



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 10, 2017 – 09:39 PM EST

PDB ID : 5LS9  
Title : Humanized Archaeal ferritin  
Authors : Baiocco, P.; Trabuco, M.C.; Boffi, A.  
Deposited on : 2016-08-23  
Resolution : 2.93 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

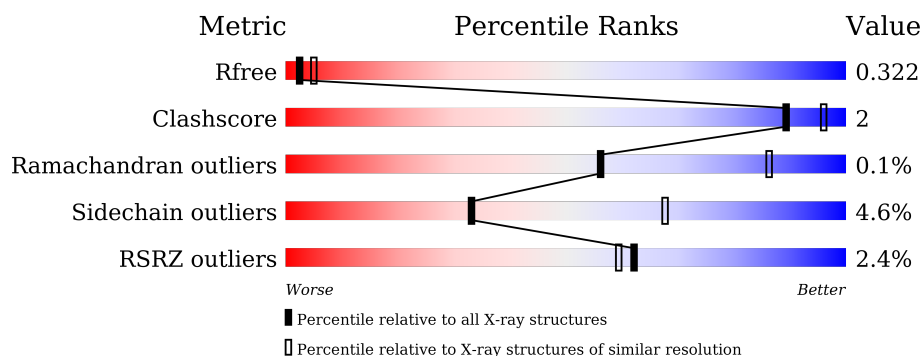
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.93 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2057 (2.98-2.90)
Clashscore	102246	2308 (2.98-2.90)
Ramachandran outliers	100387	2245 (2.98-2.90)
Sidechain outliers	100360	2247 (2.98-2.90)
RSRZ outliers	91569	2065 (2.98-2.90)

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  $\geq 3$ , 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	173	<div> <div>3%</div> <div>86% 8% 5%</div> </div>
1	B	173	<div> <div>3%</div> <div>85% 9% 6%</div> </div>
1	C	173	<div> <div></div> <div>85% 9% 6%</div> </div>
1	D	173	<div> <div></div> <div>82% 13% 6%</div> </div>
1	E	173	<div> <div>%</div> <div>86% 8% 6%</div> </div>
1	F	173	<div> <div>5%</div> <div>89% 6% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	173	<div><div></div><div>79%</div><div>15%</div><div>• 5%</div></div>
1	H	173	<div><div>8%</div><div></div><div>84%</div><div>10%</div><div>6%</div></div>
1	I	173	<div><div>%</div><div></div><div>82%</div><div>12%</div><div>• 6%</div></div>
1	J	173	<div><div></div><div>88%</div><div>6%</div><div>5%</div></div>
1	K	173	<div><div>4%</div><div></div><div>87%</div><div>8%</div><div>• 5%</div></div>
1	L	173	<div><div>3%</div><div></div><div>82%</div><div>13%</div><div>5%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16350 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, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1365	877	223	257	8			
1	B	163	Total	C	N	O	S	0	0	0
			1358	873	222	255	8			
1	C	163	Total	C	N	O	S	0	0	0
			1358	873	222	255	8			
1	D	163	Total	C	N	O	S	0	0	0
			1358	873	222	255	8			
1	E	163	Total	C	N	O	S	0	0	0
			1358	873	222	255	8			
1	F	165	Total	C	N	O	S	0	0	0
			1372	882	224	258	8			
1	G	164	Total	C	N	O	S	0	0	0
			1363	876	223	256	8			
1	H	163	Total	C	N	O	S	0	0	0
			1352	867	222	255	8			
1	I	163	Total	C	N	O	S	0	0	0
			1358	873	222	255	8			
1	J	164	Total	C	N	O	S	0	0	0
			1363	876	223	256	8			
1	K	164	Total	C	N	O	S	0	0	0
			1365	877	223	257	8			
1	L	164	Total	C	N	O	S	0	0	0
			1365	877	223	257	8			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	CYS	MET	engineered mutation	UNP O29424
A	70	ILE	VAL	engineered mutation	UNP O29424
A	71	PHE	LYS	engineered mutation	UNP O29424
A	73	GLN	TYR	engineered mutation	UNP O29424
A	74	ASP	ALA	engineered mutation	UNP O29424

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Chain	Residue	Modelled	Actual	Comment	Reference
A	75	ILE	VAL	engineered mutation	UNP O29424
A	76	LYS	GLU	engineered mutation	UNP O29424
A	77	LYS	GLU	engineered mutation	UNP O29424
A	79	ASP	PRO	engineered mutation	UNP O29424
A	83	GLU	ASP	engineered mutation	UNP O29424
B	54	CYS	MET	engineered mutation	UNP O29424
B	70	ILE	VAL	engineered mutation	UNP O29424
B	71	PHE	LYS	engineered mutation	UNP O29424
B	73	GLN	TYR	engineered mutation	UNP O29424
B	74	ASP	ALA	engineered mutation	UNP O29424
B	75	ILE	VAL	engineered mutation	UNP O29424
B	76	LYS	GLU	engineered mutation	UNP O29424
B	77	LYS	GLU	engineered mutation	UNP O29424
B	79	ASP	PRO	engineered mutation	UNP O29424
B	83	GLU	ASP	engineered mutation	UNP O29424
C	54	CYS	MET	engineered mutation	UNP O29424
C	70	ILE	VAL	engineered mutation	UNP O29424
C	71	PHE	LYS	engineered mutation	UNP O29424
C	73	GLN	TYR	engineered mutation	UNP O29424
C	74	ASP	ALA	engineered mutation	UNP O29424
C	75	ILE	VAL	engineered mutation	UNP O29424
C	76	LYS	GLU	engineered mutation	UNP O29424
C	77	LYS	GLU	engineered mutation	UNP O29424
C	79	ASP	PRO	engineered mutation	UNP O29424
C	83	GLU	ASP	engineered mutation	UNP O29424
D	54	CYS	MET	engineered mutation	UNP O29424
D	70	ILE	VAL	engineered mutation	UNP O29424
D	71	PHE	LYS	engineered mutation	UNP O29424
D	73	GLN	TYR	engineered mutation	UNP O29424
D	74	ASP	ALA	engineered mutation	UNP O29424
D	75	ILE	VAL	engineered mutation	UNP O29424
D	76	LYS	GLU	engineered mutation	UNP O29424
D	77	LYS	GLU	engineered mutation	UNP O29424
D	79	ASP	PRO	engineered mutation	UNP O29424
D	83	GLU	ASP	engineered mutation	UNP O29424
E	54	CYS	MET	engineered mutation	UNP O29424
E	70	ILE	VAL	engineered mutation	UNP O29424
E	71	PHE	LYS	engineered mutation	UNP O29424
E	73	GLN	TYR	engineered mutation	UNP O29424
E	74	ASP	ALA	engineered mutation	UNP O29424
E	75	ILE	VAL	engineered mutation	UNP O29424
E	76	LYS	GLU	engineered mutation	UNP O29424

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Chain	Residue	Modelled	Actual	Comment	Reference
E	77	LYS	GLU	engineered mutation	UNP O29424
E	79	ASP	PRO	engineered mutation	UNP O29424
E	83	GLU	ASP	engineered mutation	UNP O29424
F	54	CYS	MET	engineered mutation	UNP O29424
F	70	ILE	VAL	engineered mutation	UNP O29424
F	71	PHE	LYS	engineered mutation	UNP O29424
F	73	GLN	TYR	engineered mutation	UNP O29424
F	74	ASP	ALA	engineered mutation	UNP O29424
F	75	ILE	VAL	engineered mutation	UNP O29424
F	76	LYS	GLU	engineered mutation	UNP O29424
F	77	LYS	GLU	engineered mutation	UNP O29424
F	79	ASP	PRO	engineered mutation	UNP O29424
F	83	GLU	ASP	engineered mutation	UNP O29424
G	54	CYS	MET	engineered mutation	UNP O29424
G	70	ILE	VAL	engineered mutation	UNP O29424
G	71	PHE	LYS	engineered mutation	UNP O29424
G	73	GLN	TYR	engineered mutation	UNP O29424
G	74	ASP	ALA	engineered mutation	UNP O29424
G	75	ILE	VAL	engineered mutation	UNP O29424
G	76	LYS	GLU	engineered mutation	UNP O29424
G	77	LYS	GLU	engineered mutation	UNP O29424
G	79	ASP	PRO	engineered mutation	UNP O29424
G	83	GLU	ASP	engineered mutation	UNP O29424
H	54	CYS	MET	engineered mutation	UNP O29424
H	70	ILE	VAL	engineered mutation	UNP O29424
H	71	PHE	LYS	engineered mutation	UNP O29424
H	73	GLN	TYR	engineered mutation	UNP O29424
H	74	ASP	ALA	engineered mutation	UNP O29424
H	75	ILE	VAL	engineered mutation	UNP O29424
H	76	LYS	GLU	engineered mutation	UNP O29424
H	77	LYS	GLU	engineered mutation	UNP O29424
H	79	ASP	PRO	engineered mutation	UNP O29424
H	83	GLU	ASP	engineered mutation	UNP O29424
I	54	CYS	MET	engineered mutation	UNP O29424
I	70	ILE	VAL	engineered mutation	UNP O29424
I	71	PHE	LYS	engineered mutation	UNP O29424
I	73	GLN	TYR	engineered mutation	UNP O29424
I	74	ASP	ALA	engineered mutation	UNP O29424
I	75	ILE	VAL	engineered mutation	UNP O29424
I	76	LYS	GLU	engineered mutation	UNP O29424
I	77	LYS	GLU	engineered mutation	UNP O29424
I	79	ASP	PRO	engineered mutation	UNP O29424

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Chain	Residue	Modelled	Actual	Comment	Reference
I	83	GLU	ASP	engineered mutation	UNP O29424
J	54	CYS	MET	engineered mutation	UNP O29424
J	70	ILE	VAL	engineered mutation	UNP O29424
J	71	PHE	LYS	engineered mutation	UNP O29424
J	73	GLN	TYR	engineered mutation	UNP O29424
J	74	ASP	ALA	engineered mutation	UNP O29424
J	75	ILE	VAL	engineered mutation	UNP O29424
J	76	LYS	GLU	engineered mutation	UNP O29424
J	77	LYS	GLU	engineered mutation	UNP O29424
J	79	ASP	PRO	engineered mutation	UNP O29424
J	83	GLU	ASP	engineered mutation	UNP O29424
K	54	CYS	MET	engineered mutation	UNP O29424
K	70	ILE	VAL	engineered mutation	UNP O29424
K	71	PHE	LYS	engineered mutation	UNP O29424
K	73	GLN	TYR	engineered mutation	UNP O29424
K	74	ASP	ALA	engineered mutation	UNP O29424
K	75	ILE	VAL	engineered mutation	UNP O29424
K	76	LYS	GLU	engineered mutation	UNP O29424
K	77	LYS	GLU	engineered mutation	UNP O29424
K	79	ASP	PRO	engineered mutation	UNP O29424
K	83	GLU	ASP	engineered mutation	UNP O29424
L	54	CYS	MET	engineered mutation	UNP O29424
L	70	ILE	VAL	engineered mutation	UNP O29424
L	71	PHE	LYS	engineered mutation	UNP O29424
L	73	GLN	TYR	engineered mutation	UNP O29424
L	74	ASP	ALA	engineered mutation	UNP O29424
L	75	ILE	VAL	engineered mutation	UNP O29424
L	76	LYS	GLU	engineered mutation	UNP O29424
L	77	LYS	GLU	engineered mutation	UNP O29424
L	79	ASP	PRO	engineered mutation	UNP O29424
L	83	GLU	ASP	engineered mutation	UNP O29424

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	I	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is water.

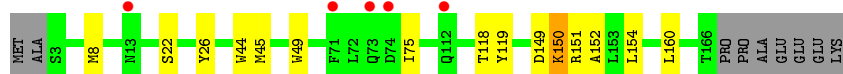
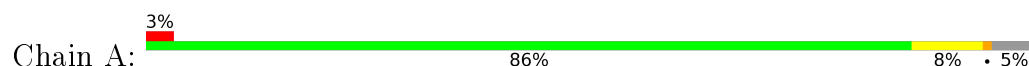
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	3	Total 3	O 3	0	0
3	D	1	Total 1	O 1	0	0
3	E	1	Total 1	O 1	0	0
3	F	2	Total 2	O 2	0	0
3	G	1	Total 1	O 1	0	0
3	H	1	Total 1	O 1	0	0
3	I	1	Total 1	O 1	0	0
3	K	1	Total 1	O 1	0	0
3	L	2	Total 2	O 2	0	0



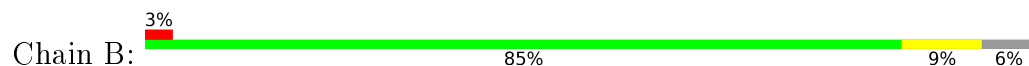
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

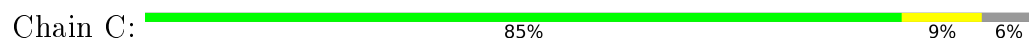
- Molecule 1: Ferritin, putative



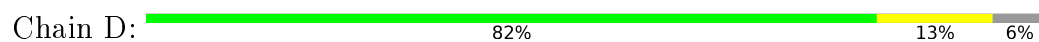
- Molecule 1: Ferritin, putative



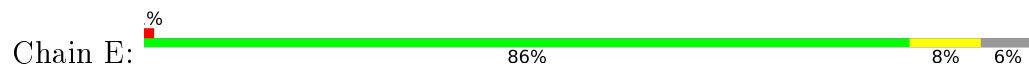
- Molecule 1: Ferritin, putative



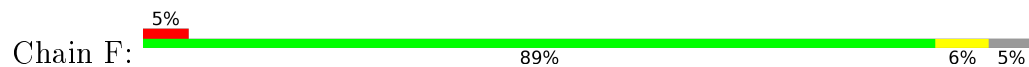
- Molecule 1: Ferritin, putative



- Molecule 1: Ferritin, putative



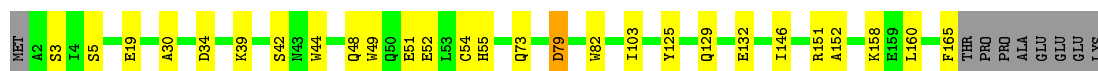
- Molecule 1: Ferritin, putative





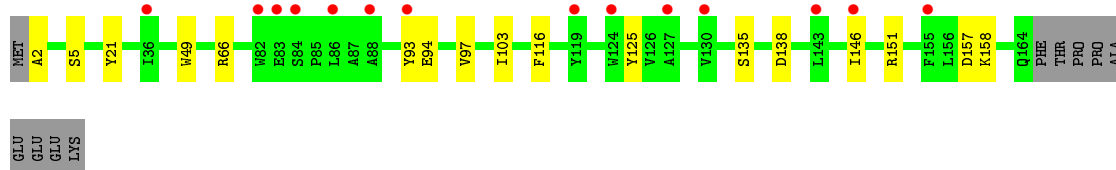
- Molecule 1: Ferritin, putative

Chain G: 79% 15% 5%



- Molecule 1: Ferritin, putative

Chain H: 8% 84% 10% 6%



- Molecule 1: Ferritin, putative

Chain I: % 82% 12% 6%



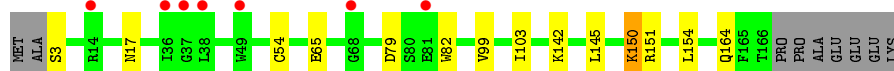
- Molecule 1: Ferritin, putative

Chain J: 88% 6% 5%



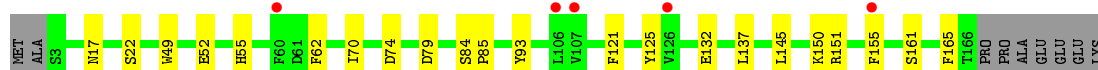
- Molecule 1: Ferritin, putative

Chain K: 4% 87% 8% 5%



- Molecule 1: Ferritin, putative

Chain L: 3% 82% 13% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.80Å 190.65Å 176.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.69 – 2.93 49.69 – 2.93	Depositor EDS
% Data completeness (in resolution range)	89.0 (49.69-2.93) 93.8 (49.69-2.93)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.277 , 0.302 0.290 , 0.322	Depositor DCC
$R_{free}$ test set	3239 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.7	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 31.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
Reported twinning fraction	0.846 for H, K, L 0.154 for K, H, -L	Depositor
Outliers	0 of 63466 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	16350	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG

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	0.37	0/1395	0.54	0/1878
1	B	0.36	0/1388	0.51	0/1868
1	C	0.40	0/1388	0.55	0/1868
1	D	0.40	0/1388	0.55	0/1868
1	E	0.36	0/1388	0.52	0/1868
1	F	0.37	0/1403	0.51	0/1890
1	G	0.38	0/1393	0.52	0/1875
1	H	0.35	0/1381	0.54	0/1859
1	I	0.39	0/1388	0.56	0/1868
1	J	0.40	0/1393	0.54	0/1875
1	K	0.37	0/1395	0.53	0/1878
1	L	0.36	0/1395	0.54	0/1878
All	All	0.38	0/16695	0.53	0/22473

There are no bond length outliers.

There are no bond angle outliers.

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	1365	0	1325	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1358	0	1318	7	0
1	C	1358	0	1318	9	0
1	D	1358	0	1318	8	0
1	E	1358	0	1318	7	1
1	F	1372	0	1332	6	0
1	G	1363	0	1323	14	0
1	H	1352	0	1314	7	0
1	I	1358	0	1318	8	0
1	J	1363	0	1323	7	0
1	K	1365	0	1325	3	0
1	L	1365	0	1325	8	0
2	F	1	0	0	0	0
2	I	1	0	0	0	0
3	C	3	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	2	0	0	0	0
3	G	1	0	0	1	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
3	L	2	0	0	0	0
All	All	16350	0	15857	78	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (78) 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:E:51:GLU:OE1	1:E:163:ARG:NH2	2.30	0.65
1:A:152:ALA:HB2	1:F:151:ARG:HB3	1.79	0.64
1:C:125:TYR:O	1:C:129:GLN:HG2	2.01	0.61
1:C:75:ILE:HB	1:D:75:ILE:HB	1.83	0.60
1:F:103:ILE:HD13	1:F:125:TYR:HB3	1.85	0.58
1:G:44:TRP:CD1	1:G:160:LEU:HD23	2.38	0.58
1:C:151:ARG:HD2	1:E:151:ARG:HB3	1.85	0.57
1:I:70:ILE:O	1:J:31:SER:OG	2.12	0.56
1:J:146:ILE:HG23	1:J:152:ALA:HB3	1.89	0.55
1:L:52:GLU:OE2	1:L:132:GLU:OE1	2.26	0.54
1:E:32:TYR:O	1:E:35:SER:OG	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:TRP:CD1	1:A:160:LEU:HD22	2.44	0.53
1:G:39:LYS:CE	1:G:39:LYS:HA	2.39	0.52
1:D:12:LEU:O	1:D:15:GLN:N	2.40	0.51
1:B:55:HIS:O	1:B:125:TYR:OH	2.24	0.51
1:G:51:GLU:O	1:G:55:HIS:CD2	2.64	0.51
1:A:26:TYR:O	1:A:45:MET:HB3	2.10	0.51
1:G:52:GLU:OE1	3:G:201:HOH:O	2.19	0.51
1:D:22:SER:O	1:D:26:TYR:CD2	2.64	0.50
1:G:30:ALA:O	1:G:34:ASP:HB2	2.12	0.50
1:B:67:GLY:HA3	1:H:2:ALA:HB3	1.92	0.50
1:I:26:TYR:OH	1:I:96:GLU:OE2	2.22	0.49
1:G:152:ALA:N	1:L:151:ARG:HG3	2.26	0.49
1:L:62:PHE:HB2	1:L:121:PHE:CE2	2.47	0.49
1:L:55:HIS:O	1:L:125:TYR:OH	2.16	0.48
1:B:93:TYR:O	1:B:97:VAL:HG23	2.13	0.48
1:G:103:ILE:HD13	1:G:125:TYR:HB3	1.94	0.48
1:G:79:ASP:O	1:G:82:TRP:CH2	2.66	0.48
1:B:67:GLY:C	1:H:2:ALA:HB3	2.34	0.48
1:C:146:ILE:HG23	1:C:152:ALA:HB3	1.94	0.48
1:G:146:ILE:HG23	1:G:152:ALA:HB3	1.95	0.48
1:C:151:ARG:HD3	1:E:151:ARG:NH2	2.29	0.48
1:H:151:ARG:HG3	1:J:152:ALA:HB2	1.95	0.47
1:I:35:SER:HB3	1:J:69:ARG:HD3	1.96	0.47
1:G:39:LYS:HE3	1:G:39:LYS:HA	1.96	0.47
1:I:51:GLU:OE1	1:I:163:ARG:NH2	2.48	0.47
1:L:93:TYR:CE2	1:L:137:LEU:HD13	2.49	0.47
1:C:81:GLU:OE2	1:D:69:ARG:NH1	2.45	0.47
1:A:151:ARG:HB3	1:F:151:ARG:CD	2.45	0.47
1:A:44:TRP:CD1	1:A:160:LEU:CD2	2.99	0.46
1:F:146:ILE:HG23	1:F:152:ALA:HB3	1.97	0.46
1:C:48:GLN:NE2	1:C:132:GLU:OE2	2.49	0.46
1:A:154:LEU:HD21	1:H:116:PHE:CD1	2.51	0.45
1:I:44:TRP:CD1	1:I:163:ARG:HD2	2.51	0.45
1:D:146:ILE:HG23	1:D:152:ALA:HB3	1.99	0.45
1:A:8:MET:CE	1:A:118:THR:HG21	2.47	0.44
1:I:146:ILE:HG23	1:I:152:ALA:HB3	1.98	0.44
1:F:51:GLU:OE2	1:F:163:ARG:NH2	2.51	0.44
1:A:119:TYR:HH	1:E:119:TYR:HE2	1.60	0.44
1:H:93:TYR:O	1:H:97:VAL:HG23	2.18	0.44
1:E:15:GLN:HA	1:E:15:GLN:OE1	2.17	0.44
1:G:125:TYR:O	1:G:129:GLN:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:GLY:N	1:C:157:ASP:OD1	2.43	0.44
1:L:84:SER:HB2	1:L:85:PRO:HD2	2.00	0.44
1:G:19:GLU:OE1	1:G:52:GLU:OE1	2.36	0.43
1:G:151:ARG:HB3	1:L:151:ARG:NE	2.32	0.43
1:I:150:LYS:HD3	1:I:150:LYS:N	2.34	0.43
1:A:150:LYS:HE3	1:A:150:LYS:N	2.34	0.43
1:G:48:GLN:NE2	1:G:132:GLU:OE2	2.50	0.43
1:B:121:PHE:C	1:B:121:PHE:CD1	2.92	0.42
1:J:155:PHE:C	1:J:155:PHE:CD1	2.91	0.42
1:E:5:SER:O	1:E:9:VAL:HG23	2.19	0.42
1:B:67:GLY:CA	1:H:2:ALA:HB3	2.49	0.42
1:D:57:MET:O	1:D:58:LYS:C	2.58	0.42
1:A:22:SER:O	1:A:26:TYR:CD2	2.73	0.42
1:C:69:ARG:NH1	1:D:35:SER:OG	2.52	0.42
1:H:103:ILE:HD13	1:H:125:TYR:HB3	2.01	0.41
1:L:93:TYR:C	1:L:93:TYR:CD1	2.94	0.41
1:K:150:LYS:O	1:K:154:LEU:N	2.48	0.41
1:D:140:VAL:O	1:D:141:GLU:C	2.58	0.41
1:J:89:PHE:CE2	1:J:139:ILE:HG21	2.55	0.41
1:K:99:VAL:O	1:K:103:ILE:HG12	2.20	0.41
1:J:86:LEU:HA	1:J:143:LEU:HD13	2.03	0.41
1:A:149:ASP:O	1:A:152:ALA:N	2.54	0.40
1:B:156:LEU:O	1:B:160:LEU:HD13	2.21	0.40
1:I:136:ALA:O	1:I:140:VAL:HG23	2.20	0.40
1:K:79:ASP:O	1:K:82:TRP:CH2	2.74	0.40
1:A:151:ARG:HB3	1:F:151:ARG:HD2	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:GLU:OE2	1:E:105:GLU:OE2[3_554]	2.09	0.11

## 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	162/173 (94%)	154 (95%)	8 (5%)	0	100	100
1	B	161/173 (93%)	157 (98%)	4 (2%)	0	100	100
1	C	161/173 (93%)	155 (96%)	5 (3%)	1 (1%)	30	66
1	D	161/173 (93%)	153 (95%)	7 (4%)	1 (1%)	30	66
1	E	161/173 (93%)	157 (98%)	4 (2%)	0	100	100
1	F	163/173 (94%)	159 (98%)	4 (2%)	0	100	100
1	G	162/173 (94%)	155 (96%)	7 (4%)	0	100	100
1	H	161/173 (93%)	154 (96%)	7 (4%)	0	100	100
1	I	161/173 (93%)	158 (98%)	3 (2%)	0	100	100
1	J	162/173 (94%)	155 (96%)	7 (4%)	0	100	100
1	K	162/173 (94%)	157 (97%)	5 (3%)	0	100	100
1	L	162/173 (94%)	156 (96%)	6 (4%)	0	100	100
All	All	1939/2076 (93%)	1870 (96%)	67 (4%)	2 (0%)	56	86

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	4	ILE
1	D	13	ASN

### 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	146/153 (95%)	143 (98%)	3 (2%)	61	87
1	B	145/153 (95%)	137 (94%)	8 (6%)	27	60
1	C	145/153 (95%)	142 (98%)	3 (2%)	61	87
1	D	145/153 (95%)	137 (94%)	8 (6%)	27	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	145/153 (95%)	141 (97%)	4 (3%)	51	83
1	F	147/153 (96%)	143 (97%)	4 (3%)	52	83
1	G	145/153 (95%)	136 (94%)	9 (6%)	23	54
1	H	144/153 (94%)	134 (93%)	10 (7%)	19	48
1	I	145/153 (95%)	135 (93%)	10 (7%)	19	48
1	J	145/153 (95%)	143 (99%)	2 (1%)	74	92
1	K	146/153 (95%)	137 (94%)	9 (6%)	23	54
1	L	146/153 (95%)	135 (92%)	11 (8%)	17	43
All	All	1744/1836 (95%)	1663 (95%)	81 (5%)	33	68

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	TRP
1	A	75	ILE
1	A	150	LYS
1	B	28	SER
1	B	49	TRP
1	B	53	LEU
1	B	79	ASP
1	B	103	ILE
1	B	120	ASN
1	B	145	LEU
1	B	151	ARG
1	C	74	ASP
1	C	148	GLU
1	C	165	PHE
1	D	10	GLU
1	D	49	TRP
1	D	54	CYS
1	D	74	ASP
1	D	138	ASP
1	D	161	SER
1	D	164	GLN
1	D	165	PHE
1	E	24	TYR
1	E	34	ASP
1	E	54	CYS
1	E	65	GLU

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Mol	Chain	Res	Type
1	F	34	ASP
1	F	49	TRP
1	F	80	SER
1	F	155	PHE
1	G	3	SER
1	G	5	SER
1	G	42	SER
1	G	49	TRP
1	G	54	CYS
1	G	73	GLN
1	G	79	ASP
1	G	158	LYS
1	G	165	PHE
1	H	5	SER
1	H	21	TYR
1	H	49	TRP
1	H	66	ARG
1	H	94	GLU
1	H	135	SER
1	H	138	ASP
1	H	146	ILE
1	H	157	ASP
1	H	158	LYS
1	I	34	ASP
1	I	42	SER
1	I	49	TRP
1	I	79	ASP
1	I	104	HIS
1	I	135	SER
1	I	138	ASP
1	I	150	LYS
1	I	151	ARG
1	I	164	GLN
1	J	94	GLU
1	J	165	PHE
1	K	3	SER
1	K	17	ASN
1	K	54	CYS
1	K	65	GLU
1	K	142	LYS
1	K	145	LEU
1	K	150	LYS

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Mol	Chain	Res	Type
1	K	151	ARG
1	K	164	GLN
1	L	17	ASN
1	L	22	SER
1	L	49	TRP
1	L	70	ILE
1	L	74	ASP
1	L	79	ASP
1	L	145	LEU
1	L	150	LYS
1	L	155	PHE
1	L	161	SER
1	L	165	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	120	ASN
1	C	104	HIS
1	D	50	GLN
1	E	48	GLN
1	E	50	GLN
1	G	43	ASN
1	G	55	HIS
1	G	95	HIS
1	H	104	HIS
1	I	95	HIS
1	J	50	GLN
1	J	112	GLN
1	J	120	ASN
1	K	123	GLN
1	K	164	GLN
1	L	50	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	164/173 (94%)	0.34	5 (3%) 54 50	45, 69, 91, 122	0
1	B	163/173 (94%)	0.43	5 (3%) 52 48	55, 80, 103, 116	0
1	C	163/173 (94%)	0.13	0 100 100	38, 58, 78, 92	0
1	D	163/173 (94%)	0.12	0 100 100	42, 65, 82, 89	0
1	E	163/173 (94%)	0.22	1 (0%) 90 90	52, 71, 97, 109	0
1	F	165/173 (95%)	0.30	9 (5%) 29 24	50, 73, 91, 102	0
1	G	164/173 (94%)	0.19	0 100 100	45, 64, 83, 105	0
1	H	163/173 (94%)	0.60	14 (8%) 13 9	53, 79, 100, 112	0
1	I	163/173 (94%)	0.17	1 (0%) 90 90	39, 67, 89, 105	0
1	J	164/173 (94%)	0.00	0 100 100	38, 56, 77, 103	0
1	K	164/173 (94%)	0.24	7 (4%) 39 35	47, 71, 94, 106	0
1	L	164/173 (94%)	0.44	5 (3%) 54 50	49, 80, 107, 121	0
All	All	1963/2076 (94%)	0.27	47 (2%) 62 59	38, 70, 97, 122	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	GLN	4.3
1	H	143	LEU	3.8
1	A	71	PHE	3.7
1	K	68	GLY	3.7
1	H	146	ILE	3.6
1	H	155	PHE	3.4
1	H	84	SER	3.2
1	B	141	GLU	3.2
1	H	127	ALA	3.1
1	B	76	LYS	3.0
1	L	60	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	83	GLU	2.9
1	H	88	ALA	2.9
1	H	124	TRP	2.8
1	F	162	LEU	2.8
1	F	137	LEU	2.8
1	L	155	PHE	2.7
1	A	74	ASP	2.7
1	K	36	ILE	2.6
1	K	49	TRP	2.6
1	F	145	LEU	2.6
1	F	136	ALA	2.6
1	A	112	GLN	2.6
1	F	4	ILE	2.6
1	H	130	VAL	2.5
1	K	81	GLU	2.4
1	H	119	TYR	2.4
1	B	89	PHE	2.4
1	H	86	LEU	2.4
1	K	38	LEU	2.3
1	L	107	VAL	2.3
1	A	13	ASN	2.3
1	H	83	GLU	2.3
1	B	145	LEU	2.3
1	F	32	TYR	2.3
1	F	6	GLU	2.2
1	L	106	LEU	2.2
1	F	5	SER	2.2
1	K	14	ARG	2.1
1	L	126	VAL	2.1
1	H	82	TRP	2.1
1	H	93	TYR	2.1
1	I	94	GLU	2.1
1	K	37	GLY	2.1
1	E	80	SER	2.1
1	H	36	ILE	2.0
1	F	86	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	MG	F	201	1/1	0.97	0.17	-0.24	64,64,64,64	0
2	MG	I	201	1/1	0.95	0.11	-2.00	51,51,51,51	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.