



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 2, 2023 – 09:34 PM EDT

PDB ID : 3RBC  
Title : Bullfrog M ferritin with iron(III) bound to the ferroxidase site  
Authors : Bertini, I.; Lalli, D.; Mangani, S.; Pozzi, C.; Rosa, C.; Turano, P.  
Deposited on : 2011-03-29  
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
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

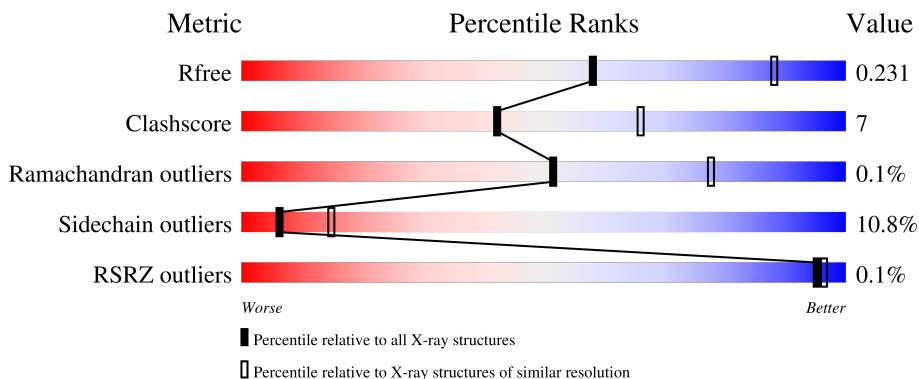
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



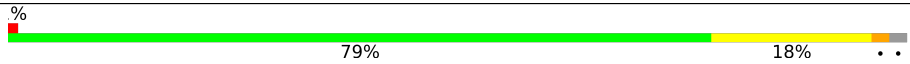
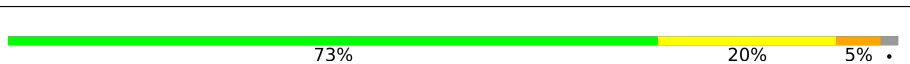

The reported resolution of this entry is 2.70 Å.

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.











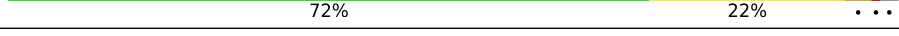


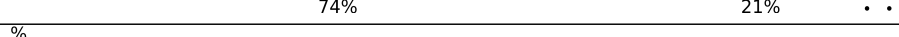

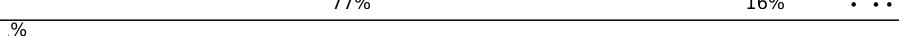


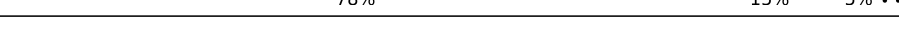

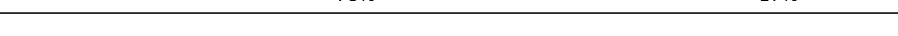
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	176	
1	B	176	
1	C	176	
1	D	176	
1	E	176	

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Mol	Chain	Length	Quality of chain
1	F	176	 80% 16% ..
1	G	176	 77% 15% 6% .
1	H	176	 75% 20% ..
1	I	176	 73% 18% 6% ..
1	J	176	 73% 20% . .
1	K	176	 80% 15% ..
1	L	176	 75% 19% . .
1	M	176	 % 74% 19% 6% .
1	N	176	 72% 22% . . .
1	O	176	 78% 17% . .
1	P	176	 81% 14% . . .
1	Q	176	 % 74% 21% . .
1	R	176	 % 72% 21% 5% . .
1	S	176	 77% 16% . . .
1	T	176	 % 82% 14% . . .
1	U	176	 74% 18% 6% .
1	V	176	 78% 15% 5% . .
1	W	176	 78% 15% . . .
1	X	176	 78% 17% . .

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 35540 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, middle subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	173	1414	890	244	273	7	0	0	0
1	B	173	1417	892	244	273	8	0	0	0
1	C	173	1417	892	244	273	8	0	0	0
1	D	173	1417	892	244	273	8	0	0	0
1	E	173	1414	890	244	273	7	0	0	0
1	F	173	1414	890	244	273	7	0	0	0
1	G	173	1419	892	247	273	7	0	0	0
1	H	173	1414	890	244	273	7	0	0	0
1	I	172	1414	889	246	272	7	0	0	0
1	J	172	1406	885	242	272	7	0	0	0
1	K	173	1414	890	244	273	7	0	0	0
1	L	172	1409	887	243	272	7	0	0	0
1	M	173	1411	888	243	273	7	0	0	0
1	N	172	1414	889	246	272	7	0	0	0
1	O	173	1411	888	243	273	7	0	0	0
1	P	172	1414	889	246	272	7	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	173	Total	C	N	O	S	0	0	0
			1414	890	244	273	7			
1	R	173	Total	C	N	O	S	0	0	0
			1423	895	248	273	7			
1	S	173	Total	C	N	O	S	0	0	0
			1416	890	246	273	7			
1	T	174	Total	C	N	O	S	0	0	0
			1419	893	245	274	7			
1	U	173	Total	C	N	O	S	0	0	0
			1411	888	243	273	7			
1	V	173	Total	C	N	O	S	0	0	0
			1411	888	243	273	7			
1	W	173	Total	C	N	O	S	0	0	0
			1418	893	245	273	7			
1	X	173	Total	C	N	O	S	0	0	0
			1414	890	244	273	7			

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	L	3	Total Fe 3 3	0	0
2	M	2	Total Fe 2 2	0	0
2	N	2	Total Fe 2 2	0	0
2	O	2	Total Fe 2 2	0	0
2	P	2	Total Fe 2 2	0	0
2	Q	2	Total Fe 2 2	0	0
2	R	2	Total Fe 2 2	0	0
2	S	2	Total Fe 2 2	0	0
2	T	2	Total Fe 2 2	0	0
2	U	2	Total Fe 2 2	0	0
2	V	2	Total Fe 2 2	0	0
2	W	2	Total Fe 2 2	0	0
2	X	2	Total Fe 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	74	Total O 74 74	0	0
3	B	83	Total O 83 83	0	0
3	C	49	Total O 49 49	0	0
3	D	81	Total O 81 81	0	0
3	E	81	Total O 81 81	0	0
3	F	60	Total O 60 60	0	0

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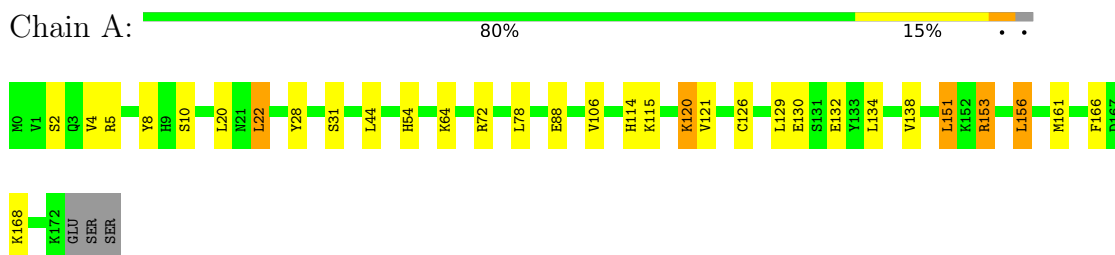
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	77	Total 77	O 77	0	0
3	H	64	Total 64	O 64	0	0
3	I	80	Total 80	O 80	0	0
3	J	49	Total 49	O 49	0	0
3	K	58	Total 58	O 58	0	0
3	L	65	Total 65	O 65	0	0
3	M	56	Total 56	O 56	0	0
3	N	51	Total 51	O 51	0	0
3	O	65	Total 65	O 65	0	0
3	P	69	Total 69	O 69	0	0
3	Q	47	Total 47	O 47	0	0
3	R	43	Total 43	O 43	0	0
3	S	49	Total 49	O 49	0	0
3	T	61	Total 61	O 61	0	0
3	U	60	Total 60	O 60	0	0
3	V	80	Total 80	O 80	0	0
3	W	80	Total 80	O 80	0	0
3	X	63	Total 63	O 63	0	0

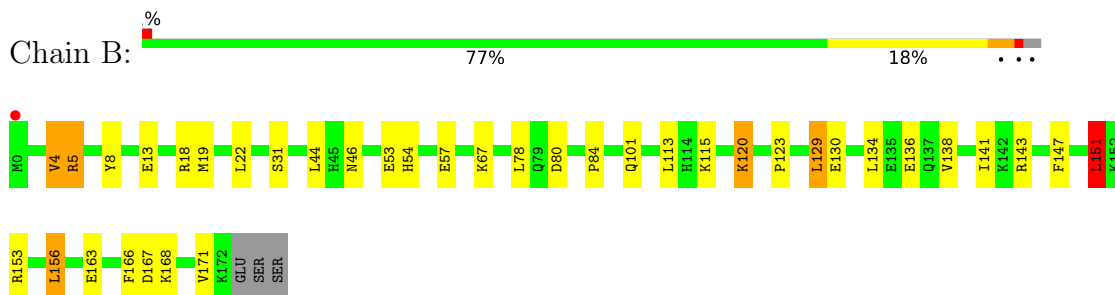
### 3 Residue-property plots [i](#)

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.

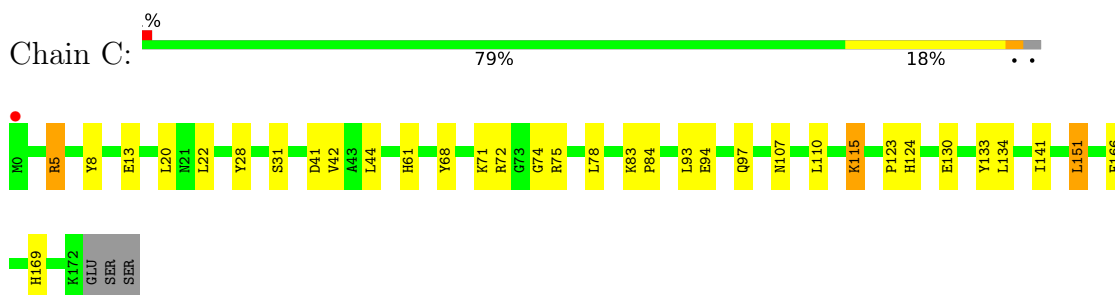
- Molecule 1: Ferritin, middle subunit



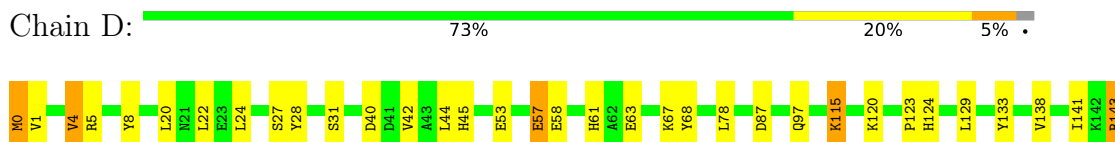
- Molecule 1: Ferritin, middle subunit



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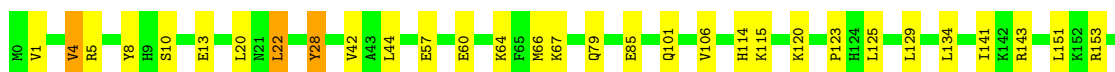
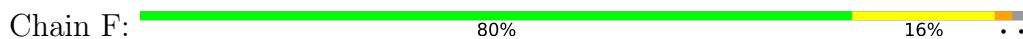




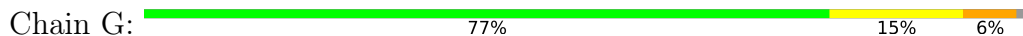
- Molecule 1: Ferritin, middle subunit



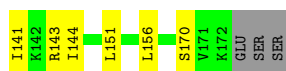
- Molecule 1: Ferritin, middle subunit



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- Molecule 1: Ferritin, middle subunit



- Molecule 1: Ferritin, middle subunit

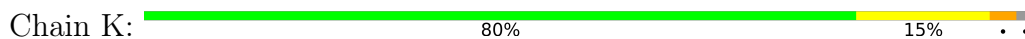




● Molecule 1: Ferritin, middle subunit



● Molecule 1: Ferritin, middle subunit



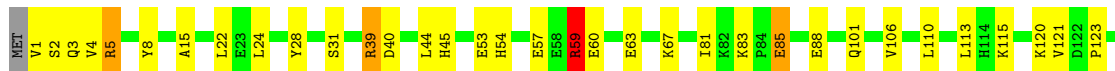
● Molecule 1: Ferritin, middle subunit

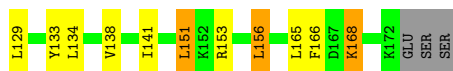


● Molecule 1: Ferritin, middle subunit



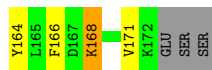
● Molecule 1: Ferritin, middle subunit





- Molecule 1: Ferritin, middle subunit

Chain O: 78% 17%



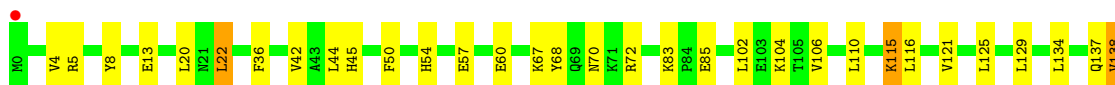
- Molecule 1: Ferritin, middle subunit

Chain P: 81% 14%



- Molecule 1: Ferritin, middle subunit

Chain Q: 74% 21%



- Molecule 1: Ferritin, middle subunit

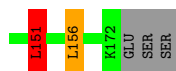
Chain R: 72% 21% 5%



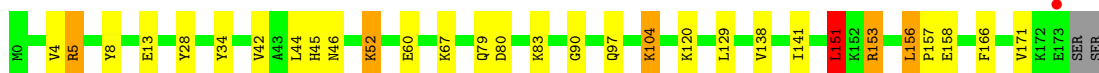
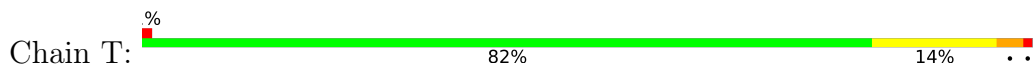
- Molecule 1: Ferritin, middle subunit

Chain S: 77% 16%

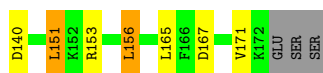




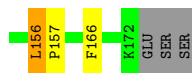
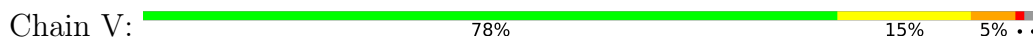
• Molecule 1: Ferritin, middle subunit



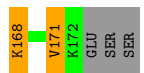
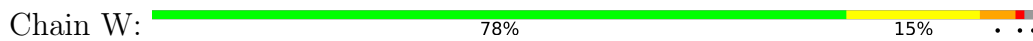
• Molecule 1: Ferritin, middle subunit



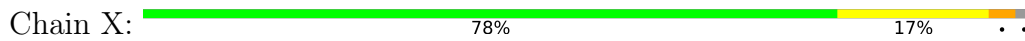
• Molecule 1: Ferritin, middle subunit



• Molecule 1: Ferritin, middle subunit



• Molecule 1: Ferritin, middle subunit



C155	L156	M161	K172	GLU	SER	SER
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.72Å 210.72Å 324.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.13 – 2.70 61.13 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.3 (61.13-2.70) 92.3 (61.13-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.173 , 0.235 0.173 , 0.231	Depositor DCC
$R_{free}$ test set	10510 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.0	Xtrriage
Anisotropy	0.082	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 33.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	35540	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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 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	0.99	0/1442	0.92	2/1941 (0.1%)
1	B	1.04	4/1445 (0.3%)	0.94	4/1944 (0.2%)
1	C	0.96	1/1445 (0.1%)	0.90	3/1944 (0.2%)
1	D	1.05	2/1445 (0.1%)	0.98	2/1944 (0.1%)
1	E	1.07	4/1442 (0.3%)	0.97	5/1941 (0.3%)
1	F	1.01	2/1442 (0.1%)	0.92	0/1941
1	G	1.07	7/1447 (0.5%)	0.98	2/1947 (0.1%)
1	H	1.02	3/1442 (0.2%)	0.95	2/1941 (0.1%)
1	I	1.09	4/1442 (0.3%)	0.95	4/1940 (0.2%)
1	J	0.97	4/1434 (0.3%)	0.85	2/1931 (0.1%)
1	K	1.05	2/1442 (0.1%)	0.91	0/1941
1	L	1.01	4/1437 (0.3%)	0.95	3/1934 (0.2%)
1	M	0.97	1/1439 (0.1%)	0.91	2/1938 (0.1%)
1	N	0.94	3/1442 (0.2%)	0.94	4/1940 (0.2%)
1	O	0.97	2/1439 (0.1%)	0.92	1/1938 (0.1%)
1	P	1.06	3/1442 (0.2%)	1.02	8/1940 (0.4%)
1	Q	0.98	1/1442 (0.1%)	0.89	1/1941 (0.1%)
1	R	0.93	1/1451 (0.1%)	0.91	3/1951 (0.2%)
1	S	1.00	4/1444 (0.3%)	0.94	4/1944 (0.2%)
1	T	0.99	3/1447 (0.2%)	0.97	7/1948 (0.4%)
1	U	1.01	4/1439 (0.3%)	0.92	1/1938 (0.1%)
1	V	0.99	3/1439 (0.2%)	0.98	4/1938 (0.2%)
1	W	1.04	4/1446 (0.3%)	0.93	3/1945 (0.2%)
1	X	1.04	4/1442 (0.3%)	0.97	4/1941 (0.2%)
All	All	1.01	70/34617 (0.2%)	0.94	71/46591 (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	D	0	1

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	57	GLU	CG-CD	10.72	1.68	1.51
1	P	60	GLU	CG-CD	10.46	1.67	1.51
1	I	57	GLU	CG-CD	9.52	1.66	1.51
1	X	57	GLU	CG-CD	9.25	1.65	1.51
1	M	57	GLU	CG-CD	9.06	1.65	1.51

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	153	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	G	153	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	C	5	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	D	153	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	X	153	ARG	NE-CZ-NH1	7.35	123.97	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	0	MET	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1414	0	1355	20	0
1	B	1417	0	1362	19	0
1	C	1417	0	1362	23	0
1	D	1417	0	1362	32	0
1	E	1414	0	1355	22	0
1	F	1414	0	1355	15	0
1	G	1419	0	1364	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1414	0	1355	21	0
1	I	1414	0	1362	23	0
1	J	1406	0	1344	29	0
1	K	1414	0	1355	26	0
1	L	1409	0	1353	23	0
1	M	1411	0	1346	28	0
1	N	1414	0	1362	26	0
1	O	1411	0	1346	19	0
1	P	1414	0	1362	22	0
1	Q	1414	0	1355	34	0
1	R	1423	0	1375	30	0
1	S	1416	0	1355	21	0
1	T	1419	0	1357	12	0
1	U	1411	0	1346	23	0
1	V	1411	0	1346	18	0
1	W	1418	0	1366	16	0
1	X	1414	0	1355	26	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	3	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	3	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
2	Q	2	0	0	0	0
2	R	2	0	0	0	0
2	S	2	0	0	0	0
2	T	2	0	0	0	0
2	U	2	0	0	0	0
2	V	2	0	0	0	0
2	W	2	0	0	0	0
2	X	2	0	0	0	0
3	A	74	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	83	0	0	8	0
3	C	49	0	0	7	0
3	D	81	0	0	2	0
3	E	81	0	0	6	0
3	F	60	0	0	3	0
3	G	77	0	0	4	0
3	H	64	0	0	9	0
3	I	80	0	0	4	0
3	J	49	0	0	11	0
3	K	58	0	0	5	0
3	L	65	0	0	3	0
3	M	56	0	0	9	0
3	N	51	0	0	11	0
3	O	65	0	0	5	0
3	P	69	0	0	3	0
3	Q	47	0	0	3	0
3	R	43	0	0	3	0
3	S	49	0	0	4	0
3	T	61	0	0	2	0
3	U	60	0	0	6	0
3	V	80	0	0	5	0
3	W	80	0	0	6	0
3	X	63	0	0	7	0
All	All	35540	0	32555	459	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 7.

The worst 5 of 459 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LYS:HE3	3:A:266:HOH:O	1.40	1.18
1:N:45:HIS:HB3	3:N:185:HOH:O	1.61	1.00
1:S:143:ARG:HG3	1:S:143:ARG:HH11	1.26	0.99
1:Q:153:ARG:NH2	1:X:42:VAL:O	1.97	0.96
1:E:153:ARG:HD3	3:L:1405:HOH:O	1.64	0.95

There are no symmetry-related clashes.

## 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	171/176 (97%)	167 (98%)	4 (2%)	0	100	100
1	B	171/176 (97%)	165 (96%)	6 (4%)	0	100	100
1	C	171/176 (97%)	163 (95%)	8 (5%)	0	100	100
1	D	171/176 (97%)	166 (97%)	4 (2%)	1 (1%)	25	50
1	E	171/176 (97%)	169 (99%)	1 (1%)	1 (1%)	25	50
1	F	171/176 (97%)	165 (96%)	6 (4%)	0	100	100
1	G	171/176 (97%)	166 (97%)	5 (3%)	0	100	100
1	H	171/176 (97%)	166 (97%)	5 (3%)	0	100	100
1	I	170/176 (97%)	166 (98%)	3 (2%)	1 (1%)	25	50
1	J	170/176 (97%)	160 (94%)	10 (6%)	0	100	100
1	K	171/176 (97%)	166 (97%)	4 (2%)	1 (1%)	25	50
1	L	170/176 (97%)	163 (96%)	7 (4%)	0	100	100
1	M	171/176 (97%)	162 (95%)	9 (5%)	0	100	100
1	N	170/176 (97%)	161 (95%)	9 (5%)	0	100	100
1	O	171/176 (97%)	168 (98%)	3 (2%)	0	100	100
1	P	170/176 (97%)	165 (97%)	5 (3%)	0	100	100
1	Q	171/176 (97%)	165 (96%)	6 (4%)	0	100	100
1	R	171/176 (97%)	167 (98%)	4 (2%)	0	100	100
1	S	171/176 (97%)	160 (94%)	11 (6%)	0	100	100
1	T	172/176 (98%)	167 (97%)	4 (2%)	1 (1%)	25	50
1	U	171/176 (97%)	164 (96%)	6 (4%)	1 (1%)	25	50
1	V	171/176 (97%)	167 (98%)	4 (2%)	0	100	100
1	W	171/176 (97%)	166 (97%)	5 (3%)	0	100	100
1	X	171/176 (97%)	164 (96%)	7 (4%)	0	100	100
All	All	4100/4224 (97%)	3958 (96%)	136 (3%)	6 (0%)	51	78

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1	VAL
1	E	90	GLY
1	K	10	SER
1	T	90	GLY
1	I	90	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	151/157 (96%)	137 (91%)	14 (9%)	9 21
1	B	152/157 (97%)	136 (90%)	16 (10%)	7 16
1	C	152/157 (97%)	143 (94%)	9 (6%)	19 43
1	D	152/157 (97%)	132 (87%)	20 (13%)	4 9
1	E	151/157 (96%)	130 (86%)	21 (14%)	3 8
1	F	151/157 (96%)	137 (91%)	14 (9%)	9 21
1	G	152/157 (97%)	135 (89%)	17 (11%)	6 13
1	H	151/157 (96%)	133 (88%)	18 (12%)	5 12
1	I	152/157 (97%)	130 (86%)	22 (14%)	3 8
1	J	150/157 (96%)	134 (89%)	16 (11%)	6 15
1	K	151/157 (96%)	136 (90%)	15 (10%)	8 18
1	L	151/157 (96%)	134 (89%)	17 (11%)	6 13
1	M	150/157 (96%)	134 (89%)	16 (11%)	6 15
1	N	152/157 (97%)	131 (86%)	21 (14%)	3 8
1	O	150/157 (96%)	132 (88%)	18 (12%)	5 11
1	P	152/157 (97%)	143 (94%)	9 (6%)	19 43
1	Q	151/157 (96%)	139 (92%)	12 (8%)	12 28
1	R	153/157 (98%)	136 (89%)	17 (11%)	6 14
1	S	151/157 (96%)	135 (89%)	16 (11%)	6 15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T	151/157 (96%)	137 (91%)	14 (9%)	9	21
1	U	150/157 (96%)	130 (87%)	20 (13%)	4	9
1	V	150/157 (96%)	133 (89%)	17 (11%)	6	13
1	W	152/157 (97%)	135 (89%)	17 (11%)	6	13
1	X	151/157 (96%)	136 (90%)	15 (10%)	8	18
All	All	3629/3768 (96%)	3238 (89%)	391 (11%)	6	15

5 of 391 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	134	LEU
1	R	129	LEU
1	O	5	ARG
1	P	151	LEU
1	S	115	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	45	HIS
1	R	56	HIS
1	X	97	GLN
1	O	97	GLN
1	Q	3	GLN

### 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 50 ligands modelled in this entry, 50 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, 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	173/176 (98%)	-0.68	0 100 100	19, 28, 40, 45	0
1	B	173/176 (98%)	-0.76	1 (0%) 89 91	18, 25, 37, 57	0
1	C	173/176 (98%)	-0.66	1 (0%) 89 91	22, 31, 42, 62	0
1	D	173/176 (98%)	-0.71	0 100 100	19, 26, 38, 53	0
1	E	173/176 (98%)	-0.79	0 100 100	17, 24, 36, 45	0
1	F	173/176 (98%)	-0.79	0 100 100	20, 27, 39, 47	0
1	G	173/176 (98%)	-0.76	0 100 100	15, 24, 37, 49	0
1	H	173/176 (98%)	-0.76	0 100 100	16, 26, 38, 49	0
1	I	172/176 (97%)	-0.77	0 100 100	16, 24, 37, 46	0
1	J	172/176 (97%)	-0.62	0 100 100	23, 33, 45, 49	0
1	K	173/176 (98%)	-0.75	0 100 100	21, 27, 39, 46	0
1	L	172/176 (97%)	-0.78	0 100 100	16, 25, 37, 42	0
1	M	173/176 (98%)	-0.67	1 (0%) 89 91	19, 30, 41, 51	0
1	N	172/176 (97%)	-0.58	0 100 100	27, 36, 45, 53	0
1	O	173/176 (98%)	-0.65	0 100 100	18, 30, 42, 48	0
1	P	172/176 (97%)	-0.78	0 100 100	16, 25, 38, 50	0
1	Q	173/176 (98%)	-0.62	1 (0%) 89 91	21, 33, 45, 51	0
1	R	173/176 (98%)	-0.59	1 (0%) 89 91	28, 35, 47, 54	0
1	S	173/176 (98%)	-0.61	0 100 100	23, 33, 45, 54	0
1	T	174/176 (98%)	-0.65	1 (0%) 89 91	19, 29, 39, 58	0
1	U	173/176 (98%)	-0.56	0 100 100	22, 30, 42, 48	0
1	V	173/176 (98%)	-0.70	0 100 100	16, 25, 38, 49	0
1	W	173/176 (98%)	-0.73	0 100 100	16, 26, 38, 54	0
1	X	173/176 (98%)	-0.67	0 100 100	23, 31, 43, 51	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	4148/4224 (98%)	-0.69	6 (0%) 95 96	15, 29, 42, 62	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	0	MET	3.6
1	C	0	MET	2.8
1	T	173	GLU	2.6
1	M	0	MET	2.1
1	R	0	MET	2.1

## 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	FE	H	176	1/1	0.95	0.11	38,38,38,38	1
2	FE	L	176	1/1	0.95	0.10	31,31,31,31	1
2	FE	F	181	1/1	0.96	0.07	45,45,45,45	0
2	FE	R	181	1/1	0.97	0.08	44,44,44,44	1
2	FE	U	181	1/1	0.97	0.06	45,45,45,45	1
2	FE	D	180	1/1	0.98	0.09	43,43,43,43	1
2	FE	K	181	1/1	0.98	0.05	42,42,42,42	1
2	FE	D	181	1/1	0.98	0.10	41,41,41,41	1
2	FE	M	180	1/1	0.98	0.08	43,43,43,43	1
2	FE	M	181	1/1	0.98	0.09	41,41,41,41	1
2	FE	N	180	1/1	0.98	0.05	46,46,46,46	1
2	FE	O	180	1/1	0.98	0.05	40,40,40,40	1
2	FE	Q	181	1/1	0.98	0.11	37,37,37,37	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FE	A	181	1/1	0.98	0.05	40,40,40,40	1
2	FE	S	181	1/1	0.98	0.09	46,46,46,46	1
2	FE	T	181	1/1	0.98	0.07	43,43,43,43	1
2	FE	G	180	1/1	0.98	0.08	47,47,47,47	0
2	FE	V	180	1/1	0.98	0.08	43,43,43,43	0
2	FE	V	181	1/1	0.98	0.06	45,45,45,45	1
2	FE	W	180	1/1	0.98	0.09	49,49,49,49	0
2	FE	W	181	1/1	0.98	0.08	48,48,48,48	0
2	FE	L	181	1/1	0.99	0.07	43,43,43,43	1
2	FE	E	181	1/1	0.99	0.09	40,40,40,40	1
2	FE	F	180	1/1	0.99	0.08	44,44,44,44	0
2	FE	C	181	1/1	0.99	0.10	43,43,43,43	1
2	FE	A	180	1/1	0.99	0.06	42,42,42,42	1
2	FE	H	180	1/1	0.99	0.07	46,46,46,46	0
2	FE	O	181	1/1	0.99	0.07	41,41,41,41	1
2	FE	P	180	1/1	0.99	0.09	40,40,40,40	0
2	FE	P	181	1/1	0.99	0.09	41,41,41,41	0
2	FE	Q	180	1/1	0.99	0.06	43,43,43,43	1
2	FE	H	181	1/1	0.99	0.07	45,45,45,45	0
2	FE	R	180	1/1	0.99	0.08	39,39,39,39	1
2	FE	B	180	1/1	0.99	0.06	44,44,44,44	1
2	FE	S	180	1/1	0.99	0.05	46,46,46,46	1
2	FE	I	180	1/1	0.99	0.07	43,43,43,43	0
2	FE	T	180	1/1	0.99	0.06	45,45,45,45	0
2	FE	I	181	1/1	0.99	0.05	40,40,40,40	0
2	FE	U	180	1/1	0.99	0.05	45,45,45,45	1
2	FE	J	180	1/1	0.99	0.08	42,42,42,42	1
2	FE	J	181	1/1	0.99	0.09	42,42,42,42	1
2	FE	K	180	1/1	0.99	0.06	38,38,38,38	1
2	FE	E	180	1/1	0.99	0.09	39,39,39,39	1
2	FE	L	180	1/1	0.99	0.08	45,45,45,45	1
2	FE	X	180	1/1	0.99	0.05	45,45,45,45	1
2	FE	X	181	1/1	0.99	0.06	44,44,44,44	1
2	FE	B	181	1/1	1.00	0.07	32,32,32,32	1
2	FE	C	180	1/1	1.00	0.08	39,39,39,39	1
2	FE	G	181	1/1	1.00	0.07	44,44,44,44	0
2	FE	N	181	1/1	1.00	0.07	40,40,40,40	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.