



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:48 PM UTC

PDB ID : 8P10 / pdb_00008p10
Title : The crystal structure of the C-terminal domain of Mengla nucleoprotein
Authors : Ferrero, D.S.; Tomas Gilabert, O.; Verdaguer, N.
Deposited on : 2023-05-11
Resolution : 3.26 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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
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

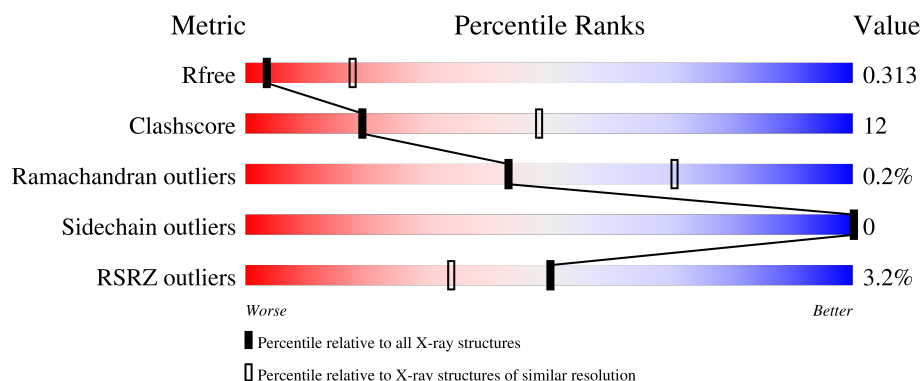
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	130	2% 39% 10% 51%
1	B	130	31% 20% 49%
1	C	130	2% 35% 14% 51%
1	D	130	2% 32% 18% 51%
1	E	130	2% 36% 14% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	130	
1	G	130	
1	H	130	
1	I	130	
1	J	130	
1	K	130	
1	L	130	
1	M	130	
1	N	130	
1	O	130	
1	P	130	
1	Q	130	
1	R	130	
1	S	130	
1	T	130	
1	U	130	
1	V	130	
1	W	130	
1	X	130	
1	Y	130	
1	Z	130	
1	a	130	
1	b	130	
2	c	10	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15285 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 Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	65	Total	C	N	O	S	0	0	0
			543	345	92	104	2			
1	L	64	Total	C	N	O	S	0	0	0
			535	341	91	101	2			
1	K	64	Total	C	N	O	S	0	0	0
			535	341	91	101	2			
1	V	66	Total	C	N	O	S	0	0	0
			552	350	94	106	2			
1	H	67	Total	C	N	O	S	0	0	0
			558	353	95	108	2			
1	Z	65	Total	C	N	O	S	0	0	0
			543	345	92	104	2			
1	B	66	Total	C	N	O	S	0	0	0
			552	350	94	106	2			
1	Y	65	Total	C	N	O	S	0	0	0
			543	345	92	104	2			
1	G	66	Total	C	N	O	S	0	0	0
			552	350	94	106	2			
1	C	64	Total	C	N	O	S	0	0	0
			535	341	91	101	2			
1	T	64	Total	C	N	O	S	0	0	0
			535	341	91	101	2			
1	P	64	Total	C	N	O	S	0	0	0
			535	341	91	101	2			
1	M	67	Total	C	N	O	S	0	0	0
			558	353	95	108	2			
1	N	66	Total	C	N	O	S	0	0	0
			552	350	94	106	2			
1	S	66	Total	C	N	O	S	0	0	0
			552	350	94	106	2			
1	I	65	Total	C	N	O	S	0	0	0
			543	345	92	104	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	64	Total	C	N	O	S	0	0	0
			535	341	91	101	2			
1	X	66	Total	C	N	O	S	0	0	0
			552	350	94	106	2			
1	W	66	Total	C	N	O	S	0	0	0
			552	350	94	106	2			
1	J	66	Total	C	N	O	S	0	0	0
			552	350	94	106	2			
1	F	64	Total	C	N	O	S	0	0	0
			535	341	91	101	2			
1	Q	65	Total	C	N	O	S	0	0	0
			543	345	92	104	2			
1	R	66	Total	C	N	O	S	0	0	0
			552	350	94	106	2			
1	U	64	Total	C	N	O	S	0	0	0
			535	341	91	101	2			
1	a	64	Total	C	N	O	S	0	0	0
			535	341	91	101	2			
1	b	64	Total	C	N	O	S	0	0	0
			535	341	91	101	2			
1	O	66	Total	C	N	O	S	0	0	0
			552	350	94	106	2			
1	D	64	Total	C	N	O	S	0	0	0
			535	341	91	101	2			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	568	GLY	-	expression tag	UNP A0A1Q1N1MU1
E	569	PRO	-	expression tag	UNP A0A1Q1N1MU1
E	570	LEU	-	expression tag	UNP A0A1Q1N1MU1
E	571	GLY	-	expression tag	UNP A0A1Q1N1MU1
E	572	SER	-	expression tag	UNP A0A1Q1N1MU1
L	568	GLY	-	expression tag	UNP A0A1Q1N1MU1
L	569	PRO	-	expression tag	UNP A0A1Q1N1MU1
L	570	LEU	-	expression tag	UNP A0A1Q1N1MU1
L	571	GLY	-	expression tag	UNP A0A1Q1N1MU1
L	572	SER	-	expression tag	UNP A0A1Q1N1MU1
K	568	GLY	-	expression tag	UNP A0A1Q1N1MU1
K	569	PRO	-	expression tag	UNP A0A1Q1N1MU1
K	570	LEU	-	expression tag	UNP A0A1Q1N1MU1
K	571	GLY	-	expression tag	UNP A0A1Q1N1MU1
K	572	SER	-	expression tag	UNP A0A1Q1N1MU1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
V	568	GLY	-	expression tag	UNP A0A1Q1NMU1
V	569	PRO	-	expression tag	UNP A0A1Q1NMU1
V	570	LEU	-	expression tag	UNP A0A1Q1NMU1
V	571	GLY	-	expression tag	UNP A0A1Q1NMU1
V	572	SER	-	expression tag	UNP A0A1Q1NMU1
H	568	GLY	-	expression tag	UNP A0A1Q1NMU1
H	569	PRO	-	expression tag	UNP A0A1Q1NMU1
H	570	LEU	-	expression tag	UNP A0A1Q1NMU1
H	571	GLY	-	expression tag	UNP A0A1Q1NMU1
H	572	SER	-	expression tag	UNP A0A1Q1NMU1
Z	568	GLY	-	expression tag	UNP A0A1Q1NMU1
Z	569	PRO	-	expression tag	UNP A0A1Q1NMU1
Z	570	LEU	-	expression tag	UNP A0A1Q1NMU1
Z	571	GLY	-	expression tag	UNP A0A1Q1NMU1
Z	572	SER	-	expression tag	UNP A0A1Q1NMU1
B	568	GLY	-	expression tag	UNP A0A1Q1NMU1
B	569	PRO	-	expression tag	UNP A0A1Q1NMU1
B	570	LEU	-	expression tag	UNP A0A1Q1NMU1
B	571	GLY	-	expression tag	UNP A0A1Q1NMU1
B	572	SER	-	expression tag	UNP A0A1Q1NMU1
Y	568	GLY	-	expression tag	UNP A0A1Q1NMU1
Y	569	PRO	-	expression tag	UNP A0A1Q1NMU1
Y	570	LEU	-	expression tag	UNP A0A1Q1NMU1
Y	571	GLY	-	expression tag	UNP A0A1Q1NMU1
Y	572	SER	-	expression tag	UNP A0A1Q1NMU1
G	568	GLY	-	expression tag	UNP A0A1Q1NMU1
G	569	PRO	-	expression tag	UNP A0A1Q1NMU1
G	570	LEU	-	expression tag	UNP A0A1Q1NMU1
G	571	GLY	-	expression tag	UNP A0A1Q1NMU1
G	572	SER	-	expression tag	UNP A0A1Q1NMU1
C	568	GLY	-	expression tag	UNP A0A1Q1NMU1
C	569	PRO	-	expression tag	UNP A0A1Q1NMU1
C	570	LEU	-	expression tag	UNP A0A1Q1NMU1
C	571	GLY	-	expression tag	UNP A0A1Q1NMU1
C	572	SER	-	expression tag	UNP A0A1Q1NMU1
T	568	GLY	-	expression tag	UNP A0A1Q1NMU1
T	569	PRO	-	expression tag	UNP A0A1Q1NMU1
T	570	LEU	-	expression tag	UNP A0A1Q1NMU1
T	571	GLY	-	expression tag	UNP A0A1Q1NMU1
T	572	SER	-	expression tag	UNP A0A1Q1NMU1
P	568	GLY	-	expression tag	UNP A0A1Q1NMU1
P	569	PRO	-	expression tag	UNP A0A1Q1NMU1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
P	570	LEU	-	expression tag	UNP A0A1Q1NMU1
P	571	GLY	-	expression tag	UNP A0A1Q1NMU1
P	572	SER	-	expression tag	UNP A0A1Q1NMU1
M	568	GLY	-	expression tag	UNP A0A1Q1NMU1
M	569	PRO	-	expression tag	UNP A0A1Q1NMU1
M	570	LEU	-	expression tag	UNP A0A1Q1NMU1
M	571	GLY	-	expression tag	UNP A0A1Q1NMU1
M	572	SER	-	expression tag	UNP A0A1Q1NMU1
N	568	GLY	-	expression tag	UNP A0A1Q1NMU1
N	569	PRO	-	expression tag	UNP A0A1Q1NMU1
N	570	LEU	-	expression tag	UNP A0A1Q1NMU1
N	571	GLY	-	expression tag	UNP A0A1Q1NMU1
N	572	SER	-	expression tag	UNP A0A1Q1NMU1
S	568	GLY	-	expression tag	UNP A0A1Q1NMU1
S	569	PRO	-	expression tag	UNP A0A1Q1NMU1
S	570	LEU	-	expression tag	UNP A0A1Q1NMU1
S	571	GLY	-	expression tag	UNP A0A1Q1NMU1
S	572	SER	-	expression tag	UNP A0A1Q1NMU1
I	568	GLY	-	expression tag	UNP A0A1Q1NMU1
I	569	PRO	-	expression tag	UNP A0A1Q1NMU1
I	570	LEU	-	expression tag	UNP A0A1Q1NMU1
I	571	GLY	-	expression tag	UNP A0A1Q1NMU1
I	572	SER	-	expression tag	UNP A0A1Q1NMU1
A	568	GLY	-	expression tag	UNP A0A1Q1NMU1
A	569	PRO	-	expression tag	UNP A0A1Q1NMU1
A	570	LEU	-	expression tag	UNP A0A1Q1NMU1
A	571	GLY	-	expression tag	UNP A0A1Q1NMU1
A	572	SER	-	expression tag	UNP A0A1Q1NMU1
X	568	GLY	-	expression tag	UNP A0A1Q1NMU1
X	569	PRO	-	expression tag	UNP A0A1Q1NMU1
X	570	LEU	-	expression tag	UNP A0A1Q1NMU1
X	571	GLY	-	expression tag	UNP A0A1Q1NMU1
X	572	SER	-	expression tag	UNP A0A1Q1NMU1
W	568	GLY	-	expression tag	UNP A0A1Q1NMU1
W	569	PRO	-	expression tag	UNP A0A1Q1NMU1
W	570	LEU	-	expression tag	UNP A0A1Q1NMU1
W	571	GLY	-	expression tag	UNP A0A1Q1NMU1
W	572	SER	-	expression tag	UNP A0A1Q1NMU1
J	568	GLY	-	expression tag	UNP A0A1Q1NMU1
J	569	PRO	-	expression tag	UNP A0A1Q1NMU1
J	570	LEU	-	expression tag	UNP A0A1Q1NMU1
J	571	GLY	-	expression tag	UNP A0A1Q1NMU1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	572	SER	-	expression tag	UNP A0A1Q1NMU1
F	568	GLY	-	expression tag	UNP A0A1Q1NMU1
F	569	PRO	-	expression tag	UNP A0A1Q1NMU1
F	570	LEU	-	expression tag	UNP A0A1Q1NMU1
F	571	GLY	-	expression tag	UNP A0A1Q1NMU1
F	572	SER	-	expression tag	UNP A0A1Q1NMU1
Q	568	GLY	-	expression tag	UNP A0A1Q1NMU1
Q	569	PRO	-	expression tag	UNP A0A1Q1NMU1
Q	570	LEU	-	expression tag	UNP A0A1Q1NMU1
Q	571	GLY	-	expression tag	UNP A0A1Q1NMU1
Q	572	SER	-	expression tag	UNP A0A1Q1NMU1
R	568	GLY	-	expression tag	UNP A0A1Q1NMU1
R	569	PRO	-	expression tag	UNP A0A1Q1NMU1
R	570	LEU	-	expression tag	UNP A0A1Q1NMU1
R	571	GLY	-	expression tag	UNP A0A1Q1NMU1
R	572	SER	-	expression tag	UNP A0A1Q1NMU1
U	568	GLY	-	expression tag	UNP A0A1Q1NMU1
U	569	PRO	-	expression tag	UNP A0A1Q1NMU1
U	570	LEU	-	expression tag	UNP A0A1Q1NMU1
U	571	GLY	-	expression tag	UNP A0A1Q1NMU1
U	572	SER	-	expression tag	UNP A0A1Q1NMU1
a	568	GLY	-	expression tag	UNP A0A1Q1NMU1
a	569	PRO	-	expression tag	UNP A0A1Q1NMU1
a	570	LEU	-	expression tag	UNP A0A1Q1NMU1
a	571	GLY	-	expression tag	UNP A0A1Q1NMU1
a	572	SER	-	expression tag	UNP A0A1Q1NMU1
b	568	GLY	-	expression tag	UNP A0A1Q1NMU1
b	569	PRO	-	expression tag	UNP A0A1Q1NMU1
b	570	LEU	-	expression tag	UNP A0A1Q1NMU1
b	571	GLY	-	expression tag	UNP A0A1Q1NMU1
b	572	SER	-	expression tag	UNP A0A1Q1NMU1
O	568	GLY	-	expression tag	UNP A0A1Q1NMU1
O	569	PRO	-	expression tag	UNP A0A1Q1NMU1
O	570	LEU	-	expression tag	UNP A0A1Q1NMU1
O	571	GLY	-	expression tag	UNP A0A1Q1NMU1
O	572	SER	-	expression tag	UNP A0A1Q1NMU1
D	568	GLY	-	expression tag	UNP A0A1Q1NMU1
D	569	PRO	-	expression tag	UNP A0A1Q1NMU1
D	570	LEU	-	expression tag	UNP A0A1Q1NMU1
D	571	GLY	-	expression tag	UNP A0A1Q1NMU1
D	572	SER	-	expression tag	UNP A0A1Q1NMU1

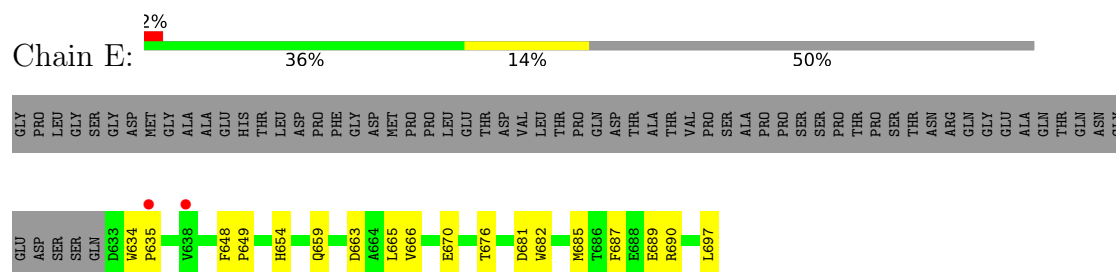
- Molecule 2 is a protein called ALA-ALA-GLY-ALA-ALA-ALA-ALA-ALA-ALA-ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	c	10	Total	C	N	O	0	0	0
			49	29	10	10			

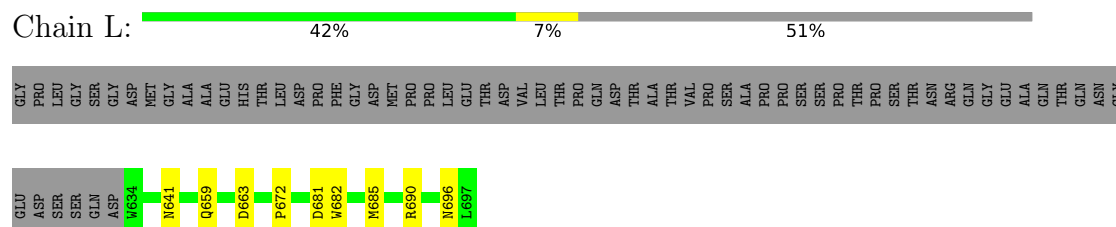
3 Residue-property plots [i](#)

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.

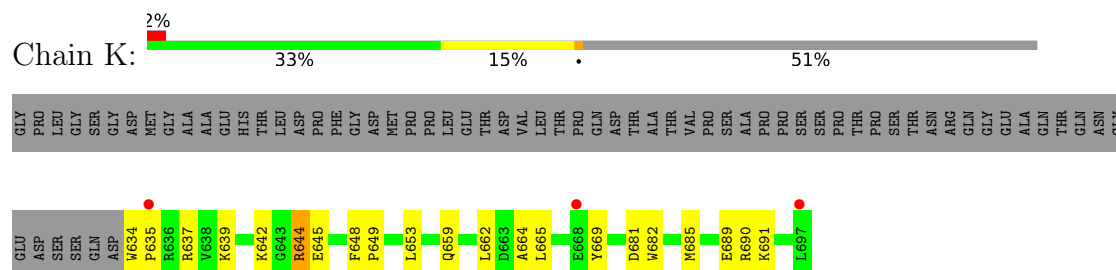
• Molecule 1: Nucleoprotein



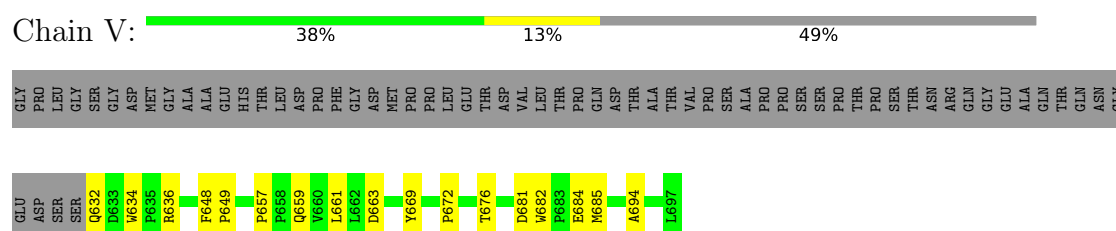
• Molecule 1: Nucleoprotein



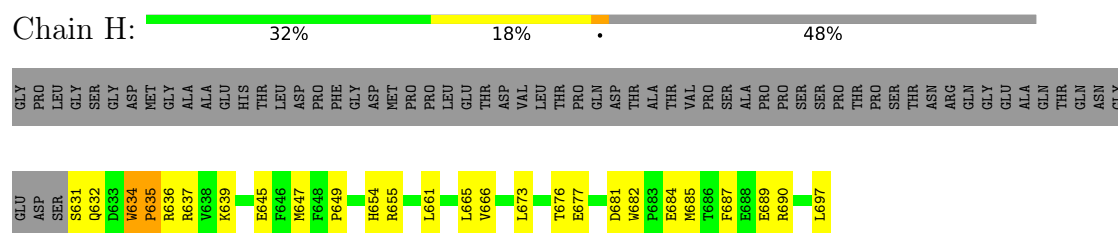
• Molecule 1: Nucleoprotein



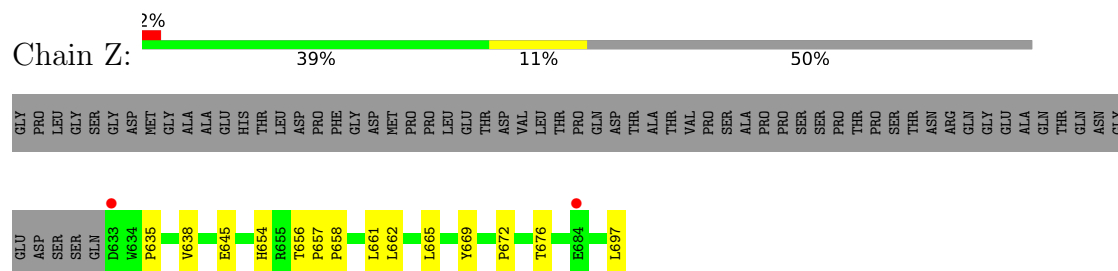
• Molecule 1: Nucleoprotein



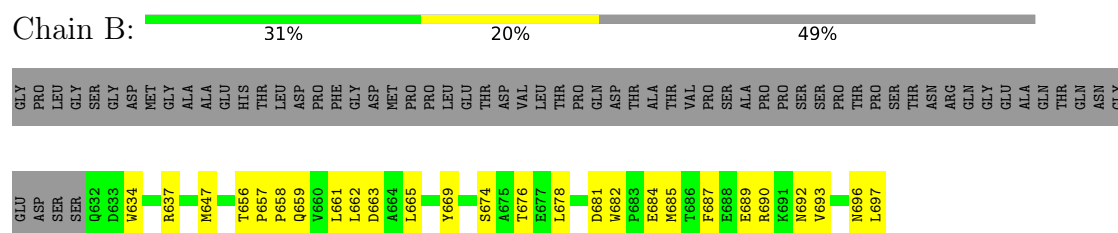
● Molecule 1: Nucleoprotein



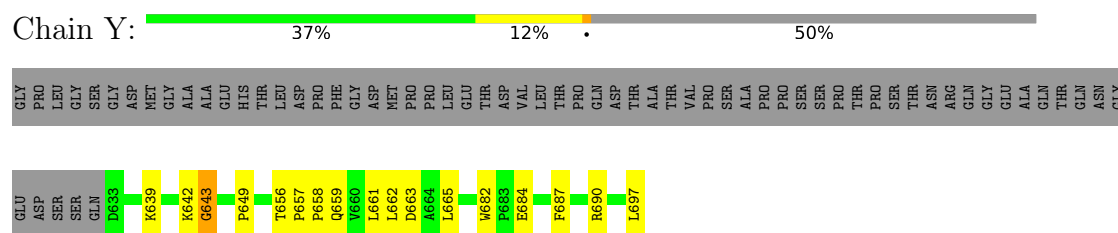
● Molecule 1: Nucleoprotein



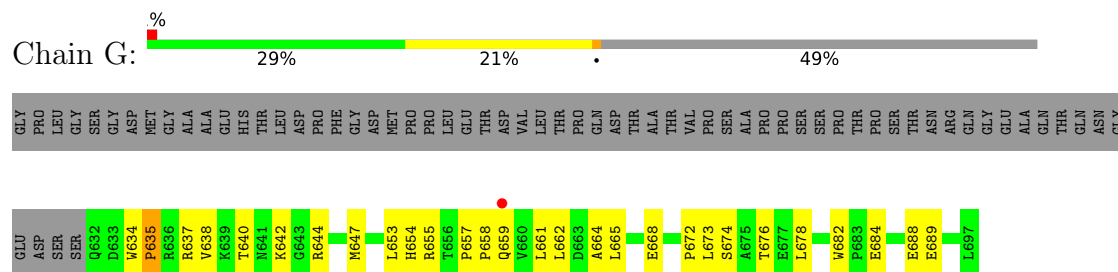
● Molecule 1: Nucleoprotein



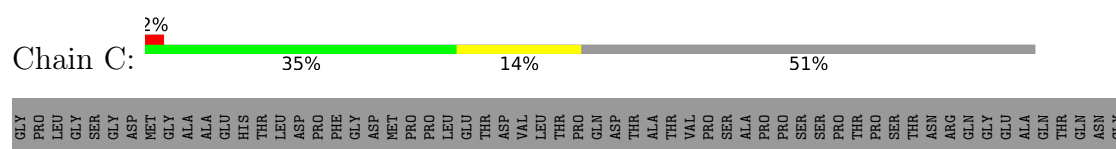
● Molecule 1: Nucleoprotein



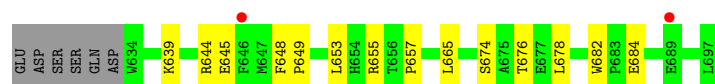
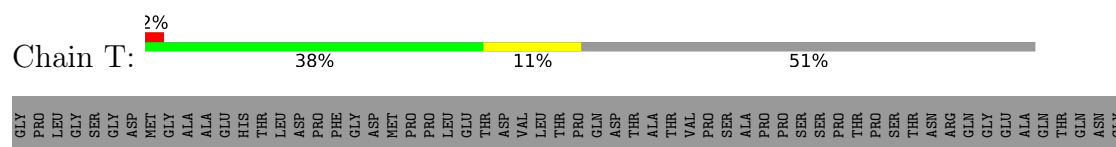
● Molecule 1: Nucleoprotein



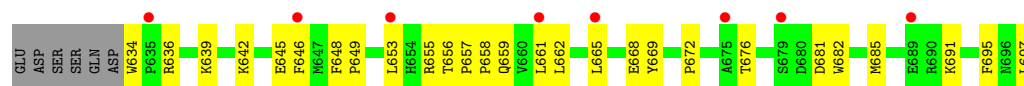
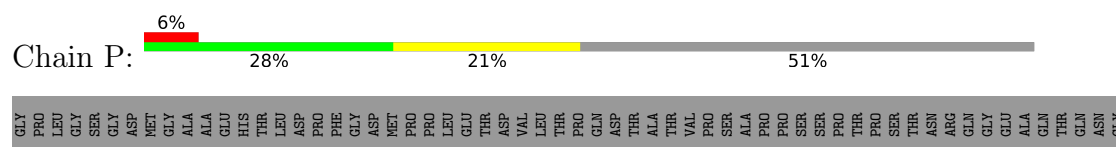
● Molecule 1: Nucleoprotein



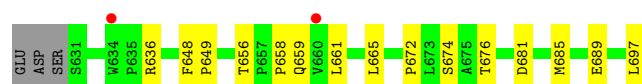
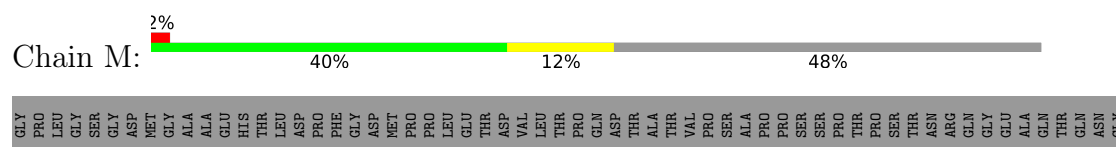
• Molecule 1: Nucleoprotein



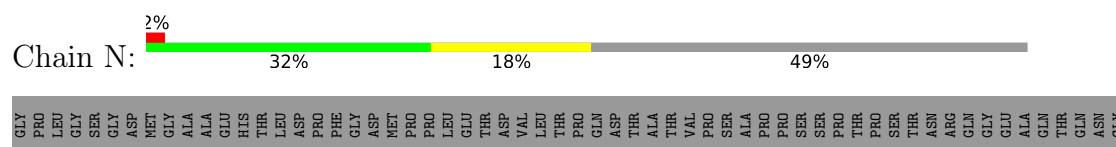
• Molecule 1: Nucleoprotein



• Molecule 1: Nucleoprotein

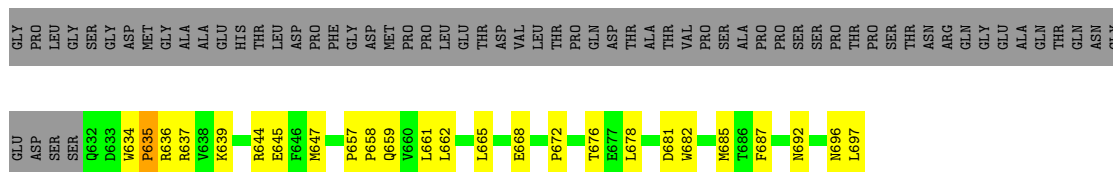


• Molecule 1: Nucleoprotein



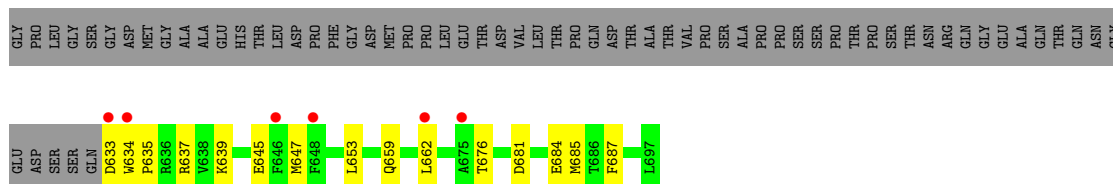
• Molecule 1: Nucleoprotein

Chain S: 

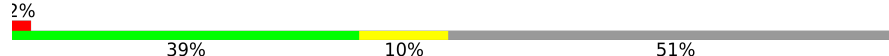


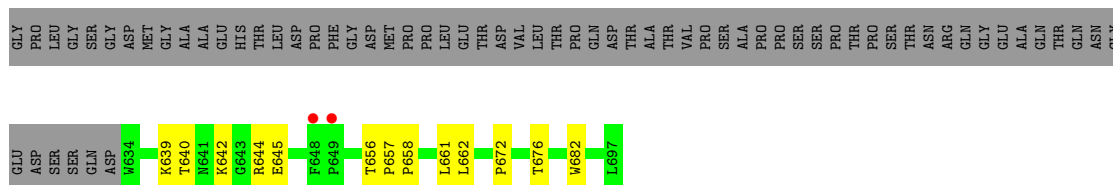
• Molecule 1: Nucleoprotein

Chain I: 



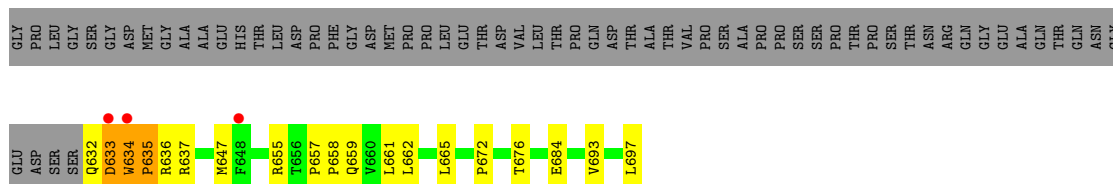
• Molecule 1: Nucleoprotein

Chain A: 

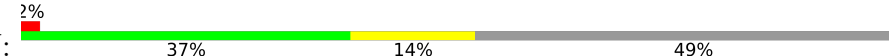


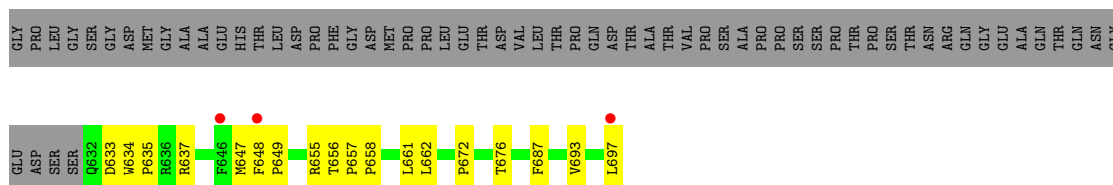
• Molecule 1: Nucleoprotein

Chain X: 



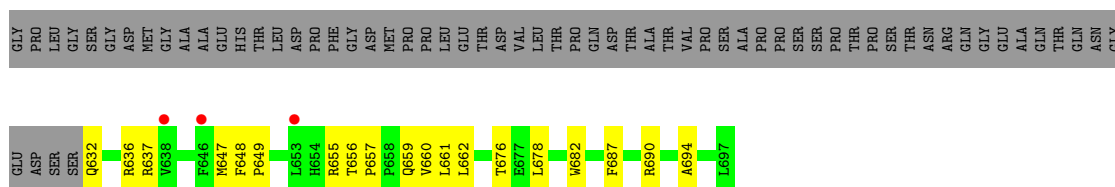
• Molecule 1: Nucleoprotein

Chain W: 

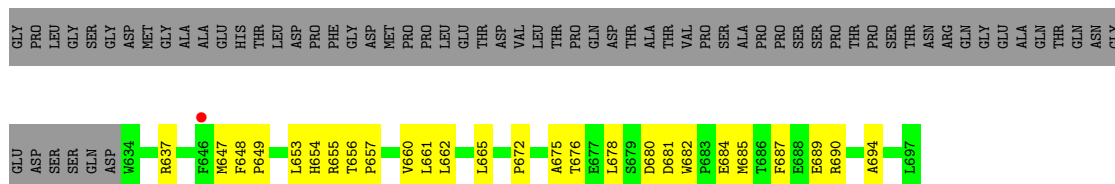
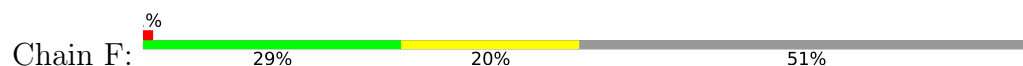


• Molecule 1: Nucleoprotein

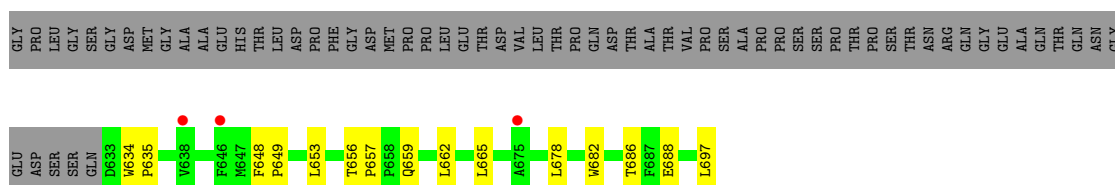
Chain J: 



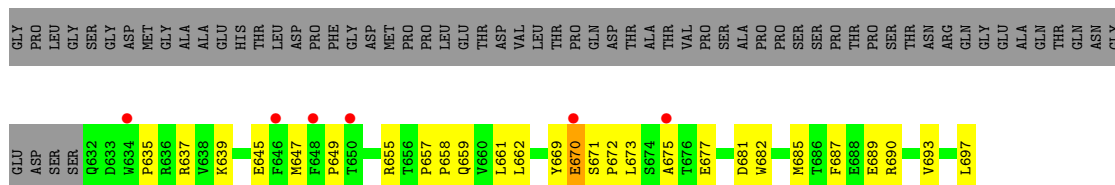
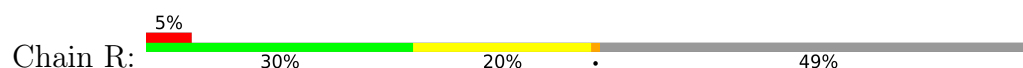
- Molecule 1: Nucleoprotein



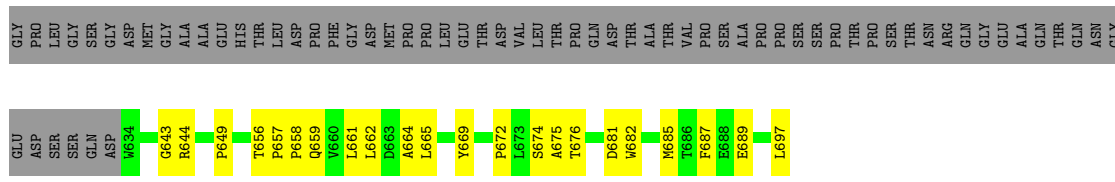
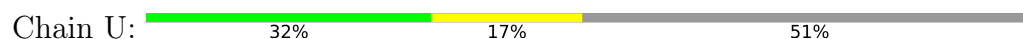
- Molecule 1: Nucleoprotein



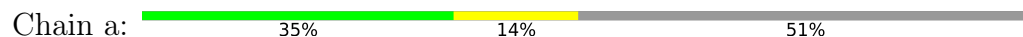
- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein



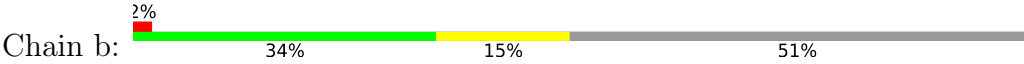
- Molecule 1: Nucleoprotein



GLY	PRO	LEU	SER	GLY	SER	GLN	ASP	ASP	MET	GLY	ALA	ALA	GLU	HIS	THR	ASP	ASP	PHE	GLY	ASP	MET	PRO	PRO	GLU	THR	ASP	VAL	THR	THR	PRO	GLN	ASP	THR	THR	THR	VAL	PRO	SER	ALA	ALA	THR	THR	THR	ASN	ARG	GLN	GLY	GLU	ALA	GLN	THR	GLN	ASN	GLY
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

GLU	ASP	SER	SER	GLN	ASP	W634	R637	R644	E645	P657	P658	Q659	L662	L665	E668	P672	L673	S674	A675	T676	D681	W682	P683	E684	M685	W686	F687	R690	L697
-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

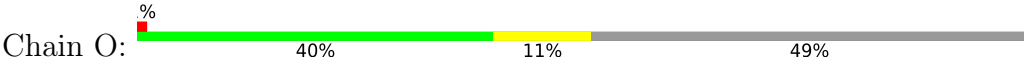
• Molecule 1: Nucleoprotein



GLY	PRO	LEU	SER	GLY	SER	GLN	ASP	ASP	MET	GLY	ALA	ALA	GLU	HIS	THR	ASP	ASP	PHE	GLY	ASP	MET	PRO	PRO	GLU	THR	ASP	VAL	THR	THR	PRO	GLN	ASP	THR	THR	THR	VAL	PRO	SER	ALA	ALA	PRO	PRO	SER	SER	PRO	THR	THR	THR	ASN	ARG	GLN	GLY	GLU	ALA	GLN	THR	GLN	ASN	GLY
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

GLU	ASP	SER	SER	GLN	ASP	W634	K639	R644	E645	F648	P649	T656	P657	P658	L661	L662	L665	E668	S674	A675	T676	S679	D680	D681	W682	M685	R690	V693	A694	F695	N696	L697
-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

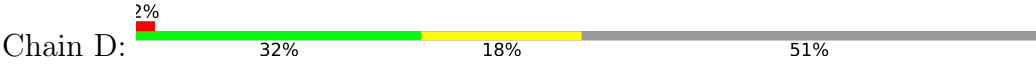
• Molecule 1: Nucleoprotein



GLY	PRO	LEU	SER	GLY	SER	GLN	ASP	ASP	MET	GLY	ALA	ALA	GLU	HIS	THR	ASP	ASP	PHE	GLY	ASP	MET	PRO	PRO	GLU	THR	ASP	VAL	THR	THR	PRO	GLN	ASP	THR	THR	THR	VAL	PRO	SER	ALA	ALA	PRO	PRO	SER	SER	PRO	THR	THR	THR	ASN	ARG	GLN	GLY	GLU	ALA	GLN	THR	GLN	ASN	GLY
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

GLU	ASP	SER	SER	GLN	ASP	W634	Q632	P649	L653	P658	Q659	V660	L661	L662	L665	S674	W682	P683	E684	M685	T686	E688	E689	R690	L697
-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

• Molecule 1: Nucleoprotein



GLY	PRO	LEU	SER	GLY	SER	GLN	ASP	ASP	MET	GLY	ALA	ALA	GLU	HIS	THR	ASP	ASP	PHE	GLY	ASP	MET	PRO	PRO	GLU	THR	ASP	VAL	THR	THR	PRO	GLN	ASP	THR	THR	THR	VAL	PRO	SER	ALA	ALA	PRO	PRO	SER	SER	PRO	THR	THR	THR	ASN	ARG	GLN	GLY	GLU	ALA	GLN	THR	GLN	ASN	GLY
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

GLU	ASP	SER	SER	GLN	ASP	W634	P635	R636	R637	R644	E645	F646	M647	F648	P649	R655	T656	P657	P658	L661	L662	L665	E668	S674	A675	T676	D681	W682	P683	E684	M685	T686	E688	E689	L697
-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

• Molecule 2: ALA-ALA-GLY-ALA-ALA-ALA-ALA-ALA-ALA-ALA



A234	A239	A240	A241	A242	A243
------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	68.31Å 85.71Å 146.24Å 88.52° 76.45° 80.26°	Depositor
Resolution (Å)	47.99 – 3.26 47.99 – 3.26	Depositor EDS
% Data completeness (in resolution range)	62.0 (47.99-3.26) 62.3 (47.99-3.26)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.26Å)	Xtriage
Refinement program	REFMAC V.5, PHENIX dev_4788	Depositor
R, R_{free}	0.274 , 0.305 0.278 , 0.313	Depositor DCC
R_{free} test set	1575 reflections (3.17%)	wwPDB-VP
Wilson B-factor (Å ²)	109.0	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 81.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.069 for -h,-k,-h+l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	15285	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.12	0/550	0.25	0/747
1	B	0.13	0/567	0.31	0/770
1	C	0.12	0/550	0.30	0/747
1	D	0.11	0/550	0.27	0/747
1	E	0.12	0/558	0.31	0/758
1	F	0.11	0/550	0.27	0/747
1	G	0.16	0/567	0.32	0/770
1	H	0.32	1/573 (0.2%)	0.56	3/778 (0.4%)
1	I	0.12	0/558	0.28	0/758
1	J	0.12	0/567	0.29	0/770
1	K	0.14	0/550	0.34	0/747
1	L	0.12	0/550	0.28	0/747
1	M	0.12	0/573	0.30	0/778
1	N	0.11	0/567	0.27	0/770
1	O	0.11	0/567	0.25	0/770
1	P	0.13	0/550	0.30	0/747
1	Q	0.13	0/558	0.32	0/758
1	R	0.52	1/567 (0.2%)	0.79	2/770 (0.3%)
1	S	0.12	0/567	0.45	2/770 (0.3%)
1	T	0.11	0/550	0.26	0/747
1	U	0.14	0/550	0.29	0/747
1	V	0.11	0/567	0.28	0/770
1	W	0.11	0/567	0.25	0/770
1	X	0.44	1/567 (0.2%)	0.96	4/770 (0.5%)
1	Y	0.79	2/558 (0.4%)	0.46	1/758 (0.1%)
1	Z	0.11	0/558	0.26	0/758
1	a	0.13	0/550	0.30	0/747
1	b	0.12	0/550	0.29	0/747
2	c	0.21	0/48	0.37	0/65
All	All	0.24	5/15704 (0.0%)	0.39	12/21328 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	1
1	X	0	2
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	643	GLY	C-N	15.77	1.55	1.33
1	R	670	GLU	C-N	11.54	1.57	1.33
1	X	632	GLN	C-N	-8.64	1.22	1.33
1	Y	642	LYS	C-N	8.03	1.45	1.33
1	H	634	TRP	C-N	7.17	1.50	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	633	ASP	N-CA-C	20.26	139.63	112.68
1	R	670	GLU	N-CA-C	-17.28	84.39	110.30
1	H	635	PRO	N-CA-C	-9.64	92.60	112.47
1	S	635	PRO	N-CA-C	-8.11	95.77	112.47
1	H	634	TRP	O-C-N	-7.37	112.85	121.32

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	644	ARG	Sidechain
1	X	633	ASP	Mainchain
1	X	636	ARG	Sidechain

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	535	0	517	9	0
1	B	552	0	529	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	535	0	517	16	0
1	D	535	0	517	18	0
1	E	543	0	521	13	0
1	F	535	0	517	21	0
1	G	552	0	529	29	0
1	H	558	0	534	25	0
1	I	543	0	521	11	0
1	J	552	0	529	12	0
1	K	535	0	517	18	0
1	L	535	0	517	9	0
1	M	558	0	534	13	0
1	N	552	0	529	19	0
1	O	552	0	529	9	0
1	P	535	0	517	19	0
1	Q	543	0	521	14	0
1	R	552	0	529	17	0
1	S	552	0	529	16	0
1	T	535	0	517	11	0
1	U	535	0	517	17	0
1	V	552	0	529	12	0
1	W	552	0	529	13	0
1	X	552	0	529	15	0
1	Y	543	0	521	14	0
1	Z	543	0	521	10	0
1	a	535	0	517	13	0
1	b	535	0	517	12	0
2	c	49	0	47	5	0
All	All	15285	0	14697	351	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 351 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:G:653:LEU:HB3	1:F:662:LEU:HD21	1.44	1.00
1:I:637:ARG:HG2	1:I:647:MET:HG2	1.68	0.75
1:S:639:LYS:HG2	1:S:645:GLU:HG2	1.70	0.73
1:M:636:ARG:O	1:M:648:PHE:N	2.23	0.71
1:R:669:TYR:O	1:R:670:GLU:C	2.32	0.71

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	62/130 (48%)	58 (94%)	4 (6%)	0	100	100
1	B	64/130 (49%)	60 (94%)	4 (6%)	0	100	100
1	C	62/130 (48%)	55 (89%)	7 (11%)	0	100	100
1	D	62/130 (48%)	59 (95%)	3 (5%)	0	100	100
1	E	63/130 (48%)	60 (95%)	3 (5%)	0	100	100
1	F	62/130 (48%)	58 (94%)	4 (6%)	0	100	100
1	G	64/130 (49%)	54 (84%)	9 (14%)	1 (2%)	7	30
1	H	65/130 (50%)	61 (94%)	4 (6%)	0	100	100
1	I	63/130 (48%)	60 (95%)	3 (5%)	0	100	100
1	J	64/130 (49%)	61 (95%)	3 (5%)	0	100	100
1	K	62/130 (48%)	59 (95%)	3 (5%)	0	100	100
1	L	62/130 (48%)	59 (95%)	3 (5%)	0	100	100
1	M	65/130 (50%)	58 (89%)	7 (11%)	0	100	100
1	N	64/130 (49%)	62 (97%)	2 (3%)	0	100	100
1	O	64/130 (49%)	61 (95%)	3 (5%)	0	100	100
1	P	62/130 (48%)	58 (94%)	4 (6%)	0	100	100
1	Q	63/130 (48%)	58 (92%)	5 (8%)	0	100	100
1	R	64/130 (49%)	58 (91%)	5 (8%)	1 (2%)	7	30
1	S	64/130 (49%)	60 (94%)	4 (6%)	0	100	100
1	T	62/130 (48%)	59 (95%)	3 (5%)	0	100	100
1	U	62/130 (48%)	57 (92%)	5 (8%)	0	100	100
1	V	64/130 (49%)	60 (94%)	4 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	64/130 (49%)	60 (94%)	4 (6%)	0	100	100
1	X	64/130 (49%)	59 (92%)	4 (6%)	1 (2%)	7	30
1	Y	63/130 (48%)	59 (94%)	4 (6%)	0	100	100
1	Z	63/130 (48%)	60 (95%)	3 (5%)	0	100	100
1	a	62/130 (48%)	59 (95%)	3 (5%)	0	100	100
1	b	62/130 (48%)	57 (92%)	5 (8%)	0	100	100
2	c	8/10 (80%)	5 (62%)	3 (38%)	0	100	100
All	All	1775/3650 (49%)	1654 (93%)	118 (7%)	3 (0%)	43	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	635	PRO
1	R	635	PRO
1	G	635	PRO

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	60/114 (53%)	60 (100%)	0	100	100
1	B	62/114 (54%)	62 (100%)	0	100	100
1	C	60/114 (53%)	60 (100%)	0	100	100
1	D	60/114 (53%)	60 (100%)	0	100	100
1	E	61/114 (54%)	61 (100%)	0	100	100
1	F	60/114 (53%)	60 (100%)	0	100	100
1	G	62/114 (54%)	62 (100%)	0	100	100
1	H	63/114 (55%)	63 (100%)	0	100	100
1	I	61/114 (54%)	61 (100%)	0	100	100
1	J	62/114 (54%)	62 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	60/114 (53%)	60 (100%)	0	100	100
1	L	60/114 (53%)	60 (100%)	0	100	100
1	M	63/114 (55%)	63 (100%)	0	100	100
1	N	62/114 (54%)	62 (100%)	0	100	100
1	O	62/114 (54%)	62 (100%)	0	100	100
1	P	60/114 (53%)	60 (100%)	0	100	100
1	Q	61/114 (54%)	61 (100%)	0	100	100
1	R	62/114 (54%)	62 (100%)	0	100	100
1	S	62/114 (54%)	62 (100%)	0	100	100
1	T	60/114 (53%)	60 (100%)	0	100	100
1	U	60/114 (53%)	60 (100%)	0	100	100
1	V	62/114 (54%)	62 (100%)	0	100	100
1	W	62/114 (54%)	62 (100%)	0	100	100
1	X	62/114 (54%)	62 (100%)	0	100	100
1	Y	61/114 (54%)	61 (100%)	0	100	100
1	Z	61/114 (54%)	61 (100%)	0	100	100
1	a	60/114 (53%)	60 (100%)	0	100	100
1	b	60/114 (53%)	60 (100%)	0	100	100
All	All	1711/3192 (54%)	1711 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	696	ASN
1	b	659	GLN
1	O	659	GLN
1	b	667	ASN
1	S	632	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	64/130 (49%)	0.22	2 (3%) 51 34	100, 128, 155, 162	0
1	B	66/130 (50%)	0.09	0 100 100	95, 117, 151, 172	0
1	C	64/130 (49%)	0.45	3 (4%) 36 24	100, 121, 147, 155	0
1	D	64/130 (49%)	0.37	2 (3%) 51 34	97, 129, 166, 180	0
1	E	65/130 (50%)	0.21	2 (3%) 51 34	87, 101, 124, 166	0
1	F	64/130 (49%)	0.37	1 (1%) 70 52	91, 128, 154, 168	0
1	G	66/130 (50%)	0.30	1 (1%) 72 53	93, 113, 165, 182	0
1	H	67/130 (51%)	0.08	0 100 100	87, 108, 137, 152	0
1	I	65/130 (50%)	0.48	6 (9%) 14 11	90, 122, 156, 189	0
1	J	66/130 (50%)	0.19	3 (4%) 38 25	81, 109, 146, 188	0
1	K	64/130 (49%)	0.30	3 (4%) 36 24	71, 94, 119, 125	0
1	L	64/130 (49%)	-0.02	0 100 100	74, 95, 119, 132	0
1	M	67/130 (51%)	0.32	2 (2%) 52 35	95, 123, 153, 168	0
1	N	66/130 (50%)	0.42	2 (3%) 52 35	113, 136, 166, 189	0
1	O	66/130 (50%)	0.42	1 (1%) 72 53	109, 145, 172, 190	0
1	P	64/130 (49%)	0.59	8 (12%) 8 7	92, 114, 130, 144	0
1	Q	65/130 (50%)	0.42	3 (4%) 37 25	103, 126, 163, 193	0
1	R	66/130 (50%)	0.52	6 (9%) 15 11	94, 151, 181, 188	0
1	S	66/130 (50%)	0.20	0 100 100	88, 118, 141, 162	0
1	T	64/130 (49%)	0.27	2 (3%) 51 34	95, 124, 162, 175	0
1	U	64/130 (49%)	0.29	0 100 100	102, 122, 147, 156	0
1	V	66/130 (50%)	0.20	0 100 100	80, 99, 137, 154	0
1	W	66/130 (50%)	0.21	3 (4%) 38 25	89, 123, 152, 164	0
1	X	66/130 (50%)	0.25	3 (4%) 38 25	84, 110, 137, 143	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	65/130 (50%)	0.09	0 100 100	79, 96, 128, 163	0
1	Z	65/130 (50%)	-0.01	2 (3%) 51 34	80, 98, 121, 144	0
1	a	64/130 (49%)	0.37	0 100 100	89, 109, 144, 158	0
1	b	64/130 (49%)	0.41	3 (4%) 36 24	107, 139, 162, 167	0
2	c	10/10 (100%)	0.46	0 100 100	87, 94, 106, 109	0
All	All	1833/3650 (50%)	0.29	58 (3%) 50 34	71, 117, 161, 193	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	648	PHE	4.2
1	Q	646	PHE	4.1
1	A	648	PHE	3.7
1	N	689	GLU	3.5
1	I	646	PHE	3.4

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

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

6.3 Carbohydrates [i](#)

There are no 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.