



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 26, 2026 – 11:16 PM UTC

PDB ID : 8P24 / pdb_00008p24
Title : The crystal structure of the C-terminal domain of Mengla nucleoprotein
Authors : Ferrero, D.S.; Tomas Gilabert, O.; Verdaguer, N.
Deposited on : 2023-05-14
Resolution : 3.73 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

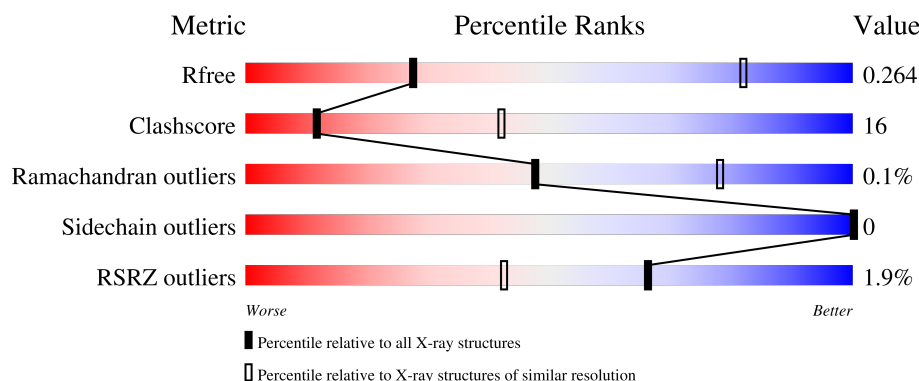
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.73 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	1234 (3.88-3.60)
Clashscore	190562	1274 (3.88-3.60)
Ramachandran outliers	187476	1226 (3.88-3.60)
Sidechain outliers	187428	1221 (3.88-3.60)
RSRZ outliers	180081	1233 (3.88-3.60)

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	41% 10% 49%
1	B	130	29% 20% 51%
1	C	130	31% 18% 51%
1	D	130	38% 12% 51%
1	E	130	30% 20% 50%

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Mol	Chain	Length	Quality of chain
1	F	130	 % 29% 20% 51%
1	G	130	 % 32% 16% 52%
1	H	130	 2% 29% 19% 52%
1	I	130	 30% 20% 50%
1	J	130	 2% 32% 18% 49%
1	K	130	 3% 30% 20% 49%
1	L	130	 2% 38% 10% 51%
1	M	130	 34% 18% 48%
1	N	130	 2% 32% 18% 49%
1	O	130	 % 37% 13% 50%
1	P	130	 2% 26% 22% 52%
1	Q	130	 % 32% 18% 50%
1	R	130	 2% 25% 23% 52%
1	S	130	 24% 24% 52%
1	T	130	 33% 16% 51%
1	U	130	 2% 32% 18% 51%
1	V	130	 35% 15% 49%
1	W	130	 % 33% 15% 52%
1	X	130	 % 33% 17% 49%
1	Y	130	 34% 16% 50%
1	Z	130	 38% 12% 50%
1	a	130	 2% 34% 15% 51%
1	b	130	 % 30% 19% 51%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15048 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	V	66	Total	C	N	O	S	0	0	0
			552	350	94	106	2			
1	Z	65	Total	C	N	O	S	0	0	0
			543	345	92	104	2			
1	Y	65	Total	C	N	O	S	0	0	0
			543	345	92	104	2			
1	T	64	Total	C	N	O	S	0	0	0
			535	341	91	101	2			
1	P	62	Total	C	N	O	S	0	0	0
			514	325	88	99	2			
1	S	62	Total	C	N	O	S	0	0	0
			514	325	88	99	2			
1	X	66	Total	C	N	O	S	0	0	0
			552	350	94	106	2			
1	W	63	Total	C	N	O	S	0	0	0
			521	330	89	100	2			
1	Q	65	Total	C	N	O	S	0	0	0
			543	345	92	104	2			
1	R	63	Total	C	N	O	S	0	0	0
			521	330	89	100	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	O	65	Total	C	N	O	S	0	0	0
			543	345	92	104	2			
1	A	66	Total	C	N	O	S	0	0	0
			552	350	94	106	2			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	K	66	Total	C	N	O	S	0	0	0
			552	350	94	106	2			
1	H	63	Total	C	N	O	S	0	0	0
			521	330	89	100	2			
1	B	64	Total	C	N	O	S	0	0	0
			535	341	91	101	2			
1	G	62	Total	C	N	O	S	0	0	0
			514	325	88	99	2			
1	C	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	I	65	Total	C	N	O	S	0	0	0
			543	345	92	104	2			
1	D	64	Total	C	N	O	S	0	0	0
			535	341	91	101	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	b	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
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
T	568	GLY	-	expression tag	UNP A0A1Q1N MU1
T	569	PRO	-	expression tag	UNP A0A1Q1N MU1
T	570	LEU	-	expression tag	UNP A0A1Q1N MU1
T	571	GLY	-	expression tag	UNP A0A1Q1N MU1
T	572	SER	-	expression tag	UNP A0A1Q1N MU1
P	568	GLY	-	expression tag	UNP A0A1Q1N MU1
P	569	PRO	-	expression tag	UNP A0A1Q1N MU1
P	570	LEU	-	expression tag	UNP A0A1Q1N MU1
P	571	GLY	-	expression tag	UNP A0A1Q1N MU1
P	572	SER	-	expression tag	UNP A0A1Q1N MU1
S	568	GLY	-	expression tag	UNP A0A1Q1N MU1
S	569	PRO	-	expression tag	UNP A0A1Q1N MU1
S	570	LEU	-	expression tag	UNP A0A1Q1N MU1
S	571	GLY	-	expression tag	UNP A0A1Q1N MU1
S	572	SER	-	expression tag	UNP A0A1Q1N MU1
X	568	GLY	-	expression tag	UNP A0A1Q1N MU1
X	569	PRO	-	expression tag	UNP A0A1Q1N MU1
X	570	LEU	-	expression tag	UNP A0A1Q1N MU1
X	571	GLY	-	expression tag	UNP A0A1Q1N MU1
X	572	SER	-	expression tag	UNP A0A1Q1N MU1
W	568	GLY	-	expression tag	UNP A0A1Q1N MU1
W	569	PRO	-	expression tag	UNP A0A1Q1N MU1
W	570	LEU	-	expression tag	UNP A0A1Q1N MU1
W	571	GLY	-	expression tag	UNP A0A1Q1N MU1
W	572	SER	-	expression tag	UNP A0A1Q1N MU1
Q	568	GLY	-	expression tag	UNP A0A1Q1N MU1
Q	569	PRO	-	expression tag	UNP A0A1Q1N MU1
Q	570	LEU	-	expression tag	UNP A0A1Q1N MU1
Q	571	GLY	-	expression tag	UNP A0A1Q1N MU1
Q	572	SER	-	expression tag	UNP A0A1Q1N MU1
R	568	GLY	-	expression tag	UNP A0A1Q1N MU1
R	569	PRO	-	expression tag	UNP A0A1Q1N MU1
R	570	LEU	-	expression tag	UNP A0A1Q1N MU1
R	571	GLY	-	expression tag	UNP A0A1Q1N MU1
R	572	SER	-	expression tag	UNP A0A1Q1N MU1
U	568	GLY	-	expression tag	UNP A0A1Q1N MU1
U	569	PRO	-	expression tag	UNP A0A1Q1N MU1
U	570	LEU	-	expression tag	UNP A0A1Q1N MU1
U	571	GLY	-	expression tag	UNP A0A1Q1N MU1
U	572	SER	-	expression tag	UNP A0A1Q1N MU1
a	568	GLY	-	expression tag	UNP A0A1Q1N MU1
a	569	PRO	-	expression tag	UNP A0A1Q1N MU1

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Chain	Residue	Modelled	Actual	Comment	Reference
a	570	LEU	-	expression tag	UNP A0A1Q1N MU1
a	571	GLY	-	expression tag	UNP A0A1Q1N MU1
a	572	SER	-	expression tag	UNP A0A1Q1N MU1
O	568	GLY	-	expression tag	UNP A0A1Q1N MU1
O	569	PRO	-	expression tag	UNP A0A1Q1N MU1
O	570	LEU	-	expression tag	UNP A0A1Q1N MU1
O	571	GLY	-	expression tag	UNP A0A1Q1N MU1
O	572	SER	-	expression tag	UNP A0A1Q1N MU1
A	568	GLY	-	expression tag	UNP A0A1Q1N MU1
A	569	PRO	-	expression tag	UNP A0A1Q1N MU1
A	570	LEU	-	expression tag	UNP A0A1Q1N MU1
A	571	GLY	-	expression tag	UNP A0A1Q1N MU1
A	572	SER	-	expression tag	UNP A0A1Q1N MU1
E	568	GLY	-	expression tag	UNP A0A1Q1N MU1
E	569	PRO	-	expression tag	UNP A0A1Q1N MU1
E	570	LEU	-	expression tag	UNP A0A1Q1N MU1
E	571	GLY	-	expression tag	UNP A0A1Q1N MU1
E	572	SER	-	expression tag	UNP A0A1Q1N MU1
L	568	GLY	-	expression tag	UNP A0A1Q1N MU1
L	569	PRO	-	expression tag	UNP A0A1Q1N MU1
L	570	LEU	-	expression tag	UNP A0A1Q1N MU1
L	571	GLY	-	expression tag	UNP A0A1Q1N MU1
L	572	SER	-	expression tag	UNP A0A1Q1N MU1
K	568	GLY	-	expression tag	UNP A0A1Q1N MU1
K	569	PRO	-	expression tag	UNP A0A1Q1N MU1
K	570	LEU	-	expression tag	UNP A0A1Q1N MU1
K	571	GLY	-	expression tag	UNP A0A1Q1N MU1
K	572	SER	-	expression tag	UNP A0A1Q1N MU1
H	568	GLY	-	expression tag	UNP A0A1Q1N MU1
H	569	PRO	-	expression tag	UNP A0A1Q1N MU1
H	570	LEU	-	expression tag	UNP A0A1Q1N MU1
H	571	GLY	-	expression tag	UNP A0A1Q1N MU1
H	572	SER	-	expression tag	UNP A0A1Q1N MU1
B	568	GLY	-	expression tag	UNP A0A1Q1N MU1
B	569	PRO	-	expression tag	UNP A0A1Q1N MU1
B	570	LEU	-	expression tag	UNP A0A1Q1N MU1
B	571	GLY	-	expression tag	UNP A0A1Q1N MU1
B	572	SER	-	expression tag	UNP A0A1Q1N MU1
G	568	GLY	-	expression tag	UNP A0A1Q1N MU1
G	569	PRO	-	expression tag	UNP A0A1Q1N MU1
G	570	LEU	-	expression tag	UNP A0A1Q1N MU1
G	571	GLY	-	expression tag	UNP A0A1Q1N MU1

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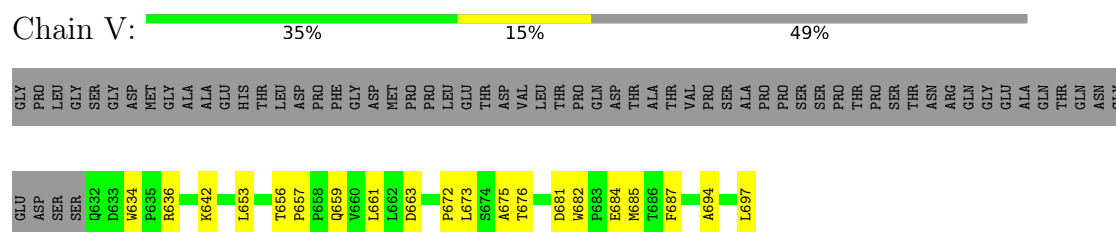
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Chain	Residue	Modelled	Actual	Comment	Reference
G	572	SER	-	expression tag	UNP A0A1Q1N MU1
C	568	GLY	-	expression tag	UNP A0A1Q1N MU1
C	569	PRO	-	expression tag	UNP A0A1Q1N MU1
C	570	LEU	-	expression tag	UNP A0A1Q1N MU1
C	571	GLY	-	expression tag	UNP A0A1Q1N MU1
C	572	SER	-	expression tag	UNP A0A1Q1N MU1
M	568	GLY	-	expression tag	UNP A0A1Q1N MU1
M	569	PRO	-	expression tag	UNP A0A1Q1N MU1
M	570	LEU	-	expression tag	UNP A0A1Q1N MU1
M	571	GLY	-	expression tag	UNP A0A1Q1N MU1
M	572	SER	-	expression tag	UNP A0A1Q1N MU1
N	568	GLY	-	expression tag	UNP A0A1Q1N MU1
N	569	PRO	-	expression tag	UNP A0A1Q1N MU1
N	570	LEU	-	expression tag	UNP A0A1Q1N MU1
N	571	GLY	-	expression tag	UNP A0A1Q1N MU1
N	572	SER	-	expression tag	UNP A0A1Q1N MU1
I	568	GLY	-	expression tag	UNP A0A1Q1N MU1
I	569	PRO	-	expression tag	UNP A0A1Q1N MU1
I	570	LEU	-	expression tag	UNP A0A1Q1N MU1
I	571	GLY	-	expression tag	UNP A0A1Q1N MU1
I	572	SER	-	expression tag	UNP A0A1Q1N MU1
D	568	GLY	-	expression tag	UNP A0A1Q1N MU1
D	569	PRO	-	expression tag	UNP A0A1Q1N MU1
D	570	LEU	-	expression tag	UNP A0A1Q1N MU1
D	571	GLY	-	expression tag	UNP A0A1Q1N MU1
D	572	SER	-	expression tag	UNP A0A1Q1N MU1
J	568	GLY	-	expression tag	UNP A0A1Q1N MU1
J	569	PRO	-	expression tag	UNP A0A1Q1N MU1
J	570	LEU	-	expression tag	UNP A0A1Q1N MU1
J	571	GLY	-	expression tag	UNP A0A1Q1N MU1
J	572	SER	-	expression tag	UNP A0A1Q1N MU1
F	568	GLY	-	expression tag	UNP A0A1Q1N MU1
F	569	PRO	-	expression tag	UNP A0A1Q1N MU1
F	570	LEU	-	expression tag	UNP A0A1Q1N MU1
F	571	GLY	-	expression tag	UNP A0A1Q1N MU1
F	572	SER	-	expression tag	UNP A0A1Q1N MU1
b	568	GLY	-	expression tag	UNP A0A1Q1N MU1
b	569	PRO	-	expression tag	UNP A0A1Q1N MU1
b	570	LEU	-	expression tag	UNP A0A1Q1N MU1
b	571	GLY	-	expression tag	UNP A0A1Q1N MU1
b	572	SER	-	expression tag	UNP A0A1Q1N MU1

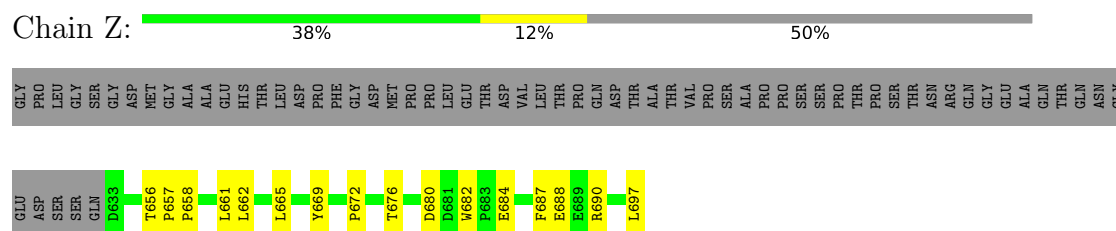
3 Residue-property plots [i](#)

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.

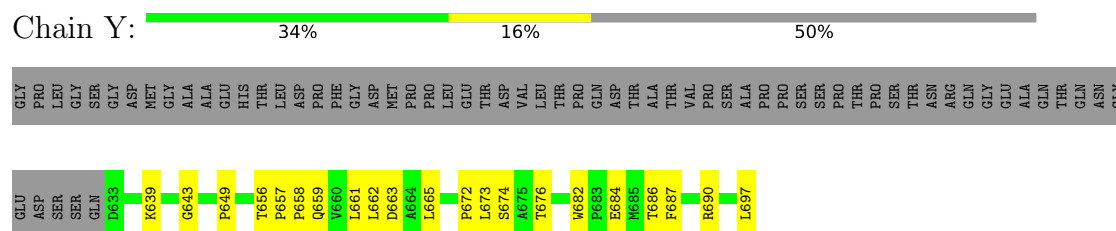
- Molecule 1: Nucleoprotein



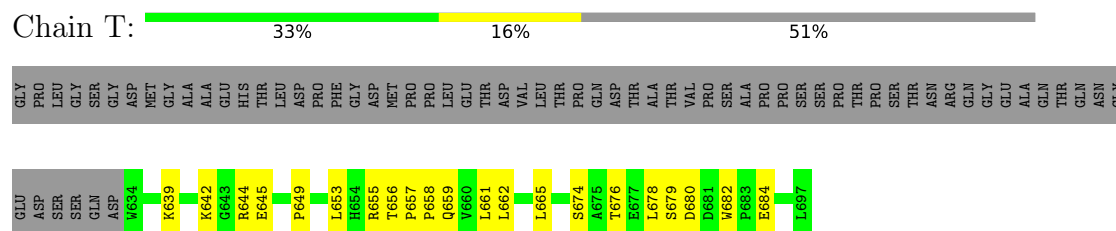
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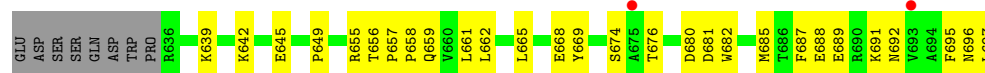
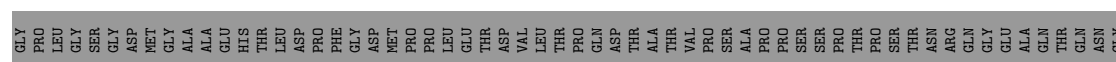
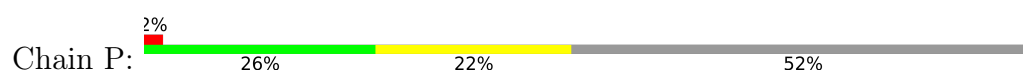
- Molecule 1: Nucleoprotein



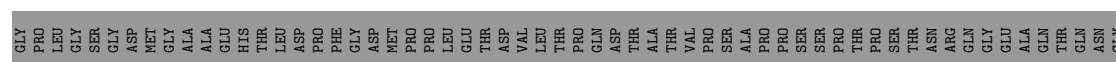
- Molecule 1: Nucleoprotein



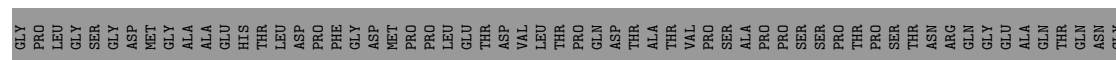
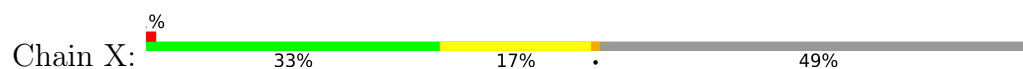
- Molecule 1: Nucleoprotein



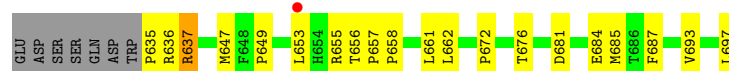
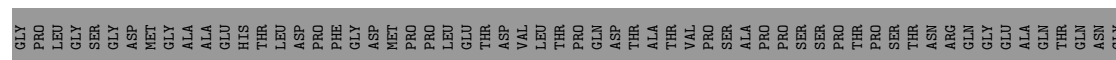
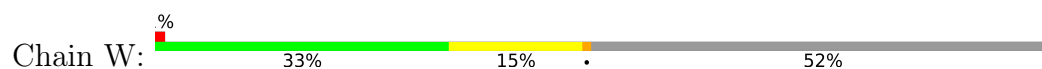
- Molecule 1: Nucleoprotein



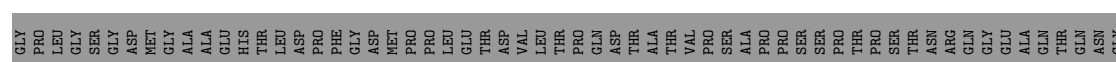
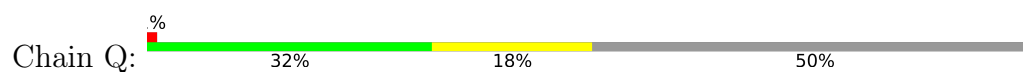
- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein



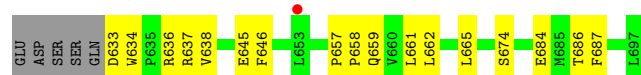
Chain U:



Chain a:



Chain O: %



Chain A: %



WORLDWIDE
PDB
PROTEIN DATA BANK



Chain L:

Amino Acid
GLY
PRO
LEU
GLY
SER
GLY
ASP
MET
GLY
ALA
GLU
HIS
THR
LEU
ASP
PHE
GLY
ASP
MET
PRO
LEU
GLU
THR
ASP
VAL
LEU
THR
PRO
GLN
ASP
THR
ALA
THR
VAL
PRO
SER
ALA
PRO
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ARG
GLN
GLY
GLU
ALA
GLN
THR
GLM
ASV

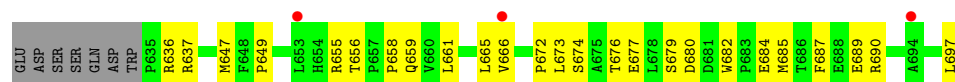


Chain K:



Chain H:

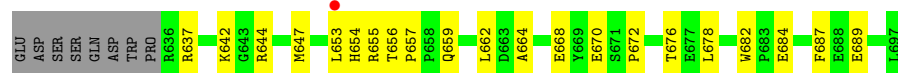
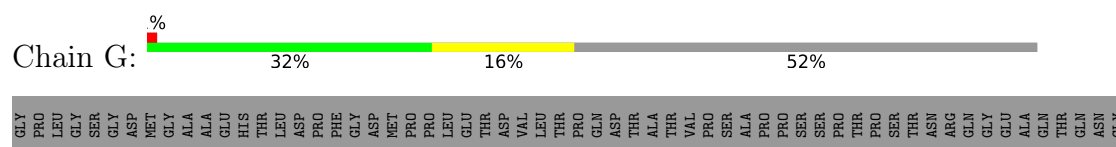
Amino Acid	Percentage
GLY	2%
PRO	29%
LEU	19%
GLY	52%
SER	
GLY	
ASP	
MET	
GLY	
ALA	
GLY	
GLU	
HIS	
THR	
LEU	
ASP	
PRO	
PHE	
GLY	
ASP	
MET	
PRO	
PRO	
LEU	
GLU	
THR	
ASP	
VAL	
LEU	
THR	
PRO	
GLN	
ASP	
THR	
THR	
ALA	
THR	
VAL	
PRO	
SER	
SER	
ALA	
PRO	
PRO	
SER	
SER	
THR	
THR	
SER	
THR	
ASN	
ASP	
ARG	
GLN	
GLY	
GLU	
GLU	
ALA	
GLN	
GLN	
THR	
GLN	
ASN	
Y	



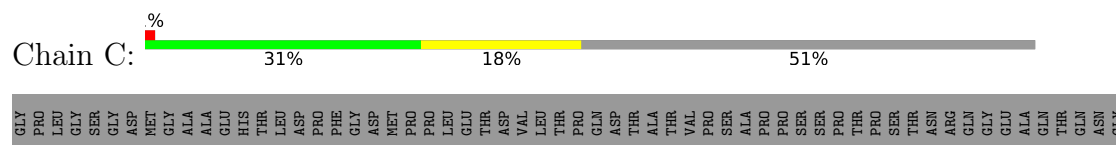
Chain B: 29% 20% 51%

Residue	Category
GLY	Green
PRO	Green
LEU	Green
GLY	Green
SER	Green
GLY	Green
ASP	Green
MET	Green
GLY	Green
ALA	Green
GLU	Green
HIS	Green
THR	Green
LEU	Green
ASP	Green
PRO	Green
PHE	Green
GLY	Green
ASP	Green
MET	Green
PRO	Green
LEU	Green
GLU	Green
ASP	Green
THR	Green
VAL	Green
LEU	Green
THR	Green
PRO	Green
GLN	Green
ASP	Green
THR	Green
ALA	Green
THR	Green
VAL	Green
PRO	Green
SER	Green
SER	Green
ALA	Green
PRO	Green
PRO	Green
SER	Green
SER	Green
THR	Green
PRO	Green
THR	Green
SER	Green
THR	Green
ASN	Green
ARG	Green
GLN	Green
GLY	Green
GLU	Green
ALA	Green
GLN	Green
GLN	Green
THR	Green
GLN	Green
ASP	Green
VAL	Green

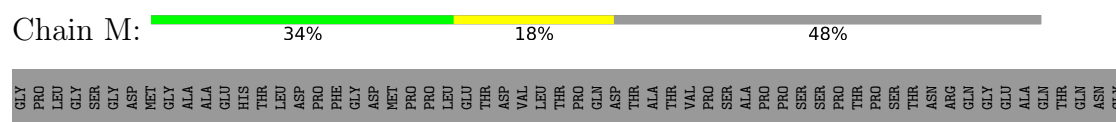




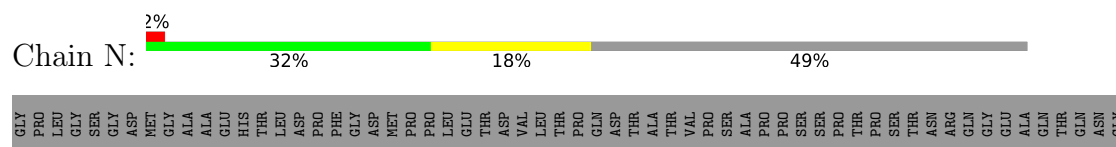
- Molecule 1: Nucleoprotein



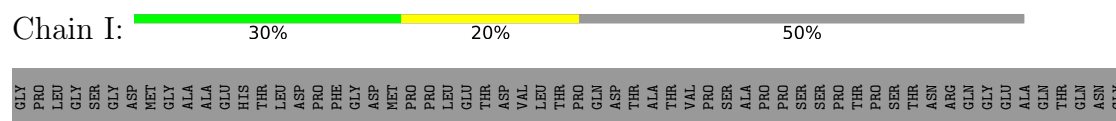
- Molecule 1: Nucleoprotein



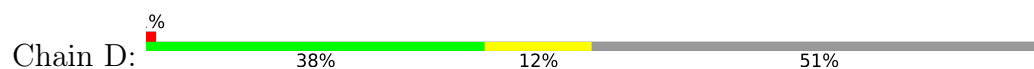
- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein



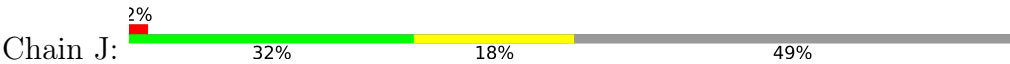
- Molecule 1: Nucleoprotein



GLY	PRO	LEU	GLY	SER	GLY	ASP	MET	GLY	ALA	ALA	GLU	HIS	THR	LEU	ASP	ASP	PHE	PRO	GLY	ASP	MET	PRO	PRO	LEU	GLU	THR	ASP	VAL	THR	PRO	GLN	ASP	THR	ALA	VAL	PRO	SER	ALA	PRO	PRO	PRO	SER	SER	PRO	THR	THR	ASN	ARG	GLN	GLY	ALA	GLN	THR	GLN	ASN	GLY
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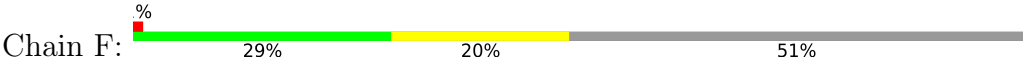
• Molecule 1: Nucleoprotein



GLY	PRO	LEU	GLY	SER	GLY	ASP	MET	GLY	ALA	ALA	GLU	HIS	THR	LEU	ASP	ASP	PHE	PRO	GLY	ASP	MET	PRO	PRO	LEU	GLU	THR	ASP	VAL	THR	PRO	GLN	ASP	THR	ALA	VAL	PRO	SER	ALA	PRO	PRO	PRO	SER	SER	PRO	THR	THR	ASN	ARG	GLN	GLY	ALA	GLN	THR	GLN	ASN	GLY
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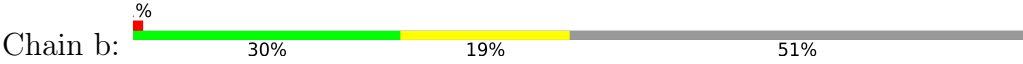
• Molecule 1: Nucleoprotein



GLY	PRO	LEU	GLY	SER	GLY	ASP	MET	GLY	ALA	ALA	GLU	HIS	THR	LEU	ASP	ASP	PHE	PRO	GLY	ASP	MET	PRO	PRO	LEU	GLU	THR	ASP	VAL	THR	PRO	GLN	ASP	THR	ALA	VAL	PRO	SER	ALA	PRO	PRO	PRO	SER	SER	PRO	THR	THR	ASN	ARG	GLN	GLY	ALA	GLN	THR	GLN	ASN	GLY
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• Molecule 1: Nucleoprotein



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.75Å 162.94Å 175.36Å 90.00° 99.15° 90.00°	Depositor
Resolution (Å)	173.13 – 3.73 173.13 – 3.73	Depositor EDS
% Data completeness (in resolution range)	25.1 (173.13-3.73) 25.0 (173.13-3.73)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.78Å)	Xtriage
Refinement program	REFMAC dev_4788, PHENIX dev_4788	Depositor
R, R_{free}	0.248 , 0.265 0.264 , 0.264	Depositor DCC
R_{free} test set	435 reflections (1.32%)	wwPDB-VP
Wilson B-factor (Å ²)	108.2	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 95.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.149 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	15048	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.18% 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	0/567	0.28	0/770
1	B	0.13	0/550	0.34	0/747
1	C	0.12	0/550	0.31	0/747
1	D	0.12	0/550	0.27	0/747
1	E	0.14	0/558	0.34	0/758
1	F	0.12	0/550	0.30	0/747
1	G	0.14	0/526	0.31	0/712
1	H	0.19	0/534	0.40	0/723
1	I	0.13	0/558	0.29	0/758
1	J	0.13	0/567	0.30	0/770
1	K	0.29	0/567	0.51	1/770 (0.1%)
1	L	0.24	0/550	0.70	1/747 (0.1%)
1	M	0.16	0/573	0.35	0/778
1	N	0.13	0/567	0.34	0/770
1	O	0.15	0/558	0.32	0/758
1	P	0.11	0/526	0.26	0/712
1	Q	0.13	0/558	0.34	0/758
1	R	0.15	0/534	0.34	0/723
1	S	0.13	0/526	0.28	0/712
1	T	0.12	0/550	0.32	0/747
1	U	0.13	0/550	0.30	0/747
1	V	0.12	0/567	0.31	0/770
1	W	0.27	0/534	0.41	0/723
1	X	0.16	0/567	0.35	0/770
1	Y	0.14	0/558	0.34	0/758
1	Z	0.12	0/558	0.27	0/758
1	a	0.15	0/550	0.37	0/747
1	b	0.12	0/550	0.30	0/747
All	All	0.16	0/15453	0.35	2/20974 (0.0%)

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	2
1	L	0	2
1	W	0	2
All	All	0	6

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	L	637	ARG	N-CA-C	-14.57	85.32	108.63
1	K	635	PRO	N-CA-C	-5.83	100.46	112.47

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	636	ARG	Sidechain
1	L	636	ARG	Sidechain
1	L	637	ARG	Sidechain
1	W	636	ARG	Sidechain
1	W	637	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	552	0	529	8	0
1	B	535	0	517	22	0
1	C	535	0	517	20	0
1	D	535	0	517	15	0
1	E	543	0	521	21	0
1	F	535	0	517	26	0
1	G	514	0	500	28	0
1	H	521	0	508	38	0
1	I	543	0	521	37	0
1	J	552	0	529	27	0
1	K	552	0	529	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	535	0	517	10	0
1	M	558	0	534	19	0
1	N	552	0	529	17	1
1	O	543	0	521	15	1
1	P	514	0	500	24	0
1	Q	543	0	521	24	0
1	R	521	0	508	28	0
1	S	514	0	500	33	0
1	T	535	0	517	27	0
1	U	535	0	517	23	0
1	V	552	0	529	17	0
1	W	521	0	508	24	0
1	X	552	0	529	26	0
1	Y	543	0	521	22	0
1	Z	543	0	521	16	0
1	a	535	0	517	17	0
1	b	535	0	517	21	0
All	All	15048	0	14511	469	1

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 16.

The worst 5 of 469 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:X:672:PRO:HB2	1:W:649:PRO:HG2	1.32	1.12
1:T:655:ARG:HB2	1:U:659:GLN:HG2	1.55	0.88
1:Y:656:THR:HB	1:X:684:GLU:HA	1.56	0.87
1:I:659:GLN:HG2	1:J:655:ARG:HB2	1.57	0.85
1:W:635:PRO:HD2	1:W:649:PRO:HD3	1.60	0.83

All (1) 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:O:633:ASP:O	1:N:692:ASN:ND2[2_444]	2.11	0.09

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	64/130 (49%)	60 (94%)	4 (6%)	0	100	100
1	B	62/130 (48%)	58 (94%)	4 (6%)	0	100	100
1	C	62/130 (48%)	56 (90%)	6 (10%)	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%)	59 (95%)	3 (5%)	0	100	100
1	G	60/130 (46%)	53 (88%)	7 (12%)	0	100	100
1	H	61/130 (47%)	59 (97%)	2 (3%)	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	64/130 (49%)	61 (95%)	3 (5%)	0	100	100
1	L	62/130 (48%)	59 (95%)	3 (5%)	0	100	100
1	M	65/130 (50%)	59 (91%)	6 (9%)	0	100	100
1	N	64/130 (49%)	62 (97%)	2 (3%)	0	100	100
1	O	63/130 (48%)	59 (94%)	4 (6%)	0	100	100
1	P	60/130 (46%)	56 (93%)	4 (7%)	0	100	100
1	Q	63/130 (48%)	58 (92%)	5 (8%)	0	100	100
1	R	61/130 (47%)	53 (87%)	8 (13%)	0	100	100
1	S	60/130 (46%)	57 (95%)	3 (5%)	0	100	100
1	T	62/130 (48%)	59 (95%)	3 (5%)	0	100	100
1	U	62/130 (48%)	58 (94%)	4 (6%)	0	100	100
1	V	64/130 (49%)	59 (92%)	5 (8%)	0	100	100
1	W	61/130 (47%)	56 (92%)	5 (8%)	0	100	100
1	X	64/130 (49%)	59 (92%)	4 (6%)	1 (2%)	7	35
1	Y	63/130 (48%)	57 (90%)	6 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	59 (95%)	3 (5%)	0	100	100
All	All	1748/3640 (48%)	1635 (94%)	112 (6%)	1 (0%)	48	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	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	62/114 (54%)	62 (100%)	0	100	100
1	B	60/114 (53%)	60 (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	58/114 (51%)	58 (100%)	0	100	100
1	H	59/114 (52%)	59 (100%)	0	100	100
1	I	61/114 (54%)	61 (100%)	0	100	100
1	J	62/114 (54%)	62 (100%)	0	100	100
1	K	62/114 (54%)	62 (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	61/114 (54%)	61 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	58/114 (51%)	58 (100%)	0	100	100
1	Q	61/114 (54%)	61 (100%)	0	100	100
1	R	59/114 (52%)	59 (100%)	0	100	100
1	S	58/114 (51%)	58 (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	59/114 (52%)	59 (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	1692/3192 (53%)	1692 (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 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	659	GLN
1	J	696	ASN
1	J	659	GLN
1	E	659	GLN
1	N	696	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 [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	66/130 (50%)	0.03	1 (1%) 72 47	80, 120, 151, 167	0
1	B	64/130 (49%)	-0.00	1 (1%) 70 45	95, 137, 169, 181	0
1	C	64/130 (49%)	-0.05	1 (1%) 70 45	82, 113, 135, 141	0
1	D	64/130 (49%)	-0.05	1 (1%) 70 45	77, 108, 129, 137	0
1	E	65/130 (50%)	-0.14	1 (1%) 72 47	122, 146, 169, 204	0
1	F	64/130 (49%)	-0.05	1 (1%) 70 45	116, 136, 164, 175	0
1	G	62/130 (47%)	0.06	1 (1%) 70 45	102, 123, 139, 148	0
1	H	63/130 (48%)	0.09	3 (4%) 35 24	96, 127, 142, 152	0
1	I	65/130 (50%)	0.11	0 100 100	74, 100, 137, 186	0
1	J	66/130 (50%)	0.15	2 (3%) 52 33	82, 111, 149, 174	0
1	K	66/130 (50%)	0.29	4 (6%) 27 19	30, 82, 122, 129	0
1	L	64/130 (49%)	0.07	2 (3%) 51 32	60, 83, 106, 132	0
1	M	67/130 (51%)	0.07	0 100 100	71, 96, 127, 192	0
1	N	66/130 (50%)	0.28	3 (4%) 38 25	56, 73, 139, 186	0
1	O	65/130 (50%)	0.19	1 (1%) 72 47	63, 85, 125, 157	0
1	P	62/130 (47%)	0.25	2 (3%) 50 32	58, 92, 143, 157	0
1	Q	65/130 (50%)	0.04	1 (1%) 72 47	62, 103, 147, 165	0
1	R	63/130 (48%)	0.14	2 (3%) 50 32	70, 99, 123, 134	0
1	S	62/130 (47%)	0.01	0 100 100	89, 121, 151, 173	0
1	T	64/130 (49%)	-0.02	0 100 100	90, 119, 136, 143	0
1	U	64/130 (49%)	-0.03	2 (3%) 51 32	94, 130, 155, 178	0
1	V	66/130 (50%)	-0.15	0 100 100	98, 131, 151, 159	0
1	W	63/130 (48%)	-0.08	1 (1%) 70 45	95, 130, 154, 166	0
1	X	66/130 (50%)	-0.07	1 (1%) 72 47	86, 116, 135, 179	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	Y	65/130 (50%)	-0.16	0	100	100	90, 137, 186, 196	0
1	Z	65/130 (50%)	-0.19	0	100	100	80, 119, 147, 158	0
1	a	64/130 (49%)	0.28	2 (3%)	51	32	62, 92, 132, 162	0
1	b	64/130 (49%)	-0.18	1 (1%)	70	45	96, 134, 160, 177	0
All	All	1804/3640 (49%)	0.03	34 (1%)	66	42	30, 116, 157, 204	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	653	LEU	4.4
1	X	653	LEU	3.7
1	K	646	PHE	3.7
1	J	653	LEU	3.5
1	B	675	ALA	3.2

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.