



Full wwPDB X-ray Structure Validation Report ⓘ

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-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

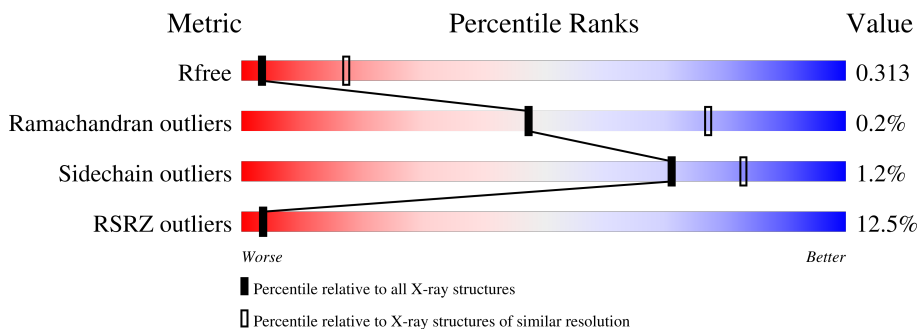
1 Overall quality at a glance

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 $\leq 5\%$. 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	
1	B	130	
1	C	130	
1	D	130	
1	E	130	
1	F	130	
1	G	130	

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Mol	Chain	Length	Quality of chain
1	H	130	% 50% 48%
1	I	130	7% 48% 50%
1	J	130	6% 51% 49%
1	K	130	5% 48% 51%
1	L	130	3% 48% 51%
1	M	130	7% 50% 48%
1	N	130	8% 50% 49%
1	O	130	14% 51% 49%
1	P	130	5% 48% 51%
1	Q	130	8% 49% 50%
1	R	130	14% 48% 49%
1	S	130	8% 50% 49%
1	T	130	8% 49% 51%
1	U	130	7% 48% 51%
1	V	130	4% 50% 49%
1	W	130	5% 51% 49%
1	X	130	3% 46% 49%
1	Y	130	5% 48% 50%
1	Z	130	2% 49% 50%
1	a	130	6% 48% 51%
1	b	130	9% 48% 51%
2	c	10	100%

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

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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

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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

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Chain	Residue	Modelled	Actual	Comment	Reference
P	570	LEU	-	expression tag	UNP A0A1Q1NMMU1
P	571	GLY	-	expression tag	UNP A0A1Q1NMMU1
P	572	SER	-	expression tag	UNP A0A1Q1NMMU1
M	568	GLY	-	expression tag	UNP A0A1Q1NMMU1
M	569	PRO	-	expression tag	UNP A0A1Q1NMMU1
M	570	LEU	-	expression tag	UNP A0A1Q1NMMU1
M	571	GLY	-	expression tag	UNP A0A1Q1NMMU1
M	572	SER	-	expression tag	UNP A0A1Q1NMMU1
N	568	GLY	-	expression tag	UNP A0A1Q1NMMU1
N	569	PRO	-	expression tag	UNP A0A1Q1NMMU1
N	570	LEU	-	expression tag	UNP A0A1Q1NMMU1
N	571	GLY	-	expression tag	UNP A0A1Q1NMMU1
N	572	SER	-	expression tag	UNP A0A1Q1NMMU1
S	568	GLY	-	expression tag	UNP A0A1Q1NMMU1
S	569	PRO	-	expression tag	UNP A0A1Q1NMMU1
S	570	LEU	-	expression tag	UNP A0A1Q1NMMU1
S	571	GLY	-	expression tag	UNP A0A1Q1NMMU1
S	572	SER	-	expression tag	UNP A0A1Q1NMMU1
I	568	GLY	-	expression tag	UNP A0A1Q1NMMU1
I	569	PRO	-	expression tag	UNP A0A1Q1NMMU1
I	570	LEU	-	expression tag	UNP A0A1Q1NMMU1
I	571	GLY	-	expression tag	UNP A0A1Q1NMMU1
I	572	SER	-	expression tag	UNP A0A1Q1NMMU1
A	568	GLY	-	expression tag	UNP A0A1Q1NMMU1
A	569	PRO	-	expression tag	UNP A0A1Q1NMMU1
A	570	LEU	-	expression tag	UNP A0A1Q1NMMU1
A	571	GLY	-	expression tag	UNP A0A1Q1NMMU1
A	572	SER	-	expression tag	UNP A0A1Q1NMMU1
X	568	GLY	-	expression tag	UNP A0A1Q1NMMU1
X	569	PRO	-	expression tag	UNP A0A1Q1NMMU1
X	570	LEU	-	expression tag	UNP A0A1Q1NMMU1
X	571	GLY	-	expression tag	UNP A0A1Q1NMMU1
X	572	SER	-	expression tag	UNP A0A1Q1NMMU1
W	568	GLY	-	expression tag	UNP A0A1Q1NMMU1
W	569	PRO	-	expression tag	UNP A0A1Q1NMMU1
W	570	LEU	-	expression tag	UNP A0A1Q1NMMU1
W	571	GLY	-	expression tag	UNP A0A1Q1NMMU1
W	572	SER	-	expression tag	UNP A0A1Q1NMMU1
J	568	GLY	-	expression tag	UNP A0A1Q1NMMU1
J	569	PRO	-	expression tag	UNP A0A1Q1NMMU1
J	570	LEU	-	expression tag	UNP A0A1Q1NMMU1
J	571	GLY	-	expression tag	UNP A0A1Q1NMMU1

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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

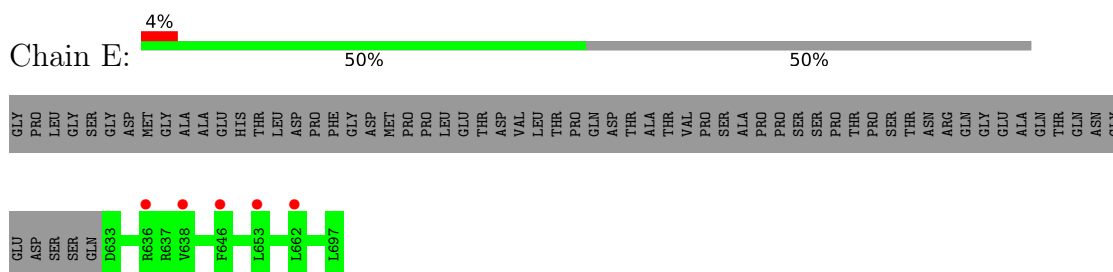
- Molecule 2 is a protein called ALA-ALA-GLY-ALA-ALA-ALA-ALA-ALA-ALA-ALA.

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

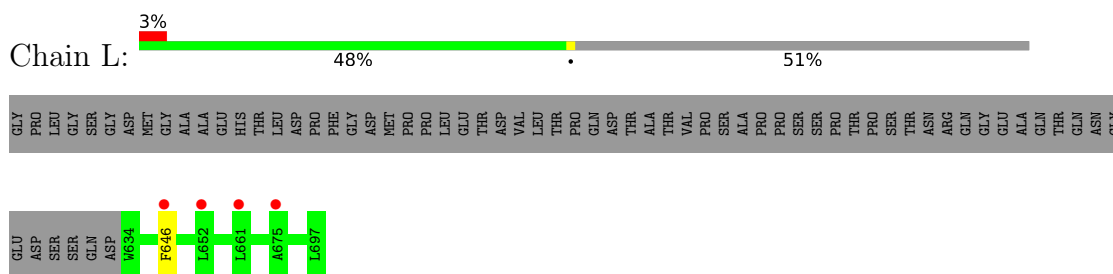
3 Residue-property plots [i](#)

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



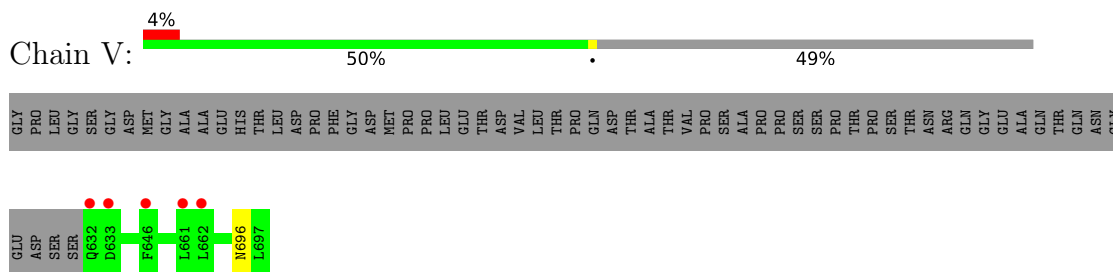
- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein



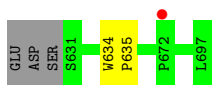
- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein



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



- Molecule 1: Nucleoprotein



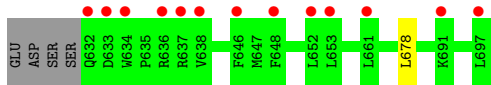
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- Molecule 1: Nucleoprotein



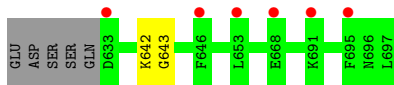
GLY PRO LEU LEU SER SER ASP MET GLY GLY ALA ALA HIS THR LEU LEU ASP ASP PHE GLY ASP MET PRO PRO LEU LEU THR ASP VAL LEU THR THR PRO GLN ASP THR ALA ALA THR VAL PRO ALA PRO SER SER PRO THR THR SER SER ASN ARG GLN GLY GLY ALA ALA THR GLN ASN GLY



- Molecule 1: Nucleoprotein



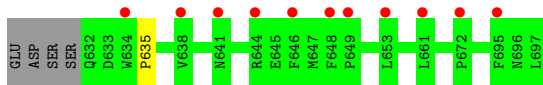
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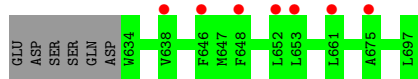
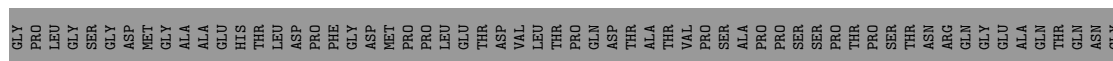
- Molecule 1: Nucleoprotein



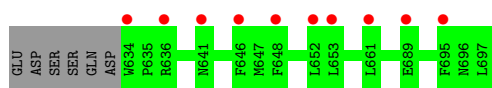
GLY PRO LEU LEU SER SER ASP MET GLY GLY ALA ALA HIS THR LEU LEU ASP ASP PHE GLY ASP MET PRO PRO LEU LEU THR ASP VAL LEU THR THR PRO GLN ASP THR ALA ALA THR VAL PRO ALA PRO SER SER PRO THR THR SER SER ASN ARG GLN GLY GLY ALA ALA THR GLN ASN GLY



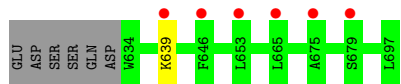
- Molecule 1: Nucleoprotein



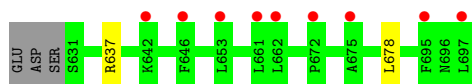
- Molecule 1: Nucleoprotein



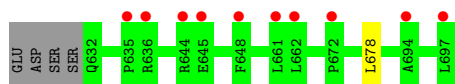
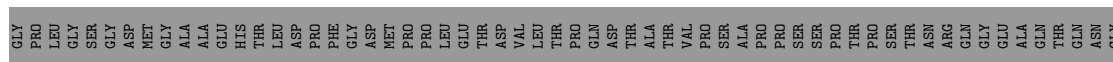
- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein



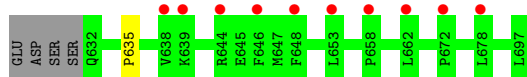
- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein



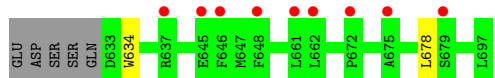
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● Molecule 1: Nucleoprotein



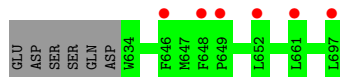
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● Molecule 1: Nucleoprotein



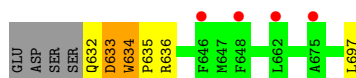
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● Molecule 1: Nucleoprotein



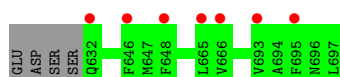
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● Molecule 1: Nucleoprotein



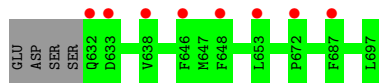
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● Molecule 1: Nucleoprotein



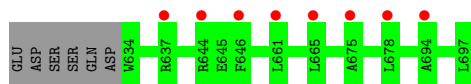
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- Molecule 1: Nucleoprotein



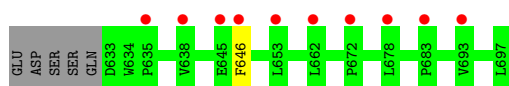
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- Molecule 1: Nucleoprotein



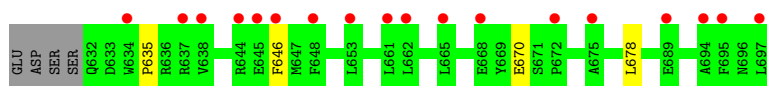
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- Molecule 1: Nucleoprotein



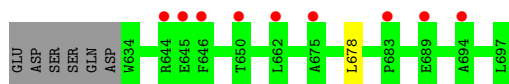
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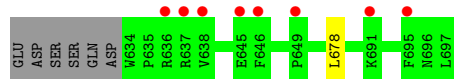
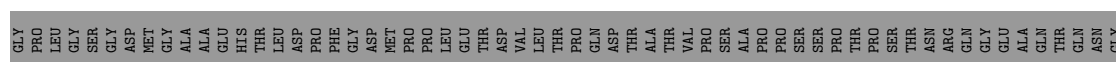
- Molecule 1: Nucleoprotein



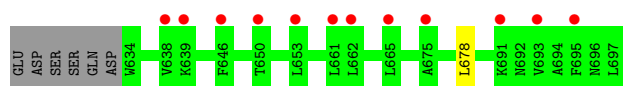
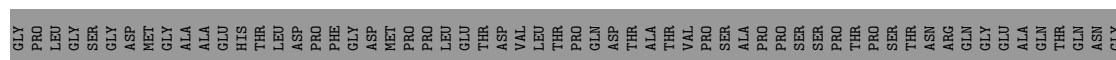
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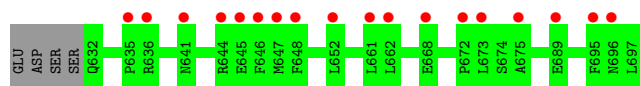
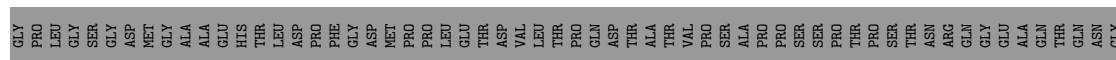
- Molecule 1: Nucleoprotein



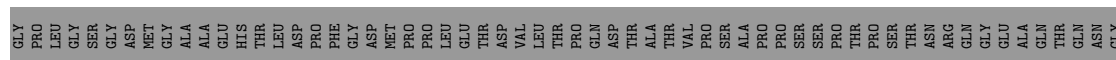
- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein



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



There are no outlier residues recorded for this chain.

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 – 3.26 142.16 – 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
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.26Å)	Xtrriage
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	Xtrriage
Anisotropy	0.082	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 75.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.069 for -h,-k,-h+1	Xtrriage
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

Xtrriage'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 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

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	R	670	GLU	O-C-N	5.32	131.21	122.70
1	X	633	ASP	CB-CG-OD2	5.24	123.01	118.30
1	X	634	TRP	N-CA-C	-5.22	96.91	111.00

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

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

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	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

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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%)	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

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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

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	646	PHE
1	K	634	TRP
1	V	696	ASN
1	Z	636	ARG
1	B	678	LEU
1	P	639	LYS
1	M	637	ARG
1	M	678	LEU
1	N	678	LEU
1	I	634	TRP
1	I	678	LEU
1	X	634	TRP
1	Q	646	PHE
1	R	646	PHE
1	R	678	LEU
1	U	678	LEU
1	a	678	LEU

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Mol	Chain	Res	Type
1	b	678	LEU
1	D	655	ARG
1	D	678	LEU

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 [i](#)

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 monosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.69	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

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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

All (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
1	R	645	GLU	5.3
1	I	646	PHE	5.2
1	Q	635	PRO	5.1
1	R	646	PHE	4.9
1	O	641	ASN	4.8
1	A	648	PHE	4.8
1	T	661	LEU	4.7
1	V	633	ASP	4.7
1	O	645	GLU	4.6
1	R	648	PHE	4.5
1	S	644	ARG	4.5
1	D	648	PHE	4.5
1	G	646	PHE	4.2
1	J	646	PHE	4.1
1	B	646	PHE	4.0
1	W	646	PHE	4.0
1	N	636	ARG	3.9
1	O	646	PHE	3.9
1	b	695	PHE	3.9
1	R	653	LEU	3.8
1	F	661	LEU	3.8
1	M	642	LYS	3.8
1	I	648	PHE	3.7
1	U	646	PHE	3.7
1	I	661	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	Z	633	ASP	3.6
1	Y	633	ASP	3.6
1	V	646	PHE	3.6
1	V	632	GLN	3.6
1	N	672	PRO	3.6
1	S	639	LYS	3.6
1	B	636	ARG	3.5
1	N	644	ARG	3.5
1	C	646	PHE	3.5
1	O	647	MET	3.5
1	I	675	ALA	3.4
1	N	648	PHE	3.4
1	X	662	LEU	3.4
1	I	662	LEU	3.4
1	T	646	PHE	3.4
1	M	672	PRO	3.4
1	G	661	LEU	3.4
1	P	646	PHE	3.3
1	R	675	ALA	3.3
1	F	646	PHE	3.3
1	O	675	ALA	3.3
1	S	646	PHE	3.3
1	V	662	LEU	3.2
1	F	675	ALA	3.2
1	R	644	ARG	3.2
1	B	661	LEU	3.2
1	A	697	LEU	3.2
1	R	662	LEU	3.2
1	O	695	PHE	3.2
1	b	646	PHE	3.2
1	O	644	ARG	3.1
1	W	693	VAL	3.0
1	L	661	LEU	3.0
1	N	697	LEU	3.0
1	M	675	ALA	3.0
1	b	693	VAL	3.0
1	Q	653	LEU	3.0
1	S	648	PHE	2.9
1	a	646	PHE	2.9
1	B	637	ARG	2.9
1	O	689	GLU	2.9
1	R	694	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	638	VAL	2.9
1	O	636	ARG	2.9
1	Q	638	VAL	2.9
1	J	653	LEU	2.9
1	U	675	ALA	2.8
1	I	645	GLU	2.8
1	E	662	LEU	2.8
1	W	665	LEU	2.8
1	R	637	ARG	2.8
1	b	661	LEU	2.8
1	a	638	VAL	2.8
1	T	641	ASN	2.8
1	G	695	PHE	2.8
1	G	649	PRO	2.8
1	X	646	PHE	2.8
1	B	648	PHE	2.8
1	G	648	PHE	2.8
1	S	672	PRO	2.7
1	T	636	ARG	2.7
1	F	644	ARG	2.7
1	A	652	LEU	2.7
1	R	661	LEU	2.7
1	I	672	PRO	2.7
1	G	653	LEU	2.7
1	Y	646	PHE	2.7
1	A	646	PHE	2.7
1	N	635	PRO	2.7
1	O	696	ASN	2.6
1	V	661	LEU	2.6
1	B	638	VAL	2.6
1	b	638	VAL	2.6
1	C	648	PHE	2.6
1	T	648	PHE	2.6
1	B	633	ASP	2.6
1	P	653	LEU	2.6
1	C	675	ALA	2.5
1	a	636	ARG	2.5
1	P	679	SER	2.5
1	K	646	PHE	2.5
1	D	665	LEU	2.5
1	B	634	TRP	2.5
1	b	639	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	646	PHE	2.5
1	N	645	GLU	2.5
1	U	689	GLU	2.5
1	H	672	PRO	2.5
1	J	672	PRO	2.5
1	M	646	PHE	2.5
1	D	695	PHE	2.5
1	G	644	ARG	2.5
1	O	652	LEU	2.5
1	Q	693	VAL	2.5
1	A	661	LEU	2.4
1	b	662	LEU	2.4
1	W	632	GLN	2.4
1	R	689	GLU	2.4
1	R	665	LEU	2.4
1	M	695	PHE	2.4
1	I	637	ARG	2.4
1	Y	691	LYS	2.4
1	P	639	LYS	2.4
1	T	689	GLU	2.4
1	a	637	ARG	2.4
1	O	661	LEU	2.4
1	U	662	LEU	2.4
1	O	672	PRO	2.4
1	K	652	LEU	2.4
1	O	635	PRO	2.4
1	B	652	LEU	2.4
1	E	653	LEU	2.4
1	P	665	LEU	2.4
1	M	662	LEU	2.4
1	C	653	LEU	2.4
1	K	637	ARG	2.3
1	b	653	LEU	2.3
1	N	694	ALA	2.3
1	X	675	ALA	2.3
1	Y	695	PHE	2.3
1	M	697	LEU	2.3
1	O	668	GLU	2.3
1	a	645	GLU	2.3
1	T	652	LEU	2.3
1	S	678	LEU	2.3
1	D	653	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	X	648	PHE	2.3
1	J	638	VAL	2.3
1	F	665	LEU	2.3
1	O	662	LEU	2.3
1	W	666	VAL	2.3
1	N	661	LEU	2.3
1	E	638	VAL	2.3
1	A	649	PRO	2.3
1	Q	683	PRO	2.3
1	J	633	ASP	2.2
1	F	678	LEU	2.2
1	S	658	PRO	2.2
1	Q	672	PRO	2.2
1	C	638	VAL	2.2
1	T	695	PHE	2.2
1	T	634	TRP	2.2
1	b	665	LEU	2.2
1	R	668	GLU	2.2
1	K	697	LEU	2.2
1	L	646	PHE	2.2
1	B	691	LYS	2.2
1	F	637	ARG	2.2
1	G	672	PRO	2.2
1	R	695	PHE	2.2
1	R	697	LEU	2.2
1	K	665	LEU	2.1
1	S	653	LEU	2.1
1	Q	678	LEU	2.1
1	O	673	LEU	2.1
1	L	675	ALA	2.1
1	Y	653	LEU	2.1
1	P	675	ALA	2.1
1	a	695	PHE	2.1
1	S	662	LEU	2.1
1	F	694	ALA	2.1
1	U	694	ALA	2.1
1	E	636	ARG	2.1
1	K	649	PRO	2.1
1	M	661	LEU	2.1
1	C	661	LEU	2.1
1	U	645	GLU	2.1
1	K	672	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	679	SER	2.1
1	U	644	ARG	2.1
1	N	662	LEU	2.1
1	D	662	LEU	2.1
1	U	650	THR	2.1
1	a	691	LYS	2.1
1	B	653	LEU	2.1
1	Q	662	LEU	2.1
1	J	648	PHE	2.1
1	C	652	LEU	2.1
1	b	691	LYS	2.0
1	R	638	VAL	2.0
1	R	672	PRO	2.0
1	b	650	THR	2.0
1	M	653	LEU	2.0
1	a	649	PRO	2.0
1	Y	668	GLU	2.0
1	Q	645	GLU	2.0
1	B	697	LEU	2.0
1	J	687	PHE	2.0
1	Z	679	SER	2.0
1	W	695	PHE	2.0
1	U	683	PRO	2.0
1	D	649	PRO	2.0
1	S	638	VAL	2.0
1	L	652	LEU	2.0
1	b	675	ALA	2.0
1	W	648	PHE	2.0
1	O	648	PHE	2.0
1	G	641	ASN	2.0
1	T	653	LEU	2.0

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.