



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:45 PM GMT

PDB ID : 3UNO  
Title : Mycobacterium tuberculosis ferritin homolog, BfrB  
Authors : McMath, L.M.; Contreras, H.; Goulding, C.W.; TB Structural Genomics Consortium (TBSGC)  
Deposited on : 2011-11-16  
Resolution : 2.50 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  
<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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

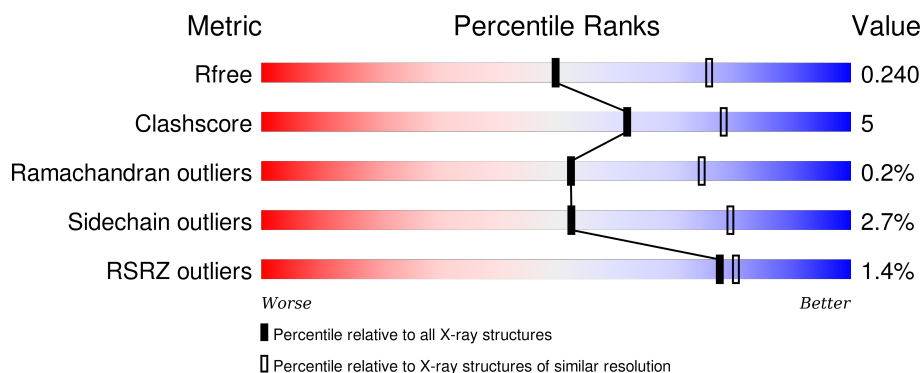
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	189	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>•</div> <div>7%</div> </div> </div>
1	B	189	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	189	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>8%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	189	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>10%</div> <div>•</div> <div>11%</div> </div> </div>
1	E	189	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div></div> <div>12%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	189	
1	G	189	
1	H	189	
1	I	189	
1	J	189	
1	K	189	
1	L	189	
1	M	189	
1	N	189	
1	O	189	
1	P	189	
1	Q	189	
1	R	189	
1	S	189	
1	T	189	
1	U	189	
1	V	189	
1	W	189	
1	X	189	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34567 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 Probable bacterioferritin BfrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1387	870	249	263	5			
1	B	169	Total	C	N	O	S	0	0	0
			1352	848	243	256	5			
1	C	169	Total	C	N	O	S	0	0	0
			1355	851	243	256	5			
1	D	169	Total	C	N	O	S	0	0	0
			1352	848	243	256	5			
1	E	167	Total	C	N	O	S	0	0	0
			1340	842	241	252	5			
1	F	168	Total	C	N	O	S	0	0	0
			1348	846	242	255	5			
1	G	170	Total	C	N	O	S	0	0	0
			1358	851	244	258	5			
1	H	168	Total	C	N	O	S	0	0	0
			1348	846	242	255	5			
1	I	168	Total	C	N	O	S	0	0	0
			1348	846	242	255	5			
1	J	168	Total	C	N	O	S	0	0	0
			1348	846	242	255	5			
1	K	168	Total	C	N	O	S	0	0	0
			1346	846	242	253	5			
1	L	168	Total	C	N	O	S	0	0	0
			1348	846	242	255	5			
1	M	168	Total	C	N	O	S	0	0	0
			1348	846	242	255	5			
1	N	172	Total	C	N	O	S	0	0	0
			1370	859	246	260	5			
1	O	168	Total	C	N	O	S	0	0	0
			1348	846	242	255	5			
1	P	168	Total	C	N	O	S	0	0	0
			1348	846	242	255	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	168	Total	C	N	O	S	0	0	0
			1342	843	239	255	5			
1	R	170	Total	C	N	O	S	0	0	0
			1358	851	244	258	5			
1	S	168	Total	C	N	O	S	0	0	0
			1344	842	242	255	5			
1	T	168	Total	C	N	O	S	0	0	0
			1348	846	242	255	5			
1	U	169	Total	C	N	O	S	0	0	0
			1352	848	243	256	5			
1	V	168	Total	C	N	O	S	0	0	0
			1348	846	242	255	5			
1	W	168	Total	C	N	O	S	0	0	0
			1348	846	242	255	5			
1	X	167	Total	C	N	O	S	0	0	0
			1340	842	241	252	5			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	GLY	-	EXPRESSION TAG	UNP P96237
A	183	SER	-	EXPRESSION TAG	UNP P96237
A	184	HIS	-	EXPRESSION TAG	UNP P96237
A	185	HIS	-	EXPRESSION TAG	UNP P96237
A	186	HIS	-	EXPRESSION TAG	UNP P96237
A	187	HIS	-	EXPRESSION TAG	UNP P96237
A	188	HIS	-	EXPRESSION TAG	UNP P96237
A	189	HIS	-	EXPRESSION TAG	UNP P96237
B	182	GLY	-	EXPRESSION TAG	UNP P96237
B	183	SER	-	EXPRESSION TAG	UNP P96237
B	184	HIS	-	EXPRESSION TAG	UNP P96237
B	185	HIS	-	EXPRESSION TAG	UNP P96237
B	186	HIS	-	EXPRESSION TAG	UNP P96237
B	187	HIS	-	EXPRESSION TAG	UNP P96237
B	188	HIS	-	EXPRESSION TAG	UNP P96237
B	189	HIS	-	EXPRESSION TAG	UNP P96237
C	182	GLY	-	EXPRESSION TAG	UNP P96237
C	183	SER	-	EXPRESSION TAG	UNP P96237
C	184	HIS	-	EXPRESSION TAG	UNP P96237
C	185	HIS	-	EXPRESSION TAG	UNP P96237
C	186	HIS	-	EXPRESSION TAG	UNP P96237
C	187	HIS	-	EXPRESSION TAG	UNP P96237
C	188	HIS	-	EXPRESSION TAG	UNP P96237

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Chain	Residue	Modelled	Actual	Comment	Reference
C	189	HIS	-	EXPRESSION TAG	UNP P96237
D	182	GLY	-	EXPRESSION TAG	UNP P96237
D	183	SER	-	EXPRESSION TAG	UNP P96237
D	184	HIS	-	EXPRESSION TAG	UNP P96237
D	185	HIS	-	EXPRESSION TAG	UNP P96237
D	186	HIS	-	EXPRESSION TAG	UNP P96237
D	187	HIS	-	EXPRESSION TAG	UNP P96237
D	188	HIS	-	EXPRESSION TAG	UNP P96237
D	189	HIS	-	EXPRESSION TAG	UNP P96237
E	182	GLY	-	EXPRESSION TAG	UNP P96237
E	183	SER	-	EXPRESSION TAG	UNP P96237
E	184	HIS	-	EXPRESSION TAG	UNP P96237
E	185	HIS	-	EXPRESSION TAG	UNP P96237
E	186	HIS	-	EXPRESSION TAG	UNP P96237
E	187	HIS	-	EXPRESSION TAG	UNP P96237
E	188	HIS	-	EXPRESSION TAG	UNP P96237
E	189	HIS	-	EXPRESSION TAG	UNP P96237
F	182	GLY	-	EXPRESSION TAG	UNP P96237
F	183	SER	-	EXPRESSION TAG	UNP P96237
F	184	HIS	-	EXPRESSION TAG	UNP P96237
F	185	HIS	-	EXPRESSION TAG	UNP P96237
F	186	HIS	-	EXPRESSION TAG	UNP P96237
F	187	HIS	-	EXPRESSION TAG	UNP P96237
F	188	HIS	-	EXPRESSION TAG	UNP P96237
F	189	HIS	-	EXPRESSION TAG	UNP P96237
G	182	GLY	-	EXPRESSION TAG	UNP P96237
G	183	SER	-	EXPRESSION TAG	UNP P96237
G	184	HIS	-	EXPRESSION TAG	UNP P96237
G	185	HIS	-	EXPRESSION TAG	UNP P96237
G	186	HIS	-	EXPRESSION TAG	UNP P96237
G	187	HIS	-	EXPRESSION TAG	UNP P96237
G	188	HIS	-	EXPRESSION TAG	UNP P96237
G	189	HIS	-	EXPRESSION TAG	UNP P96237
H	182	GLY	-	EXPRESSION TAG	UNP P96237
H	183	SER	-	EXPRESSION TAG	UNP P96237
H	184	HIS	-	EXPRESSION TAG	UNP P96237
H	185	HIS	-	EXPRESSION TAG	UNP P96237
H	186	HIS	-	EXPRESSION TAG	UNP P96237
H	187	HIS	-	EXPRESSION TAG	UNP P96237
H	188	HIS	-	EXPRESSION TAG	UNP P96237
H	189	HIS	-	EXPRESSION TAG	UNP P96237
I	182	GLY	-	EXPRESSION TAG	UNP P96237

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Chain	Residue	Modelled	Actual	Comment	Reference
I	183	SER	-	EXPRESSION TAG	UNP P96237
I	184	HIS	-	EXPRESSION TAG	UNP P96237
I	185	HIS	-	EXPRESSION TAG	UNP P96237
I	186	HIS	-	EXPRESSION TAG	UNP P96237
I	187	HIS	-	EXPRESSION TAG	UNP P96237
I	188	HIS	-	EXPRESSION TAG	UNP P96237
I	189	HIS	-	EXPRESSION TAG	UNP P96237
J	182	GLY	-	EXPRESSION TAG	UNP P96237
J	183	SER	-	EXPRESSION TAG	UNP P96237
J	184	HIS	-	EXPRESSION TAG	UNP P96237
J	185	HIS	-	EXPRESSION TAG	UNP P96237
J	186	HIS	-	EXPRESSION TAG	UNP P96237
J	187	HIS	-	EXPRESSION TAG	UNP P96237
J	188	HIS	-	EXPRESSION TAG	UNP P96237
J	189	HIS	-	EXPRESSION TAG	UNP P96237
K	182	GLY	-	EXPRESSION TAG	UNP P96237
K	183	SER	-	EXPRESSION TAG	UNP P96237
K	184	HIS	-	EXPRESSION TAG	UNP P96237
K	185	HIS	-	EXPRESSION TAG	UNP P96237
K	186	HIS	-	EXPRESSION TAG	UNP P96237
K	187	HIS	-	EXPRESSION TAG	UNP P96237
K	188	HIS	-	EXPRESSION TAG	UNP P96237
K	189	HIS	-	EXPRESSION TAG	UNP P96237
L	182	GLY	-	EXPRESSION TAG	UNP P96237
L	183	SER	-	EXPRESSION TAG	UNP P96237
L	184	HIS	-	EXPRESSION TAG	UNP P96237
L	185	HIS	-	EXPRESSION TAG	UNP P96237
L	186	HIS	-	EXPRESSION TAG	UNP P96237
L	187	HIS	-	EXPRESSION TAG	UNP P96237
L	188	HIS	-	EXPRESSION TAG	UNP P96237
L	189	HIS	-	EXPRESSION TAG	UNP P96237
M	182	GLY	-	EXPRESSION TAG	UNP P96237
M	183	SER	-	EXPRESSION TAG	UNP P96237
M	184	HIS	-	EXPRESSION TAG	UNP P96237
M	185	HIS	-	EXPRESSION TAG	UNP P96237
M	186	HIS	-	EXPRESSION TAG	UNP P96237
M	187	HIS	-	EXPRESSION TAG	UNP P96237
M	188	HIS	-	EXPRESSION TAG	UNP P96237
M	189	HIS	-	EXPRESSION TAG	UNP P96237
N	182	GLY	-	EXPRESSION TAG	UNP P96237
N	183	SER	-	EXPRESSION TAG	UNP P96237
N	184	HIS	-	EXPRESSION TAG	UNP P96237

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Chain	Residue	Modelled	Actual	Comment	Reference
N	185	HIS	-	EXPRESSION TAG	UNP P96237
N	186	HIS	-	EXPRESSION TAG	UNP P96237
N	187	HIS	-	EXPRESSION TAG	UNP P96237
N	188	HIS	-	EXPRESSION TAG	UNP P96237
N	189	HIS	-	EXPRESSION TAG	UNP P96237
O	182	GLY	-	EXPRESSION TAG	UNP P96237
O	183	SER	-	EXPRESSION TAG	UNP P96237
O	184	HIS	-	EXPRESSION TAG	UNP P96237
O	185	HIS	-	EXPRESSION TAG	UNP P96237
O	186	HIS	-	EXPRESSION TAG	UNP P96237
O	187	HIS	-	EXPRESSION TAG	UNP P96237
O	188	HIS	-	EXPRESSION TAG	UNP P96237
O	189	HIS	-	EXPRESSION TAG	UNP P96237
P	182	GLY	-	EXPRESSION TAG	UNP P96237
P	183	SER	-	EXPRESSION TAG	UNP P96237
P	184	HIS	-	EXPRESSION TAG	UNP P96237
P	185	HIS	-	EXPRESSION TAG	UNP P96237
P	186	HIS	-	EXPRESSION TAG	UNP P96237
P	187	HIS	-	EXPRESSION TAG	UNP P96237
P	188	HIS	-	EXPRESSION TAG	UNP P96237
P	189	HIS	-	EXPRESSION TAG	UNP P96237
Q	182	GLY	-	EXPRESSION TAG	UNP P96237
Q	183	SER	-	EXPRESSION TAG	UNP P96237
Q	184	HIS	-	EXPRESSION TAG	UNP P96237
Q	185	HIS	-	EXPRESSION TAG	UNP P96237
Q	186	HIS	-	EXPRESSION TAG	UNP P96237
Q	187	HIS	-	EXPRESSION TAG	UNP P96237
Q	188	HIS	-	EXPRESSION TAG	UNP P96237
Q	189	HIS	-	EXPRESSION TAG	UNP P96237
R	182	GLY	-	EXPRESSION TAG	UNP P96237
R	183	SER	-	EXPRESSION TAG	UNP P96237
R	184	HIS	-	EXPRESSION TAG	UNP P96237
R	185	HIS	-	EXPRESSION TAG	UNP P96237
R	186	HIS	-	EXPRESSION TAG	UNP P96237
R	187	HIS	-	EXPRESSION TAG	UNP P96237
R	188	HIS	-	EXPRESSION TAG	UNP P96237
R	189	HIS	-	EXPRESSION TAG	UNP P96237
S	182	GLY	-	EXPRESSION TAG	UNP P96237
S	183	SER	-	EXPRESSION TAG	UNP P96237
S	184	HIS	-	EXPRESSION TAG	UNP P96237
S	185	HIS	-	EXPRESSION TAG	UNP P96237
S	186	HIS	-	EXPRESSION TAG	UNP P96237

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Chain	Residue	Modelled	Actual	Comment	Reference
S	187	HIS	-	EXPRESSION TAG	UNP P96237
S	188	HIS	-	EXPRESSION TAG	UNP P96237
S	189	HIS	-	EXPRESSION TAG	UNP P96237
T	182	GLY	-	EXPRESSION TAG	UNP P96237
T	183	SER	-	EXPRESSION TAG	UNP P96237
T	184	HIS	-	EXPRESSION TAG	UNP P96237
T	185	HIS	-	EXPRESSION TAG	UNP P96237
T	186	HIS	-	EXPRESSION TAG	UNP P96237
T	187	HIS	-	EXPRESSION TAG	UNP P96237
T	188	HIS	-	EXPRESSION TAG	UNP P96237
T	189	HIS	-	EXPRESSION TAG	UNP P96237
U	182	GLY	-	EXPRESSION TAG	UNP P96237
U	183	SER	-	EXPRESSION TAG	UNP P96237
U	184	HIS	-	EXPRESSION TAG	UNP P96237
U	185	HIS	-	EXPRESSION TAG	UNP P96237
U	186	HIS	-	EXPRESSION TAG	UNP P96237
U	187	HIS	-	EXPRESSION TAG	UNP P96237
U	188	HIS	-	EXPRESSION TAG	UNP P96237
U	189	HIS	-	EXPRESSION TAG	UNP P96237
V	182	GLY	-	EXPRESSION TAG	UNP P96237
V	183	SER	-	EXPRESSION TAG	UNP P96237
V	184	HIS	-	EXPRESSION TAG	UNP P96237
V	185	HIS	-	EXPRESSION TAG	UNP P96237
V	186	HIS	-	EXPRESSION TAG	UNP P96237
V	187	HIS	-	EXPRESSION TAG	UNP P96237
V	188	HIS	-	EXPRESSION TAG	UNP P96237
V	189	HIS	-	EXPRESSION TAG	UNP P96237
W	182	GLY	-	EXPRESSION TAG	UNP P96237
W	183	SER	-	EXPRESSION TAG	UNP P96237
W	184	HIS	-	EXPRESSION TAG	UNP P96237
W	185	HIS	-	EXPRESSION TAG	UNP P96237
W	186	HIS	-	EXPRESSION TAG	UNP P96237
W	187	HIS	-	EXPRESSION TAG	UNP P96237
W	188	HIS	-	EXPRESSION TAG	UNP P96237
W	189	HIS	-	EXPRESSION TAG	UNP P96237
X	182	GLY	-	EXPRESSION TAG	UNP P96237
X	183	SER	-	EXPRESSION TAG	UNP P96237
X	184	HIS	-	EXPRESSION TAG	UNP P96237
X	185	HIS	-	EXPRESSION TAG	UNP P96237
X	186	HIS	-	EXPRESSION TAG	UNP P96237
X	187	HIS	-	EXPRESSION TAG	UNP P96237
X	188	HIS	-	EXPRESSION TAG	UNP P96237

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Chain	Residue	Modelled	Actual	Comment	Reference
X	189	HIS	-	EXPRESSION TAG	UNP P96237

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	76	Total O 76 76	0	0
2	B	90	Total O 90 90	0	0
2	C	84	Total O 84 84	0	0
2	D	93	Total O 93 93	0	0
2	E	78	Total O 78 78	0	0
2	F	79	Total O 79 79	0	0
2	G	83	Total O 83 83	0	0
2	H	100	Total O 100 100	0	0
2	I	92	Total O 92 92	0	0
2	J	101	Total O 101 101	0	0
2	K	97	Total O 97 97	0	0
2	L	104	Total O 104 104	0	0
2	M	80	Total O 80 80	0	0
2	N	90	Total O 90 90	0	0
2	O	100	Total O 100 100	0	0
2	P	88	Total O 88 88	0	0
2	Q	100	Total O 100 100	0	0
2	R	89	Total O 89 89	0	0
2	S	87	Total O 87 87	0	0

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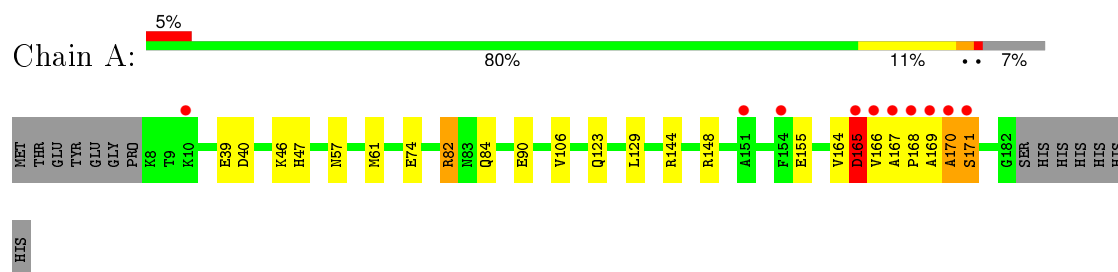
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	T	88	Total 88	O 88	0	0
2	U	90	Total 90	O 90	0	0
2	V	89	Total 89	O 89	0	0
2	W	77	Total 77	O 77	0	0
2	X	88	Total 88	O 88	0	0

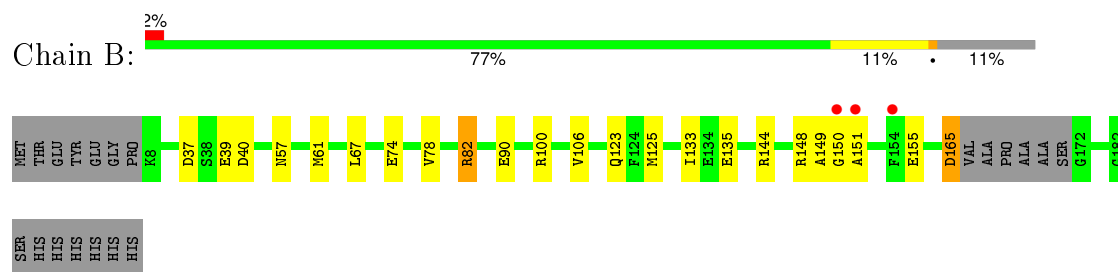
### 3 Residue-property plots [i](#)

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.

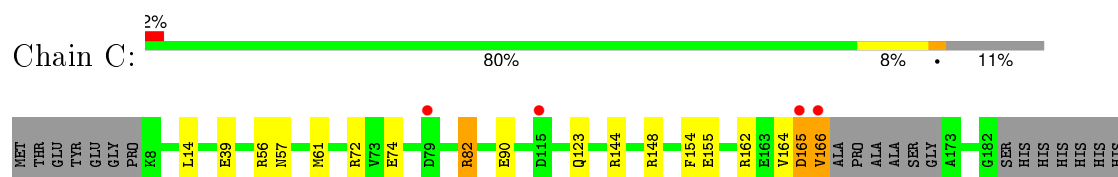
- Molecule 1: Probable bacterioferritin BfrB



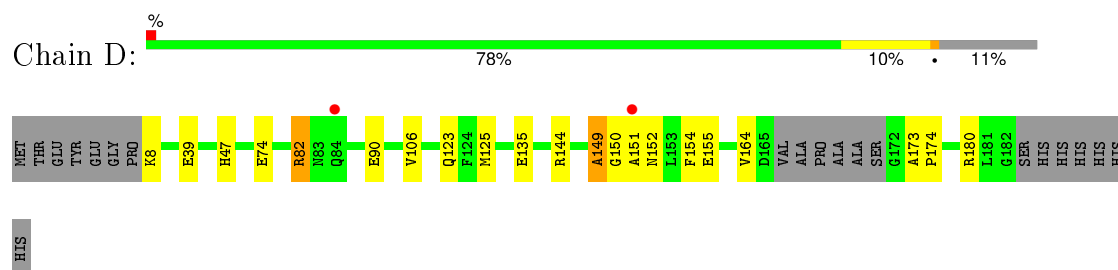
- Molecule 1: Probable bacterioferritin BfrB



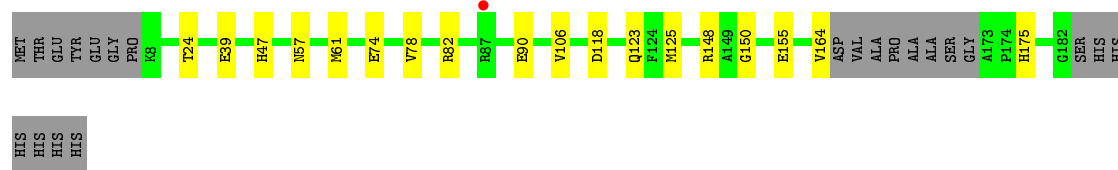
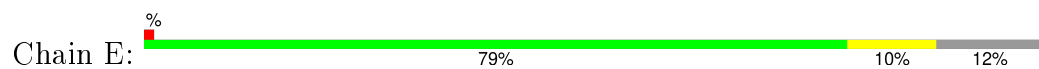
- Molecule 1: Probable bacterioferritin BfrB



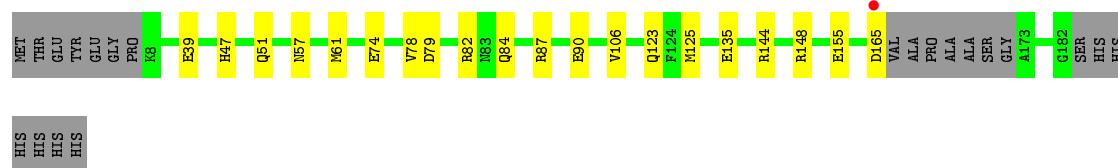
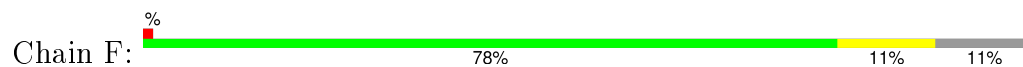
- Molecule 1: Probable bacterioferritin BfrB



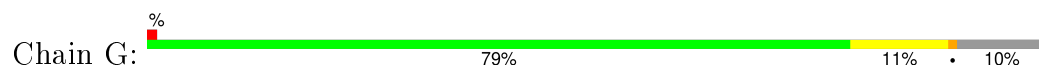
- Molecule 1: Probable bacterioferritin BfrB



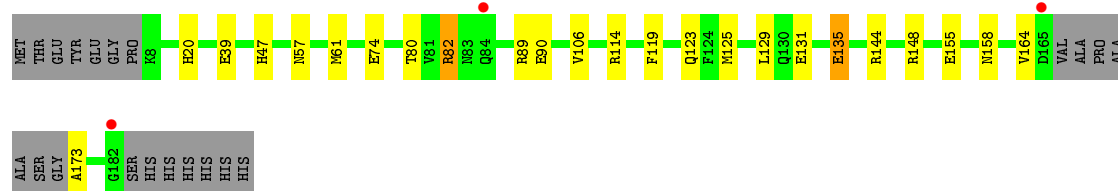
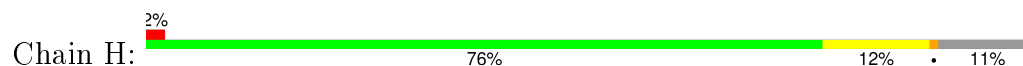
- Molecule 1: Probable bacterioferritin BfrB



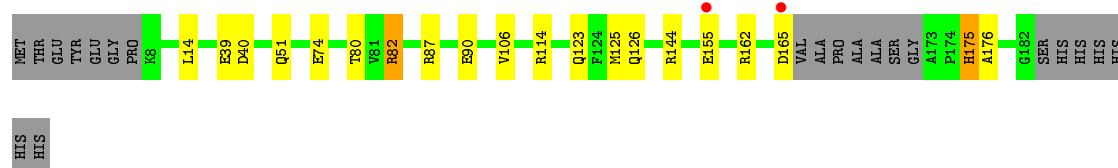
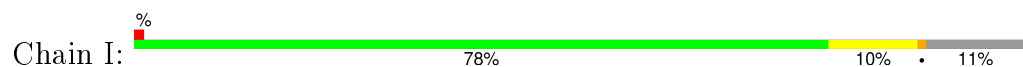
- Molecule 1: Probable bacterioferritin BfrB



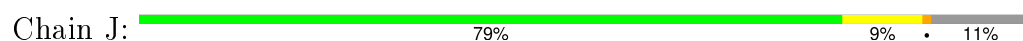
- Molecule 1: Probable bacterioferritin BfrB



- Molecule 1: Probable bacterioferritin BfrB

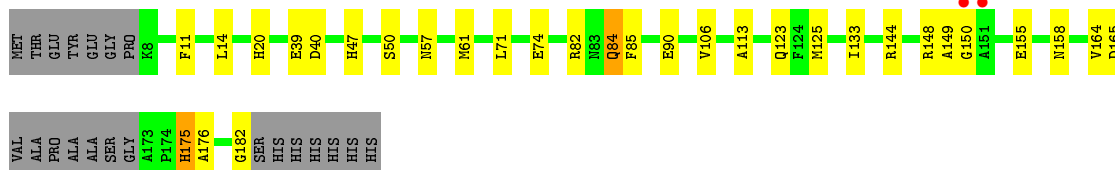
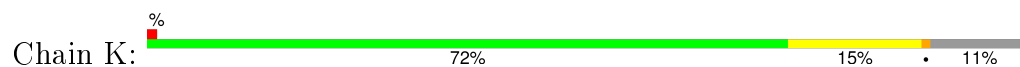


- Molecule 1: Probable bacterioferritin BfrB

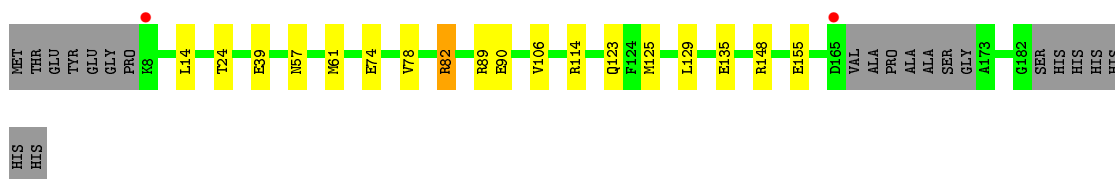
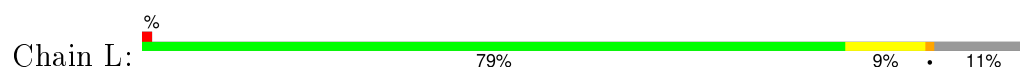




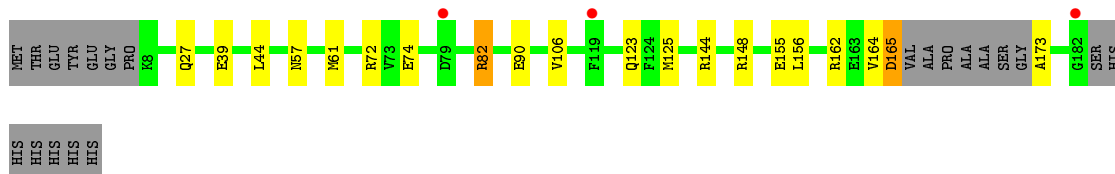
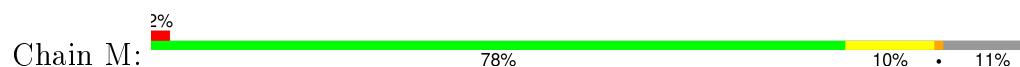
- Molecule 1: Probable bacterioferritin BfrB



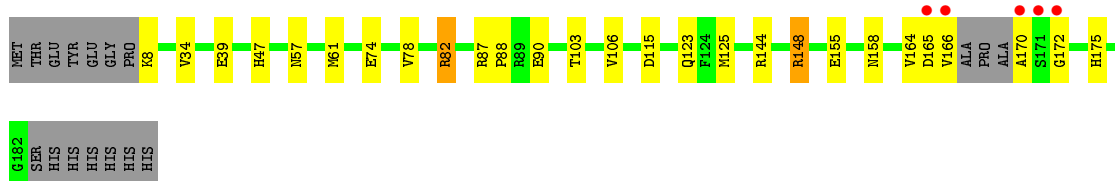
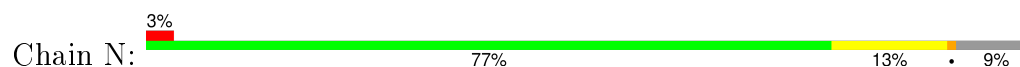
- Molecule 1: Probable bacterioferritin BfrB



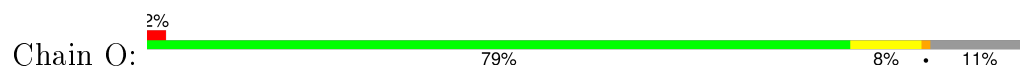
- Molecule 1: Probable bacterioferritin BfrB



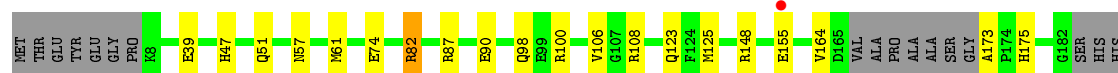
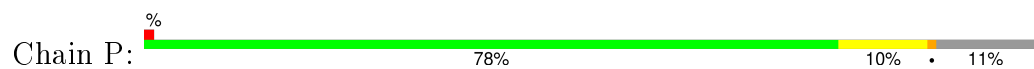
- Molecule 1: Probable bacterioferritin BfrB



- Molecule 1: Probable bacterioferritin BfrB

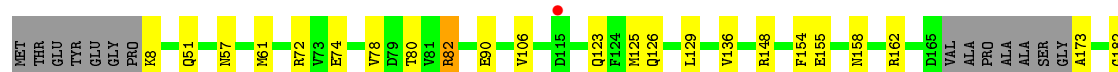
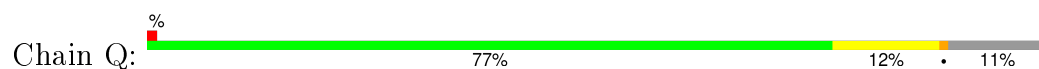


- Molecule 1: Probable bacterioferritin BfrB



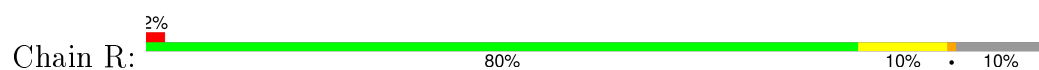
HIS  
HIS  
HIS

- Molecule 1: Probable bacterioferritin BfrB



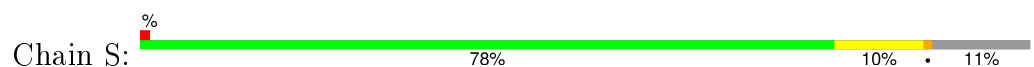
SER  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS

- Molecule 1: Probable bacterioferritin BfrB



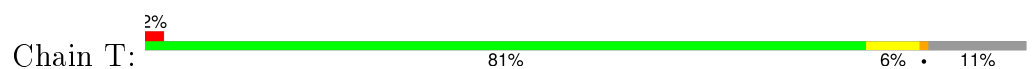
HIS  
HIS  
HIS

- Molecule 1: Probable bacterioferritin BfrB

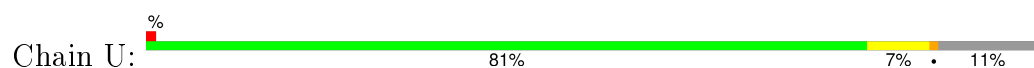


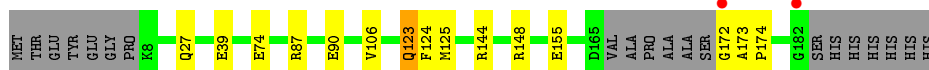
HIS  
HIS

- Molecule 1: Probable bacterioferritin BfrB



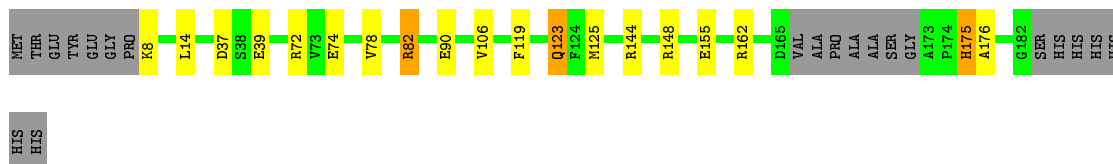
- Molecule 1: Probable bacterioferritin BfrB





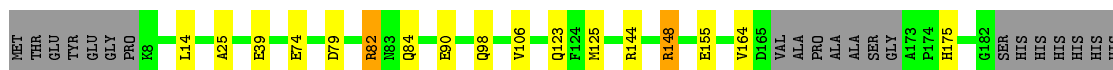
- Molecule 1: Probable bacterioferritin BfrB

Chain V: 79% 8% 11%



- Molecule 1: Probable bacterioferritin BfrB

Chain W: 80% 8% 11%



- Molecule 1: Probable bacterioferritin BfrB

Chain X: 80% 8% 12%





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	226.23Å 226.75Å 113.68Å 90.00° 94.75° 90.00°	Depositor
Resolution (Å)	49.35 – 2.50 49.35 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.35-2.50) 99.3 (49.35-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.66 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.206 , 0.247 0.199 , 0.240	Depositor DCC
$R_{free}$ test set	19314 reflections (9.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.7	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.55$ , $\langle L^2 \rangle = 0.39$	Xtriage
Outliers	4 of 194309 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	34567	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	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 51.92 % 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 5.2357e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.75	0/1412	0.63	0/1912
1	B	0.80	0/1375	0.75	2/1858 (0.1%)
1	C	0.78	0/1378	0.64	1/1863 (0.1%)
1	D	0.78	0/1375	0.64	0/1858
1	E	0.79	0/1363	0.62	0/1842
1	F	0.81	1/1371 (0.1%)	0.66	1/1853 (0.1%)
1	G	0.76	0/1381	0.64	0/1866
1	H	0.79	0/1371	0.63	0/1853
1	I	0.79	0/1371	0.66	0/1853
1	J	0.87	3/1371 (0.2%)	0.65	0/1853
1	K	0.78	0/1369	0.67	1/1850 (0.1%)
1	L	0.80	0/1371	0.65	0/1853
1	M	0.75	0/1371	0.62	0/1853
1	N	0.80	1/1393 (0.1%)	0.76	2/1883 (0.1%)
1	O	0.79	0/1371	0.65	0/1853
1	P	0.87	2/1371 (0.1%)	0.65	0/1853
1	Q	0.78	0/1365	0.65	0/1846
1	R	0.77	0/1381	0.64	0/1866
1	S	0.77	0/1367	0.63	0/1847
1	T	0.81	1/1371 (0.1%)	0.70	1/1853 (0.1%)
1	U	0.76	0/1375	0.61	0/1858
1	V	0.77	0/1371	0.64	0/1853
1	W	0.80	2/1371 (0.1%)	0.71	2/1853 (0.1%)
1	X	0.76	0/1363	0.63	0/1842
All	All	0.79	10/32978 (0.0%)	0.66	10/44574 (0.0%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	130	GLN	CD-NE2	-9.85	1.08	1.32
1	P	98	GLN	CD-NE2	-9.48	1.09	1.32
1	J	130	GLN	CD-OE1	-8.84	1.04	1.24
1	F	87	ARG	CZ-NH1	8.45	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	98	GLN	CD-OE1	-8.35	1.05	1.24

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	ARG	NE-CZ-NH2	-14.41	113.09	120.30
1	N	148	ARG	NE-CZ-NH2	-13.66	113.47	120.30
1	W	148	ARG	NE-CZ-NH2	-12.68	113.96	120.30
1	T	148	ARG	NE-CZ-NH2	-10.79	114.91	120.30
1	B	148	ARG	NE-CZ-NH1	9.20	124.90	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1387	0	1344	21	0
1	B	1352	0	1307	17	0
1	C	1355	0	1313	16	0
1	D	1352	0	1307	15	0
1	E	1340	0	1300	11	0
1	F	1348	0	1304	14	0
1	G	1358	0	1312	17	0
1	H	1348	0	1304	19	0
1	I	1348	0	1304	16	6
1	J	1348	0	1304	14	0
1	K	1346	0	1304	23	0
1	L	1348	0	1304	13	0
1	M	1348	0	1304	13	0
1	N	1370	0	1326	17	0
1	O	1348	0	1304	18	0
1	P	1348	0	1304	14	6
1	Q	1342	0	1293	20	0
1	R	1358	0	1312	23	0
1	S	1344	0	1294	14	4

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	1348	0	1304	11	0
1	U	1352	0	1307	21	0
1	V	1348	0	1304	15	0
1	W	1348	0	1304	14	0
1	X	1340	0	1300	11	0
2	A	76	0	0	3	0
2	B	90	0	0	7	0
2	C	84	0	0	3	0
2	D	93	0	0	5	0
2	E	78	0	0	3	0
2	F	79	0	0	5	0
2	G	83	0	0	5	0
2	H	100	0	0	6	0
2	I	92	0	0	9	0
2	J	101	0	0	6	0
2	K	97	0	0	6	0
2	L	104	0	0	4	0
2	M	80	0	0	6	0
2	N	90	0	0	7	0
2	O	100	0	0	8	0
2	P	88	0	0	4	0
2	Q	100	0	0	9	0
2	R	89	0	0	2	0
2	S	87	0	0	5	0
2	T	88	0	0	5	0
2	U	90	0	0	4	0
2	V	89	0	0	7	0
2	W	77	0	0	5	0
2	X	88	0	0	1	0
All	All	34567	0	31363	347	10

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 5.

The worst 5 of 347 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:82:ARG:NH2	1:E:90:GLU:OE1	1.68	1.25
1:O:87:ARG:HG2	1:O:88:PRO:CD	1.69	1.21
1:B:67:LEU:HD11	2:N:268:HOH:O	1.45	1.16
1:I:144:ARG:NH2	2:I:270:HOH:O	1.80	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:158:ASN:HB3	2:N:287:HOH:O	1.61	0.99

The worst 5 of 10 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:S:87:ARG:CZ	1:S:87:ARG:NH2[2_656]	1.80	0.40
1:I:87:ARG:CZ	1:P:87:ARG:NH2[4_556]	1.83	0.37
1:I:87:ARG:NH2	1:P:87:ARG:CZ[4_556]	1.85	0.35
1:I:87:ARG:NE	1:P:87:ARG:NH2[4_556]	1.90	0.30
1:I:87:ARG:NH2	1:P:87:ARG:NE[4_556]	1.92	0.28

## 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	173/189 (92%)	166 (96%)	3 (2%)	4 (2%)	8	12
1	B	165/189 (87%)	164 (99%)	1 (1%)	0	100	100
1	C	165/189 (87%)	162 (98%)	2 (1%)	1 (1%)	30	50
1	D	165/189 (87%)	160 (97%)	3 (2%)	2 (1%)	16	29
1	E	163/189 (86%)	162 (99%)	1 (1%)	0	100	100
1	F	164/189 (87%)	163 (99%)	1 (1%)	0	100	100
1	G	166/189 (88%)	164 (99%)	2 (1%)	0	100	100
1	H	164/189 (87%)	161 (98%)	3 (2%)	0	100	100
1	I	164/189 (87%)	162 (99%)	2 (1%)	0	100	100
1	J	164/189 (87%)	162 (99%)	2 (1%)	0	100	100
1	K	164/189 (87%)	162 (99%)	2 (1%)	0	100	100
1	L	164/189 (87%)	162 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	164/189 (87%)	162 (99%)	2 (1%)	0	100	100
1	N	168/189 (89%)	165 (98%)	2 (1%)	1 (1%)	30	50
1	O	164/189 (87%)	161 (98%)	3 (2%)	0	100	100
1	P	164/189 (87%)	162 (99%)	2 (1%)	0	100	100
1	Q	164/189 (87%)	162 (99%)	2 (1%)	0	100	100
1	R	166/189 (88%)	164 (99%)	2 (1%)	0	100	100
1	S	164/189 (87%)	163 (99%)	1 (1%)	0	100	100
1	T	164/189 (87%)	162 (99%)	2 (1%)	0	100	100
1	U	165/189 (87%)	164 (99%)	1 (1%)	0	100	100
1	V	164/189 (87%)	162 (99%)	2 (1%)	0	100	100
1	W	164/189 (87%)	162 (99%)	2 (1%)	0	100	100
1	X	163/189 (86%)	161 (99%)	2 (1%)	0	100	100
All	All	3955/4536 (87%)	3900 (99%)	47 (1%)	8 (0%)	52	75

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	ASP
1	A	170	ALA
1	A	171	SER
1	C	165	ASP
1	D	150	GLY

### 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	141/154 (92%)	136 (96%)	5 (4%)	43	70
1	B	138/154 (90%)	134 (97%)	4 (3%)	50	77
1	C	139/154 (90%)	135 (97%)	4 (3%)	50	77
1	D	138/154 (90%)	135 (98%)	3 (2%)	60	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	137/154 (89%)	134 (98%)	3 (2%)	60	84
1	F	138/154 (90%)	135 (98%)	3 (2%)	60	84
1	G	139/154 (90%)	134 (96%)	5 (4%)	42	69
1	H	138/154 (90%)	134 (97%)	4 (3%)	50	77
1	I	138/154 (90%)	134 (97%)	4 (3%)	50	77
1	J	138/154 (90%)	135 (98%)	3 (2%)	60	84
1	K	137/154 (89%)	134 (98%)	3 (2%)	60	84
1	L	138/154 (90%)	135 (98%)	3 (2%)	60	84
1	M	138/154 (90%)	134 (97%)	4 (3%)	50	77
1	N	140/154 (91%)	135 (96%)	5 (4%)	42	69
1	O	138/154 (90%)	133 (96%)	5 (4%)	42	69
1	P	138/154 (90%)	134 (97%)	4 (3%)	50	77
1	Q	137/154 (89%)	134 (98%)	3 (2%)	60	84
1	R	139/154 (90%)	136 (98%)	3 (2%)	60	84
1	S	137/154 (89%)	133 (97%)	4 (3%)	50	77
1	T	138/154 (90%)	135 (98%)	3 (2%)	60	84
1	U	138/154 (90%)	136 (99%)	2 (1%)	74	91
1	V	138/154 (90%)	134 (97%)	4 (3%)	50	77
1	W	138/154 (90%)	135 (98%)	3 (2%)	60	84
1	X	137/154 (89%)	133 (97%)	4 (3%)	50	77
All	All	3315/3696 (90%)	3227 (97%)	88 (3%)	52	79

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	123	GLN
1	N	82	ARG
1	W	74	GLU
1	K	175	HIS
1	M	74	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	47	HIS
1	N	47	HIS
1	V	47	HIS
1	M	47	HIS
1	O	47	HIS

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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	175/189 (92%)	0.04	10 (5%) 27 31	17, 27, 56, 98	0
1	B	169/189 (89%)	-0.05	3 (1%) 71 75	17, 27, 49, 63	0
1	C	169/189 (89%)	-0.13	4 (2%) 62 66	18, 27, 50, 73	0
1	D	169/189 (89%)	-0.05	2 (1%) 81 83	18, 27, 49, 60	0
1	E	167/189 (88%)	-0.18	1 (0%) 90 91	17, 26, 48, 57	0
1	F	168/189 (88%)	-0.13	1 (0%) 90 91	17, 27, 49, 72	0
1	G	170/189 (89%)	-0.15	1 (0%) 90 91	18, 27, 49, 72	0
1	H	168/189 (88%)	-0.12	3 (1%) 71 75	17, 26, 49, 72	0
1	I	168/189 (88%)	-0.07	2 (1%) 81 83	17, 26, 49, 67	0
1	J	168/189 (88%)	-0.14	0 100 100	16, 26, 48, 73	0
1	K	168/189 (88%)	-0.06	2 (1%) 81 83	17, 27, 49, 57	0
1	L	168/189 (88%)	-0.09	2 (1%) 81 83	17, 26, 48, 72	0
1	M	168/189 (88%)	-0.18	3 (1%) 71 75	18, 27, 48, 67	0
1	N	172/189 (91%)	-0.06	5 (2%) 55 60	18, 26, 50, 79	0
1	O	168/189 (88%)	-0.02	3 (1%) 71 75	18, 26, 47, 71	0
1	P	168/189 (88%)	-0.10	1 (0%) 90 91	18, 26, 48, 68	0
1	Q	168/189 (88%)	-0.20	1 (0%) 90 91	17, 26, 48, 84	0
1	R	170/189 (89%)	-0.13	4 (2%) 62 66	17, 27, 48, 60	0
1	S	168/189 (88%)	-0.07	2 (1%) 81 83	18, 26, 47, 70	0
1	T	168/189 (88%)	-0.12	3 (1%) 71 75	17, 27, 47, 57	0
1	U	169/189 (89%)	-0.06	2 (1%) 81 83	18, 27, 48, 70	0
1	V	168/189 (88%)	-0.19	0 100 100	17, 26, 49, 74	0
1	W	168/189 (88%)	-0.19	0 100 100	18, 27, 49, 69	0
1	X	167/189 (88%)	-0.22	0 100 100	18, 26, 48, 57	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	4049/4536 (89%)	-0.11	55 (1%) 78 80	16, 27, 49, 98	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	151	ALA	8.2
1	N	171	SER	7.6
1	K	151	ALA	6.8
1	A	169	ALA	6.2
1	A	167	ALA	5.5

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.