



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 02:59 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

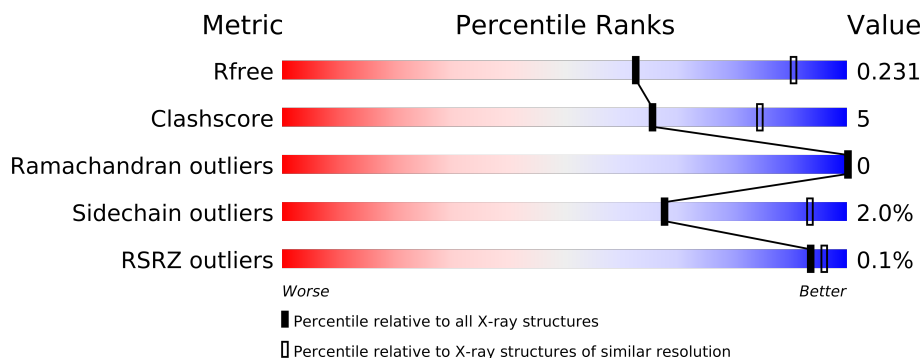
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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.








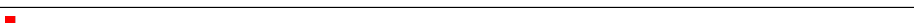




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2270 (2.88-2.80)
Clashscore	79885	2848 (2.88-2.80)
Ramachandran outliers	78287	2786 (2.88-2.80)
Sidechain outliers	78261	2789 (2.88-2.80)
RSRZ outliers	66119	2274 (2.88-2.80)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	189	
1	B	189	
1	C	189	
1	D	189	
1	E	189	
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	

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Mol	Chain	Length	Quality of chain
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 hydrogen and 0 are deuterium.

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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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

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

- Molecule 1: Ferritin family protein

Chain A: 



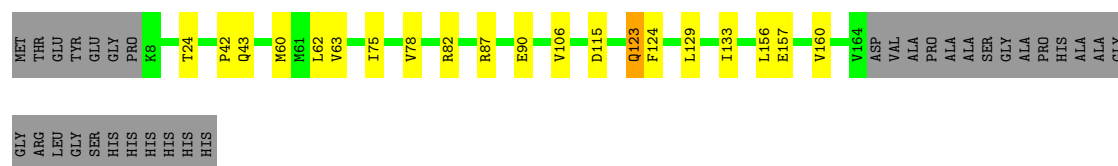
- Molecule 1: Ferritin family protein

Chain B: 



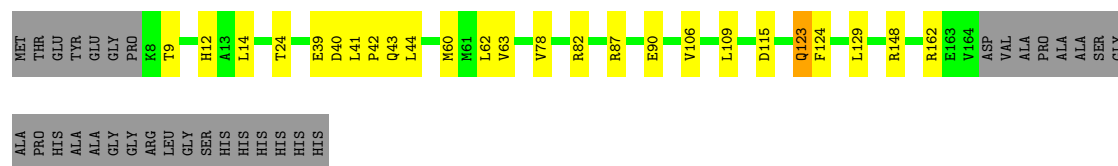
- Molecule 1: Ferritin family protein

Chain C: 



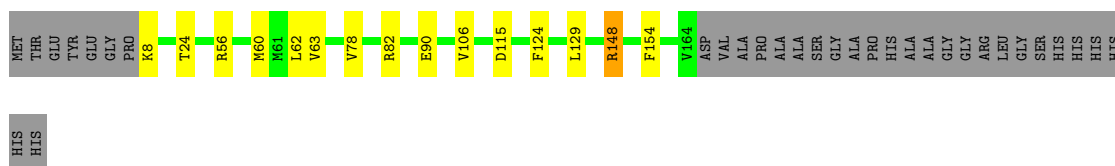
- Molecule 1: Ferritin family protein

Chain D: 



- Molecule 1: Ferritin family protein

Chain E: 



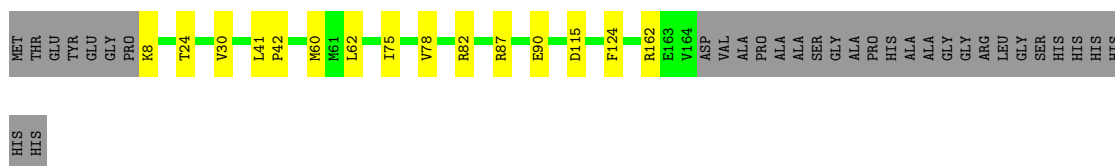
- Molecule 1: Ferritin family protein

Chain F:



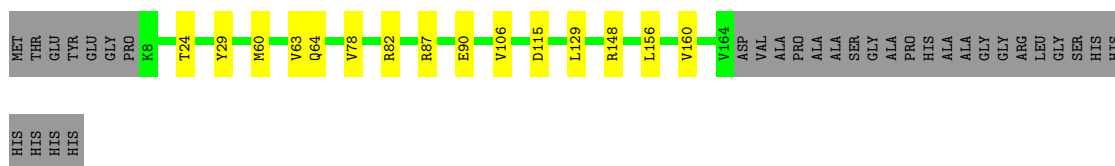
- Molecule 1: Ferritin family protein

Chain G:



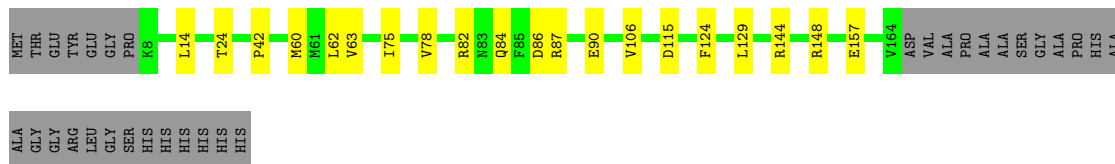
- Molecule 1: Ferritin family protein

Chain H:



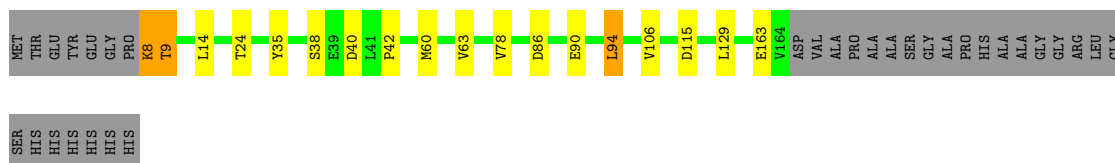
- Molecule 1: Ferritin family protein

Chain I:



- Molecule 1: Ferritin family protein

Chain J:



- Molecule 1: Ferritin family protein

Chain K:



- Molecule 1: Ferritin family protein

Chain L:



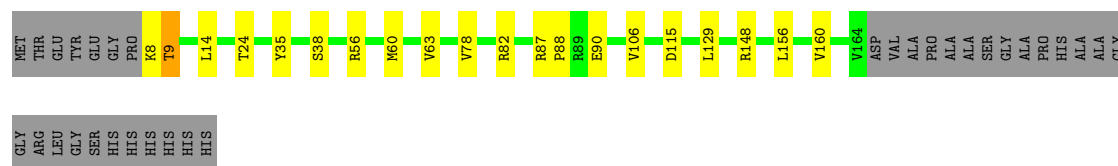
- Molecule 1: Ferritin family protein

Chain M:



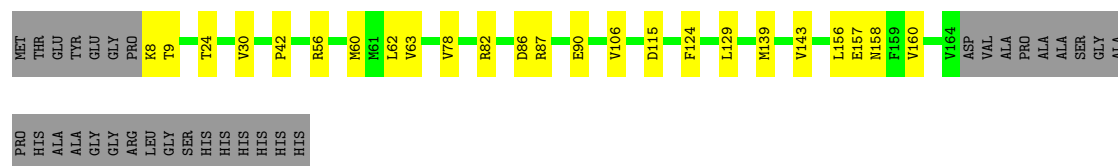
- Molecule 1: Ferritin family protein

Chain N:



- Molecule 1: Ferritin family protein

Chain O:



- Molecule 1: Ferritin family protein

Chain P:



SER
HIS
HIS
HIS
HIS
HIS
HIS

- Molecule 1: Ferritin family protein

Chain Q:

MET THR GLU TYR GLY PRO K8 Q18 T24 P42 M60 V63 V78 R82 R87 E90 V106 D115 Q123 F124 L129 R148 E157 V164 ASP VAL ALA PRO ALA ALA SER GLY ALA PRO HIS ALA ALA GLY ARG LEU SER

HIS
HIS
HIS
HIS
HIS

- Molecule 1: Ferritin family protein

Chain R:

MET THR GLU TYR GLY PRO K8 L14 T24 E39 D40 L41 P42 M60 M61 L62 V63 V78 R82 R87 E90 V106 D115 Q123 F124 L129 E157 V164 ASP VAL ALA PRO PRO ALA ALA SER GLY ALA PRO HIS ALA ALA GLY ARG LEU

GLY
SER
HIS
HIS
HIS
HIS
HIS

- Molecule 1: Ferritin family protein

Chain S:

MET THR GLU TYR GLY PRO K8 L14 T24 V30 Y35 S38 M60 M61 L62 V63 I75 V78 R82 E90 V106 D115 F124 L129 L156 E157 N158 F159 V160 V164 ASP VAL ALA PRO ALA ALA SER GLY PRO HIS ALA

GLY
GLY
ARG
HIS
LEU
GLY
SER
HIS
HIS
HIS
HIS

- Molecule 1: Ferritin family protein

Chain T:

MET THR GLU TYR GLY PRO K8 L14 T24 M60 V63 V78 R82 R87 E90 V106 D115 L129 Q130 A149 G150 A151 N152 L153 F154 E155 L156 E157 N158 F159 V160 A161 R162 E163 V164 ASP VAL ALA PRO ALA ALA SER GLY ALA PRO HIS ALA

ALA
GLY
GLY
ARG
HIS
LEU
GLY
SER
HIS
HIS
HIS
HIS

- Molecule 1: Ferritin family protein

Chain U:

MET THR GLU TYR GLY PRO K8 T9 L14 F23 T24 V30 Q43 M60 M61 L62 V78 R82 R87 E90 V106 D115 F124 L129 E163 V164 ASP VAL ALA PRO PRO ALA ALA SER GLY ALA PRO HIS ALA ALA GLY ARG LEU SER

HIS
HIS
HIS
HIS
HIS

- Molecule 1: Ferritin family protein

Chain V:



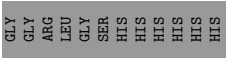
● Molecule 1: Ferritin family protein

Chain W: 



● Molecule 1: Ferritin family protein

Chain X: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.207 , 0.239 0.201 , 0.231	Depositor DCC
R_{free} test set	6981 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.635	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 9.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 139164 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	30954	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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	0.76	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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	V	1277	0	1239	10	0
1	W	1277	0	1239	8	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (315) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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:X:82:ARG:NH2	1:X:90:GLU:OE2	2.24	0.71
1:S:82:ARG:NH2	1:S:90:GLU:OE2	2.23	0.71
1:B:82:ARG:NH2	1:B:90:GLU:OE2	2.23	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:V:82:ARG:NH2	1:V:90:GLU:OE2	2.24	0.70
1:U:82:ARG:NH2	1:U:90:GLU:OE2	2.23	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:U:23:PHE:CZ	1:U:60:MET:HE3	2.29	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:H:148:ARG:HD3	2:M:335:HOH:O	1.93	0.67
1:T:152:ASN:ND2	1:X:155:GLU:OE2	2.27	0.67
1:I:86:ASP:HB2	1:I:90:GLU:OE1	1.95	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:H:82:ARG:NH2	1:H:90:GLU:OE2	2.29	0.66
1:F:82:ARG:NH2	1:F: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:R:123:GLN:C	1:R:123:GLN:NE2	2.48	0.62
1:N:148:ARG:HD2	2:N:342:HOH:O	2.00	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:Q:123:GLN:HE21	1:Q:124:PHE:CA	2.14	0.60
1:K:148:ARG:HD3	2:K:338:HOH:O	2.01	0.60
1:U:23:PHE:CZ	1:U:60:MET:HE1	2.30	0.60
1:M:65:HIS:ND1	1:M:124:PHE:CG	2.67	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:P:152:ASN:ND2	1:P:155:GLU:HG2	2.17	0.59
1:B:148:ARG:HD3	2:S:326:HOH:O	2.01	0.59
1:P:152:ASN:HD22	1:P:153:LEU:H	1.47	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: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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:D:162:ARG:NH1	1:O:158:ASN:OD1	2.30	0.55
1:J:94:LEU:O	1:J:94:LEU:HD23	2.07	0.55
1:I:60:MET:CE	1:I:63:VAL:HG21	2.35	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:X:155:GLU:HA	1:X:155:GLU:OE1	2.08	0.54
1:C:123:GLN:NE2	1:C:124:PHE:HA	2.22	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:N:8:LYS:O	1:N:8:LYS:HG2	2.06	0.53
1:K:123:GLN:NE2	1:K:124:PHE:HA	2.24	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:23:PHE:CZ	1:K:60:MET:HE3	2.45	0.52
1:K:42:PRO:HD2	1:K:157:GLU:OE1	2.09	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:S:60:MET:CE	1:S:63:VAL:HG21	2.41	0.51
1:J:163:GLU:OE2	1:U:43:GLN:NE2	2.36	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
1:O:139:MET:O	1:O:143:VAL:HG13	2.11	0.50
2:G:344:HOH:O	1:Q:148:ARG:HD3	2.11	0.50
1:Q:106:VAL:HG12	1:Q:129:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:V:60:MET:HA	1:V:60:MET:CE	2.42	0.49
1:Q:60:MET:CE	1:Q:63:VAL:HG21	2.41	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:U:8:LYS:O	1:U:8:LYS:CG	2.59	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: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:F:106:VAL:HG12	1:F:129:LEU:HD21	1.95	0.48
1:C:133:ILE:HG13	1:W:120:LEU:HD22	1.96	0.48
1:R:106:VAL:HG12	1:R:129:LEU:HD21	1.96	0.48
1:N:87:ARG:HB2	1:N:88:PRO:HD2	1.95	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:D:60:MET:CE	1:D:63:VAL:HG21	2.43	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:60:MET:CE	1:L:63:VAL:HG21	2.44	0.47
1:L:24:THR:HA	1:L:78:VAL:HG13	1.96	0.47
1:W:24:THR:HA	1:W:78:VAL:HG13	1.96	0.47
1:O:156:LEU:O	1:O:160:VAL:HG23	2.15	0.47
1:C:106:VAL:HG12	1:C:129:LEU:HD21	1.95	0.47
1:B:39:GLU:O	1:B:40:ASP:HB2	2.15	0.47
1:T:60:MET:HA	1:T:60:MET:CE	2.44	0.47
1:C:24:THR:HA	1:C:78:VAL:HG13	1.97	0.47
1:T:106:VAL:HG12	1:T:129:LEU:HD21	1.95	0.47
1:A:156:LEU:O	1:A:160:VAL:HG23	2.14	0.47
1:O:62:LEU:HD23	1:O:124:PHE:HE2	1.79	0.47
1:F:24:THR:HA	1:F:78:VAL:HG13	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Q:123:GLN:OE1	1:T:130:GLN:HB2	2.15	0.47
1:R:123:GLN:NE2	1:R:124:PHE:HA	2.29	0.47
1:E:24:THR:HA	1:E:78:VAL:HG13	1.96	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:T:24:THR:HA	1:T:78:VAL:HG13	1.97	0.46
1:F:60:MET:CE	1:F:63:VAL:HG21	2.45	0.46
1:N:24:THR:HA	1:N:78:VAL:HG13	1.97	0.46
1:F:14:LEU:HD23	1:F:14:LEU:HA	1.81	0.46
1:N:60:MET:CE	1:N:60:MET:HA	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:J:60:MET:CE	1:J:63:VAL:HG21	2.45	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:T:152:ASN:OD1	1:T:154:PHE:HB2	2.16	0.46
1:J:35:TYR:O	1:J:38:SER:OG	2.24	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:Q:123:GLN:NE2	1:Q:124:PHE:CA	2.80	0.45
1:H:24:THR:HA	1:H:78:VAL:HG13	1.98	0.45
1:D:24:THR:HA	1:D:78:VAL:HG13	1.98	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:U:24:THR:HA	1:U:78:VAL:HG13	1.99	0.45
1:I:84:GLN:HG2	2:U:276:HOH:O	2.15	0.45
1:A:60:MET:CE	1:A:60:MET:HA	2.47	0.45
1:K:23:PHE:CZ	1:K:60:MET:CE	3.00	0.45
1:R:62:LEU:HD23	1:R:124:PHE:HE2	1.82	0.45
1:M:62:LEU:HD23	1:M: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:Q:123:GLN:C	1:Q:123:GLN:NE2	2.71	0.44
1:C:43:GLN:NE2	1:L:163:GLU:OE2	2.36	0.44
1:I:82:ARG:NH2	1:I:90:GLU:OE2	2.51	0.44
1:F:65:HIS:NE2	1:F:69:ARG:CD	2.80	0.44
1:D:41:LEU:HD13	1:D:44:LEU:HD12	1.99	0.44
1:F:20:HIS:HE1	2:F:200:HOH:O	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:123:GLN:HE21	1:R:124:PHE:HA	1.83	0.44
1:A:106:VAL:HG12	1:A:129:LEU:CD2	2.47	0.44
1:U:62:LEU:HD23	1:U:124:PHE:HE2	1.82	0.44
1:I:62:LEU:HD23	1:I:124:PHE:HE2	1.83	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:E:106:VAL:HG12	1:E:129:LEU:HD21	2.00	0.44
1:A:24:THR:HA	1:A:78:VAL:HG13	1.98	0.44
1:F:84:GLN:HG2	2:R:250:HOH:O	2.16	0.44
1:B:106:VAL:HG12	1:B:129:LEU:HD21	1.98	0.44
1:N:148:ARG:HH21	1:W:40:ASP:HB2	1.83	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:G:24:THR:HA	1:G:78:VAL:HG13	1.99	0.44
1:P:152:ASN:HD21	1:P:155:GLU:N	2.06	0.43
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:X:97:ASP:OD1	2:X:285:HOH:O	2.21	0.43
1:V:24:THR:HA	1:V:78:VAL:HG13	1.99	0.43
1:Q:60:MET:HE2	1:Q:63:VAL:HG21	2.01	0.43
1:L:8:LYS:HB2	1:L:8:LYS:HE3	1.67	0.43
1:E:56:ARG:NH1	2:E:197:HOH:O	2.47	0.43
1:S:106:VAL:HG12	1:S:129:LEU:HD21	2.01	0.43
1:X:40:ASP:O	1:X:42:PRO:HD3	2.18	0.43
1:S:60:MET:CE	1:S:60:MET:HA	2.49	0.43
1:D:148:ARG:HD3	2:O:329:HOH:O	2.19	0.43
1:S:62:LEU:HD23	1:S:124:PHE:HE2	1.83	0.43
1:L:106:VAL:HG12	1:L:129:LEU:HD21	2.01	0.43
1:M:14:LEU:HD23	1:M:14:LEU:HA	1.91	0.43
1:D:123:GLN:OE1	1:W:130:GLN:HB2	2.19	0.43
1:M:65:HIS:CD2	1:M:69:ARG:HD3	2.54	0.43
1:B:24:THR:HA	1:B:78:VAL:HG13	2.01	0.43
1:T:152:ASN:HD21	1:X:155:GLU:CD	2.16	0.42
1:E:60:MET:CE	1:E:63:VAL:HG21	2.48	0.42
1:O:24:THR:HA	1:O:78:VAL:HG13	2.01	0.42
1:K:8:LYS:HG3	1:K:8:LYS:O	2.19	0.42
1:B:40:ASP:C	1:B:42:PRO:HD3	2.40	0.42
1:A:60:MET:HE3	1:A:60:MET:HA	2.01	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:I:14:LEU:HA	1:I:14:LEU:HD23	1.91	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:60:MET:CE	1:C:63:VAL:HG21	2.49	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:K:40:ASP:C	1:K:42:PRO:HD3	2.39	0.42
1:D:14:LEU:HB3	1:D:109:LEU:HD21	2.02	0.42
1:E:154:PHE:CZ	1:T:149:ALA:HB2	2.55	0.42
1:C:75:ILE:HG13	1:O:30:VAL:HG12	2.01	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: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:B:14:LEU:HA	1:B:14:LEU:HD23	1.88	0.42
1:T:60:MET:HE2	1:T:63:VAL:HG21	2.02	0.42
1:S:35:TYR:O	1:S:38:SER:OG	2.27	0.42
1:C:62:LEU:HD23	1:C: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:A:62:LEU:HD23	1:A:124:PHE:HE2	1.85	0.41
1:X:14:LEU:HD23	1:X:14:LEU:HA	1.87	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: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:O:60:MET:CE	1:O:60:MET:HA	2.51	0.41
1:K:23:PHE:HZ	1:K:60:MET:HE1	1.86	0.41
1:R:39:GLU:O	1:R:40:ASP:HB2	2.21	0.41
1:N:156:LEU:O	1:N:160:VAL:HG23	2.20	0.41
1:F:65:HIS:CD2	1:F:69:ARG:HD3	2.56	0.41
1:W:60:MET:HA	1:W:60:MET:CE	2.51	0.41
1:G:75:ILE:HG13	1:S:30:VAL:HG12	2.03	0.41
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:P:130:GLN:HB2	1:R:123:GLN:OE1	2.21	0.41
1:E:62:LEU:HD23	1:E:124:PHE:HE2	1.86	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:60:MET:HA	1:C:60:MET:CE	2.51	0.40
2:L:296:HOH:O	1:X:84:GLN:HG2	2.21	0.40
1:Q:18:GLN:OE1	1:Q:18:GLN:HA	2.21	0.40
1:H:29:TYR:HA	1:H:29:TYR:HD1	1.72	0.40
1:P:14:LEU:HA	1:P:14:LEU:HD23	1.84	0.40
1:J:40:ASP:C	1:J:42:PRO:HD3	2.41	0.40
1:S:24:THR:HA	1:S:78:VAL:HG13	2.02	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:R:14:LEU:HA	1:R:14:LEU:HD23	1.86	0.40
1:L:14:LEU:HD23	1:L:14:LEU:HA	1.81	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	89	98
1	B	133/154 (86%)	131 (98%)	2 (2%)	76	96
1	C	133/154 (86%)	130 (98%)	3 (2%)	63	92
1	D	133/154 (86%)	130 (98%)	3 (2%)	63	92
1	E	132/154 (86%)	129 (98%)	3 (2%)	63	92
1	F	133/154 (86%)	130 (98%)	3 (2%)	63	92
1	G	133/154 (86%)	130 (98%)	3 (2%)	63	92
1	H	133/154 (86%)	131 (98%)	2 (2%)	76	96
1	I	133/154 (86%)	132 (99%)	1 (1%)	89	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	133/154 (86%)	129 (97%)	4 (3%)	53	86
1	K	133/154 (86%)	130 (98%)	3 (2%)	63	92
1	L	133/154 (86%)	130 (98%)	3 (2%)	63	92
1	M	133/154 (86%)	131 (98%)	2 (2%)	76	96
1	N	133/154 (86%)	131 (98%)	2 (2%)	76	96
1	O	132/154 (86%)	129 (98%)	3 (2%)	63	92
1	P	133/154 (86%)	128 (96%)	5 (4%)	44	80
1	Q	133/154 (86%)	129 (97%)	4 (3%)	53	86
1	R	133/154 (86%)	129 (97%)	4 (3%)	53	86
1	S	132/154 (86%)	131 (99%)	1 (1%)	89	98
1	T	133/154 (86%)	131 (98%)	2 (2%)	76	96
1	U	133/154 (86%)	130 (98%)	3 (2%)	63	92
1	V	133/154 (86%)	132 (99%)	1 (1%)	89	98
1	W	133/154 (86%)	130 (98%)	3 (2%)	63	92
1	X	133/154 (86%)	131 (98%)	2 (2%)	76	96
All	All	3188/3696 (86%)	3125 (98%)	63 (2%)	68	93

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	157/189 (83%)	-0.32	0 100 100	17, 26, 47, 60	0
1	B	157/189 (83%)	-0.27	0 100 100	17, 27, 50, 61	0
1	C	157/189 (83%)	-0.28	0 100 100	17, 27, 49, 60	0
1	D	157/189 (83%)	-0.25	0 100 100	18, 27, 51, 61	0
1	E	157/189 (83%)	-0.27	0 100 100	17, 27, 49, 61	0
1	F	157/189 (83%)	-0.31	0 100 100	17, 27, 50, 59	0
1	G	157/189 (83%)	-0.29	0 100 100	16, 27, 49, 59	0
1	H	157/189 (83%)	-0.31	0 100 100	17, 27, 49, 60	0
1	I	157/189 (83%)	-0.32	0 100 100	16, 26, 48, 60	0
1	J	157/189 (83%)	-0.29	0 100 100	17, 27, 49, 58	0
1	K	157/189 (83%)	-0.30	0 100 100	18, 27, 49, 61	0
1	L	157/189 (83%)	-0.33	0 100 100	16, 27, 48, 60	0
1	M	157/189 (83%)	-0.30	0 100 100	16, 27, 50, 61	0
1	N	157/189 (83%)	-0.31	0 100 100	16, 27, 49, 61	0
1	O	157/189 (83%)	-0.30	0 100 100	17, 26, 48, 60	0
1	P	157/189 (83%)	-0.27	1 (0%) 86 88	16, 28, 49, 60	0
1	Q	157/189 (83%)	-0.33	0 100 100	16, 27, 50, 60	0
1	R	157/189 (83%)	-0.34	0 100 100	17, 27, 50, 59	0
1	S	157/189 (83%)	-0.31	0 100 100	17, 26, 50, 59	0
1	T	157/189 (83%)	-0.18	1 (0%) 86 88	17, 27, 50, 60	0
1	U	157/189 (83%)	-0.31	0 100 100	16, 27, 50, 58	0
1	V	157/189 (83%)	-0.23	0 100 100	17, 27, 49, 63	0
1	W	157/189 (83%)	-0.36	0 100 100	17, 28, 51, 62	0
1	X	157/189 (83%)	-0.32	1 (0%) 86 88	16, 27, 50, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3768/4536 (83%)	-0.30	3 (0%) 93 96	16, 27, 50, 63	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	84	GLN	2.1
1	T	151	ALA	2.0
1	P	152	ASN	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 carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.