



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:22 am GMT

PDB ID : 3OJ5  
Title : Mycobacterium tuberculosis ferritin homolog, BfrB  
Authors : McMath, L.M.; Goulding, C.W.  
Deposited on : 2010-08-20  
Resolution : 2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

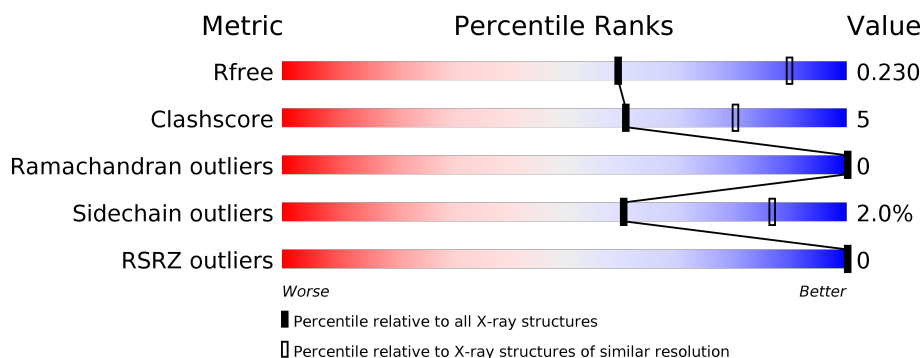
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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))
$R_{free}$	100719	3466 (2.88-2.80)
Clashscore	112137	3975 (2.88-2.80)
Ramachandran outliers	110173	3902 (2.88-2.80)
Sidechain outliers	110143	3905 (2.88-2.80)
RSRZ outliers	101464	3501 (2.88-2.80)

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>74%</div> <div>9%</div> <div>17%</div> </div>
1	B	189	<div> <div>72%</div> <div>11%</div> <div>17%</div> </div>
1	C	189	<div> <div>72%</div> <div>10%</div> <div>•</div> <div>17%</div> </div>
1	D	189	<div> <div>70%</div> <div>13%</div> <div>•</div> <div>17%</div> </div>
1	E	189	<div> <div>75%</div> <div>7%</div> <div>•</div> <div>17%</div> </div>
1	F	189	<div> <div>70%</div> <div>12%</div> <div>•</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
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 30954 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 family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	0	0
			1271	801	223	242	5			
1	B	157	Total	C	N	O	S	0	0	0
			1277	804	226	242	5			
1	C	157	Total	C	N	O	S	0	0	0
			1277	804	226	242	5			
1	D	157	Total	C	N	O	S	0	0	0
			1277	804	226	242	5			
1	E	157	Total	C	N	O	S	0	0	0
			1271	801	223	242	5			
1	F	157	Total	C	N	O	S	0	0	0
			1277	804	226	242	5			
1	G	157	Total	C	N	O	S	0	0	0
			1277	804	226	242	5			
1	H	157	Total	C	N	O	S	0	0	0
			1277	804	226	242	5			
1	I	157	Total	C	N	O	S	0	0	0
			1277	804	226	242	5			
1	J	157	Total	C	N	O	S	0	0	0
			1277	804	226	242	5			
1	K	157	Total	C	N	O	S	0	0	0
			1277	804	226	242	5			
1	L	157	Total	C	N	O	S	0	0	0
			1277	804	226	242	5			
1	M	157	Total	C	N	O	S	0	0	0
			1277	804	226	242	5			
1	N	157	Total	C	N	O	S	0	0	0
			1277	804	226	242	5			
1	O	157	Total	C	N	O	S	0	0	0
			1271	801	223	242	5			
1	P	157	Total	C	N	O	S	0	0	0
			1277	804	226	242	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	157	Total	C	N	O	S	0	0	0
			1277	804	226	242	5			
1	R	157	Total	C	N	O	S	0	0	0
			1277	804	226	242	5			
1	S	157	Total	C	N	O	S	0	0	0
			1271	801	223	242	5			
1	T	157	Total	C	N	O	S	0	0	0
			1277	804	226	242	5			
1	U	157	Total	C	N	O	S	0	0	0
			1277	804	226	242	5			
1	V	157	Total	C	N	O	S	0	0	0
			1277	804	226	242	5			
1	W	157	Total	C	N	O	S	0	0	0
			1277	804	226	242	5			
1	X	157	Total	C	N	O	S	0	0	0
			1277	804	226	242	5			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	GLY	-	EXPRESSION TAG	UNP A5U9H0
A	183	SER	-	EXPRESSION TAG	UNP A5U9H0
A	184	HIS	-	EXPRESSION TAG	UNP A5U9H0
A	185	HIS	-	EXPRESSION TAG	UNP A5U9H0
A	186	HIS	-	EXPRESSION TAG	UNP A5U9H0
A	187	HIS	-	EXPRESSION TAG	UNP A5U9H0
A	188	HIS	-	EXPRESSION TAG	UNP A5U9H0
A	189	HIS	-	EXPRESSION TAG	UNP A5U9H0
B	182	GLY	-	EXPRESSION TAG	UNP A5U9H0
B	183	SER	-	EXPRESSION TAG	UNP A5U9H0
B	184	HIS	-	EXPRESSION TAG	UNP A5U9H0
B	185	HIS	-	EXPRESSION TAG	UNP A5U9H0
B	186	HIS	-	EXPRESSION TAG	UNP A5U9H0
B	187	HIS	-	EXPRESSION TAG	UNP A5U9H0
B	188	HIS	-	EXPRESSION TAG	UNP A5U9H0
B	189	HIS	-	EXPRESSION TAG	UNP A5U9H0
C	182	GLY	-	EXPRESSION TAG	UNP A5U9H0
C	183	SER	-	EXPRESSION TAG	UNP A5U9H0
C	184	HIS	-	EXPRESSION TAG	UNP A5U9H0
C	185	HIS	-	EXPRESSION TAG	UNP A5U9H0
C	186	HIS	-	EXPRESSION TAG	UNP A5U9H0
C	187	HIS	-	EXPRESSION TAG	UNP A5U9H0
C	188	HIS	-	EXPRESSION TAG	UNP A5U9H0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	189	HIS	-	EXPRESSION TAG	UNP A5U9H0
D	182	GLY	-	EXPRESSION TAG	UNP A5U9H0
D	183	SER	-	EXPRESSION TAG	UNP A5U9H0
D	184	HIS	-	EXPRESSION TAG	UNP A5U9H0
D	185	HIS	-	EXPRESSION TAG	UNP A5U9H0
D	186	HIS	-	EXPRESSION TAG	UNP A5U9H0
D	187	HIS	-	EXPRESSION TAG	UNP A5U9H0
D	188	HIS	-	EXPRESSION TAG	UNP A5U9H0
D	189	HIS	-	EXPRESSION TAG	UNP A5U9H0
E	182	GLY	-	EXPRESSION TAG	UNP A5U9H0
E	183	SER	-	EXPRESSION TAG	UNP A5U9H0
E	184	HIS	-	EXPRESSION TAG	UNP A5U9H0
E	185	HIS	-	EXPRESSION TAG	UNP A5U9H0
E	186	HIS	-	EXPRESSION TAG	UNP A5U9H0
E	187	HIS	-	EXPRESSION TAG	UNP A5U9H0
E	188	HIS	-	EXPRESSION TAG	UNP A5U9H0
E	189	HIS	-	EXPRESSION TAG	UNP A5U9H0
F	182	GLY	-	EXPRESSION TAG	UNP A5U9H0
F	183	SER	-	EXPRESSION TAG	UNP A5U9H0
F	184	HIS	-	EXPRESSION TAG	UNP A5U9H0
F	185	HIS	-	EXPRESSION TAG	UNP A5U9H0
F	186	HIS	-	EXPRESSION TAG	UNP A5U9H0
F	187	HIS	-	EXPRESSION TAG	UNP A5U9H0
F	188	HIS	-	EXPRESSION TAG	UNP A5U9H0
F	189	HIS	-	EXPRESSION TAG	UNP A5U9H0
G	182	GLY	-	EXPRESSION TAG	UNP A5U9H0
G	183	SER	-	EXPRESSION TAG	UNP A5U9H0
G	184	HIS	-	EXPRESSION TAG	UNP A5U9H0
G	185	HIS	-	EXPRESSION TAG	UNP A5U9H0
G	186	HIS	-	EXPRESSION TAG	UNP A5U9H0
G	187	HIS	-	EXPRESSION TAG	UNP A5U9H0
G	188	HIS	-	EXPRESSION TAG	UNP A5U9H0
G	189	HIS	-	EXPRESSION TAG	UNP A5U9H0
H	182	GLY	-	EXPRESSION TAG	UNP A5U9H0
H	183	SER	-	EXPRESSION TAG	UNP A5U9H0
H	184	HIS	-	EXPRESSION TAG	UNP A5U9H0
H	185	HIS	-	EXPRESSION TAG	UNP A5U9H0
H	186	HIS	-	EXPRESSION TAG	UNP A5U9H0
H	187	HIS	-	EXPRESSION TAG	UNP A5U9H0
H	188	HIS	-	EXPRESSION TAG	UNP A5U9H0
H	189	HIS	-	EXPRESSION TAG	UNP A5U9H0
I	182	GLY	-	EXPRESSION TAG	UNP A5U9H0

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Chain	Residue	Modelled	Actual	Comment	Reference
I	183	SER	-	EXPRESSION TAG	UNP A5U9H0
I	184	HIS	-	EXPRESSION TAG	UNP A5U9H0
I	185	HIS	-	EXPRESSION TAG	UNP A5U9H0
I	186	HIS	-	EXPRESSION TAG	UNP A5U9H0
I	187	HIS	-	EXPRESSION TAG	UNP A5U9H0
I	188	HIS	-	EXPRESSION TAG	UNP A5U9H0
I	189	HIS	-	EXPRESSION TAG	UNP A5U9H0
J	182	GLY	-	EXPRESSION TAG	UNP A5U9H0
J	183	SER	-	EXPRESSION TAG	UNP A5U9H0
J	184	HIS	-	EXPRESSION TAG	UNP A5U9H0
J	185	HIS	-	EXPRESSION TAG	UNP A5U9H0
J	186	HIS	-	EXPRESSION TAG	UNP A5U9H0
J	187	HIS	-	EXPRESSION TAG	UNP A5U9H0
J	188	HIS	-	EXPRESSION TAG	UNP A5U9H0
J	189	HIS	-	EXPRESSION TAG	UNP A5U9H0
K	182	GLY	-	EXPRESSION TAG	UNP A5U9H0
K	183	SER	-	EXPRESSION TAG	UNP A5U9H0
K	184	HIS	-	EXPRESSION TAG	UNP A5U9H0
K	185	HIS	-	EXPRESSION TAG	UNP A5U9H0
K	186	HIS	-	EXPRESSION TAG	UNP A5U9H0
K	187	HIS	-	EXPRESSION TAG	UNP A5U9H0
K	188	HIS	-	EXPRESSION TAG	UNP A5U9H0
K	189	HIS	-	EXPRESSION TAG	UNP A5U9H0
L	182	GLY	-	EXPRESSION TAG	UNP A5U9H0
L	183	SER	-	EXPRESSION TAG	UNP A5U9H0
L	184	HIS	-	EXPRESSION TAG	UNP A5U9H0
L	185	HIS	-	EXPRESSION TAG	UNP A5U9H0
L	186	HIS	-	EXPRESSION TAG	UNP A5U9H0
L	187	HIS	-	EXPRESSION TAG	UNP A5U9H0
L	188	HIS	-	EXPRESSION TAG	UNP A5U9H0
L	189	HIS	-	EXPRESSION TAG	UNP A5U9H0
M	182	GLY	-	EXPRESSION TAG	UNP A5U9H0
M	183	SER	-	EXPRESSION TAG	UNP A5U9H0
M	184	HIS	-	EXPRESSION TAG	UNP A5U9H0
M	185	HIS	-	EXPRESSION TAG	UNP A5U9H0
M	186	HIS	-	EXPRESSION TAG	UNP A5U9H0
M	187	HIS	-	EXPRESSION TAG	UNP A5U9H0
M	188	HIS	-	EXPRESSION TAG	UNP A5U9H0
M	189	HIS	-	EXPRESSION TAG	UNP A5U9H0
N	182	GLY	-	EXPRESSION TAG	UNP A5U9H0
N	183	SER	-	EXPRESSION TAG	UNP A5U9H0
N	184	HIS	-	EXPRESSION TAG	UNP A5U9H0

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Chain	Residue	Modelled	Actual	Comment	Reference
N	185	HIS	-	EXPRESSION TAG	UNP A5U9H0
N	186	HIS	-	EXPRESSION TAG	UNP A5U9H0
N	187	HIS	-	EXPRESSION TAG	UNP A5U9H0
N	188	HIS	-	EXPRESSION TAG	UNP A5U9H0
N	189	HIS	-	EXPRESSION TAG	UNP A5U9H0
O	182	GLY	-	EXPRESSION TAG	UNP A5U9H0
O	183	SER	-	EXPRESSION TAG	UNP A5U9H0
O	184	HIS	-	EXPRESSION TAG	UNP A5U9H0
O	185	HIS	-	EXPRESSION TAG	UNP A5U9H0
O	186	HIS	-	EXPRESSION TAG	UNP A5U9H0
O	187	HIS	-	EXPRESSION TAG	UNP A5U9H0
O	188	HIS	-	EXPRESSION TAG	UNP A5U9H0
O	189	HIS	-	EXPRESSION TAG	UNP A5U9H0
P	182	GLY	-	EXPRESSION TAG	UNP A5U9H0
P	183	SER	-	EXPRESSION TAG	UNP A5U9H0
P	184	HIS	-	EXPRESSION TAG	UNP A5U9H0
P	185	HIS	-	EXPRESSION TAG	UNP A5U9H0
P	186	HIS	-	EXPRESSION TAG	UNP A5U9H0
P	187	HIS	-	EXPRESSION TAG	UNP A5U9H0
P	188	HIS	-	EXPRESSION TAG	UNP A5U9H0
P	189	HIS	-	EXPRESSION TAG	UNP A5U9H0
Q	182	GLY	-	EXPRESSION TAG	UNP A5U9H0
Q	183	SER	-	EXPRESSION TAG	UNP A5U9H0
Q	184	HIS	-	EXPRESSION TAG	UNP A5U9H0
Q	185	HIS	-	EXPRESSION TAG	UNP A5U9H0
Q	186	HIS	-	EXPRESSION TAG	UNP A5U9H0
Q	187	HIS	-	EXPRESSION TAG	UNP A5U9H0
Q	188	HIS	-	EXPRESSION TAG	UNP A5U9H0
Q	189	HIS	-	EXPRESSION TAG	UNP A5U9H0
R	182	GLY	-	EXPRESSION TAG	UNP A5U9H0
R	183	SER	-	EXPRESSION TAG	UNP A5U9H0
R	184	HIS	-	EXPRESSION TAG	UNP A5U9H0
R	185	HIS	-	EXPRESSION TAG	UNP A5U9H0
R	186	HIS	-	EXPRESSION TAG	UNP A5U9H0
R	187	HIS	-	EXPRESSION TAG	UNP A5U9H0
R	188	HIS	-	EXPRESSION TAG	UNP A5U9H0
R	189	HIS	-	EXPRESSION TAG	UNP A5U9H0
S	182	GLY	-	EXPRESSION TAG	UNP A5U9H0
S	183	SER	-	EXPRESSION TAG	UNP A5U9H0
S	184	HIS	-	EXPRESSION TAG	UNP A5U9H0
S	185	HIS	-	EXPRESSION TAG	UNP A5U9H0
S	186	HIS	-	EXPRESSION TAG	UNP A5U9H0

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Chain	Residue	Modelled	Actual	Comment	Reference
S	187	HIS	-	EXPRESSION TAG	UNP A5U9H0
S	188	HIS	-	EXPRESSION TAG	UNP A5U9H0
S	189	HIS	-	EXPRESSION TAG	UNP A5U9H0
T	182	GLY	-	EXPRESSION TAG	UNP A5U9H0
T	183	SER	-	EXPRESSION TAG	UNP A5U9H0
T	184	HIS	-	EXPRESSION TAG	UNP A5U9H0
T	185	HIS	-	EXPRESSION TAG	UNP A5U9H0
T	186	HIS	-	EXPRESSION TAG	UNP A5U9H0
T	187	HIS	-	EXPRESSION TAG	UNP A5U9H0
T	188	HIS	-	EXPRESSION TAG	UNP A5U9H0
T	189	HIS	-	EXPRESSION TAG	UNP A5U9H0
U	182	GLY	-	EXPRESSION TAG	UNP A5U9H0
U	183	SER	-	EXPRESSION TAG	UNP A5U9H0
U	184	HIS	-	EXPRESSION TAG	UNP A5U9H0
U	185	HIS	-	EXPRESSION TAG	UNP A5U9H0
U	186	HIS	-	EXPRESSION TAG	UNP A5U9H0
U	187	HIS	-	EXPRESSION TAG	UNP A5U9H0
U	188	HIS	-	EXPRESSION TAG	UNP A5U9H0
U	189	HIS	-	EXPRESSION TAG	UNP A5U9H0
V	182	GLY	-	EXPRESSION TAG	UNP A5U9H0
V	183	SER	-	EXPRESSION TAG	UNP A5U9H0
V	184	HIS	-	EXPRESSION TAG	UNP A5U9H0
V	185	HIS	-	EXPRESSION TAG	UNP A5U9H0
V	186	HIS	-	EXPRESSION TAG	UNP A5U9H0
V	187	HIS	-	EXPRESSION TAG	UNP A5U9H0
V	188	HIS	-	EXPRESSION TAG	UNP A5U9H0
V	189	HIS	-	EXPRESSION TAG	UNP A5U9H0
W	182	GLY	-	EXPRESSION TAG	UNP A5U9H0
W	183	SER	-	EXPRESSION TAG	UNP A5U9H0
W	184	HIS	-	EXPRESSION TAG	UNP A5U9H0
W	185	HIS	-	EXPRESSION TAG	UNP A5U9H0
W	186	HIS	-	EXPRESSION TAG	UNP A5U9H0
W	187	HIS	-	EXPRESSION TAG	UNP A5U9H0
W	188	HIS	-	EXPRESSION TAG	UNP A5U9H0
W	189	HIS	-	EXPRESSION TAG	UNP A5U9H0
X	182	GLY	-	EXPRESSION TAG	UNP A5U9H0
X	183	SER	-	EXPRESSION TAG	UNP A5U9H0
X	184	HIS	-	EXPRESSION TAG	UNP A5U9H0
X	185	HIS	-	EXPRESSION TAG	UNP A5U9H0
X	186	HIS	-	EXPRESSION TAG	UNP A5U9H0
X	187	HIS	-	EXPRESSION TAG	UNP A5U9H0
X	188	HIS	-	EXPRESSION TAG	UNP A5U9H0

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Chain	Residue	Modelled	Actual	Comment	Reference
X	189	HIS	-	EXPRESSION TAG	UNP A5U9H0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	21	Total O 21 21	0	0
2	B	9	Total O 9 9	0	0
2	C	11	Total O 11 11	0	0
2	D	10	Total O 10 10	0	0
2	E	18	Total O 18 18	0	0
2	F	21	Total O 21 21	0	0
2	G	13	Total O 13 13	0	0
2	H	14	Total O 14 14	0	0
2	I	14	Total O 14 14	0	0
2	J	13	Total O 13 13	0	0
2	K	9	Total O 9 9	0	0
2	L	14	Total O 14 14	0	0
2	M	12	Total O 12 12	0	0
2	N	20	Total O 20 20	0	0
2	O	17	Total O 17 17	0	0
2	P	14	Total O 14 14	0	0
2	Q	15	Total O 15 15	0	0
2	R	9	Total O 9 9	0	0
2	S	16	Total O 16 16	0	0

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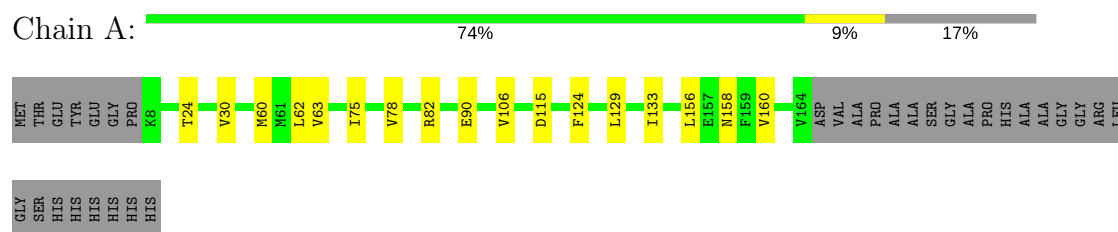
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	T	8	Total 8	O 8	0	0
2	U	14	Total 14	O 14	0	0
2	V	8	Total 8	O 8	0	0
2	W	15	Total 15	O 15	0	0
2	X	15	Total 15	O 15	0	0

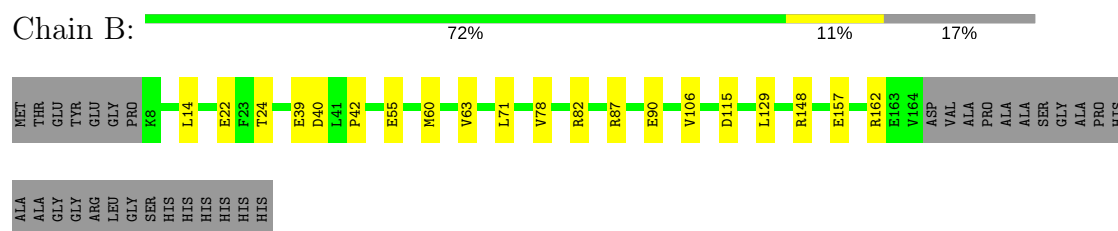
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

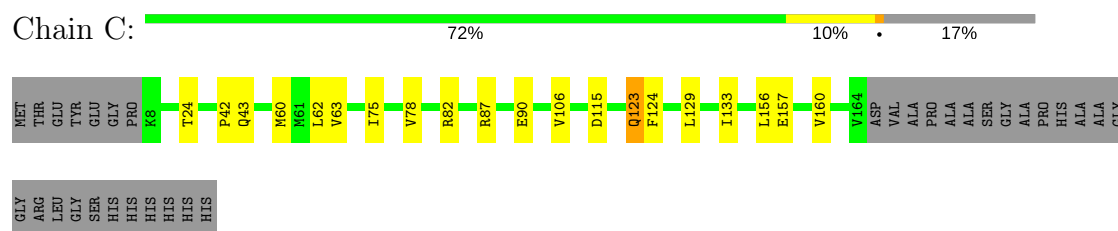
#### • Molecule 1: Ferritin family protein



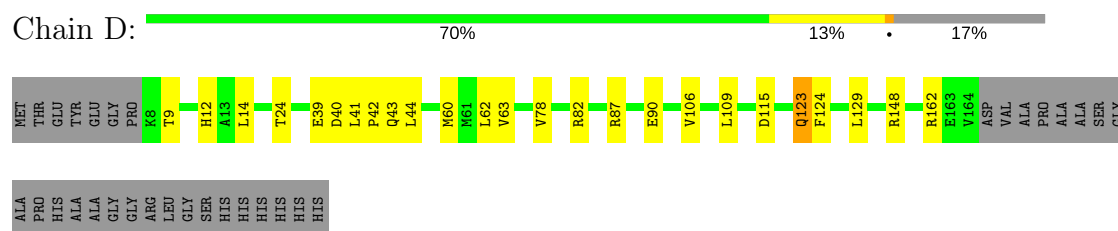
#### • Molecule 1: Ferritin family protein



#### • Molecule 1: Ferritin family protein

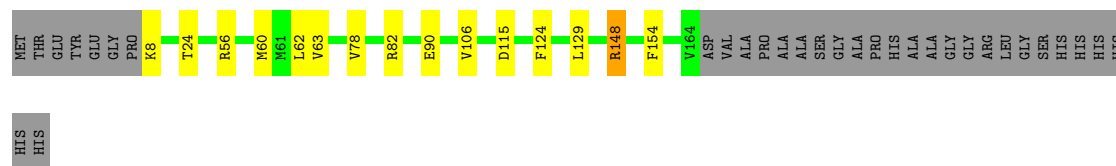


#### • Molecule 1: Ferritin family protein



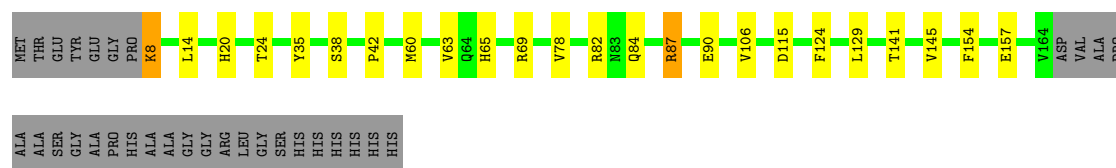
- Molecule 1: Ferritin family protein

Chain E: 




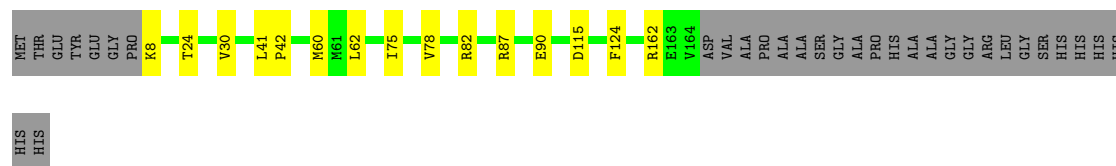
- Molecule 1: Ferritin family protein

Chain F: 




- Molecule 1: Ferritin family protein

Chain G: 



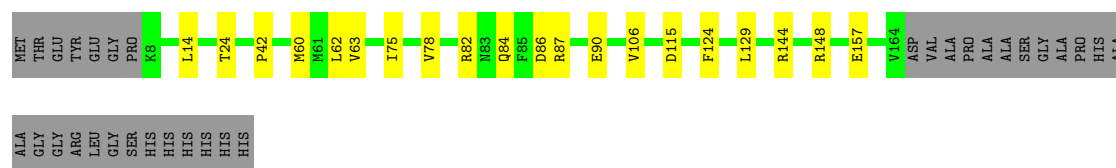
- Molecule 1: Ferritin family protein

Chain H: 

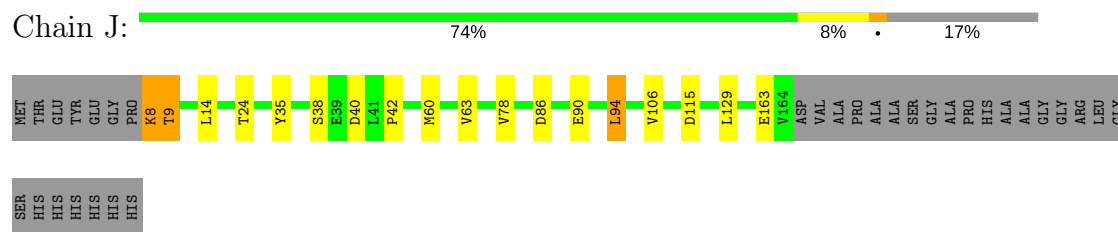


- Molecule 1: Ferritin family protein

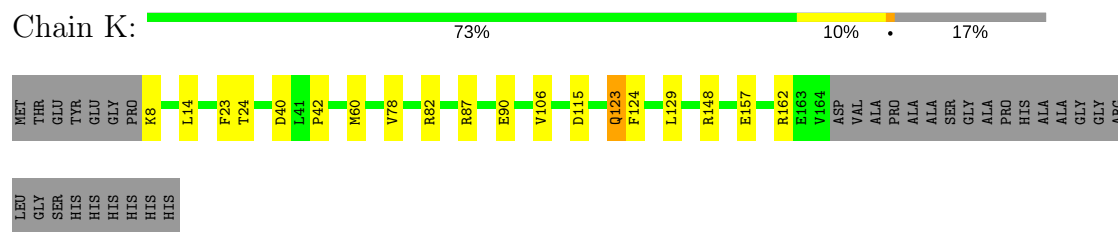
Chain I: 



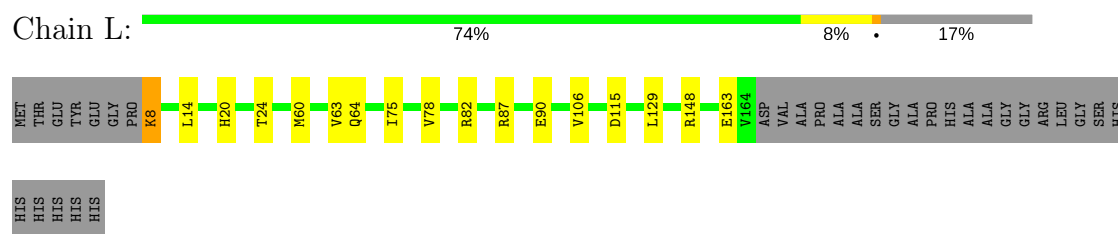
- Molecule 1: Ferritin family protein



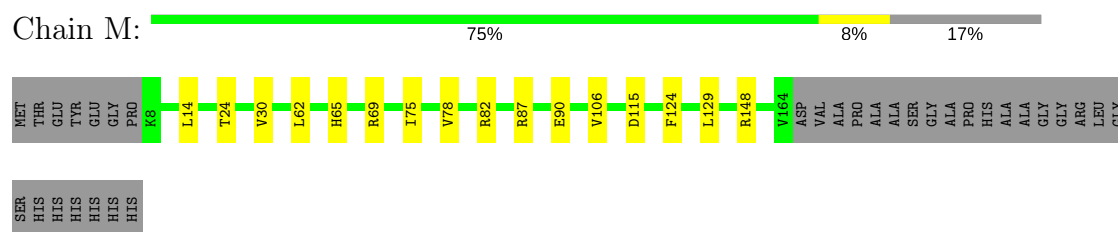
- Molecule 1: Ferritin family protein



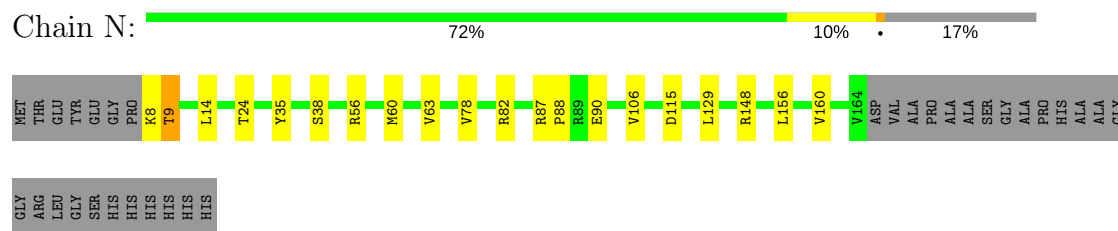
- Molecule 1: Ferritin family protein



- Molecule 1: Ferritin family protein



- Molecule 1: Ferritin family protein



- Molecule 1: Ferritin family protein





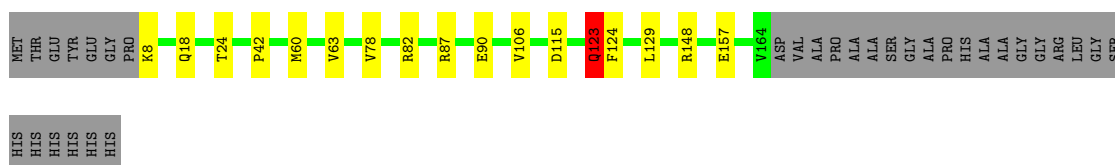
• Molecule 1: Ferritin family protein

Chain P: 73% 9% 17%



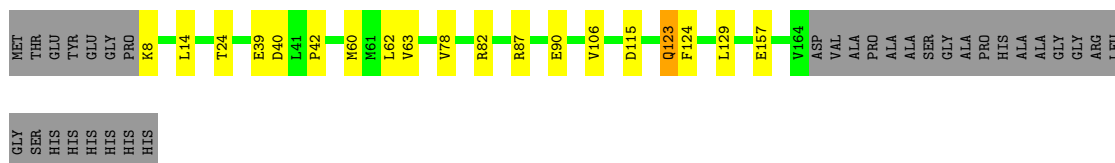
• Molecule 1: Ferritin family protein

Chain Q: 74% 8% 17%



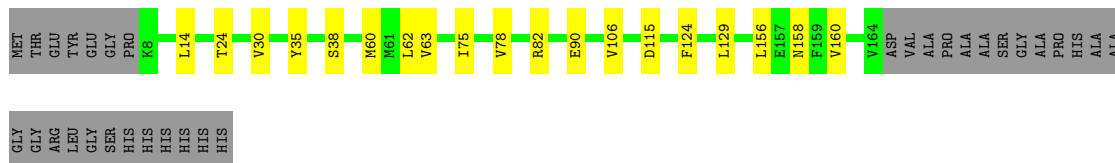
• Molecule 1: Ferritin family protein

Chain R: 73% 10% 17%



• Molecule 1: Ferritin family protein

Chain S: 73% 10% 17%



• Molecule 1: Ferritin family protein

Chain T: 72% 11% 17%



GLY  
GLY  
ARG  
LEU  
GLY  
SER  
HIS  
HIS  
HIS  
HIS  
HIS

● Molecule 1: Ferritin family protein



HIS  
HIS  
HIS  
HIS  
HIS  
HIS

● Molecule 1: Ferritin family protein



● Molecule 1: Ferritin family protein



● Molecule 1: Ferritin family protein



GLY  
GLY  
ARG  
LEU  
GLY  
SER  
HIS  
HIS  
HIS  
HIS  
HIS



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	231.77Å 232.00Å 114.32Å 90.00° 94.67° 90.00°	Depositor
Resolution (Å)	49.90 – 2.85 49.90 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.90-2.85) 99.0 (49.90-2.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.67 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.207 , 0.239 0.200 , 0.230	Depositor DCC
$R_{free}$ test set	6981 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	0.635	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	30954	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.45% 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](#)

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	0.76	0/1293	0.61	0/1750
1	B	0.73	0/1299	0.65	0/1757
1	C	0.77	0/1299	0.64	0/1757
1	D	0.87	0/1299	0.67	0/1757
1	E	0.73	0/1293	0.65	0/1750
1	F	0.79	1/1299 (0.1%)	0.65	1/1757 (0.1%)
1	G	0.73	0/1299	0.62	1/1757 (0.1%)
1	H	0.75	0/1299	0.65	0/1757
1	I	0.76	0/1299	0.63	0/1757
1	J	0.82	0/1299	0.65	0/1757
1	K	0.76	0/1299	0.63	0/1757
1	L	0.73	0/1299	0.63	0/1757
1	M	0.75	0/1299	0.62	0/1757
1	N	0.79	0/1299	0.67	1/1757 (0.1%)
1	O	0.86	0/1293	0.66	0/1750
1	P	0.77	0/1299	0.68	0/1757
1	Q	0.77	0/1299	0.69	2/1757 (0.1%)
1	R	0.72	0/1299	0.64	0/1757
1	S	0.76	0/1293	0.61	0/1750
1	T	0.74	0/1299	0.69	1/1757 (0.1%)
1	U	0.78	0/1299	0.64	1/1757 (0.1%)
1	V	0.73	0/1299	0.65	0/1757
1	W	0.75	0/1299	0.64	0/1757
1	X	0.73	0/1299	0.63	0/1757
All	All	0.77	1/31152 (0.0%)	0.64	7/42140 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	87	ARG	CZ-NH2	5.30	1.40	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	162	ARG	NE-CZ-NH1	-5.99	117.31	120.30
1	U	9	THR	N-CA-C	-5.84	95.24	111.00
1	F	87	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	Q	123	GLN	N-CA-CB	-5.43	100.82	110.60
1	N	9	THR	N-CA-C	-5.42	96.37	111.00
1	Q	123	GLN	CB-CG-CD	5.29	125.34	111.60
1	T	162	ARG	NE-CZ-NH1	-5.19	117.70	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	1271	0	1228	13	0
1	B	1277	0	1239	15	0
1	C	1277	0	1239	17	0
1	D	1277	0	1239	20	0
1	E	1271	0	1228	9	0
1	F	1277	0	1239	18	0
1	G	1277	0	1239	7	0
1	H	1277	0	1239	9	0
1	I	1277	0	1239	15	0
1	J	1277	0	1239	10	0
1	K	1277	0	1239	17	0
1	L	1277	0	1239	11	0
1	M	1277	0	1239	14	0
1	N	1277	0	1239	17	0
1	O	1271	0	1228	17	0
1	P	1277	0	1239	23	0
1	Q	1277	0	1239	15	0
1	R	1277	0	1239	15	0
1	S	1271	0	1228	12	0
1	T	1277	0	1239	19	0
1	U	1277	0	1239	16	0
1	V	1277	0	1239	10	0
1	W	1277	0	1239	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	1277	0	1239	16	0
2	A	21	0	0	0	0
2	B	9	0	0	3	0
2	C	11	0	0	1	0
2	D	10	0	0	0	0
2	E	18	0	0	2	0
2	F	21	0	0	1	0
2	G	13	0	0	1	0
2	H	14	0	0	1	0
2	I	14	0	0	0	0
2	J	13	0	0	0	0
2	K	9	0	0	1	0
2	L	14	0	0	3	0
2	M	12	0	0	4	0
2	N	20	0	0	4	0
2	O	17	0	0	2	0
2	P	14	0	0	0	0
2	Q	15	0	0	0	0
2	R	9	0	0	1	0
2	S	16	0	0	1	0
2	T	8	0	0	0	0
2	U	14	0	0	2	0
2	V	8	0	0	0	0
2	W	15	0	0	0	0
2	X	15	0	0	1	0
All	All	30954	0	29692	315	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 5.

All (315) 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:P:152:ASN:ND2	1:P:154:PHE:H	1.47	1.12
1:P:152:ASN:HD21	1:P:154:PHE:H	0.97	0.97
1:D:123:GLN:HE21	1:D:124:PHE:N	1.64	0.95
1:R:123:GLN:C	1:R:123:GLN:HE21	1.70	0.94
1:Q:123:GLN:HE21	1:Q:124:PHE:N	1.67	0.93
1:P:152:ASN:HD22	1:P:153:LEU:N	1.67	0.92
1:T:152:ASN:OD1	1:T:154:PHE:HD2	1.53	0.90
1:P:152:ASN:HD21	1:P:154:PHE:N	1.71	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:23:PHE:HZ	1:U:60:MET:HE1	1.41	0.85
1:U:23:PHE:HZ	1:U:60:MET:CE	1.92	0.83
1:R:123:GLN:HE21	1:R:124:PHE:N	1.77	0.82
1:C:123:GLN:HE21	1:C:124:PHE:N	1.78	0.81
1:P:152:ASN:ND2	1:P:153:LEU:N	2.29	0.80
1:C:42:PRO:HD2	1:C:157:GLU:OE1	1.82	0.79
1:D:40:ASP:O	1:D:42:PRO:HD3	1.82	0.77
1:N:8:LYS:O	1:N:8:LYS:CG	2.32	0.76
1:O:42:PRO:HD2	1:O:157:GLU:OE1	1.86	0.75
1:I:42:PRO:HD2	1:I:157:GLU:OE1	1.87	0.74
1:P:152:ASN:HD21	1:P:155:GLU:H	1.33	0.74
1:P:82:ARG:NH2	1:P:90:GLU:OE2	2.20	0.74
1:U:23:PHE:CZ	1:U:60:MET:CE	2.70	0.74
1:T:152:ASN:OD1	1:T:154:PHE:CD2	2.41	0.74
1:D:82:ARG:NH2	1:D:90:GLU:OE2	2.22	0.72
1:P:152:ASN:ND2	1:P:154:PHE:N	2.30	0.71
1:W:82:ARG:NH2	1:W:90:GLU:OE2	2.22	0.71
1:D:123:GLN:HE21	1:D:123:GLN:C	1.92	0.71
1:B:82:ARG:NH2	1:B:90:GLU:OE2	2.23	0.71
1:S:82:ARG:NH2	1:S:90:GLU:OE2	2.23	0.71
1:X:82:ARG:NH2	1:X:90:GLU:OE2	2.24	0.71
1:G:82:ARG:NH2	1:G:90:GLU:OE2	2.23	0.71
1:P:152:ASN:C	1:P:152:ASN:ND2	2.44	0.70
1:U:82:ARG:NH2	1:U:90:GLU:OE2	2.23	0.70
1:V:82:ARG:NH2	1:V:90:GLU:OE2	2.24	0.70
1:M:82:ARG:NH2	1:M:90:GLU:OE2	2.24	0.70
1:R:82:ARG:NH2	1:R:90:GLU:OE2	2.25	0.70
1:A:82:ARG:NH2	1:A:90:GLU:OE2	2.24	0.70
1:N:148:ARG:NE	2:N:342:HOH:O	2.25	0.70
1:C:82:ARG:NH2	1:C:90:GLU:OE2	2.24	0.69
1:N:82:ARG:NH2	1:N:90:GLU:OE2	2.25	0.69
1:E:82:ARG:NH2	1:E:90:GLU:OE2	2.24	0.69
1:C:123:GLN:HE21	1:C:124:PHE:CA	2.06	0.69
1:O:82:ARG:NH2	1:O:90:GLU:OE2	2.26	0.68
1:Q:82:ARG:NH2	1:Q:90:GLU:OE2	2.27	0.68
1:D:123:GLN:HE21	1:D:124:PHE:CA	2.05	0.68
1:O:86:ASP:N	1:O:90:GLU:OE1	2.27	0.68
1:T:82:ARG:NH2	1:T:90:GLU:OE2	2.25	0.68
1:U:23:PHE:CZ	1:U:60:MET:HE3	2.29	0.68
1:H:148:ARG:HD3	2:M:335:HOH:O	1.93	0.67
1:I:86:ASP:HB2	1:I:90:GLU:OE1	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:152:ASN:ND2	1:X:155:GLU:OE2	2.27	0.67
1:N:35:TYR:O	1:N:38:SER:HB2	1.94	0.67
1:P:152:ASN:ND2	1:P:155:GLU:H	1.92	0.67
1:M:148:ARG:HD2	2:M:340:HOH:O	1.95	0.66
1:F:82:ARG:NH2	1:F:90:GLU:OE2	2.29	0.66
1:H:82:ARG:NH2	1:H:90:GLU:OE2	2.29	0.66
1:F:154:PHE:CZ	1:P:149:ALA:HB2	2.30	0.65
1:U:8:LYS:O	1:U:8:LYS:HG3	1.96	0.65
1:D:43:GLN:NE2	1:U:163:GLU:OE2	2.29	0.65
1:K:82:ARG:NH2	1:K:90:GLU:OE2	2.31	0.64
1:B:162:ARG:NH1	1:S:158:ASN:OD1	2.24	0.64
1:J:86:ASP:HB2	1:J:90:GLU:OE1	1.98	0.63
1:V:148:ARG:NH1	1:X:39:GLU:O	2.31	0.62
1:K:123:GLN:HE21	1:K:124:PHE:N	1.97	0.62
1:N:148:ARG:HD2	2:N:342:HOH:O	2.00	0.62
1:R:123:GLN:C	1:R:123:GLN:NE2	2.48	0.62
1:F:65:HIS:NE2	1:F:69:ARG:HD2	2.15	0.61
1:B:55:GLU:HG2	2:B:191:HOH:O	1.99	0.61
1:K:148:ARG:HD3	2:K:338:HOH:O	2.01	0.60
1:Q:123:GLN:HE21	1:Q:124:PHE:CA	2.14	0.60
1:M:65:HIS:ND1	1:M:124:PHE:CG	2.67	0.60
1:U:23:PHE:CZ	1:U:60:MET:HE1	2.30	0.60
1:A:158:ASN:OD1	1:K:162:ARG:NH1	2.27	0.60
1:P:152:ASN:O	1:P:153:LEU:HB2	2.02	0.60
1:E:148:ARG:NH1	1:V:39:GLU:O	2.35	0.59
1:O:60:MET:CE	1:O:63:VAL:HG21	2.33	0.59
1:I:86:ASP:N	1:I:90:GLU:OE1	2.35	0.59
1:L:82:ARG:NH2	1:L:90:GLU:OE2	2.35	0.59
1:T:158:ASN:OD1	1:X:162:ARG:NH1	2.26	0.59
1:B:148:ARG:HD3	2:S:326:HOH:O	2.01	0.59
1:P:152:ASN:ND2	1:P:155:GLU:HG2	2.17	0.59
1:D:123:GLN:NE2	1:D:123:GLN:C	2.56	0.59
1:D:39:GLU:O	1:D:40:ASP:HB2	2.02	0.59
1:P:152:ASN:HD22	1:P:153:LEU:H	1.47	0.59
1:F:141:THR:O	1:F:145:VAL:HG23	2.03	0.58
1:H:148:ARG:CD	2:M:335:HOH:O	2.50	0.58
1:K:123:GLN:HE21	1:K:124:PHE:CA	2.16	0.58
1:F:65:HIS:ND1	1:F:124:PHE:CG	2.70	0.58
1:Q:42:PRO:HD2	1:Q:157:GLU:OE1	2.04	0.58
1:C:123:GLN:HE21	1:C:124:PHE:HA	1.68	0.57
1:O:86:ASP:HB2	1:O:90:GLU:OE1	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:40:ASP:C	1:X:42:PRO:HD3	2.25	0.57
1:B:42:PRO:HD2	1:B:157:GLU:OE1	2.04	0.56
1:N:56:ARG:NH1	2:N:194:HOH:O	2.37	0.56
1:I:87:ARG:O	1:I:90:GLU:HB3	2.04	0.56
1:N:8:LYS:O	1:N:8:LYS:HG3	2.05	0.56
1:P:156:LEU:O	1:P:160:VAL:HG23	2.06	0.56
1:A:60:MET:CE	1:A:63:VAL:HG21	2.36	0.56
1:Q:123:GLN:C	1:Q:123:GLN:HE21	2.09	0.56
1:H:64:GLN:HB3	2:H:192:HOH:O	2.06	0.55
1:D:123:GLN:HE21	1:D:124:PHE:HA	1.72	0.55
1:I:60:MET:CE	1:I:63:VAL:HG21	2.35	0.55
1:J:94:LEU:O	1:J:94:LEU:HD23	2.07	0.55
1:D:162:ARG:NH1	1:O:158:ASN:OD1	2.30	0.55
1:U:82:ARG:NH1	2:U:195:HOH:O	2.32	0.55
1:D:123:GLN:NE2	1:D:124:PHE:HA	2.23	0.54
1:C:123:GLN:NE2	1:C:124:PHE:HA	2.22	0.54
1:X:155:GLU:HA	1:X:155:GLU:OE1	2.08	0.54
1:R:123:GLN:HE21	1:R:124:PHE:CA	2.20	0.54
1:A:75:ILE:HG13	1:M:30:VAL:HG12	1.90	0.53
1:T:60:MET:CE	1:T:63:VAL:HG21	2.38	0.53
1:T:155:GLU:HA	1:T:155:GLU:OE1	2.08	0.53
1:K:123:GLN:NE2	1:K:124:PHE:HA	2.24	0.53
1:N:8:LYS:O	1:N:8:LYS:HG2	2.06	0.53
1:F:42:PRO:HD2	1:F:157:GLU:OE1	2.08	0.53
1:C:123:GLN:HE21	1:C:123:GLN:C	2.12	0.52
1:N:148:ARG:CD	2:N:342:HOH:O	2.53	0.52
1:N:60:MET:CE	1:N:63:VAL:HG21	2.40	0.52
1:K:42:PRO:HD2	1:K:157:GLU:OE1	2.09	0.52
1:K:23:PHE:CZ	1:K:60:MET:HE3	2.45	0.52
2:C:339:HOH:O	1:L:148:ARG:HD3	2.09	0.52
1:F:35:TYR:O	1:F:38:SER:OG	2.21	0.52
1:N:106:VAL:HG12	1:N:129:LEU:HD21	1.92	0.51
1:K:106:VAL:HG12	1:K:129:LEU:HD21	1.93	0.51
1:M:106:VAL:HG12	1:M:129:LEU:HD21	1.92	0.51
1:A:106:VAL:HG12	1:A:129:LEU:HD21	1.92	0.51
1:K:24:THR:HA	1:K:78:VAL:HG13	1.93	0.51
1:O:56:ARG:NH1	2:O:323:HOH:O	2.40	0.51
1:J:163:GLU:OE2	1:U:43:GLN:NE2	2.36	0.51
1:S:60:MET:CE	1:S:63:VAL:HG21	2.41	0.51
1:M:65:HIS:NE2	1:M:69:ARG:HD2	2.25	0.50
1:L:20:HIS:HE1	2:L:194:HOH:O	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:139:MET:O	1:O:143:VAL:HG13	2.11	0.50
1:Q:106:VAL:HG12	1:Q:129:LEU:HD21	1.93	0.50
2:G:344:HOH:O	1:Q:148:ARG:HD3	2.11	0.50
1:Q:60:MET:CE	1:Q:63:VAL:HG21	2.41	0.49
1:V:60:MET:HA	1:V:60:MET:CE	2.42	0.49
1:W:40:ASP:C	1:W:42:PRO:HD3	2.32	0.49
1:I:106:VAL:HG12	1:I:129:LEU:HD21	1.93	0.49
1:B:60:MET:CE	1:B:63:VAL:HG21	2.42	0.49
1:H:106:VAL:HG12	1:H:129:LEU:HD21	1.94	0.49
1:U:8:LYS:O	1:U:8:LYS:CG	2.59	0.49
1:K:23:PHE:HZ	1:K:60:MET:CE	2.26	0.49
1:K:123:GLN:HE21	1:K:124:PHE:HA	1.77	0.49
1:L:64:GLN:HB3	2:L:196:HOH:O	2.13	0.49
1:J:106:VAL:HG12	1:J:129:LEU:HD21	1.95	0.49
1:P:60:MET:CE	1:P:63:VAL:HG21	2.43	0.49
1:V:106:VAL:HG12	1:V:129:LEU:HD21	1.95	0.49
1:M:148:ARG:CD	2:M:340:HOH:O	2.55	0.48
1:R:60:MET:CE	1:R:63:VAL:HG21	2.43	0.48
1:F:8:LYS:HB2	1:F:8:LYS:HE2	1.65	0.48
1:R:24:THR:HA	1:R:78:VAL:HG13	1.95	0.48
1:O:87:ARG:O	1:O:90:GLU:HB3	2.13	0.48
1:Q:24:THR:HA	1:Q:78:VAL:HG13	1.95	0.48
1:T:60:MET:HA	1:T:60:MET:HE3	1.95	0.48
1:C:133:ILE:HG13	1:W:120:LEU:HD22	1.96	0.48
1:F:106:VAL:HG12	1:F:129:LEU:HD21	1.95	0.48
1:N:87:ARG:HB2	1:N:88:PRO:HD2	1.95	0.48
1:R:106:VAL:HG12	1:R:129:LEU:HD21	1.96	0.48
1:D:60:MET:CE	1:D:63:VAL:HG21	2.43	0.48
1:F:154:PHE:CE2	1:P:149:ALA:HB2	2.48	0.48
1:I:144:ARG:HB3	1:I:148:ARG:NH2	2.28	0.48
1:T:156:LEU:O	1:T:160:VAL:HG23	2.14	0.48
1:X:24:THR:HA	1:X:78:VAL:HG13	1.96	0.47
1:Q:123:GLN:NE2	1:Q:124:PHE:HA	2.29	0.47
1:L:24:THR:HA	1:L:78:VAL:HG13	1.96	0.47
1:L:60:MET:CE	1:L:63:VAL:HG21	2.44	0.47
1:W:24:THR:HA	1:W:78:VAL:HG13	1.96	0.47
1:C:106:VAL:HG12	1:C:129:LEU:HD21	1.95	0.47
1:O:156:LEU:O	1:O:160:VAL:HG23	2.15	0.47
1:A:156:LEU:O	1:A:160:VAL:HG23	2.14	0.47
1:B:39:GLU:O	1:B:40:ASP:HB2	2.15	0.47
1:C:24:THR:HA	1:C:78:VAL:HG13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:106:VAL:HG12	1:T:129:LEU:HD21	1.95	0.47
1:F:24:THR:HA	1:F:78:VAL:HG13	1.97	0.47
1:O:62:LEU:HD23	1:O:124:PHE:HE2	1.79	0.47
1:T:60:MET:HA	1:T:60:MET:CE	2.44	0.47
1:Q:123:GLN:OE1	1:T:130:GLN:HB2	2.15	0.47
1:E:24:THR:HA	1:E:78:VAL:HG13	1.96	0.47
1:R:123:GLN:NE2	1:R:124:PHE:HA	2.29	0.47
1:J:24:THR:HA	1:J:78:VAL:HG13	1.96	0.47
1:D:106:VAL:HG12	1:D:129:LEU:HD21	1.97	0.46
1:F:60:MET:CE	1:F:63:VAL:HG21	2.45	0.46
1:T:24:THR:HA	1:T:78:VAL:HG13	1.97	0.46
1:F:14:LEU:HD23	1:F:14:LEU:HA	1.81	0.46
1:N:24:THR:HA	1:N:78:VAL:HG13	1.97	0.46
1:J:60:MET:CE	1:J:63:VAL:HG21	2.45	0.46
1:N:60:MET:HA	1:N:60:MET:CE	2.45	0.46
1:P:24:THR:HA	1:P:78:VAL:HG13	1.96	0.46
1:R:42:PRO:HD2	1:R:157:GLU:OE1	2.15	0.46
1:C:123:GLN:NE2	1:C:123:GLN:C	2.68	0.46
1:J:14:LEU:HD23	1:J:14:LEU:HA	1.79	0.46
1:W:60:MET:CE	1:W:63:VAL:HG21	2.45	0.46
1:G:30:VAL:HG12	1:S:75:ILE:HG13	1.97	0.46
1:J:35:TYR:O	1:J:38:SER:OG	2.24	0.46
1:T:152:ASN:OD1	1:T:154:PHE:HB2	2.16	0.46
1:H:60:MET:CE	1:H:63:VAL:HG21	2.46	0.45
1:A:30:VAL:HG12	1:M:75:ILE:HG13	1.98	0.45
1:C:156:LEU:O	1:C:160:VAL:HG23	2.17	0.45
1:N:14:LEU:HD23	1:N:14:LEU:HA	1.81	0.45
1:D:24:THR:HA	1:D:78:VAL:HG13	1.98	0.45
1:H:24:THR:HA	1:H:78:VAL:HG13	1.98	0.45
1:Q:123:GLN:NE2	1:Q:124:PHE:CA	2.80	0.45
1:F:65:HIS:CD2	1:F:69:ARG:CD	2.99	0.45
1:T:153:LEU:HD23	1:T:153:LEU:HA	1.47	0.45
1:I:84:GLN:HG2	2:U:276:HOH:O	2.15	0.45
1:U:24:THR:HA	1:U:78:VAL:HG13	1.99	0.45
1:A:60:MET:HA	1:A:60:MET:CE	2.47	0.45
1:K:23:PHE:CZ	1:K:60:MET:CE	3.00	0.45
1:M:62:LEU:HD23	1:M:124:PHE:HE2	1.82	0.45
1:R:62:LEU:HD23	1:R:124:PHE:HE2	1.82	0.45
1:U:106:VAL:HG12	1:U:129:LEU:HD21	1.97	0.45
1:J:8:LYS:HB2	1:J:9:THR:H	1.58	0.44
1:C:43:GLN:NE2	1:L:163:GLU:OE2	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:123:GLN:C	1:Q:123:GLN:NE2	2.71	0.44
1:D:41:LEU:HD13	1:D:44:LEU:HD12	1.99	0.44
1:F:65:HIS:NE2	1:F:69:ARG:CD	2.80	0.44
1:I:82:ARG:NH2	1:I:90:GLU:OE2	2.51	0.44
1:F:20:HIS:HE1	2:F:200:HOH:O	1.99	0.44
1:A:106:VAL:HG12	1:A:129:LEU:CD2	2.47	0.44
1:I:62:LEU:HD23	1:I:124:PHE:HE2	1.83	0.44
1:R:123:GLN:HE21	1:R:124:PHE:HA	1.83	0.44
1:U:62:LEU:HD23	1:U:124:PHE:HE2	1.82	0.44
1:E:106:VAL:HG12	1:E:129:LEU:HD21	2.00	0.44
1:M:106:VAL:HG12	1:M:129:LEU:CD2	2.47	0.44
1:O:106:VAL:HG12	1:O:129:LEU:HD21	1.98	0.44
1:A:24:THR:HA	1:A:78:VAL:HG13	1.98	0.44
1:B:106:VAL:HG12	1:B:129:LEU:HD21	1.98	0.44
1:F:84:GLN:HG2	2:R:250:HOH:O	2.16	0.44
1:N:148:ARG:HH21	1:W:40:ASP:HB2	1.83	0.44
1:G:24:THR:HA	1:G:78:VAL:HG13	1.99	0.44
1:I:75:ILE:HG13	1:U:30:VAL:HG12	2.00	0.44
1:L:75:ILE:HG13	1:X:30:VAL:HG12	1.98	0.44
1:B:22:GLU:OE2	2:B:194:HOH:O	2.21	0.43
1:G:60:MET:HA	1:G:60:MET:CE	2.48	0.43
1:P:152:ASN:HD21	1:P:155:GLU:N	2.06	0.43
1:V:24:THR:HA	1:V:78:VAL:HG13	1.99	0.43
1:X:97:ASP:OD1	2:X:285:HOH:O	2.21	0.43
1:Q:60:MET:HE2	1:Q:63:VAL:HG21	2.01	0.43
1:E:56:ARG:NH1	2:E:197:HOH:O	2.47	0.43
1:L:8:LYS:HB2	1:L:8:LYS:HE3	1.67	0.43
1:S:106:VAL:HG12	1:S:129:LEU:HD21	2.01	0.43
1:D:148:ARG:HD3	2:O:329:HOH:O	2.19	0.43
1:L:106:VAL:HG12	1:L:129:LEU:HD21	2.01	0.43
1:S:60:MET:CE	1:S:60:MET:HA	2.49	0.43
1:S:62:LEU:HD23	1:S:124:PHE:HE2	1.83	0.43
1:X:40:ASP:O	1:X:42:PRO:HD3	2.18	0.43
1:M:14:LEU:HD23	1:M:14:LEU:HA	1.91	0.43
1:B:24:THR:HA	1:B:78:VAL:HG13	2.01	0.43
1:M:65:HIS:CD2	1:M:69:ARG:HD3	2.54	0.43
1:D:123:GLN:OE1	1:W:130:GLN:HB2	2.19	0.43
1:E:60:MET:CE	1:E:63:VAL:HG21	2.48	0.42
1:K:8:LYS:HG3	1:K:8:LYS:O	2.19	0.42
1:O:24:THR:HA	1:O:78:VAL:HG13	2.01	0.42
1:T:152:ASN:HD21	1:X:155:GLU:CD	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:MET:HA	1:A:60:MET:HE3	2.01	0.42
1:B:40:ASP:C	1:B:42:PRO:HD3	2.40	0.42
1:G:62:LEU:HD23	1:G:124:PHE:HE2	1.84	0.42
1:E:148:ARG:HD2	2:E:330:HOH:O	2.20	0.42
1:I:24:THR:HA	1:I:78:VAL:HG13	2.00	0.42
1:C:60:MET:CE	1:C:63:VAL:HG21	2.49	0.42
1:I:14:LEU:HA	1:I:14:LEU:HD23	1.91	0.42
1:M:24:THR:HA	1:M:78:VAL:HG13	2.01	0.42
1:P:152:ASN:O	1:P:153:LEU:CB	2.66	0.42
1:P:29:TYR:HA	1:P:29:TYR:HD1	1.74	0.42
1:D:14:LEU:HB3	1:D:109:LEU:HD21	2.02	0.42
1:K:40:ASP:C	1:K:42:PRO:HD3	2.39	0.42
1:C:75:ILE:HG13	1:O:30:VAL:HG12	2.01	0.42
1:E:154:PHE:CZ	1:T:149:ALA:HB2	2.55	0.42
1:B:55:GLU:CG	2:B:191:HOH:O	2.62	0.42
1:K:14:LEU:HD23	1:K:14:LEU:HA	1.84	0.42
1:U:14:LEU:HA	1:U:14:LEU:HD23	1.87	0.42
1:B:14:LEU:HA	1:B:14:LEU:HD23	1.88	0.42
1:I:106:VAL:HG12	1:I:129:LEU:CD2	2.50	0.42
1:V:8:LYS:HB3	1:V:8:LYS:HE3	1.88	0.42
1:S:35:TYR:O	1:S:38:SER:OG	2.27	0.42
1:T:60:MET:HE2	1:T:63:VAL:HG21	2.02	0.42
1:C:62:LEU:HD23	1:C:124:PHE:HE2	1.85	0.41
1:A:62:LEU:HD23	1:A:124:PHE:HE2	1.85	0.41
1:B:39:GLU:O	1:M:148:ARG:NH1	2.52	0.41
1:V:60:MET:HE3	1:V:60:MET:HA	2.03	0.41
1:V:60:MET:CE	1:V:63:VAL:HG21	2.49	0.41
1:S:14:LEU:HA	1:S:14:LEU:HD23	1.83	0.41
1:T:14:LEU:HD23	1:T:14:LEU:HA	1.86	0.41
1:X:14:LEU:HD23	1:X:14:LEU:HA	1.87	0.41
1:H:156:LEU:O	1:H:160:VAL:HG23	2.21	0.41
1:D:9:THR:OG1	1:D:12:HIS:HB2	2.20	0.41
1:B:71:LEU:HD23	1:B:71:LEU:HA	1.92	0.41
1:I:60:MET:CE	1:I:60:MET:HA	2.51	0.41
1:K:23:PHE:HZ	1:K:60:MET:HE1	1.86	0.41
1:N:156:LEU:O	1:N:160:VAL:HG23	2.20	0.41
1:O:60:MET:CE	1:O:60:MET:HA	2.51	0.41
1:R:39:GLU:O	1:R:40:ASP:HB2	2.21	0.41
1:G:75:ILE:HG13	1:S:30:VAL:HG12	2.03	0.41
1:W:60:MET:HA	1:W:60:MET:CE	2.51	0.41
1:F:65:HIS:CD2	1:F:69:ARG:HD3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:156:LEU:O	1:S:160:VAL:HG23	2.20	0.41
1:D:62:LEU:HD23	1:D:124:PHE:HE2	1.86	0.41
1:E:62:LEU:HD23	1:E:124:PHE:HE2	1.86	0.41
1:P:130:GLN:HB2	1:R:123:GLN:OE1	2.21	0.41
1:X:60:MET:CE	1:X:60:MET:HA	2.51	0.41
1:G:41:LEU:N	1:G:42:PRO:CD	2.84	0.40
1:X:62:LEU:HD23	1:X:124:PHE:HE2	1.85	0.40
1:C:60:MET:HA	1:C:60:MET:CE	2.51	0.40
1:H:29:TYR:HA	1:H:29:TYR:HD1	1.72	0.40
1:J:40:ASP:C	1:J:42:PRO:HD3	2.41	0.40
1:P:14:LEU:HA	1:P:14:LEU:HD23	1.84	0.40
1:Q:18:GLN:OE1	1:Q:18:GLN:HA	2.21	0.40
1:S:24:THR:HA	1:S:78:VAL:HG13	2.02	0.40
2:L:296:HOH:O	1:X:84:GLN:HG2	2.21	0.40
1:L:14:LEU:HD23	1:L:14:LEU:HA	1.81	0.40
1:R:14:LEU:HA	1:R:14:LEU:HD23	1.86	0.40
1:V:35:TYR:O	1:V:38:SER:OG	2.32	0.40
1:A:133:ILE:HG13	1:X:120:LEU:HD22	2.04	0.40
1:O:60:MET:HE3	1:O:60:MET:HA	2.02	0.40
1:O:106:VAL:HG12	1:O:129:LEU:CD2	2.51	0.40

There are no symmetry-related clashes.

## 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	155/189 (82%)	155 (100%)	0	0	100	100
1	B	155/189 (82%)	155 (100%)	0	0	100	100
1	C	155/189 (82%)	155 (100%)	0	0	100	100
1	D	155/189 (82%)	154 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	155/189 (82%)	155 (100%)	0	0	100	100
1	F	155/189 (82%)	155 (100%)	0	0	100	100
1	G	155/189 (82%)	155 (100%)	0	0	100	100
1	H	155/189 (82%)	155 (100%)	0	0	100	100
1	I	155/189 (82%)	155 (100%)	0	0	100	100
1	J	155/189 (82%)	155 (100%)	0	0	100	100
1	K	155/189 (82%)	155 (100%)	0	0	100	100
1	L	155/189 (82%)	155 (100%)	0	0	100	100
1	M	155/189 (82%)	155 (100%)	0	0	100	100
1	N	155/189 (82%)	155 (100%)	0	0	100	100
1	O	155/189 (82%)	155 (100%)	0	0	100	100
1	P	155/189 (82%)	154 (99%)	1 (1%)	0	100	100
1	Q	155/189 (82%)	155 (100%)	0	0	100	100
1	R	155/189 (82%)	155 (100%)	0	0	100	100
1	S	155/189 (82%)	155 (100%)	0	0	100	100
1	T	155/189 (82%)	155 (100%)	0	0	100	100
1	U	155/189 (82%)	155 (100%)	0	0	100	100
1	V	155/189 (82%)	155 (100%)	0	0	100	100
1	W	155/189 (82%)	155 (100%)	0	0	100	100
1	X	155/189 (82%)	155 (100%)	0	0	100	100
All	All	3720/4536 (82%)	3718 (100%)	2 (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	132/154 (86%)	131 (99%)	1 (1%)	85	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	133/154 (86%)	131 (98%)	2 (2%)	70	90
1	C	133/154 (86%)	130 (98%)	3 (2%)	56	84
1	D	133/154 (86%)	130 (98%)	3 (2%)	56	84
1	E	132/154 (86%)	129 (98%)	3 (2%)	56	84
1	F	133/154 (86%)	130 (98%)	3 (2%)	56	84
1	G	133/154 (86%)	130 (98%)	3 (2%)	56	84
1	H	133/154 (86%)	131 (98%)	2 (2%)	70	90
1	I	133/154 (86%)	132 (99%)	1 (1%)	85	95
1	J	133/154 (86%)	129 (97%)	4 (3%)	46	78
1	K	133/154 (86%)	130 (98%)	3 (2%)	56	84
1	L	133/154 (86%)	130 (98%)	3 (2%)	56	84
1	M	133/154 (86%)	131 (98%)	2 (2%)	70	90
1	N	133/154 (86%)	131 (98%)	2 (2%)	70	90
1	O	132/154 (86%)	129 (98%)	3 (2%)	56	84
1	P	133/154 (86%)	128 (96%)	5 (4%)	38	70
1	Q	133/154 (86%)	129 (97%)	4 (3%)	46	78
1	R	133/154 (86%)	129 (97%)	4 (3%)	46	78
1	S	132/154 (86%)	131 (99%)	1 (1%)	85	95
1	T	133/154 (86%)	131 (98%)	2 (2%)	70	90
1	U	133/154 (86%)	130 (98%)	3 (2%)	56	84
1	V	133/154 (86%)	132 (99%)	1 (1%)	85	95
1	W	133/154 (86%)	130 (98%)	3 (2%)	56	84
1	X	133/154 (86%)	131 (98%)	2 (2%)	70	90
All	All	3188/3696 (86%)	3125 (98%)	63 (2%)	60	87

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	ASP
1	B	87	ARG
1	B	115	ASP
1	C	87	ARG
1	C	115	ASP
1	C	123	GLN

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Mol	Chain	Res	Type
1	D	87	ARG
1	D	115	ASP
1	D	123	GLN
1	E	8	LYS
1	E	115	ASP
1	E	148	ARG
1	F	8	LYS
1	F	87	ARG
1	F	115	ASP
1	G	8	LYS
1	G	87	ARG
1	G	115	ASP
1	H	87	ARG
1	H	115	ASP
1	I	115	ASP
1	J	8	LYS
1	J	9	THR
1	J	94	LEU
1	J	115	ASP
1	K	87	ARG
1	K	115	ASP
1	K	123	GLN
1	L	8	LYS
1	L	87	ARG
1	L	115	ASP
1	M	87	ARG
1	M	115	ASP
1	N	9	THR
1	N	115	ASP
1	O	8	LYS
1	O	9	THR
1	O	115	ASP
1	P	8	LYS
1	P	87	ARG
1	P	115	ASP
1	P	152	ASN
1	P	153	LEU
1	Q	8	LYS
1	Q	87	ARG
1	Q	115	ASP
1	Q	123	GLN
1	R	8	LYS

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Mol	Chain	Res	Type
1	R	87	ARG
1	R	115	ASP
1	R	123	GLN
1	S	115	ASP
1	T	87	ARG
1	T	115	ASP
1	U	9	THR
1	U	87	ARG
1	U	115	ASP
1	V	115	ASP
1	W	8	LYS
1	W	87	ARG
1	W	115	ASP
1	X	87	ARG
1	X	115	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	123	GLN
1	D	123	GLN
1	F	20	HIS
1	K	123	GLN
1	L	20	HIS
1	N	130	GLN
1	P	84	GLN
1	P	130	GLN
1	P	152	ASN
1	Q	123	GLN
1	R	123	GLN
1	T	130	GLN
1	X	84	GLN

### 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 [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	157/189 (83%)	-0.21	0 100 100	17, 26, 47, 60	0
1	B	157/189 (83%)	-0.19	0 100 100	17, 27, 50, 61	0
1	C	157/189 (83%)	-0.18	0 100 100	17, 27, 49, 60	0
1	D	157/189 (83%)	-0.11	0 100 100	18, 27, 51, 61	0
1	E	157/189 (83%)	-0.17	0 100 100	17, 27, 49, 61	0
1	F	157/189 (83%)	-0.21	0 100 100	17, 27, 50, 59	0
1	G	157/189 (83%)	-0.19	0 100 100	16, 27, 49, 59	0
1	H	157/189 (83%)	-0.20	0 100 100	17, 27, 49, 60	0
1	I	157/189 (83%)	-0.23	0 100 100	16, 26, 48, 60	0
1	J	157/189 (83%)	-0.19	0 100 100	17, 27, 49, 58	0
1	K	157/189 (83%)	-0.19	0 100 100	18, 27, 49, 61	0
1	L	157/189 (83%)	-0.22	0 100 100	16, 27, 48, 60	0
1	M	157/189 (83%)	-0.21	0 100 100	16, 27, 50, 61	0
1	N	157/189 (83%)	-0.21	0 100 100	16, 27, 49, 61	0
1	O	157/189 (83%)	-0.21	0 100 100	17, 26, 48, 60	0
1	P	157/189 (83%)	-0.18	0 100 100	16, 28, 49, 60	0
1	Q	157/189 (83%)	-0.22	0 100 100	16, 27, 50, 60	0
1	R	157/189 (83%)	-0.25	0 100 100	17, 27, 50, 59	0
1	S	157/189 (83%)	-0.21	0 100 100	17, 26, 50, 59	0
1	T	157/189 (83%)	-0.11	0 100 100	17, 27, 50, 60	0
1	U	157/189 (83%)	-0.19	0 100 100	16, 27, 50, 58	0
1	V	157/189 (83%)	-0.15	0 100 100	17, 27, 49, 63	0
1	W	157/189 (83%)	-0.28	0 100 100	17, 28, 51, 62	0
1	X	157/189 (83%)	-0.24	0 100 100	16, 27, 50, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3768/4536 (83%)	-0.20	0 100 100	16, 27, 50, 63	0

There are no RSRZ outliers to report.

## 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.