Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:23 PM GMT

PDB ID	:	4ENR
Title	:	Structure of E530I variant 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:

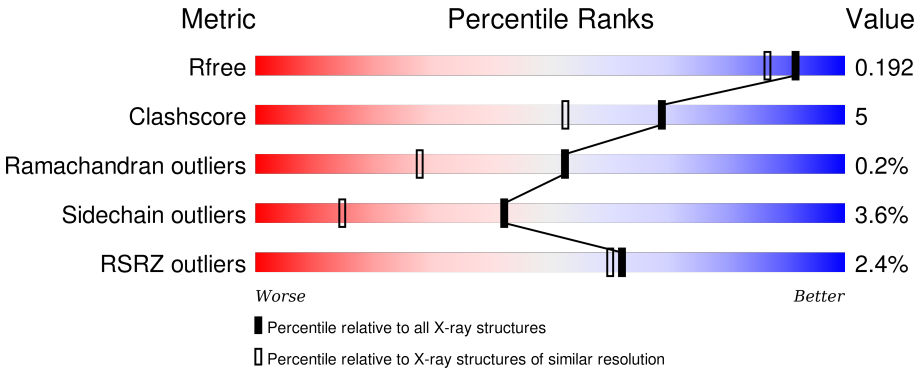
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	2% 85% 10%
1	B	753	4% 82% 12%
1	C	753	2% 84% 10%
1	D	753	2% 82% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26152 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.

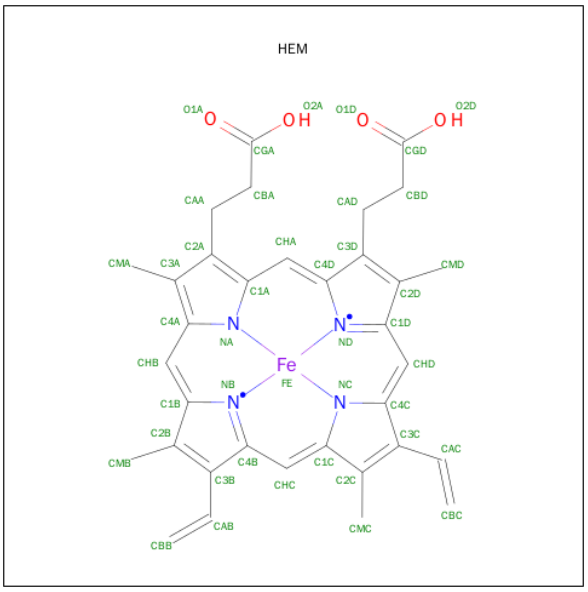
- Molecule 1 is a protein called Catalase HPII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	4	0
			5758	3658	1006	1082	12			
1	B	726	Total	C	N	O	S	0	4	0
			5761	3661	1007	1081	12			
1	C	726	Total	C	N	O	S	0	3	0
			5755	3656	1006	1081	12			
1	D	726	Total	C	N	O	S	0	4	0
			5758	3658	1006	1082	12			

There are 4 discrepancies between the modelled and reference sequences:

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

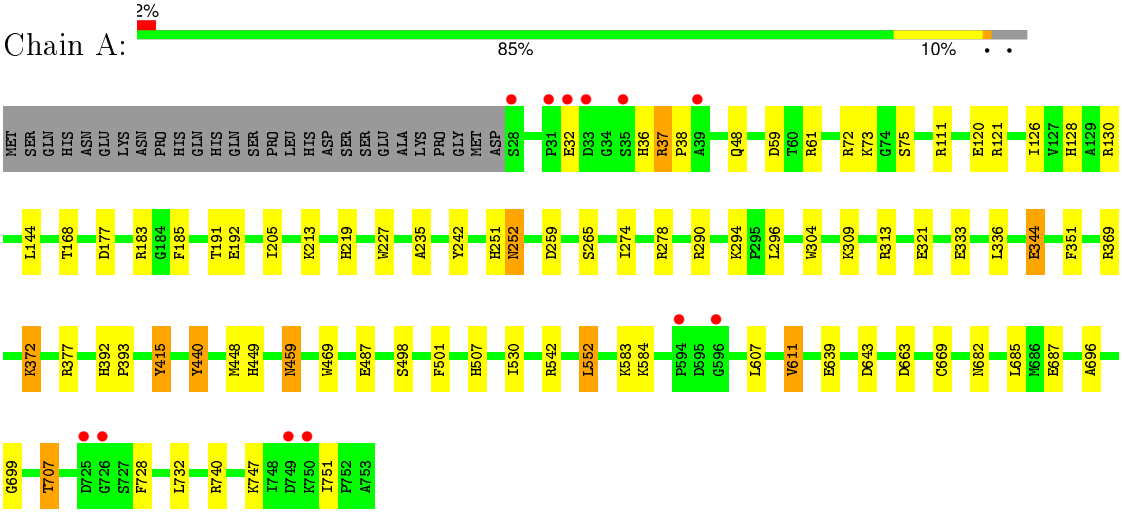
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	747	Total	O	0	0
			747	747		
3	B	690	Total	O	0	0
			690	690		
3	C	733	Total	O	0	0
			733	733		
3	D	778	Total	O	0	0
			778	778		

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.

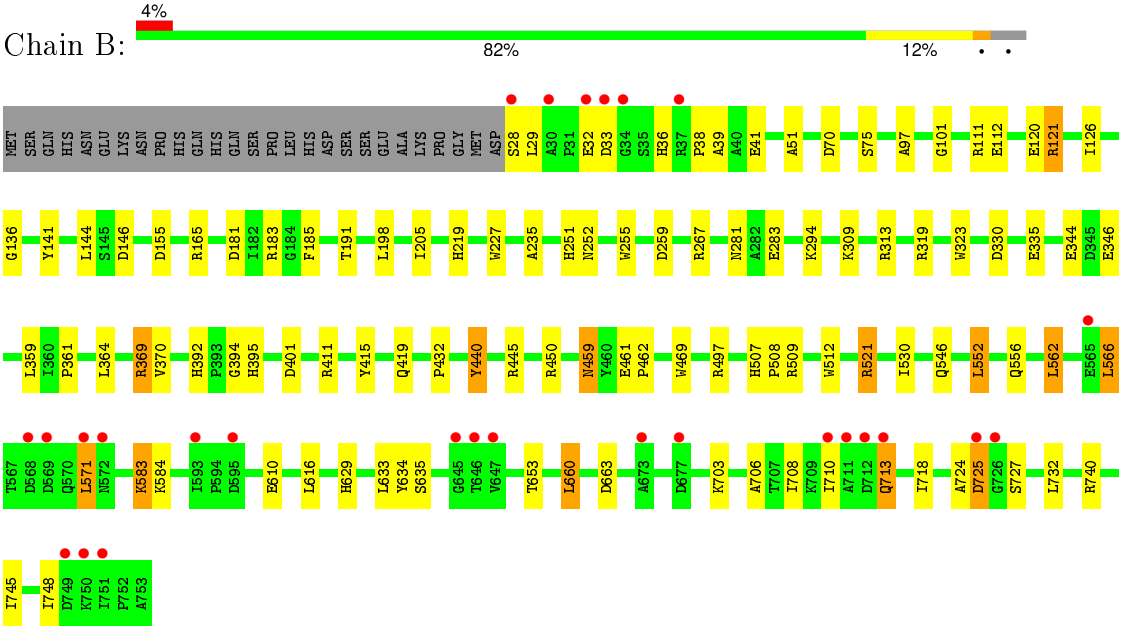
- Molecule 1: Catalase HPII

Chain A:



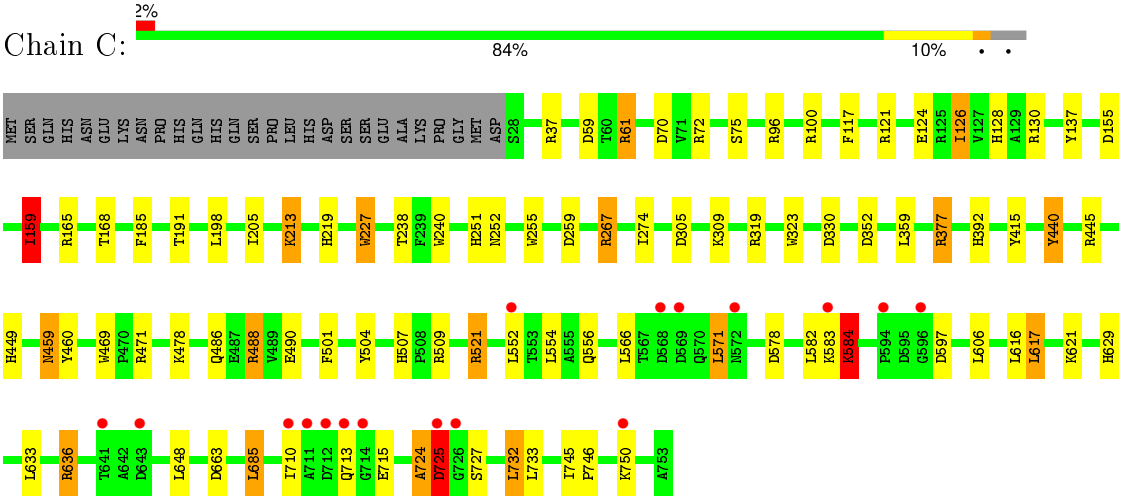
- Molecule 1: Catalase HPII

Chain B:



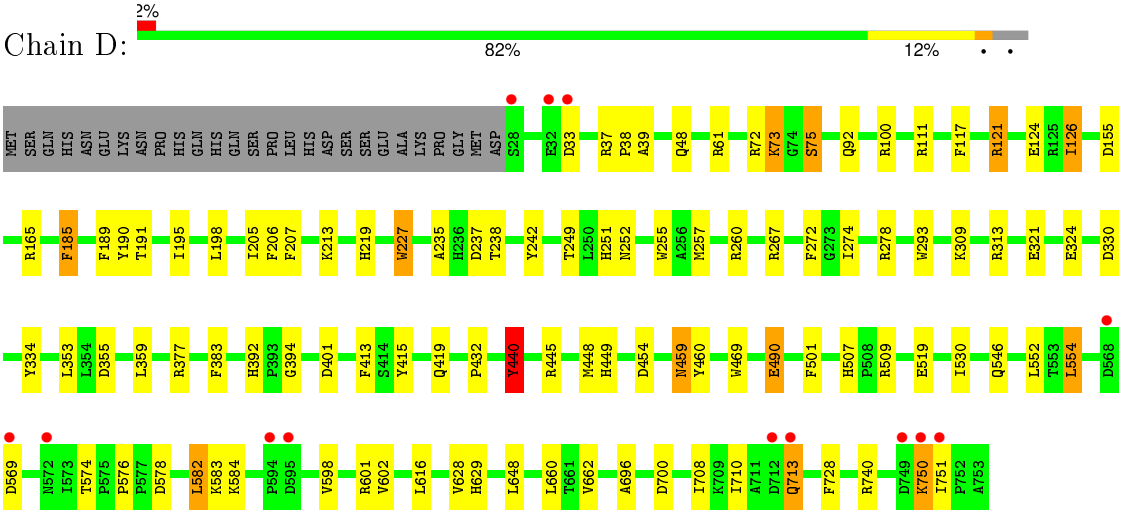
- Molecule 1: Catalase HPII

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	93.58Å 132.78Å 122.81Å 90.00° 109.35° 90.00°	Depositor
Resolution (Å)	33.20 – 1.60 33.20 – 1.60	Depositor EDS
% Data completeness (in resolution range)	96.2 (33.20-1.60) 96.2 (33.20-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.158 , 0.193 0.156 , 0.192	Depositor DCC
R_{free} test set	18012 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	12.2	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 357264 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	26152	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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, OCS

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	12/5917 (0.2%)	1.18	28/8043 (0.3%)
1	B	1.22	10/5920 (0.2%)	1.16	27/8046 (0.3%)
1	C	1.21	9/5911 (0.2%)	1.17	31/8035 (0.4%)
1	D	1.29	20/5917 (0.3%)	1.20	34/8043 (0.4%)
All	All	1.24	51/23665 (0.2%)	1.18	120/32167 (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	C	0	2

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	124	GLU	CD-OE1	7.83	1.34	1.25
1	C	469	TRP	CD2-CE2	7.79	1.50	1.41
1	A	469	TRP	CD2-CE2	7.50	1.50	1.41
1	D	519	GLU	CD-OE1	7.14	1.33	1.25
1	D	440	TYR	CE1-CZ	7.12	1.47	1.38
1	D	272	PHE	CG-CD1	7.00	1.49	1.38
1	D	75	SER	CB-OG	6.90	1.51	1.42
1	A	415	TYR	CG-CD2	6.87	1.48	1.39
1	D	413	PHE	CG-CD1	6.72	1.48	1.38
1	B	440	TYR	CE1-CZ	6.67	1.47	1.38
1	A	377	ARG	CZ-NH1	6.59	1.41	1.33
1	A	242	TYR	CE1-CZ	6.54	1.47	1.38
1	B	323	TRP	CD2-CE2	6.49	1.49	1.41
1	B	255	TRP	CD2-CE2	6.34	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	383	PHE	CG-CD1	6.29	1.48	1.38
1	D	121	ARG	CZ-NH2	6.19	1.41	1.33
1	B	346	GLU	CD-OE1	6.02	1.32	1.25
1	A	321	GLU	CD-OE1	5.96	1.32	1.25
1	D	321	GLU	CD-OE1	5.84	1.32	1.25
1	A	498	SER	CB-OG	5.75	1.49	1.42
1	A	192	GLU	CD-OE2	5.74	1.31	1.25
1	B	112	GLU	CD-OE2	5.72	1.31	1.25
1	A	440	TYR	CE1-CZ	5.71	1.46	1.38
1	C	504	TYR	CG-CD2	5.67	1.46	1.39
1	D	377	ARG	CZ-NH2	5.65	1.40	1.33
1	C	323	TRP	CD2-CE2	5.57	1.48	1.41
1	D	324	GLU	CD-OE1	5.56	1.31	1.25
1	D	255	TRP	CD2-CE2	5.54	1.48	1.41
1	D	377	ARG	CZ-NH1	5.50	1.40	1.33
1	D	260	ARG	CZ-NH2	5.50	1.40	1.33
1	C	159	ILE	CB-CG1	-5.49	1.38	1.54
1	D	469	TRP	CD2-CE2	5.43	1.47	1.41
1	C	319	ARG	CZ-NH1	5.43	1.40	1.33
1	B	181	ASP	CB-CG	5.42	1.63	1.51
1	D	419	GLN	CD-NE2	5.33	1.46	1.32
1	D	293	TRP	CD2-CE2	5.33	1.47	1.41
1	C	124	GLU	CD-OE1	5.31	1.31	1.25
1	A	290	ARG	CZ-NH2	5.30	1.40	1.33
1	A	351	PHE	CB-CG	-5.29	1.42	1.51
1	B	136	GLY	N-CA	5.27	1.53	1.46
1	B	469	TRP	CE3-CZ3	5.21	1.47	1.38
1	C	240	TRP	CD2-CE2	5.21	1.47	1.41
1	C	440	TYR	CE1-CZ	5.19	1.45	1.38
1	D	227	TRP	CD2-CE2	5.18	1.47	1.41
1	A	304	TRP	CD2-CE2	5.15	1.47	1.41
1	B	512	TRP	CD2-CE2	5.06	1.47	1.41
1	C	255	TRP	CD2-CE2	5.06	1.47	1.41
1	D	334	TYR	CG-CD2	5.04	1.45	1.39
1	D	206	PHE	CE1-CZ	5.03	1.47	1.37
1	A	344	GLU	CD-OE2	5.02	1.31	1.25
1	B	469	TRP	CD2-CE2	5.02	1.47	1.41

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	401	ASP	CB-CG-OD2	12.12	129.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	740	ARG	NE-CZ-NH1	10.68	125.64	120.30
1	A	740	ARG	NE-CZ-NH2	-10.29	115.16	120.30
1	B	70	ASP	CB-CG-OD1	9.78	127.10	118.30
1	A	377	ARG	NE-CZ-NH2	-9.50	115.55	120.30
1	B	369	ARG	NE-CZ-NH1	-9.39	115.61	120.30
1	C	471	ARG	NE-CZ-NH2	-9.31	115.64	120.30
1	C	445	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	D	401	ASP	CB-CG-OD1	-8.38	110.76	118.30
1	D	554	LEU	CB-CG-CD2	8.27	125.06	111.00
1	C	130	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	D	740	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	C	509	ARG	NE-CZ-NH2	8.09	124.34	120.30
1	C	96	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	C	165	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	B	165	ARG	NE-CZ-NH1	-7.66	116.47	120.30
1	A	643	ASP	CB-CG-OD1	7.65	125.18	118.30
1	B	33	ASP	CB-CG-OD1	7.59	125.13	118.30
1	C	37	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	B	509	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	C	96	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	D	582	LEU	CB-CG-CD1	7.31	123.43	111.00
1	C	732	LEU	CB-CG-CD1	-7.21	98.73	111.00
1	C	267	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	A	259	ASP	CB-CG-OD2	7.07	124.67	118.30
1	A	663	ASP	CB-CG-OD1	6.95	124.55	118.30
1	D	377	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	C	159	ILE	CB-CG1-CD1	-6.83	94.76	113.90
1	C	59	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	B	509	ARG	NE-CZ-NH1	-6.77	116.92	120.30
1	B	663	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	A	72	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	B	521	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	D	165	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	111	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	B	198	LEU	CB-CG-CD2	-6.58	99.81	111.00
1	C	100	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	A	130	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	C	663	ASP	CB-CG-OD2	-6.45	112.49	118.30
1	B	155	ASP	CB-CG-OD2	6.45	124.11	118.30
1	B	369	ARG	NE-CZ-NH2	6.31	123.45	120.30
1	D	117	PHE	CB-CG-CD1	-6.29	116.40	120.80
1	D	189	PHE	CB-CG-CD2	-6.26	116.42	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	353	LEU	CB-CG-CD1	-6.23	100.41	111.00
1	D	377	ARG	NE-CZ-NH1	-6.23	117.19	120.30
1	A	552	LEU	CB-CG-CD2	6.22	121.58	111.00
1	D	100	ARG	NE-CZ-NH1	-6.14	117.23	120.30
1	B	660	LEU	CB-CG-CD1	-6.13	100.58	111.00
1	A	377	ARG	CG-CD-NE	-6.12	98.95	111.80
1	B	445	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	C	685	LEU	CB-CG-CD1	6.08	121.33	111.00
1	B	401	ASP	CB-CG-OD1	-6.06	112.84	118.30
1	C	155	ASP	CB-CG-OD2	6.03	123.73	118.30
1	A	121	ARG	NE-CZ-NH1	-6.03	117.28	120.30
1	B	450	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	D	601	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	D	111	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	D	377	ARG	NH1-CZ-NH2	5.92	125.91	119.40
1	C	584	LYS	CD-CE-NZ	5.89	125.24	111.70
1	D	185	PHE	CB-CG-CD2	-5.79	116.75	120.80
1	B	419	GLN	CB-CA-C	5.76	121.92	110.40
1	C	554	LEU	CB-CG-CD2	-5.75	101.22	111.00
1	C	509	ARG	NE-CZ-NH1	-5.75	117.43	120.30
1	B	259	ASP	CB-CG-OD2	5.74	123.47	118.30
1	D	445	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	D	155	ASP	CB-CG-OD2	5.73	123.46	118.30
1	C	213	LYS	CD-CE-NZ	-5.70	98.60	111.70
1	C	126[A]	ILE	CB-CG1-CD1	-5.67	98.02	113.90
1	C	126[B]	ILE	CB-CG1-CD1	-5.67	98.02	113.90
1	A	685	LEU	CB-CG-CD1	-5.67	101.36	111.00
1	B	740	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	183	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	B	146	ASP	CB-CG-OD2	5.57	123.32	118.30
1	A	372	LYS	CD-CE-NZ	-5.57	98.89	111.70
1	B	111	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	313	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	B	562	LEU	CB-CG-CD1	5.54	120.43	111.00
1	A	501	PHE	CB-CG-CD2	-5.54	116.92	120.80
1	C	61	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	C	59	ASP	CB-CG-OD1	5.49	123.25	118.30
1	A	611	VAL	CG1-CB-CG2	-5.49	102.11	110.90
1	A	144	LEU	CB-CG-CD1	-5.45	101.74	111.00
1	D	213	LYS	CA-CB-CG	-5.45	101.42	113.40
1	C	305	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	A	61	ARG	NE-CZ-NH2	-5.42	117.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	177	ASP	CB-CG-OD1	-5.41	113.43	118.30
1	B	411	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	C	259	ASP	CB-CG-OD2	5.34	123.10	118.30
1	C	377	ARG	NE-CZ-NH1	-5.33	117.64	120.30
1	C	501	PHE	CB-CG-CD2	-5.32	117.08	120.80
1	D	126[A]	ILE	CB-CG1-CD1	-5.30	99.06	113.90
1	D	126[B]	ILE	CB-CG1-CD1	-5.30	99.06	113.90
1	D	198	LEU	CB-CG-CD2	-5.29	102.00	111.00
1	D	278	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	A	663	ASP	CB-CG-OD2	-5.27	113.55	118.30
1	D	454	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	336	LEU	CB-CG-CD2	-5.26	102.05	111.00
1	A	265	SER	N-CA-CB	-5.26	102.61	110.50
1	D	700	ASP	CB-CG-OD1	5.25	123.02	118.30
1	B	121	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	183	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	C	72	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	D	501	PHE	CB-CG-CD2	-5.19	117.16	120.80
1	D	355	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	A	37	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	C	617	LEU	CA-CB-CG	5.15	127.14	115.30
1	D	61	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	D	72	ARG	CG-CD-NE	-5.13	101.02	111.80
1	D	569	ASP	CB-CG-OD1	5.12	122.91	118.30
1	B	497	ARG	NE-CZ-NH2	5.11	122.85	120.30
1	A	542	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	B	141	TYR	CZ-CE2-CD2	-5.10	115.21	119.80
1	A	294	LYS	CD-CE-NZ	-5.06	100.07	111.70
1	D	33	ASP	CB-CG-OD1	5.04	122.83	118.30
1	D	189	PHE	CB-CG-CD1	5.04	124.33	120.80
1	B	571	LEU	CA-CB-CG	5.03	126.87	115.30
1	D	111	ARG	NE-CZ-NH2	5.03	122.81	120.30
1	D	242	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	C	352	ASP	CB-CG-OD2	5.02	122.82	118.30
1	A	259	ASP	CB-CG-OD1	-5.01	113.79	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	5758	0	5606	41	1
1	B	5761	0	5615	73	1
1	C	5755	0	5601	56	0
1	D	5758	0	5606	59	0
2	A	43	0	30	2	0
2	B	43	0	30	0	0
2	C	43	0	30	3	0
2	D	43	0	30	3	0
3	A	747	0	0	6	0
3	B	690	0	0	15	0
3	C	733	0	0	13	0
3	D	778	0	0	16	0
All	All	26152	0	22548	209	1

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 (209) 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:CB	1.71	1.53
1:B:392:HIS:ND1	1:B:415:TYR:CB	1.69	1.51
1:D:392:HIS:ND1	1:D:415:TYR:CB	1.72	1.48
1:C:392:HIS:ND1	1:C:415:TYR:CB	1.73	1.48
3:B:1494:HOH:O	1:D:73:LYS:HD3	1.18	1.30
1:D:449[B]:HIS:NE2	3:D:1517:HOH:O	1.66	1.27
1:C:392:HIS:CE1	1:C:415:TYR:HB2	1.70	1.24
1:D:392:HIS:CE1	1:D:415:TYR:HB2	1.73	1.22
1:B:521:ARG:HD3	3:B:1560:HOH:O	1.41	1.20
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:D:392:HIS:ND1	1:D:415:TYR:HB2	0.83	1.16
1:C:392:HIS:ND1	1:C:415:TYR:HB2	0.83	1.15
1:B:392:HIS:ND1	1:B:415:TYR:HB2	0.78	1.10
1:A:392:HIS:ND1	1:A:415:TYR:HB2	0.77	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:ARG:HG3	3:D:1372:HOH:O	1.61	1.00
1:B:309[A]:LYS:HE2	1:C:309:LYS:HE3	1.48	0.92
1:A:392:HIS:CG	1:A:415:TYR:HB2	2.05	0.91
1:D:546:GLN:HG3	3:D:1570:HOH:O	1.73	0.89
1:B:267:ARG:HG3	3:B:1372:HOH:O	1.74	0.86
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.58	0.86
1:C:267:ARG:HG3	3:C:1558:HOH:O	1.78	0.82
1:B:552:LEU:HD23	1:B:552:LEU:O	1.80	0.81
1:B:309[A]:LYS:CE	1:C:309:LYS:HE3	2.11	0.81
1:B:309[A]:LYS:HG2	1:B:660:LEU:HD11	1.65	0.79
1:C:552:LEU:HD11	1:C:556:GLN:NE2	2.01	0.76
1:C:578:ASP:HB2	1:C:582:LEU:O	1.86	0.75
1:A:392:HIS:ND1	1:A:415:TYR:CG	2.53	0.75
1:C:521:ARG:NH1	1:C:521:ARG:HG2	2.01	0.73
1:B:724:ALA:O	1:B:725:ASP:O	2.05	0.73
1:B:309[A]:LYS:NZ	1:B:313:ARG:HE	1.87	0.73
3:A:1641:HOH:O	1:D:126[B]:ILE:HD11	1.89	0.73
1:B:392:HIS:ND1	1:B:415:TYR:HB3	2.02	0.69
1:B:521:ARG:NH2	1:B:745:ILE:HD13	2.06	0.69
1:B:708:ILE:HD12	1:B:710:ILE:HD11	1.75	0.69
1:C:583:LYS:O	1:C:584:LYS:HB3	1.93	0.69
3:B:1585:HOH:O	1:C:126[B]:ILE:HD11	1.92	0.68
1:B:281:ASN:OD1	1:B:283:GLU:HG2	1.93	0.68
1:B:126[B]:ILE:HD11	3:C:1628:HOH:O	1.93	0.68
1:D:392:HIS:ND1	1:D:415:TYR:CG	2.61	0.68
1:C:392:HIS:ND1	1:C:415:TYR:CG	2.58	0.68
1:B:126[A]:ILE:HD12	1:C:121:ARG:CZ	2.24	0.67
1:D:449[B]:HIS:CE1	3:D:1517:HOH:O	2.26	0.67
1:C:486:GLN:OE1	3:C:1555:HOH:O	2.13	0.66
1:D:309:LYS:CE	3:D:1676:HOH:O	2.44	0.66
1:B:144:LEU:HD11	1:B:370:VAL:HG13	1.76	0.66
1:B:710:ILE:CD1	1:B:718:ILE:HG13	2.25	0.65
1:C:597:ASP:OD2	3:C:1423:HOH:O	2.14	0.65
1:A:36:HIS:CD2	1:A:36:HIS:H	2.16	0.64
1:C:552:LEU:CD1	1:C:556:GLN:HE21	2.10	0.64
1:D:629:HIS:HD2	3:D:1262:HOH:O	1.81	0.63
1:B:521:ARG:NH2	1:B:745:ILE:CD1	2.61	0.63
1:B:521:ARG:HH21	1:B:745:ILE:HD13	1.60	0.63
1:B:369:ARG:HG2	3:B:1303:HOH:O	1.97	0.63
1:A:120:GLU:HB2	1:D:126[A]:ILE:HD11	1.82	0.62
1:B:556:GLN:HG2	1:B:566:LEU:CD2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:521:ARG:HG2	1:C:521:ARG:HH11	1.64	0.62
1:D:440:TYR:HD1	3:D:1660:HOH:O	1.83	0.61
1:B:120:GLU:HB2	1:C:126[A]:ILE:HD11	1.83	0.61
1:C:521:ARG:CG	1:C:521:ARG:HH11	2.14	0.60
1:C:629:HIS:HD2	3:C:1209:HOH:O	1.84	0.60
1:D:38:PRO:HA	1:D:48:GLN:HE21	1.67	0.58
1:B:552:LEU:HD23	1:B:552:LEU:C	2.24	0.58
1:C:552:LEU:CD1	1:C:556:GLN:NE2	2.66	0.58
1:D:392:HIS:ND1	1:D:415:TYR:HB3	2.04	0.57
1:D:546:GLN:CG	3:D:1570:HOH:O	2.40	0.57
1:B:294:LYS:NZ	3:B:1513:HOH:O	2.33	0.57
1:D:546:GLN:CD	3:D:1570:HOH:O	2.43	0.56
1:B:309[A]:LYS:HZ1	1:B:313:ARG:HH21	1.51	0.56
1:B:552:LEU:CD2	1:B:552:LEU:C	2.75	0.55
1:B:583:LYS:O	1:B:584:LYS:HB3	2.07	0.55
1:D:359:LEU:H	1:D:507:HIS:HD2	1.54	0.55
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.90	0.54
1:A:639:GLU:HG3	3:A:1485:HOH:O	2.06	0.54
1:D:190:TYR:CD1	1:D:195:ILE:HD11	2.43	0.54
1:C:490:GLU:HG3	1:D:490:GLU:HG3	1.88	0.54
3:A:1335:HOH:O	1:C:449[B]:HIS:HE1	1.89	0.54
1:A:126[B]:ILE:CD1	3:D:1009:HOH:O	2.55	0.54
1:A:126[A]:ILE:HD12	1:D:121:ARG:CZ	2.38	0.54
1:C:724:ALA:O	1:C:725:ASP:HB2	2.07	0.54
1:D:708:ILE:HG13	1:D:710:ILE:HG12	1.88	0.54
1:C:621:LYS:HG2	3:C:1608:HOH:O	2.07	0.54
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.91	0.54
1:B:392:HIS:ND1	1:B:415:TYR:CG	2.65	0.53
1:B:546:GLN:NE2	3:B:1467:HOH:O	2.41	0.53
1:B:309[A]:LYS:HG3	3:B:1588:HOH:O	2.08	0.53
1:B:38:PRO:HG2	1:B:51:ALA:HB2	1.91	0.53
1:B:521:ARG:HH22	1:B:745:ILE:HD12	1.74	0.53
1:D:598:VAL:HG22	1:D:628:VAL:HG22	1.90	0.53
1:A:120:GLU:HB2	1:D:126[A]:ILE:CD1	2.39	0.52
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.13	0.52
1:C:727:SER:HA	3:C:1526:HOH:O	2.08	0.52
1:C:552:LEU:HD13	1:C:556:GLN:HE21	1.74	0.52
1:B:395:HIS:HE1	3:B:1589:HOH:O	1.92	0.52
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.92	0.52
1:A:449[B]:HIS:HE1	3:A:1335:HOH:O	1.92	0.52
1:D:448:MET:O	1:D:449[A]:HIS:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:LEU:HD23	1:B:556:GLN:HG3	1.91	0.51
1:B:144:LEU:HD11	1:B:370:VAL:CG1	2.40	0.51
1:D:309:LYS:HE3	3:D:1676:HOH:O	2.07	0.51
1:D:190:TYR:HA	1:D:195:ILE:HD13	1.93	0.50
1:D:190:TYR:HD1	1:D:195:ILE:HD11	1.76	0.50
1:B:725:ASP:OD2	1:B:727:SER:HB3	2.11	0.50
1:A:344:GLU:HB3	3:A:1569:HOH:O	2.11	0.50
1:C:636:ARG:NH1	3:C:1527:HOH:O	2.35	0.50
1:C:126[A]:ILE:CG2	2:C:801:HEM:HMD1	2.41	0.50
1:B:126[B]:ILE:HG21	1:C:117:PHE:CE2	2.46	0.50
1:C:274:ILE:HD12	2:C:801:HEM:HMB1	1.94	0.50
1:C:732:LEU:HD13	1:C:732:LEU:C	2.32	0.50
1:D:309:LYS:HE2	3:D:1676:HOH:O	2.08	0.49
1:A:126[B]:ILE:HD11	3:D:1009:HOH:O	2.11	0.49
1:B:359:LEU:H	1:B:507:HIS:HD2	1.59	0.49
1:A:682:ASN:HB3	1:A:707:THR:HG21	1.95	0.49
1:A:459:ASN:HD22	1:A:459:ASN:H	1.60	0.49
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.42	0.49
1:A:126[A]:ILE:CG2	2:A:801:HEM:HMD1	2.43	0.49
1:B:521:ARG:HH22	1:B:745:ILE:CD1	2.26	0.49
1:C:745:ILE:HD13	3:C:1560:HOH:O	2.13	0.49
1:B:121:ARG:HG2	1:C:126[A]:ILE:HD12	1.94	0.49
2:C:801:HEM:HBC2	2:C:801:HEM:CMC	2.43	0.49
1:C:70:ASP:OD1	3:C:1495:HOH:O	2.20	0.49
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.28	0.49
3:B:1494:HOH:O	1:D:73:LYS:CD	2.02	0.49
1:B:309[A]:LYS:HZ1	1:B:313:ARG:NH2	2.11	0.48
1:C:392:HIS:CE1	1:C:415:TYR:CB	2.63	0.48
1:D:274:ILE:HD12	2:D:801:HEM:HMB1	1.95	0.48
1:C:392:HIS:ND1	1:C:415:TYR:HB3	2.05	0.48
1:D:126[A]:ILE:HG22	2:D:801:HEM:HMD1	1.94	0.48
1:A:38:PRO:HA	1:A:48:GLN:OE1	2.13	0.47
1:B:461:GLU:HA	1:B:462:PRO:C	2.33	0.47
1:B:251:HIS:HA	1:B:508:PRO:HG3	1.97	0.47
1:A:235:ALA:HA	1:A:530:ILE:HG23	1.95	0.47
1:A:309:LYS:NZ	1:A:687:GLU:OE2	2.40	0.47
1:D:235:ALA:HA	1:D:530:ILE:HG23	1.97	0.47
1:D:251:HIS:CE1	1:D:507:HIS:HB3	2.50	0.47
1:C:488:ARG:CD	3:C:1466:HOH:O	2.62	0.47
1:C:488:ARG:HD3	3:C:1466:HOH:O	2.14	0.47
1:A:392:HIS:CG	1:A:415:TYR:CB	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:750:LYS:NZ	3:D:1383:HOH:O	2.41	0.47
1:C:460:TYR:CE2	1:D:238:THR:HB	2.50	0.46
1:B:629:HIS:HD2	3:B:1158:HOH:O	1.98	0.46
1:C:128:HIS:HA	1:C:168:THR:O	2.15	0.46
1:B:267:ARG:HD2	3:B:1132:HOH:O	2.14	0.46
1:D:37:ARG:HD2	3:D:1429:HOH:O	2.16	0.45
1:B:335:GLU:OE1	1:B:369:ARG:HD2	2.17	0.45
1:C:710:ILE:HG23	1:C:715:GLU:HG2	1.98	0.45
1:A:274:ILE:HD12	2:A:801:HEM:HMB1	1.99	0.45
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.31	0.45
1:B:126[B]:ILE:HG12	3:B:1040:HOH:O	2.16	0.45
1:A:36:HIS:HD2	1:A:36:HIS:H	1.63	0.45
1:A:372:LYS:NZ	3:A:1612:HOH:O	2.50	0.45
1:B:392:HIS:CD2	1:B:394:GLY:H	2.35	0.45
1:B:309[A]:LYS:NZ	1:B:313:ARG:NE	2.60	0.45
1:A:449[A]:HIS:CD2	1:C:449[A]:HIS:CD2	3.05	0.45
1:B:745:ILE:O	1:B:748:ILE:HG12	2.18	0.44
1:B:319:ARG:HD3	1:C:227:TRP:O	2.16	0.44
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.52	0.44
1:D:713:GLN:O	1:D:713:GLN:HG2	2.17	0.44
1:B:556:GLN:HG2	1:B:566:LEU:HD22	1.99	0.44
1:B:634:TYR:O	1:B:653:THR:HA	2.17	0.44
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.33	0.44
1:D:602:VAL:HG13	1:D:662:VAL:HA	2.00	0.44
1:C:583:LYS:O	1:C:584:LYS:CB	2.64	0.43
1:D:207:PHE:O	1:D:249:THR:HA	2.17	0.43
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.34	0.43
1:A:128:HIS:HA	1:A:168:THR:O	2.17	0.43
1:A:213:LYS:HD2	1:D:92:GLN:OE1	2.18	0.43
1:D:313:ARG:HG3	1:D:660:LEU:HD12	2.01	0.43
1:A:251:HIS:CE1	1:A:507:HIS:HB3	2.54	0.43
1:A:607:LEU:HD22	1:A:611:VAL:HG21	2.00	0.43
1:C:359:LEU:H	1:C:507:HIS:HD2	1.66	0.43
1:D:126[A]:ILE:CG2	2:D:801:HEM:HMD1	2.49	0.42
1:D:257:MET:SD	1:D:530:ILE:HD12	2.58	0.42
1:C:566:LEU:HB2	1:C:571:LEU:HD13	2.01	0.42
1:B:39:ALA:HB1	1:B:41:GLU:HG2	2.00	0.42
1:B:126[B]:ILE:HG21	1:C:117:PHE:CZ	2.53	0.42
1:B:344:GLU:H	1:B:344:GLU:CD	2.22	0.42
1:B:708:ILE:CD1	1:B:710:ILE:HD11	2.48	0.42
1:C:251:HIS:CE1	1:C:507:HIS:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:PRO:HA	1:D:48:GLN:NE2	2.33	0.42
1:A:448:MET:O	1:A:449[B]:HIS:HB2	2.19	0.42
1:D:696:ALA:HB1	1:D:728:PHE:CZ	2.55	0.42
1:D:459:ASN:HD22	1:D:459:ASN:H	1.68	0.42
1:C:746:PRO:HB2	3:C:1579:HOH:O	2.19	0.42
1:D:392:HIS:CD2	1:D:394:GLY:H	2.38	0.42
1:A:449[B]:HIS:CG	1:C:449[B]:HIS:CG	2.34	0.42
1:B:459:ASN:H	1:B:459:ASN:HD22	1.66	0.42
1:D:392:HIS:CE1	1:D:415:TYR:CB	2.67	0.41
1:D:39:ALA:H	1:D:48:GLN:NE2	2.19	0.41
1:B:36:HIS:HD1	1:B:36:HIS:H	1.68	0.41
1:B:713:GLN:H	1:B:713:GLN:HG3	1.47	0.41
1:D:359:LEU:H	1:D:507:HIS:CD2	2.37	0.41
1:B:359:LEU:H	1:B:507:HIS:CD2	2.37	0.41
1:B:235:ALA:HA	1:B:530:ILE:HG23	2.02	0.41
1:A:583:LYS:O	1:A:584:LYS:HB3	2.20	0.41
1:D:509:ARG:HD2	1:D:576:PRO:HD2	2.01	0.41
1:B:97:ALA:O	1:B:101:GLY:HA3	2.21	0.41
1:A:393:PRO:HD2	1:A:415:TYR:CD2	2.55	0.41
1:A:36:HIS:N	1:A:36:HIS:CD2	2.85	0.41
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.56	0.41
1:D:578:ASP:OD1	1:D:583:LYS:HE3	2.20	0.41
1:A:296:LEU:HD12	1:A:333:GLU:HB3	2.03	0.41
1:D:267:ARG:HD2	3:D:1237:HOH:O	2.20	0.40
1:B:29:LEU:N	3:B:1478:HOH:O	2.38	0.40
1:A:669:OCS:OD3	1:A:699:GLY:HA3	2.22	0.40
1:A:252:ASN:HD22	1:A:252:ASN:HA	1.71	0.40
1:C:238:THR:HB	1:D:460:TYR:CE2	2.56	0.40
1:B:361:PRO:HD2	1:B:364:LEU:HD12	2.03	0.40
1:B:706:ALA:HB3	3:B:1438:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASP:OD1	1:B:369:ARG:NH2[2_545]	1.94	0.26

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	727/753 (96%)	709 (98%)	17 (2%)	1 (0%)	56	31
1	B	727/753 (96%)	710 (98%)	15 (2%)	2 (0%)	46	23
1	C	726/753 (96%)	710 (98%)	13 (2%)	3 (0%)	39	17
1	D	727/753 (96%)	708 (97%)	18 (2%)	1 (0%)	56	31
All	All	2907/3012 (96%)	2837 (98%)	63 (2%)	7 (0%)	52	28

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	725	ASP
1	A	75	SER
1	C	75	SER
1	C	725	ASP
1	D	75	SER
1	C	584	LYS
1	B	75	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	614/635 (97%)	598 (97%)	16 (3%)	54	25
1	B	614/635 (97%)	592 (96%)	22 (4%)	42	15
1	C	613/635 (96%)	585 (95%)	28 (5%)	33	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	614/635 (97%)	593 (97%)	21 (3%)	44 16
All	All	2455/2540 (97%)	2368 (96%)	87 (4%)	42 16

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	37	ARG
1	A	73	LYS
1	A	185	PHE
1	A	191	THR
1	A	205	ILE
1	A	227	TRP
1	A	252	ASN
1	A	369	ARG
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	707	THR
1	A	732	LEU
1	A	747	LYS
1	A	751	ILE
1	B	28	SER
1	B	32	GLU
1	B	185	PHE
1	B	191	THR
1	B	205	ILE
1	B	227	TRP
1	B	252	ASN
1	B	432	PRO
1	B	440	TYR
1	B	459	ASN
1	B	552	LEU
1	B	562	LEU
1	B	566	LEU
1	B	571	LEU
1	B	583	LYS
1	B	610	GLU
1	B	616	LEU
1	B	633	LEU
1	B	635	SER
1	B	703	LYS

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Mol	Chain	Res	Type
1	B	713	GLN
1	B	732	LEU
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	213	LYS
1	C	227	TRP
1	C	252	ASN
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	571	LEU
1	C	584	LYS
1	C	606	LEU
1	C	616	LEU
1	C	617	LEU
1	C	633	LEU
1	C	636	ARG
1	C	648	LEU
1	C	685	LEU
1	C	713	GLN
1	C	725	ASP
1	C	733	LEU
1	C	750	LYS
1	D	73	LYS
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	227	TRP
1	D	237	ASP
1	D	252	ASN
1	D	432	PRO
1	D	440	TYR
1	D	459	ASN
1	D	490	GLU
1	D	552	LEU

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Mol	Chain	Res	Type
1	D	554	LEU
1	D	574	THR
1	D	582	LEU
1	D	584	LYS
1	D	616	LEU
1	D	648	LEU
1	D	713	GLN
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	368	GLN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	B	713	GLN
1	C	252	ASN
1	C	459	ASN
1	C	486	GLN
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	459	ASN
1	D	507	HIS
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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	OCS	A	669	1	7,8,9	3.05	2 (28%)	7,11,13	2.07	2 (28%)
1	OCS	B	669	1	7,8,9	3.28	2 (28%)	7,11,13	4.60	2 (28%)
1	OCS	C	669	1	7,8,9	2.98	2 (28%)	7,11,13	1.27	1 (14%)
1	OCS	D	669	1	7,8,9	2.31	2 (28%)	7,11,13	4.00	2 (28%)

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
1	OCS	A	669	1	-	1/4/7/9	0/0/0/0
1	OCS	B	669	1	-	1/4/7/9	0/0/0/0
1	OCS	C	669	1	-	1/4/7/9	0/0/0/0
1	OCS	D	669	1	-	1/4/7/9	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	669	OCS	CB-SG	-5.42	1.69	1.77
1	C	669	OCS	CB-SG	-4.75	1.70	1.77
1	A	669	OCS	CB-SG	-3.78	1.72	1.77
1	D	669	OCS	CB-SG	-3.09	1.73	1.77
1	D	669	OCS	OD2-SG	5.01	1.59	1.46
1	C	669	OCS	OD2-SG	6.12	1.62	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	669	OCS	OD2-SG	6.55	1.63	1.46
1	A	669	OCS	OD2-SG	6.85	1.64	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	669	OCS	OD3-SG-CB	-11.59	97.17	106.94
1	D	669	OCS	OD3-SG-CB	-10.01	98.50	106.94
1	A	669	OCS	OD3-SG-CB	-4.36	103.27	106.94
1	C	669	OCS	OD1-SG-CB	-2.33	104.98	106.94
1	D	669	OCS	OD3-SG-OD1	2.40	122.23	113.48
1	B	669	OCS	OD1-SG-CB	2.42	108.98	106.94
1	A	669	OCS	OD1-SG-CB	2.94	109.42	106.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	669	OCS	SG-CB-CA-N
1	C	669	OCS	SG-CB-CA-N
1	B	669	OCS	SG-CB-CA-N
1	D	669	OCS	SG-CB-CA-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	669	OCS	1	0

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	801	1	30,50,50	3.24	13 (43%)	24,82,82	3.13	14 (58%)
2	HEM	B	801	1	30,50,50	2.78	12 (40%)	24,82,82	3.10	12 (50%)
2	HEM	C	801	1	30,50,50	3.00	12 (40%)	24,82,82	3.38	12 (50%)
2	HEM	D	801	1	30,50,50	2.61	11 (36%)	24,82,82	3.35	14 (58%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	801	1	-	0/10/54/54	0/0/8/8
2	HEM	B	801	1	-	0/10/54/54	0/0/8/8
2	HEM	C	801	1	-	0/10/54/54	0/0/8/8
2	HEM	D	801	1	-	0/10/54/54	0/0/8/8

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C3B-C4B	-9.77	1.43	1.51
2	B	801	HEM	C3B-C4B	-8.27	1.44	1.51
2	C	801	HEM	C3B-C4B	-6.94	1.45	1.51
2	A	801	HEM	C3D-C4D	-5.76	1.44	1.51
2	C	801	HEM	C2D-C3D	-5.09	1.39	1.54
2	B	801	HEM	C2D-C3D	-4.73	1.40	1.54
2	D	801	HEM	C3D-C4D	-4.63	1.45	1.51
2	D	801	HEM	C2D-C3D	-4.11	1.42	1.54
2	C	801	HEM	C2C-C1C	-3.66	1.45	1.52
2	B	801	HEM	C3C-CAC	-3.55	1.44	1.51
2	A	801	HEM	C2C-C1C	-3.44	1.46	1.52
2	A	801	HEM	C2D-C3D	-3.40	1.44	1.54
2	D	801	HEM	CMB-C2B	-3.31	1.45	1.53
2	B	801	HEM	C2C-C1C	-2.95	1.47	1.52
2	A	801	HEM	CMB-C2B	-2.87	1.46	1.53
2	B	801	HEM	C3B-CAB	-2.83	1.46	1.51
2	C	801	HEM	C2D-C1D	-2.34	1.44	1.51
2	A	801	HEM	C2D-C1D	-2.17	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	HEM	C2C-C1C	-2.08	1.48	1.52
2	B	801	HEM	C2D-C1D	-2.03	1.45	1.51
2	C	801	HEM	C4A-CHB	2.09	1.45	1.39
2	A	801	HEM	CHD-C1D	2.14	1.44	1.38
2	B	801	HEM	CHC-C4B	2.18	1.44	1.38
2	B	801	HEM	FE-NB	2.27	2.09	1.97
2	A	801	HEM	CHC-C4B	2.33	1.45	1.38
2	C	801	HEM	CHC-C1C	2.48	1.42	1.36
2	C	801	HEM	CHD-C4C	2.56	1.42	1.36
2	C	801	HEM	C2A-C3A	2.59	1.45	1.37
2	B	801	HEM	CHD-C1D	2.62	1.46	1.38
2	D	801	HEM	CHC-C4B	2.67	1.46	1.38
2	B	801	HEM	CHD-C4C	2.68	1.42	1.36
2	A	801	HEM	CHC-C1C	2.78	1.42	1.36
2	C	801	HEM	CHC-C4B	2.80	1.46	1.38
2	A	801	HEM	CHD-C4C	2.83	1.43	1.36
2	D	801	HEM	CHC-C1C	2.94	1.43	1.36
2	D	801	HEM	C4A-CHB	2.96	1.48	1.39
2	A	801	HEM	C2A-C3A	3.06	1.46	1.37
2	D	801	HEM	CHD-C1D	3.17	1.47	1.38
2	C	801	HEM	CHD-C1D	3.29	1.48	1.38
2	B	801	HEM	C4C-NC	3.36	1.40	1.36
2	D	801	HEM	CHD-C4C	3.91	1.45	1.36
2	D	801	HEM	C1C-NC	5.34	1.42	1.36
2	C	801	HEM	C4C-NC	5.37	1.42	1.36
2	A	801	HEM	C4C-NC	5.63	1.43	1.36
2	D	801	HEM	C4C-NC	6.72	1.44	1.36
2	B	801	HEM	C1C-NC	6.72	1.44	1.36
2	A	801	HEM	C1C-NC	8.19	1.46	1.36
2	C	801	HEM	C1C-NC	8.77	1.46	1.36

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	801	HEM	C3B-CAB-CBB	-8.44	111.50	124.46
2	B	801	HEM	CAA-CBA-CGA	-6.91	100.08	112.75
2	D	801	HEM	CAA-CBA-CGA	-6.53	100.77	112.75
2	D	801	HEM	C3C-CAC-CBC	-5.62	115.84	124.46
2	A	801	HEM	CAA-CBA-CGA	-5.02	103.54	112.75
2	A	801	HEM	C3B-CAB-CBB	-4.94	116.87	124.46
2	C	801	HEM	CAA-CBA-CGA	-4.90	103.76	112.75
2	A	801	HEM	C3C-CAC-CBC	-4.76	117.16	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	801	HEM	C1D-CHD-C4C	-4.49	118.32	125.82
2	C	801	HEM	CBD-CAD-C3D	-4.42	100.69	113.55
2	A	801	HEM	CBD-CAD-C3D	-4.13	101.52	113.55
2	B	801	HEM	CBD-CAD-C3D	-4.08	101.67	113.55
2	D	801	HEM	C3B-CAB-CBB	-3.41	119.23	124.46
2	A	801	HEM	C1D-CHD-C4C	-3.23	120.43	125.82
2	D	801	HEM	CBD-CAD-C3D	-3.09	104.55	113.55
2	C	801	HEM	C3C-CAC-CBC	-3.06	119.77	124.46
2	A	801	HEM	C2C-C1C-CHC	-2.78	119.45	123.68
2	B	801	HEM	CBA-CAA-C2A	-2.65	107.79	112.53
2	D	801	HEM	CMA-C3A-C4A	-2.55	124.15	128.36
2	B	801	HEM	CMA-C3A-C4A	-2.51	124.22	128.36
2	C	801	HEM	C4B-CHC-C1C	-2.46	121.71	125.82
2	A	801	HEM	CMA-C3A-C4A	-2.35	124.47	128.36
2	C	801	HEM	C2C-C1C-CHC	-2.33	120.14	123.68
2	A	801	HEM	C4B-CHC-C1C	-2.06	122.38	125.82
2	C	801	HEM	C2C-C1C-NC	2.00	113.59	110.21
2	D	801	HEM	CMA-C3A-C2A	2.28	130.00	125.24
2	B	801	HEM	CAA-C2A-C1A	2.36	129.56	127.01
2	D	801	HEM	C2D-C3D-C4D	2.47	105.69	101.50
2	D	801	HEM	CAD-C3D-C4D	2.64	121.78	112.47
2	B	801	HEM	CMA-C3A-C2A	2.68	130.84	125.24
2	A	801	HEM	CMD-C2D-C3D	2.77	126.61	114.35
2	B	801	HEM	C2C-C1C-NC	3.12	115.48	110.21
2	D	801	HEM	CMD-C2D-C3D	3.23	128.62	114.35
2	A	801	HEM	C2C-C1C-NC	3.52	116.14	110.21
2	A	801	HEM	CAD-C3D-C2D	3.52	123.35	113.22
2	B	801	HEM	CMD-C2D-C3D	3.55	130.06	114.35
2	D	801	HEM	C2C-C1C-NC	3.62	116.31	110.21
2	C	801	HEM	CMC-C2C-C3C	3.65	125.65	116.53
2	A	801	HEM	CMC-C2C-C3C	4.00	126.51	116.53
2	C	801	HEM	CMD-C2D-C3D	4.07	132.34	114.35
2	B	801	HEM	CAD-C3D-C4D	4.23	127.38	112.47
2	C	801	HEM	CAD-C3D-C4D	4.28	127.55	112.47
2	D	801	HEM	CMC-C2C-C3C	4.79	128.48	116.53
2	B	801	HEM	CMC-C2C-C3C	5.11	129.30	116.53
2	C	801	HEM	CAD-C3D-C2D	5.20	128.16	113.22
2	B	801	HEM	CAD-C3D-C2D	5.21	128.19	113.22
2	D	801	HEM	CMB-C2B-C3B	5.45	130.12	116.53
2	A	801	HEM	CMB-C2B-C3B	5.45	130.13	116.53
2	A	801	HEM	CAD-C3D-C4D	5.58	132.15	112.47
2	B	801	HEM	CMB-C2B-C3B	5.77	130.92	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	801	HEM	CAD-C3D-C2D	6.49	131.86	113.22
2	C	801	HEM	CMB-C2B-C3B	6.53	132.83	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	HEM	2	0
2	C	801	HEM	3	0
2	D	801	HEM	3	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	725/753 (96%)	-0.30	12 (1%)	73	71	5, 11, 27, 57	1 (0%)
1	B	725/753 (96%)	-0.15	27 (3%)	45	43	5, 13, 35, 68	1 (0%)
1	C	725/753 (96%)	-0.22	17 (2%)	64	62	6, 13, 36, 53	1 (0%)
1	D	725/753 (96%)	-0.27	13 (1%)	71	70	5, 11, 29, 68	1 (0%)
All	All	2900/3012 (96%)	-0.23	69 (2%)	62	60	5, 12, 33, 68	4 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	726	GLY	7.3
1	D	749	ASP	4.6
1	B	749	ASP	4.5
1	A	32	GLU	4.5
1	B	28	SER	4.3
1	B	32	GLU	4.1
1	B	673	ALA	4.1
1	B	712	ASP	4.0
1	A	28	SER	3.8
1	C	711	ALA	3.7
1	D	28	SER	3.6
1	D	750	LYS	3.5
1	C	726	GLY	3.5
1	A	726	GLY	3.5
1	B	711	ALA	3.3
1	C	594	PRO	3.3
1	D	712	ASP	3.3
1	B	713	GLN	3.2
1	B	725	ASP	3.2
1	B	568	ASP	3.2
1	C	568	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	35	SER	3.0
1	A	594	PRO	2.9
1	D	713	GLN	2.9
1	C	713	GLN	2.8
1	D	594	PRO	2.8
1	B	750	LYS	2.7
1	B	677	ASP	2.7
1	C	641	THR	2.7
1	C	712	ASP	2.7
1	C	714	GLY	2.6
1	C	583	LYS	2.6
1	D	751	ILE	2.5
1	B	34	GLY	2.5
1	B	572	ASN	2.5
1	B	33	ASP	2.4
1	A	33	ASP	2.4
1	C	569	ASP	2.4
1	D	32	GLU	2.3
1	D	568	ASP	2.3
1	B	647	VAL	2.3
1	B	595	ASP	2.3
1	D	33	ASP	2.3
1	C	552	LEU	2.3
1	D	572	ASN	2.3
1	C	710	ILE	2.3
1	B	30	ALA	2.3
1	C	643	ASP	2.3
1	C	725	ASP	2.3
1	A	596	GLY	2.2
1	C	596	GLY	2.2
1	A	750	LYS	2.2
1	A	39	ALA	2.2
1	B	646	THR	2.2
1	B	645	GLY	2.2
1	A	749	ASP	2.2
1	C	572	ASN	2.2
1	B	571	LEU	2.2
1	B	593	ILE	2.2
1	A	31	PRO	2.1
1	B	569	ASP	2.1
1	B	751	ILE	2.1
1	B	565	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	750	LYS	2.1
1	B	37	ARG	2.1
1	D	595	ASP	2.1
1	D	569	ASP	2.1
1	A	725	ASP	2.0
1	B	710	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	OCS	D	669	9/10	0.96	0.14	-	17,21,24,30	0
1	OCS	C	669	9/10	0.92	0.16	-	26,29,36,37	0
1	OCS	B	669	9/10	0.92	0.15	-	25,29,34,42	0
1	OCS	A	669	9/10	0.95	0.10	-	17,20,28,29	0

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	A	801	43/43	0.99	0.09	0.22	5,6,8,11	0
2	HEM	B	801	43/43	0.99	0.08	-0.19	6,7,9,12	0
2	HEM	C	801	43/43	0.99	0.08	-0.39	5,6,9,11	0
2	HEM	D	801	43/43	0.99	0.07	-0.71	5,6,8,10	0

6.5 Other polymers (i)

There are no such residues in this entry.