	335	GLU	CD-OE2	7.52	1.33	1.25
1	D	377	ARG	CZ-NH1	7.12	1.42	1.33
1	C	497	ARG	CZ-NH2	6.94	1.42	1.33
1	A	469	TRP	CD2-CE2	6.85	1.49	1.41
1	A	240	TRP	CD2-CE2	6.72	1.49	1.41
1	B	471	ARG	CZ-NH2	6.70	1.41	1.33
1	C	193	GLU	CD-OE2	6.68	1.32	1.25
1	A	321	GLU	CD-OE1	6.66	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	323	TRP	CD2-CE2	6.50	1.49	1.41
1	D	255	TRP	CD2-CE2	6.48	1.49	1.41
1	A	498	SER	CB-OG	6.42	1.50	1.42
1	A	112	GLU	CD-OE2	6.37	1.32	1.25
1	D	323	TRP	CD2-CE2	6.34	1.49	1.41
1	B	497	ARG	CZ-NH2	6.33	1.41	1.33
1	D	112	GLU	CD-OE2	6.20	1.32	1.25
1	A	338	PHE	CG-CD2	6.10	1.47	1.38
1	C	440	TYR	CE1-CZ	6.06	1.46	1.38
1	C	742	TRP	CD2-CE2	5.87	1.48	1.41
1	A	377	ARG	CZ-NH1	5.87	1.40	1.33
1	D	70	ASP	CB-CG	5.86	1.64	1.51
1	C	293	TRP	CG-CD1	5.78	1.44	1.36
1	D	338	PHE	CG-CD2	5.75	1.47	1.38
1	B	320	ARG	CZ-NH2	5.74	1.40	1.33
1	A	344	GLU	CD-OE1	5.72	1.31	1.25
1	C	740	ARG	CZ-NH2	5.69	1.40	1.33
1	B	293	TRP	CG-CD1	5.68	1.44	1.36
1	D	469	TRP	CD2-CE2	5.65	1.48	1.41
1	B	346	GLU	CD-OE1	5.55	1.31	1.25
1	D	530	GLU	CD-OE1	5.51	1.31	1.25
1	D	277	PHE	CG-CD2	5.45	1.47	1.38
1	D	518	PHE	CG-CD2	5.45	1.47	1.38
1	B	185	PHE	CE1-CZ	5.44	1.47	1.37
1	A	512	TRP	CD2-CE2	5.35	1.47	1.41
1	B	224	GLU	CD-OE2	5.31	1.31	1.25
1	A	387	GLU	CG-CD	5.29	1.59	1.51
1	A	293	TRP	CD2-CE2	5.29	1.47	1.41
1	D	320	ARG	CZ-NH1	5.25	1.39	1.33
1	A	290	ARG	CZ-NH2	5.24	1.39	1.33
1	D	193	GLU	CD-OE1	5.23	1.31	1.25
1	B	70	ASP	CB-CG	5.23	1.62	1.51
1	D	124	GLU	CD-OE1	5.21	1.31	1.25
1	B	293	TRP	CD2-CE2	5.13	1.47	1.41
1	D	542	ARG	CZ-NH2	5.11	1.39	1.33
1	C	469	TRP	CD2-CE2	5.11	1.47	1.41
1	A	502	GLY	N-CA	5.09	1.53	1.46
1	A	324	GLU	CD-OE2	5.08	1.31	1.25
1	C	181	ASP	CB-CG	5.05	1.62	1.51
1	D	742	TRP	CD2-CE2	5.04	1.47	1.41
1	B	304	TRP	CD2-CE2	5.04	1.47	1.41
1	C	472	GLU	CD-OE2	5.02	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	414	SER	C-O	5.00	1.32	1.23

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	ARG	NE-CZ-NH2	-13.22	113.69	120.30
1	D	61	ARG	NE-CZ-NH2	10.34	125.47	120.30
1	C	471	ARG	NE-CZ-NH2	-10.03	115.28	120.30
1	D	377	ARG	NE-CZ-NH2	-9.57	115.52	120.30
1	C	165	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	A	740	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	C	422	ARG	NE-CZ-NH1	-9.22	115.69	120.30
1	C	278	ARG	NE-CZ-NH1	-9.06	115.77	120.30
1	D	401	ASP	CB-CG-OD2	8.72	126.15	118.30
1	D	313	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	B	370	VAL	CG1-CB-CG2	8.24	124.09	110.90
1	A	130	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	C	37	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	A	377	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	B	479	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	C	159	ILE	CB-CG1-CD1	-7.88	91.85	113.90
1	B	320	ARG	NE-CZ-NH1	-7.80	116.40	120.30
1	D	740	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	D	582	LEU	CB-CG-CD1	7.59	123.91	111.00
1	D	401	ASP	CB-CG-OD1	-7.51	111.54	118.30
1	C	660	LEU	CB-CG-CD2	7.31	123.42	111.00
1	C	497	ARG	NE-CZ-NH1	-7.24	116.68	120.30
1	D	165	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	B	521	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	C	72	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	A	90	ASP	CB-CG-OD1	6.88	124.49	118.30
1	C	509	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	A	540	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	D	320	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	D	180	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	D	183	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	C	185	PHE	CB-CG-CD2	-6.61	116.17	120.80
1	D	278	ARG	NE-CZ-NH1	-6.55	117.03	120.30
1	A	552	LEU	CB-CG-CD1	6.49	122.04	111.00
1	D	643	ASP	CB-CG-OD1	6.48	124.14	118.30
1	D	497	ARG	NE-CZ-NH2	6.45	123.52	120.30
1	A	740	ARG	NE-CZ-NH2	-6.42	117.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	165	ARG	NE-CZ-NH1	-6.40	117.10	120.30
1	A	479	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	D	740	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	B	571	LEU	CA-CB-CG	6.27	129.72	115.30
1	B	495	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	B	595	ASP	CB-CG-OD1	6.16	123.84	118.30
1	D	183	ARG	NE-CZ-NH1	-6.13	117.24	120.30
1	D	213	LYS	CD-CE-NZ	-6.12	97.62	111.70
1	A	185	PHE	CB-CG-CD2	-6.10	116.53	120.80
1	D	290	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	554	LEU	CB-CG-CD2	-6.03	100.74	111.00
1	A	422	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	A	313	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	D	377	ARG	NH1-CZ-NH2	5.98	125.98	119.40
1	C	181	ASP	CB-CG-OD2	5.96	123.67	118.30
1	C	725	ASP	N-CA-C	5.96	127.09	111.00
1	A	422	ARG	NE-CZ-NH1	-5.93	117.34	120.30
1	A	663	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	633	LEU	CB-CG-CD2	-5.89	100.99	111.00
1	C	446	ASP	CB-CG-OD1	5.88	123.60	118.30
1	C	254	MET	CG-SD-CE	-5.88	90.79	100.20
1	D	497	ARG	NE-CZ-NH1	-5.87	117.36	120.30
1	B	497	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	D	121	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	D	144	LEU	CB-CG-CD1	-5.79	101.16	111.00
1	C	733	LEU	CB-CG-CD1	5.78	120.82	111.00
1	A	421	SER	N-CA-CB	5.77	119.16	110.50
1	D	189	PHE	CB-CG-CD2	-5.75	116.78	120.80
1	B	259	ASP	CB-CG-OD1	-5.73	113.14	118.30
1	B	601	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	C	660	LEU	CB-CG-CD1	5.67	120.65	111.00
1	B	582	LEU	CB-CG-CD1	-5.66	101.37	111.00
1	D	636	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	501	PHE	CB-CG-CD2	-5.65	116.85	120.80
1	B	440	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	D	445	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	C	87	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	D	509	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	595	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	B	309	LYS	CD-CE-NZ	-5.58	98.88	111.70
1	A	55	LEU	CB-CG-CD2	5.57	120.47	111.00
1	B	509	ARG	NE-CZ-NH2	5.56	123.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	733	LEU	CA-CB-CG	5.55	128.06	115.30
1	D	345	ASP	CB-CG-OD1	5.55	123.29	118.30
1	A	377	ARG	NH1-CZ-NH2	5.53	125.48	119.40
1	A	210	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	338	PHE	CB-CG-CD1	-5.50	116.95	120.80
1	C	571	LEU	CA-CB-CG	5.49	127.93	115.30
1	A	260	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	495	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	D	355	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	421	SER	N-CA-CB	5.44	118.67	110.50
1	C	401	ASP	CB-CG-OD2	5.44	123.19	118.30
1	A	626	LYS	CD-CE-NZ	-5.43	99.20	111.70
1	C	740	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	C	320	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	D	61	ARG	NE-CZ-NH1	-5.43	117.59	120.30
1	B	87	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	D	368	GLN	CA-CB-CG	-5.42	101.48	113.40
1	B	33	ASP	CB-CG-OD1	5.42	123.17	118.30
1	B	130	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	C	445	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	D	554	LEU	CB-CG-CD1	5.30	120.01	111.00
1	B	195	ILE	CA-CB-CG1	-5.29	100.95	111.00
1	D	419	GLN	CB-CA-C	5.28	120.95	110.40
1	D	511	PHE	CB-CG-CD2	-5.27	117.11	120.80
1	D	55	LEU	CB-CG-CD1	-5.26	102.06	111.00
1	A	595	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	397	VAL	CG1-CB-CG2	-5.24	102.52	110.90
1	B	562	LEU	CB-CG-CD1	5.24	119.90	111.00
1	B	542	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	D	189	PHE	CB-CG-CD1	5.20	124.44	120.80
1	C	615	ASP	CB-CG-OD2	5.18	122.97	118.30
1	D	377	ARG	CA-CB-CG	-5.16	102.05	113.40
1	A	582	LEU	CB-CG-CD1	-5.15	102.24	111.00
1	B	401	ASP	CB-CG-OD1	-5.15	113.67	118.30
1	C	501	PHE	CB-CG-CD2	-5.14	117.20	120.80
1	D	421	SER	N-CA-CB	5.12	118.19	110.50
1	A	352	ASP	CB-CG-OD1	5.12	122.91	118.30
1	C	449[A]	HIS	CB-CA-C	5.11	120.62	110.40
1	C	449[B]	HIS	CB-CA-C	5.11	120.62	110.40
1	A	177	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	D	125	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	D	504	TYR	CG-CD2-CE2	-5.09	117.23	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	445	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	D	454	ASP	CB-CG-OD1	-5.06	113.75	118.30
1	B	479	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	C	159	ILE	CA-CB-CG2	5.02	120.94	110.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	ARG	Sidechain
1	A	708	ILE	Peptide
1	C	121	ARG	Sidechain
1	C	724	ALA	Peptide
1	C	725	ASP	Peptide

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	5745	0	5576	40	0
1	B	5746	0	5581	54	0
1	C	5745	0	5577	55	0
1	D	5746	0	5581	61	0
2	A	43	0	30	1	0
2	B	43	0	30	3	0
2	C	43	0	30	2	0
2	D	43	0	30	1	0
3	A	815	0	0	6	2
3	B	673	0	0	14	1
3	C	737	0	0	18	0
3	D	783	0	0	17	1
All	All	26162	0	22435	193	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 4.

All (193) 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:449[B]:HIS:CE1	3:D:2501:HOH:O	1.80	1.29
1:B:521:ARG:HD3	3:B:3047:HOH:O	1.41	1.14
1:D:546:GLN:HG3	3:D:2742:HOH:O	1.53	1.05
1:D:267:ARG:HG3	3:D:1920:HOH:O	1.56	1.02
1:C:267:ARG:HG3	3:C:2916:HOH:O	1.59	1.02
1:A:413:TYR:HE2	1:B:413:TYR:CE2	1.80	0.98
1:A:413:TYR:CE2	1:B:413:TYR:HE2	1.83	0.96
1:B:267:ARG:HG3	3:B:1921:HOH:O	1.64	0.94
3:B:2705:HOH:O	1:D:73:LYS:HE3	1.68	0.93
1:C:413:TYR:CE2	1:D:413:TYR:HE2	1.87	0.92
1:C:612:ARG:HG3	1:C:612:ARG:HH11	1.34	0.92
1:A:413:TYR:CE2	1:B:413:TYR:CE2	2.59	0.90
1:A:29:LEU:HB2	3:C:2405:HOH:O	1.71	0.89
1:C:413:TYR:CE2	1:D:413:TYR:CE2	2.63	0.86
1:C:636:ARG:NH1	3:C:2717:HOH:O	2.07	0.85
1:A:111:ARG:O	1:A:115:THR:HG23	1.80	0.81
1:B:583:LYS:NZ	1:B:583:LYS:H	1.76	0.81
1:C:621:LYS:HE3	3:C:3116:HOH:O	1.80	0.81
1:A:541:GLU:OE2	3:A:2550:HOH:O	2.01	0.78
1:D:490:GLU:OE1	3:D:2308:HOH:O	2.02	0.77
1:C:612:ARG:HH11	1:C:612:ARG:CG	1.97	0.76
1:B:583:LYS:HZ2	1:B:583:LYS:H	1.30	0.74
1:D:574:THR:HG22	3:D:1614:HOH:O	1.86	0.74
1:C:413:TYR:HE2	1:D:413:TYR:CE2	2.04	0.73
1:B:533:LYS:HE2	3:B:3100:HOH:O	1.90	0.71
1:A:449[A]:HIS:CD2	1:C:449[A]:HIS:CD2	2.79	0.71
1:A:710:ILE:HG12	1:A:715:GLU:OE1	1.91	0.71
1:D:111:ARG:O	1:D:115:THR:HG23	1.91	0.70
1:A:28:SER:OG	1:A:28:SER:O	2.09	0.70
1:C:486:GLN:OE1	3:C:2892:HOH:O	2.09	0.69
1:B:449[B]:HIS:CD2	1:D:449[B]:HIS:CD2	2.81	0.68
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.77	0.67
1:D:750:LYS:HD2	1:D:751:ILE:H	1.61	0.66
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.78	0.66
1:A:479:ARG:NH2	3:A:2607:HOH:O	2.27	0.65
1:D:449[B]:HIS:NE2	3:D:2501:HOH:O	2.09	0.65
1:A:369:ARG:NH2	3:A:2403:HOH:O	2.03	0.65
1:C:552:LEU:HD11	1:C:571:LEU:HD12	1.78	0.64
1:C:344:GLU:OE1	3:C:2887:HOH:O	2.15	0.64
1:B:521:ARG:NH2	1:B:745:ILE:HD13	2.13	0.64
1:C:748:ILE:O	1:C:751:ILE:HG22	2.00	0.62
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:TYR:HE2	1:D:413:TYR:CD2	2.18	0.62
1:B:111:ARG:O	1:B:115:THR:HG23	2.00	0.62
1:C:610:GLU:O	1:C:610:GLU:HG3	2.00	0.62
1:A:29:LEU:HD12	1:A:29:LEU:H	1.65	0.61
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.83	0.61
1:D:583:LYS:HB2	1:D:583:LYS:NZ	2.16	0.61
1:A:36:HIS:CD2	1:A:36:HIS:H	2.18	0.60
1:B:350:ASP:HB2	3:B:1940:HOH:O	2.00	0.59
1:D:546:GLN:CG	3:D:2742:HOH:O	2.26	0.59
1:D:750:LYS:CD	1:D:751:ILE:H	2.16	0.59
1:D:750:LYS:HD2	1:D:751:ILE:N	2.18	0.58
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.85	0.58
1:C:521:ARG:HG2	3:C:2920:HOH:O	2.04	0.58
1:D:597:ASP:OD2	3:D:2709:HOH:O	2.17	0.57
1:A:750:LYS:HE2	1:D:677:ASP:HB3	1.86	0.57
1:C:111:ARG:O	1:C:115:THR:HG23	2.05	0.56
1:D:546:GLN:CD	3:D:2742:HOH:O	2.42	0.56
1:B:281:ASN:OD1	1:B:283:GLU:HG3	2.05	0.56
1:B:629:HIS:HD2	3:B:1045:HOH:O	1.88	0.56
1:B:552:LEU:HD22	1:B:556:GLN:HG3	1.87	0.56
1:D:61:ARG:HH11	1:D:66:ASN:HA	1.70	0.56
1:A:603:VAL:HG11	1:A:666:ILE:HD12	1.88	0.56
1:B:521:ARG:HH21	1:B:745:ILE:HD13	1.71	0.55
1:D:363:GLU:HB2	1:D:582:LEU:HD21	1.88	0.55
1:C:115:THR:O	1:C:119:HIS:HD2	1.89	0.54
1:D:478:LYS:HD2	3:D:2968:HOH:O	2.06	0.54
1:C:274:ILE:HD12	2:C:760:HEM:HMB1	1.89	0.54
1:C:629:HIS:HD2	3:C:1129:HOH:O	1.91	0.53
1:D:629:HIS:HD2	3:D:1554:HOH:O	1.91	0.53
1:B:420:ILE:HG21	1:D:119:HIS:CE1	2.42	0.53
1:C:503:GLU:OE1	3:C:1142:HOH:O	2.18	0.53
1:D:750:LYS:O	1:D:751:ILE:O	2.26	0.52
1:B:449[A]:HIS:CG	1:D:449[A]:HIS:CG	2.42	0.52
1:C:612:ARG:NH1	1:C:612:ARG:CG	2.65	0.52
1:C:359:LEU:H	1:C:507:HIS:HD2	1.57	0.52
1:C:488:ARG:HD2	3:C:2379:HOH:O	2.10	0.51
1:C:283:GLU:OE1	1:C:283:GLU:N	2.43	0.51
1:C:556:GLN:HG2	1:C:566:LEU:HD12	1.93	0.51
1:B:359:LEU:H	1:B:507:HIS:HD2	1.59	0.51
1:A:29:LEU:CB	3:C:2405:HOH:O	2.45	0.51
1:C:596:GLY:HA3	1:C:737:ALA:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:760:HEM:HMC2	2:C:760:HEM:HBC2	1.94	0.50
1:A:448:MET:O	1:A:449[B]:HIS:HB2	2.12	0.50
1:C:578:ASP:HB2	1:C:582:LEU:O	2.12	0.50
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.94	0.49
1:D:521:ARG:HD2	3:D:2912:HOH:O	2.11	0.49
1:C:610:GLU:OE1	1:C:643:ASP:HA	2.12	0.49
1:C:478:LYS:HG3	3:C:3207:HOH:O	2.12	0.49
1:A:751:ILE:O	1:A:751:ILE:HD12	2.12	0.49
1:C:745:ILE:HD13	3:C:2920:HOH:O	2.11	0.49
1:B:521:ARG:NH2	1:B:745:ILE:HG21	2.28	0.49
1:C:195:ILE:HD11	1:C:436:PRO:HA	1.94	0.49
1:D:321:GLU:HG3	3:D:2151:HOH:O	2.11	0.48
1:A:578:ASP:OD1	1:A:583:LYS:NZ	2.43	0.48
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.43	0.48
1:D:61:ARG:NH1	1:D:66:ASN:HA	2.28	0.48
1:D:283:GLU:OE2	3:D:2496:HOH:O	2.20	0.48
1:B:571:LEU:HD22	3:B:2758:HOH:O	2.14	0.48
1:A:449[B]:HIS:CG	1:C:449[B]:HIS:CG	2.54	0.47
1:B:369:ARG:HB2	1:B:369:ARG:HE	1.47	0.47
1:C:584:LYS:NZ	3:C:1767:HOH:O	2.46	0.47
1:C:634:TYR:O	1:C:653:THR:HA	2.14	0.47
1:C:612:ARG:HB2	1:C:612:ARG:NH1	2.29	0.47
1:A:682:ASN:HB3	1:A:707:THR:HG21	1.97	0.47
3:B:2705:HOH:O	1:D:73:LYS:CD	2.63	0.47
1:C:552:LEU:HD13	1:C:556:GLN:HG3	1.97	0.47
1:A:115:THR:O	1:A:119:HIS:HD2	1.97	0.46
1:C:713:GLN:HG2	3:C:2154:HOH:O	2.15	0.46
1:C:686:MET:HB3	1:C:751:ILE:HD11	1.96	0.46
1:B:36:HIS:HD1	1:B:36:HIS:H	1.63	0.46
1:A:603:VAL:HG11	1:A:666:ILE:CD1	2.45	0.46
1:A:461:GLU:OE1	1:C:91:ASP:OD1	2.33	0.46
1:C:621:LYS:HG2	3:C:3116:HOH:O	2.16	0.46
1:A:128:HIS:CE1	1:A:169:VAL:HG22	2.50	0.46
1:C:128:HIS:HA	1:C:168:THR:O	2.15	0.46
1:B:634:TYR:O	1:B:653:THR:HA	2.16	0.46
1:B:646:THR:HA	3:B:1822:HOH:O	2.16	0.46
1:C:583:LYS:HE2	1:C:583:LYS:HB2	1.60	0.46
2:B:760:HEM:CMC	2:B:760:HEM:HBC2	2.45	0.45
1:B:91:ASP:OD1	1:D:461:GLU:OE1	2.34	0.45
1:D:115:THR:O	1:D:119:HIS:HD2	2.00	0.45
1:B:115:THR:O	1:B:119:HIS:HD2	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:LEU:HD23	3:B:812:HOH:O	2.16	0.45
1:D:583:LYS:HB2	1:D:583:LYS:HZ2	1.82	0.45
1:A:607:LEU:HD11	1:A:632:LEU:HB3	1.99	0.45
1:A:459:ASN:HD22	1:A:459:ASN:H	1.65	0.44
1:B:566:LEU:HD22	1:B:566:LEU:N	2.32	0.44
1:B:128:HIS:HA	1:B:168:THR:O	2.18	0.44
1:B:372:LYS:NZ	3:B:2242:HOH:O	2.41	0.44
1:D:222:LYS:HB3	1:D:223:PRO:CD	2.48	0.44
1:B:29:LEU:N	3:B:2571:HOH:O	2.24	0.44
1:D:252:ASN:HD22	1:D:252:ASN:HA	1.63	0.44
1:D:313:ARG:HG3	1:D:660:LEU:HD12	1.99	0.44
1:D:751:ILE:HA	1:D:752:PRO:HD3	1.75	0.43
1:C:128:HIS:CE1	1:C:169:VAL:HG22	2.53	0.43
1:B:344:GLU:H	1:B:344:GLU:CD	2.22	0.43
1:C:727:SER:HA	3:C:2714:HOH:O	2.17	0.43
1:D:359:LEU:H	1:D:507:HIS:HD2	1.67	0.43
2:B:760:HEM:HMC1	2:B:760:HEM:HBC2	1.99	0.43
1:B:359:LEU:H	1:B:507:HIS:CD2	2.35	0.43
1:C:105:LEU:HD12	1:C:105:LEU:HA	1.76	0.43
1:A:274:ILE:HD12	2:A:760:HEM:HMB1	1.99	0.43
1:B:267:ARG:HD2	3:B:1023:HOH:O	2.18	0.43
1:D:583:LYS:HB2	1:D:583:LYS:HZ3	1.83	0.43
1:A:440:TYR:HD1	3:A:1918:HOH:O	2.01	0.43
1:D:556:GLN:NE2	3:D:2773:HOH:O	2.51	0.43
1:A:610:GLU:CG	3:A:2551:HOH:O	2.67	0.43
1:C:38:PRO:HG2	1:C:51:ALA:HB2	2.01	0.42
1:D:744:ARG:HA	1:D:747:LYS:HD3	2.01	0.42
1:B:119:HIS:CE1	1:D:420:ILE:HG21	2.54	0.42
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.55	0.42
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.35	0.42
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.50	0.42
1:B:459:ASN:H	1:B:459:ASN:HD22	1.67	0.42
1:A:703:LYS:HA	1:A:703:LYS:HD2	1.96	0.41
1:A:214:PHE:HB3	1:A:215:PRO:HD3	2.01	0.41
1:B:583:LYS:HZ3	1:B:583:LYS:H	1.60	0.41
1:B:128:HIS:CE1	1:B:169:VAL:HG22	2.55	0.41
1:B:335:GLU:OE1	1:B:369:ARG:HG2	2.20	0.41
1:B:289:VAL:HA	1:B:339:GLN:O	2.20	0.41
1:B:717:GLY:HA3	1:B:741:VAL:HG11	2.02	0.41
2:B:760:HEM:CMB	2:B:760:HEM:HBB2	2.50	0.41
1:C:207:PHE:O	1:C:249:THR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ALA:O	1:C:101:GLY:HA3	2.20	0.41
1:B:105:LEU:HD11	1:D:413:TYR:HB2	2.02	0.41
1:D:488:ARG:NE	3:D:2698:HOH:O	2.01	0.41
1:A:251:HIS:CE1	1:A:507:HIS:HB3	2.55	0.41
1:A:610:GLU:HG2	3:A:2551:HOH:O	2.21	0.41
1:D:274:ILE:HD12	2:D:760:HEM:HMB1	2.01	0.41
1:A:392:HIS:CE1	1:A:415:TYR:H	2.39	0.41
1:A:115:THR:HG22	1:D:413:TYR:OH	2.21	0.41
1:D:459:ASN:HD22	1:D:459:ASN:H	1.68	0.41
1:D:48:GLN:HB3	1:D:48:GLN:HE21	1.65	0.41
1:B:393:PRO:HD2	1:B:415:TYR:CG	2.56	0.41
1:A:626:LYS:HA	1:A:626:LYS:HD3	1.88	0.41
1:B:417:ASP:O	1:B:420:ILE:HB	2.21	0.41
1:C:556:GLN:HG2	1:C:566:LEU:CD1	2.51	0.41
1:C:459:ASN:H	1:C:459:ASN:HD22	1.68	0.41
1:D:696:ALA:HB1	1:D:728:PHE:CZ	2.56	0.41
1:C:144:LEU:HD11	1:C:370:VAL:HG13	2.02	0.41
3:B:2705:HOH:O	1:D:73:LYS:CE	2.44	0.41
1:D:634:TYR:CG	1:D:635:SER:N	2.88	0.41
1:D:361:PRO:HD2	1:D:364:LEU:HD12	2.02	0.41
1:A:413:TYR:CD2	1:B:413:TYR:HE2	2.34	0.40
1:B:533:LYS:CD	3:C:2623:HOH:O	2.69	0.40
1:D:222:LYS:HB3	1:D:223:PRO:HD2	2.02	0.40
1:D:476:GLY:HA3	3:D:1112:HOH:O	2.20	0.40
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.36	0.40
1:B:745:ILE:O	1:B:748:ILE:HG12	2.21	0.40
1:B:372:LYS:HB3	1:B:372:LYS:HE3	1.78	0.40
1:D:535:VAL:O	1:D:537:PRO:HD3	2.20	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)
3:A:2627:HOH:O	3:B:2418:HOH:O[2_545]	2.14	0.06
3:A:2402:HOH:O	3:D:2299:HOH:O[1_455]	2.14	0.06

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	725/753 (96%)	707 (98%)	16 (2%)	2 (0%)	46	22
1	B	725/753 (96%)	703 (97%)	20 (3%)	2 (0%)	46	22
1	C	725/753 (96%)	710 (98%)	14 (2%)	1 (0%)	56	29
1	D	725/753 (96%)	707 (98%)	15 (2%)	3 (0%)	39	16
All	All	2900/3012 (96%)	2827 (98%)	65 (2%)	8 (0%)	46	22

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	711	ALA
1	B	725	ASP
1	D	751	ILE
1	B	75	SER
1	D	75	SER
1	D	750	LYS
1	A	75	SER
1	C	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	612/636 (96%)	592 (97%)	20 (3%)	45	16
1	B	612/636 (96%)	586 (96%)	26 (4%)	36	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	612/636 (96%)	579 (95%)	33 (5%)	27	5
1	D	612/636 (96%)	587 (96%)	25 (4%)	37	10
All	All	2448/2544 (96%)	2344 (96%)	104 (4%)	35	9

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	29	LEU
1	A	32	GLU
1	A	37	ARG
1	A	73	LYS
1	A	185	PHE
1	A	205	ILE
1	A	227	TRP
1	A	252	ASN
1	A	369	ARG
1	A	420	ILE
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	710	ILE
1	A	712	ASP
1	A	713	GLN
1	A	732	LEU
1	A	750	LYS
1	B	185	PHE
1	B	191	THR
1	B	195	ILE
1	B	205	ILE
1	B	227	TRP
1	B	237	ASP
1	B	252	ASN
1	B	370	VAL
1	B	432	PRO
1	B	440	TYR
1	B	459	ASN
1	B	552	LEU
1	B	562	LEU
1	B	568	ASP

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Mol	Chain	Res	Type
1	B	571	LEU
1	B	583	LYS
1	B	595	ASP
1	B	610	GLU
1	B	612	ARG
1	B	616	LEU
1	B	633	LEU
1	B	703	LYS
1	B	707	THR
1	B	709	LYS
1	B	749	ASP
1	B	751	ILE
1	C	37	ARG
1	C	61	ARG
1	C	159	ILE
1	C	185	PHE
1	C	191	THR
1	C	198	LEU
1	C	205	ILE
1	C	227	TRP
1	C	237	ASP
1	C	252	ASN
1	C	369	ARG
1	C	377	ARG
1	C	440	TYR
1	C	459	ASN
1	C	478	LYS
1	C	488	ARG
1	C	521	ARG
1	C	552	LEU
1	C	568	ASP
1	C	571	LEU
1	C	584	LYS
1	C	606	LEU
1	C	610	GLU
1	C	612	ARG
1	C	613	SER
1	C	616	LEU
1	C	633	LEU
1	C	648	LEU
1	C	660	LEU
1	C	685	LEU

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Mol	Chain	Res	Type
1	C	709	LYS
1	C	733	LEU
1	C	750	LYS
1	D	32	GLU
1	D	41	GLU
1	D	48	GLN
1	D	73	LYS
1	D	127	VAL
1	D	185	PHE
1	D	205	ILE
1	D	227	TRP
1	D	237	ASP
1	D	252	ASN
1	D	263	PRO
1	D	369	ARG
1	D	440	TYR
1	D	459	ASN
1	D	490	GLU
1	D	552	LEU
1	D	554	LEU
1	D	574	THR
1	D	582	LEU
1	D	616	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 (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	252	ASN
1	A	459	ASN
1	A	515	GLN
1	A	713	GLN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	C	119	HIS

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Mol	Chain	Res	Type
1	C	252	ASN
1	C	368	GLN
1	C	459	ASN
1	C	486	GLN
1	C	507	HIS
1	C	572	ASN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	252	ASN
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)

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	30,50,50	2.90	10 (33%)	24,82,82	3.08	10 (41%)
2	HEM	B	760	1	30,50,50	2.52	13 (43%)	24,82,82	3.54	13 (54%)
2	HEM	C	760	1	30,50,50	3.25	12 (40%)	24,82,82	3.25	9 (37%)
2	HEM	D	760	1	30,50,50	2.66	10 (33%)	24,82,82	3.37	12 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	760	1	-	0/10/54/54	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 (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	760	HEM	C3B-C4B	-13.16	1.40	1.51
2	A	760	HEM	C3B-C4B	-7.50	1.45	1.51
2	D	760	HEM	C3B-C4B	-7.17	1.45	1.51
2	B	760	HEM	C3B-C4B	-6.92	1.45	1.51
2	A	760	HEM	C3D-C4D	-6.33	1.43	1.51
2	C	760	HEM	C2D-C3D	-4.13	1.42	1.54
2	B	760	HEM	C2D-C3D	-4.12	1.42	1.54
2	A	760	HEM	C2D-C3D	-3.87	1.42	1.54
2	D	760	HEM	C2D-C3D	-3.69	1.43	1.54
2	A	760	HEM	CMB-C2B	-3.58	1.44	1.53
2	D	760	HEM	C2D-C1D	-3.40	1.40	1.51
2	C	760	HEM	C3C-CAC	-3.40	1.45	1.51
2	B	760	HEM	C3D-C4D	-3.36	1.47	1.51
2	D	760	HEM	C2C-C1C	-3.28	1.46	1.52
2	B	760	HEM	C2C-C1C	-3.27	1.46	1.52
2	D	760	HEM	CAA-C2A	-3.10	1.46	1.52
2	A	760	HEM	C2C-C1C	-3.07	1.46	1.52
2	B	760	HEM	C2D-C1D	-2.93	1.42	1.51
2	D	760	HEM	C3D-C4D	-2.73	1.48	1.51
2	B	760	HEM	C3C-CAC	-2.50	1.46	1.51
2	C	760	HEM	C3D-C4D	-2.31	1.48	1.51
2	C	760	HEM	CMB-C2B	-2.26	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	760	HEM	C2C-C1C	-2.23	1.48	1.52
2	D	760	HEM	CMD-C2D	-2.19	1.48	1.53
2	B	760	HEM	CAA-C2A	-2.02	1.48	1.52
2	A	760	HEM	C2D-C1D	-2.02	1.45	1.51
2	B	760	HEM	FE-NB	2.03	2.08	1.97
2	C	760	HEM	C4A-CHB	2.06	1.45	1.39
2	B	760	HEM	FE-NC	2.21	2.04	1.95
2	D	760	HEM	CHD-C1D	2.29	1.45	1.38
2	B	760	HEM	CHD-C1D	2.37	1.45	1.38
2	C	760	HEM	C2A-C3A	2.40	1.44	1.37
2	B	760	HEM	CHD-C4C	2.56	1.42	1.36
2	B	760	HEM	CHC-C4B	2.60	1.46	1.38
2	C	760	HEM	CHC-C4B	2.64	1.46	1.38
2	A	760	HEM	C2A-C3A	2.64	1.45	1.37
2	A	760	HEM	CHD-C4C	2.86	1.43	1.36
2	C	760	HEM	CHC-C1C	2.89	1.43	1.36
2	D	760	HEM	C4C-NC	3.02	1.39	1.36
2	A	760	HEM	CHD-C1D	3.06	1.47	1.38
2	C	760	HEM	C4C-NC	3.28	1.40	1.36
2	B	760	HEM	C1C-NC	6.30	1.43	1.36
2	C	760	HEM	C1C-NC	6.35	1.43	1.36
2	D	760	HEM	C1C-NC	8.11	1.46	1.36
2	A	760	HEM	C1C-NC	8.14	1.46	1.36

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	760	HEM	C3C-CAC-CBC	-6.49	114.50	124.46
2	D	760	HEM	CBD-CAD-C3D	-6.40	94.94	113.55
2	C	760	HEM	CBD-CAD-C3D	-6.20	95.51	113.55
2	A	760	HEM	CBD-CAD-C3D	-5.78	96.72	113.55
2	B	760	HEM	CBD-CAD-C3D	-5.56	97.38	113.55
2	D	760	HEM	C3C-CAC-CBC	-5.35	116.25	124.46
2	A	760	HEM	CAA-CBA-CGA	-5.19	103.23	112.75
2	D	760	HEM	CAA-CBA-CGA	-4.98	103.62	112.75
2	C	760	HEM	C3B-CAB-CBB	-4.97	116.83	124.46
2	A	760	HEM	C3C-CAC-CBC	-4.93	116.89	124.46
2	C	760	HEM	CAA-CBA-CGA	-4.82	103.92	112.75
2	B	760	HEM	CAA-CBA-CGA	-4.45	104.60	112.75
2	D	760	HEM	C3B-CAB-CBB	-4.44	117.65	124.46
2	A	760	HEM	CBA-CAA-C2A	-2.87	107.38	112.53
2	D	760	HEM	CMA-C3A-C4A	-2.78	123.76	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	760	HEM	C3B-CAB-CBB	-2.65	120.39	124.46
2	C	760	HEM	C3C-CAC-CBC	-2.47	120.67	124.46
2	D	760	HEM	CAA-C2A-C1A	-2.40	124.40	127.01
2	B	760	HEM	CBA-CAA-C2A	-2.24	108.52	112.53
2	A	760	HEM	C1D-CHD-C4C	-2.22	122.10	125.82
2	D	760	HEM	CMD-C2D-C3D	2.18	124.01	114.35
2	A	760	HEM	CMD-C2D-C3D	2.20	124.06	114.35
2	B	760	HEM	C3B-C4B-CHC	2.43	126.59	123.16
2	B	760	HEM	CMA-C3A-C2A	2.52	130.50	125.24
2	B	760	HEM	C2C-C1C-NC	2.63	114.64	110.21
2	D	760	HEM	C2C-C1C-NC	2.63	114.65	110.21
2	C	760	HEM	CMD-C2D-C3D	3.49	129.79	114.35
2	B	760	HEM	CMD-C2D-C3D	3.54	130.01	114.35
2	C	760	HEM	CAD-C3D-C4D	4.11	126.96	112.47
2	D	760	HEM	CMC-C2C-C3C	4.15	126.89	116.53
2	D	760	HEM	CAD-C3D-C4D	4.19	127.24	112.47
2	B	760	HEM	CAD-C3D-C4D	4.59	128.65	112.47
2	A	760	HEM	CAD-C3D-C2D	5.06	127.77	113.22
2	A	760	HEM	CMB-C2B-C3B	5.12	129.31	116.53
2	A	760	HEM	CAD-C3D-C4D	5.28	131.08	112.47
2	D	760	HEM	CAD-C3D-C2D	5.39	128.70	113.22
2	B	760	HEM	CAD-C3D-C2D	5.59	129.28	113.22
2	A	760	HEM	CMC-C2C-C3C	5.75	130.88	116.53
2	C	760	HEM	CAD-C3D-C2D	5.88	130.11	113.22
2	C	760	HEM	CMC-C2C-C3C	5.97	131.44	116.53
2	C	760	HEM	CMB-C2B-C3B	6.74	133.36	116.53
2	B	760	HEM	CMB-C2B-C3B	6.91	133.78	116.53
2	B	760	HEM	CMC-C2C-C3C	7.34	134.85	116.53
2	D	760	HEM	CMB-C2B-C3B	7.44	135.09	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	760	HEM	1	0
2	B	760	HEM	3	0
2	C	760	HEM	2	0
2	D	760	HEM	1	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(Å^2)	Q<0.9
1	A	726/753 (96%)	-0.17	20 (2%)	56	56	4, 11, 29, 84	1 (0%)
1	B	726/753 (96%)	-0.02	36 (4%)	32	31	5, 14, 39, 61	1 (0%)
1	C	726/753 (96%)	-0.10	28 (3%)	43	42	5, 14, 36, 56	1 (0%)
1	D	726/753 (96%)	-0.17	18 (2%)	61	61	4, 12, 29, 58	1 (0%)
All	All	2904/3012 (96%)	-0.12	102 (3%)	48	47	4, 13, 34, 84	4 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	711	ALA	9.2
1	A	710	ILE	7.4
1	B	726	GLY	6.8
1	B	32	GLU	6.0
1	B	673	ALA	4.7
1	D	28	SER	4.5
1	A	712	ASP	4.4
1	D	711	ALA	4.4
1	B	712	ASP	4.3
1	A	32	GLU	4.3
1	A	29	LEU	4.2
1	B	711	ALA	3.9
1	C	711	ALA	3.8
1	B	28	SER	3.7
1	B	647	VAL	3.7
1	A	28	SER	3.6
1	B	646	THR	3.6
1	B	710	ILE	3.6
1	C	750	LYS	3.6
1	D	750	LYS	3.2
1	B	617	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	726	GLY	3.2
1	B	713	GLN	3.2
1	C	677	ASP	3.2
1	B	645	GLY	3.2
1	A	713	GLN	3.2
1	D	712	ASP	3.2
1	A	726	GLY	3.1
1	B	727	SER	3.1
1	D	749	ASP	3.1
1	D	32	GLU	3.1
1	C	596	GLY	3.1
1	B	750	LYS	3.1
1	B	641	THR	3.0
1	C	645	GLY	3.0
1	C	594	PRO	3.0
1	D	713	GLN	3.0
1	B	34	GLY	2.9
1	D	710	ILE	2.9
1	D	751	ILE	2.9
1	C	568	ASP	2.9
1	A	725	ASP	2.8
1	A	709	LYS	2.8
1	B	709	LYS	2.8
1	C	712	ASP	2.8
1	A	749	ASP	2.7
1	B	572	ASN	2.7
1	B	552	LEU	2.7
1	B	583	LYS	2.7
1	D	413	TYR	2.7
1	B	677	ASP	2.7
1	A	596	GLY	2.7
1	C	749	ASP	2.6
1	C	413	TYR	2.6
1	B	722	ASP	2.6
1	C	625	ALA	2.6
1	C	646	THR	2.6
1	B	644	ASP	2.6
1	A	33	ASP	2.5
1	B	568	ASP	2.5
1	C	641	THR	2.5
1	B	569	ASP	2.5
1	B	610	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	725	ASP	2.5
1	C	751	ILE	2.5
1	B	347	PHE	2.5
1	C	643	ASP	2.5
1	C	714	GLY	2.4
1	A	39	ALA	2.4
1	A	751	ILE	2.4
1	C	571	LEU	2.4
1	C	673	ALA	2.3
1	B	612	ARG	2.3
1	B	609	ASP	2.3
1	C	595	ASP	2.3
1	D	33	ASP	2.2
1	D	569	ASP	2.2
1	A	594	PRO	2.2
1	D	714	GLY	2.2
1	C	706	ALA	2.2
1	A	568	ASP	2.2
1	B	749	ASP	2.2
1	B	33	ASP	2.2
1	D	725	ASP	2.2
1	A	35	SER	2.2
1	C	569	ASP	2.2
1	B	348	LYS	2.1
1	C	32	GLU	2.1
1	D	583	LYS	2.1
1	D	594	PRO	2.1
1	C	572	ASN	2.1
1	C	644	ASP	2.1
1	A	37	ARG	2.1
1	D	595	ASP	2.1
1	C	703	LYS	2.1
1	C	725	ASP	2.1
1	C	730	ASP	2.1
1	B	37	ARG	2.0
1	B	716	GLU	2.0
1	B	574	THR	2.0
1	D	597	ASP	2.0
1	A	283	GLU	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	HEM	A	760	43/43	0.99	0.07	-0.29	4,6,10,13	0
2	HEM	B	760	43/43	0.99	0.07	-0.34	6,8,12,15	0
2	HEM	C	760	43/43	0.99	0.06	-0.66	6,8,12,15	0
2	HEM	D	760	43/43	0.99	0.06	-0.70	5,7,11,16	0

6.5 Other polymers (i)

There are no such residues in this entry.