Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 10:44 am GMT

PDB ID	:	5N5E
Title	:	Crystal structure of encapsulated ferritin domain from Pyrococcus furiosus PFC_05175
Authors	:	Marles-Wright, J.; He, D.
Deposited on	:	2017-02-13
Resolution	:	2.03 Å(reported)

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

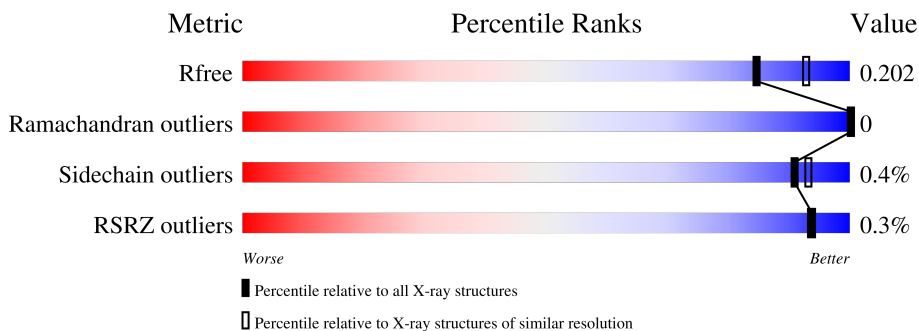|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.03 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.
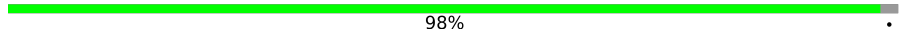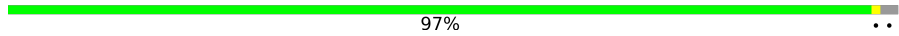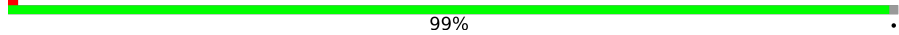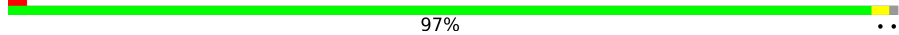
Metric	Percentile Ranks	Value
Rfree		0.202
Ramachandran outliers		0
Sidechain outliers		0.4%
RSRZ outliers		0.3%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution
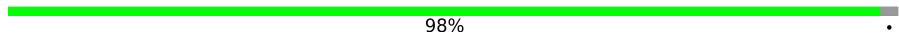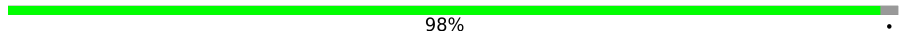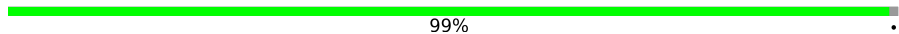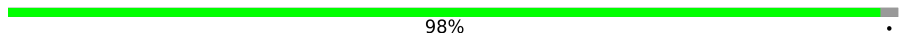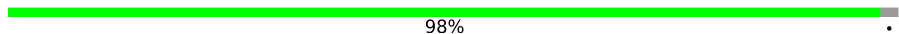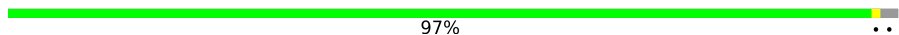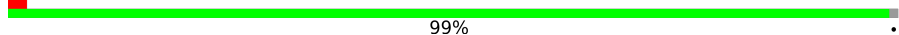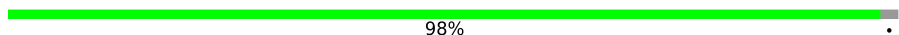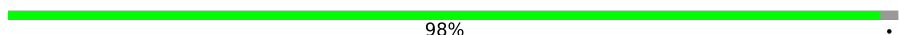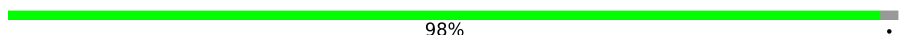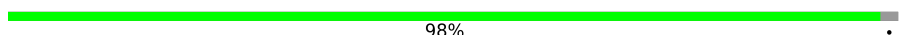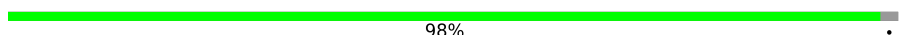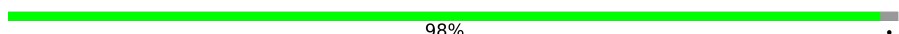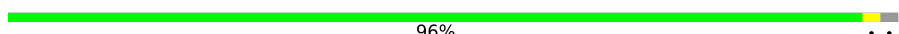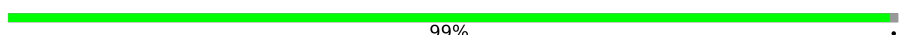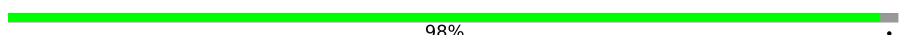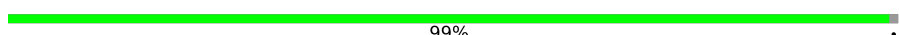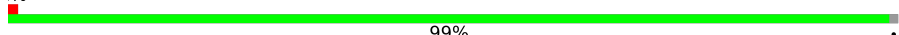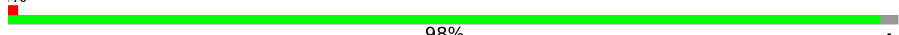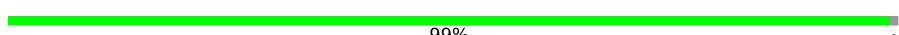
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	10434 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	99	99%
1	B	99	99%
1	C	99	98%
1	D	99	97%
1	E	99	98%
1	F	99	98%

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Mol	Chain	Length	Quality of chain
1	G	99	98%
1	H	99	97%
1	I	99	.% 99%
1	J	99	2% 97%
1	K	99	98%
1	L	99	98%
1	M	99	99%
1	N	99	98%
1	O	99	98%
1	P	99	97%
1	Q	99	2% 99%
1	R	99	98%
1	T	99	98%
1	U	99	98%
1	V	99	98%
1	W	99	98%
1	X	99	98%
1	Y	99	96%
1	Z	99	99%
1	a	99	98%
1	b	99	99%
1	c	99	.% 99%
1	d	99	.% 98%
1	e	99	99%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 49851 atoms, of which 24116 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 PFC_05175.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	e	98	Total	C	H	N	O	S	0	1	0
			1591	500	803	128	156	4			
1	A	98	Total	C	H	N	O	S	0	1	0
			1588	500	799	128	158	3			
1	B	98	Total	C	H	N	O	S	0	1	0
			1592	500	804	128	156	4			
1	C	98	Total	C	H	N	O	S	0	1	0
			1598	501	807	131	156	3			
1	D	97	Total	C	H	N	O	S	0	2	0
			1596	502	804	128	158	4			
1	E	98	Total	C	H	N	O	S	0	2	0
			1606	505	809	131	158	3			
1	F	97	Total	C	H	N	O	S	0	1	0
			1579	497	795	127	157	3			
1	G	97	Total	C	H	N	O	S	0	1	0
			1585	498	799	128	156	4			
1	H	97	Total	C	H	N	O	S	0	1	0
			1579	497	795	127	157	3			
1	I	98	Total	C	H	N	O	S	0	1	0
			1589	500	800	128	158	3			
1	J	98	Total	C	H	N	O	S	0	2	0
			1619	506	820	134	156	3			
1	K	97	Total	C	H	N	O	S	0	3	0
			1612	506	815	130	157	4			
1	L	97	Total	C	H	N	O	S	0	4	0
			1625	510	823	130	157	5			
1	M	98	Total	C	H	N	O	S	0	2	0
			1602	504	808	128	158	4			
1	N	97	Total	C	H	N	O	S	0	2	0
			1592	501	803	127	157	4			
1	O	97	Total	C	H	N	O	S	0	2	0
			1603	503	808	131	158	3			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	P	97	Total	C	H	N	O	S	0	2	0
			1587	499	801	127	156	4			
1	Q	98	Total	C	H	N	O	S	0	1	0
			1591	500	803	128	156	4			
1	R	97	Total	C	H	N	O	S	0	1	0
			1581	497	798	127	155	4			
1	T	97	Total	C	H	N	O	S	0	3	0
			1609	506	812	128	158	5			
1	U	97	Total	C	H	N	O	S	0	1	0
			1581	497	798	127	155	4			
1	V	97	Total	C	H	N	O	S	0	2	0
			1587	499	800	127	158	3			
1	W	97	Total	C	H	N	O	S	0	2	0
			1592	501	803	127	157	4			
1	X	97	Total	C	H	N	O	S	0	1	0
			1579	497	795	127	157	3			
1	Y	97	Total	C	H	N	O	S	0	2	0
			1599	502	807	130	157	3			
1	Z	98	Total	C	H	N	O	S	0	1	0
			1589	500	800	128	158	3			
1	a	97	Total	C	H	N	O	S	0	1	0
			1579	497	795	127	157	3			
1	b	98	Total	C	H	N	O	S	0	0	0
			1578	496	795	128	156	3			
1	c	98	Total	C	H	N	O	S	0	3	0
			1631	510	827	134	156	4			
1	d	97	Total	C	H	N	O	S	0	0	0
			1568	493	790	127	155	3			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	1	MET	-	initiating methionine	UNP I6U7J4
e	2	GLY	-	expression tag	UNP I6U7J4
A	1	MET	-	initiating methionine	UNP I6U7J4
A	2	GLY	-	expression tag	UNP I6U7J4
B	1	MET	-	initiating methionine	UNP I6U7J4
B	2	GLY	-	expression tag	UNP I6U7J4
C	1	MET	-	initiating methionine	UNP I6U7J4
C	2	GLY	-	expression tag	UNP I6U7J4
D	1	MET	-	initiating methionine	UNP I6U7J4
D	2	GLY	-	expression tag	UNP I6U7J4
E	1	MET	-	initiating methionine	UNP I6U7J4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	2	GLY	-	expression tag	UNP I6U7J4
F	1	MET	-	initiating methionine	UNP I6U7J4
F	2	GLY	-	expression tag	UNP I6U7J4
G	1	MET	-	initiating methionine	UNP I6U7J4
G	2	GLY	-	expression tag	UNP I6U7J4
H	1	MET	-	initiating methionine	UNP I6U7J4
H	2	GLY	-	expression tag	UNP I6U7J4
I	1	MET	-	initiating methionine	UNP I6U7J4
I	2	GLY	-	expression tag	UNP I6U7J4
J	1	MET	-	initiating methionine	UNP I6U7J4
J	2	GLY	-	expression tag	UNP I6U7J4
K	1	MET	-	initiating methionine	UNP I6U7J4
K	2	GLY	-	expression tag	UNP I6U7J4
L	1	MET	-	initiating methionine	UNP I6U7J4
L	2	GLY	-	expression tag	UNP I6U7J4
M	1	MET	-	initiating methionine	UNP I6U7J4
M	2	GLY	-	expression tag	UNP I6U7J4
N	1	MET	-	initiating methionine	UNP I6U7J4
N	2	GLY	-	expression tag	UNP I6U7J4
O	1	MET	-	initiating methionine	UNP I6U7J4
O	2	GLY	-	expression tag	UNP I6U7J4
P	1	MET	-	initiating methionine	UNP I6U7J4
P	2	GLY	-	expression tag	UNP I6U7J4
Q	1	MET	-	initiating methionine	UNP I6U7J4
Q	2	GLY	-	expression tag	UNP I6U7J4
R	1	MET	-	initiating methionine	UNP I6U7J4
R	2	GLY	-	expression tag	UNP I6U7J4
T	1	MET	-	initiating methionine	UNP I6U7J4
T	2	GLY	-	expression tag	UNP I6U7J4
U	1	MET	-	initiating methionine	UNP I6U7J4
U	2	GLY	-	expression tag	UNP I6U7J4
V	1	MET	-	initiating methionine	UNP I6U7J4
V	2	GLY	-	expression tag	UNP I6U7J4
W	1	MET	-	initiating methionine	UNP I6U7J4
W	2	GLY	-	expression tag	UNP I6U7J4
X	1	MET	-	initiating methionine	UNP I6U7J4
X	2	GLY	-	expression tag	UNP I6U7J4
Y	1	MET	-	initiating methionine	UNP I6U7J4
Y	2	GLY	-	expression tag	UNP I6U7J4
Z	1	MET	-	initiating methionine	UNP I6U7J4
Z	2	GLY	-	expression tag	UNP I6U7J4
a	1	MET	-	initiating methionine	UNP I6U7J4

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Chain	Residue	Modelled	Actual	Comment	Reference
a	2	GLY	-	expression tag	UNP I6U7J4
b	1	MET	-	initiating methionine	UNP I6U7J4
b	2	GLY	-	expression tag	UNP I6U7J4
c	1	MET	-	initiating methionine	UNP I6U7J4
c	2	GLY	-	expression tag	UNP I6U7J4
d	1	MET	-	initiating methionine	UNP I6U7J4
d	2	GLY	-	expression tag	UNP I6U7J4

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	e	2	Total 2	Fe 2	0	0
2	A	2	Total 2	Fe 2	0	0
2	B	2	Total 2	Fe 2	0	0
2	C	2	Total 2	Fe 2	0	0
2	D	2	Total 2	Fe 2	0	0
2	E	2	Total 2	Fe 2	0	0
2	F	2	Total 2	Fe 2	0	0
2	G	2	Total 2	Fe 2	0	0
2	L	2	Total 2	Fe 2	0	0
2	M	2	Total 2	Fe 2	0	0
2	P	2	Total 2	Fe 2	0	0
2	Q	2	Total 2	Fe 2	0	0
2	T	2	Total 2	Fe 2	0	0
2	X	2	Total 2	Fe 2	0	0
2	a	2	Total 2	Fe 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	e	62	Total 62	O 62	0	0
3	A	76	Total 76	O 76	0	0
3	B	68	Total 68	O 68	0	0
3	C	57	Total 57	O 57	0	0
3	D	59	Total 59	O 59	0	0
3	E	58	Total 58	O 58	0	0
3	F	70	Total 70	O 70	0	0
3	G	72	Total 72	O 72	0	0
3	H	59	Total 59	O 59	0	0
3	I	73	Total 73	O 73	0	0
3	J	61	Total 61	O 61	0	0
3	K	52	Total 52	O 52	0	0
3	L	72	Total 72	O 72	0	0
3	M	91	Total 91	O 91	0	0
3	N	74	Total 74	O 74	0	0
3	O	62	Total 62	O 62	0	0
3	P	56	Total 56	O 56	0	0
3	Q	59	Total 59	O 59	0	0
3	R	53	Total 53	O 53	0	0
3	T	92	Total 92	O 92	0	0
3	U	69	Total 69	O 69	0	0
3	V	80	Total 80	O 80	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	W	66	Total 66	O 66	0	0
3	X	70	Total 70	O 70	0	0
3	Y	71	Total 71	O 71	0	0
3	Z	74	Total 74	O 74	0	0
3	a	71	Total 71	O 71	0	0
3	b	69	Total 69	O 69	0	0
3	c	68	Total 68	O 68	0	0
3	d	50	Total 50	O 50	0	0

3 Residue-property plots ⓘ

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: PFC_05175

Chain e:

- Molecule 1: PFC_05175

Chain A:

- Molecule 1: PFC_05175

Chain B:

- Molecule 1: PFC_05175

Chain C:

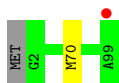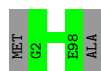- Molecule 1: PFC_05175

Chain D:

- Molecule 1: PFC_05175

Chain E:

98%

• Molecule 1: PFC_05175

Chain F:

98%

• Molecule 1: PFC_05175

Chain G:

98%
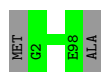
• Molecule 1: PFC_05175

Chain H:

97%

• Molecule 1: PFC_05175

Chain I:

99%

• Molecule 1: PFC_05175

Chain J:

97%

• Molecule 1: PFC_05175

Chain K:

98%
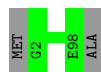
• Molecule 1: PFC_05175

Chain L:

98%

MET G2 E98 ALA
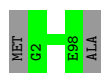
• Molecule 1: PFC_05175

Chain M:

99%

MET G2 A99
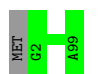
• Molecule 1: PFC_05175

Chain N:

98%

MET G2 E98 ALA
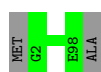
• Molecule 1: PFC_05175

Chain O:

98%

MET G2 E98 ALA

• Molecule 1: PFC_05175

Chain P:

97%

MET G2 E93 E98 ALA

• Molecule 1: PFC_05175

2%

Chain Q:

99%

MET G2 K18 A99
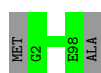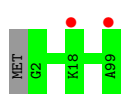
• Molecule 1: PFC_05175

Chain R:

98%

MET G2 E98 ALA
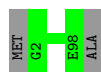
• Molecule 1: PFC_05175

Chain T:

98%

.

MET G2 E98 ALA
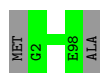
• Molecule 1: PFC_05175

Chain U:

98%

.

MET G2 E98 ALA
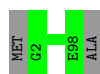
• Molecule 1: PFC_05175

Chain V:

98%

.

MET G2 E98 ALA
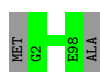
• Molecule 1: PFC_05175

Chain W:

98%

.

MET G2 E98 ALA
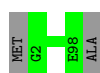
• Molecule 1: PFC_05175

Chain X:

98%

.

MET G2 E98 ALA
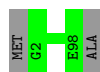
• Molecule 1: PFC_05175

Chain Y:

96%

. .

MET G2 E47 M70 E98 ALA

• Molecule 1: PFC_05175

Chain Z:

99%

.

MET G2 A99

• Molecule 1: PFC_05175

Chain a:

98%

MET G2 E98 ALA
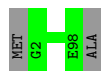
• Molecule 1: PFC_05175

Chain b:

99%

MET G2 A99

• Molecule 1: PFC_05175

%

Chain c:

99%

MET G2 A99

• Molecule 1: PFC_05175

%

Chain d:

98%

MET G2 E89 E98 ALA
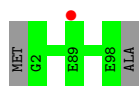
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	99.85Å 110.06Å 136.27Å 90.00° 91.22° 90.00°	Depositor
Resolution (Å)	47.19 – 2.03 49.71 – 2.03	Depositor EDS
% Data completeness (in resolution range)	97.0 (47.19-2.03) 99.7 (49.71-2.03)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	4.52 (at 2.03Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.174 , 0.202 0.174 , 0.202	Depositor DCC
R_{free} test set	9396 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	22.6	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 48.5	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	49851	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.9620e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

---

[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	0.25	0/800	0.39	0/1078
1	B	0.25	0/799	0.39	0/1076
1	C	0.24	0/802	0.39	0/1080
1	D	0.25	0/803	0.39	0/1081
1	E	0.25	0/811	0.41	0/1092
1	F	0.25	0/795	0.40	0/1071
1	G	0.25	0/794	0.40	0/1069
1	H	0.24	0/795	0.39	0/1071
1	I	0.24	0/800	0.39	0/1078
1	J	0.24	0/813	0.39	0/1094
1	K	0.25	0/814	0.40	0/1095
1	L	0.24	0/822	0.39	0/1105
1	M	0.25	0/808	0.39	0/1088
1	N	0.24	0/803	0.39	0/1081
1	O	0.24	0/806	0.38	0/1085
1	P	0.24	0/800	0.38	0/1077
1	Q	0.24	0/799	0.38	0/1076
1	R	0.24	0/794	0.38	0/1069
1	T	0.24	0/811	0.38	0/1091
1	U	0.24	0/794	0.39	0/1069
1	V	0.25	0/801	0.39	0/1079
1	W	0.25	0/803	0.39	0/1081
1	X	0.24	0/795	0.39	0/1071
1	Y	0.24	0/806	0.40	0/1085
1	Z	0.24	0/800	0.38	0/1078
1	a	0.25	0/795	0.40	0/1071
1	b	0.24	0/791	0.38	0/1066
1	c	0.24	0/821	0.39	0/1104
1	d	0.24	0/786	0.37	0/1059
1	e	0.24	0/799	0.39	0/1076
All	All	0.24	0/24060	0.39	0/32396

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 ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	97/99 (98%)	97 (100%)	0	0	100	100
1	B	97/99 (98%)	97 (100%)	0	0	100	100
1	C	97/99 (98%)	97 (100%)	0	0	100	100
1	D	97/99 (98%)	97 (100%)	0	0	100	100
1	E	98/99 (99%)	98 (100%)	0	0	100	100
1	F	96/99 (97%)	96 (100%)	0	0	100	100
1	G	96/99 (97%)	96 (100%)	0	0	100	100
1	H	96/99 (97%)	96 (100%)	0	0	100	100
1	I	97/99 (98%)	97 (100%)	0	0	100	100
1	J	98/99 (99%)	98 (100%)	0	0	100	100
1	K	98/99 (99%)	98 (100%)	0	0	100	100
1	L	99/99 (100%)	99 (100%)	0	0	100	100
1	M	98/99 (99%)	98 (100%)	0	0	100	100
1	N	97/99 (98%)	97 (100%)	0	0	100	100
1	O	97/99 (98%)	97 (100%)	0	0	100	100
1	P	97/99 (98%)	96 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	97/99 (98%)	97 (100%)	0	0	100	100
1	R	96/99 (97%)	96 (100%)	0	0	100	100
1	T	98/99 (99%)	98 (100%)	0	0	100	100
1	U	96/99 (97%)	96 (100%)	0	0	100	100
1	V	97/99 (98%)	97 (100%)	0	0	100	100
1	W	97/99 (98%)	97 (100%)	0	0	100	100
1	X	96/99 (97%)	95 (99%)	1 (1%)	0	100	100
1	Y	97/99 (98%)	97 (100%)	0	0	100	100
1	Z	97/99 (98%)	97 (100%)	0	0	100	100
1	a	96/99 (97%)	96 (100%)	0	0	100	100
1	b	96/99 (97%)	96 (100%)	0	0	100	100
1	c	99/99 (100%)	98 (99%)	1 (1%)	0	100	100
1	d	95/99 (96%)	95 (100%)	0	0	100	100
1	e	97/99 (98%)	97 (100%)	0	0	100	100
All	All	2909/2970 (98%)	2906 (100%)	3 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	86/86 (100%)	86 (100%)	0	100	100
1	B	86/86 (100%)	86 (100%)	0	100	100
1	C	86/86 (100%)	85 (99%)	1 (1%)	71	75
1	D	87/86 (101%)	86 (99%)	1 (1%)	73	77
1	E	87/86 (101%)	86 (99%)	1 (1%)	73	77
1	F	86/86 (100%)	86 (100%)	0	100	100
1	G	86/86 (100%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	86/86 (100%)	85 (99%)	1 (1%)	71	75
1	I	86/86 (100%)	86 (100%)	0	100	100
1	J	87/86 (101%)	85 (98%)	2 (2%)	50	51
1	K	88/86 (102%)	88 (100%)	0	100	100
1	L	89/86 (104%)	89 (100%)	0	100	100
1	M	87/86 (101%)	87 (100%)	0	100	100
1	N	87/86 (101%)	87 (100%)	0	100	100
1	O	87/86 (101%)	87 (100%)	0	100	100
1	P	87/86 (101%)	86 (99%)	1 (1%)	73	77
1	Q	86/86 (100%)	86 (100%)	0	100	100
1	R	86/86 (100%)	86 (100%)	0	100	100
1	T	88/86 (102%)	88 (100%)	0	100	100
1	U	86/86 (100%)	86 (100%)	0	100	100
1	V	87/86 (101%)	87 (100%)	0	100	100
1	W	87/86 (101%)	87 (100%)	0	100	100
1	X	86/86 (100%)	86 (100%)	0	100	100
1	Y	87/86 (101%)	85 (98%)	2 (2%)	50	51
1	Z	86/86 (100%)	86 (100%)	0	100	100
1	a	86/86 (100%)	86 (100%)	0	100	100
1	b	85/86 (99%)	85 (100%)	0	100	100
1	c	88/86 (102%)	88 (100%)	0	100	100
1	d	85/86 (99%)	85 (100%)	0	100	100
1	e	86/86 (100%)	86 (100%)	0	100	100
All	All	2597/2580 (101%)	2588 (100%)	9 (0%)	91	94

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	70	MET
1	D	13	ASP
1	E	13	ASP
1	H	70	MET
1	J	18	LYS
1	J	70	MET

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Mol	Chain	Res	Type
1	P	93	GLU
1	Y	47	GLU
1	Y	70	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 30 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 ⓘ

There are no such residues in this entry.

5.8   Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	98/99 (98%)	-0.40	1 (1%)	82	82	18, 27, 46, 62	0
1	B	98/99 (98%)	-0.47	0	100	100	15, 25, 44, 62	0
1	C	98/99 (98%)	-0.42	1 (1%)	82	82	16, 30, 49, 63	0
1	D	97/99 (97%)	-0.29	0	100	100	19, 27, 48, 58	0
1	E	98/99 (98%)	-0.50	1 (1%)	82	82	14, 26, 45, 59	0
1	F	97/99 (97%)	-0.39	0	100	100	16, 25, 44, 56	0
1	G	97/99 (97%)	-0.36	0	100	100	14, 23, 41, 53	0
1	H	97/99 (97%)	-0.47	0	100	100	18, 26, 46, 63	0
1	I	98/99 (98%)	-0.29	1 (1%)	82	82	15, 25, 45, 62	0
1	J	98/99 (98%)	-0.40	2 (2%)	65	64	17, 27, 46, 63	0
1	K	97/99 (97%)	-0.39	0	100	100	17, 26, 48, 59	0
1	L	97/99 (97%)	-0.40	0	100	100	14, 23, 44, 52	0
1	M	98/99 (98%)	-0.46	0	100	100	15, 25, 47, 58	0
1	N	97/99 (97%)	-0.44	0	100	100	16, 26, 44, 61	0
1	O	97/99 (97%)	-0.41	0	100	100	18, 25, 44, 59	0
1	P	97/99 (97%)	-0.36	0	100	100	19, 29, 51, 76	0
1	Q	98/99 (98%)	-0.33	2 (2%)	65	64	19, 30, 52, 70	0
1	R	97/99 (97%)	-0.42	0	100	100	19, 30, 47, 58	0
1	T	97/99 (97%)	-0.42	0	100	100	14, 23, 42, 56	0
1	U	97/99 (97%)	-0.41	0	100	100	16, 25, 44, 60	0
1	V	97/99 (97%)	-0.42	0	100	100	14, 23, 40, 57	0
1	W	97/99 (97%)	-0.45	0	100	100	16, 24, 44, 62	0
1	X	97/99 (97%)	-0.47	0	100	100	14, 23, 43, 52	0
1	Y	97/99 (97%)	-0.49	0	100	100	15, 24, 43, 58	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	Z	98/99 (98%)	-0.46	0	100	100	17, 27, 48, 62	0
1	a	97/99 (97%)	-0.45	0	100	100	17, 26, 43, 61	0
1	b	98/99 (98%)	-0.47	0	100	100	16, 26, 49, 66	0
1	c	98/99 (98%)	-0.31	1 (1%)	82	82	15, 24, 49, 67	0
1	d	97/99 (97%)	-0.33	1 (1%)	82	82	18, 29, 48, 63	0
1	e	98/99 (98%)	-0.36	0	100	100	17, 28, 48, 62	0
All	All	2922/2970 (98%)	-0.41	10 (0%)	94	93	14, 26, 47, 76	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	99	ALA	6.7
1	c	99	ALA	6.5
1	Q	99	ALA	3.0
1	J	99	ALA	2.9
1	A	99	ALA	2.8
1	C	99	ALA	2.2
1	J	13	ASP	2.2
1	E	99	ALA	2.1
1	d	89	GLU	2.0
1	Q	18	LYS	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	D	101	1/1	0.91	0.32	19,19,19,19	0
2	FE	P	101	1/1	0.92	0.36	20,20,20,20	1
2	FE	D	102	1/1	0.93	0.29	20,20,20,20	0
2	FE	G	102	1/1	0.93	0.29	15,15,15,15	1
2	FE	A	101	1/1	0.93	0.38	17,17,17,17	0
2	FE	e	101	1/1	0.94	0.30	19,19,19,19	1
2	FE	P	102	1/1	0.94	0.33	19,19,19,19	0
2	FE	a	102	1/1	0.94	0.32	16,16,16,16	0
2	FE	B	102	1/1	0.95	0.31	20,20,20,20	0
2	FE	L	102	1/1	0.95	0.26	21,21,21,21	0
2	FE	C	101	1/1	0.95	0.32	19,19,19,19	0
2	FE	e	102	1/1	0.95	0.34	16,16,16,16	0
2	FE	Q	102	1/1	0.95	0.30	20,20,20,20	0
2	FE	X	102	1/1	0.95	0.29	18,18,18,18	0
2	FE	a	101	1/1	0.95	0.32	18,18,18,18	0
2	FE	B	101	1/1	0.95	0.30	21,21,21,21	0
2	FE	G	101	1/1	0.96	0.31	14,14,14,14	0
2	FE	Q	101	1/1	0.96	0.28	27,27,27,27	0
2	FE	A	102	1/1	0.96	0.32	18,18,18,18	0
2	FE	E	101	1/1	0.96	0.30	23,23,23,23	0
2	FE	M	101	1/1	0.96	0.30	20,20,20,20	0
2	FE	F	102	1/1	0.96	0.30	16,16,16,16	0
2	FE	C	102	1/1	0.97	0.28	23,23,23,23	0
2	FE	E	102	1/1	0.97	0.29	20,20,20,20	0
2	FE	T	101	1/1	0.97	0.27	21,21,21,21	0
2	FE	T	102	1/1	0.97	0.25	19,19,19,19	0
2	FE	X	101	1/1	0.97	0.29	24,24,24,24	0
2	FE	M	102	1/1	0.97	0.27	22,22,22,22	0
2	FE	F	101	1/1	0.97	0.35	14,14,14,14	0
2	FE	L	101	1/1	0.97	0.24	20,20,20,20	0

6.5　Other polymers ⓘ

There are no such residues in this entry.