Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 05:38 PM EDT

PDB ID	:	1SQ3
Title	:	Crystal structures of a novel open pore ferritin from the hyperthermophilic Archaeon Archaeoglobus fulgidus.
Authors	:	Johnson, E.; Cascio, D.; Michael, S.; Schroder, I.
Deposited on	:	2004-03-17
Resolution	:	2.70 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

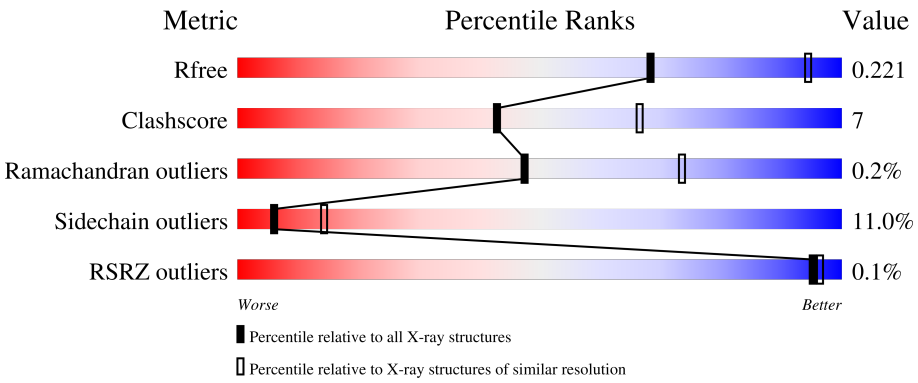
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	173	75% 17% • 6%
1	B	173	75% 17% • 6%
1	C	173	73% 16% • 6%
1	D	173	75% 17% • 6%
1	E	173	77% 16% • 6%

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Mol	Chain	Length	Quality of chain
1	F	173	75% 14% 6%
1	G	173	68% 21% 6%
1	H	173	% 74% 17% 6%
1	I	173	76% 16% 6%
1	J	173	77% 15% 6%
1	K	173	68% 23% 6%
1	L	173	76% 15% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16665 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 ferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	162	1343	862	219	254	8	0	0	0
1	B	162	1343	862	219	254	8	0	0	0
1	C	162	1343	862	219	254	8	0	0	0
1	D	162	1343	862	219	254	8	0	0	0
1	E	162	1343	862	219	254	8	0	0	0
1	F	162	1342	862	218	254	8	0	0	0
1	G	162	1343	862	219	254	8	0	0	0
1	H	162	1343	862	219	254	8	0	0	0
1	I	162	1343	862	219	254	8	0	0	0
1	J	162	1342	862	218	254	8	0	0	0
1	K	162	1342	862	218	254	8	0	0	0
1	L	162	1343	862	219	254	8	0	0	0

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	A	3	3	3	0	0
2	B	3	3	3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	C	3	3	3	0	0
2	D	3	3	3	0	0
2	E	3	3	3	0	0
2	F	3	3	3	0	0
2	G	3	3	3	0	0
2	H	3	3	3	0	0
2	I	3	3	3	0	0
2	J	3	3	3	0	0
2	K	3	3	3	0	0
2	L	3	3	3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	43	44	44	0	1
3	B	18	18	18	0	0
3	C	16	16	16	0	0
3	D	44	44	44	0	0
3	E	69	69	69	0	0
3	F	54	54	54	0	0
3	G	42	42	42	0	0
3	H	19	19	19	0	0
3	I	29	29	29	0	0

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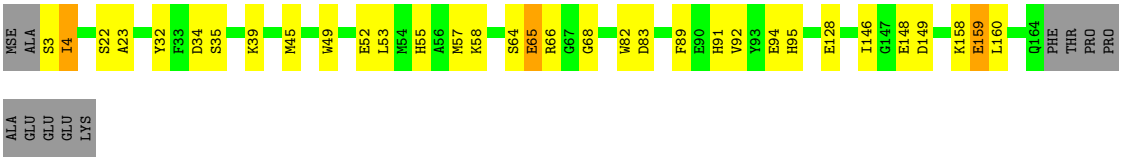
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	J	45	45	45	0	0
			Total	O		
3	K	69	69	69	0	0
			Total	O		
3	L	67	67	67	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

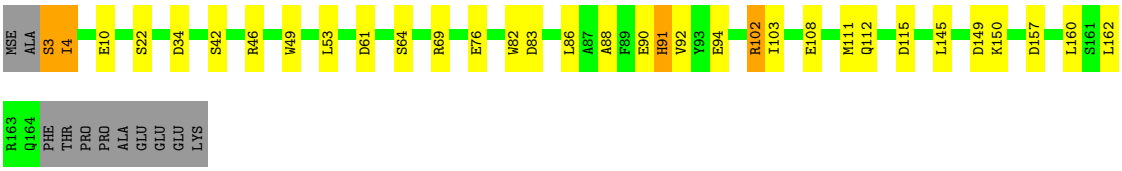
• Molecule 1: ferritin

Chain A:



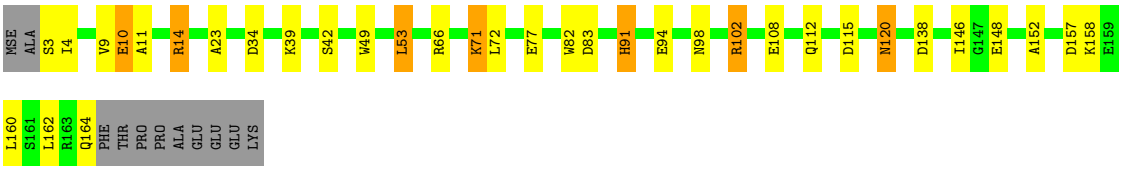
• Molecule 1: ferritin

Chain B:



• Molecule 1: ferritin

Chain C:

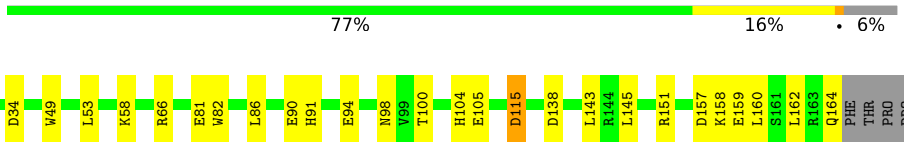


• Molecule 1: ferritin

Chain D:

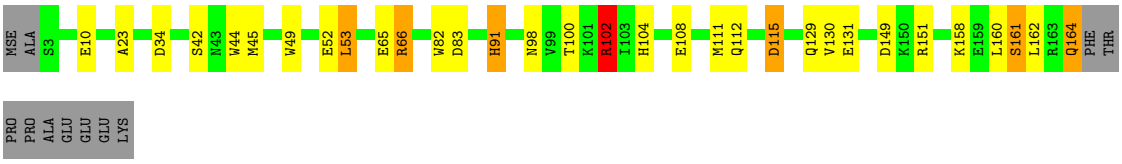
• Molecule 1: ferritin

Chain E:



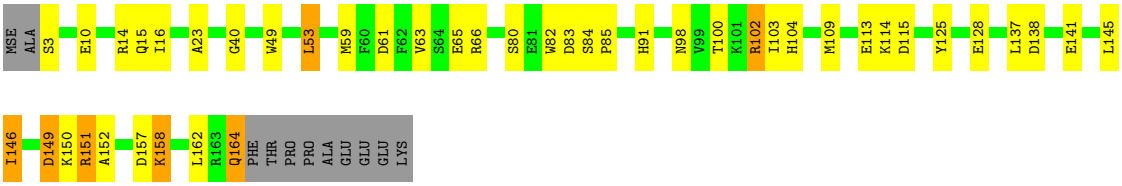
• Molecule 1: ferritin

Chain F:



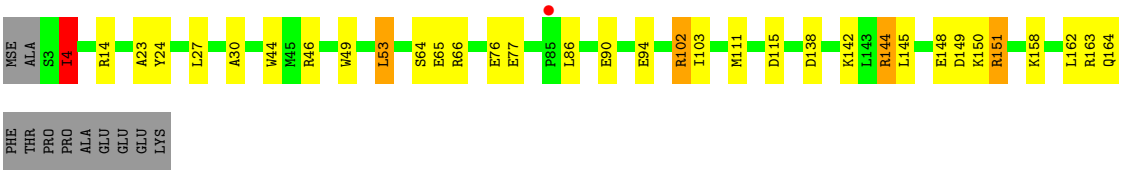
• Molecule 1: ferritin

Chain G:



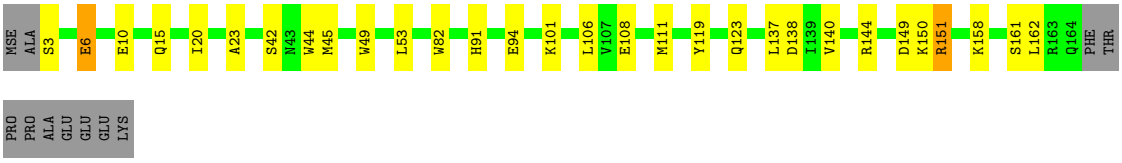
• Molecule 1: ferritin

Chain H:



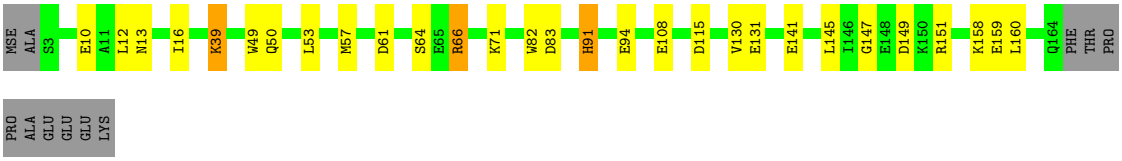
• Molecule 1: ferritin

Chain I:



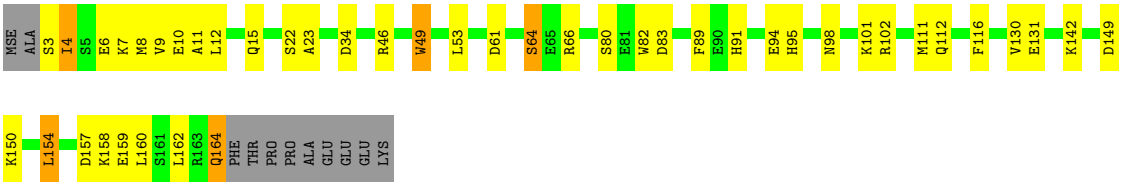
• Molecule 1: ferritin

Chain J:



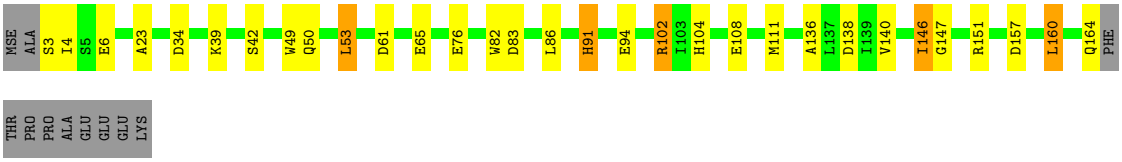
• Molecule 1: ferritin

Chain K:



• Molecule 1: ferritin

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	184.50Å 190.24Å 179.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 74.27 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.70) 99.8 (74.27-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.33 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.177 , 0.218 0.185 , 0.221	Depositor DCC
R_{free} test set	4330 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16665	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FE

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	0.56	0/1365	0.76	3/1827 (0.2%)
1	B	0.80	3/1365 (0.2%)	0.82	6/1827 (0.3%)
1	C	0.60	0/1365	0.76	3/1827 (0.2%)
1	D	0.60	1/1365 (0.1%)	0.79	2/1827 (0.1%)
1	E	0.66	0/1365	0.79	4/1827 (0.2%)
1	F	0.66	0/1363	0.83	6/1822 (0.3%)
1	G	0.59	0/1365	0.83	4/1827 (0.2%)
1	H	0.60	0/1365	0.79	2/1827 (0.1%)
1	I	0.60	0/1365	0.74	2/1827 (0.1%)
1	J	0.61	0/1363	0.78	2/1822 (0.1%)
1	K	0.64	0/1363	0.85	6/1822 (0.3%)
1	L	0.65	0/1365	0.82	5/1827 (0.3%)
All	All	0.63	4/16374 (0.0%)	0.80	45/21909 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4	ILE	N-CA	-16.07	1.14	1.46
1	B	3	SER	N-CA	8.38	1.63	1.46
1	B	3	SER	C-N	6.89	1.49	1.34
1	D	19	GLU	CD-OE1	5.25	1.31	1.25

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	34	ASP	CB-CG-OD2	8.35	125.82	118.30
1	G	61	ASP	CB-CG-OD2	7.85	125.37	118.30
1	J	61	ASP	CB-CG-OD2	7.77	125.30	118.30
1	L	157	ASP	CB-CG-OD2	7.53	125.07	118.30
1	D	61	ASP	CB-CG-OD2	7.39	124.95	118.30
1	H	138	ASP	CB-CG-OD2	7.24	124.81	118.30
1	L	34	ASP	CB-CG-OD2	6.98	124.59	118.30
1	C	138	ASP	CB-CG-OD2	6.87	124.48	118.30
1	E	34	ASP	CB-CG-OD2	6.85	124.46	118.30
1	K	83	ASP	CB-CG-OD2	6.80	124.42	118.30
1	K	149	ASP	CB-CG-OD2	6.76	124.39	118.30
1	F	83	ASP	CB-CG-OD2	6.64	124.28	118.30
1	B	46	ARG	NE-CZ-NH1	-6.59	117.01	120.30
1	K	46	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	E	138	ASP	CB-CG-OD2	6.47	124.12	118.30
1	A	149	ASP	CB-CG-OD2	6.30	123.97	118.30
1	B	83	ASP	CB-CG-OD2	6.27	123.95	118.30
1	K	34	ASP	CB-CG-OD2	6.24	123.91	118.30
1	G	149	ASP	CB-CG-OD2	6.23	123.91	118.30
1	L	138	ASP	CB-CG-OD2	5.96	123.67	118.30
1	G	115	ASP	CB-CG-OD2	5.95	123.66	118.30
1	C	157	ASP	CB-CG-OD2	5.95	123.65	118.30
1	L	61	ASP	CB-CG-OD2	5.94	123.65	118.30
1	D	138	ASP	CB-CG-OD2	5.85	123.57	118.30
1	F	149	ASP	CB-CG-OD2	5.84	123.56	118.30
1	B	149	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	34	ASP	CB-CG-OD2	5.71	123.44	118.30
1	K	61	ASP	CB-CG-OD2	5.67	123.41	118.30
1	B	61	ASP	CB-CG-OD2	5.66	123.39	118.30
1	H	149	ASP	CB-CG-OD2	5.63	123.37	118.30
1	F	115	ASP	CB-CG-OD2	5.49	123.24	118.30
1	K	157	ASP	CB-CG-OD2	5.48	123.23	118.30
1	F	102	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	I	138	ASP	CB-CG-OD2	5.42	123.18	118.30
1	E	157	ASP	CB-CG-OD2	5.41	123.17	118.30
1	C	83	ASP	CB-CG-OD2	5.29	123.06	118.30
1	F	66	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	115	ASP	CB-CG-OD2	5.29	123.06	118.30
1	J	83	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	34	ASP	CB-CG-OD2	5.24	123.01	118.30
1	L	83	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	83	ASP	CB-CG-OD2	5.20	122.97	118.30
1	E	115	ASP	CB-CG-OD2	5.13	122.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	83	ASP	CB-CG-OD2	5.04	122.84	118.30
1	I	149	ASP	CB-CG-OD2	5.04	122.83	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	3	SER	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1343	0	1302	16	0
1	B	1343	0	1302	10	0
1	C	1343	0	1302	22	0
1	D	1343	0	1302	16	0
1	E	1343	0	1302	15	0
1	F	1342	0	1300	19	0
1	G	1343	0	1302	33	0
1	H	1343	0	1302	17	0
1	I	1343	0	1302	18	0
1	J	1342	0	1300	12	0
1	K	1342	0	1300	33	0
1	L	1343	0	1302	22	1
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
2	I	3	0	0	0	0
2	J	3	0	0	0	0
2	K	3	0	0	0	0
2	L	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	44	0	0	2	0
3	B	18	0	0	0	0
3	C	16	0	0	1	0
3	D	44	0	0	1	0
3	E	69	0	0	3	0
3	F	54	0	0	5	0
3	G	42	0	0	4	0
3	H	19	0	0	1	0
3	I	29	0	0	1	1
3	J	45	0	0	0	0
3	K	69	0	0	7	1
3	L	67	0	0	7	0
All	All	16665	0	15618	215	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (215) 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:I:158:LYS:NZ	1:K:159:GLU:HG3	1.27	1.39
1:F:98:ASN:HB2	3:F:957:HOH:O	1.23	1.33
1:K:130:VAL:C	1:K:131:GLU:CA	2.06	1.24
1:F:130:VAL:C	1:F:131:GLU:CA	2.12	1.18
1:J:130:VAL:C	1:J:131:GLU:CA	2.20	1.08
1:C:102:ARG:HH11	1:C:102:ARG:HG3	1.22	1.05
1:I:158:LYS:NZ	1:K:159:GLU:CG	2.24	1.00
1:H:164:GLN:O	3:H:941:HOH:O	1.81	0.97
1:L:102:ARG:CB	3:L:992:HOH:O	2.17	0.93
1:C:39:LYS:HD2	3:E:973:HOH:O	1.71	0.90
1:L:3:SER:HB2	3:L:965:HOH:O	1.71	0.88
1:I:158:LYS:HZ2	1:K:159:GLU:CG	1.87	0.86
1:G:104:HIS:HD1	1:K:116:PHE:HD2	1.15	0.85
1:G:151:ARG:NH2	3:G:942:HOH:O	1.99	0.85
1:I:158:LYS:HZ2	1:K:159:GLU:HG3	1.07	0.85
1:G:114:LYS:HE2	1:J:108:GLU:OE2	1.76	0.85
1:I:158:LYS:HZ1	1:K:159:GLU:HG3	1.04	0.84
1:L:102:ARG:HG3	1:L:102:ARG:HH11	1.39	0.84
1:L:82:TRP:HE1	1:L:91:HIS:HD2	1.22	0.83
1:I:158:LYS:HZ1	1:K:159:GLU:CG	1.87	0.83
1:L:82:TRP:HE1	1:L:91:HIS:CD2	1.97	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:102:ARG:O	1:L:102:ARG:HD2	1.78	0.83
1:F:102:ARG:HH11	1:F:102:ARG:HG3	1.44	0.81
1:E:151:ARG:HD2	3:E:971:HOH:O	1.82	0.79
1:L:3:SER:CB	3:L:965:HOH:O	2.26	0.79
1:F:130:VAL:O	1:F:131:GLU:CA	2.32	0.77
1:F:66:ARG:NH2	1:F:115:ASP:OD1	2.17	0.77
1:F:158:LYS:O	1:F:161:SER:HB2	1.84	0.76
1:F:164:GLN:O	3:F:942:HOH:O	2.04	0.75
1:K:164:GLN:O	3:K:973:HOH:O	2.04	0.75
1:C:164:GLN:O	3:C:923:HOH:O	2.05	0.74
1:A:4:ILE:HG12	1:A:66:ARG:HB3	1.69	0.73
1:J:130:VAL:O	1:J:131:GLU:CA	2.36	0.73
1:L:102:ARG:CG	3:L:992:HOH:O	2.36	0.73
1:E:90:GLU:O	1:E:94:GLU:HG2	1.89	0.73
1:L:102:ARG:HB2	3:L:992:HOH:O	1.81	0.70
1:K:130:VAL:O	1:K:131:GLU:CA	2.42	0.68
1:F:98:ASN:CB	3:F:957:HOH:O	2.05	0.66
1:K:22:SER:OG	1:K:95:HIS:HE1	1.78	0.66
1:B:82:TRP:HE1	1:B:91:HIS:HD2	1.43	0.66
1:G:102:ARG:HH11	1:G:102:ARG:HG3	1.62	0.65
1:D:145:LEU:HD23	1:D:145:LEU:O	1.97	0.64
1:G:104:HIS:CE1	1:K:116:PHE:HB2	2.31	0.64
1:D:39:LYS:HD3	3:D:955:HOH:O	1.97	0.64
1:G:100:THR:HG22	1:G:104:HIS:CD2	2.33	0.64
1:J:82:TRP:HE1	1:J:91:HIS:HD2	1.46	0.64
1:A:82:TRP:HE1	1:A:91:HIS:HD2	1.47	0.63
1:G:102:ARG:HH11	1:G:102:ARG:CG	2.12	0.63
1:G:104:HIS:ND1	1:K:116:PHE:HD2	1.92	0.63
1:A:3:SER:HB3	3:A:943:HOH:O	1.97	0.63
1:C:77:GLU:OE2	1:D:71:LYS:NZ	2.24	0.61
1:B:86:LEU:O	1:B:90:GLU:HG3	2.01	0.60
1:G:164:GLN:O	3:G:959:HOH:O	2.16	0.60
1:C:146:ILE:HG12	1:C:152:ALA:HB1	1.82	0.60
1:F:102:ARG:HG3	1:F:102:ARG:NH1	2.17	0.60
1:D:82:TRP:HE1	1:D:91:HIS:HD2	1.49	0.60
1:K:112:GLN:NE2	3:K:986:HOH:O	2.31	0.59
1:K:91:HIS:HE1	3:K:976:HOH:O	1.85	0.59
1:L:86:LEU:HD12	1:L:86:LEU:O	2.03	0.59
1:L:102:ARG:HG3	3:L:992:HOH:O	2.00	0.58
1:D:88:ALA:O	1:D:92:VAL:HG23	2.04	0.58
1:G:137:LEU:O	1:G:141:GLU:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:GLU:OE1	1:F:158:LYS:HE3	2.04	0.57
1:E:100:THR:O	1:E:104:HIS:HD2	1.87	0.57
1:D:82:TRP:HE1	1:D:91:HIS:CD2	2.22	0.57
1:L:102:ARG:HG3	1:L:102:ARG:NH1	2.16	0.57
1:K:82:TRP:HE1	1:K:91:HIS:HD2	1.53	0.57
1:A:55:HIS:CE1	1:A:128:GLU:HG2	2.39	0.57
1:B:102:ARG:HH11	1:B:102:ARG:HG3	1.69	0.56
1:G:100:THR:HG22	1:G:104:HIS:HD2	1.70	0.56
1:E:82:TRP:HE1	1:E:91:HIS:CD2	2.24	0.56
1:J:66:ARG:NH2	1:J:115:ASP:OD1	2.38	0.56
1:H:27:LEU:O	1:H:30:ALA:HB3	2.06	0.56
1:I:6:GLU:HA	1:I:6:GLU:OE1	2.05	0.56
1:H:151:ARG:HB3	1:H:151:ARG:HH11	1.69	0.55
1:H:4:ILE:HG13	1:H:66:ARG:HB3	1.89	0.55
1:G:82:TRP:HE1	1:G:91:HIS:HD2	1.53	0.55
1:A:58:LYS:NZ	3:A:936:HOH:O	2.35	0.55
1:A:82:TRP:HE1	1:A:91:HIS:CD2	2.23	0.55
1:K:4:ILE:HG23	1:K:66:ARG:NH1	2.22	0.54
1:H:4:ILE:HD12	1:H:4:ILE:N	2.23	0.54
1:L:102:ARG:HD2	1:L:102:ARG:C	2.26	0.54
1:C:102:ARG:HG3	1:C:102:ARG:NH1	2.02	0.54
1:B:82:TRP:HE1	1:B:91:HIS:CD2	2.24	0.54
1:G:104:HIS:HE1	1:K:116:PHE:HB2	1.73	0.54
1:A:22:SER:OG	1:A:95:HIS:HE1	1.90	0.54
1:K:82:TRP:HE1	1:K:91:HIS:CD2	2.25	0.54
1:G:102:ARG:HG3	1:G:102:ARG:NH1	2.23	0.53
1:C:4:ILE:O	1:C:4:ILE:HG23	2.09	0.52
1:G:109:MSE:O	1:G:113:GLU:HG3	2.09	0.52
1:K:66:ARG:HH11	1:K:66:ARG:HG3	1.74	0.52
1:J:57:MSE:HA	1:J:57:MSE:HE2	1.92	0.52
1:I:82:TRP:HE1	1:I:91:HIS:HD2	1.59	0.51
1:K:11:ALA:O	1:K:102:ARG:NH2	2.43	0.51
1:F:82:TRP:HE1	1:F:91:HIS:HD2	1.58	0.51
1:E:82:TRP:HE1	1:E:91:HIS:HD2	1.59	0.50
1:J:12:LEU:O	1:J:16:ILE:HG13	2.10	0.50
1:J:39:LYS:HA	1:J:39:LYS:HE3	1.92	0.50
1:A:57:MSE:HA	1:A:57:MSE:HE2	1.93	0.50
1:F:104:HIS:HB3	3:F:954:HOH:O	2.10	0.50
1:G:103:ILE:HG12	1:G:125:TYR:HB3	1.93	0.50
1:D:159:GLU:O	1:D:162:LEU:HB2	2.12	0.50
1:A:4:ILE:HD11	1:A:68:GLY:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:39:LYS:HA	1:J:39:LYS:CE	2.42	0.49
1:J:82:TRP:HE1	1:J:91:HIS:CD2	2.27	0.49
1:C:23:ALA:CB	1:C:53:LEU:HD13	2.43	0.49
1:H:86:LEU:O	1:H:90:GLU:HG3	2.13	0.49
1:D:100:THR:OG1	1:D:129:GLN:HB3	2.13	0.49
1:E:100:THR:HG22	1:E:104:HIS:CD2	2.48	0.49
1:K:150:LYS:HB2	3:K:1002:HOH:O	2.12	0.49
1:C:82:TRP:HE1	1:C:91:HIS:CD2	2.31	0.48
1:D:116:PHE:CD2	1:E:104:HIS:ND1	2.82	0.48
1:A:4:ILE:H	1:A:4:ILE:HG13	1.47	0.48
1:L:4:ILE:HG23	1:L:4:ILE:O	2.13	0.48
1:F:44:TRP:CE3	1:F:45:MSE:HE2	2.49	0.47
1:E:4:ILE:HG23	1:E:4:ILE:O	2.13	0.47
1:F:23:ALA:HB2	1:F:52:GLU:HB2	1.96	0.47
1:K:8:MSE:HE2	1:K:12:LEU:HG	1.96	0.47
1:H:102:ARG:HA	1:H:102:ARG:HD2	1.67	0.47
1:C:11:ALA:O	1:C:14:ARG:HB2	2.15	0.47
1:I:15:GLN:OE1	1:I:15:GLN:HA	2.13	0.47
1:G:14:ARG:HB2	1:G:102:ARG:HH22	1.79	0.47
1:G:146:ILE:HG12	1:G:152:ALA:HB1	1.96	0.47
1:I:82:TRP:HE1	1:I:91:HIS:CD2	2.32	0.47
1:A:35:SER:HB3	1:B:69:ARG:HD3	1.96	0.47
1:D:116:PHE:HB2	1:E:104:HIS:CE1	2.49	0.47
1:I:158:LYS:O	1:I:161:SER:HB2	2.15	0.47
1:G:82:TRP:HE1	1:G:91:HIS:CD2	2.32	0.47
1:K:150:LYS:HD2	3:K:1002:HOH:O	2.15	0.46
1:B:94:GLU:HA	1:B:94:GLU:OE1	2.14	0.46
1:H:90:GLU:OE1	1:H:144:ARG:NH1	2.49	0.46
1:C:66:ARG:HB3	1:C:66:ARG:NH1	2.30	0.46
1:L:136:ALA:O	1:L:140:VAL:HG23	2.15	0.46
1:D:145:LEU:HD23	1:D:145:LEU:C	2.36	0.46
1:D:116:PHE:HD2	1:E:104:HIS:ND1	2.14	0.45
1:H:102:ARG:HH11	1:H:102:ARG:HG3	1.81	0.45
1:C:102:ARG:HH11	1:C:102:ARG:CG	2.10	0.45
1:B:4:ILE:O	1:B:4:ILE:HG23	2.16	0.45
1:G:40:GLY:HA3	1:G:157:ASP:O	2.16	0.45
1:F:82:TRP:HE1	1:F:91:HIS:CD2	2.35	0.45
1:L:50:GLN:NE2	3:L:1000:HOH:O	2.43	0.45
1:E:66:ARG:NH2	1:E:115:ASP:OD1	2.49	0.44
1:F:66:ARG:HH22	1:F:115:ASP:CG	2.21	0.44
1:G:15:GLN:OE1	1:G:102:ARG:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:LEU:HA	1:E:143:LEU:HD13	1.98	0.44
1:G:16:ILE:HG12	1:G:59:MSE:HB3	1.99	0.44
1:H:102:ARG:HG3	1:H:102:ARG:NH1	2.33	0.44
1:G:150:LYS:NZ	3:G:946:HOH:O	2.48	0.44
1:H:115:ASP:OD1	1:H:115:ASP:C	2.55	0.44
1:K:154:LEU:HD12	1:K:154:LEU:HA	1.80	0.44
1:L:23:ALA:CB	1:L:53:LEU:HD13	2.48	0.44
1:E:81:GLU:OE1	3:E:979:HOH:O	2.21	0.44
1:L:146:ILE:HG22	1:L:147:GLY:O	2.18	0.43
1:G:149:ASP:OD1	1:G:149:ASP:C	2.56	0.43
1:A:45:MSE:HE1	1:A:92:VAL:HG21	2.00	0.43
1:H:151:ARG:HB3	1:H:151:ARG:NH1	2.34	0.43
1:B:88:ALA:O	1:B:92:VAL:HG23	2.18	0.43
1:D:40:GLY:HA3	1:D:157:ASP:O	2.18	0.43
1:C:102:ARG:HA	1:C:102:ARG:HD2	1.77	0.43
1:D:60:PHE:CD2	1:D:70:VAL:HG11	2.53	0.43
1:G:59:MSE:O	1:G:63:VAL:HG23	2.17	0.43
1:A:65:GLU:O	1:A:65:GLU:HG3	2.19	0.43
1:I:151:ARG:HD3	1:I:151:ARG:C	2.39	0.43
1:G:128:GLU:OE1	3:G:948:HOH:O	2.21	0.42
1:D:102:ARG:HE	1:D:102:ARG:HB3	1.55	0.42
1:H:44:TRP:CD1	1:H:163:ARG:HD2	2.54	0.42
1:G:23:ALA:CB	1:G:53:LEU:HD13	2.50	0.42
1:K:4:ILE:CD1	1:K:9:VAL:CG2	2.98	0.42
1:C:39:LYS:HE2	1:C:39:LYS:HA	2.02	0.42
1:G:158:LYS:HB2	1:G:158:LYS:HE3	1.61	0.42
1:J:13:ASN:ND2	1:J:71:LYS:H	2.18	0.42
1:G:84:SER:HB2	1:G:85:PRO:HD2	2.00	0.42
1:F:98:ASN:CG	3:F:957:HOH:O	2.44	0.42
1:G:100:THR:CG2	1:G:104:HIS:CD2	3.01	0.42
1:D:14:ARG:HD3	1:D:14:ARG:HA	1.91	0.42
1:G:66:ARG:HG3	1:G:66:ARG:HH11	1.85	0.42
1:C:10:GLU:HG3	1:C:11:ALA:N	2.34	0.42
1:G:164:GLN:HE21	1:G:164:GLN:HB3	1.48	0.41
1:J:149:ASP:C	1:J:149:ASP:OD1	2.56	0.41
1:B:102:ARG:HG3	1:B:102:ARG:NH1	2.35	0.41
1:L:4:ILE:O	1:L:4:ILE:CG2	2.68	0.41
1:A:23:ALA:HB2	1:A:52:GLU:HB2	2.02	0.41
1:C:91:HIS:HD1	1:C:91:HIS:C	2.24	0.41
1:I:20:ILE:O	1:I:23:ALA:HB3	2.20	0.41
1:K:64:SER:HB3	3:K:966:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:102:ARG:O	1:L:102:ARG:CD	2.59	0.41
1:E:143:LEU:HD23	1:E:143:LEU:HA	1.94	0.41
1:K:4:ILE:HD12	1:K:9:VAL:CG2	2.51	0.41
1:C:115:ASP:OD1	1:C:115:ASP:C	2.59	0.41
1:F:23:ALA:CB	1:F:53:LEU:HD13	2.50	0.41
1:H:23:ALA:CB	1:H:53:LEU:HD13	2.50	0.41
1:H:14:ARG:HB2	1:H:102:ARG:HH22	1.86	0.41
1:I:44:TRP:CE3	1:I:45:MSE:HE2	2.55	0.41
1:F:100:THR:HA	1:F:129:GLN:HG3	2.03	0.41
1:G:138:ASP:OD2	1:L:39:LYS:HE2	2.20	0.41
1:H:46:ARG:HD2	1:H:46:ARG:HA	1.94	0.41
1:H:102:ARG:HH11	1:H:102:ARG:CG	2.34	0.41
1:I:91:HIS:HE1	3:I:945:HOH:O	2.03	0.41
1:I:119:TYR:O	1:I:123:GLN:HG2	2.20	0.41
1:I:137:LEU:O	1:I:140:VAL:HB	2.21	0.41
1:K:23:ALA:HB1	1:K:49:TRP:CE3	2.56	0.41
1:L:160:LEU:HD12	1:L:160:LEU:HA	1.94	0.41
1:A:32:TYR:O	1:A:35:SER:OG	2.32	0.41
1:K:15:GLN:OE1	1:K:102:ARG:HG3	2.20	0.41
1:C:120:ASN:HD22	1:C:120:ASN:HA	1.62	0.40
1:B:69:ARG:HG2	1:B:69:ARG:NH1	2.37	0.40
1:K:150:LYS:CB	3:K:1002:HOH:O	2.67	0.40
1:C:146:ILE:HG12	1:C:152:ALA:CB	2.51	0.40
1:E:4:ILE:O	1:E:4:ILE:CG2	2.69	0.40
1:K:102:ARG:HG2	1:K:102:ARG:HH11	1.86	0.40
1:C:4:ILE:O	1:C:4:ILE:CG2	2.70	0.40
1:C:9:VAL:O	1:C:10:GLU:C	2.60	0.40
1:C:71:LYS:HE3	1:C:72:LEU:O	2.22	0.40
1:K:15:GLN:OE1	1:K:102:ARG:CG	2.69	0.40
1:I:15:GLN:HB2	1:I:106:LEU:HD11	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:952:HOH:O	3:I:952:HOH:O[3_557]	1.85	0.35
1:L:111:MSE:SE	3:K:1002:HOH:O[4_567]	1.91	0.29

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	160/173 (92%)	157 (98%)	3 (2%)	0	100	100
1	B	160/173 (92%)	158 (99%)	2 (1%)	0	100	100
1	C	160/173 (92%)	159 (99%)	1 (1%)	0	100	100
1	D	160/173 (92%)	159 (99%)	1 (1%)	0	100	100
1	E	160/173 (92%)	158 (99%)	2 (1%)	0	100	100
1	F	158/173 (91%)	156 (99%)	2 (1%)	0	100	100
1	G	160/173 (92%)	158 (99%)	2 (1%)	0	100	100
1	H	160/173 (92%)	157 (98%)	2 (1%)	1 (1%)	25	50
1	I	160/173 (92%)	157 (98%)	3 (2%)	0	100	100
1	J	158/173 (91%)	154 (98%)	2 (1%)	2 (1%)	12	30
1	K	158/173 (91%)	155 (98%)	3 (2%)	0	100	100
1	L	160/173 (92%)	160 (100%)	0	0	100	100
All	All	1914/2076 (92%)	1888 (99%)	23 (1%)	3 (0%)	47	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	4	ILE
1	J	145	LEU
1	J	147	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	143/143 (100%)	130 (91%)	13 (9%)	9 21
1	B	143/143 (100%)	125 (87%)	18 (13%)	4 10
1	C	143/143 (100%)	124 (87%)	19 (13%)	4 9
1	D	143/143 (100%)	129 (90%)	14 (10%)	8 18
1	E	143/143 (100%)	130 (91%)	13 (9%)	9 21
1	F	142/143 (99%)	127 (89%)	15 (11%)	6 15
1	G	143/143 (100%)	129 (90%)	14 (10%)	8 18
1	H	143/143 (100%)	123 (86%)	20 (14%)	3 8
1	I	143/143 (100%)	129 (90%)	14 (10%)	8 18
1	J	142/143 (99%)	128 (90%)	14 (10%)	8 18
1	K	142/143 (99%)	122 (86%)	20 (14%)	3 8
1	L	143/143 (100%)	128 (90%)	15 (10%)	7 16
All	All	1713/1716 (100%)	1524 (89%)	189 (11%)	6 14

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	39	LYS
1	A	49	TRP
1	A	53	LEU
1	A	64	SER
1	A	65	GLU
1	A	89	PHE
1	A	94	GLU
1	A	146	ILE
1	A	148	GLU
1	A	158	LYS
1	A	159	GLU
1	A	160	LEU
1	B	10	GLU
1	B	22	SER
1	B	42	SER
1	B	49	TRP
1	B	53	LEU
1	B	64	SER
1	B	76	GLU
1	B	91	HIS
1	B	102	ARG

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Mol	Chain	Res	Type
1	B	103	ILE
1	B	108	GLU
1	B	111	MSE
1	B	112	GLN
1	B	145	LEU
1	B	150	LYS
1	B	157	ASP
1	B	160	LEU
1	B	162	LEU
1	C	3	SER
1	C	10	GLU
1	C	14	ARG
1	C	34	ASP
1	C	42	SER
1	C	49	TRP
1	C	53	LEU
1	C	71	LYS
1	C	91	HIS
1	C	94	GLU
1	C	98	ASN
1	C	102	ARG
1	C	108	GLU
1	C	112	GLN
1	C	120	ASN
1	C	148	GLU
1	C	158	LYS
1	C	160	LEU
1	C	162	LEU
1	D	3	SER
1	D	49	TRP
1	D	53	LEU
1	D	64	SER
1	D	65	GLU
1	D	71	LYS
1	D	94	GLU
1	D	98	ASN
1	D	102	ARG
1	D	103	ILE
1	D	146	ILE
1	D	151	ARG
1	D	158	LYS
1	D	162	LEU

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Mol	Chain	Res	Type
1	E	3	SER
1	E	10	GLU
1	E	49	TRP
1	E	53	LEU
1	E	58	LYS
1	E	98	ASN
1	E	105	GLU
1	E	145	LEU
1	E	158	LYS
1	E	159	GLU
1	E	160	LEU
1	E	162	LEU
1	E	164	GLN
1	F	10	GLU
1	F	42	SER
1	F	49	TRP
1	F	53	LEU
1	F	65	GLU
1	F	91	HIS
1	F	102	ARG
1	F	108	GLU
1	F	111	MSE
1	F	112	GLN
1	F	151	ARG
1	F	160	LEU
1	F	161	SER
1	F	162	LEU
1	F	164	GLN
1	G	3	SER
1	G	10	GLU
1	G	49	TRP
1	G	53	LEU
1	G	65	GLU
1	G	80	SER
1	G	98	ASN
1	G	102	ARG
1	G	145	LEU
1	G	146	ILE
1	G	151	ARG
1	G	158	LYS
1	G	162	LEU
1	G	164	GLN

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Mol	Chain	Res	Type
1	H	4	ILE
1	H	24	TYR
1	H	49	TRP
1	H	53	LEU
1	H	64	SER
1	H	65	GLU
1	H	76	GLU
1	H	77	GLU
1	H	94	GLU
1	H	102	ARG
1	H	103	ILE
1	H	111	MSE
1	H	142	LYS
1	H	144	ARG
1	H	145	LEU
1	H	148	GLU
1	H	150	LYS
1	H	151	ARG
1	H	158	LYS
1	H	162	LEU
1	I	3	SER
1	I	6	GLU
1	I	10	GLU
1	I	42	SER
1	I	49	TRP
1	I	53	LEU
1	I	94	GLU
1	I	101	LYS
1	I	108	GLU
1	I	111	MSE
1	I	144	ARG
1	I	150	LYS
1	I	151	ARG
1	I	162	LEU
1	J	10	GLU
1	J	39	LYS
1	J	49	TRP
1	J	50	GLN
1	J	53	LEU
1	J	64	SER
1	J	66	ARG
1	J	91	HIS

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Mol	Chain	Res	Type
1	J	94	GLU
1	J	141	GLU
1	J	151	ARG
1	J	158	LYS
1	J	159	GLU
1	J	160	LEU
1	K	3	SER
1	K	4	ILE
1	K	6	GLU
1	K	7	LYS
1	K	10	GLU
1	K	49	TRP
1	K	53	LEU
1	K	64	SER
1	K	80	SER
1	K	89	PHE
1	K	94	GLU
1	K	98	ASN
1	K	101	LYS
1	K	111	MSE
1	K	142	LYS
1	K	154	LEU
1	K	158	LYS
1	K	160	LEU
1	K	162	LEU
1	K	164	GLN
1	L	6	GLU
1	L	42	SER
1	L	49	TRP
1	L	53	LEU
1	L	65	GLU
1	L	76	GLU
1	L	91	HIS
1	L	94	GLU
1	L	102	ARG
1	L	104	HIS
1	L	108	GLU
1	L	146	ILE
1	L	151	ARG
1	L	160	LEU
1	L	164	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	50	GLN
1	A	55	HIS
1	A	91	HIS
1	A	95	HIS
1	B	91	HIS
1	B	95	HIS
1	B	120	ASN
1	B	164	GLN
1	C	17	ASN
1	C	120	ASN
1	C	123	GLN
1	D	17	ASN
1	D	112	GLN
1	E	17	ASN
1	E	91	HIS
1	F	17	ASN
1	F	120	ASN
1	G	91	HIS
1	G	164	GLN
1	H	120	ASN
1	H	123	GLN
1	I	17	ASN
1	I	91	HIS
1	I	120	ASN
1	J	43	ASN
1	J	91	HIS
1	K	17	ASN
1	K	91	HIS
1	K	95	HIS
1	K	98	ASN
1	L	43	ASN
1	L	91	HIS
1	L	120	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 36 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	154/173 (89%)	-0.07	0	100	100	10, 18, 30, 35	0
1	B	154/173 (89%)	-0.02	0	100	100	14, 20, 33, 40	0
1	C	154/173 (89%)	-0.08	0	100	100	13, 20, 34, 39	0
1	D	154/173 (89%)	-0.02	0	100	100	12, 18, 32, 37	0
1	E	154/173 (89%)	-0.15	0	100	100	10, 17, 31, 37	0
1	F	154/173 (89%)	-0.08	0	100	100	11, 19, 33, 38	0
1	G	154/173 (89%)	-0.08	0	100	100	12, 18, 31, 37	0
1	H	154/173 (89%)	0.21	1 (0%)	89	91	14, 21, 34, 45	0
1	I	154/173 (89%)	-0.15	0	100	100	13, 21, 32, 37	0
1	J	154/173 (89%)	-0.00	0	100	100	11, 19, 31, 36	0
1	K	154/173 (89%)	-0.06	0	100	100	8, 16, 30, 37	0
1	L	154/173 (89%)	-0.16	0	100	100	11, 18, 32, 38	0
All	All	1848/2076 (89%)	-0.05	1 (0%)	95	96	8, 19, 32, 45	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	85	PRO	2.2

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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
2	FE	B	904	1/1	0.91	0.16	55,55,55,55	0
2	FE	B	906	1/1	0.92	0.15	68,68,68,68	0
2	FE	B	905	1/1	0.95	0.15	57,57,57,57	0
2	FE	I	925	1/1	0.95	0.17	50,50,50,50	0
2	FE	J	928	1/1	0.95	0.18	51,51,51,51	0
2	FE	H	924	1/1	0.96	0.13	60,60,60,60	0
2	FE	E	913	1/1	0.96	0.19	42,42,42,42	0
2	FE	I	926	1/1	0.96	0.13	56,56,56,56	0
2	FE	I	927	1/1	0.96	0.10	67,67,67,67	0
2	FE	H	922	1/1	0.96	0.17	51,51,51,51	0
2	FE	D	911	1/1	0.97	0.15	51,51,51,51	0
2	FE	C	909	1/1	0.97	0.14	55,55,55,55	0
2	FE	G	919	1/1	0.97	0.19	49,49,49,49	0
2	FE	G	920	1/1	0.97	0.14	49,49,49,49	0
2	FE	D	910	1/1	0.97	0.17	50,50,50,50	0
2	FE	J	929	1/1	0.97	0.14	50,50,50,50	0
2	FE	L	934	1/1	0.97	0.15	43,43,43,43	0
2	FE	A	903	1/1	0.98	0.15	55,55,55,55	0
2	FE	H	923	1/1	0.98	0.14	58,58,58,58	0
2	FE	E	915	1/1	0.98	0.16	49,49,49,49	0
2	FE	F	916	1/1	0.98	0.17	44,44,44,44	0
2	FE	F	917	1/1	0.98	0.18	46,46,46,46	0
2	FE	F	918	1/1	0.98	0.10	57,57,57,57	0
2	FE	A	901	1/1	0.98	0.17	50,50,50,50	0
2	FE	C	908	1/1	0.98	0.17	58,58,58,58	0
2	FE	J	930	1/1	0.98	0.15	56,56,56,56	0
2	FE	G	921	1/1	0.98	0.14	50,50,50,50	0
2	FE	L	935	1/1	0.98	0.18	44,44,44,44	0
2	FE	A	902	1/1	0.99	0.15	47,47,47,47	0
2	FE	E	914	1/1	0.99	0.15	42,42,42,42	0
2	FE	K	931	1/1	0.99	0.14	43,43,43,43	0
2	FE	K	932	1/1	0.99	0.16	42,42,42,42	0
2	FE	K	933	1/1	0.99	0.13	47,47,47,47	0
2	FE	C	907	1/1	0.99	0.17	52,52,52,52	0
2	FE	D	912	1/1	0.99	0.12	54,54,54,54	0
2	FE	L	936	1/1	0.99	0.13	52,52,52,52	0

6.5 Other polymers (i)

There are no such residues in this entry.