



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2017 – 12:20 AM EDT

PDB ID : 3IS7
Title : Structure of mineralized Bfrb from Pseudomonas aeruginosa to 2.1A Resolution
Authors : Lovell, S.; Weeratunga, S.K.; Battaile, K.P.; Rivera, M.
Deposited on : unknown
Resolution : 2.10 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

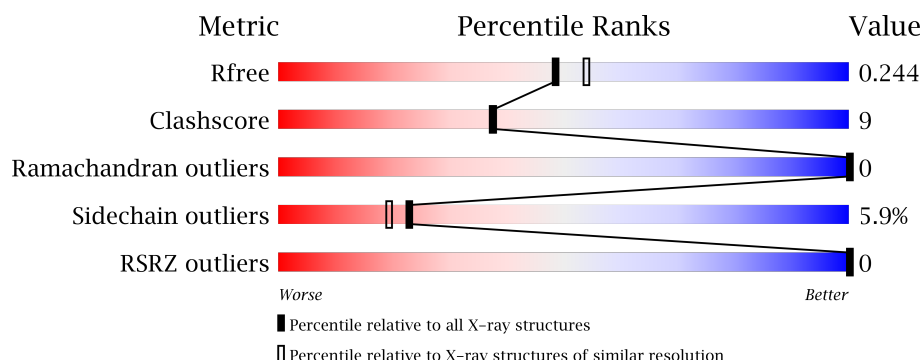
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.
















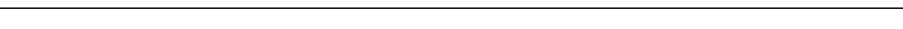





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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 $\leq 5\%$. 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	158	
1	B	158	
1	C	158	
1	D	158	
1	E	158	

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Mol	Chain	Length	Quality of chain
1	F	158	 83% 11% . . .
1	G	158	 73% 20% . . .
1	H	158	 83% 11% . . .
1	I	158	 78% 15% . . .
1	J	158	 80% 15% . .
1	K	158	 74% 18% . . .
1	L	158	 80% 13% . . .
1	M	158	 84% 11% . . .
1	N	158	 84% 11% . . .
1	O	158	 78% 16% . . .
1	P	158	 81% 12% . . .
1	Q	158	 83% 11% . . .
1	R	158	 75% 21% . .
1	S	158	 77% 16% . . .
1	T	158	 77% 18% . . .
1	U	158	 81% 13% . . .
1	V	158	 77% 17% . .
1	W	158	 75% 19% . . .
1	X	158	 82% 13% . . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	K	B	159	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32332 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 Bacterioferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1251	791	213	241	6			
1	B	154	Total	C	N	O	S	0	0	0
			1262	798	216	242	6			
1	C	155	Total	C	N	O	S	0	0	0
			1261	797	215	243	6			
1	D	154	Total	C	N	O	S	0	0	0
			1266	801	217	242	6			
1	E	154	Total	C	N	O	S	0	0	0
			1259	797	214	242	6			
1	F	154	Total	C	N	O	S	0	0	0
			1260	797	215	242	6			
1	G	154	Total	C	N	O	S	0	0	0
			1266	801	217	242	6			
1	H	155	Total	C	N	O	S	0	0	0
			1270	804	217	243	6			
1	I	154	Total	C	N	O	S	0	0	0
			1262	798	216	242	6			
1	J	154	Total	C	N	O	S	0	0	0
			1259	796	215	242	6			
1	K	154	Total	C	N	O	S	0	0	0
			1267	801	218	242	6			
1	L	154	Total	C	N	O	S	0	0	0
			1263	799	216	242	6			
1	M	154	Total	C	N	O	S	0	0	0
			1260	798	216	240	6			
1	N	154	Total	C	N	O	S	0	0	0
			1260	798	214	242	6			
1	O	154	Total	C	N	O	S	0	0	0
			1259	796	215	242	6			
1	P	154	Total	C	N	O	S	0	0	0
			1262	798	216	242	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	154	Total 1260	C 798	N 214	O 242	S 6	0	0	0
1	R	155	Total 1272	C 805	N 218	O 243	S 6	0	0	0
1	S	154	Total 1259	C 796	N 215	O 242	S 6	0	0	0
1	T	154	Total 1259	C 796	N 215	O 242	S 6	0	0	0
1	U	154	Total 1264	C 799	N 217	O 242	S 6	0	0	0
1	V	154	Total 1260	C 797	N 215	O 242	S 6	0	0	0
1	W	155	Total 1274	C 806	N 219	O 243	S 6	0	0	0
1	X	154	Total 1263	C 799	N 216	O 242	S 6	0	0	0

- # HEM

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



WORLD WIDE
PDB
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	S	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	X	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total 1	K 1	0	0
3	E	1	Total 1	K 1	0	0
3	B	1	Total 1	K 1	0	0
3	C	1	Total 1	K 1	0	0
3	A	1	Total 1	K 1	0	0
3	N	1	Total 1	K 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	68	Total 68	O 68	0	0
4	B	78	Total 78	O 78	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	72	Total O 72 72	0	0
4	D	80	Total O 80 80	0	0
4	E	53	Total O 53 53	0	0
4	F	66	Total O 66 66	0	0
4	G	74	Total O 74 74	0	0
4	H	78	Total O 78 78	0	0
4	I	61	Total O 61 61	0	0
4	J	49	Total O 49 49	0	0
4	K	67	Total O 67 67	0	0
4	L	63	Total O 63 63	0	0
4	M	60	Total O 60 60	0	0
4	N	68	Total O 68 68	0	0
4	O	59	Total O 59 59	0	0
4	P	53	Total O 53 53	0	0
4	Q	40	Total O 40 40	0	0
4	R	43	Total O 43 43	0	0
4	S	47	Total O 47 47	0	0
4	T	46	Total O 46 46	0	0
4	U	64	Total O 64 64	0	0
4	V	52	Total O 52 52	0	0
4	W	85	Total O 85 85	0	0

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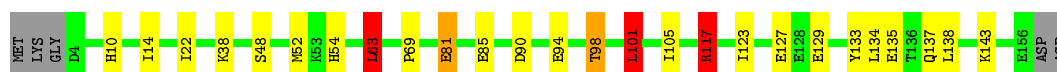
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	X	86	Total	O	0	0
			86	86		

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 the various outlier classes 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: Bacterioferritin

Chain A: 




• Molecule 1: Bacterioferritin

Chain B: 




• Molecule 1: Bacterioferritin

Chain C: 




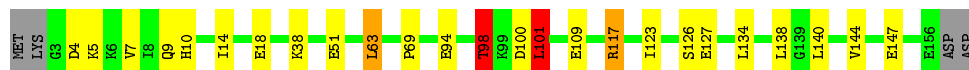
• Molecule 1: Bacterioferritin

Chain D: 




• Molecule 1: Bacterioferritin

Chain E: 

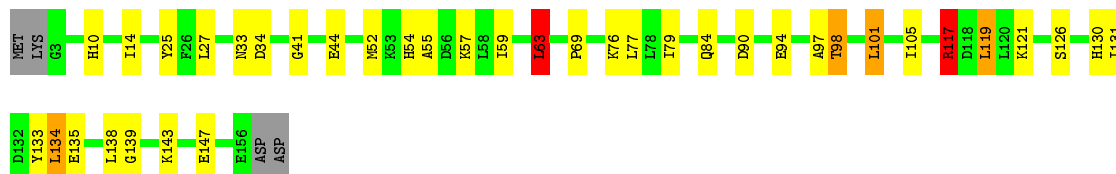


• Molecule 1: Bacterioferritin

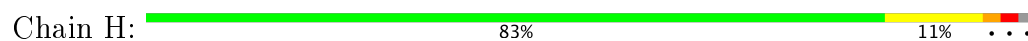
Chain F: 



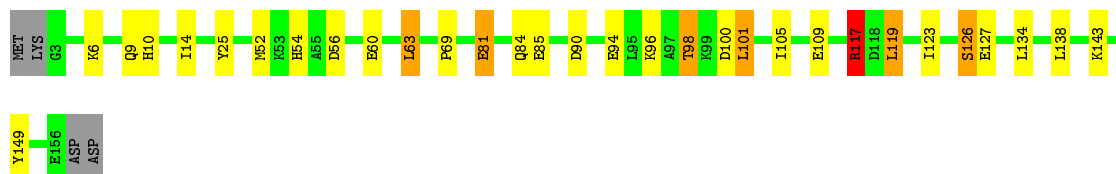
• Molecule 1: Bacterioferritin



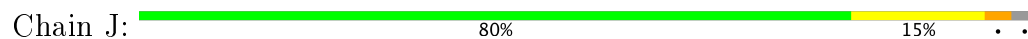
• Molecule 1: Bacterioferritin



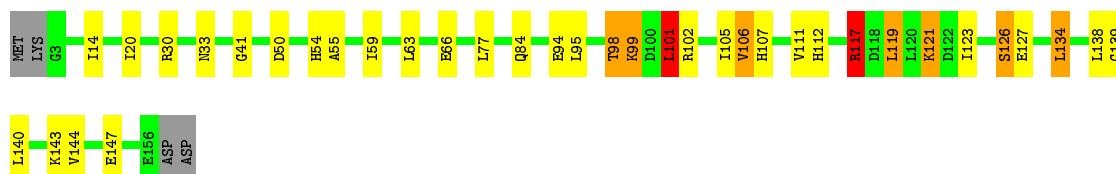
• Molecule 1: Bacterioferritin



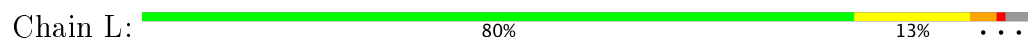
• Molecule 1: Bacterioferritin



• Molecule 1: Bacterioferritin



• Molecule 1: Bacterioferritin





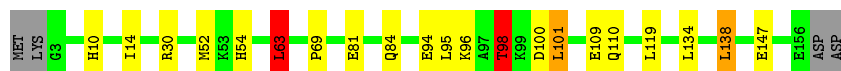
- Molecule 1: Bacterioferritin

Chain M: 84% 11% . . .



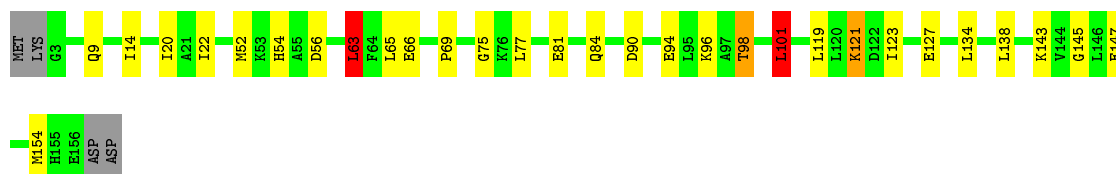
- Molecule 1: Bacterioferritin

Chain N: 84% 11% . . .



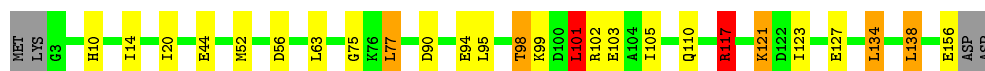
- Molecule 1: Bacterioferritin

Chain O: 78% 16% . . .



- Molecule 1: Bacterioferritin

Chain P: 81% 12% . . .



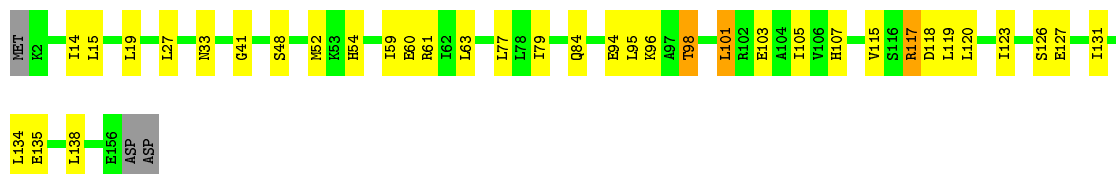
- Molecule 1: Bacterioferritin

Chain Q: 83% 11% . . .

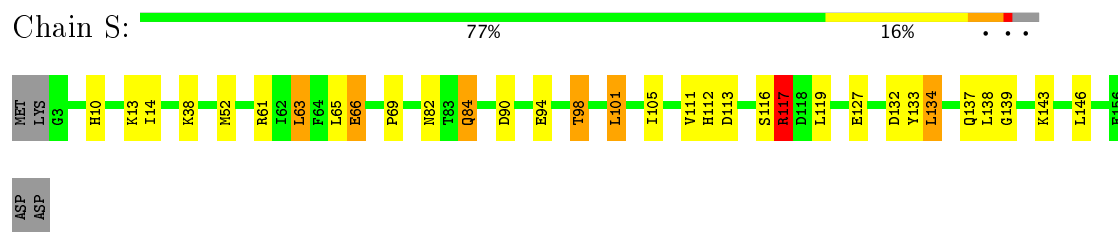


- Molecule 1: Bacterioferritin

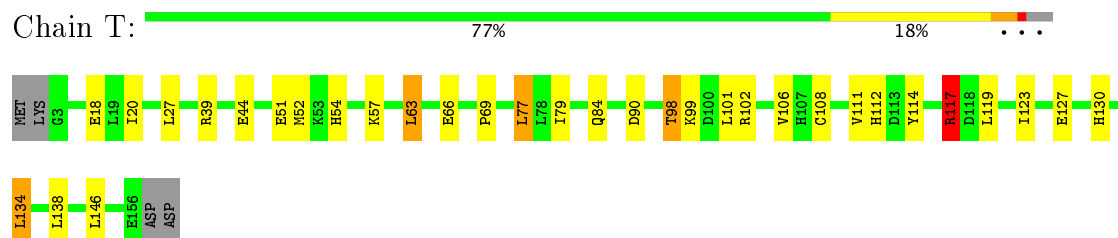
Chain R: 75% 21% . .



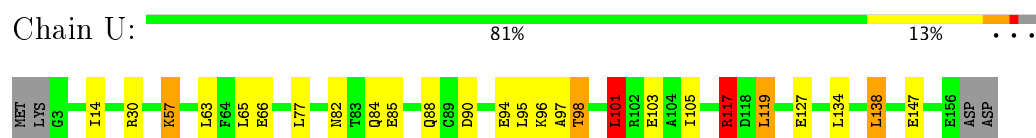
- Molecule 1: Bacterioferritin



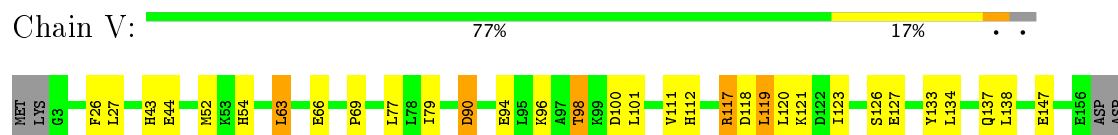
- Molecule 1: Bacterioferritin



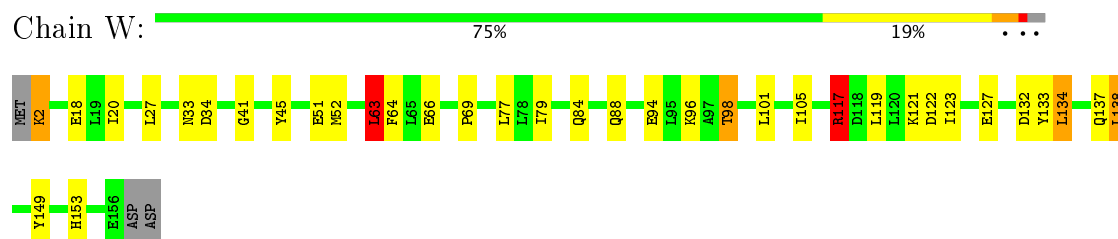
- Molecule 1: Bacterioferritin



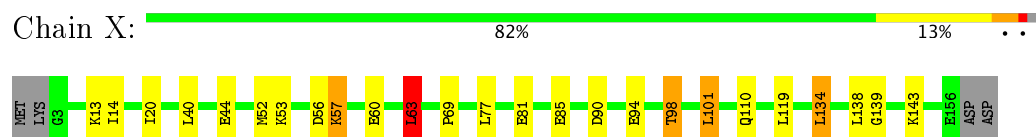
- Molecule 1: Bacterioferritin



- Molecule 1: Bacterioferritin



- Molecule 1: Bacterioferritin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.81Å 202.76Å 207.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.04 – 2.10 47.02 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.04-2.10) 99.9 (47.02-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.10Å)	Xtriage
Refinement program	REFMAC refmac _5.5.0066	Depositor
R, R_{free}	0.193 , 0.244 0.200 , 0.244	Depositor DCC
R_{free} test set	15512 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.002 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32332	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, K

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	0.98	1/1272 (0.1%)	0.96	5/1717 (0.3%)
1	B	0.97	0/1283	0.91	2/1729 (0.1%)
1	C	0.98	1/1282 (0.1%)	0.92	5/1730 (0.3%)
1	D	1.03	1/1287 (0.1%)	0.94	4/1733 (0.2%)
1	E	1.01	0/1280	0.95	5/1726 (0.3%)
1	F	1.01	0/1281	1.03	8/1727 (0.5%)
1	G	1.00	1/1287 (0.1%)	0.96	5/1733 (0.3%)
1	H	1.02	1/1291 (0.1%)	1.06	10/1739 (0.6%)
1	I	0.96	1/1283 (0.1%)	0.88	2/1729 (0.1%)
1	J	0.96	0/1280	0.89	4/1726 (0.2%)
1	K	0.96	0/1288	0.93	4/1734 (0.2%)
1	L	0.97	1/1284 (0.1%)	0.90	5/1730 (0.3%)
1	M	0.94	0/1281	0.95	6/1726 (0.3%)
1	N	1.03	4/1281 (0.3%)	0.87	4/1727 (0.2%)
1	O	0.96	0/1280	0.90	6/1726 (0.3%)
1	P	0.94	0/1283	0.89	6/1729 (0.3%)
1	Q	0.93	0/1281	0.94	5/1727 (0.3%)
1	R	0.91	1/1293 (0.1%)	0.90	2/1741 (0.1%)
1	S	0.96	0/1280	0.94	5/1726 (0.3%)
1	T	1.01	1/1280 (0.1%)	0.90	2/1726 (0.1%)
1	U	0.94	0/1285	1.02	6/1731 (0.3%)
1	V	0.94	0/1281	0.93	3/1727 (0.2%)
1	W	0.99	0/1295	0.98	7/1743 (0.4%)
1	X	1.01	0/1284	0.94	5/1730 (0.3%)
All	All	0.98	13/30802 (0.0%)	0.94	116/41512 (0.3%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	81	GLU	CG-CD	5.87	1.60	1.51
1	R	60	GLU	CG-CD	5.57	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	129	GLU	CG-CD	5.31	1.59	1.51
1	I	149	TYR	CD1-CE1	-5.28	1.31	1.39
1	L	114	TYR	CD1-CE1	5.27	1.47	1.39
1	D	127	GLU	CB-CG	5.27	1.62	1.52
1	N	147	GLU	CB-CG	5.27	1.62	1.52
1	G	97	ALA	CA-CB	5.14	1.63	1.52
1	H	108	CYS	CB-SG	-5.14	1.73	1.81
1	C	81	GLU	CG-CD	5.11	1.59	1.51
1	N	109	GLU	CG-CD	5.09	1.59	1.51
1	T	108	CYS	CB-SG	-5.09	1.73	1.81
1	N	98	THR	CB-CG2	-5.05	1.35	1.52

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	117	ARG	NE-CZ-NH1	15.74	128.17	120.30
1	U	117	ARG	NE-CZ-NH1	12.74	126.67	120.30
1	H	117	ARG	NE-CZ-NH1	11.95	126.27	120.30
1	F	117	ARG	NE-CZ-NH2	-11.29	114.65	120.30
1	E	117	ARG	NE-CZ-NH1	10.53	125.57	120.30
1	K	117	ARG	NE-CZ-NH1	10.50	125.55	120.30
1	Q	117	ARG	NE-CZ-NH1	10.33	125.47	120.30
1	H	117	ARG	NE-CZ-NH2	-9.45	115.58	120.30
1	V	117	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	W	117	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	B	117	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	U	117	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	S	117	ARG	NE-CZ-NH1	8.93	124.77	120.30
1	G	117	ARG	NE-CZ-NH1	8.75	124.67	120.30
1	W	117	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	A	117	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	Q	117	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	D	117	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	B	117	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	W	132	ASP	CB-CG-OD1	7.90	125.41	118.30
1	C	101	LEU	CB-CG-CD1	7.87	124.38	111.00
1	T	117	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	L	56	ASP	CB-CG-OD1	7.49	125.04	118.30
1	H	63	LEU	CB-CG-CD1	7.49	123.73	111.00
1	M	117	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	M	56	ASP	CB-CG-OD1	6.92	124.53	118.30
1	L	56	ASP	CB-CG-OD2	-6.84	112.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	30	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	J	117	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	K	101	LEU	CA-CB-CG	6.80	130.95	115.30
1	R	117	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	H	63	LEU	CA-CB-CG	6.73	130.78	115.30
1	G	63	LEU	CA-CB-CG	6.64	130.57	115.30
1	K	117	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	63	LEU	CB-CG-CD1	6.49	122.04	111.00
1	K	30	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	A	90	ASP	CB-CG-OD1	6.49	124.14	118.30
1	D	101	LEU	CA-CB-CG	6.49	130.22	115.30
1	V	117	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	O	101	LEU	CA-CB-CG	6.44	130.11	115.30
1	X	56	ASP	CB-CG-OD1	6.44	124.09	118.30
1	G	117	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	T	117	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	X	134	LEU	CA-CB-CG	6.29	129.77	115.30
1	J	90	ASP	CB-CG-OD1	6.25	123.92	118.30
1	P	117	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	F	134	LEU	CA-CB-CG	6.13	129.40	115.30
1	F	30	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	O	63	LEU	CA-CB-CG	6.04	129.20	115.30
1	M	63	LEU	CB-CG-CD1	6.04	121.27	111.00
1	U	90	ASP	CB-CG-OD1	6.01	123.71	118.30
1	E	117	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	R	117	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	F	63	LEU	CB-CG-CD1	5.97	121.15	111.00
1	H	101	LEU	CA-CB-CG	5.96	129.00	115.30
1	U	101	LEU	CA-CB-CG	5.95	128.99	115.30
1	G	63	LEU	CB-CG-CD1	5.95	121.11	111.00
1	X	134	LEU	CB-CG-CD1	5.94	121.10	111.00
1	H	138	LEU	CB-CG-CD1	5.94	121.10	111.00
1	W	63	LEU	CB-CG-CD1	5.92	121.07	111.00
1	M	63	LEU	CA-CB-CG	5.91	128.88	115.30
1	C	134	LEU	CB-CG-CD1	5.89	121.01	111.00
1	W	138	LEU	CB-CG-CD1	5.88	120.99	111.00
1	C	63	LEU	CA-CB-CG	5.85	128.76	115.30
1	W	134	LEU	CB-CG-CD1	5.78	120.82	111.00
1	Q	134	LEU	CB-CG-CD1	5.76	120.80	111.00
1	N	138	LEU	CA-CB-CG	5.74	128.50	115.30
1	A	117	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	N	101	LEU	CA-CB-CG	5.60	128.17	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	61	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	C	101	LEU	CA-CB-CG	5.59	128.16	115.30
1	F	134	LEU	CB-CG-CD1	5.59	120.50	111.00
1	N	63	LEU	CB-CG-CD1	5.55	120.44	111.00
1	E	98	THR	N-CA-CB	-5.55	99.76	110.30
1	M	101	LEU	CA-CB-CG	5.54	128.05	115.30
1	I	90	ASP	CB-CG-OD1	5.54	123.28	118.30
1	U	138	LEU	CB-CG-CD1	5.54	120.41	111.00
1	M	134	LEU	CB-CG-CD1	5.53	120.40	111.00
1	O	90	ASP	CB-CG-OD1	5.48	123.23	118.30
1	P	56	ASP	CB-CG-OD1	5.48	123.23	118.30
1	I	117	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	V	90	ASP	CB-CG-OD1	5.46	123.21	118.30
1	P	138	LEU	CB-CG-CD1	5.46	120.28	111.00
1	H	98	THR	N-CA-CB	-5.43	99.97	110.30
1	Q	101	LEU	CA-CB-CG	5.42	127.76	115.30
1	H	102	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	W	63	LEU	CA-CB-CG	5.39	127.70	115.30
1	Q	132	ASP	CB-CG-OD1	5.39	123.15	118.30
1	G	101	LEU	CA-CB-CG	5.37	127.66	115.30
1	O	101	LEU	CB-CG-CD1	5.37	120.13	111.00
1	E	101	LEU	CA-CB-CG	5.35	127.61	115.30
1	H	90	ASP	CB-CG-OD1	5.35	123.11	118.30
1	S	90	ASP	CB-CG-OD1	5.35	123.11	118.30
1	N	101	LEU	CB-CG-CD1	5.31	120.03	111.00
1	X	63	LEU	CA-CB-CG	5.29	127.47	115.30
1	P	134	LEU	CA-CB-CG	5.27	127.42	115.30
1	J	56	ASP	CB-CG-OD1	5.25	123.02	118.30
1	L	117	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	E	100	ASP	CB-CG-OD2	5.19	122.97	118.30
1	L	63	LEU	CA-CB-CG	5.17	127.18	115.30
1	H	134	LEU	CA-CB-CG	5.13	127.10	115.30
1	O	56	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	98	THR	N-CA-CB	-5.10	100.61	110.30
1	X	13	LYS	CD-CE-NZ	-5.09	100.00	111.70
1	J	101	LEU	CA-CB-CG	5.06	126.94	115.30
1	S	132	ASP	CB-CG-OD1	5.06	122.86	118.30
1	S	134	LEU	CA-CB-CG	5.06	126.93	115.30
1	A	101	LEU	CA-CB-CG	5.05	126.91	115.30
1	F	101	LEU	CA-CB-CG	5.05	126.91	115.30
1	F	93	LEU	CB-CG-CD1	-5.04	102.43	111.00
1	O	77	LEU	CB-CG-CD1	5.04	119.57	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	101	LEU	CB-CG-CD1	5.04	119.56	111.00
1	L	134	LEU	CA-CB-CG	5.02	126.85	115.30
1	D	134	LEU	CB-CG-CD1	5.02	119.53	111.00
1	P	56	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	D	117	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1251	0	1211	20	0
1	B	1262	0	1234	19	0
1	C	1261	0	1218	16	0
1	D	1266	0	1245	18	0
1	E	1259	0	1222	13	0
1	F	1260	0	1227	11	0
1	G	1266	0	1245	21	0
1	H	1270	0	1242	14	0
1	I	1262	0	1234	26	0
1	J	1259	0	1225	19	0
1	K	1267	0	1250	33	0
1	L	1263	0	1236	19	0
1	M	1260	0	1234	16	0
1	N	1260	0	1224	13	0
1	O	1259	0	1225	20	0
1	P	1262	0	1234	14	0
1	Q	1260	0	1224	15	0
1	R	1272	0	1249	25	0
1	S	1259	0	1225	24	0
1	T	1259	0	1225	27	0
1	U	1264	0	1241	20	0
1	V	1260	0	1227	30	0
1	W	1274	0	1256	23	0
1	X	1263	0	1236	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	43	0	30	6	0
2	C	43	0	30	10	0
2	F	43	0	30	10	0
2	H	43	0	30	10	0
2	J	43	0	30	12	0
2	K	43	0	30	8	0
2	N	43	0	30	9	0
2	P	43	0	30	8	0
2	Q	43	0	30	7	0
2	S	43	0	30	6	0
2	V	43	0	30	5	0
2	X	43	0	30	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	N	1	0	0	0	0
4	A	68	0	0	5	0
4	B	78	0	0	5	0
4	C	72	0	0	3	0
4	D	80	0	0	4	0
4	E	53	0	0	3	0
4	F	66	0	0	5	0
4	G	74	0	0	7	0
4	H	78	0	0	5	0
4	I	61	0	0	6	0
4	J	49	0	0	5	0
4	K	67	0	0	7	0
4	L	63	0	0	3	0
4	M	60	0	0	5	0
4	N	68	0	0	2	0
4	O	59	0	0	8	0
4	P	53	0	0	1	0
4	Q	40	0	0	1	0
4	R	43	0	0	7	0
4	S	47	0	0	4	0
4	T	46	0	0	3	0
4	U	64	0	0	6	0
4	V	52	0	0	6	0
4	W	85	0	0	7	0
4	X	86	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	32332	0	29949	537	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 9.

All (537) 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:J:98:THR:HG21	4:J:452:HOH:O	1.18	1.27
1:I:98:THR:HG21	4:I:1235:HOH:O	1.38	1.22
1:L:119:LEU:HD23	1:L:119:LEU:C	1.55	1.20
1:V:119:LEU:HD23	1:V:119:LEU:C	1.66	1.15
1:K:99:LYS:NZ	1:K:99:LYS:HB3	1.60	1.11
1:K:98:THR:HG21	4:K:356:HOH:O	1.52	1.08
1:K:99:LYS:HZ2	1:K:99:LYS:HB3	0.91	1.07
2:N:159:HEM:HMB2	2:N:159:HEM:HBB2	1.08	1.07
1:G:98:THR:HG21	4:G:667:HOH:O	1.52	1.06
2:N:159:HEM:CMB	2:N:159:HEM:HBB2	1.79	1.06
1:I:119:LEU:HD23	1:I:119:LEU:C	1.76	1.06
1:X:98:THR:HG21	4:X:518:HOH:O	1.58	1.04
1:W:98:THR:HG21	4:W:450:HOH:O	1.59	1.02
1:R:98:THR:HG21	4:R:655:HOH:O	1.60	1.01
1:T:84:GLN:OE1	1:T:146:LEU:HD11	1.60	1.00
2:X:159:HEM:CMB	2:X:159:HEM:HBB2	1.86	1.00
1:T:98:THR:HG21	4:T:732:HOH:O	1.60	0.99
1:O:98:THR:HG21	4:O:1029:HOH:O	1.60	0.99
1:V:119:LEU:C	1:V:119:LEU:CD2	2.30	0.98
1:U:98:THR:HG21	4:U:459:HOH:O	1.63	0.97
1:V:119:LEU:HD23	1:V:119:LEU:O	1.65	0.97
2:P:159:HEM:HBC2	2:P:159:HEM:HHD	1.47	0.97
2:X:159:HEM:HBB2	2:X:159:HEM:HMB1	1.47	0.95
2:A:159:HEM:HMC2	2:A:159:HEM:HBC2	1.46	0.94
1:L:119:LEU:CD2	1:L:119:LEU:C	2.35	0.94
1:V:98:THR:HG21	4:V:391:HOH:O	1.66	0.93
1:A:135:GLU:OE1	1:W:2:LYS:NZ	2.01	0.91
1:L:119:LEU:HD23	1:L:119:LEU:O	1.67	0.91
2:C:159:HEM:HBC2	2:C:159:HEM:HHD	1.51	0.90
2:H:159:HEM:HBC2	2:H:159:HEM:HMC2	1.50	0.90
1:J:98:THR:CG2	4:J:452:HOH:O	1.89	0.90
1:V:98:THR:CG2	4:V:391:HOH:O	2.18	0.90
1:R:27:LEU:HD23	1:R:79:ILE:HD12	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:98:THR:CG2	4:K:356:HOH:O	2.13	0.89
1:M:46:HIS:HE1	4:M:462:HOH:O	1.56	0.88
2:F:159:HEM:HHD	2:F:159:HEM:HBC2	1.56	0.87
2:P:159:HEM:HBC2	2:P:159:HEM:CHD	1.99	0.87
2:C:159:HEM:HBB2	2:C:159:HEM:CMB	2.03	0.86
2:H:159:HEM:HBC2	2:H:159:HEM:CMC	2.05	0.86
1:T:84:GLN:OE1	1:T:146:LEU:CD1	2.24	0.86
1:B:98:THR:HG21	4:B:829:HOH:O	1.75	0.86
1:G:54:HIS:HD2	4:G:636:HOH:O	1.58	0.85
2:P:159:HEM:CBC	2:P:159:HEM:HHD	2.07	0.85
2:F:159:HEM:HBB2	2:F:159:HEM:CMB	2.07	0.84
2:A:159:HEM:CMC	2:A:159:HEM:HBC2	2.03	0.84
1:G:34:ASP:OD1	4:G:1089:HOH:O	1.93	0.84
2:X:159:HEM:HHD	2:X:159:HEM:HBC2	1.58	0.84
1:D:98:THR:HG21	4:D:775:HOH:O	1.78	0.83
1:I:98:THR:CG2	4:I:1235:HOH:O	2.07	0.83
1:U:98:THR:CG2	4:U:459:HOH:O	2.21	0.83
2:J:159:HEM:HBC2	2:J:159:HEM:HHD	1.61	0.82
1:F:98:THR:HG21	4:F:1435:HOH:O	1.80	0.82
1:I:119:LEU:CD2	1:I:119:LEU:C	2.49	0.81
1:U:119:LEU:C	1:U:119:LEU:HD23	2.00	0.81
1:S:84:GLN:HE22	1:S:146:LEU:HD11	1.46	0.80
1:H:98:THR:HG21	4:H:906:HOH:O	1.83	0.79
1:K:99:LYS:CB	1:K:99:LYS:HZ2	1.83	0.79
2:V:159:HEM:HHD	2:V:159:HEM:HBC2	1.65	0.79
1:I:54:HIS:HD2	4:I:429:HOH:O	1.65	0.79
1:V:43:HIS:HD2	4:V:868:HOH:O	1.64	0.78
2:H:159:HEM:CMB	2:H:159:HEM:HBB2	2.14	0.78
1:N:96:LYS:NZ	1:N:100:ASP:OD2	2.17	0.77
1:X:98:THR:CG2	4:X:518:HOH:O	2.24	0.77
1:E:18:GLU:OE1	1:E:51:GLU:OE1	2.02	0.77
2:X:159:HEM:HMB1	2:X:159:HEM:CBB	2.15	0.76
2:N:159:HEM:HBC2	2:N:159:HEM:HMC1	1.68	0.76
1:T:27:LEU:HD23	1:T:79:ILE:HD12	1.67	0.76
1:K:84:GLN:NE2	4:K:541:HOH:O	2.18	0.75
1:W:2:LYS:HE3	1:W:64:PHE:O	1.87	0.75
1:A:81:GLU:HG2	1:A:85:GLU:OE2	1.87	0.74
2:J:159:HEM:CMB	2:J:159:HEM:HBB2	2.17	0.73
2:H:159:HEM:HMB1	2:H:159:HEM:HBB2	1.70	0.73
1:I:119:LEU:O	1:I:119:LEU:HD23	1.87	0.73
2:K:159:HEM:HBB2	2:K:159:HEM:CMB	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:GLN:OE1	4:B:733:HOH:O	2.06	0.73
1:P:121:LYS:HD2	1:P:121:LYS:C	2.09	0.73
1:W:27:LEU:HD23	1:W:79:ILE:HD12	1.71	0.72
1:T:102:ARG:O	1:T:106:VAL:HG23	1.89	0.72
2:Q:159:HEM:HBB2	2:Q:159:HEM:HHC	1.70	0.72
1:V:119:LEU:HD21	1:V:123:ILE:CD1	2.19	0.72
1:K:119:LEU:CD2	1:K:119:LEU:C	2.58	0.71
1:B:84:GLN:NE2	4:B:443:HOH:O	2.24	0.71
2:P:159:HEM:HBB2	2:P:159:HEM:CMB	2.18	0.71
1:M:119:LEU:C	1:M:119:LEU:HD23	2.11	0.71
1:S:65:LEU:O	1:S:66:GLU:HG2	1.91	0.70
1:R:98:THR:CG2	4:R:655:HOH:O	2.25	0.70
1:W:88:GLN:OE1	4:W:1474:HOH:O	2.09	0.70
1:G:98:THR:CG2	4:G:667:HOH:O	2.25	0.70
1:I:14:ILE:HD12	1:I:101:LEU:HD13	1.72	0.70
2:C:159:HEM:CBB	2:C:159:HEM:HMB1	2.22	0.70
1:W:84:GLN:NE2	4:W:665:HOH:O	2.25	0.70
2:N:159:HEM:HMB2	2:N:159:HEM:CBB	2.04	0.69
1:U:119:LEU:HD23	1:U:119:LEU:O	1.92	0.69
1:D:121:LYS:C	1:D:121:LYS:HE2	2.13	0.69
2:C:159:HEM:CBB	2:C:159:HEM:CMB	2.66	0.69
2:Q:159:HEM:CBB	2:Q:159:HEM:HHC	2.21	0.69
1:S:84:GLN:HE22	1:S:146:LEU:CD1	2.05	0.69
1:B:99:LYS:HB3	1:B:99:LYS:HZ2	1.58	0.69
1:K:119:LEU:HD23	1:K:119:LEU:C	2.12	0.69
2:K:159:HEM:HBC2	2:K:159:HEM:HHH	1.73	0.68
1:K:99:LYS:CB	1:K:99:LYS:NZ	2.34	0.68
1:I:109:GLU:OE1	1:Q:117:ARG:NH2	2.26	0.68
1:T:119:LEU:HD23	1:T:119:LEU:C	2.13	0.68
1:W:105:ILE:HG23	1:W:117:ARG:HG3	1.76	0.67
1:S:84:GLN:CD	1:S:84:GLN:H	1.96	0.67
1:S:65:LEU:C	1:S:66:GLU:HG2	2.15	0.67
1:W:98:THR:CG2	4:W:450:HOH:O	2.29	0.67
1:A:127:GLU:OE1	4:A:1216:HOH:O	2.13	0.67
1:M:46:HIS:CE1	4:M:462:HOH:O	2.38	0.67
1:O:14:ILE:HD12	1:O:101:LEU:HD13	1.77	0.67
1:H:119:LEU:C	1:H:119:LEU:HD23	2.15	0.67
1:O:84:GLN:NE2	4:O:423:HOH:O	2.27	0.67
1:S:10:HIS:ND1	4:S:1079:HOH:O	2.22	0.67
1:N:84:GLN:NE2	4:N:1285:HOH:O	2.21	0.67
1:T:119:LEU:HD23	1:T:119:LEU:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:156:GLU:HG3	4:P:540:HOH:O	1.94	0.66
1:H:54:HIS:HE1	4:H:1301:HOH:O	1.78	0.66
2:F:159:HEM:CBB	2:F:159:HEM:CMB	2.73	0.66
4:A:801:HOH:O	1:L:143:LYS:HE3	1.95	0.65
1:U:119:LEU:C	1:U:119:LEU:CD2	2.64	0.65
1:V:43:HIS:CD2	4:V:868:HOH:O	2.44	0.65
2:C:159:HEM:HBB2	2:C:159:HEM:HMB3	1.79	0.65
1:K:119:LEU:O	1:K:119:LEU:HD23	1.97	0.65
1:A:14:ILE:HD12	1:A:101:LEU:HD13	1.78	0.65
1:B:38:LYS:HE2	4:B:163:HOH:O	1.97	0.65
1:U:147:GLU:HG3	4:U:160:HOH:O	1.96	0.64
1:F:84:GLN:NE2	4:F:408:HOH:O	2.30	0.64
1:V:119:LEU:HD21	1:V:123:ILE:HD11	1.78	0.64
1:P:10:HIS:O	1:P:14:ILE:HG12	1.98	0.64
1:D:63:LEU:HD13	1:D:69:PRO:HD3	1.80	0.63
1:D:98:THR:CG2	4:D:775:HOH:O	2.39	0.63
1:I:9:GLN:NE2	4:I:1476:HOH:O	2.28	0.63
1:U:88:GLN:OE1	4:U:216:HOH:O	2.15	0.63
1:I:56:ASP:O	1:I:60:GLU:HG3	1.97	0.63
1:R:94:GLU:O	1:R:98:THR:HB	1.98	0.63
1:K:50:ASP:OD1	4:K:1293:HOH:O	2.16	0.62
1:Q:119:LEU:HD23	1:Q:119:LEU:C	2.19	0.62
2:X:159:HEM:CHD	2:X:159:HEM:HBC2	2.28	0.62
1:C:94:GLU:O	1:C:98:THR:HB	2.00	0.62
1:P:44:GLU:OE2	1:P:90:ASP:OD2	2.17	0.62
1:R:118:ASP:OD1	1:V:121:LYS:HE3	1.99	0.61
1:R:59:ILE:O	1:R:63:LEU:CD2	2.49	0.61
1:X:119:LEU:HD23	1:X:119:LEU:C	2.20	0.61
1:K:95:LEU:O	1:K:98:THR:HG22	2.01	0.61
1:S:84:GLN:NE2	1:S:146:LEU:CD1	2.64	0.60
1:V:96:LYS:NZ	1:V:100:ASP:OD2	2.34	0.60
1:B:99:LYS:HB3	1:B:99:LYS:NZ	2.16	0.60
1:E:147:GLU:HG3	4:E:581:HOH:O	1.99	0.60
1:N:94:GLU:O	1:N:98:THR:HB	2.00	0.60
1:A:94:GLU:O	1:A:98:THR:HB	2.01	0.60
1:E:38:LYS:HD3	4:E:721:HOH:O	2.01	0.60
1:J:52:MET:HB3	2:J:159:HEM:CHB	2.31	0.60
1:M:94:GLU:O	1:M:98:THR:HB	2.02	0.60
1:N:119:LEU:C	1:N:119:LEU:HD23	2.21	0.60
1:U:82:ASN:OD1	1:U:84:GLN:HG2	2.01	0.60
2:A:159:HEM:HBB2	2:A:159:HEM:CMB	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:159:HEM:CBB	2:H:159:HEM:HMB1	2.31	0.60
2:J:159:HEM:CHD	2:J:159:HEM:HBC2	2.24	0.60
1:U:94:GLU:OE1	1:U:127:GLU:HB3	2.01	0.60
1:F:20:ILE:HD11	1:F:75:GLY:HA3	1.83	0.60
1:D:10:HIS:O	1:D:14:ILE:HG12	2.03	0.59
2:F:159:HEM:CBB	2:F:159:HEM:HMB1	2.32	0.59
2:N:159:HEM:HBC2	2:N:159:HEM:CMC	2.32	0.59
2:S:159:HEM:CMB	2:S:159:HEM:HBB2	2.32	0.59
1:W:2:LYS:HE2	1:W:66:GLU:OE2	2.02	0.59
2:K:159:HEM:CBB	2:K:159:HEM:CMB	2.79	0.59
1:Q:20:ILE:HD11	1:Q:75:GLY:HA3	1.84	0.59
1:G:27:LEU:HD23	1:G:79:ILE:HD12	1.84	0.59
1:V:94:GLU:O	1:V:98:THR:HB	2.01	0.59
1:D:94:GLU:O	1:D:98:THR:HB	2.02	0.59
1:I:94:GLU:O	1:I:98:THR:HB	2.02	0.59
1:T:20:ILE:HG23	1:T:77:LEU:HD12	1.84	0.59
1:U:82:ASN:OD1	1:U:85:GLU:HG3	2.03	0.58
1:V:119:LEU:HD21	1:V:123:ILE:HD12	1.85	0.58
1:K:147:GLU:HG3	4:K:633:HOH:O	2.03	0.58
1:X:14:ILE:HD12	1:X:101:LEU:HD13	1.85	0.58
1:O:123:ILE:O	1:O:127:GLU:HG2	2.03	0.58
1:K:20:ILE:HG23	1:K:77:LEU:HD12	1.84	0.58
1:X:139:GLY:O	1:X:143:LYS:HG3	2.04	0.58
1:F:105:ILE:HG23	1:F:117:ARG:HG3	1.86	0.58
1:H:94:GLU:O	1:H:98:THR:HB	2.04	0.58
2:X:159:HEM:HMB3	2:X:159:HEM:HBB2	1.83	0.58
1:J:20:ILE:HD11	1:J:75:GLY:HA3	1.86	0.57
1:L:147:GLU:HG3	4:L:798:HOH:O	2.03	0.57
1:B:20:ILE:HG23	1:B:77:LEU:HD12	1.86	0.57
1:N:52:MET:HB3	2:N:159:HEM:CHB	2.34	0.57
1:V:119:LEU:CD2	1:V:123:ILE:HD12	2.33	0.57
1:T:63:LEU:HD13	1:T:69:PRO:CG	2.34	0.57
1:Q:94:GLU:O	1:Q:98:THR:HB	2.05	0.56
1:A:48:SER:O	1:A:52:MET:HG3	2.05	0.56
2:Q:159:HEM:HBB2	2:Q:159:HEM:CHC	2.31	0.56
1:T:84:GLN:H	1:T:84:GLN:NE2	2.03	0.56
1:X:63:LEU:HD13	1:X:69:PRO:HD3	1.86	0.56
1:E:5:LYS:O	1:E:9:GLN:HG3	2.06	0.56
2:J:159:HEM:HBB2	2:J:159:HEM:HMB1	1.88	0.56
1:N:119:LEU:O	1:N:119:LEU:HD23	2.06	0.56
1:S:94:GLU:O	1:S:98:THR:HB	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:GLU:HG3	4:G:164:HOH:O	2.06	0.56
1:A:81:GLU:CG	1:A:85:GLU:OE2	2.53	0.56
1:J:119:LEU:C	1:J:119:LEU:HD23	2.26	0.56
1:S:94:GLU:OE1	1:S:127:GLU:HB3	2.06	0.55
1:W:52:MET:HB3	2:X:159:HEM:CHB	2.36	0.55
1:X:53:LYS:O	1:X:57:LYS:HG2	2.06	0.55
1:U:94:GLU:O	1:U:98:THR:HB	2.06	0.55
1:U:57:LYS:N	1:U:57:LYS:HD2	2.20	0.55
2:H:159:HEM:CBB	2:H:159:HEM:CMB	2.84	0.55
1:E:38:LYS:HG2	4:E:721:HOH:O	2.06	0.55
1:K:101:LEU:O	1:K:105:ILE:HG13	2.06	0.55
1:R:103:GLU:HG3	4:R:1287:HOH:O	2.07	0.55
2:F:159:HEM:HMB3	2:F:159:HEM:HBB2	1.89	0.55
2:N:159:HEM:CMB	2:N:159:HEM:CBB	2.65	0.55
1:W:18:GLU:OE1	1:W:51:GLU:OE1	2.25	0.55
1:M:52:MET:HB3	2:N:159:HEM:CHD	2.37	0.54
1:S:84:GLN:NE2	1:S:146:LEU:HD13	2.22	0.54
1:A:52:MET:HB3	2:A:159:HEM:CHD	2.37	0.54
1:I:143:LYS:HE3	4:O:674:HOH:O	2.07	0.54
1:F:81:GLU:HG2	1:F:85:GLU:OE2	2.07	0.54
1:K:98:THR:O	1:K:102:ARG:HG3	2.06	0.54
1:O:20:ILE:HD11	1:O:75:GLY:HA3	1.89	0.54
1:T:123:ILE:O	1:T:127:GLU:HG2	2.07	0.54
1:D:147:GLU:HG3	4:D:159:HOH:O	2.06	0.54
1:I:96:LYS:NZ	1:I:100:ASP:OD2	2.40	0.54
1:B:98:THR:HG23	4:B:175:HOH:O	2.07	0.54
1:C:105:ILE:HG23	1:C:117:ARG:HG3	1.89	0.54
1:K:134:LEU:HD11	4:K:1144:HOH:O	2.08	0.54
1:B:38:LYS:HE3	1:B:154:MET:O	2.07	0.54
1:T:84:GLN:CD	1:T:84:GLN:H	2.10	0.54
1:A:143:LYS:HE3	4:X:410:HOH:O	2.07	0.53
1:H:147:GLU:HG3	4:H:160:HOH:O	2.07	0.53
1:I:10:HIS:O	1:I:14:ILE:HG12	2.08	0.53
1:R:59:ILE:O	1:R:63:LEU:HD23	2.08	0.53
1:X:81:GLU:HG2	1:X:85:GLU:OE2	2.07	0.53
1:L:105:ILE:HG23	1:L:117:ARG:HG3	1.90	0.53
1:B:10:HIS:O	1:B:14:ILE:HG12	2.08	0.53
1:D:123:ILE:O	1:D:127:GLU:HG2	2.08	0.53
1:S:63:LEU:HD13	1:S:69:PRO:HD3	1.90	0.53
1:G:63:LEU:HD13	1:G:69:PRO:HD3	1.91	0.53
2:J:159:HEM:CBC	2:J:159:HEM:HHD	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:57:LYS:HD3	4:U:579:HOH:O	2.08	0.53
1:V:111:VAL:O	1:V:112:HIS:HB2	2.09	0.53
1:D:81:GLU:HG2	1:D:85:GLU:OE2	2.08	0.53
2:K:159:HEM:CBB	2:K:159:HEM:HMB1	2.37	0.53
1:B:96:LYS:NZ	1:B:100:ASP:OD2	2.42	0.52
1:C:119:LEU:HD23	1:C:119:LEU:C	2.30	0.52
2:H:159:HEM:CBC	2:H:159:HEM:HMC2	2.32	0.52
2:Q:159:HEM:HHD	2:Q:159:HEM:HBC2	1.91	0.52
1:J:84:GLN:NE2	4:J:927:HOH:O	2.42	0.52
1:O:147:GLU:HG3	4:O:167:HOH:O	2.08	0.52
1:S:119:LEU:HD23	1:S:119:LEU:C	2.30	0.52
1:S:119:LEU:HD23	1:S:119:LEU:O	2.09	0.52
1:B:105:ILE:HG23	1:B:117:ARG:HG3	1.92	0.52
1:C:119:LEU:O	1:C:119:LEU:HD23	2.10	0.52
2:F:159:HEM:CHD	2:F:159:HEM:HBC2	2.33	0.52
1:L:111:VAL:O	1:L:112:HIS:HB2	2.10	0.52
1:G:139:GLY:O	1:G:143:LYS:HG3	2.10	0.52
2:V:159:HEM:CMB	2:V:159:HEM:HBB2	2.40	0.52
1:K:14:ILE:HD12	1:K:101:LEU:HD13	1.91	0.52
1:T:119:LEU:CD2	1:T:119:LEU:C	2.79	0.52
1:S:13:LYS:HD3	4:S:1251:HOH:O	2.09	0.51
1:A:94:GLU:OE2	4:A:1216:HOH:O	2.17	0.51
1:K:105:ILE:HG23	1:K:117:ARG:HG3	1.93	0.51
1:K:139:GLY:O	1:K:143:LYS:HG3	2.11	0.51
2:C:159:HEM:CBC	2:C:159:HEM:HHD	2.32	0.51
1:L:119:LEU:HD23	1:L:120:LEU:N	2.22	0.51
1:G:94:GLU:O	1:G:98:THR:HB	2.10	0.51
2:S:159:HEM:HMB1	2:S:159:HEM:HBB2	1.92	0.51
1:J:18:GLU:OE1	1:J:51:GLU:OE2	2.27	0.51
1:I:84:GLN:NE2	4:I:1248:HOH:O	2.44	0.51
1:X:52:MET:HB3	2:X:159:HEM:CHD	2.41	0.51
1:J:33:ASN:ND2	1:J:41:GLY:HA3	2.26	0.51
1:J:68:LEU:HB3	4:J:739:HOH:O	2.10	0.51
2:K:159:HEM:CHB	1:L:52:MET:HB3	2.41	0.51
4:I:1317:HOH:O	1:O:154:MET:HE3	2.11	0.51
1:K:121:LYS:HE2	1:K:121:LYS:C	2.31	0.50
2:C:159:HEM:CHD	2:C:159:HEM:HBC2	2.20	0.50
1:E:123:ILE:O	1:E:127:GLU:HG2	2.11	0.50
1:X:44:GLU:OE2	1:X:90:ASP:OD2	2.28	0.50
1:J:48:SER:O	1:J:52:MET:HG3	2.12	0.50
1:N:54:HIS:HE1	4:N:1375:HOH:O	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:107:HIS:HE1	4:R:1169:HOH:O	1.92	0.50
1:T:63:LEU:HD13	1:T:69:PRO:CD	2.42	0.50
1:G:76:LYS:O	4:G:1360:HOH:O	2.19	0.50
1:I:54:HIS:HE1	1:I:126:SER:OG	1.94	0.50
1:N:63:LEU:HD13	1:N:69:PRO:CD	2.41	0.50
1:J:9:GLN:HG3	4:J:1457:HOH:O	2.11	0.50
1:O:98:THR:CG2	4:O:1029:HOH:O	2.37	0.50
1:O:94:GLU:O	1:O:98:THR:HB	2.11	0.50
2:P:159:HEM:CBB	2:P:159:HEM:CMB	2.87	0.50
1:R:59:ILE:O	1:R:63:LEU:HD22	2.12	0.50
1:W:119:LEU:HD23	1:W:119:LEU:C	2.32	0.50
2:C:159:HEM:HBB2	2:C:159:HEM:HMB1	1.83	0.50
2:P:159:HEM:HBB2	2:P:159:HEM:HMB1	1.92	0.50
1:S:133:TYR:O	1:S:137:GLN:HG2	2.11	0.50
1:T:98:THR:HG22	1:T:99:LYS:N	2.26	0.50
2:F:159:HEM:O2D	4:F:1019:HOH:O	2.18	0.50
1:Q:52:MET:HB3	2:Q:159:HEM:CHD	2.42	0.50
1:T:63:LEU:HD13	1:T:69:PRO:HD3	1.94	0.50
1:V:52:MET:HB3	2:V:159:HEM:CHB	2.42	0.50
1:R:105:ILE:HG23	1:R:117:ARG:HG3	1.94	0.49
1:S:111:VAL:O	1:S:112:HIS:HB2	2.12	0.49
1:L:22:ILE:HD11	1:L:52:MET:HA	1.93	0.49
1:X:110:GLN:NE2	4:X:1164:HOH:O	2.38	0.49
1:L:14:ILE:HD12	1:L:101:LEU:HD13	1.94	0.49
1:R:33:ASN:ND2	1:R:41:GLY:HA3	2.27	0.49
1:U:105:ILE:HG23	1:U:117:ARG:HG3	1.94	0.49
1:D:121:LYS:HE2	1:D:122:ASP:N	2.27	0.49
1:I:123:ILE:O	1:I:127:GLU:HG2	2.13	0.49
1:U:96:LYS:HD2	1:U:96:LYS:O	2.12	0.49
1:M:130:HIS:CD2	1:M:134:LEU:HD22	2.47	0.49
1:P:105:ILE:HG23	1:P:117:ARG:HG3	1.94	0.48
2:S:159:HEM:CHB	1:T:52:MET:HB3	2.43	0.48
1:C:52:MET:HB3	2:C:159:HEM:CHD	2.43	0.48
1:G:52:MET:HB3	2:H:159:HEM:CHD	2.43	0.48
1:L:95:LEU:O	1:L:98:THR:HG22	2.14	0.48
1:U:14:ILE:HD12	1:U:101:LEU:HD13	1.94	0.48
1:V:63:LEU:HD21	1:V:69:PRO:HG2	1.94	0.48
1:A:63:LEU:HD13	1:A:69:PRO:CD	2.42	0.48
1:D:121:LYS:HB3	1:D:121:LYS:HE2	1.46	0.48
1:S:82:ASN:OD1	1:S:84:GLN:HG2	2.12	0.48
1:J:44:GLU:OE2	1:J:90:ASP:OD2	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:63:LEU:HD13	1:N:69:PRO:HD3	1.95	0.48
1:P:123:ILE:O	1:P:127:GLU:HG2	2.13	0.48
1:U:97:ALA:O	1:U:101:LEU:HD22	2.13	0.48
1:X:57:LYS:NZ	4:X:1040:HOH:O	2.47	0.48
1:T:54:HIS:HE1	4:T:780:HOH:O	1.95	0.48
1:E:10:HIS:O	1:E:14:ILE:HG12	2.14	0.48
1:K:106:VAL:HG23	1:T:114:TYR:OH	2.13	0.48
1:A:22:ILE:HD11	1:A:52:MET:HA	1.96	0.48
2:K:159:HEM:HBB2	2:K:159:HEM:HMB3	1.95	0.47
1:Q:133:TYR:O	1:Q:137:GLN:HG2	2.14	0.47
1:X:94:GLU:O	1:X:98:THR:HB	2.14	0.47
1:H:52:MET:HB3	2:H:159:HEM:CHB	2.44	0.47
1:W:123:ILE:O	1:W:127:GLU:HG2	2.14	0.47
1:I:63:LEU:HD13	1:I:69:PRO:HD3	1.96	0.47
1:M:71:LEU:HD12	1:M:71:LEU:N	2.29	0.47
1:R:107:HIS:CE1	4:R:1169:HOH:O	2.67	0.47
1:R:118:ASP:CG	1:V:121:LYS:HE3	2.35	0.47
1:I:105:ILE:HG23	1:I:117:ARG:HG3	1.96	0.47
1:Q:105:ILE:HG23	1:Q:117:ARG:HG3	1.96	0.47
1:D:63:LEU:HD13	1:D:69:PRO:CD	2.45	0.47
1:M:101:LEU:HD12	1:M:120:LEU:HD22	1.95	0.47
1:O:121:LYS:HB3	1:O:121:LYS:HZ3	1.80	0.47
1:H:98:THR:CG2	4:H:906:HOH:O	2.50	0.47
1:W:45:TYR:OH	4:W:1493:HOH:O	2.20	0.47
1:B:44:GLU:OE2	1:B:90:ASP:OD2	2.33	0.47
1:P:20:ILE:HD11	1:P:75:GLY:HA3	1.96	0.47
1:A:105:ILE:HG23	1:A:117:ARG:HG3	1.97	0.47
2:J:159:HEM:CBB	2:J:159:HEM:HMB1	2.44	0.47
1:D:48:SER:O	1:D:52:MET:HG3	2.14	0.47
1:F:52:MET:HB3	2:F:159:HEM:CHB	2.45	0.47
1:G:55:ALA:O	1:G:59:ILE:HG13	2.15	0.47
1:O:143:LYS:HE3	4:W:1500:HOH:O	2.15	0.47
1:V:119:LEU:CD2	1:V:123:ILE:CD1	2.90	0.47
1:B:140:LEU:O	1:B:144:VAL:HG22	2.15	0.46
1:O:63:LEU:HD13	1:O:69:PRO:HD3	1.95	0.46
1:I:81:GLU:HG2	1:I:85:GLU:OE2	2.16	0.46
1:L:33:ASN:ND2	1:L:41:GLY:HA3	2.30	0.46
1:V:147:GLU:HG3	4:V:409:HOH:O	2.13	0.46
1:V:27:LEU:HD23	1:V:79:ILE:HD12	1.96	0.46
1:B:94:GLU:O	1:B:98:THR:HB	2.15	0.46
2:A:159:HEM:CBB	2:A:159:HEM:CMB	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:159:HEM:CBB	2:P:159:HEM:HMB1	2.44	0.46
1:P:94:GLU:OE1	1:P:127:GLU:OE1	2.34	0.46
1:L:119:LEU:CD2	1:L:120:LEU:N	2.78	0.46
1:W:117:ARG:HD2	4:W:1511:HOH:O	2.16	0.46
1:A:133:TYR:O	1:A:137:GLN:HG2	2.16	0.46
1:V:119:LEU:HD22	1:V:120:LEU:N	2.31	0.46
1:K:94:GLU:O	1:K:98:THR:HB	2.16	0.46
1:T:84:GLN:OE1	1:T:146:LEU:HD13	2.13	0.46
1:S:14:ILE:HD12	1:S:101:LEU:HD13	1.98	0.45
1:B:33:ASN:ND2	1:B:41:GLY:HA3	2.32	0.45
1:I:52:MET:HB3	2:J:159:HEM:C1D	2.51	0.45
1:R:15:LEU:O	1:R:19:LEU:HG	2.16	0.45
1:C:84:GLN:CB	4:C:1467:HOH:O	2.63	0.45
1:L:20:ILE:HD11	1:L:75:GLY:HA3	1.99	0.45
1:X:20:ILE:HG23	1:X:77:LEU:HD12	1.97	0.45
1:C:10:HIS:O	1:C:14:ILE:HG12	2.16	0.45
1:H:63:LEU:HD13	1:H:69:PRO:CD	2.47	0.45
1:L:154:MET:HE3	4:M:522:HOH:O	2.14	0.45
1:K:111:VAL:O	1:K:112:HIS:HB2	2.16	0.45
1:H:38:LYS:HG2	4:H:288:HOH:O	2.17	0.45
1:I:63:LEU:HD13	1:I:69:PRO:CD	2.47	0.45
2:K:159:HEM:CBC	2:K:159:HEM:HHD	2.45	0.45
1:Q:63:LEU:HD13	1:Q:69:PRO:HD3	1.99	0.45
2:X:159:HEM:HHD	2:X:159:HEM:CBC	2.39	0.45
1:X:63:LEU:HD13	1:X:69:PRO:CD	2.47	0.45
1:T:57:LYS:HG2	4:T:923:HOH:O	2.15	0.45
1:V:119:LEU:C	1:V:119:LEU:HD22	2.31	0.45
1:A:54:HIS:HE1	4:A:761:HOH:O	1.98	0.44
1:G:44:GLU:OE2	1:G:90:ASP:OD2	2.35	0.44
1:P:98:THR:O	1:P:102:ARG:HG3	2.17	0.44
2:J:159:HEM:CHD	2:J:159:HEM:CBC	2.95	0.44
2:S:159:HEM:CBB	2:S:159:HEM:HMB1	2.47	0.44
1:U:95:LEU:HD23	1:U:95:LEU:HA	1.72	0.44
1:A:123:ILE:O	1:A:127:GLU:HG2	2.18	0.44
1:H:10:HIS:O	1:H:14:ILE:HG12	2.18	0.44
1:I:52:MET:HB3	2:J:159:HEM:CHD	2.47	0.44
1:R:14:ILE:HD12	4:R:160:HOH:O	2.16	0.44
1:W:33:ASN:ND2	1:W:41:GLY:HA3	2.32	0.44
1:E:4:ASP:HB3	1:E:7:VAL:HB	1.99	0.44
1:K:121:LYS:HE2	1:K:121:LYS:HB3	1.46	0.44
1:Q:84:GLN:NE2	4:Q:497:HOH:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:131:ILE:O	1:R:135:GLU:HG3	2.17	0.44
1:T:18:GLU:OE1	1:T:51:GLU:OE1	2.36	0.44
1:T:44:GLU:OE2	1:T:90:ASP:OD2	2.36	0.44
1:C:20:ILE:HD11	1:C:75:GLY:HA3	1.99	0.44
1:M:54:HIS:HE1	4:M:809:HOH:O	2.00	0.44
1:Q:119:LEU:CD2	1:Q:119:LEU:C	2.84	0.44
2:S:159:HEM:O1D	4:S:1286:HOH:O	2.21	0.44
1:C:98:THR:HG23	4:C:752:HOH:O	2.18	0.44
1:J:117:ARG:HG2	1:J:117:ARG:O	2.11	0.44
1:K:33:ASN:ND2	1:K:41:GLY:HA3	2.33	0.44
1:M:109:GLU:OE1	1:T:117:ARG:NH2	2.44	0.44
2:C:159:HEM:CHB	1:D:52:MET:HB3	2.48	0.44
1:E:94:GLU:O	1:E:98:THR:HB	2.17	0.44
1:F:44:GLU:OE2	1:F:90:ASP:OD2	2.36	0.44
1:V:54:HIS:HE1	1:V:126:SER:OG	2.01	0.44
1:D:38:LYS:HB3	1:D:156:GLU:HG3	1.99	0.44
1:O:121:LYS:HB3	1:O:121:LYS:NZ	2.33	0.44
1:J:27:LEU:HD23	1:J:79:ILE:HD12	2.00	0.43
1:M:119:LEU:C	1:M:119:LEU:CD2	2.84	0.43
1:M:119:LEU:O	1:M:119:LEU:HD23	2.18	0.43
1:S:139:GLY:O	1:S:143:LYS:HG3	2.18	0.43
1:C:133:TYR:O	1:C:137:GLN:HG2	2.17	0.43
1:G:10:HIS:O	1:G:14:ILE:HG12	2.18	0.43
1:W:63:LEU:HD13	1:W:69:PRO:HD3	2.00	0.43
1:B:38:LYS:CE	1:B:154:MET:O	2.66	0.43
1:R:119:LEU:HD23	1:R:119:LEU:C	2.39	0.43
1:X:60:GLU:OE1	4:X:1040:HOH:O	2.21	0.43
1:B:81:GLU:HG2	1:B:85:GLU:OE2	2.19	0.43
1:D:134:LEU:O	1:D:138:LEU:HD22	2.19	0.43
1:E:140:LEU:O	1:E:144:VAL:HG22	2.19	0.43
2:H:159:HEM:CBC	2:H:159:HEM:CMC	2.87	0.43
1:K:123:ILE:O	1:K:127:GLU:HG2	2.19	0.43
1:G:131:ILE:O	1:G:135:GLU:HG3	2.19	0.43
1:G:33:ASN:ND2	1:G:41:GLY:HA3	2.34	0.43
1:J:119:LEU:O	1:J:119:LEU:HD23	2.19	0.43
1:K:119:LEU:C	1:K:119:LEU:HD22	2.35	0.43
1:M:117:ARG:HG2	1:M:117:ARG:O	2.17	0.43
1:V:123:ILE:O	1:V:127:GLU:HG2	2.19	0.43
1:V:44:GLU:OE2	1:V:90:ASP:OD2	2.37	0.43
1:I:54:HIS:CE1	1:I:126:SER:OG	2.71	0.43
1:N:52:MET:HB3	2:N:159:HEM:C4A	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:54:HIS:CE1	1:V:126:SER:OG	2.71	0.43
1:G:133:TYR:HD2	1:G:134:LEU:HD13	1.84	0.43
1:G:57:LYS:HB3	1:G:119:LEU:HD21	1.99	0.43
1:O:54:HIS:HE1	4:O:644:HOH:O	2.01	0.43
1:J:111:VAL:O	1:J:112:HIS:HB2	2.19	0.42
1:P:14:ILE:HD12	1:P:101:LEU:HD13	1.99	0.42
1:V:133:TYR:O	1:V:137:GLN:HG2	2.19	0.42
1:D:117:ARG:NH2	1:E:109:GLU:OE1	2.51	0.42
1:K:140:LEU:O	1:K:144:VAL:HG22	2.19	0.42
1:O:65:LEU:O	1:O:66:GLU:HB2	2.19	0.42
1:Q:63:LEU:HD13	1:Q:69:PRO:CD	2.49	0.42
1:Q:74:LEU:CD2	4:R:1391:HOH:O	2.67	0.42
1:R:123:ILE:O	1:R:127:GLU:HG2	2.19	0.42
1:V:119:LEU:CD2	1:V:120:LEU:N	2.81	0.42
1:F:70:ASN:HA	4:F:1021:HOH:O	2.18	0.42
1:N:119:LEU:CD2	1:N:119:LEU:C	2.87	0.42
1:G:25:TYR:CZ	1:G:130:HIS:HE1	2.38	0.42
1:D:60:GLU:OE1	4:D:1139:HOH:O	2.22	0.42
1:P:52:MET:HB3	2:P:159:HEM:CHB	2.49	0.42
1:H:146:LEU:O	1:H:150:LEU:HG	2.20	0.42
1:A:10:HIS:O	1:A:14:ILE:HG12	2.20	0.42
1:C:119:LEU:CD2	1:C:119:LEU:C	2.88	0.42
1:K:98:THR:HG23	4:K:356:HOH:O	2.02	0.42
1:J:52:MET:HB3	2:J:159:HEM:C4A	2.55	0.42
1:M:33:ASN:ND2	1:M:41:GLY:HA3	2.35	0.42
1:O:119:LEU:HD23	1:O:123:ILE:HD12	2.01	0.42
1:R:101:LEU:HD12	1:R:120:LEU:HD22	2.01	0.42
1:S:119:LEU:CD2	1:S:119:LEU:C	2.88	0.42
1:A:81:GLU:H	1:A:81:GLU:HG2	1.68	0.42
1:C:63:LEU:HD13	1:C:69:PRO:HD3	2.02	0.42
1:Q:52:MET:HB3	2:Q:159:HEM:C4C	2.54	0.42
1:I:25:TYR:OH	1:I:94:GLU:OE2	2.30	0.41
1:L:107:HIS:CE1	4:L:163:HOH:O	2.73	0.41
1:P:95:LEU:HD23	1:P:95:LEU:HA	1.73	0.41
1:T:111:VAL:O	1:T:112:HIS:HB2	2.20	0.41
1:W:94:GLU:O	1:W:98:THR:HB	2.20	0.41
1:X:40:LEU:HA	1:X:40:LEU:HD23	1.94	0.41
1:G:105:ILE:HG23	1:G:117:ARG:HG3	2.02	0.41
1:L:84:GLN:NE2	4:L:1284:HOH:O	2.37	0.41
2:Q:159:HEM:CHB	1:R:52:MET:HB3	2.50	0.41
1:A:38:LYS:HE3	4:A:375:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:GLN:HB3	4:C:1467:HOH:O	2.20	0.41
1:F:117:ARG:O	1:F:117:ARG:HG2	2.19	0.41
1:P:99:LYS:O	1:P:103:GLU:HG3	2.20	0.41
1:U:103:GLU:HG3	4:U:1221:HOH:O	2.20	0.41
1:M:14:ILE:HD12	1:M:101:LEU:HD13	2.03	0.41
1:Q:154:MET:HE3	4:V:530:HOH:O	2.20	0.41
1:R:48:SER:O	1:R:52:MET:HG3	2.21	0.41
1:H:109:GLU:OE1	1:W:117:ARG:NH2	2.47	0.41
1:K:54:HIS:HE1	1:K:126:SER:OG	2.03	0.41
1:S:38:LYS:HD3	4:S:1229:HOH:O	2.19	0.41
1:V:26:PHE:CE1	2:V:159:HEM:CBC	3.02	0.41
1:W:20:ILE:HG23	1:W:77:LEU:HD12	2.03	0.41
1:F:123:ILE:O	1:F:127:GLU:HG2	2.21	0.41
1:F:26:PHE:CE1	2:F:159:HEM:CBC	3.03	0.41
1:Q:15:LEU:O	1:Q:19:LEU:HG	2.21	0.41
1:N:10:HIS:O	1:N:14:ILE:HG12	2.20	0.41
1:O:22:ILE:HD11	1:O:52:MET:HA	2.02	0.41
1:P:20:ILE:HG23	1:P:77:LEU:HD12	2.01	0.41
1:R:61:ARG:NH2	1:R:115:VAL:HB	2.36	0.41
1:U:65:LEU:O	1:U:66:GLU:HB2	2.20	0.41
1:R:54:HIS:HE1	1:R:126:SER:OG	2.03	0.41
1:S:113:ASP:CG	1:S:116:SER:HB2	2.41	0.41
1:C:20:ILE:HG23	1:C:77:LEU:HD12	2.01	0.41
1:E:63:LEU:HD13	1:E:69:PRO:CG	2.50	0.41
1:J:140:LEU:O	1:J:144:VAL:HG22	2.20	0.41
1:N:95:LEU:HA	1:N:95:LEU:HD23	1.89	0.41
1:O:145:GLY:HA2	4:O:776:HOH:O	2.20	0.41
1:O:63:LEU:HD13	1:O:69:PRO:CD	2.51	0.41
1:G:84:GLN:HB2	4:G:165:HOH:O	2.20	0.41
1:L:20:ILE:HG23	1:L:77:LEU:HD12	2.03	0.41
1:W:133:TYR:O	1:W:137:GLN:HG2	2.21	0.41
1:J:52:MET:HB3	2:J:159:HEM:C1B	2.56	0.41
1:R:95:LEU:HA	1:R:95:LEU:HD23	1.85	0.41
2:K:159:HEM:HBC2	2:K:159:HEM:CHD	2.39	0.40
1:B:117:ARG:NH2	1:C:109:GLU:OE1	2.50	0.40
1:H:140:LEU:O	1:H:144:VAL:HG22	2.21	0.40
1:S:52:MET:HB3	2:S:159:HEM:CHD	2.51	0.40
1:T:39:ARG:HD2	1:T:39:ARG:HH11	1.72	0.40
1:E:14:ILE:HD12	1:E:101:LEU:HD13	2.03	0.40
1:H:105:ILE:HG23	1:H:117:ARG:HG3	2.03	0.40
1:K:55:ALA:O	1:K:59:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:9:GLN:HA	4:M:244:HOH:O	2.22	0.40
2:V:159:HEM:CMB	2:V:159:HEM:CBB	2.99	0.40
1:W:121:LYS:HE2	1:W:122:ASP:OD2	2.22	0.40
1:C:39:ARG:HH11	1:C:39:ARG:HD2	1.67	0.40
1:T:130:HIS:O	1:T:134:LEU:HD22	2.22	0.40
1:A:52:MET:HB3	2:A:159:HEM:C4C	2.57	0.40
2:F:159:HEM:O1D	4:F:1204:HOH:O	2.21	0.40
1:I:119:LEU:HD21	1:I:123:ILE:CD1	2.52	0.40
1:K:106:VAL:HG12	1:K:107:HIS:N	2.37	0.40
1:O:9:GLN:HG3	4:O:159:HOH:O	2.20	0.40
1:S:105:ILE:HG23	1:S:117:ARG:HG3	2.03	0.40
1:W:149:TYR:CE1	1:W:153:HIS:CE1	3.10	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	151/158 (96%)	150 (99%)	1 (1%)	0	100	100
1	B	152/158 (96%)	151 (99%)	1 (1%)	0	100	100
1	C	153/158 (97%)	152 (99%)	1 (1%)	0	100	100
1	D	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
1	E	152/158 (96%)	149 (98%)	3 (2%)	0	100	100
1	F	152/158 (96%)	152 (100%)	0	0	100	100
1	G	152/158 (96%)	152 (100%)	0	0	100	100
1	H	153/158 (97%)	153 (100%)	0	0	100	100
1	I	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
1	J	152/158 (96%)	151 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	152/158 (96%)	152 (100%)	0	0	100	100
1	L	152/158 (96%)	151 (99%)	1 (1%)	0	100	100
1	M	152/158 (96%)	151 (99%)	1 (1%)	0	100	100
1	N	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
1	O	152/158 (96%)	151 (99%)	1 (1%)	0	100	100
1	P	152/158 (96%)	151 (99%)	1 (1%)	0	100	100
1	Q	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
1	R	153/158 (97%)	152 (99%)	1 (1%)	0	100	100
1	S	152/158 (96%)	151 (99%)	1 (1%)	0	100	100
1	T	152/158 (96%)	151 (99%)	1 (1%)	0	100	100
1	U	152/158 (96%)	149 (98%)	3 (2%)	0	100	100
1	V	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
1	W	153/158 (97%)	153 (100%)	0	0	100	100
1	X	152/158 (96%)	151 (99%)	1 (1%)	0	100	100
All	All	3651/3792 (96%)	3623 (99%)	28 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	135/144 (94%)	128 (95%)	7 (5%)	27	24
1	B	137/144 (95%)	129 (94%)	8 (6%)	23	20
1	C	135/144 (94%)	128 (95%)	7 (5%)	27	24
1	D	138/144 (96%)	130 (94%)	8 (6%)	23	20
1	E	135/144 (94%)	128 (95%)	7 (5%)	27	24
1	F	136/144 (94%)	127 (93%)	9 (7%)	19	16
1	G	138/144 (96%)	128 (93%)	10 (7%)	17	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	137/144 (95%)	131 (96%)	6 (4%)	33	31
1	I	137/144 (95%)	127 (93%)	10 (7%)	16	13
1	J	136/144 (94%)	131 (96%)	5 (4%)	39	39
1	K	139/144 (96%)	127 (91%)	12 (9%)	12	8
1	L	137/144 (95%)	130 (95%)	7 (5%)	28	25
1	M	136/144 (94%)	128 (94%)	8 (6%)	23	19
1	N	135/144 (94%)	128 (95%)	7 (5%)	27	24
1	O	136/144 (94%)	128 (94%)	8 (6%)	23	19
1	P	137/144 (95%)	128 (93%)	9 (7%)	19	16
1	Q	135/144 (94%)	127 (94%)	8 (6%)	23	19
1	R	138/144 (96%)	131 (95%)	7 (5%)	28	25
1	S	136/144 (94%)	128 (94%)	8 (6%)	23	19
1	T	136/144 (94%)	128 (94%)	8 (6%)	23	19
1	U	138/144 (96%)	129 (94%)	9 (6%)	20	16
1	V	136/144 (94%)	126 (93%)	10 (7%)	16	12
1	W	139/144 (96%)	130 (94%)	9 (6%)	20	16
1	X	137/144 (95%)	131 (96%)	6 (4%)	33	31
All	All	3279/3456 (95%)	3086 (94%)	193 (6%)	23	19

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LEU
1	A	81	GLU
1	A	98	THR
1	A	101	LEU
1	A	117	ARG
1	A	134	LEU
1	A	138	LEU
1	B	63	LEU
1	B	77	LEU
1	B	98	THR
1	B	99	LYS
1	B	101	LEU
1	B	117	ARG
1	B	134	LEU

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Mol	Chain	Res	Type
1	B	138	LEU
1	C	63	LEU
1	C	98	THR
1	C	101	LEU
1	C	118	ASP
1	C	134	LEU
1	C	138	LEU
1	C	156	GLU
1	D	63	LEU
1	D	81	GLU
1	D	98	THR
1	D	101	LEU
1	D	117	ARG
1	D	121	LYS
1	D	134	LEU
1	D	138	LEU
1	E	63	LEU
1	E	98	THR
1	E	101	LEU
1	E	117	ARG
1	E	126	SER
1	E	134	LEU
1	E	138	LEU
1	F	63	LEU
1	F	81	GLU
1	F	98	THR
1	F	99	LYS
1	F	101	LEU
1	F	117	ARG
1	F	126	SER
1	F	134	LEU
1	F	138	LEU
1	G	63	LEU
1	G	77	LEU
1	G	98	THR
1	G	101	LEU
1	G	117	ARG
1	G	119	LEU
1	G	121	LYS
1	G	126	SER
1	G	134	LEU
1	G	138	LEU

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Mol	Chain	Res	Type
1	H	63	LEU
1	H	98	THR
1	H	101	LEU
1	H	117	ARG
1	H	134	LEU
1	H	138	LEU
1	I	6	LYS
1	I	63	LEU
1	I	81	GLU
1	I	98	THR
1	I	101	LEU
1	I	117	ARG
1	I	119	LEU
1	I	126	SER
1	I	134	LEU
1	I	138	LEU
1	J	63	LEU
1	J	101	LEU
1	J	119	LEU
1	J	134	LEU
1	J	138	LEU
1	K	63	LEU
1	K	66	GLU
1	K	98	THR
1	K	99	LYS
1	K	101	LEU
1	K	106	VAL
1	K	117	ARG
1	K	119	LEU
1	K	121	LYS
1	K	126	SER
1	K	134	LEU
1	K	138	LEU
1	L	63	LEU
1	L	77	LEU
1	L	101	LEU
1	L	117	ARG
1	L	119	LEU
1	L	134	LEU
1	L	138	LEU
1	M	63	LEU
1	M	77	LEU

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Mol	Chain	Res	Type
1	M	98	THR
1	M	101	LEU
1	M	117	ARG
1	M	118	ASP
1	M	134	LEU
1	M	138	LEU
1	N	30	ARG
1	N	63	LEU
1	N	98	THR
1	N	101	LEU
1	N	110	GLN
1	N	134	LEU
1	N	138	LEU
1	O	63	LEU
1	O	81	GLU
1	O	96	LYS
1	O	98	THR
1	O	101	LEU
1	O	121	LYS
1	O	134	LEU
1	O	138	LEU
1	P	63	LEU
1	P	77	LEU
1	P	98	THR
1	P	101	LEU
1	P	110	GLN
1	P	117	ARG
1	P	121	LYS
1	P	134	LEU
1	P	138	LEU
1	Q	34	ASP
1	Q	63	LEU
1	Q	77	LEU
1	Q	98	THR
1	Q	101	LEU
1	Q	117	ARG
1	Q	134	LEU
1	Q	138	LEU
1	R	77	LEU
1	R	84	GLN
1	R	96	LYS
1	R	98	THR

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Mol	Chain	Res	Type
1	R	101	LEU
1	R	134	LEU
1	R	138	LEU
1	S	63	LEU
1	S	66	GLU
1	S	84	GLN
1	S	98	THR
1	S	101	LEU
1	S	117	ARG
1	S	134	LEU
1	S	138	LEU
1	T	63	LEU
1	T	66	GLU
1	T	77	LEU
1	T	98	THR
1	T	101	LEU
1	T	117	ARG
1	T	134	LEU
1	T	138	LEU
1	U	57	LYS
1	U	63	LEU
1	U	77	LEU
1	U	98	THR
1	U	101	LEU
1	U	117	ARG
1	U	119	LEU
1	U	134	LEU
1	U	138	LEU
1	V	63	LEU
1	V	66	GLU
1	V	77	LEU
1	V	98	THR
1	V	101	LEU
1	V	117	ARG
1	V	118	ASP
1	V	119	LEU
1	V	134	LEU
1	V	138	LEU
1	W	2	LYS
1	W	34	ASP
1	W	63	LEU
1	W	96	LYS

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Mol	Chain	Res	Type
1	W	98	THR
1	W	101	LEU
1	W	117	ARG
1	W	134	LEU
1	W	138	LEU
1	X	57	LYS
1	X	63	LEU
1	X	98	THR
1	X	101	LEU
1	X	134	LEU
1	X	138	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	54	HIS
1	A	84	GLN
1	A	112	HIS
1	B	33	ASN
1	B	112	HIS
1	C	33	ASN
1	C	54	HIS
1	D	33	ASN
1	D	112	HIS
1	D	130	HIS
1	E	33	ASN
1	E	54	HIS
1	F	33	ASN
1	F	54	HIS
1	G	33	ASN
1	G	54	HIS
1	G	112	HIS
1	G	130	HIS
1	H	33	ASN
1	H	54	HIS
1	H	84	GLN
1	H	112	HIS
1	I	33	ASN
1	I	54	HIS
1	I	84	GLN
1	I	112	HIS

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Mol	Chain	Res	Type
1	J	33	ASN
1	J	54	HIS
1	J	84	GLN
1	K	33	ASN
1	K	54	HIS
1	K	112	HIS
1	L	33	ASN
1	L	112	HIS
1	M	33	ASN
1	M	43	HIS
1	M	155	HIS
1	N	33	ASN
1	N	54	HIS
1	N	110	GLN
1	N	112	HIS
1	O	33	ASN
1	O	54	HIS
1	O	112	HIS
1	P	9	GLN
1	P	33	ASN
1	P	54	HIS
1	Q	33	ASN
1	Q	54	HIS
1	Q	84	GLN
1	R	33	ASN
1	R	54	HIS
1	S	33	ASN
1	S	54	HIS
1	T	33	ASN
1	T	54	HIS
1	U	33	ASN
1	U	54	HIS
1	U	112	HIS
1	V	33	ASN
1	V	54	HIS
1	V	84	GLN
1	V	130	HIS
1	W	33	ASN
1	W	84	GLN
1	W	88	GLN
1	X	33	ASN
1	X	54	HIS

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Mol	Chain	Res	Type
1	X	110	GLN
1	X	112	HIS

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 ⓘ

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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	159	1	28,50,50	1.97	8 (28%)	17,82,82	2.24	9 (52%)
2	HEM	C	159	1	28,50,50	2.02	6 (21%)	17,82,82	3.12	8 (47%)
2	HEM	F	159	1	28,50,50	2.41	10 (35%)	17,82,82	2.54	6 (35%)
2	HEM	H	159	1	28,50,50	2.03	8 (28%)	17,82,82	2.80	8 (47%)
2	HEM	J	159	1	28,50,50	2.23	7 (25%)	17,82,82	2.53	5 (29%)
2	HEM	K	159	1	28,50,50	2.08	8 (28%)	17,82,82	2.55	7 (41%)
2	HEM	N	159	1	28,50,50	2.18	8 (28%)	17,82,82	2.29	7 (41%)
2	HEM	P	159	1	28,50,50	2.26	10 (35%)	17,82,82	2.64	8 (47%)
2	HEM	Q	159	1	28,50,50	2.23	7 (25%)	17,82,82	2.17	9 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	S	159	1	28,50,50	2.54	12 (42%)	17,82,82	2.18	7 (41%)
2	HEM	V	159	1	28,50,50	2.38	12 (42%)	17,82,82	1.98	5 (29%)
2	HEM	X	159	1	28,50,50	2.25	9 (32%)	17,82,82	2.00	4 (23%)

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	159	1	-	0/6/54/54	0/0/8/8
2	HEM	C	159	1	-	0/6/54/54	0/0/8/8
2	HEM	F	159	1	-	0/6/54/54	0/0/8/8
2	HEM	H	159	1	-	0/6/54/54	0/0/8/8
2	HEM	J	159	1	-	0/6/54/54	0/0/8/8
2	HEM	K	159	1	-	0/6/54/54	0/0/8/8
2	HEM	N	159	1	-	0/6/54/54	0/0/8/8
2	HEM	P	159	1	-	0/6/54/54	0/0/8/8
2	HEM	Q	159	1	-	0/6/54/54	0/0/8/8
2	HEM	S	159	1	-	0/6/54/54	0/0/8/8
2	HEM	V	159	1	-	0/6/54/54	0/0/8/8
2	HEM	X	159	1	-	0/6/54/54	0/0/8/8

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	159	HEM	C3C-C2C	-7.20	1.30	1.40
2	V	159	HEM	C3C-C2C	-6.34	1.32	1.40
2	Q	159	HEM	C3B-C2B	-6.15	1.32	1.40
2	P	159	HEM	C3C-C2C	-6.10	1.32	1.40
2	X	159	HEM	C3B-C2B	-6.04	1.32	1.40
2	J	159	HEM	C3C-C2C	-5.99	1.32	1.40
2	N	159	HEM	C3B-C2B	-5.81	1.32	1.40
2	Q	159	HEM	C3C-C2C	-5.66	1.32	1.40
2	S	159	HEM	C3C-C2C	-5.64	1.32	1.40
2	X	159	HEM	C3C-C2C	-5.30	1.33	1.40
2	H	159	HEM	C3B-C2B	-5.24	1.33	1.40
2	J	159	HEM	C3B-C2B	-4.99	1.33	1.40
2	K	159	HEM	C3B-C2B	-4.77	1.34	1.40
2	C	159	HEM	C3B-C2B	-4.70	1.34	1.40
2	C	159	HEM	C3C-C2C	-4.65	1.34	1.40
2	A	159	HEM	C3B-C2B	-4.53	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	159	HEM	C3B-C2B	-4.43	1.34	1.40
2	P	159	HEM	C3B-C2B	-4.42	1.34	1.40
2	F	159	HEM	C3B-C2B	-4.17	1.34	1.40
2	H	159	HEM	C3C-C2C	-3.90	1.35	1.40
2	N	159	HEM	C3C-C2C	-3.69	1.35	1.40
2	A	159	HEM	C3C-C2C	-3.68	1.35	1.40
2	V	159	HEM	C3B-C2B	-3.41	1.35	1.40
2	K	159	HEM	C3C-C2C	-3.31	1.36	1.40
2	X	159	HEM	C4A-CHB	-2.26	1.34	1.40
2	Q	159	HEM	C4A-CHB	-2.21	1.34	1.40
2	X	159	HEM	C1C-NC	2.02	1.39	1.36
2	H	159	HEM	C4C-NC	2.02	1.39	1.36
2	A	159	HEM	C4B-NB	2.04	1.40	1.36
2	J	159	HEM	C3B-CAB	2.05	1.51	1.47
2	P	159	HEM	CMA-C3A	2.07	1.55	1.51
2	V	159	HEM	C1D-ND	2.08	1.40	1.36
2	N	159	HEM	CMC-C2C	2.09	1.56	1.51
2	V	159	HEM	CMB-C2B	2.10	1.56	1.51
2	A	159	HEM	CMA-C3A	2.11	1.55	1.51
2	F	159	HEM	C1A-NA	2.11	1.40	1.36
2	N	159	HEM	CMA-C3A	2.12	1.56	1.51
2	V	159	HEM	CMA-C3A	2.15	1.56	1.51
2	S	159	HEM	C1D-ND	2.15	1.40	1.36
2	X	159	HEM	C3C-CAC	2.16	1.52	1.47
2	F	159	HEM	C4A-NA	2.16	1.40	1.36
2	Q	159	HEM	C3C-CAC	2.18	1.52	1.47
2	H	159	HEM	C3C-CAC	2.22	1.52	1.47
2	Q	159	HEM	CAA-C2A	2.23	1.55	1.52
2	P	159	HEM	C1C-NC	2.26	1.39	1.36
2	K	159	HEM	C4D-ND	2.26	1.39	1.36
2	P	159	HEM	C1D-ND	2.27	1.41	1.36
2	V	159	HEM	C4A-NA	2.28	1.41	1.36
2	S	159	HEM	C3C-CAC	2.28	1.52	1.47
2	F	159	HEM	C3B-CAB	2.29	1.52	1.47
2	X	159	HEM	C4C-NC	2.30	1.39	1.36
2	H	159	HEM	C3B-CAB	2.31	1.52	1.47
2	V	159	HEM	C1B-NB	2.31	1.39	1.36
2	P	159	HEM	C4D-ND	2.31	1.39	1.36
2	X	159	HEM	CMA-C3A	2.33	1.56	1.51
2	K	159	HEM	C3C-CAC	2.34	1.52	1.47
2	F	159	HEM	CAA-C2A	2.35	1.56	1.52
2	V	159	HEM	C1C-NC	2.36	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	159	HEM	C1B-NB	2.42	1.39	1.36
2	C	159	HEM	C4B-NB	2.42	1.41	1.36
2	X	159	HEM	C3B-CAB	2.43	1.52	1.47
2	A	159	HEM	C3B-CAB	2.44	1.52	1.47
2	J	159	HEM	C1B-NB	2.44	1.39	1.36
2	V	159	HEM	CAA-C2A	2.47	1.56	1.52
2	S	159	HEM	C4A-NA	2.49	1.41	1.36
2	P	159	HEM	C3B-CAB	2.55	1.52	1.47
2	J	159	HEM	C4D-ND	2.56	1.39	1.36
2	K	159	HEM	C1D-ND	2.62	1.41	1.36
2	Q	159	HEM	C1C-NC	2.62	1.39	1.36
2	S	159	HEM	C1B-NB	2.66	1.39	1.36
2	C	159	HEM	CMD-C2D	2.66	1.57	1.51
2	S	159	HEM	C4D-ND	2.67	1.39	1.36
2	N	159	HEM	C4B-NB	2.67	1.41	1.36
2	K	159	HEM	C3B-CAB	2.70	1.53	1.47
2	P	159	HEM	C1B-NB	2.75	1.40	1.36
2	S	159	HEM	C4B-NB	2.78	1.42	1.36
2	A	159	HEM	C3C-CAC	2.78	1.53	1.47
2	S	159	HEM	C3B-CAB	2.88	1.53	1.47
2	N	159	HEM	C3C-CAC	2.91	1.53	1.47
2	K	159	HEM	C1C-NC	2.99	1.40	1.36
2	P	159	HEM	C4C-NC	3.06	1.40	1.36
2	V	159	HEM	C3C-CAC	3.12	1.53	1.47
2	H	159	HEM	C4D-ND	3.13	1.40	1.36
2	H	159	HEM	CMD-C2D	3.16	1.58	1.51
2	V	159	HEM	C3B-CAB	3.27	1.54	1.47
2	A	159	HEM	C1C-NC	3.45	1.40	1.36
2	J	159	HEM	C1C-NC	3.46	1.40	1.36
2	S	159	HEM	C4C-NC	3.46	1.40	1.36
2	F	159	HEM	C3C-CAC	3.50	1.54	1.47
2	C	159	HEM	C1C-NC	3.50	1.40	1.36
2	N	159	HEM	C1C-NC	3.62	1.41	1.36
2	F	159	HEM	C1C-NC	3.78	1.41	1.36
2	C	159	HEM	C3D-C2D	4.18	1.50	1.37
2	H	159	HEM	C3D-C2D	4.29	1.50	1.37
2	A	159	HEM	C3D-C2D	4.37	1.50	1.37
2	F	159	HEM	C3D-C2D	4.38	1.50	1.37
2	N	159	HEM	C3D-C2D	4.52	1.51	1.37
2	X	159	HEM	C3D-C2D	4.66	1.51	1.37
2	Q	159	HEM	C3D-C2D	4.82	1.51	1.37
2	J	159	HEM	C3D-C2D	4.83	1.52	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	159	HEM	C3D-C2D	4.91	1.52	1.37
2	V	159	HEM	C3D-C2D	5.04	1.52	1.37
2	K	159	HEM	C3D-C2D	5.04	1.52	1.37
2	P	159	HEM	C3D-C2D	5.29	1.53	1.37
2	S	159	HEM	C1C-NC	5.29	1.43	1.36

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	159	HEM	C1D-C2D-C3D	-6.37	102.56	107.00
2	F	159	HEM	CBD-CAD-C3D	-5.35	102.26	112.47
2	F	159	HEM	C1D-C2D-C3D	-5.35	103.28	107.00
2	A	159	HEM	CBD-CAD-C3D	-5.26	102.44	112.47
2	H	159	HEM	CBD-CAD-C3D	-5.22	102.51	112.47
2	N	159	HEM	CBD-CAD-C3D	-5.13	102.68	112.47
2	K	159	HEM	CBD-CAD-C3D	-5.07	102.80	112.47
2	J	159	HEM	CBD-CAD-C3D	-4.97	102.98	112.47
2	X	159	HEM	CBA-CAA-C2A	-4.95	103.01	112.48
2	P	159	HEM	CMA-C3A-C4A	-4.86	120.99	128.46
2	K	159	HEM	CBA-CAA-C2A	-4.78	103.34	112.48
2	H	159	HEM	C1D-C2D-C3D	-4.74	103.70	107.00
2	C	159	HEM	CMA-C3A-C4A	-4.54	121.49	128.46
2	H	159	HEM	CMA-C3A-C4A	-4.42	121.66	128.46
2	Q	159	HEM	CBD-CAD-C3D	-4.25	104.36	112.47
2	P	159	HEM	C1D-C2D-C3D	-4.16	104.10	107.00
2	S	159	HEM	CBD-CAD-C3D	-4.15	104.55	112.47
2	J	159	HEM	C1D-C2D-C3D	-4.06	104.17	107.00
2	S	159	HEM	CBA-CAA-C2A	-3.81	105.20	112.48
2	C	159	HEM	CAD-CBD-CGD	-3.75	106.25	112.66
2	N	159	HEM	C1D-C2D-C3D	-3.75	104.39	107.00
2	X	159	HEM	CBD-CAD-C3D	-3.69	105.42	112.47
2	H	159	HEM	CBA-CAA-C2A	-3.67	105.47	112.48
2	S	159	HEM	C1D-C2D-C3D	-3.62	104.48	107.00
2	H	159	HEM	CAD-CBD-CGD	-3.61	106.50	112.66
2	C	159	HEM	CBA-CAA-C2A	-3.43	105.92	112.48
2	V	159	HEM	CBD-CAD-C3D	-3.42	105.95	112.47
2	K	159	HEM	C1D-C2D-C3D	-3.36	104.66	107.00
2	P	159	HEM	CBA-CAA-C2A	-3.32	106.13	112.48
2	C	159	HEM	CBD-CAD-C3D	-3.29	106.20	112.47
2	V	159	HEM	C1D-C2D-C3D	-3.27	104.72	107.00
2	J	159	HEM	CBA-CAA-C2A	-3.19	106.38	112.48
2	K	159	HEM	CMA-C3A-C4A	-3.11	123.68	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	159	HEM	C1D-C2D-C3D	-2.98	104.92	107.00
2	C	159	HEM	C3C-C4C-NC	-2.95	105.37	110.94
2	Q	159	HEM	CAD-CBD-CGD	-2.94	107.64	112.66
2	K	159	HEM	C3C-C4C-NC	-2.92	105.44	110.94
2	Q	159	HEM	CBA-CAA-C2A	-2.87	106.99	112.48
2	A	159	HEM	CAD-CBD-CGD	-2.86	107.78	112.66
2	N	159	HEM	CBA-CAA-C2A	-2.79	107.14	112.48
2	P	159	HEM	C3C-C4C-NC	-2.71	105.83	110.94
2	P	159	HEM	CBD-CAD-C3D	-2.68	107.35	112.47
2	S	159	HEM	CMA-C3A-C4A	-2.65	124.39	128.46
2	J	159	HEM	C3C-C4C-NC	-2.63	105.98	110.94
2	F	159	HEM	C3C-C4C-NC	-2.60	106.04	110.94
2	Q	159	HEM	C3C-C4C-NC	-2.38	106.46	110.94
2	P	159	HEM	CAD-CBD-CGD	-2.36	108.64	112.66
2	V	159	HEM	CMC-C2C-C3C	-2.31	120.61	124.89
2	Q	159	HEM	CMA-C3A-C4A	-2.26	125.00	128.46
2	A	159	HEM	C1D-C2D-C3D	-2.20	105.47	107.00
2	F	159	HEM	C3B-C4B-NB	-2.16	106.42	109.21
2	A	159	HEM	CBA-CAA-C2A	-2.15	108.38	112.48
2	S	159	HEM	C3C-C4C-NC	-2.12	106.94	110.94
2	V	159	HEM	C4A-C3A-C2A	-2.08	105.55	107.00
2	F	159	HEM	CBA-CAA-C2A	-2.06	108.54	112.48
2	A	159	HEM	CMA-C3A-C4A	-2.05	125.31	128.46
2	N	159	HEM	C4A-C3A-C2A	-2.05	105.57	107.00
2	Q	159	HEM	C1D-C2D-C3D	-2.05	105.57	107.00
2	N	159	HEM	C3C-C4C-NC	-2.04	107.08	110.94
2	A	159	HEM	C3C-C4C-NC	-2.01	107.14	110.94
2	H	159	HEM	C3C-C4C-NC	-2.01	107.15	110.94
2	A	159	HEM	CMD-C2D-C3D	2.05	128.80	124.94
2	S	159	HEM	CMA-C3A-C2A	2.05	128.81	124.94
2	N	159	HEM	CMC-C2C-C3C	2.08	128.75	124.89
2	X	159	HEM	C4C-C3C-C2C	2.11	108.38	106.90
2	Q	159	HEM	CMA-C3A-C2A	2.15	128.99	124.94
2	Q	159	HEM	CMB-C2B-C3B	2.16	128.90	124.89
2	A	159	HEM	CMC-C2C-C3C	2.41	129.36	124.89
2	K	159	HEM	CMA-C3A-C2A	2.69	130.02	124.94
2	C	159	HEM	CMA-C3A-C2A	2.97	130.54	124.94
2	H	159	HEM	CMA-C3A-C2A	3.41	131.38	124.94
2	S	159	HEM	C4C-C3C-C2C	3.43	109.30	106.90
2	A	159	HEM	C4C-C3C-C2C	3.50	109.34	106.90
2	H	159	HEM	C4C-C3C-C2C	3.57	109.39	106.90
2	P	159	HEM	CMA-C3A-C2A	3.58	131.69	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	159	HEM	C4C-C3C-C2C	3.61	109.42	106.90
2	N	159	HEM	C4C-C3C-C2C	3.62	109.43	106.90
2	V	159	HEM	C4C-C3C-C2C	3.69	109.47	106.90
2	K	159	HEM	C4C-C3C-C2C	4.01	109.70	106.90
2	F	159	HEM	C4C-C3C-C2C	4.80	110.25	106.90
2	P	159	HEM	C4C-C3C-C2C	5.01	110.40	106.90
2	J	159	HEM	C4C-C3C-C2C	5.79	110.94	106.90
2	C	159	HEM	C4C-C3C-C2C	6.14	111.19	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 100 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	159	HEM	6	0
2	C	159	HEM	10	0
2	F	159	HEM	10	0
2	H	159	HEM	10	0
2	J	159	HEM	12	0
2	K	159	HEM	8	0
2	N	159	HEM	9	0
2	P	159	HEM	8	0
2	Q	159	HEM	7	0
2	S	159	HEM	6	0
2	V	159	HEM	5	0
2	X	159	HEM	9	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, 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	153/158 (96%)	-0.47	0 100 100	17, 24, 33, 42	0
1	B	154/158 (97%)	-0.51	0 100 100	16, 24, 33, 39	0
1	C	155/158 (98%)	-0.53	0 100 100	18, 25, 34, 43	0
1	D	154/158 (97%)	-0.55	0 100 100	17, 23, 32, 40	0
1	E	154/158 (97%)	-0.52	0 100 100	18, 26, 34, 41	0
1	F	154/158 (97%)	-0.52	0 100 100	17, 24, 33, 39	0
1	G	154/158 (97%)	-0.47	0 100 100	18, 26, 35, 41	0
1	H	155/158 (98%)	-0.47	0 100 100	15, 23, 33, 42	0
1	I	154/158 (97%)	-0.48	0 100 100	19, 29, 37, 42	0
1	J	154/158 (97%)	-0.49	0 100 100	21, 28, 37, 43	0
1	K	154/158 (97%)	-0.46	0 100 100	20, 28, 38, 42	0
1	L	154/158 (97%)	-0.46	0 100 100	20, 26, 35, 44	0
1	M	154/158 (97%)	-0.52	0 100 100	19, 27, 35, 45	0
1	N	154/158 (97%)	-0.57	0 100 100	19, 25, 34, 43	0
1	O	154/158 (97%)	-0.52	0 100 100	19, 24, 33, 42	0
1	P	154/158 (97%)	-0.48	0 100 100	21, 28, 37, 42	0
1	Q	154/158 (97%)	-0.47	0 100 100	22, 30, 38, 44	0
1	R	155/158 (98%)	-0.45	0 100 100	23, 30, 39, 44	0
1	S	154/158 (97%)	-0.45	0 100 100	22, 28, 36, 41	0
1	T	154/158 (97%)	-0.41	0 100 100	22, 28, 38, 45	0
1	U	154/158 (97%)	-0.51	0 100 100	21, 26, 34, 42	0
1	V	154/158 (97%)	-0.49	0 100 100	21, 29, 38, 43	0
1	W	155/158 (98%)	-0.57	0 100 100	17, 24, 33, 41	0
1	X	154/158 (97%)	-0.59	0 100 100	16, 23, 31, 39	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3699/3792 (97%)	-0.50	0 100 100	15, 26, 36, 45	0

There are no RSRZ outliers to report.

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
3	K	B	159	1/1	1.00	0.11	2.05	20,20,20,20	0
3	K	C	160	1/1	0.99	0.10	1.82	23,23,23,23	0
3	K	A	160	1/1	1.00	0.09	1.65	22,22,22,22	0
2	HEM	X	159	43/43	0.97	0.11	1.63	18,23,34,37	0
3	K	G	159	1/1	1.00	0.09	0.94	23,23,23,23	0
2	HEM	P	159	43/43	0.96	0.10	0.90	24,29,36,38	0
2	HEM	Q	159	43/43	0.97	0.10	0.52	25,31,36,40	0
2	HEM	N	159	43/43	0.97	0.10	0.47	20,26,35,39	0
2	HEM	H	159	43/43	0.97	0.10	0.14	16,22,36,38	0
2	HEM	V	159	43/43	0.96	0.10	0.10	24,28,35,38	0
2	HEM	S	159	43/43	0.97	0.10	0.09	23,28,38,43	0
2	HEM	A	159	43/43	0.97	0.10	0.05	18,22,31,37	0
2	HEM	J	159	43/43	0.96	0.10	-0.11	23,29,37,42	0
2	HEM	C	159	43/43	0.97	0.09	-0.53	18,23,31,35	0
2	HEM	F	159	43/43	0.97	0.10	-0.61	19,25,35,38	0
2	HEM	K	159	43/43	0.96	0.10	-0.62	21,27,34,40	0
3	K	E	159	1/1	0.99	0.07	-1.58	27,27,27,27	0
3	K	N	160	1/1	0.99	0.06	-2.03	26,26,26,26	0

6.5 Other polymers

There are no such residues in this entry.