wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2023 – 04:28 pm BST

PDB ID	:	8P10
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 (i) 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 (i)) were used in the production of this report:

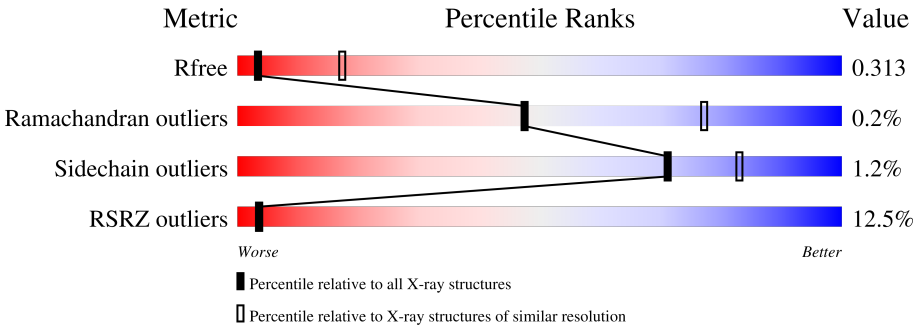
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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.



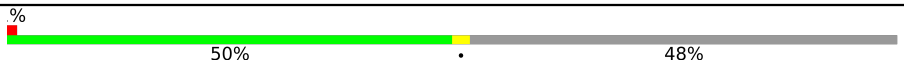
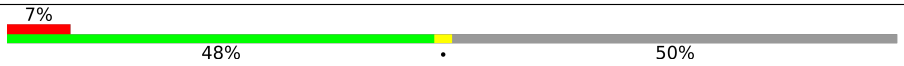
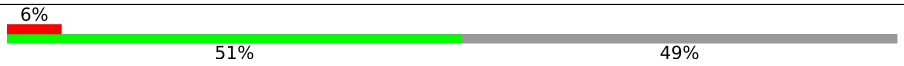
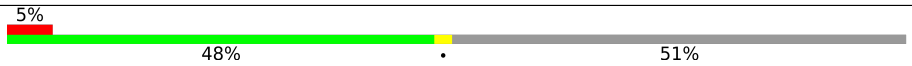
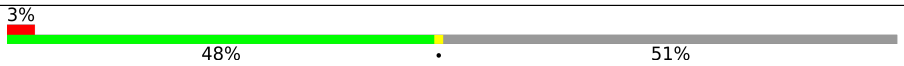
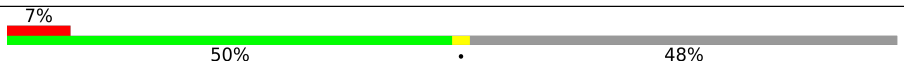
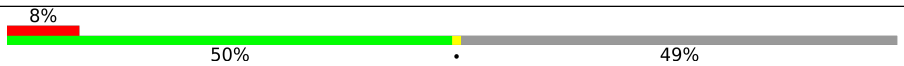
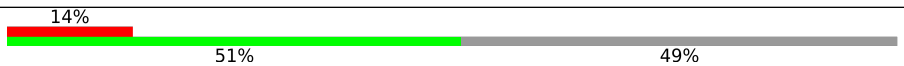
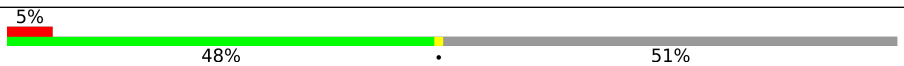
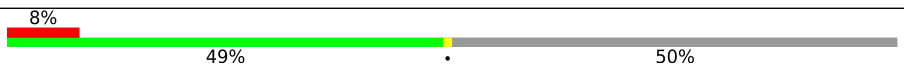
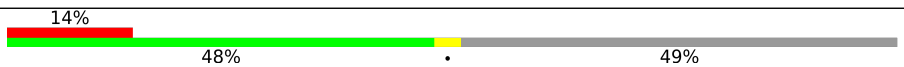
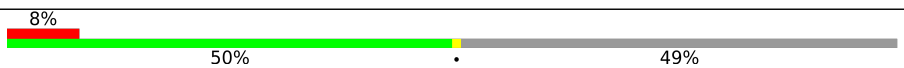
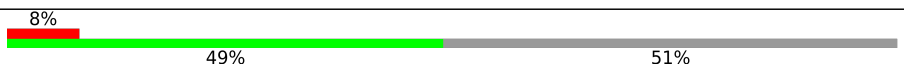
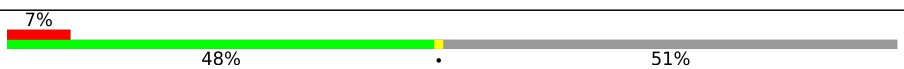
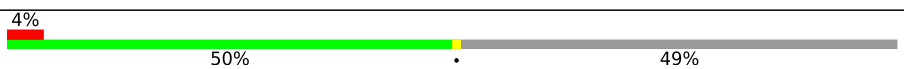
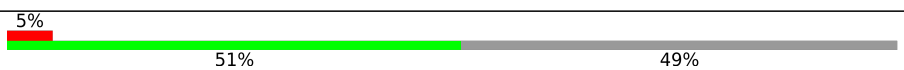
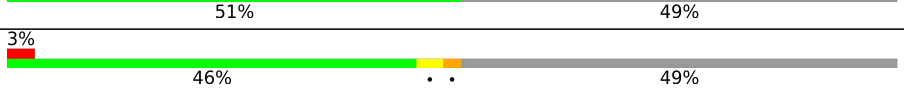
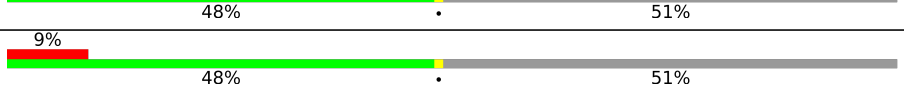
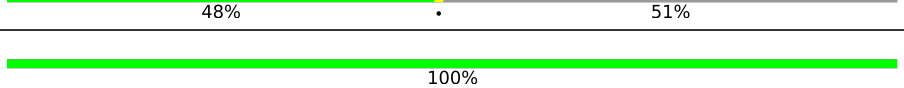
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1191 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 <=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	5% 49% 51%
1	B	130	10% 50% 49%
1	C	130	5% 49% 51%
1	D	130	5% 48% 51%
1	E	130	4% 50% 50%
1	F	130	6% 49% 51%
1	G	130	8% 50% 49%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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 (i)

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 A0A1Q1NMU1
E	569	PRO	-	expression tag	UNP A0A1Q1NMU1
E	570	LEU	-	expression tag	UNP A0A1Q1NMU1
E	571	GLY	-	expression tag	UNP A0A1Q1NMU1
E	572	SER	-	expression tag	UNP A0A1Q1NMU1
L	568	GLY	-	expression tag	UNP A0A1Q1NMU1
L	569	PRO	-	expression tag	UNP A0A1Q1NMU1
L	570	LEU	-	expression tag	UNP A0A1Q1NMU1
L	571	GLY	-	expression tag	UNP A0A1Q1NMU1
L	572	SER	-	expression tag	UNP A0A1Q1NMU1
K	568	GLY	-	expression tag	UNP A0A1Q1NMU1
K	569	PRO	-	expression tag	UNP A0A1Q1NMU1
K	570	LEU	-	expression tag	UNP A0A1Q1NMU1
K	571	GLY	-	expression tag	UNP A0A1Q1NMU1
K	572	SER	-	expression tag	UNP A0A1Q1NMU1

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.

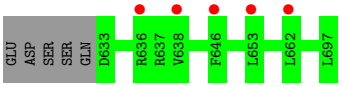
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	c	10	Total	C	N	O	0	0	0
			49	29	10	10			

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.

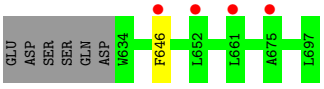
- Molecule 1: Nucleoprotein

Chain E:



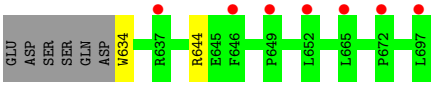
- Molecule 1: Nucleoprotein

Chain L:



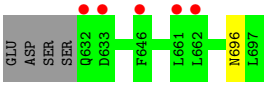
- Molecule 1: Nucleoprotein

Chain K:



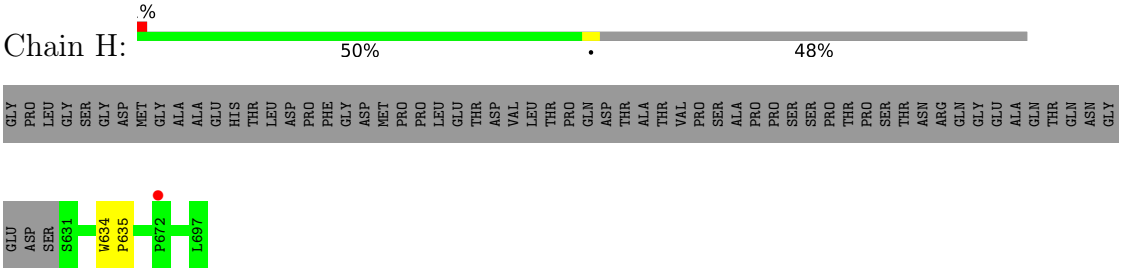
- Molecule 1: Nucleoprotein

Chain V:



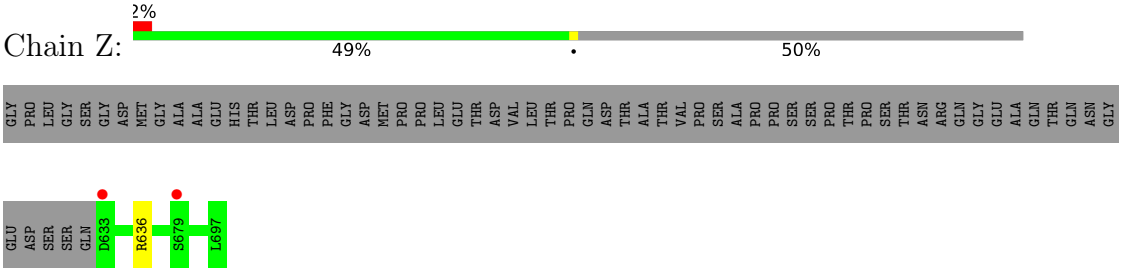
• Molecule 1: Nucleoprotein

Chain H:



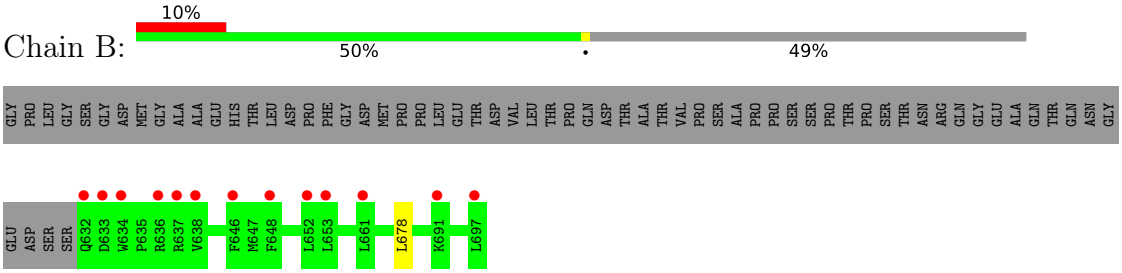
• Molecule 1: Nucleoprotein

Chain Z:



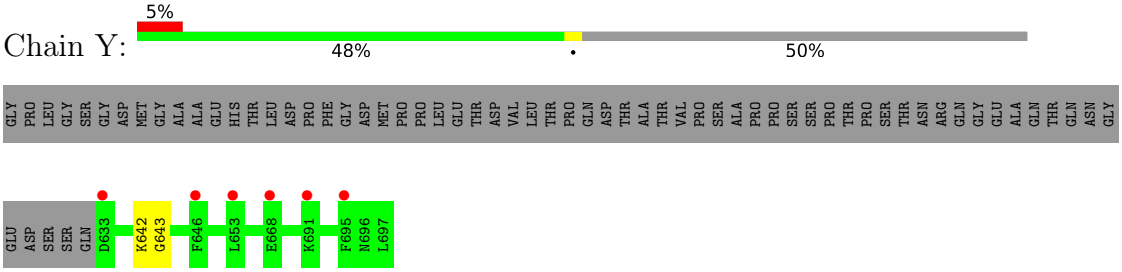
• Molecule 1: Nucleoprotein

Chain B:



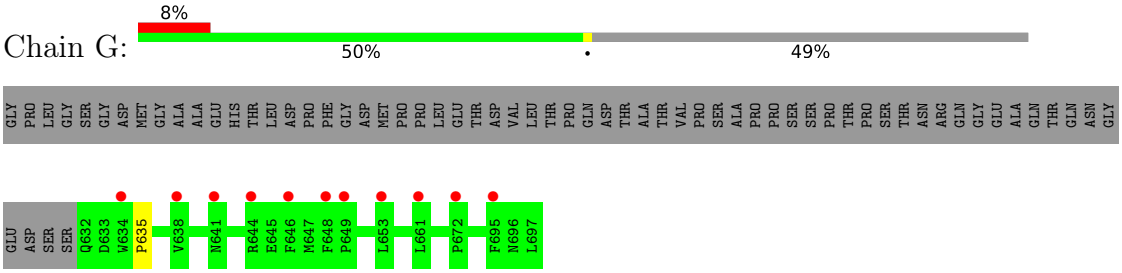
• Molecule 1: Nucleoprotein

Chain Y:



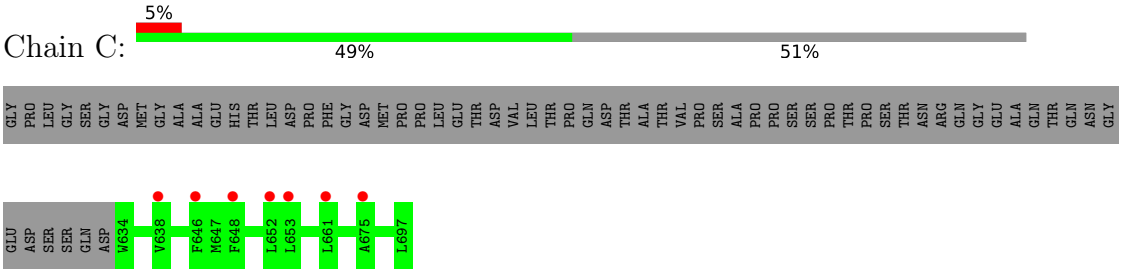
• Molecule 1: Nucleoprotein

Chain G:



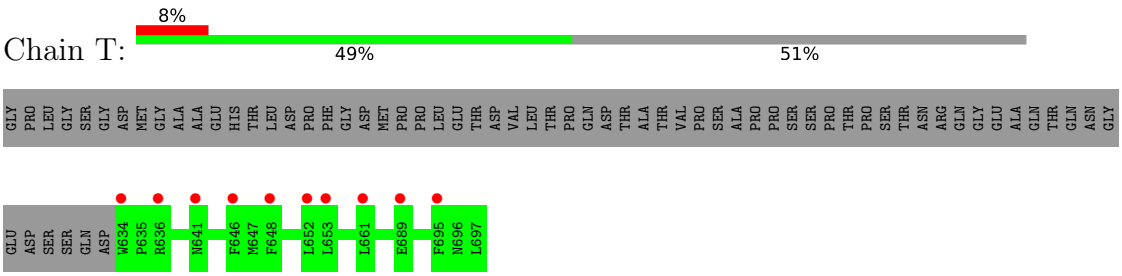
• Molecule 1: Nucleoprotein

Chain C:



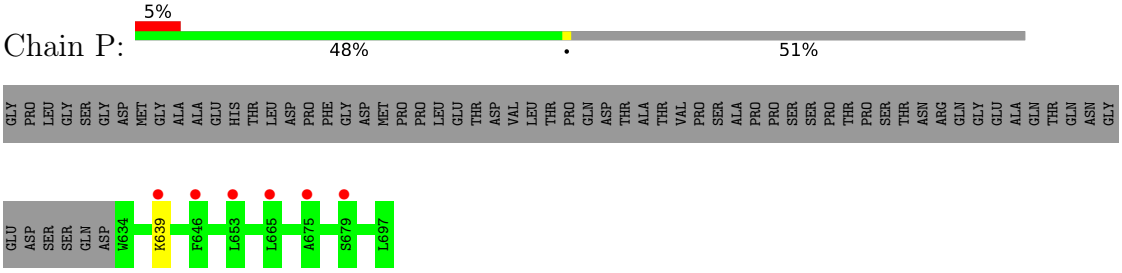
• Molecule 1: Nucleoprotein

Chain T:



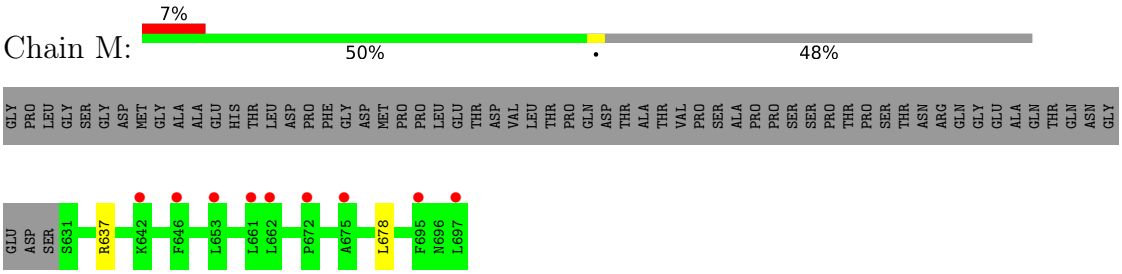
• Molecule 1: Nucleoprotein

Chain P:



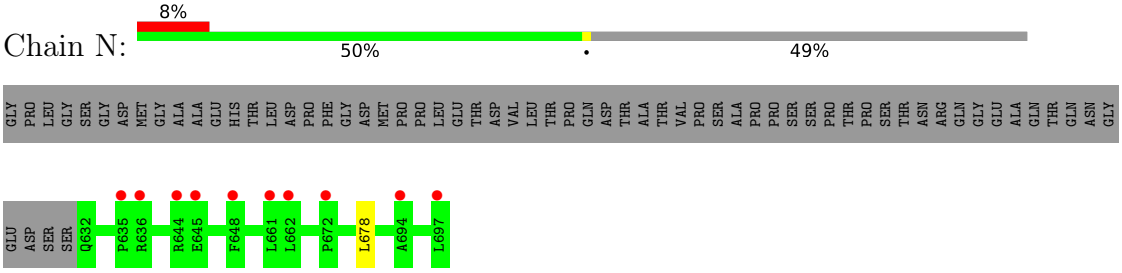
• Molecule 1: Nucleoprotein

Chain M:



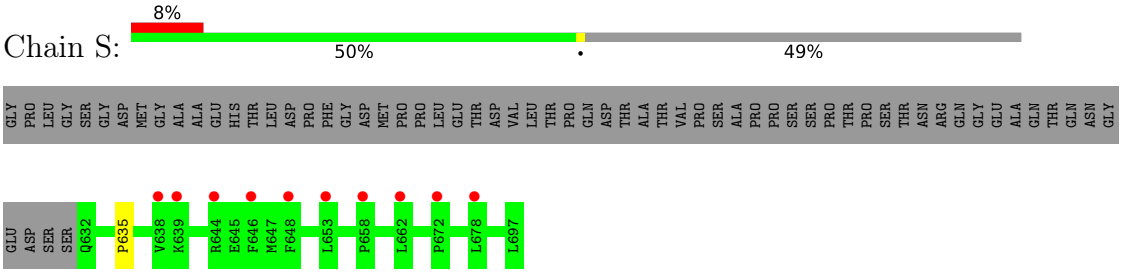
• Molecule 1: Nucleoprotein

Chain N:



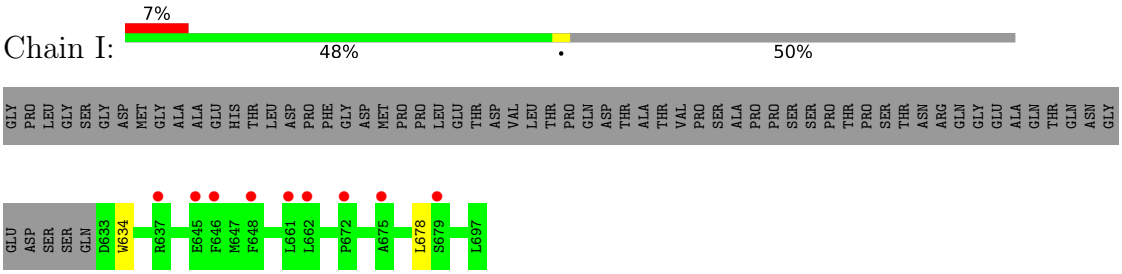
• Molecule 1: Nucleoprotein

Chain S:



• Molecule 1: Nucleoprotein

Chain I:

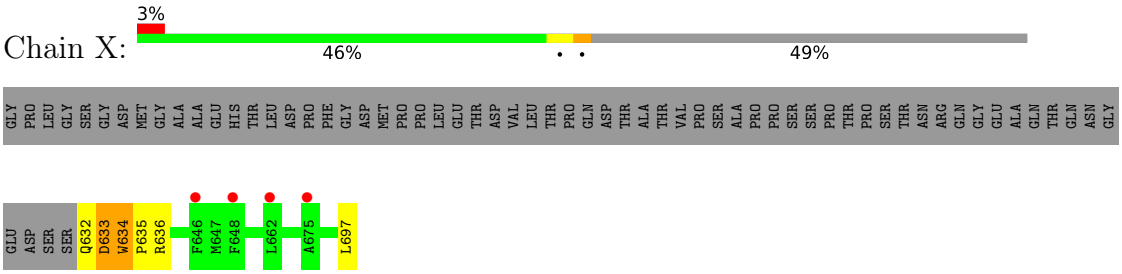


• Molecule 1: Nucleoprotein

Chain A:

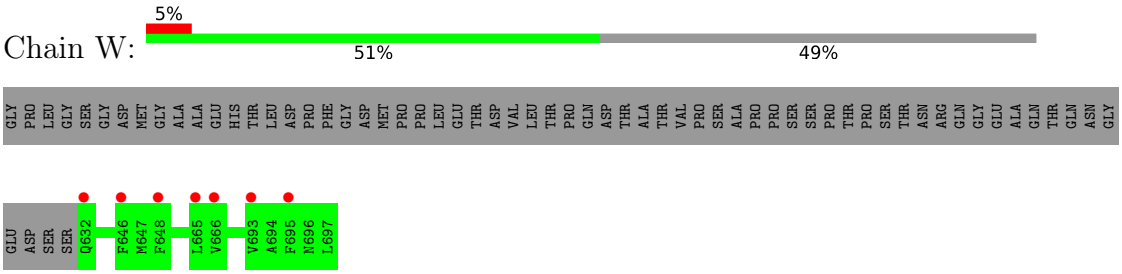
• Molecule 1: Nucleoprotein

Chain X:



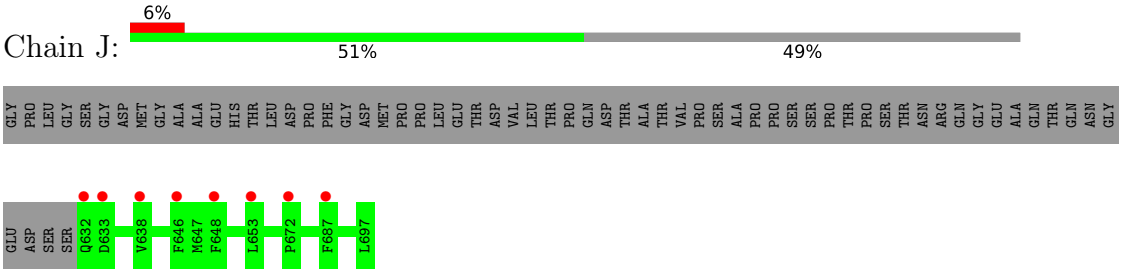
• Molecule 1: Nucleoprotein

Chain W:



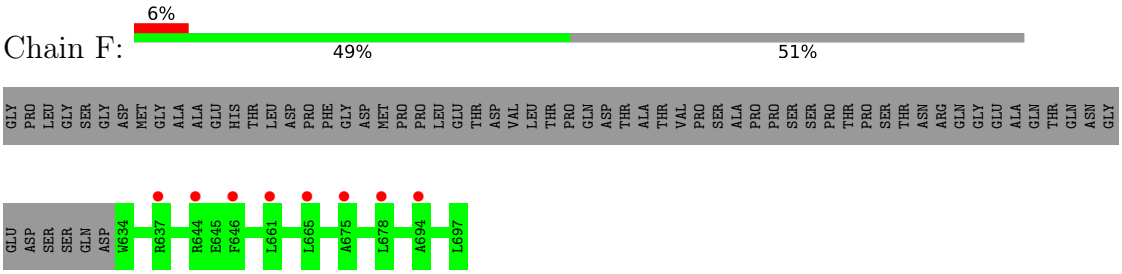
• Molecule 1: Nucleoprotein

Chain J:



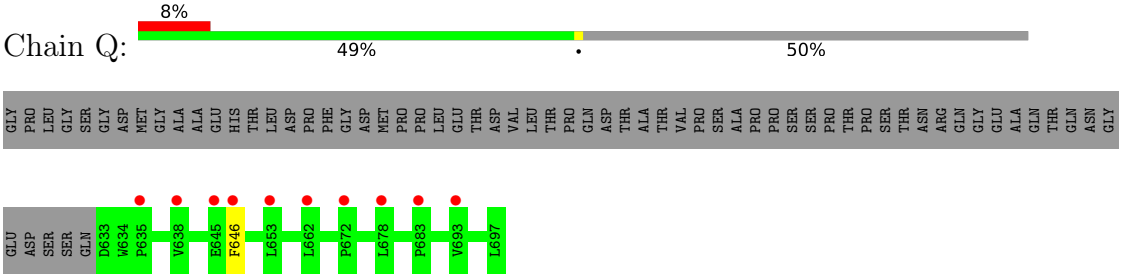
• Molecule 1: Nucleoprotein

Chain F:



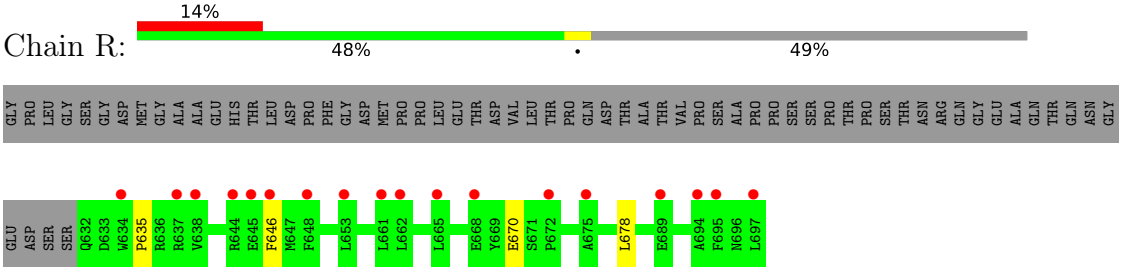
• Molecule 1: Nucleoprotein

Chain Q:



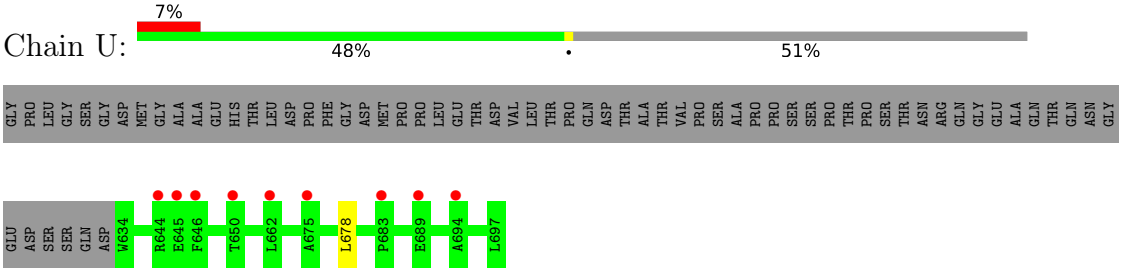
• Molecule 1: Nucleoprotein

Chain R:



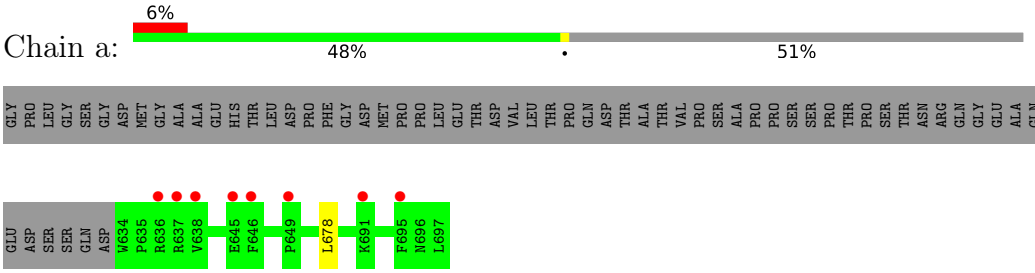
• Molecule 1: Nucleoprotein

Chain U:



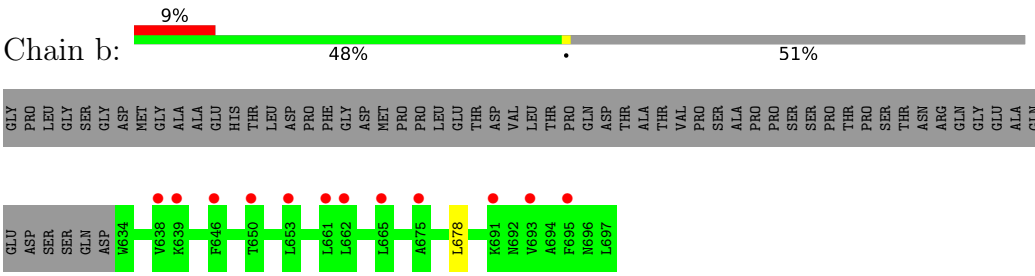
• Molecule 1: Nucleoprotein

Chain a:



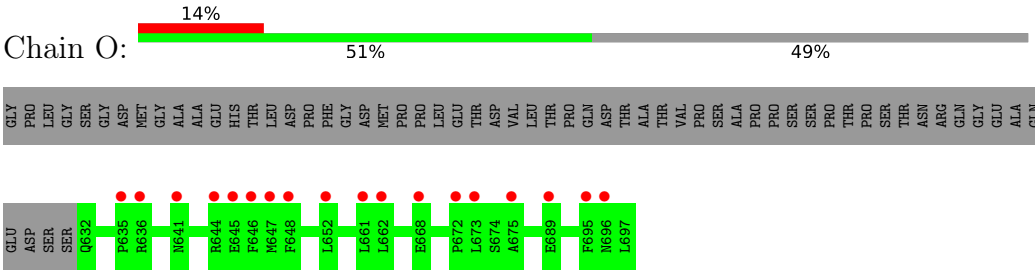
• Molecule 1: Nucleoprotein

Chain b:



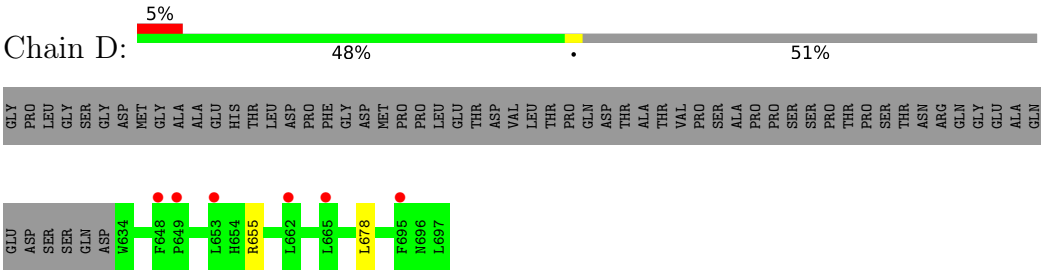
• Molecule 1: Nucleoprotein

Chain O:



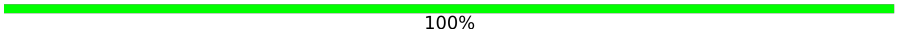
• Molecule 1: Nucleoprotein

Chain D:



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

Chain c:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

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 – 3.26 142.16 – 3.26	Depositor EDS
% Data completeness (in resolution range)	62.0 (47.99-3.26) 62.1 (142.16-3.26)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.10%)	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)	0.36 , 75.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.069 for -h,-k,-h+l	Xtriage
F_o,F_c correlation	0.89	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.25	0/550	0.45	0/747
1	B	0.25	0/567	0.49	0/770
1	C	0.24	0/550	0.48	0/747
1	D	0.24	0/550	0.49	0/747
1	E	0.24	0/558	0.48	0/758
1	F	0.24	0/550	0.49	0/747
1	G	0.25	0/567	0.48	0/770
1	H	0.44	1/573 (0.2%)	0.60	1/778 (0.1%)
1	I	0.24	0/558	0.47	0/758
1	J	0.24	0/567	0.49	0/770
1	K	0.26	0/550	0.51	0/747
1	L	0.24	0/550	0.48	0/747
1	M	0.24	0/573	0.48	0/778
1	N	0.24	0/567	0.47	0/770
1	O	0.24	0/567	0.46	0/770
1	P	0.24	0/550	0.49	0/747
1	Q	0.24	0/558	0.50	0/758
1	R	0.50	1/567 (0.2%)	0.69	2/770 (0.3%)
1	S	0.24	0/567	0.55	1/770 (0.1%)
1	T	0.23	0/550	0.47	0/747
1	U	0.24	0/550	0.49	0/747
1	V	0.25	0/567	0.48	0/770
1	W	0.24	0/567	0.47	0/770
1	X	0.35	1/567 (0.2%)	0.76	4/770 (0.5%)
1	Y	0.55	2/558 (0.4%)	0.53	0/758
1	Z	0.24	0/558	0.45	0/758
1	a	0.24	0/550	0.48	0/747
1	b	0.24	0/550	0.49	0/747
2	c	0.26	0/48	0.64	0/65
All	All	0.29	5/15704 (0.0%)	0.51	8/21328 (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	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	R	670	GLU	C-N	10.17	1.57	1.34
1	Y	643	GLY	C-N	9.25	1.55	1.34
1	H	634	TRP	C-N	8.62	1.50	1.34
1	Y	642	LYS	C-N	6.76	1.45	1.33
1	X	632	GLN	C-N	-5.00	1.22	1.34

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	633	ASP	N-CA-C	10.60	139.63	111.00
1	R	670	GLU	N-CA-C	-9.86	84.39	111.00
1	H	635	PRO	N-CA-C	-7.50	92.60	112.10
1	S	635	PRO	N-CA-C	-6.28	95.77	112.10
1	X	697	LEU	CA-CB-CG	5.46	127.85	115.30

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 (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	9	37
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%)	9	37
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
1	W	64/130 (49%)	60 (94%)	4 (6%)	0	100	100
1	X	64/130 (49%)	59 (92%)	4 (6%)	1 (2%)	9	37
1	Y	63/130 (48%)	59 (94%)	4 (6%)	0	100	100

Continued on next page...

Continued from previous page...

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%)	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%)	47	77

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 (i)

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%)	61 (98%)	1 (2%)	62	79
1	C	60/114 (53%)	60 (100%)	0	100	100
1	D	60/114 (53%)	58 (97%)	2 (3%)	38	65
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%)	59 (97%)	2 (3%)	38	65
1	J	62/114 (54%)	62 (100%)	0	100	100
1	K	60/114 (53%)	59 (98%)	1 (2%)	60	78
1	L	60/114 (53%)	59 (98%)	1 (2%)	60	78
1	M	63/114 (55%)	61 (97%)	2 (3%)	39	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	N	62/114 (54%)	61 (98%)	1 (2%)	62 79
1	O	62/114 (54%)	62 (100%)	0	100 100
1	P	60/114 (53%)	59 (98%)	1 (2%)	60 78
1	Q	61/114 (54%)	60 (98%)	1 (2%)	62 79
1	R	62/114 (54%)	60 (97%)	2 (3%)	39 66
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%)	59 (98%)	1 (2%)	60 78
1	V	62/114 (54%)	61 (98%)	1 (2%)	62 79
1	W	62/114 (54%)	62 (100%)	0	100 100
1	X	62/114 (54%)	61 (98%)	1 (2%)	62 79
1	Y	61/114 (54%)	61 (100%)	0	100 100
1	Z	61/114 (54%)	60 (98%)	1 (2%)	62 79
1	a	60/114 (53%)	59 (98%)	1 (2%)	60 78
1	b	60/114 (53%)	59 (98%)	1 (2%)	60 78
All	All	1711/3192 (54%)	1691 (99%)	20 (1%)	71 83

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	678	LEU
1	b	678	LEU
1	D	678	LEU
1	D	655	ARG
1	M	637	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	696	ASN
1	L	641	ASN
1	G	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.69	6 (9%) 8 9	100, 128, 155, 162	0
1	B	66/130 (50%)	1.08	13 (19%) 1 1	95, 117, 151, 172	0
1	C	64/130 (49%)	0.77	7 (10%) 5 5	100, 121, 147, 155	0
1	D	64/130 (49%)	0.74	6 (9%) 8 9	97, 129, 166, 180	0
1	E	65/130 (50%)	0.81	5 (7%) 13 12	87, 101, 124, 166	0
1	F	64/130 (49%)	0.79	8 (12%) 3 3	91, 128, 154, 168	0
1	G	66/130 (50%)	1.04	11 (16%) 1 1	93, 113, 165, 182	0
1	H	67/130 (51%)	0.54	1 (1%) 73 71	87, 108, 137, 152	0
1	I	65/130 (50%)	0.87	9 (13%) 2 2	90, 122, 156, 189	0
1	J	66/130 (50%)	0.85	8 (12%) 4 4	81, 109, 146, 188	0
1	K	64/130 (49%)	0.77	7 (10%) 5 5	71, 94, 119, 125	0
1	L	64/130 (49%)	0.71	4 (6%) 20 19	74, 95, 119, 132	0
1	M	67/130 (51%)	0.74	9 (13%) 3 3	95, 123, 153, 168	0
1	N	66/130 (50%)	0.89	10 (15%) 2 2	113, 136, 166, 189	0
1	O	66/130 (50%)	1.22	18 (27%) 0 0	109, 145, 172, 190	0
1	P	64/130 (49%)	0.68	6 (9%) 8 9	92, 114, 130, 144	0
1	Q	65/130 (50%)	0.94	10 (15%) 2 2	103, 126, 163, 193	0
1	R	66/130 (50%)	1.28	18 (27%) 0 0	94, 151, 181, 188	0
1	S	66/130 (50%)	0.76	10 (15%) 2 2	88, 118, 141, 162	0
1	T	64/130 (49%)	0.89	10 (15%) 2 2	95, 124, 162, 175	0
1	U	64/130 (49%)	0.77	9 (14%) 2 2	102, 122, 147, 156	0
1	V	66/130 (50%)	0.82	5 (7%) 13 12	80, 99, 137, 154	0
1	W	66/130 (50%)	0.67	7 (10%) 6 6	89, 123, 152, 164	0
1	X	66/130 (50%)	0.67	4 (6%) 21 20	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%)	0.80	6 (9%) 9 10	79, 96, 128, 163	0
1	Z	65/130 (50%)	0.61	2 (3%) 49 47	80, 98, 121, 144	0
1	a	64/130 (49%)	0.81	8 (12%) 3 3	89, 109, 144, 158	0
1	b	64/130 (49%)	0.93	12 (18%) 1 1	107, 139, 162, 167	0
2	c	10/10 (100%)	0.32	0 100 100	87, 94, 106, 109	0
All	All	1833/3650 (50%)	0.82	229 (12%) 3 3	71, 117, 161, 193	0

The worst 5 of 229 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	632	GLN	8.7
1	G	634	TRP	8.3
1	R	634	TRP	6.4
1	J	632	GLN	5.9
1	Q	646	PHE	5.7

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 monosaccharides 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.