



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 05:00 PM UTC

PDB ID : 4EMH / pdb_00004emh
Title : Crystal structure of SpLsm4
Authors : Jiang, S.M.; Wu, D.H.; Song, H.W.
Deposited on : 2012-04-12
Resolution : 2.20 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

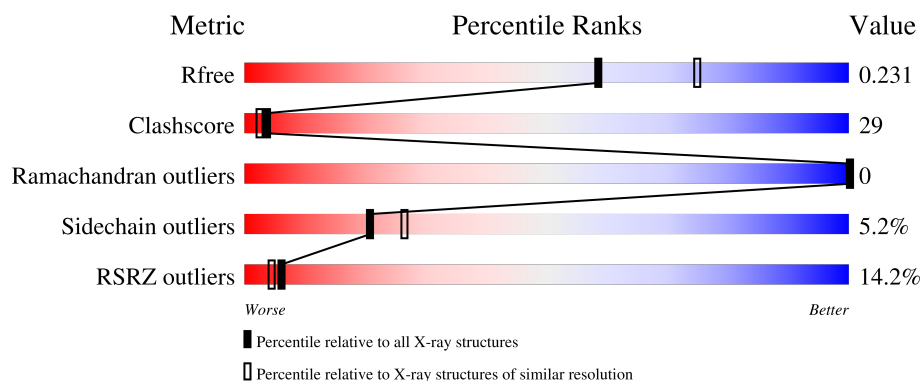
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	105	10% 40% 15% • 43%
1	B	105	8% 35% 20% • 43%
1	C	105	8% 38% 18% • 43%
1	D	105	8% 42% 14% • 43%
1	E	105	9% 36% 20% • 43%

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Mol	Chain	Length	Quality of chain
1	F	105	
1	G	105	
1	H	105	
1	I	105	
1	J	105	
1	K	105	
1	L	105	
1	M	105	
1	N	105	
1	O	105	
1	P	105	
1	Q	105	
1	R	105	
1	T	105	
1	U	105	
1	V	105	
1	W	105	
1	X	105	
1	Y	105	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 12991 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 U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	60	Total	C	N	O	S	Se	0	0	0
			497	314	90	89	2	2			
1	B	60	Total	C	N	O	S	Se	0	0	0
			497	314	90	89	2	2			
1	C	60	Total	C	N	O	S	Se	0	0	0
			497	314	90	89	2	2			
1	D	60	Total	C	N	O	S	Se	0	0	0
			497	314	90	89	2	2			
1	E	60	Total	C	N	O	S	Se	0	0	0
			497	314	90	89	2	2			
1	F	60	Total	C	N	O	S	Se	0	0	0
			497	314	90	89	2	2			
1	G	60	Total	C	N	O	S	Se	0	0	0
			497	314	90	89	2	2			
1	H	60	Total	C	N	O	S	Se	0	0	0
			497	314	90	89	2	2			
1	I	60	Total	C	N	O	S	Se	0	0	0
			497	314	90	89	2	2			
1	J	60	Total	C	N	O	S	Se	0	0	0
			497	314	90	89	2	2			
1	K	60	Total	C	N	O	S	Se	0	0	0
			497	314	90	89	2	2			
1	L	60	Total	C	N	O	S	Se	0	0	0
			497	314	90	89	2	2			
1	M	60	Total	C	N	O	S	Se	0	0	0
			497	314	90	89	2	2			
1	N	60	Total	C	N	O	S	Se	0	0	0
			497	314	90	89	2	2			
1	O	60	Total	C	N	O	S	Se	0	0	0
			497	314	90	89	2	2			
1	P	60	Total	C	N	O	S	Se	0	0	0
			497	314	90	89	2	2			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	60	Total	C	N	O	S	Se	0	0	0
			497	314	90	89	2	2			
1	R	60	Total	C	N	O	S	Se	0	0	0
			497	314	90	89	2	2			
1	T	60	Total	C	N	O	S	Se	0	0	0
			497	314	90	89	2	2			
1	U	60	Total	C	N	O	S	Se	0	0	0
			497	314	90	89	2	2			
1	V	60	Total	C	N	O	S	Se	0	0	0
			497	314	90	89	2	2			
1	W	60	Total	C	N	O	S	Se	0	0	0
			497	314	90	89	2	2			
1	X	60	Total	C	N	O	S	Se	0	0	0
			497	314	90	89	2	2			
1	Y	60	Total	C	N	O	S	Se	0	0	0
			497	314	90	89	2	2			

There are 336 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MSE	-	expression tag	UNP O14352
A	-12	GLY	-	expression tag	UNP O14352
A	-11	SER	-	expression tag	UNP O14352
A	-10	SER	-	expression tag	UNP O14352
A	-9	HIS	-	expression tag	UNP O14352
A	-8	HIS	-	expression tag	UNP O14352
A	-7	HIS	-	expression tag	UNP O14352
A	-6	HIS	-	expression tag	UNP O14352
A	-5	HIS	-	expression tag	UNP O14352
A	-4	HIS	-	expression tag	UNP O14352
A	-3	SER	-	expression tag	UNP O14352
A	-2	GLN	-	expression tag	UNP O14352
A	-1	ASP	-	expression tag	UNP O14352
A	0	PRO	-	expression tag	UNP O14352
B	-13	MSE	-	expression tag	UNP O14352
B	-12	GLY	-	expression tag	UNP O14352
B	-11	SER	-	expression tag	UNP O14352
B	-10	SER	-	expression tag	UNP O14352
B	-9	HIS	-	expression tag	UNP O14352
B	-8	HIS	-	expression tag	UNP O14352
B	-7	HIS	-	expression tag	UNP O14352
B	-6	HIS	-	expression tag	UNP O14352
B	-5	HIS	-	expression tag	UNP O14352

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	expression tag	UNP O14352
B	-3	SER	-	expression tag	UNP O14352
B	-2	GLN	-	expression tag	UNP O14352
B	-1	ASP	-	expression tag	UNP O14352
B	0	PRO	-	expression tag	UNP O14352
C	-13	MSE	-	expression tag	UNP O14352
C	-12	GLY	-	expression tag	UNP O14352
C	-11	SER	-	expression tag	UNP O14352
C	-10	SER	-	expression tag	UNP O14352
C	-9	HIS	-	expression tag	UNP O14352
C	-8	HIS	-	expression tag	UNP O14352
C	-7	HIS	-	expression tag	UNP O14352
C	-6	HIS	-	expression tag	UNP O14352
C	-5	HIS	-	expression tag	UNP O14352
C	-4	HIS	-	expression tag	UNP O14352
C	-3	SER	-	expression tag	UNP O14352
C	-2	GLN	-	expression tag	UNP O14352
C	-1	ASP	-	expression tag	UNP O14352
C	0	PRO	-	expression tag	UNP O14352
D	-13	MSE	-	expression tag	UNP O14352
D	-12	GLY	-	expression tag	UNP O14352
D	-11	SER	-	expression tag	UNP O14352
D	-10	SER	-	expression tag	UNP O14352
D	-9	HIS	-	expression tag	UNP O14352
D	-8	HIS	-	expression tag	UNP O14352
D	-7	HIS	-	expression tag	UNP O14352
D	-6	HIS	-	expression tag	UNP O14352
D	-5	HIS	-	expression tag	UNP O14352
D	-4	HIS	-	expression tag	UNP O14352
D	-3	SER	-	expression tag	UNP O14352
D	-2	GLN	-	expression tag	UNP O14352
D	-1	ASP	-	expression tag	UNP O14352
D	0	PRO	-	expression tag	UNP O14352
E	-13	MSE	-	expression tag	UNP O14352
E	-12	GLY	-	expression tag	UNP O14352
E	-11	SER	-	expression tag	UNP O14352
E	-10	SER	-	expression tag	UNP O14352
E	-9	HIS	-	expression tag	UNP O14352
E	-8	HIS	-	expression tag	UNP O14352
E	-7	HIS	-	expression tag	UNP O14352
E	-6	HIS	-	expression tag	UNP O14352
E	-5	HIS	-	expression tag	UNP O14352

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP O14352
E	-3	SER	-	expression tag	UNP O14352
E	-2	GLN	-	expression tag	UNP O14352
E	-1	ASP	-	expression tag	UNP O14352
E	0	PRO	-	expression tag	UNP O14352
F	-13	MSE	-	expression tag	UNP O14352
F	-12	GLY	-	expression tag	UNP O14352
F	-11	SER	-	expression tag	UNP O14352
F	-10	SER	-	expression tag	UNP O14352
F	-9	HIS	-	expression tag	UNP O14352
F	-8	HIS	-	expression tag	UNP O14352
F	-7	HIS	-	expression tag	UNP O14352
F	-6	HIS	-	expression tag	UNP O14352
F	-5	HIS	-	expression tag	UNP O14352
F	-4	HIS	-	expression tag	UNP O14352
F	-3	SER	-	expression tag	UNP O14352
F	-2	GLN	-	expression tag	UNP O14352
F	-1	ASP	-	expression tag	UNP O14352
F	0	PRO	-	expression tag	UNP O14352
G	-13	MSE	-	expression tag	UNP O14352
G	-12	GLY	-	expression tag	UNP O14352
G	-11	SER	-	expression tag	UNP O14352
G	-10	SER	-	expression tag	UNP O14352
G	-9	HIS	-	expression tag	UNP O14352
G	-8	HIS	-	expression tag	UNP O14352
G	-7	HIS	-	expression tag	UNP O14352
G	-6	HIS	-	expression tag	UNP O14352
G	-5	HIS	-	expression tag	UNP O14352
G	-4	HIS	-	expression tag	UNP O14352
G	-3	SER	-	expression tag	UNP O14352
G	-2	GLN	-	expression tag	UNP O14352
G	-1	ASP	-	expression tag	UNP O14352
G	0	PRO	-	expression tag	UNP O14352
H	-13	MSE	-	expression tag	UNP O14352
H	-12	GLY	-	expression tag	UNP O14352
H	-11	SER	-	expression tag	UNP O14352
H	-10	SER	-	expression tag	UNP O14352
H	-9	HIS	-	expression tag	UNP O14352
H	-8	HIS	-	expression tag	UNP O14352
H	-7	HIS	-	expression tag	UNP O14352
H	-6	HIS	-	expression tag	UNP O14352
H	-5	HIS	-	expression tag	UNP O14352

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-4	HIS	-	expression tag	UNP O14352
H	-3	SER	-	expression tag	UNP O14352
H	-2	GLN	-	expression tag	UNP O14352
H	-1	ASP	-	expression tag	UNP O14352
H	0	PRO	-	expression tag	UNP O14352
I	-13	MSE	-	expression tag	UNP O14352
I	-12	GLY	-	expression tag	UNP O14352
I	-11	SER	-	expression tag	UNP O14352
I	-10	SER	-	expression tag	UNP O14352
I	-9	HIS	-	expression tag	UNP O14352
I	-8	HIS	-	expression tag	UNP O14352
I	-7	HIS	-	expression tag	UNP O14352
I	-6	HIS	-	expression tag	UNP O14352
I	-5	HIS	-	expression tag	UNP O14352
I	-4	HIS	-	expression tag	UNP O14352
I	-3	SER	-	expression tag	UNP O14352
I	-2	GLN	-	expression tag	UNP O14352
I	-1	ASP	-	expression tag	UNP O14352
I	0	PRO	-	expression tag	UNP O14352
J	-13	MSE	-	expression tag	UNP O14352
J	-12	GLY	-	expression tag	UNP O14352
J	-11	SER	-	expression tag	UNP O14352
J	-10	SER	-	expression tag	UNP O14352
J	-9	HIS	-	expression tag	UNP O14352
J	-8	HIS	-	expression tag	UNP O14352
J	-7	HIS	-	expression tag	UNP O14352
J	-6	HIS	-	expression tag	UNP O14352
J	-5	HIS	-	expression tag	UNP O14352
J	-4	HIS	-	expression tag	UNP O14352
J	-3	SER	-	expression tag	UNP O14352
J	-2	GLN	-	expression tag	UNP O14352
J	-1	ASP	-	expression tag	UNP O14352
J	0	PRO	-	expression tag	UNP O14352
K	-13	MSE	-	expression tag	UNP O14352
K	-12	GLY	-	expression tag	UNP O14352
K	-11	SER	-	expression tag	UNP O14352
K	-10	SER	-	expression tag	UNP O14352
K	-9	HIS	-	expression tag	UNP O14352
K	-8	HIS	-	expression tag	UNP O14352
K	-7	HIS	-	expression tag	UNP O14352
K	-6	HIS	-	expression tag	UNP O14352
K	-5	HIS	-	expression tag	UNP O14352

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	HIS	-	expression tag	UNP O14352
K	-3	SER	-	expression tag	UNP O14352
K	-2	GLN	-	expression tag	UNP O14352
K	-1	ASP	-	expression tag	UNP O14352
K	0	PRO	-	expression tag	UNP O14352
L	-13	MSE	-	expression tag	UNP O14352
L	-12	GLY	-	expression tag	UNP O14352
L	-11	SER	-	expression tag	UNP O14352
L	-10	SER	-	expression tag	UNP O14352
L	-9	HIS	-	expression tag	UNP O14352
L	-8	HIS	-	expression tag	UNP O14352
L	-7	HIS	-	expression tag	UNP O14352
L	-6	HIS	-	expression tag	UNP O14352
L	-5	HIS	-	expression tag	UNP O14352
L	-4	HIS	-	expression tag	UNP O14352
L	-3	SER	-	expression tag	UNP O14352
L	-2	GLN	-	expression tag	UNP O14352
L	-1	ASP	-	expression tag	UNP O14352
L	0	PRO	-	expression tag	UNP O14352
M	-13	MSE	-	expression tag	UNP O14352
M	-12	GLY	-	expression tag	UNP O14352
M	-11	SER	-	expression tag	UNP O14352
M	-10	SER	-	expression tag	UNP O14352
M	-9	HIS	-	expression tag	UNP O14352
M	-8	HIS	-	expression tag	UNP O14352
M	-7	HIS	-	expression tag	UNP O14352
M	-6	HIS	-	expression tag	UNP O14352
M	-5	HIS	-	expression tag	UNP O14352
M	-4	HIS	-	expression tag	UNP O14352
M	-3	SER	-	expression tag	UNP O14352
M	-2	GLN	-	expression tag	UNP O14352
M	-1	ASP	-	expression tag	UNP O14352
M	0	PRO	-	expression tag	UNP O14352
N	-13	MSE	-	expression tag	UNP O14352
N	-12	GLY	-	expression tag	UNP O14352
N	-11	SER	-	expression tag	UNP O14352
N	-10	SER	-	expression tag	UNP O14352
N	-9	HIS	-	expression tag	UNP O14352
N	-8	HIS	-	expression tag	UNP O14352
N	-7	HIS	-	expression tag	UNP O14352
N	-6	HIS	-	expression tag	UNP O14352
N	-5	HIS	-	expression tag	UNP O14352

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-4	HIS	-	expression tag	UNP O14352
N	-3	SER	-	expression tag	UNP O14352
N	-2	GLN	-	expression tag	UNP O14352
N	-1	ASP	-	expression tag	UNP O14352
N	0	PRO	-	expression tag	UNP O14352
O	-13	MSE	-	expression tag	UNP O14352
O	-12	GLY	-	expression tag	UNP O14352
O	-11	SER	-	expression tag	UNP O14352
O	-10	SER	-	expression tag	UNP O14352
O	-9	HIS	-	expression tag	UNP O14352
O	-8	HIS	-	expression tag	UNP O14352
O	-7	HIS	-	expression tag	UNP O14352
O	-6	HIS	-	expression tag	UNP O14352
O	-5	HIS	-	expression tag	UNP O14352
O	-4	HIS	-	expression tag	UNP O14352
O	-3	SER	-	expression tag	UNP O14352
O	-2	GLN	-	expression tag	UNP O14352
O	-1	ASP	-	expression tag	UNP O14352
O	0	PRO	-	expression tag	UNP O14352
P	-13	MSE	-	expression tag	UNP O14352
P	-12	GLY	-	expression tag	UNP O14352
P	-11	SER	-	expression tag	UNP O14352
P	-10	SER	-	expression tag	UNP O14352
P	-9	HIS	-	expression tag	UNP O14352
P	-8	HIS	-	expression tag	UNP O14352
P	-7	HIS	-	expression tag	UNP O14352
P	-6	HIS	-	expression tag	UNP O14352
P	-5	HIS	-	expression tag	UNP O14352
P	-4	HIS	-	expression tag	UNP O14352
P	-3	SER	-	expression tag	UNP O14352
P	-2	GLN	-	expression tag	UNP O14352
P	-1	ASP	-	expression tag	UNP O14352
P	0	PRO	-	expression tag	UNP O14352
Q	-13	MSE	-	expression tag	UNP O14352
Q	-12	GLY	-	expression tag	UNP O14352
Q	-11	SER	-	expression tag	UNP O14352
Q	-10	SER	-	expression tag	UNP O14352
Q	-9	HIS	-	expression tag	UNP O14352
Q	-8	HIS	-	expression tag	UNP O14352
Q	-7	HIS	-	expression tag	UNP O14352
Q	-6	HIS	-	expression tag	UNP O14352
Q	-5	HIS	-	expression tag	UNP O14352

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-4	HIS	-	expression tag	UNP O14352
Q	-3	SER	-	expression tag	UNP O14352
Q	-2	GLN	-	expression tag	UNP O14352
Q	-1	ASP	-	expression tag	UNP O14352
Q	0	PRO	-	expression tag	UNP O14352
R	-13	MSE	-	expression tag	UNP O14352
R	-12	GLY	-	expression tag	UNP O14352
R	-11	SER	-	expression tag	UNP O14352
R	-10	SER	-	expression tag	UNP O14352
R	-9	HIS	-	expression tag	UNP O14352
R	-8	HIS	-	expression tag	UNP O14352
R	-7	HIS	-	expression tag	UNP O14352
R	-6	HIS	-	expression tag	UNP O14352
R	-5	HIS	-	expression tag	UNP O14352
R	-4	HIS	-	expression tag	UNP O14352
R	-3	SER	-	expression tag	UNP O14352
R	-2	GLN	-	expression tag	UNP O14352
R	-1	ASP	-	expression tag	UNP O14352
R	0	PRO	-	expression tag	UNP O14352
T	-13	MSE	-	expression tag	UNP O14352
T	-12	GLY	-	expression tag	UNP O14352
T	-11	SER	-	expression tag	UNP O14352
T	-10	SER	-	expression tag	UNP O14352
T	-9	HIS	-	expression tag	UNP O14352
T	-8	HIS	-	expression tag	UNP O14352
T	-7	HIS	-	expression tag	UNP O14352
T	-6	HIS	-	expression tag	UNP O14352
T	-5	HIS	-	expression tag	UNP O14352
T	-4	HIS	-	expression tag	UNP O14352
T	-3	SER	-	expression tag	UNP O14352
T	-2	GLN	-	expression tag	UNP O14352
T	-1	ASP	-	expression tag	UNP O14352
T	0	PRO	-	expression tag	UNP O14352
U	-13	MSE	-	expression tag	UNP O14352
U	-12	GLY	-	expression tag	UNP O14352
U	-11	SER	-	expression tag	UNP O14352
U	-10	SER	-	expression tag	UNP O14352
U	-9	HIS	-	expression tag	UNP O14352
U	-8	HIS	-	expression tag	UNP O14352
U	-7	HIS	-	expression tag	UNP O14352
U	-6	HIS	-	expression tag	UNP O14352
U	-5	HIS	-	expression tag	UNP O14352

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Chain	Residue	Modelled	Actual	Comment	Reference
U	-4	HIS	-	expression tag	UNP O14352
U	-3	SER	-	expression tag	UNP O14352
U	-2	GLN	-	expression tag	UNP O14352
U	-1	ASP	-	expression tag	UNP O14352
U	0	PRO	-	expression tag	UNP O14352
V	-13	MSE	-	expression tag	UNP O14352
V	-12	GLY	-	expression tag	UNP O14352
V	-11	SER	-	expression tag	UNP O14352
V	-10	SER	-	expression tag	UNP O14352
V	-9	HIS	-	expression tag	UNP O14352
V	-8	HIS	-	expression tag	UNP O14352
V	-7	HIS	-	expression tag	UNP O14352
V	-6	HIS	-	expression tag	UNP O14352
V	-5	HIS	-	expression tag	UNP O14352
V	-4	HIS	-	expression tag	UNP O14352
V	-3	SER	-	expression tag	UNP O14352
V	-2	GLN	-	expression tag	UNP O14352
V	-1	ASP	-	expression tag	UNP O14352
V	0	PRO	-	expression tag	UNP O14352
W	-13	MSE	-	expression tag	UNP O14352
W	-12	GLY	-	expression tag	UNP O14352
W	-11	SER	-	expression tag	UNP O14352
W	-10	SER	-	expression tag	UNP O14352
W	-9	HIS	-	expression tag	UNP O14352
W	-8	HIS	-	expression tag	UNP O14352
W	-7	HIS	-	expression tag	UNP O14352
W	-6	HIS	-	expression tag	UNP O14352
W	-5	HIS	-	expression tag	UNP O14352
W	-4	HIS	-	expression tag	UNP O14352
W	-3	SER	-	expression tag	UNP O14352
W	-2	GLN	-	expression tag	UNP O14352
W	-1	ASP	-	expression tag	UNP O14352
W	0	PRO	-	expression tag	UNP O14352
X	-13	MSE	-	expression tag	UNP O14352
X	-12	GLY	-	expression tag	UNP O14352
X	-11	SER	-	expression tag	UNP O14352
X	-10	SER	-	expression tag	UNP O14352
X	-9	HIS	-	expression tag	UNP O14352
X	-8	HIS	-	expression tag	UNP O14352
X	-7	HIS	-	expression tag	UNP O14352
X	-6	HIS	-	expression tag	UNP O14352
X	-5	HIS	-	expression tag	UNP O14352

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Chain	Residue	Modelled	Actual	Comment	Reference
X	-4	HIS	-	expression tag	UNP O14352
X	-3	SER	-	expression tag	UNP O14352
X	-2	GLN	-	expression tag	UNP O14352
X	-1	ASP	-	expression tag	UNP O14352
X	0	PRO	-	expression tag	UNP O14352
Y	-13	MSE	-	expression tag	UNP O14352
Y	-12	GLY	-	expression tag	UNP O14352
Y	-11	SER	-	expression tag	UNP O14352
Y	-10	SER	-	expression tag	UNP O14352
Y	-9	HIS	-	expression tag	UNP O14352
Y	-8	HIS	-	expression tag	UNP O14352
Y	-7	HIS	-	expression tag	UNP O14352
Y	-6	HIS	-	expression tag	UNP O14352
Y	-5	HIS	-	expression tag	UNP O14352
Y	-4	HIS	-	expression tag	UNP O14352
Y	-3	SER	-	expression tag	UNP O14352
Y	-2	GLN	-	expression tag	UNP O14352
Y	-1	ASP	-	expression tag	UNP O14352
Y	0	PRO	-	expression tag	UNP O14352

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	50	Total O 50 50	0	0
2	B	48	Total O 48 48	0	0
2	C	49	Total O 49 49	0	0
2	D	42	Total O 42 42	0	0
2	E	45	Total O 45 45	0	0
2	F	33	Total O 33 33	0	0
2	G	65	Total O 65 65	0	0
2	H	49	Total O 49 49	0	0
2	I	59	Total O 59 59	0	0
2	J	53	Total O 53 53	0	0

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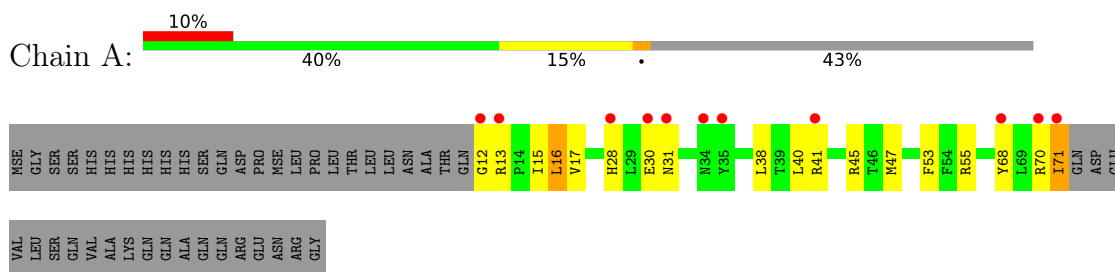
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	K	31	Total 31	O 31	0	0
2	L	43	Total 43	O 43	0	0
2	M	42	Total 42	O 42	0	0
2	N	37	Total 37	O 37	0	0
2	O	27	Total 27	O 27	0	0
2	P	49	Total 49	O 49	0	0
2	Q	54	Total 54	O 54	0	0
2	R	48	Total 48	O 48	0	0
2	T	36	Total 36	O 36	0	0
2	U	24	Total 24	O 24	0	0
2	V	28	Total 28	O 28	0	0
2	W	56	Total 56	O 56	0	0
2	X	39	Total 39	O 39	0	0
2	Y	56	Total 56	O 56	0	0

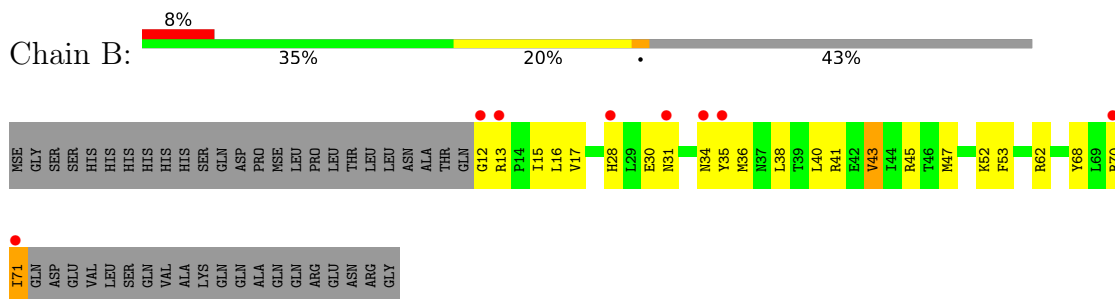
3 Residue-property plots

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

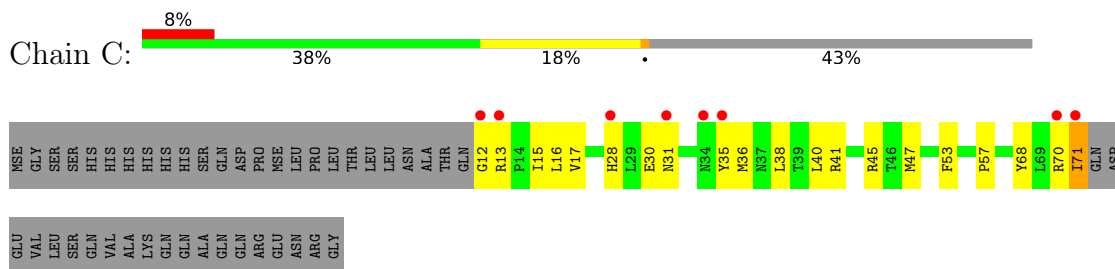
- Molecule 1: Probable U6 snRNA-associated Sm-like protein LSm4



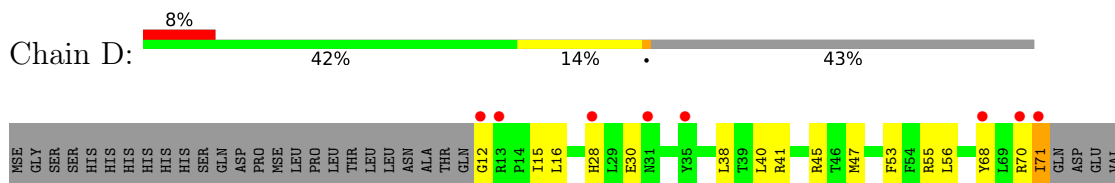
- Molecule 1: Probable U6 snRNA-associated Sm-like protein LSm4



- Molecule 1: Probable U6 snRNA-associated Sm-like protein LSm4

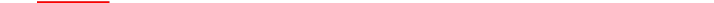


- Molecule 1: Probable U6 snRNA-associated Sm-like protein LSm4



VAL
LEU
SER
GLN
VAL
ALA
LYS
GLN
GLN
ALA
GLN
GLN
ARG
GLU
ASN
ARG
GLY

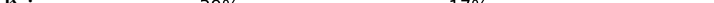
- Molecule 1: Probable U6 snRNA-associated Sm-like protein LSm4

Chain J: 

Category	Item	Value	Color
Nucleic Acids	MSE	128	Red
	GLY	129	Red
	SER	130	Red
	SER	131	Red
	HIS	132	Red
	HIS	133	Red
	HIS	134	Red
	HIS	135	Red
	HIS	136	Red
	HIS	137	Red
Amino Acids	SER	138	Red
	GLN	139	Red
	ASP	140	Red
	PRO	141	Red
	MSE	142	Red
	LEU	143	Red
	PRO	144	Red
	LEU	145	Red
	THR	146	Red
	LEU	147	Red
Other	ASN	148	Red
	ALA	149	Red
	ALA	150	Red
	THR	151	Red
	GLN	152	Red
	G12	153	Red
	R13	154	Red
	P14	155	Red
	I15	156	Red
	L16	157	Red
Lipids	V17	158	Red
	H28	159	Red
	L29	160	Red
	E30	161	Red
	R31	162	Red
	Y35	163	Red
	L38	164	Red
	T39	165	Red
	L40	166	Red
	R41	167	Red
Carbohydrates	E42	168	Red
	V43	169	Red
	I44	170	Red
	L45	171	Red
	R46	172	Red
	M47	173	Red
	F53	174	Red
	Y68	175	Red
	L69	176	Red
	R70	177	Red
Miscellaneous	I71	178	Red
	GLN	179	Red
	ASP	180	Red
	GLU	181	Red
	VAL	182	Red

LEU
SER
GLN
VAL
ALA
LYS
GLN
GLN
ALA
GLN
GLN
ARG
GLU
ASN
ARG
GLY

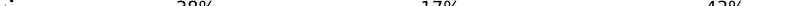
- Molecule 1: Probable U6 snRNA-associated Sm-like protein LSm4

Chain K: 

Label	Value	Color	Category
MSE	12	Green	Good
GLY	13	Green	Good
SER	14	Green	Good
SER	15	Green	Good
HIS	16	Green	Good
HIS	17	Green	Good
HIS	18	Green	Good
HIS	19	Green	Good
HIS	20	Green	Good
SER	21	Green	Good
GLN	22	Green	Good
ASP	23	Green	Good
PRO	24	Green	Good
NSE	25	Green	Good
LEU	26	Green	Good
PRO	27	Green	Good
LEU	28	Green	Good
LEU	29	Green	Good
THR	30	Green	Good
LEU	31	Green	Good
ASN	32	Green	Good
ALA	33	Green	Good
THR	34	Green	Good
GLN	35	Green	Good
G12	36	Red	Bad
R13	37	Red	Bad
P14	38	Yellow	Warning
I15	39	Yellow	Warning
L16	40	Yellow	Warning
H28	41	Red	Bad
L29	42	Green	Good
E30	43	Green	Good
N31	44	Red	Bad
N34	45	Red	Bad
Y35	46	Red	Bad
N36	47	Green	Good
N37	48	Green	Good
L38	49	Green	Good
T39	50	Green	Good
L40	51	Green	Good
R41	52	Green	Good
E42	53	Green	Good
V43	54	Green	Good
I44	55	Green	Good
R45	56	Green	Good
T46	57	Green	Good
M47	58	Yellow	Warning
F53	59	Yellow	Warning
E58	60	Green	Good
Y68	61	Red	Bad
L70	62	Green	Good
R79	63	Yellow	Warning
I71	64	Red	Bad
GLN	65	Green	Good

ASP
GLU
VAL
LEU
SER
GLN
VAL
ALA
LYS
GLN
GLN
ALA
GLN
GLN
ARG
GLU
ASN
ARG
GLY

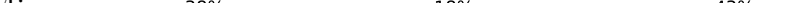
- Molecule 1: Probable U6 snRNA-associated Sm-like protein LSm4

Chain L: 

[illegible]

LEU
SER
GLN
VAL
ALA
LYS
GLN
GLN
ALA
GLN
GLN
ARG
GLU
ASN
ARG
GLY

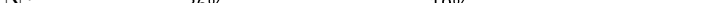
- Molecule 1: Probable U6 snRNA-associated Sm-like protein LSm4

Chain M: 

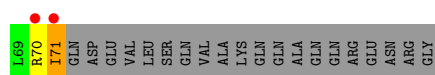
Gene	Chromosome	Position (kb)	Strand	Transcript	Length (bp)	GC Content (%)	GC Content (95% CI)	GC Content (99% CI)
NSE	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
GLY	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
SER	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
SER	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
HIS	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
HIS	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
HIS	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
HIS	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
HIS	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
SER	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
GLN	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
ASP	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
PRO	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
NSE	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
LEU	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
PRO	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
LEU	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
LEU	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
THR	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
LEU	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
LEU	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
ASN	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
ALA	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
THR	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
GLN	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
G12	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
R13	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
P14	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
I15	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
L16	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
V17	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
E18	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
H28	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
E29	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
E30	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
Y35	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
N36	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
N37	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
L38	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
T39	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
L40	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
R41	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
E42	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
V43	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
L44	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
R45	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
T46	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
M47	1	100	+	1	100	40.0	39.5-40.5	39.0-41.0
F53	1	100	+	1	100	40.0	39.5-40.5	39

GLU
VAL
LEU
SER
GLN
VAL
ALA
LYS
GLN
GLN
ALA
GLN
GLN
ARG
GLU
ASN
ARG
GLY

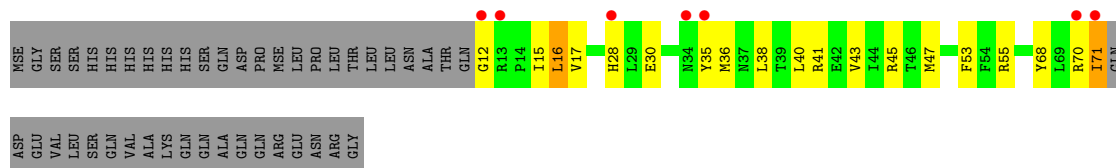
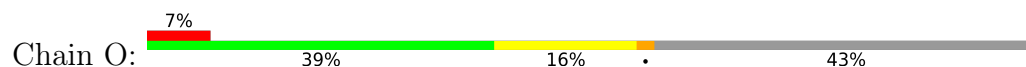
- Molecule 1: Probable U6 snRNA-associated Sm-like protein LSm4

Chain N: 

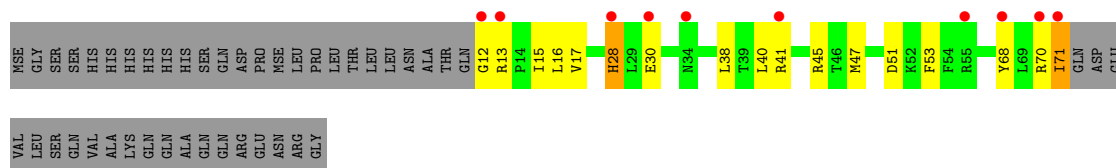
Category	Count
MSE	1
GLY	2
SER	3
SER	4
HIS	5
HIS	6
HIS	7
HIS	8
HIS	9
SER	10
GLN	11
ASP	12
PRO	13
MSE	14
LEU	15
PRO	16
LEU	17
THR	18
LEU	19
ASN	20
ALA	21
THR	22
GLN	23
R12	24
G13	25
P14	26
I15	27
L16	28
V17	29
K20	30
M26	31
G27	32
H28	33
L29	34
E30	35
D33	36
H34	37
F35	38
M36	39
N37	40
L38	41
T39	42
L40	43
R41	44
R45	45
T46	46
M47	47
F53	48
P57	49
K67	50
V69	51



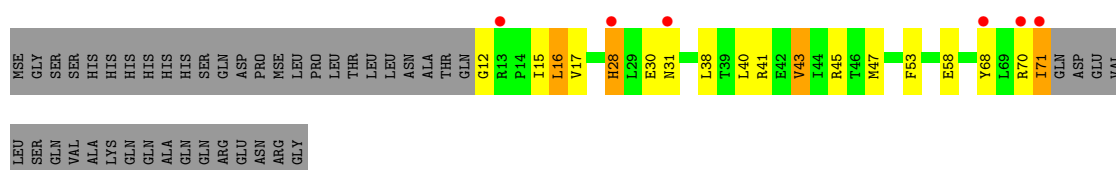
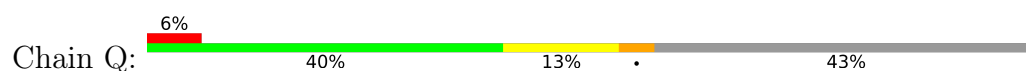
- Molecule 1: Probable U6 snRNA-associated Sm-like protein LSm4



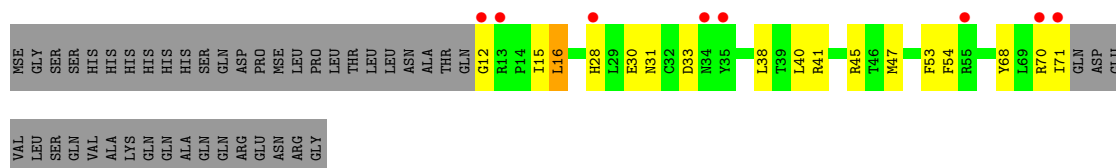
- Molecule 1: Probable U6 snRNA-associated Sm-like protein LSm4



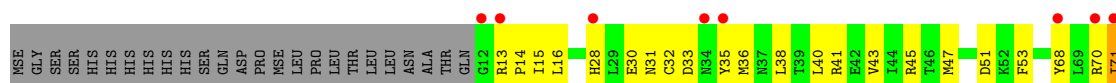
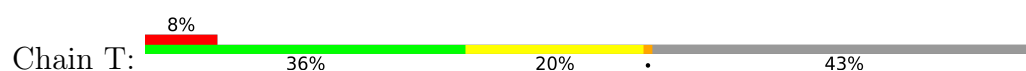
- Molecule 1: Probable U6 snRNA-associated Sm-like protein LSm4



- Molecule 1: Probable U6 snRNA-associated Sm-like protein LSm4



- Molecule 1: Probable U6 snRNA-associated Sm-like protein LSm4



Category	Value	Color
MSE	12	Red
GLY	13	Red
SER	14	Green
SER	15	Green
HIS	16	Orange
HIS	17	Orange
HIS	18	Green
HIS	19	Green
HIS	20	Green
HIS	21	Green
SER	22	Green
GLN	23	Green
ASP	24	Green
PRO	25	Green
MSE	26	Green
LEU	27	Green
PRO	28	Green
LEU	29	Green
THR	30	Green
LEU	31	Green
LEU	32	Green
ASN	33	Green
ALA	34	Green
THR	35	Green
GLN	36	Green
G12	37	Red
R13	38	Red
P14	39	Green
I15	40	Green
L16	41	Orange
V17	42	Orange
H28	43	Orange
L29	44	Red
E30	45	Red
N31	46	Red
C32	47	Red
D33	48	Red
N34	49	Red
L38	50	Green
T39	51	Green
L40	52	Green
R41	53	Red
E42	54	Green
V43	55	Green
I44	56	Green
R45	57	Green
T46	58	Green
M47	59	Green
F53	60	Green
F54	61	Green
R55	62	Red
Y68	63	Red
L69	64	Green
R70	65	Red
I71	66	Orange
GLN	67	Orange

ASP	GLU	VAL	SER	GLN	VAL	ALA	LYS	GLN	ALA	GLN	GLN	ARG	GLU	ASN	ARG	GLY
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.12Å 124.47Å 131.57Å 90.00° 135.07° 90.00°	Depositor
Resolution (Å)	92.56 – 2.20 92.56 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (92.56-2.20) 99.2 (92.56-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.237 , 0.253 0.234 , 0.231	Depositor DCC
R_{free} test set	6586 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.045 for -h-2*k,h+1 0.024 for h,-k,-h-l 0.026 for h+2*k,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12991	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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 23.82 % 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 4.3200e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

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	0.65	0/504	0.84	0/674
1	B	0.57	0/504	0.84	1/674 (0.1%)
1	C	0.58	0/504	0.82	0/674
1	D	0.56	0/504	0.83	0/674
1	E	0.59	0/504	0.77	0/674
1	F	0.55	0/504	0.83	0/674
1	G	0.59	0/504	0.85	0/674
1	H	0.59	0/504	0.83	0/674
1	I	0.60	0/504	0.84	1/674 (0.1%)
1	J	0.58	0/504	0.81	0/674
1	K	0.54	0/504	0.82	0/674
1	L	0.57	0/504	0.85	0/674
1	M	0.57	0/504	0.85	0/674
1	N	0.57	0/504	0.82	0/674
1	O	0.56	0/504	0.82	0/674
1	P	0.56	0/504	0.82	0/674
1	Q	0.61	0/504	0.86	1/674 (0.1%)
1	R	0.58	0/504	0.80	0/674
1	T	0.58	0/504	0.83	0/674
1	U	0.52	0/504	0.80	0/674
1	V	0.58	0/504	0.82	0/674
1	W	0.59	0/504	0.86	0/674
1	X	0.55	0/504	0.79	0/674
1	Y	0.59	0/504	0.84	0/674
All	All	0.58	0/12096	0.83	3/16176 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	43	VAL	N-CA-C	5.58	117.03	108.71
1	I	43	VAL	N-CA-C	5.07	115.89	108.53
1	B	43	VAL	N-CA-C	5.04	116.54	108.89

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	497	0	496	29	0
1	B	497	0	496	29	2
1	C	497	0	496	30	0
1	D	497	0	496	31	0
1	E	497	0	496	29	2
1	F	497	0	496	23	0
1	G	497	0	496	40	0
1	H	497	0	496	23	1
1	I	497	0	496	26	0
1	J	497	0	496	25	0
1	K	497	0	496	26	1
1	L	497	0	496	24	0
1	M	497	0	496	27	1
1	N	497	0	496	32	2
1	O	497	0	496	23	0
1	P	497	0	496	27	0
1	Q	497	0	496	28	0
1	R	497	0	496	29	0
1	T	497	0	496	28	1
1	U	497	0	496	30	0
1	V	497	0	496	31	0
1	W	497	0	496	36	0
1	X	497	0	496	38	0
1	Y	497	0	496	34	1
2	A	50	0	0	4	0
2	B	48	0	0	4	0
2	C	49	0	0	10	0
2	D	42	0	0	10	0
2	E	45	0	0	7	0
2	F	33	0	0	4	0
2	G	65	0	0	17	0
2	H	49	0	0	6	1
2	I	59	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	53	0	0	4	0
2	K	31	0	0	7	0
2	L	43	0	0	4	0
2	M	42	0	0	7	0
2	N	37	0	0	9	0
2	O	27	0	0	0	0
2	P	49	0	0	9	0
2	Q	54	0	0	10	0
2	R	48	0	0	8	0
2	T	36	0	0	7	0
2	U	24	0	0	4	0
2	V	28	0	0	7	0
2	W	56	0	0	12	0
2	X	39	0	0	13	0
2	Y	56	0	0	15	0
All	All	12991	0	11904	689	6

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 29.

All (689) 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:I:12:GLY:N	2:I:134:HOH:O	1.93	1.00
1:B:13:ARG:HG3	2:E:118:HOH:O	1.62	0.98
1:J:47:MSE:SE	2:J:139:HOH:O	2.32	0.97
1:B:47:MSE:SE	2:B:121:HOH:O	2.31	0.96
1:M:47:MSE:SE	2:M:117:HOH:O	2.34	0.95
1:D:12:GLY:N	1:D:71:ILE:HD13	1.82	0.94
1:U:47:MSE:HE3	1:U:53:PHE:CE2	2.02	0.94
1:W:35:TYR:O	2:W:130:HOH:O	1.87	0.93
1:C:71:ILE:O	2:C:119:HOH:O	1.86	0.93
1:N:28:HIS:HB3	2:N:120:HOH:O	1.67	0.93
1:V:13:ARG:NH2	2:V:128:HOH:O	1.99	0.93
1:I:12:GLY:CA	2:I:134:HOH:O	2.17	0.93
1:H:47:MSE:HE3	1:H:53:PHE:CE2	2.03	0.93
1:T:36:MSE:SE	2:T:119:HOH:O	2.35	0.92
1:K:47:MSE:HE3	1:K:53:PHE:CE2	2.05	0.92
1:A:12:GLY:HA3	1:A:71:ILE:HD13	1.51	0.92
1:M:47:MSE:HE3	1:M:53:PHE:CE2	2.05	0.92
1:R:31:ASN:HB2	2:R:138:HOH:O	1.67	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:47:MSE:HE3	1:X:53:PHE:CE2	2.05	0.92
1:K:41:ARG:HG2	2:K:129:HOH:O	1.71	0.91
1:R:47:MSE:HE3	1:R:53:PHE:CE2	2.05	0.91
1:N:47:MSE:HE3	1:N:53:PHE:CE2	2.06	0.91
1:G:47:MSE:HE3	1:G:53:PHE:CE2	2.05	0.90
1:B:47:MSE:HE3	1:B:53:PHE:CE2	2.07	0.90
1:Y:28:HIS:NE2	2:Y:110:HOH:O	2.03	0.90
1:E:47:MSE:HE3	1:E:53:PHE:CE2	2.07	0.90
1:A:47:MSE:HE3	1:A:53:PHE:CE2	2.08	0.89
1:I:47:MSE:SE	2:I:140:HOH:O	2.39	0.89
1:M:70:ARG:NH1	2:M:115:HOH:O	2.04	0.89
1:I:12:GLY:HA3	1:I:71:ILE:HD13	1.53	0.88
1:C:47:MSE:HE3	1:C:53:PHE:CE2	2.08	0.88
1:A:47:MSE:SE	2:A:132:HOH:O	2.40	0.88
1:C:12:GLY:HA3	1:C:71:ILE:HD13	1.56	0.88
1:W:47:MSE:HE3	1:W:53:PHE:CE2	2.09	0.88
1:E:36:MSE:SE	2:E:124:HOH:O	2.40	0.88
1:G:70:ARG:NH1	2:G:148:HOH:O	2.07	0.87
1:D:47:MSE:HE3	1:D:53:PHE:CE2	2.10	0.87
1:J:47:MSE:HE3	1:J:53:PHE:CE2	2.10	0.87
1:D:12:GLY:HA2	2:D:115:HOH:O	1.72	0.87
1:F:47:MSE:HE3	1:F:53:PHE:CE2	2.08	0.87
1:I:47:MSE:HE3	1:I:53:PHE:CE2	2.11	0.86
1:F:47:MSE:SE	2:F:116:HOH:O	2.44	0.86
1:Q:47:MSE:HE3	1:Q:53:PHE:CE2	2.11	0.86
1:O:47:MSE:HE3	1:O:53:PHE:CE2	2.10	0.85
1:Y:41:ARG:NE	2:Y:151:HOH:O	2.08	0.85
1:U:33:ASP:OD2	2:U:120:HOH:O	1.94	0.85
1:D:68:TYR:CE1	2:D:116:HOH:O	2.29	0.84
1:D:12:GLY:CA	2:D:115:HOH:O	2.24	0.84
1:C:47:MSE:SE	2:C:136:HOH:O	2.46	0.84
1:T:47:MSE:HE3	1:T:53:PHE:CE2	2.12	0.84
1:J:28:HIS:HB3	2:J:124:HOH:O	1.77	0.84
1:L:47:MSE:HE3	1:L:53:PHE:CE2	2.13	0.83
1:K:58:GLU:HB2	2:K:129:HOH:O	1.77	0.83
1:G:12:GLY:N	2:G:127:HOH:O	2.12	0.83
1:Q:12:GLY:CA	2:Q:144:HOH:O	2.27	0.82
1:W:35:TYR:HE1	2:W:153:HOH:O	1.63	0.81
1:D:12:GLY:N	2:D:115:HOH:O	2.13	0.81
1:T:13:ARG:NH2	2:T:134:HOH:O	2.12	0.81
1:P:47:MSE:HE3	1:P:53:PHE:CE2	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:41:ARG:CZ	2:W:150:HOH:O	2.30	0.80
1:W:41:ARG:NH1	2:W:150:HOH:O	2.14	0.80
1:D:70:ARG:NH1	2:D:116:HOH:O	2.13	0.79
1:B:31:ASN:HA	1:E:34:ASN:ND2	1.98	0.79
1:V:47:MSE:HE3	1:V:53:PHE:CE2	2.17	0.79
1:C:12:GLY:N	2:C:146:HOH:O	2.14	0.79
1:G:12:GLY:CA	2:G:127:HOH:O	2.30	0.78
1:Y:47:MSE:HE3	1:Y:53:PHE:CE2	2.17	0.78
1:P:71:ILE:O	2:P:145:HOH:O	2.01	0.78
1:X:35:TYR:O	2:X:127:HOH:O	2.02	0.78
1:P:28:HIS:NE2	2:P:126:HOH:O	2.16	0.78
1:W:35:TYR:CE1	2:W:153:HOH:O	2.35	0.77
1:V:15:ILE:HG22	1:V:71:ILE:HG12	1.66	0.77
1:F:31:ASN:ND2	2:F:115:HOH:O	2.18	0.76
1:G:12:GLY:HA2	2:G:127:HOH:O	1.86	0.76
1:V:42:GLU:OE2	2:V:106:HOH:O	2.03	0.76
1:V:12:GLY:N	1:V:71:ILE:HG21	2.01	0.76
1:A:55:ARG:HD2	2:C:143:HOH:O	1.86	0.75
1:X:30:GLU:OE2	2:X:137:HOH:O	2.03	0.75
1:L:12:GLY:N	2:L:122:HOH:O	2.18	0.75
1:X:13:ARG:HD3	2:X:109:HOH:O	1.87	0.75
1:N:47:MSE:SE	2:N:128:HOH:O	2.53	0.75
1:D:68:TYR:CZ	2:D:116:HOH:O	2.39	0.75
1:Q:12:GLY:N	2:Q:144:HOH:O	2.20	0.74
1:B:34:ASN:ND2	1:E:31:ASN:HA	2.03	0.74
1:M:45:ARG:NH2	2:M:138:HOH:O	2.21	0.73
1:N:26:ASN:ND2	2:N:133:HOH:O	2.19	0.73
1:G:37:ASN:O	2:G:153:HOH:O	2.07	0.73
1:R:31:ASN:ND2	2:R:112:HOH:O	2.20	0.73
1:Y:45:ARG:NE	1:Y:47:MSE:HE1	2.04	0.73
1:P:12:GLY:N	1:P:71:ILE:HD13	2.04	0.73
1:M:68:TYR:CE1	2:M:115:HOH:O	2.41	0.73
1:H:47:MSE:HE3	1:H:53:PHE:HE2	1.52	0.73
1:U:47:MSE:HE3	1:U:53:PHE:HE2	1.52	0.73
1:X:37:ASN:OD1	2:X:118:HOH:O	2.07	0.73
1:G:45:ARG:CZ	1:G:47:MSE:HE1	2.18	0.73
1:G:47:MSE:SE	2:G:137:HOH:O	2.57	0.72
1:K:47:MSE:SE	2:K:110:HOH:O	2.56	0.72
1:Q:45:ARG:NE	1:Q:47:MSE:HE1	2.04	0.72
2:Q:143:HOH:O	1:R:47:MSE:SE	2.57	0.72
1:D:45:ARG:NE	1:D:47:MSE:HE1	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:35:TYR:OH	2:W:144:HOH:O	2.06	0.72
1:Y:12:GLY:N	2:Y:101:HOH:O	2.23	0.72
1:N:28:HIS:HB2	2:N:114:HOH:O	1.88	0.72
1:E:45:ARG:NE	1:E:47:MSE:HE1	2.05	0.72
1:M:45:ARG:NE	1:M:47:MSE:HE1	2.04	0.72
1:M:45:ARG:CZ	1:M:47:MSE:HE1	2.20	0.72
1:T:45:ARG:NE	1:T:47:MSE:HE1	2.03	0.72
1:B:45:ARG:CZ	1:B:47:MSE:HE1	2.20	0.72
1:N:45:ARG:CZ	1:N:47:MSE:HE1	2.19	0.72
1:I:45:ARG:NE	1:I:47:MSE:HE1	2.04	0.71
1:N:45:ARG:NE	1:N:47:MSE:HE1	2.05	0.71
1:A:31:ASN:OD1	2:A:136:HOH:O	2.08	0.71
1:R:47:MSE:HE3	1:R:53:PHE:HE2	1.55	0.71
1:L:45:ARG:CZ	1:L:47:MSE:HE1	2.20	0.71
1:N:47:MSE:HE3	1:N:53:PHE:HE2	1.55	0.71
1:F:45:ARG:CZ	1:F:47:MSE:HE1	2.20	0.71
1:F:55:ARG:O	2:F:130:HOH:O	2.07	0.71
1:K:41:ARG:NE	2:K:129:HOH:O	2.17	0.71
1:V:45:ARG:CZ	1:V:47:MSE:HE1	2.20	0.71
1:E:47:MSE:HE3	1:E:53:PHE:HE2	1.54	0.71
1:C:45:ARG:NE	1:C:47:MSE:HE1	2.06	0.71
1:R:12:GLY:N	2:R:113:HOH:O	2.23	0.71
1:D:45:ARG:CZ	1:D:47:MSE:HE1	2.21	0.70
1:C:30:GLU:HG3	1:C:41:ARG:HG3	1.72	0.70
1:I:45:ARG:CZ	1:I:47:MSE:HE1	2.21	0.70
1:G:45:ARG:NE	1:G:47:MSE:HE1	2.05	0.70
1:X:45:ARG:CZ	1:X:47:MSE:HE1	2.21	0.70
1:C:45:ARG:CZ	1:C:47:MSE:HE1	2.22	0.70
1:A:30:GLU:HG3	1:A:41:ARG:HG3	1.74	0.70
1:V:30:GLU:HG3	1:V:41:ARG:HG3	1.74	0.70
1:L:45:ARG:NE	1:L:47:MSE:HE1	2.07	0.70
1:Y:47:MSE:SE	2:Y:142:HOH:O	2.60	0.70
1:W:45:ARG:CZ	1:W:47:MSE:HE1	2.22	0.70
1:E:45:ARG:CZ	1:E:47:MSE:HE1	2.21	0.70
1:K:45:ARG:CZ	1:K:47:MSE:HE1	2.22	0.69
1:K:47:MSE:HE3	1:K:53:PHE:HE2	1.53	0.69
1:N:30:GLU:HG3	1:N:41:ARG:HG3	1.74	0.69
1:T:45:ARG:CZ	1:T:47:MSE:HE1	2.21	0.69
1:J:30:GLU:HG3	1:J:41:ARG:HG3	1.74	0.69
1:V:45:ARG:NE	1:V:47:MSE:HE1	2.07	0.69
1:Q:45:ARG:CZ	1:Q:47:MSE:HE1	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:ARG:HD2	2:D:116:HOH:O	1.92	0.69
1:G:37:ASN:OD1	2:G:112:HOH:O	2.10	0.69
1:G:47:MSE:HE3	1:G:53:PHE:HE2	1.55	0.69
1:O:45:ARG:CZ	1:O:47:MSE:HE1	2.22	0.69
1:J:28:HIS:HB2	2:J:128:HOH:O	1.93	0.69
1:J:45:ARG:NE	1:J:47:MSE:HE1	2.08	0.69
1:F:45:ARG:NE	1:F:47:MSE:HE1	2.08	0.69
1:W:45:ARG:NE	1:W:47:MSE:HE1	2.07	0.69
1:Y:45:ARG:CZ	1:Y:47:MSE:HE1	2.23	0.69
1:D:30:GLU:HG3	1:D:41:ARG:HG3	1.75	0.68
1:G:70:ARG:NE	2:G:106:HOH:O	2.25	0.68
1:P:45:ARG:CZ	1:P:47:MSE:HE1	2.22	0.68
1:Q:47:MSE:HE3	1:Q:53:PHE:HE2	1.59	0.68
1:F:47:MSE:HE3	1:F:53:PHE:HE2	1.58	0.68
1:Y:30:GLU:HG3	1:Y:41:ARG:HG3	1.74	0.68
1:B:45:ARG:NE	1:B:47:MSE:HE1	2.08	0.68
1:P:13:ARG:NH1	2:P:136:HOH:O	2.20	0.68
1:J:45:ARG:CZ	1:J:47:MSE:HE1	2.24	0.68
1:X:47:MSE:HE3	1:X:53:PHE:HE2	1.58	0.68
1:E:30:GLU:HG3	1:E:41:ARG:HG3	1.76	0.68
1:O:45:ARG:NE	1:O:47:MSE:HE1	2.09	0.68
1:Q:30:GLU:HG3	1:Q:41:ARG:HG3	1.76	0.68
1:R:45:ARG:CZ	1:R:47:MSE:HE1	2.24	0.68
1:A:45:ARG:CZ	1:A:47:MSE:HE1	2.24	0.67
1:H:45:ARG:CZ	1:H:47:MSE:HE1	2.24	0.67
1:P:45:ARG:NE	1:P:47:MSE:HE1	2.09	0.67
1:I:30:GLU:HG3	1:I:41:ARG:HG3	1.76	0.67
1:L:12:GLY:CA	2:L:122:HOH:O	2.43	0.67
1:O:47:MSE:HE3	1:O:53:PHE:HE2	1.59	0.67
1:T:36:MSE:CE	2:T:119:HOH:O	2.43	0.67
1:H:45:ARG:NE	1:H:47:MSE:HE1	2.10	0.67
1:G:70:ARG:CZ	2:G:106:HOH:O	2.43	0.67
1:G:30:GLU:HG3	1:G:41:ARG:HG3	1.75	0.67
1:X:45:ARG:NE	1:X:47:MSE:HE1	2.10	0.67
1:Y:41:ARG:CZ	2:Y:151:HOH:O	2.41	0.67
1:V:12:GLY:N	1:V:71:ILE:CG2	2.58	0.67
1:F:30:GLU:HG3	1:F:41:ARG:HG3	1.77	0.67
1:O:30:GLU:HG3	1:O:41:ARG:HG3	1.77	0.67
1:M:68:TYR:CZ	2:M:115:HOH:O	2.48	0.66
1:X:28:HIS:HE1	2:X:137:HOH:O	1.79	0.66
1:M:30:GLU:HG3	1:M:41:ARG:HG3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:47:MSE:HE3	1:M:53:PHE:HE2	1.56	0.66
1:Q:47:MSE:SE	2:Q:152:HOH:O	2.63	0.66
1:A:45:ARG:NE	1:A:47:MSE:HE1	2.10	0.66
1:C:47:MSE:HE3	1:C:53:PHE:HE2	1.55	0.66
1:K:45:ARG:NE	1:K:47:MSE:HE1	2.10	0.66
1:K:30:GLU:HG3	1:K:41:ARG:HG3	1.76	0.66
1:V:71:ILE:O	2:V:101:HOH:O	2.12	0.66
1:X:30:GLU:HG3	1:X:41:ARG:HG3	1.77	0.66
1:B:47:MSE:HE3	1:B:53:PHE:HE2	1.54	0.66
1:R:41:ARG:NH2	2:R:120:HOH:O	2.28	0.66
1:J:12:GLY:HA3	1:J:71:ILE:HD13	1.77	0.66
1:W:47:MSE:HE3	1:W:53:PHE:HE2	1.55	0.66
1:P:13:ARG:NH2	2:P:136:HOH:O	2.28	0.65
1:H:57:PRO:HG2	1:I:55:ARG:HB2	1.78	0.65
1:L:47:MSE:HE3	1:L:53:PHE:HE2	1.61	0.65
1:P:30:GLU:HG3	1:P:41:ARG:HG3	1.79	0.65
1:T:30:GLU:HG3	1:T:41:ARG:HG3	1.78	0.65
1:U:30:GLU:HG3	1:U:41:ARG:HG3	1.76	0.65
1:H:30:GLU:HG3	1:H:41:ARG:HG3	1.78	0.65
1:V:34:ASN:CG	2:V:115:HOH:O	2.38	0.65
1:G:70:ARG:NH2	2:G:106:HOH:O	2.29	0.65
1:R:45:ARG:NE	1:R:47:MSE:HE1	2.11	0.65
1:W:30:GLU:HG3	1:W:41:ARG:HG3	1.77	0.65
1:W:30:GLU:HG3	1:W:41:ARG:HD2	1.79	0.65
1:L:30:GLU:HG3	1:L:41:ARG:HG3	1.77	0.65
1:U:55:ARG:NH1	2:U:121:HOH:O	2.29	0.65
1:D:47:MSE:HE3	1:D:53:PHE:HE2	1.60	0.64
1:I:47:MSE:HE3	1:I:53:PHE:HE2	1.60	0.64
1:N:70:ARG:NH1	2:N:119:HOH:O	2.28	0.64
1:A:55:ARG:CD	2:C:143:HOH:O	2.44	0.64
1:U:45:ARG:CZ	1:U:47:MSE:HE1	2.28	0.64
1:V:32:CYS:N	2:V:116:HOH:O	2.30	0.64
1:L:13:ARG:NE	2:L:124:HOH:O	2.30	0.64
1:L:16:LEU:HD23	1:L:16:LEU:C	2.23	0.64
1:Q:12:GLY:HA3	1:Q:71:ILE:HD13	1.78	0.64
1:U:45:ARG:NE	1:U:47:MSE:HE1	2.12	0.64
1:R:30:GLU:HG3	1:R:41:ARG:HD2	1.80	0.64
1:A:47:MSE:HE3	1:A:53:PHE:HE2	1.56	0.64
1:P:47:MSE:HE3	1:P:53:PHE:HE2	1.63	0.64
1:W:13:ARG:NH2	2:W:141:HOH:O	2.13	0.63
1:F:16:LEU:C	1:F:16:LEU:HD23	2.22	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:47:MSE:CE	1:K:53:PHE:CE2	2.82	0.63
1:X:13:ARG:NH1	2:X:109:HOH:O	2.11	0.63
1:V:30:GLU:HG3	1:V:41:ARG:HD2	1.80	0.63
1:X:28:HIS:HB3	2:X:131:HOH:O	1.97	0.63
1:B:30:GLU:HG3	1:B:41:ARG:HG3	1.78	0.63
1:B:30:GLU:HG3	1:B:41:ARG:HD2	1.81	0.63
1:W:16:LEU:C	1:W:16:LEU:HD23	2.23	0.63
1:X:30:GLU:HG3	1:X:41:ARG:HD2	1.81	0.63
1:H:13:ARG:NH1	2:H:145:HOH:O	2.31	0.63
1:M:12:GLY:HA3	1:M:71:ILE:HD13	1.78	0.63
1:A:47:MSE:CE	1:A:53:PHE:CE2	2.82	0.62
1:M:16:LEU:C	1:M:16:LEU:HD23	2.24	0.62
1:R:16:LEU:C	1:R:16:LEU:HD23	2.24	0.62
1:J:47:MSE:HE3	1:J:53:PHE:HE2	1.60	0.62
1:P:16:LEU:C	1:P:16:LEU:HD23	2.24	0.62
1:A:30:GLU:HG3	1:A:41:ARG:HD2	1.80	0.62
1:R:30:GLU:HG3	1:R:41:ARG:HG3	1.80	0.62
1:J:30:GLU:HG3	1:J:41:ARG:HD2	1.82	0.62
1:G:30:GLU:HG3	1:G:41:ARG:HD2	1.80	0.62
1:Q:16:LEU:HD23	1:Q:16:LEU:C	2.25	0.61
1:D:71:ILE:O	2:D:121:HOH:O	2.16	0.61
1:C:13:ARG:NH2	2:C:121:HOH:O	2.31	0.61
1:D:30:GLU:HG3	1:D:41:ARG:HD2	1.82	0.61
1:T:16:LEU:C	1:T:16:LEU:HD23	2.25	0.61
1:U:12:GLY:HA3	1:U:71:ILE:HD13	1.83	0.61
1:M:30:GLU:HG3	1:M:41:ARG:HD2	1.82	0.61
1:R:47:MSE:CE	1:R:53:PHE:CE2	2.83	0.61
1:X:16:LEU:HD23	1:X:16:LEU:C	2.25	0.61
1:E:16:LEU:HD23	1:E:16:LEU:C	2.25	0.61
1:C:31:ASN:ND2	2:C:145:HOH:O	2.32	0.60
1:M:45:ARG:CZ	2:M:138:HOH:O	2.48	0.60
1:N:15:ILE:HD11	1:N:40:LEU:HD21	1.84	0.60
1:O:30:GLU:HG3	1:O:41:ARG:HD2	1.83	0.60
1:Y:30:GLU:HG3	1:Y:41:ARG:HD2	1.83	0.60
1:C:30:GLU:HG3	1:C:41:ARG:HD2	1.83	0.60
1:D:16:LEU:C	1:D:16:LEU:HD23	2.26	0.60
1:K:30:GLU:HG3	1:K:41:ARG:HD2	1.83	0.60
1:O:12:GLY:HA3	1:O:71:ILE:HD13	1.83	0.60
1:H:30:GLU:OE2	2:H:120:HOH:O	2.17	0.60
1:R:41:ARG:CZ	2:R:121:HOH:O	2.50	0.60
1:D:12:GLY:N	1:D:71:ILE:CD1	2.62	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:16:LEU:C	1:O:16:LEU:HD23	2.26	0.60
1:Q:28:HIS:HB3	2:Q:147:HOH:O	2.01	0.60
1:F:30:GLU:HG3	1:F:41:ARG:HD2	1.84	0.60
1:K:15:ILE:HD11	1:K:40:LEU:HD21	1.84	0.60
1:U:30:GLU:HG3	1:U:41:ARG:HD2	1.83	0.60
1:Y:15:ILE:HD11	1:Y:40:LEU:HD21	1.84	0.60
1:I:30:GLU:HG3	1:I:41:ARG:HD2	1.84	0.59
1:A:16:LEU:C	1:A:16:LEU:HD23	2.27	0.59
1:B:16:LEU:HD23	1:B:16:LEU:C	2.27	0.59
1:E:30:GLU:HG3	1:E:41:ARG:HD2	1.84	0.59
1:Y:16:LEU:C	1:Y:16:LEU:HD23	2.28	0.59
1:E:36:MSE:CE	2:E:124:HOH:O	2.51	0.59
1:P:51:ASP:OD2	2:P:133:HOH:O	2.17	0.59
1:K:58:GLU:CB	2:K:129:HOH:O	2.44	0.59
1:X:15:ILE:HD11	1:X:40:LEU:HD21	1.84	0.59
1:U:16:LEU:C	1:U:16:LEU:HD23	2.26	0.59
1:H:16:LEU:C	1:H:16:LEU:HD23	2.27	0.59
1:V:16:LEU:HD23	1:V:16:LEU:C	2.28	0.59
1:C:16:LEU:C	1:C:16:LEU:HD23	2.28	0.59
1:T:30:GLU:HG3	1:T:41:ARG:HD2	1.85	0.58
1:N:16:LEU:C	1:N:16:LEU:HD23	2.28	0.58
1:N:30:GLU:HG3	1:N:41:ARG:HD2	1.84	0.58
1:Y:13:ARG:NH2	2:Y:129:HOH:O	2.33	0.58
1:B:12:GLY:HA3	1:B:71:ILE:HD13	1.85	0.58
1:G:12:GLY:HA3	1:G:71:ILE:HD13	1.85	0.58
1:G:16:LEU:HD23	1:G:16:LEU:C	2.27	0.58
1:V:15:ILE:HD11	1:V:40:LEU:HD21	1.84	0.58
1:V:34:ASN:HB2	2:V:115:HOH:O	2.02	0.58
1:Q:30:GLU:HG3	1:Q:41:ARG:HD2	1.84	0.58
1:Y:12:GLY:CA	2:Y:127:HOH:O	2.50	0.58
1:Q:47:MSE:CE	1:Q:53:PHE:CE2	2.85	0.58
1:U:15:ILE:HD11	1:U:40:LEU:HD21	1.85	0.58
1:T:47:MSE:HE3	1:T:53:PHE:HE2	1.62	0.58
1:K:16:LEU:C	1:K:16:LEU:HD23	2.29	0.58
1:X:12:GLY:HA3	1:X:71:ILE:HD13	1.85	0.58
1:E:15:ILE:HD11	1:E:40:LEU:HD21	1.86	0.58
1:J:16:LEU:C	1:J:16:LEU:HD23	2.29	0.58
2:H:139:HOH:O	1:I:55:ARG:CD	2.52	0.57
1:Y:47:MSE:HE3	1:Y:53:PHE:HE2	1.67	0.57
1:F:15:ILE:HD11	1:F:40:LEU:HD21	1.85	0.57
1:Q:15:ILE:HD11	1:Q:40:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:GLY:CA	2:C:146:HOH:O	2.51	0.57
1:I:12:GLY:HA2	2:I:134:HOH:O	1.93	0.57
1:W:15:ILE:HD11	1:W:40:LEU:HD21	1.85	0.57
1:I:47:MSE:CE	1:I:53:PHE:CE2	2.87	0.57
1:G:47:MSE:CE	1:G:53:PHE:CE2	2.83	0.57
1:R:15:ILE:HD11	1:R:40:LEU:HD21	1.87	0.57
1:V:34:ASN:CB	2:V:115:HOH:O	2.51	0.57
1:W:13:ARG:NE	2:W:141:HOH:O	2.36	0.57
1:A:13:ARG:NH1	2:A:141:HOH:O	2.38	0.56
1:H:30:GLU:HG3	1:H:41:ARG:HD2	1.88	0.56
1:W:12:GLY:HA3	1:W:71:ILE:HD13	1.88	0.56
1:I:15:ILE:HD11	1:I:40:LEU:HD21	1.87	0.56
1:T:47:MSE:CE	1:T:53:PHE:CE2	2.87	0.56
1:H:15:ILE:HD11	1:H:40:LEU:HD21	1.87	0.55
1:D:47:MSE:CE	1:D:53:PHE:CE2	2.88	0.55
1:E:47:MSE:CE	1:E:53:PHE:CE2	2.85	0.55
1:I:16:LEU:C	1:I:16:LEU:HD23	2.32	0.55
1:K:58:GLU:CG	2:K:129:HOH:O	2.53	0.55
1:Q:28:HIS:HB2	2:Q:151:HOH:O	2.05	0.55
1:Y:12:GLY:N	2:Y:127:HOH:O	2.38	0.55
1:P:30:GLU:HG3	1:P:41:ARG:HD2	1.87	0.55
1:Q:31:ASN:CB	2:Q:130:HOH:O	2.55	0.55
1:C:15:ILE:HD11	1:C:40:LEU:HD21	1.88	0.55
1:L:15:ILE:HD11	1:L:40:LEU:HD21	1.89	0.55
1:M:15:ILE:HD11	1:M:40:LEU:HD21	1.87	0.55
1:R:41:ARG:NH1	2:R:121:HOH:O	2.39	0.55
1:A:15:ILE:HD11	1:A:40:LEU:HD21	1.87	0.55
1:L:30:GLU:HG3	1:L:41:ARG:HD2	1.88	0.55
1:N:47:MSE:CE	1:N:53:PHE:CE2	2.85	0.54
1:V:47:MSE:HE3	1:V:53:PHE:HE2	1.66	0.54
1:O:15:ILE:HD11	1:O:40:LEU:HD21	1.89	0.54
1:W:47:MSE:CE	1:W:53:PHE:CE2	2.89	0.54
1:B:52:LYS:NZ	2:B:114:HOH:O	2.18	0.54
1:J:70:ARG:NE	2:J:135:HOH:O	2.02	0.54
1:T:32:CYS:SG	2:T:119:HOH:O	2.44	0.54
1:W:31:ASN:HB2	2:W:129:HOH:O	2.07	0.54
1:W:35:TYR:CE2	2:W:144:HOH:O	2.53	0.54
1:Y:30:GLU:CG	1:Y:41:ARG:HG3	2.37	0.54
1:G:15:ILE:HD11	1:G:40:LEU:HD21	1.90	0.54
1:T:36:MSE:HE1	2:T:119:HOH:O	2.06	0.54
1:C:41:ARG:HD2	2:C:147:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:ILE:HD11	1:D:40:LEU:HD21	1.89	0.53
1:P:15:ILE:HD11	1:P:40:LEU:HD21	1.89	0.53
1:B:15:ILE:HD11	1:B:40:LEU:HD21	1.89	0.53
1:J:47:MSE:CE	1:J:53:PHE:CE2	2.89	0.53
1:G:55:ARG:CZ	2:G:144:HOH:O	2.56	0.53
1:Q:58:GLU:HB3	1:R:54:PHE:HB2	1.90	0.53
1:P:12:GLY:N	1:P:71:ILE:CD1	2.72	0.53
1:E:13:ARG:NH1	2:E:139:HOH:O	1.96	0.53
1:T:15:ILE:HD11	1:T:40:LEU:HD21	1.89	0.53
1:Y:41:ARG:NH2	2:Y:151:HOH:O	2.40	0.52
1:C:47:MSE:CE	1:C:53:PHE:CE2	2.88	0.52
1:P:41:ARG:NH2	2:P:129:HOH:O	2.35	0.52
1:Q:31:ASN:HB3	2:Q:130:HOH:O	2.10	0.52
1:Q:38:LEU:C	1:Q:38:LEU:HD12	2.35	0.52
1:Y:13:ARG:NH1	2:Y:152:HOH:O	2.27	0.52
1:Y:30:GLU:HG3	1:Y:41:ARG:CG	2.40	0.52
1:V:47:MSE:CE	1:V:53:PHE:CE2	2.90	0.52
1:G:30:GLU:HG3	1:G:41:ARG:CG	2.40	0.52
1:J:30:GLU:CG	1:J:41:ARG:HG3	2.40	0.52
1:G:55:ARG:NH2	2:G:144:HOH:O	2.42	0.51
1:B:47:MSE:CE	1:B:53:PHE:CE2	2.87	0.51
1:V:30:GLU:HG3	1:V:41:ARG:CG	2.39	0.51
1:Y:12:GLY:N	1:Y:71:ILE:HD13	2.24	0.51
1:Y:28:HIS:CD2	2:Y:110:HOH:O	2.56	0.51
1:H:47:MSE:CE	1:H:53:PHE:CE2	2.87	0.51
1:C:30:GLU:HG3	1:C:41:ARG:CG	2.40	0.51
2:H:139:HOH:O	1:I:55:ARG:HD2	2.09	0.51
1:E:12:GLY:HA3	1:E:71:ILE:HD13	1.93	0.51
1:E:36:MSE:HE1	2:E:124:HOH:O	2.10	0.50
1:Q:45:ARG:CD	1:Q:47:MSE:HE1	2.41	0.50
1:R:31:ASN:ND2	2:R:138:HOH:O	2.32	0.50
1:J:30:GLU:HG3	1:J:41:ARG:CG	2.40	0.50
1:D:30:GLU:CG	1:D:41:ARG:HG3	2.41	0.50
2:D:132:HOH:O	1:E:55:ARG:HD3	2.11	0.50
1:G:34:ASN:CB	2:G:159:HOH:O	2.58	0.50
1:V:30:GLU:CG	1:V:41:ARG:HG3	2.41	0.50
1:A:30:GLU:HG3	1:A:41:ARG:CG	2.41	0.50
1:X:30:GLU:HG3	1:X:41:ARG:CG	2.42	0.50
1:G:70:ARG:HD2	2:G:148:HOH:O	2.11	0.50
1:W:30:GLU:HG3	1:W:41:ARG:CG	2.42	0.50
1:U:47:MSE:CE	1:U:53:PHE:CE2	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:12:GLY:HA3	1:F:71:ILE:HD13	1.93	0.49
1:G:30:GLU:CG	1:G:41:ARG:HG3	2.41	0.49
1:I:45:ARG:CD	1:I:47:MSE:HE1	2.41	0.49
1:I:30:GLU:CG	1:I:41:ARG:HG3	2.41	0.49
1:U:45:ARG:CD	1:U:47:MSE:HE1	2.43	0.49
1:W:16:LEU:HD23	1:W:17:VAL:N	2.27	0.49
1:W:30:GLU:CG	1:W:41:ARG:HG3	2.42	0.49
1:X:34:ASN:CG	2:X:138:HOH:O	2.55	0.49
1:Y:55:ARG:NH1	2:Y:143:HOH:O	2.45	0.49
1:B:35:TYR:O	1:B:36:MSE:HB2	2.12	0.49
1:F:35:TYR:O	1:F:36:MSE:HB2	2.13	0.49
1:N:30:GLU:HG3	1:N:41:ARG:CG	2.41	0.49
1:V:30:GLU:HG3	1:V:41:ARG:CD	2.43	0.49
1:W:55:ARG:CD	2:Y:147:HOH:O	2.61	0.49
1:D:30:GLU:HG3	1:D:41:ARG:CG	2.41	0.49
1:K:30:GLU:HG3	1:K:41:ARG:CG	2.41	0.48
1:K:30:GLU:CG	1:K:41:ARG:HG3	2.42	0.48
1:O:30:GLU:HG3	1:O:41:ARG:CG	2.43	0.48
1:H:13:ARG:NH2	2:H:140:HOH:O	2.46	0.48
1:J:15:ILE:HD11	1:J:40:LEU:HD21	1.94	0.48
1:L:16:LEU:HD23	1:L:17:VAL:N	2.28	0.48
1:T:38:LEU:HD12	1:T:38:LEU:C	2.39	0.48
1:F:30:GLU:HG3	1:F:41:ARG:CG	2.43	0.48
1:P:30:GLU:CG	1:P:41:ARG:HG3	2.43	0.48
1:P:47:MSE:CE	1:P:53:PHE:CE2	2.91	0.48
1:N:30:GLU:CG	1:N:41:ARG:HG3	2.41	0.48
1:X:31:ASN:ND2	2:X:126:HOH:O	2.31	0.48
1:E:45:ARG:CD	1:E:47:MSE:HE1	2.43	0.48
1:M:30:GLU:CG	1:M:41:ARG:HG3	2.42	0.48
1:N:38:LEU:C	1:N:38:LEU:HD12	2.38	0.48
1:U:57:PRO:HG2	1:V:55:ARG:HB2	1.94	0.48
1:G:34:ASN:HB3	2:G:159:HOH:O	2.13	0.48
1:H:30:GLU:CG	1:H:41:ARG:HG3	2.42	0.48
1:W:38:LEU:HD12	1:W:38:LEU:C	2.39	0.48
1:C:41:ARG:NH2	2:C:129:HOH:O	2.29	0.47
1:G:30:GLU:HG3	1:G:41:ARG:CD	2.44	0.47
1:P:13:ARG:CZ	2:P:136:HOH:O	2.54	0.47
1:R:30:GLU:CG	1:R:41:ARG:HG3	2.44	0.47
1:U:30:GLU:HG3	1:U:41:ARG:CG	2.42	0.47
1:I:30:GLU:HG3	1:I:41:ARG:CG	2.42	0.47
1:I:31:ASN:HB3	2:I:157:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:38:LEU:HD12	1:M:38:LEU:C	2.40	0.47
1:O:35:TYR:O	1:O:36:MSE:HB2	2.14	0.47
1:Y:47:MSE:CE	1:Y:53:PHE:CE2	2.93	0.47
1:B:68:TYR:CE1	1:B:70:ARG:HD2	2.50	0.47
1:I:38:LEU:C	1:I:38:LEU:HD12	2.40	0.47
1:M:30:GLU:HG3	1:M:41:ARG:CG	2.42	0.47
1:A:30:GLU:HG3	1:A:41:ARG:CD	2.44	0.47
1:A:30:GLU:CG	1:A:41:ARG:HG3	2.44	0.47
1:Q:30:GLU:CG	1:Q:41:ARG:HG3	2.43	0.47
1:K:45:ARG:CD	1:K:47:MSE:HE1	2.45	0.47
1:O:30:GLU:CG	1:O:41:ARG:HG3	2.43	0.47
1:W:16:LEU:C	1:W:16:LEU:CD2	2.87	0.47
1:Q:30:GLU:HG3	1:Q:41:ARG:CG	2.42	0.47
1:H:30:GLU:HG3	1:H:41:ARG:CG	2.44	0.47
1:L:16:LEU:C	1:L:16:LEU:CD2	2.88	0.47
1:W:30:GLU:HG3	1:W:41:ARG:CD	2.44	0.46
1:X:35:TYR:O	1:X:36:MSE:HB2	2.14	0.46
1:G:45:ARG:CD	1:G:47:MSE:HE1	2.44	0.46
1:W:35:TYR:HE2	2:W:144:HOH:O	1.94	0.46
1:A:38:LEU:HD12	1:A:38:LEU:C	2.40	0.46
1:H:12:GLY:HA3	1:H:71:ILE:HD13	1.96	0.46
1:J:30:GLU:HG3	1:J:41:ARG:CD	2.45	0.46
1:J:45:ARG:CD	1:J:47:MSE:HE1	2.45	0.46
1:L:47:MSE:CE	1:L:53:PHE:CE2	2.94	0.46
1:U:38:LEU:C	1:U:38:LEU:HD12	2.41	0.46
1:Y:12:GLY:HA2	2:Y:127:HOH:O	2.11	0.46
1:D:45:ARG:CD	1:D:47:MSE:HE1	2.45	0.46
1:E:30:GLU:HG3	1:E:41:ARG:CG	2.43	0.46
1:F:16:LEU:C	1:F:16:LEU:CD2	2.88	0.46
1:F:30:GLU:CG	1:F:41:ARG:HG3	2.44	0.46
1:W:55:ARG:HD2	2:Y:147:HOH:O	2.15	0.46
1:X:47:MSE:CE	1:X:53:PHE:CE2	2.89	0.46
1:B:30:GLU:HG3	1:B:41:ARG:CG	2.44	0.46
1:D:55:ARG:HD3	2:F:125:HOH:O	2.14	0.46
1:K:35:TYR:O	1:K:36:MSE:HB2	2.15	0.46
1:T:45:ARG:CD	1:T:47:MSE:HE1	2.45	0.46
1:C:30:GLU:HG3	1:C:41:ARG:CD	2.46	0.46
1:E:30:GLU:CG	1:E:41:ARG:HG3	2.45	0.46
1:R:30:GLU:HG3	1:R:41:ARG:CG	2.45	0.46
1:G:35:TYR:O	1:G:36:MSE:HB2	2.16	0.46
1:K:38:LEU:C	1:K:38:LEU:HD12	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:30:GLU:CG	1:U:41:ARG:HG3	2.43	0.46
1:F:47:MSE:CE	1:F:53:PHE:CE2	2.91	0.46
1:M:30:GLU:HG3	1:M:41:ARG:CD	2.46	0.46
1:L:38:LEU:C	1:L:38:LEU:HD12	2.41	0.45
1:T:30:GLU:HG3	1:T:41:ARG:CG	2.44	0.45
1:W:68:TYR:HE1	1:W:70:ARG:HD2	1.81	0.45
1:Q:12:GLY:HA2	2:Q:144:HOH:O	2.02	0.45
1:R:38:LEU:HD12	1:R:38:LEU:C	2.41	0.45
1:F:38:LEU:HD12	1:F:38:LEU:C	2.42	0.45
1:G:38:LEU:C	1:G:38:LEU:HD12	2.42	0.45
1:J:71:ILE:HD12	1:J:71:ILE:C	2.41	0.45
1:N:35:TYR:O	1:N:36:MSE:HB2	2.17	0.45
1:Q:16:LEU:HD23	1:Q:17:VAL:N	2.30	0.45
1:R:16:LEU:C	1:R:16:LEU:CD2	2.89	0.45
1:W:68:TYR:CE1	1:W:70:ARG:HD2	2.52	0.45
1:X:45:ARG:CD	1:X:47:MSE:HE1	2.45	0.45
1:X:68:TYR:CE1	1:X:70:ARG:HD2	2.52	0.45
1:R:30:GLU:HG3	1:R:41:ARG:CD	2.46	0.45
1:D:30:GLU:HG3	1:D:41:ARG:CD	2.46	0.45
1:E:35:TYR:O	1:E:36:MSE:HB2	2.17	0.45
1:E:67:LYS:NZ	2:E:114:HOH:O	2.44	0.45
1:J:38:LEU:HD12	1:J:38:LEU:C	2.42	0.45
1:L:30:GLU:HG3	1:L:41:ARG:CG	2.45	0.45
1:X:38:LEU:C	1:X:38:LEU:HD12	2.41	0.45
1:B:71:ILE:C	1:B:71:ILE:HD12	2.41	0.45
1:F:71:ILE:C	1:F:71:ILE:HD12	2.42	0.45
1:M:47:MSE:CE	1:M:53:PHE:CE2	2.90	0.45
1:P:30:GLU:HG3	1:P:41:ARG:CG	2.45	0.45
1:T:16:LEU:C	1:T:16:LEU:CD2	2.90	0.45
1:K:47:MSE:CE	1:K:53:PHE:CD2	3.00	0.45
1:M:18:GLU:CD	2:M:136:HOH:O	2.60	0.45
1:M:35:TYR:O	1:M:36:MSE:HB2	2.17	0.45
1:N:57:PRO:HG2	1:O:55:ARG:HB2	1.98	0.45
1:P:71:ILE:C	1:P:71:ILE:HD12	2.42	0.45
1:W:35:TYR:CZ	2:W:144:HOH:O	2.65	0.45
1:Y:30:GLU:HG3	1:Y:41:ARG:CD	2.46	0.45
1:B:45:ARG:CD	1:B:47:MSE:HE1	2.47	0.45
1:C:30:GLU:CG	1:C:41:ARG:HG3	2.44	0.45
1:E:68:TYR:OH	2:E:135:HOH:O	2.20	0.45
1:G:12:GLY:CA	1:G:71:ILE:HD13	2.47	0.45
1:M:45:ARG:CD	1:M:47:MSE:HE1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:30:GLU:CG	1:V:41:ARG:HD2	2.47	0.45
1:B:30:GLU:HG3	1:B:41:ARG:CD	2.46	0.44
1:D:68:TYR:CE1	1:D:70:ARG:HD2	2.52	0.44
1:D:71:ILE:C	1:D:71:ILE:HD12	2.42	0.44
1:N:12:GLY:N	1:N:71:ILE:HD13	2.31	0.44
1:Q:16:LEU:C	1:Q:16:LEU:CD2	2.90	0.44
1:G:68:TYR:CE1	1:G:70:ARG:HD2	2.52	0.44
1:U:68:TYR:CE1	1:U:70:ARG:HD2	2.51	0.44
1:O:16:LEU:C	1:O:16:LEU:CD2	2.91	0.44
1:P:16:LEU:C	1:P:16:LEU:CD2	2.90	0.44
1:D:38:LEU:C	1:D:38:LEU:HD12	2.42	0.44
1:K:13:ARG:NH2	2:K:119:HOH:O	2.49	0.44
1:O:68:TYR:CE1	1:O:70:ARG:HD2	2.52	0.44
1:Q:31:ASN:HB2	2:Q:130:HOH:O	2.15	0.44
1:T:13:ARG:NE	2:T:114:HOH:O	2.33	0.44
1:T:30:GLU:CG	1:T:41:ARG:HG3	2.44	0.44
1:U:30:GLU:HG3	1:U:41:ARG:CD	2.47	0.44
1:C:38:LEU:HD12	1:C:38:LEU:C	2.43	0.44
1:K:30:GLU:HG3	1:K:41:ARG:CD	2.47	0.44
1:O:47:MSE:CE	1:O:53:PHE:CE2	2.93	0.44
1:P:38:LEU:C	1:P:38:LEU:HD12	2.42	0.44
1:C:12:GLY:CA	1:C:71:ILE:HD13	2.38	0.44
1:L:12:GLY:HA3	1:L:71:ILE:HD13	1.99	0.44
1:X:16:LEU:C	1:X:16:LEU:CD2	2.90	0.44
1:X:30:GLU:HG3	1:X:41:ARG:CD	2.45	0.44
1:L:69:LEU:C	1:L:69:LEU:HD23	2.43	0.44
1:U:35:TYR:O	1:U:36:MSE:HB2	2.18	0.44
1:U:47:MSE:HE3	1:U:53:PHE:CD2	2.52	0.44
1:C:45:ARG:CD	1:C:47:MSE:HE1	2.48	0.44
1:M:68:TYR:CE1	1:M:70:ARG:HD2	2.52	0.44
1:N:30:GLU:HG3	1:N:41:ARG:CD	2.48	0.44
1:T:31:ASN:HB2	2:T:112:HOH:O	2.18	0.44
1:T:33:ASP:OD1	1:T:33:ASP:C	2.60	0.44
1:T:35:TYR:O	1:T:36:MSE:HB2	2.18	0.44
1:Y:38:LEU:HD12	1:Y:38:LEU:C	2.43	0.44
1:G:16:LEU:HD23	1:G:17:VAL:N	2.34	0.43
1:H:16:LEU:HD23	1:H:17:VAL:N	2.33	0.43
1:P:41:ARG:HD3	2:P:126:HOH:O	2.18	0.43
1:R:30:GLU:CG	1:R:41:ARG:HD2	2.47	0.43
1:U:71:ILE:C	1:U:71:ILE:HD12	2.43	0.43
1:A:16:LEU:HD23	1:A:17:VAL:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:LEU:C	1:B:38:LEU:HD12	2.43	0.43
1:E:16:LEU:C	1:E:16:LEU:CD2	2.91	0.43
1:E:68:TYR:CE1	1:E:70:ARG:HD2	2.53	0.43
1:I:30:GLU:HG3	1:I:41:ARG:CD	2.48	0.43
1:J:13:ARG:N	1:J:14:PRO:HD2	2.33	0.43
1:N:45:ARG:CD	1:N:47:MSE:HE1	2.47	0.43
1:R:47:MSE:CE	1:R:53:PHE:CD2	3.02	0.43
1:U:33:ASP:HB3	2:U:120:HOH:O	2.17	0.43
1:W:30:GLU:CG	1:W:41:ARG:HD2	2.47	0.43
1:X:30:GLU:CG	1:X:41:ARG:HG3	2.45	0.43
1:F:16:LEU:HD23	1:F:17:VAL:N	2.33	0.43
1:F:68:TYR:CE1	1:F:70:ARG:HD2	2.53	0.43
1:Y:68:TYR:CE1	1:Y:70:ARG:HD2	2.54	0.43
1:B:16:LEU:C	1:B:16:LEU:CD2	2.92	0.43
1:G:16:LEU:C	1:G:16:LEU:CD2	2.91	0.43
1:E:30:GLU:HG3	1:E:41:ARG:CD	2.48	0.43
1:T:13:ARG:H	1:T:14:PRO:HD2	1.84	0.43
1:X:19:LEU:HB3	2:X:105:HOH:O	2.18	0.43
1:Y:16:LEU:HD23	1:Y:17:VAL:N	2.33	0.43
1:H:16:LEU:C	1:H:16:LEU:CD2	2.92	0.43
1:I:71:ILE:C	1:I:71:ILE:HD12	2.43	0.43
1:L:35:TYR:O	1:L:36:MSE:HB2	2.19	0.43
1:N:68:TYR:CE1	1:N:70:ARG:HD2	2.53	0.43
1:X:16:LEU:HD23	1:X:17:VAL:N	2.33	0.43
1:A:30:GLU:CG	1:A:41:ARG:HD2	2.48	0.43
1:L:71:ILE:HD12	2:L:117:HOH:O	2.19	0.43
1:V:38:LEU:C	1:V:38:LEU:HD12	2.44	0.43
1:M:16:LEU:C	1:M:16:LEU:CD2	2.91	0.43
1:N:12:GLY:HA3	1:N:71:ILE:HD13	2.01	0.43
1:O:38:LEU:HD12	1:O:38:LEU:C	2.44	0.43
1:W:71:ILE:C	1:W:71:ILE:HD12	2.44	0.43
1:Y:30:GLU:CG	1:Y:41:ARG:HD2	2.47	0.43
1:A:16:LEU:C	1:A:16:LEU:CD2	2.92	0.43
1:A:47:MSE:CE	1:A:53:PHE:CD2	3.02	0.43
1:B:30:GLU:CG	1:B:41:ARG:HG3	2.47	0.43
1:B:68:TYR:HE1	1:B:70:ARG:HD2	1.83	0.43
1:E:38:LEU:HD12	1:E:38:LEU:C	2.43	0.43
1:N:33:ASP:C	1:N:33:ASP:OD1	2.60	0.43
1:T:68:TYR:CE1	1:T:70:ARG:HD2	2.54	0.43
1:U:16:LEU:HD23	1:U:17:VAL:N	2.33	0.43
1:A:55:ARG:HB2	1:C:57:PRO:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:30:GLU:HG3	1:O:41:ARG:CD	2.47	0.42
1:W:45:ARG:CD	1:W:47:MSE:HE1	2.49	0.42
1:H:71:ILE:HD12	1:H:71:ILE:C	2.44	0.42
2:H:139:HOH:O	1:I:55:ARG:HD3	2.14	0.42
1:L:71:ILE:HD12	1:L:71:ILE:C	2.44	0.42
1:O:45:ARG:CD	1:O:47:MSE:HE1	2.50	0.42
1:R:31:ASN:CB	2:R:138:HOH:O	2.46	0.42
1:X:13:ARG:CD	2:X:109:HOH:O	2.56	0.42
1:B:16:LEU:HD23	1:B:17:VAL:N	2.34	0.42
1:B:62:ARG:NE	2:B:140:HOH:O	1.85	0.42
1:D:56:LEU:HD12	1:D:56:LEU:N	2.34	0.42
1:G:47:MSE:CE	1:G:53:PHE:CD2	3.02	0.42
1:U:16:LEU:C	1:U:16:LEU:CD2	2.91	0.42
1:X:33:ASP:OD1	1:X:33:ASP:C	2.63	0.42
1:B:30:GLU:CG	1:B:41:ARG:HD2	2.49	0.42
1:C:16:LEU:HD23	1:C:17:VAL:N	2.35	0.42
1:K:68:TYR:CE1	1:K:70:ARG:HD2	2.54	0.42
1:N:68:TYR:CE1	2:N:119:HOH:O	2.71	0.42
1:O:71:ILE:HD12	1:O:71:ILE:C	2.45	0.42
1:C:71:ILE:HD12	1:C:71:ILE:C	2.44	0.42
1:F:30:GLU:HG3	1:F:41:ARG:CD	2.48	0.42
1:O:30:GLU:CG	1:O:41:ARG:HD2	2.49	0.42
1:P:12:GLY:N	2:P:122:HOH:O	2.52	0.42
1:P:16:LEU:HD23	1:P:17:VAL:N	2.35	0.42
1:Q:68:TYR:CE1	1:Q:70:ARG:HD2	2.55	0.42
1:H:68:TYR:CE1	1:H:70:ARG:HD2	2.54	0.42
1:L:30:GLU:CG	1:L:41:ARG:HG3	2.44	0.42
1:L:68:TYR:CE1	1:L:70:ARG:HD2	2.54	0.42
1:A:68:TYR:CE1	1:A:70:ARG:HD2	2.53	0.42
1:H:45:ARG:CD	1:H:47:MSE:HE1	2.50	0.42
1:J:16:LEU:HD23	1:J:17:VAL:N	2.35	0.42
1:V:16:LEU:C	1:V:16:LEU:CD2	2.92	0.42
1:Y:16:LEU:C	1:Y:16:LEU:CD2	2.93	0.42
1:C:16:LEU:C	1:C:16:LEU:CD2	2.92	0.42
1:G:71:ILE:HD12	2:G:142:HOH:O	2.18	0.42
1:N:16:LEU:C	1:N:16:LEU:CD2	2.92	0.42
1:R:45:ARG:CD	1:R:47:MSE:HE1	2.50	0.42
1:X:28:HIS:CB	2:X:130:HOH:O	2.68	0.42
1:U:47:MSE:CE	1:U:53:PHE:CD2	3.03	0.42
1:V:35:TYR:O	1:V:36:MSE:HB2	2.20	0.42
1:X:47:MSE:HE3	1:X:53:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:68:TYR:HE1	1:X:70:ARG:HD2	1.85	0.42
1:H:35:TYR:O	1:H:36:MSE:HB2	2.20	0.41
1:Y:45:ARG:CD	1:Y:47:MSE:HE1	2.50	0.41
1:G:69:LEU:C	1:G:69:LEU:HD23	2.45	0.41
1:A:13:ARG:NH1	2:A:113:HOH:O	2.52	0.41
1:K:71:ILE:C	1:K:71:ILE:HD12	2.44	0.41
1:R:33:ASP:OD1	1:R:33:ASP:C	2.63	0.41
1:N:71:ILE:C	1:N:71:ILE:HD12	2.45	0.41
1:X:30:GLU:CG	1:X:41:ARG:HD2	2.49	0.41
1:X:71:ILE:C	1:X:71:ILE:HD12	2.45	0.41
1:C:68:TYR:CE1	1:C:70:ARG:HD2	2.55	0.41
1:D:30:GLU:CG	1:D:41:ARG:HD2	2.49	0.41
1:J:12:GLY:CA	1:J:71:ILE:HD13	2.47	0.41
1:U:31:ASN:ND2	2:U:118:HOH:O	2.52	0.41
1:V:68:TYR:CE1	1:V:70:ARG:HD2	2.55	0.41
1:R:68:TYR:CE1	1:R:70:ARG:HD2	2.55	0.41
1:X:47:MSE:CE	1:X:53:PHE:CD2	3.04	0.41
1:A:45:ARG:CD	1:A:47:MSE:HE1	2.50	0.41
1:E:16:LEU:HD23	1:E:17:VAL:N	2.36	0.41
1:I:68:TYR:CE1	1:I:70:ARG:HD2	2.56	0.41
1:M:69:LEU:C	1:M:69:LEU:HD23	2.46	0.41
1:O:16:LEU:HD23	1:O:17:VAL:N	2.36	0.41
1:Q:30:GLU:HG3	1:Q:41:ARG:CD	2.48	0.41
1:W:35:TYR:O	1:W:36:MSE:HB2	2.20	0.41
1:G:71:ILE:CD1	2:G:142:HOH:O	2.69	0.41
1:N:68:TYR:CZ	2:N:119:HOH:O	2.56	0.41
1:A:47:MSE:HE2	1:A:53:PHE:CD2	2.56	0.41
1:B:12:GLY:CA	2:B:144:HOH:O	2.69	0.41
1:D:16:LEU:C	1:D:16:LEU:CD2	2.93	0.41
2:D:132:HOH:O	1:E:55:ARG:CD	2.67	0.41
1:H:38:LEU:HD12	1:H:38:LEU:C	2.46	0.41
1:K:16:LEU:C	1:K:16:LEU:CD2	2.93	0.41
1:T:51:ASP:CG	1:V:65:ASN:HD22	2.28	0.41
1:Y:71:ILE:HD12	1:Y:71:ILE:C	2.46	0.41
1:U:30:GLU:CG	1:U:41:ARG:HD2	2.50	0.41
1:V:45:ARG:CD	1:V:47:MSE:HE1	2.51	0.41
1:D:68:TYR:HE1	1:D:70:ARG:HD2	1.87	0.40
1:G:71:ILE:HD12	1:G:71:ILE:C	2.46	0.40
1:J:30:GLU:CG	1:J:41:ARG:HD2	2.49	0.40
1:L:30:GLU:HG3	1:L:41:ARG:CD	2.52	0.40
1:P:68:TYR:CE1	1:P:70:ARG:HD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:30:GLU:HG3	1:T:41:ARG:CD	2.49	0.40
1:J:68:TYR:CE1	1:J:70:ARG:HD2	2.56	0.40
1:N:16:LEU:HD23	1:N:17:VAL:N	2.36	0.40
1:U:33:ASP:C	1:U:33:ASP:OD1	2.64	0.40
1:U:58:GLU:HB3	1:V:54:PHE:HB2	2.04	0.40
1:Y:68:TYR:HE1	1:Y:70:ARG:HD2	1.86	0.40
1:M:30:GLU:CG	1:M:41:ARG:HD2	2.49	0.40
1:X:28:HIS:HB3	2:X:130:HOH:O	2.20	0.40
1:A:71:ILE:HD12	1:A:71:ILE:C	2.46	0.40
1:O:68:TYR:HE1	1:O:70:ARG:HD2	1.85	0.40
1:T:71:ILE:HD12	1:T:71:ILE:C	2.46	0.40
1:C:35:TYR:O	1:C:36:MSE:HB2	2.21	0.40
1:F:68:TYR:HE1	1:F:70:ARG:HD2	1.86	0.40
1:N:20:LYS:CE	2:N:121:HOH:O	2.70	0.40
1:N:28:HIS:CB	2:N:120:HOH:O	2.46	0.40

All (6) 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:B:31:ASN:OD1	1:E:30:GLU:OE1[2_657]	1.95	0.25
1:M:67:LYS:NZ	1:Y:30:GLU:OE2[4_556]	2.11	0.09
1:N:67:LYS:NZ	2:H:120:HOH:O[4_556]	2.12	0.08
1:H:41:ARG:NH1	1:N:67:LYS:NZ[4_546]	2.16	0.04
1:K:31:ASN:OD1	1:T:30:GLU:OE1[3_454]	2.16	0.04
1:B:31:ASN:OD1	1:E:30:GLU:CD[2_657]	2.19	0.01

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	58/105 (55%)	57 (98%)	1 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	58/105 (55%)	56 (97%)	2 (3%)	0	100	100
1	C	58/105 (55%)	56 (97%)	2 (3%)	0	100	100
1	D	58/105 (55%)	58 (100%)	0	0	100	100
1	E	58/105 (55%)	56 (97%)	2 (3%)	0	100	100
1	F	58/105 (55%)	56 (97%)	2 (3%)	0	100	100
1	G	58/105 (55%)	56 (97%)	2 (3%)	0	100	100
1	H	58/105 (55%)	56 (97%)	2 (3%)	0	100	100
1	I	58/105 (55%)	57 (98%)	1 (2%)	0	100	100
1	J	58/105 (55%)	56 (97%)	2 (3%)	0	100	100
1	K	58/105 (55%)	56 (97%)	2 (3%)	0	100	100
1	L	58/105 (55%)	56 (97%)	2 (3%)	0	100	100
1	M	58/105 (55%)	58 (100%)	0	0	100	100
1	N	58/105 (55%)	57 (98%)	1 (2%)	0	100	100
1	O	58/105 (55%)	57 (98%)	1 (2%)	0	100	100
1	P	58/105 (55%)	57 (98%)	1 (2%)	0	100	100
1	Q	58/105 (55%)	56 (97%)	2 (3%)	0	100	100
1	R	58/105 (55%)	56 (97%)	2 (3%)	0	100	100
1	T	58/105 (55%)	56 (97%)	2 (3%)	0	100	100
1	U	58/105 (55%)	57 (98%)	1 (2%)	0	100	100
1	V	58/105 (55%)	57 (98%)	1 (2%)	0	100	100
1	W	58/105 (55%)	57 (98%)	1 (2%)	0	100	100
1	X	58/105 (55%)	56 (97%)	2 (3%)	0	100	100
1	Y	58/105 (55%)	57 (98%)	1 (2%)	0	100	100
All	All	1392/2520 (55%)	1357 (98%)	35 (2%)	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	55/91 (60%)	52 (94%)	3 (6%)	19	24
1	B	55/91 (60%)	52 (94%)	3 (6%)	19	24
1	C	55/91 (60%)	53 (96%)	2 (4%)	31	42
1	D	55/91 (60%)	53 (96%)	2 (4%)	31	42
1	E	55/91 (60%)	53 (96%)	2 (4%)	31	42
1	F	55/91 (60%)	52 (94%)	3 (6%)	19	24
1	G	55/91 (60%)	51 (93%)	4 (7%)	13	15
1	H	55/91 (60%)	53 (96%)	2 (4%)	31	42
1	I	55/91 (60%)	52 (94%)	3 (6%)	19	24
1	J	55/91 (60%)	52 (94%)	3 (6%)	19	24
1	K	55/91 (60%)	52 (94%)	3 (6%)	19	24
1	L	55/91 (60%)	51 (93%)	4 (7%)	13	15
1	M	55/91 (60%)	52 (94%)	3 (6%)	19	24
1	N	55/91 (60%)	53 (96%)	2 (4%)	31	42
1	O	55/91 (60%)	51 (93%)	4 (7%)	13	15
1	P	55/91 (60%)	53 (96%)	2 (4%)	31	42
1	Q	55/91 (60%)	51 (93%)	4 (7%)	13	15
1	R	55/91 (60%)	52 (94%)	3 (6%)	19	24
1	T	55/91 (60%)	52 (94%)	3 (6%)	19	24
1	U	55/91 (60%)	53 (96%)	2 (4%)	31	42
1	V	55/91 (60%)	53 (96%)	2 (4%)	31	42
1	W	55/91 (60%)	51 (93%)	4 (7%)	13	15
1	X	55/91 (60%)	53 (96%)	2 (4%)	31	42
1	Y	55/91 (60%)	51 (93%)	4 (7%)	13	15
All	All	1320/2184 (60%)	1251 (95%)	69 (5%)	21	26

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	28	HIS
1	A	71	ILE
1	B	28	HIS
1	B	43	VAL
1	B	71	ILE

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Mol	Chain	Res	Type
1	C	28	HIS
1	C	71	ILE
1	D	28	HIS
1	D	71	ILE
1	E	28	HIS
1	E	71	ILE
1	F	28	HIS
1	F	43	VAL
1	F	71	ILE
1	G	16	LEU
1	G	28	HIS
1	G	43	VAL
1	G	71	ILE
1	H	28	HIS
1	H	71	ILE
1	I	28	HIS
1	I	43	VAL
1	I	71	ILE
1	J	28	HIS
1	J	43	VAL
1	J	71	ILE
1	K	28	HIS
1	K	43	VAL
1	K	71	ILE
1	L	16	LEU
1	L	28	HIS
1	L	43	VAL
1	L	71	ILE
1	M	28	HIS
1	M	43	VAL
1	M	71	ILE
1	N	28	HIS
1	N	71	ILE
1	O	16	LEU
1	O	28	HIS
1	O	43	VAL
1	O	71	ILE
1	P	28	HIS
1	P	71	ILE
1	Q	16	LEU
1	Q	28	HIS
1	Q	43	VAL

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Mol	Chain	Res	Type
1	Q	71	ILE
1	R	16	LEU
1	R	28	HIS
1	R	71	ILE
1	T	28	HIS
1	T	43	VAL
1	T	71	ILE
1	U	28	HIS
1	U	71	ILE
1	V	16	LEU
1	V	28	HIS
1	W	16	LEU
1	W	28	HIS
1	W	43	VAL
1	W	71	ILE
1	X	28	HIS
1	X	71	ILE
1	Y	16	LEU
1	Y	28	HIS
1	Y	43	VAL
1	Y	71	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	64	ASN
1	B	34	ASN
1	B	64	ASN
1	C	34	ASN
1	C	64	ASN
1	D	34	ASN
1	D	64	ASN
1	E	34	ASN
1	E	64	ASN
1	F	34	ASN
1	F	64	ASN
1	F	65	ASN
1	G	34	ASN
1	G	64	ASN
1	H	64	ASN
1	I	64	ASN

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Mol	Chain	Res	Type
1	J	64	ASN
1	K	34	ASN
1	K	64	ASN
1	K	65	ASN
1	L	34	ASN
1	L	64	ASN
1	M	64	ASN
1	N	34	ASN
1	N	64	ASN
1	O	34	ASN
1	O	64	ASN
1	Q	34	ASN
1	Q	64	ASN
1	R	34	ASN
1	R	64	ASN
1	T	34	ASN
1	T	64	ASN
1	U	34	ASN
1	U	64	ASN
1	V	34	ASN
1	V	64	ASN
1	W	34	ASN
1	W	64	ASN
1	W	65	ASN
1	X	34	ASN
1	X	64	ASN
1	Y	34	ASN
1	Y	64	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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, 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	58/105 (55%)	0.65	11 (18%) 3 2	19, 26, 43, 49	0
1	B	58/105 (55%)	0.76	8 (13%) 6 5	19, 26, 44, 50	0
1	C	58/105 (55%)	0.53	8 (13%) 6 5	19, 26, 43, 49	0
1	D	58/105 (55%)	0.61	8 (13%) 6 5	19, 26, 43, 49	0
1	E	58/105 (55%)	0.64	9 (15%) 5 4	20, 26, 43, 51	0
1	F	58/105 (55%)	0.63	8 (13%) 6 5	20, 27, 44, 50	0
1	G	58/105 (55%)	0.67	8 (13%) 6 5	18, 25, 43, 49	0
1	H	58/105 (55%)	0.61	9 (15%) 5 4	18, 24, 42, 48	0
1	I	58/105 (55%)	0.63	9 (15%) 5 4	17, 24, 42, 48	0
1	J	58/105 (55%)	0.50	8 (13%) 6 5	18, 25, 43, 49	0
1	K	58/105 (55%)	0.74	8 (13%) 6 5	21, 26, 46, 51	0
1	L	58/105 (55%)	0.66	6 (10%) 12 9	19, 25, 43, 50	0
1	M	58/105 (55%)	0.56	8 (13%) 6 5	19, 26, 44, 50	0
1	N	58/105 (55%)	0.83	9 (15%) 5 4	18, 26, 44, 50	0
1	O	58/105 (55%)	0.56	7 (12%) 8 6	21, 28, 44, 50	0
1	P	58/105 (55%)	0.75	10 (17%) 4 3	18, 25, 43, 49	0
1	Q	58/105 (55%)	0.56	6 (10%) 12 9	19, 25, 43, 49	0
1	R	58/105 (55%)	0.67	8 (13%) 6 5	20, 27, 46, 52	0
1	T	58/105 (55%)	0.85	8 (13%) 6 5	22, 27, 45, 52	0
1	U	58/105 (55%)	0.67	6 (10%) 12 9	21, 28, 45, 50	0
1	V	58/105 (55%)	0.72	8 (13%) 6 5	20, 27, 43, 50	0
1	W	58/105 (55%)	0.78	9 (15%) 5 4	18, 24, 43, 49	0
1	X	58/105 (55%)	0.54	7 (12%) 8 6	20, 26, 44, 50	0
1	Y	58/105 (55%)	0.77	12 (20%) 2 2	18, 25, 43, 49	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	1392/2520 (55%)	0.66	198 (14%) 6 4	17, 26, 45, 52	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	68	TYR	7.1
1	M	68	TYR	7.0
1	D	68	TYR	7.0
1	G	68	TYR	6.5
1	I	70	ARG	6.3
1	W	70	ARG	6.0
1	Q	70	ARG	5.4
1	J	70	ARG	5.3
1	J	28	HIS	5.3
1	M	71	ILE	5.1
1	V	71	ILE	5.1
1	L	68	TYR	5.0
1	W	28	HIS	4.9
1	P	12	GLY	4.8
1	U	28	HIS	4.8
1	W	34	ASN	4.7
1	I	28	HIS	4.7
1	Q	28	HIS	4.7
1	R	13	ARG	4.7
1	D	71	ILE	4.7
1	A	12	GLY	4.6
1	J	12	GLY	4.5
1	T	34	ASN	4.5
1	P	28	HIS	4.5
1	D	28	HIS	4.5
1	E	13	ARG	4.5
1	E	34	ASN	4.5
1	E	12	GLY	4.4
1	M	12	GLY	4.4
1	B	71	ILE	4.4
1	A	28	HIS	4.4
1	Y	30	GLU	4.4
1	W	71	ILE	4.4
1	A	31	ASN	4.4
1	G	28	HIS	4.3
1	K	71	ILE	4.3
1	B	35	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	I	12	GLY	4.2
1	C	34	ASN	4.2
1	N	28	HIS	4.2
1	X	28	HIS	4.2
1	N	70	ARG	4.2
1	Y	13	ARG	4.2
1	T	12	GLY	4.2
1	G	71	ILE	4.1
1	P	30	GLU	4.1
1	O	12	GLY	4.1
1	G	12	GLY	4.0
1	P	68	TYR	4.0
1	H	28	HIS	4.0
1	K	12	GLY	4.0
1	R	34	ASN	4.0
1	F	71	ILE	4.0
1	B	28	HIS	4.0
1	H	12	GLY	3.9
1	A	34	ASN	3.9
1	M	28	HIS	3.9
1	Y	28	HIS	3.9
1	K	13	ARG	3.9
1	B	13	ARG	3.9
1	K	28	HIS	3.8
1	L	13	ARG	3.8
1	Q	68	TYR	3.8
1	Y	68	TYR	3.8
1	X	12	GLY	3.8
1	D	12	GLY	3.8
1	N	12	GLY	3.8
1	Y	34	ASN	3.7
1	X	70	ARG	3.7
1	J	71	ILE	3.7
1	N	71	ILE	3.7
1	T	35	TYR	3.6
1	C	28	HIS	3.6
1	R	28	HIS	3.6
1	L	71	ILE	3.6
1	J	68	TYR	3.6
1	A	30	GLU	3.6
1	J	35	TYR	3.5
1	V	34	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	34	ASN	3.5
1	L	70	ARG	3.5
1	R	12	GLY	3.5
1	W	35	TYR	3.5
1	M	70	ARG	3.5
1	D	70	ARG	3.4
1	I	71	ILE	3.4
1	F	28	HIS	3.4
1	M	13	ARG	3.4
1	P	13	ARG	3.4
1	K	35	TYR	3.4
1	N	35	TYR	3.4
1	E	28	HIS	3.4
1	R	71	ILE	3.3
1	C	35	TYR	3.3
1	L	28	HIS	3.3
1	R	70	ARG	3.3
1	O	28	HIS	3.3
1	V	28	HIS	3.3
1	H	68	TYR	3.3
1	H	41	ARG	3.3
1	Y	71	ILE	3.3
1	K	34	ASN	3.2
1	E	31	ASN	3.2
1	G	35	TYR	3.2
1	T	71	ILE	3.2
1	G	13	ARG	3.2
1	I	68	TYR	3.2
1	L	12	GLY	3.2
1	F	13	ARG	3.1
1	I	31	ASN	3.1
1	E	71	ILE	3.1
1	H	34	ASN	3.1
1	O	35	TYR	3.0
1	F	31	ASN	3.0
1	Y	41	ARG	3.0
1	Q	71	ILE	3.0
1	U	71	ILE	3.0
1	V	13	ARG	3.0
1	X	13	ARG	3.0
1	F	12	GLY	3.0
1	N	34	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	M	18	GLU	3.0
1	C	70	ARG	3.0
1	V	70	ARG	3.0
1	G	31	ASN	3.0
1	C	71	ILE	2.9
1	P	70	ARG	2.9
1	F	35	TYR	2.9
1	W	12	GLY	2.9
1	I	13	ARG	2.9
1	B	31	ASN	2.8
1	U	34	ASN	2.8
1	V	12	GLY	2.8
1	H	70	ARG	2.8
1	X	71	ILE	2.8
1	R	35	TYR	2.8
1	P	41	ARG	2.8
1	P	34	ASN	2.7
1	A	35	TYR	2.7
1	E	35	TYR	2.7
1	E	70	ARG	2.7
1	O	13	ARG	2.7
1	K	31	ASN	2.7
1	O	71	ILE	2.7
1	X	31	ASN	2.7
1	W	13	ARG	2.7
1	X	68	TYR	2.6
1	Y	31	ASN	2.6
1	U	12	GLY	2.6
1	B	70	ARG	2.6
1	D	13	ARG	2.6
1	H	13	ARG	2.6
1	G	70	ARG	2.6
1	V	35	TYR	2.6
1	A	71	ILE	2.6
1	I	35	TYR	2.6
1	N	13	ARG	2.6
1	T	68	TYR	2.6
1	V	68	TYR	2.6
1	H	30	GLU	2.5
1	C	12	GLY	2.5
1	O	34	ASN	2.5
1	P	71	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	T	13	ARG	2.5
1	U	13	ARG	2.4
1	D	35	TYR	2.4
1	A	13	ARG	2.4
1	A	68	TYR	2.4
1	Y	55	ARG	2.4
1	A	70	ARG	2.4
1	K	68	TYR	2.3
1	I	55	ARG	2.3
1	W	68	TYR	2.3
1	T	28	HIS	2.3
1	D	31	ASN	2.3
1	E	68	TYR	2.3
1	F	55	ARG	2.3
1	H	31	ASN	2.3
1	Y	12	GLY	2.3
1	J	13	ARG	2.2
1	T	70	ARG	2.2
1	M	35	TYR	2.2
1	U	35	TYR	2.2
1	Q	31	ASN	2.2
1	A	41	ARG	2.2
1	C	13	ARG	2.2
1	Q	13	ARG	2.2
1	B	12	GLY	2.2
1	Y	70	ARG	2.1
1	C	31	ASN	2.1
1	J	31	ASN	2.1
1	Y	32	CYS	2.1
1	F	68	TYR	2.1
1	P	55	ARG	2.1
1	N	57	PRO	2.0
1	W	31	ASN	2.0
1	O	70	ARG	2.0
1	R	55	ARG	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 [i](#)

There are no oligosaccharides 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.