



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:55 AM UTC

PDB ID : 8P0Y / pdb_00008p0y
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 : 4.12 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
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

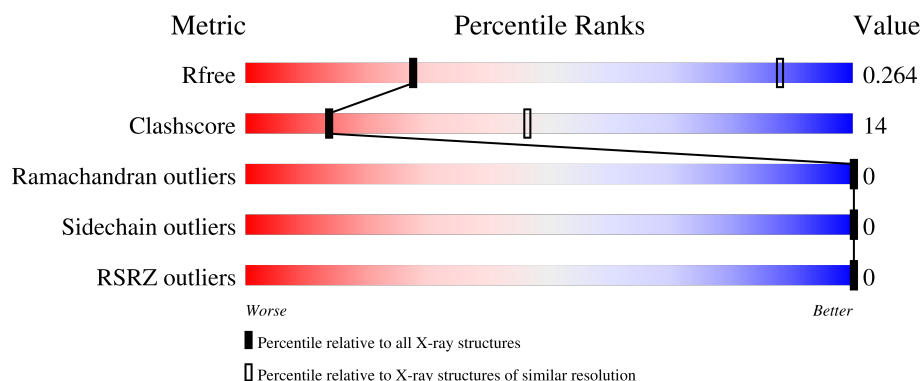
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.12 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.



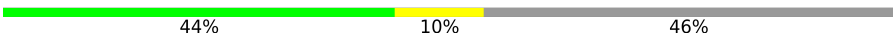
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1249 (4.44-3.80)
Clashscore	190562	1031 (4.42-3.82)
Ramachandran outliers	187476	1211 (4.44-3.80)
Sidechain outliers	187428	1198 (4.44-3.80)
RSRZ outliers	180081	1246 (4.44-3.80)

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	37% 14% 49%
1	O	130	37% 13% 50%
1	P	130	35% 15% 50%
1	Q	130	33% 17% 50%
1	R	130	28% 21% 52%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
2	C	5	
3	B	33	
4	D	34	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8000 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	64	Total	C	N	O	S	0	0	0
			535	341	91	101	2			
1	Y	65	Total	C	N	O	S	0	0	0
			543	345	92	104	2			
1	T	66	Total	C	N	O	S	0	0	0
			552	350	94	106	2			
1	P	65	Total	C	N	O	S	0	0	0
			543	345	92	104	2			
1	S	64	Total	C	N	O	S	0	0	0
			535	341	91	101	2			
1	X	65	Total	C	N	O	S	0	0	0
			543	345	92	104	2			
1	W	66	Total	C	N	O	S	0	0	0
			552	350	94	106	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	69	Total	C	N	O	S	0	0	0
			572	360	97	113	2			
1	a	70	Total	C	N	O	S	0	0	0
			565	359	97	107	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			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	568	GLY	-	expression tag	UNP A0A1Q1NMU1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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
P	570	LEU	-	expression tag	UNP A0A1Q1NMU1
P	571	GLY	-	expression tag	UNP A0A1Q1NMU1
P	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
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
Q	568	GLY	-	expression tag	UNP A0A1Q1NMU1
Q	569	PRO	-	expression tag	UNP A0A1Q1NMU1
Q	570	LEU	-	expression tag	UNP A0A1Q1NMU1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

- Molecule 2 is a protein called C-terminal domain of Mengla nucleoprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			25	15	5	5			

- Molecule 3 is a protein called C-terminal domain of Mengla nucleoprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	33	Total	C	N	O	0	0	0
			164	98	33	33			

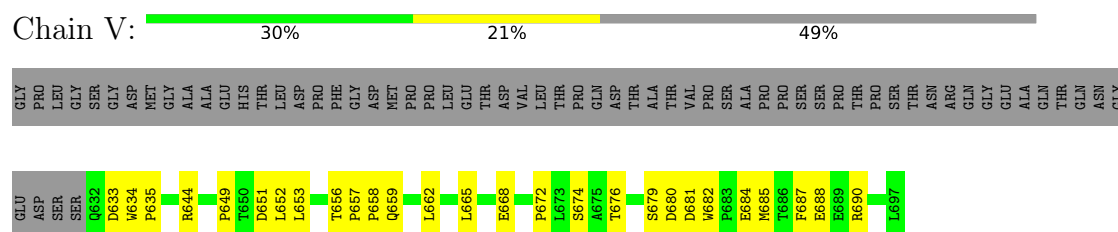
- Molecule 4 is a protein called C-terminal domain of Mengla nucleoprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	32	Total	C	N	O	0	0	0
			160	96	32	32			

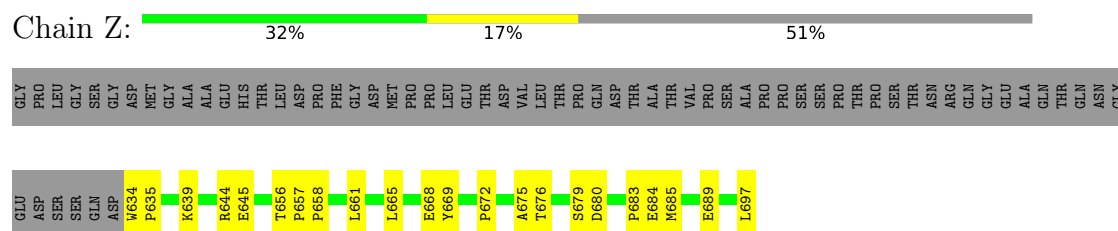
3 Residue-property plots [i](#)

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.

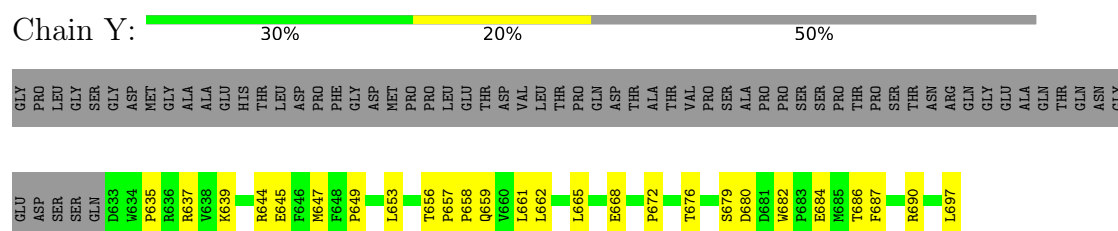
- Molecule 1: Nucleoprotein



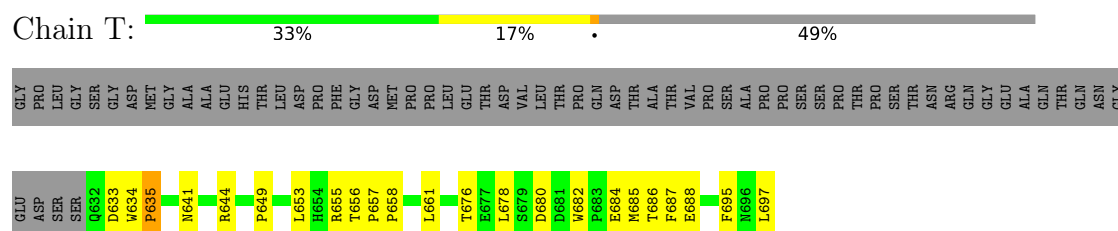
- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein

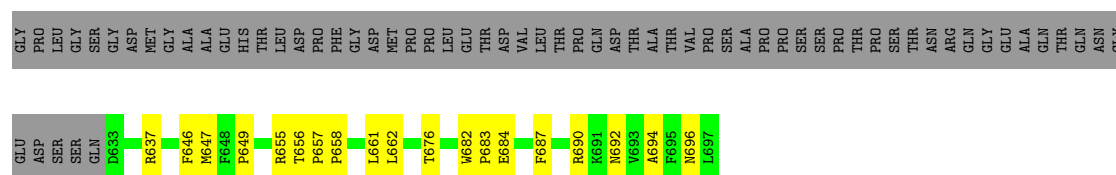


- Molecule 1: Nucleoprotein

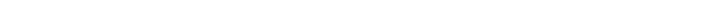


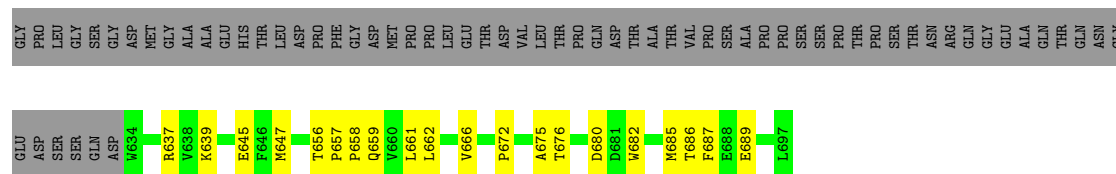
- Molecule 1: Nucleoprotein

Chain P:

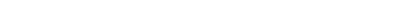


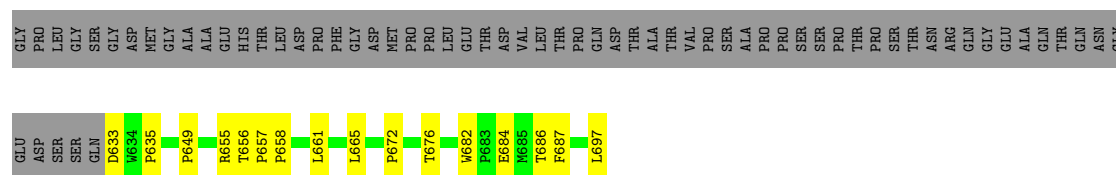
- Molecule 1: Nucleoprotein

Chain S:  34% 15% 51%

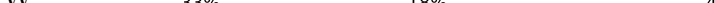


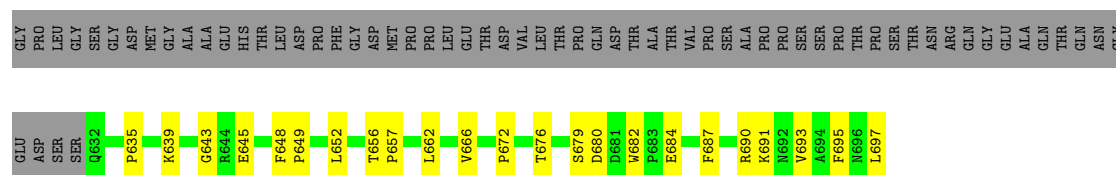
- Molecule 1: Nucleoprotein

Chain X:  38% 12% 50%



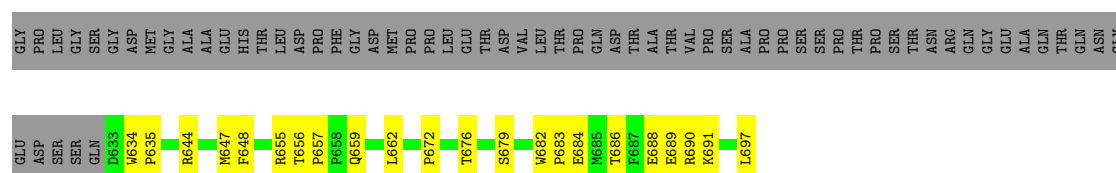
- Molecule 1: Nucleoprotein

Chain W:  33% 18% 49%



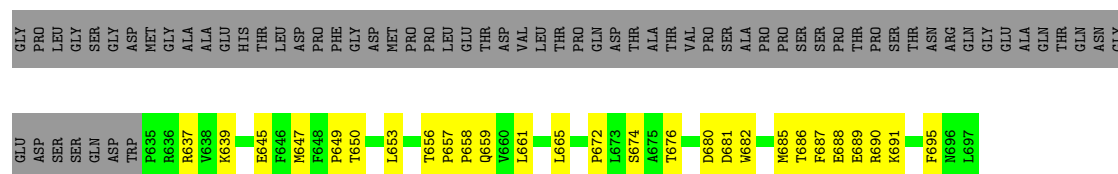
- Molecule 1: Nucleoprotein

Chain Q:  33% 17% 50%

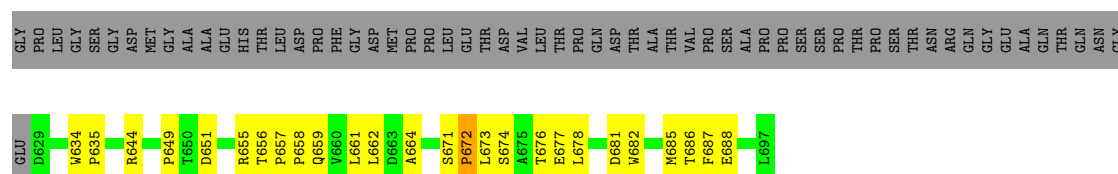
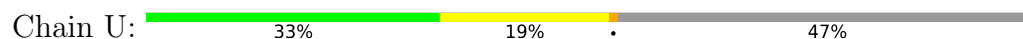


- Molecule 1: Nucleoprotein

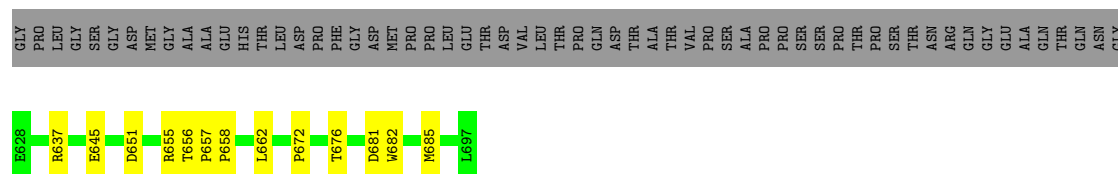
Chain R: 28% 21% 52%



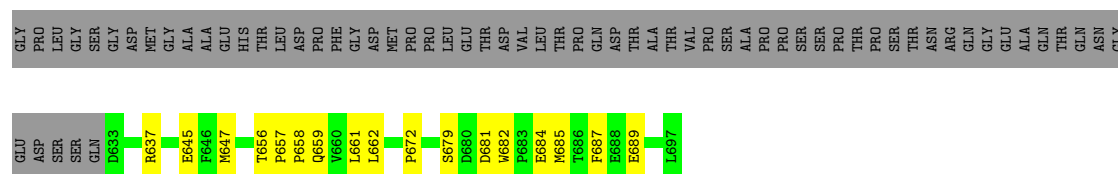
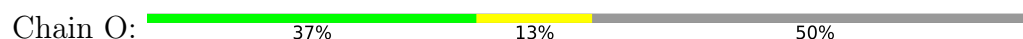
- Molecule 1: Nucleoprotein



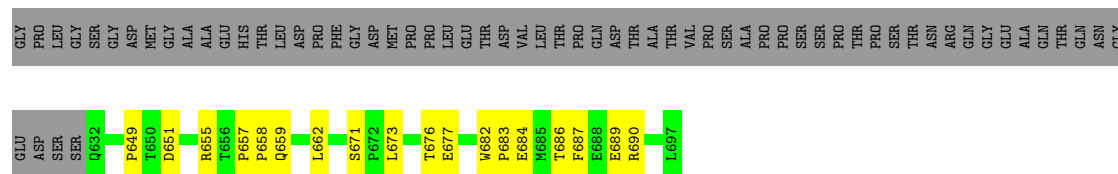
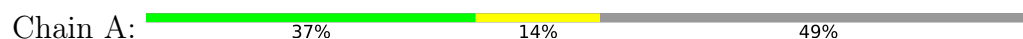
- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein



- Molecule 2: C-terminal domain of Mengla nucleoprotein



There are no outlier residues recorded for this chain.

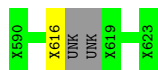
- Molecule 3: C-terminal domain of Mengla nucleoprotein

Chain B:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: C-terminal domain of Mengla nucleoprotein

Chain D:  91% • 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	177.18Å 177.18Å 90.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.90 – 4.12 48.90 – 4.12	Depositor EDS
% Data completeness (in resolution range)	51.0 (48.90-4.12) 51.6 (48.90-4.12)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 4.14Å)	Xtriage
Refinement program	REFMAC dev_4788, PHENIX dev_4788	Depositor
R, R_{free}	0.236 , 0.268 0.244 , 0.264	Depositor DCC
R_{free} test set	672 reflections (2.73%)	wwPDB-VP
Wilson B-factor (Å ²)	153.6	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 195.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.057 for -h,-k,l 0.328 for h,-h-k,-l 0.046 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8000	wwPDB-VP
Average B, all atoms (Å ²)	176.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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	0.20	0/567	0.47	0/770
1	O	0.14	0/558	0.39	0/758
1	P	0.15	0/558	0.32	0/758
1	Q	0.16	0/558	0.39	0/758
1	R	0.16	0/534	0.36	0/723
1	S	0.26	0/550	0.40	0/747
1	T	0.33	1/567 (0.2%)	0.44	0/770
1	U	0.19	0/587	0.57	2/797 (0.3%)
1	V	0.15	0/567	0.42	0/770
1	W	0.15	0/567	0.30	0/770
1	X	0.17	0/558	0.39	0/758
1	Y	0.15	0/558	0.37	0/758
1	Z	0.15	0/550	0.37	0/747
1	a	0.15	0/580	0.38	0/789
All	All	0.19	1/7859 (0.0%)	0.40	2/10673 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	635	PRO	N-CD	6.41	1.56	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	672	PRO	N-CA-C	6.88	126.63	112.47
1	U	672	PRO	CB-CA-C	-6.72	100.47	111.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	552	0	529	15	1
1	O	543	0	521	18	0
1	P	543	0	521	15	0
1	Q	543	0	521	27	0
1	R	521	0	508	30	0
1	S	535	0	517	18	0
1	T	552	0	529	22	0
1	U	572	0	543	27	1
1	V	552	0	529	29	0
1	W	552	0	529	21	0
1	X	543	0	521	19	0
1	Y	543	0	521	28	0
1	Z	535	0	517	20	0
1	a	565	0	529	11	1
2	C	25	0	7	0	0
3	B	164	0	40	0	0
4	D	160	0	45	0	1
All	All	8000	0	7427	223	2

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 14.

All (223) 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:R:686:THR:HG23	1:R:689:GLU:H	1.11	1.13
1:Y:676:THR:HG23	1:X:687:PHE:CD2	1.93	1.03
1:Q:684:GLU:HA	1:R:656:THR:HB	1.40	0.98
1:R:686:THR:HG22	1:R:689:GLU:HB2	1.49	0.94
1:Q:655:ARG:HB2	1:R:659:GLN:HG2	1.52	0.90
1:Y:659:GLN:HG2	1:X:655:ARG:HB2	1.51	0.88
1:Y:656:THR:HB	1:X:684:GLU:HA	1.52	0.88
1:Q:686:THR:HG23	1:R:680:ASP:HA	1.60	0.82
1:U:672:PRO:O	1:U:676:THR:HG23	1.81	0.81
1:X:656:THR:HB	1:W:684:GLU:HA	1.63	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:653:LEU:HD21	1:U:676:THR:HG22	1.65	0.78
1:R:686:THR:CG2	1:R:689:GLU:HB2	2.12	0.78
1:O:659:GLN:HG2	1:A:655:ARG:HB2	1.65	0.77
1:T:655:ARG:HB2	1:U:659:GLN:HG2	1.66	0.75
1:Q:684:GLU:HA	1:R:656:THR:CB	2.17	0.74
1:Z:672:PRO:HB2	1:Y:649:PRO:HG2	1.70	0.74
1:V:644:ARG:NH2	1:V:668:GLU:OE1	2.22	0.72
1:a:637:ARG:NH1	1:a:645:GLU:OE2	2.22	0.71
1:Y:656:THR:HG22	1:X:684:GLU:HG3	1.72	0.70
1:P:655:ARG:HB2	1:Q:659:GLN:HG2	1.74	0.68
1:U:634:TRP:HB3	1:U:635:PRO:HD2	1.74	0.68
1:R:686:THR:HG23	1:R:689:GLU:N	1.96	0.67
1:R:639:LYS:HB3	1:R:645:GLU:HG2	1.75	0.67
1:X:672:PRO:HG3	1:W:635:PRO:HG3	1.77	0.66
1:O:656:THR:HB	1:A:684:GLU:HA	1.75	0.66
1:R:686:THR:HG22	1:R:689:GLU:CB	2.24	0.66
1:R:686:THR:CG2	1:R:689:GLU:H	2.00	0.66
1:T:684:GLU:HA	1:U:656:THR:HB	1.77	0.65
1:V:684:GLU:HA	1:W:656:THR:HB	1.77	0.65
1:V:633:ASP:OD1	1:V:634:TRP:N	2.29	0.65
1:Y:672:PRO:HB2	1:X:649:PRO:HG2	1.79	0.64
1:P:656:THR:HB	1:O:684:GLU:HA	1.78	0.64
1:Z:656:THR:HB	1:Y:684:GLU:HA	1.80	0.64
1:A:651:ASP:HB3	1:A:658:PRO:HG3	1.79	0.63
1:P:657:PRO:HG2	1:P:662:LEU:HD11	1.81	0.63
1:Y:644:ARG:NH2	1:Y:668:GLU:OE1	2.27	0.62
1:S:672:PRO:HB2	1:R:649:PRO:HG2	1.81	0.62
1:P:687:PHE:CD2	1:Q:676:THR:HG23	2.35	0.62
1:W:639:LYS:HD2	1:W:643:GLY:HA2	1.82	0.62
1:S:637:ARG:HA	1:S:647:MET:HA	1.82	0.61
1:Y:676:THR:HG23	1:X:687:PHE:HD2	1.60	0.61
1:T:655:ARG:NH2	1:S:689:GLU:OE2	2.34	0.61
1:O:658:PRO:HD2	1:O:661:LEU:HD12	1.83	0.60
1:Y:662:LEU:HD21	1:Y:679:SER:HB2	1.82	0.60
1:T:634:TRP:CG	1:T:635:PRO:HD3	2.37	0.60
1:U:635:PRO:HB3	1:U:649:PRO:HD2	1.84	0.60
1:Z:672:PRO:HG3	1:Y:635:PRO:HG3	1.83	0.60
1:P:649:PRO:HG2	1:Q:672:PRO:HB2	1.84	0.59
1:T:634:TRP:CD1	1:T:635:PRO:HD3	2.38	0.58
1:T:678:LEU:HD12	1:T:685:MET:HE1	1.84	0.58
1:Z:680:ASP:HA	1:Y:686:THR:HG23	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:657:PRO:HG2	1:W:662:LEU:HD11	1.86	0.58
1:T:633:ASP:HB3	1:T:635:PRO:HD2	1.86	0.57
1:Q:686:THR:HG22	1:Q:688:GLU:H	1.68	0.56
1:X:665:LEU:HD21	1:X:697:LEU:HD11	1.86	0.56
1:A:659:GLN:HA	1:A:662:LEU:HD12	1.88	0.56
1:T:680:ASP:HA	1:S:686:THR:OG1	2.05	0.56
1:O:662:LEU:HD21	1:O:679:SER:HB2	1.88	0.56
1:S:686:THR:HG22	1:S:689:GLU:HG3	1.87	0.56
1:Z:676:THR:HG23	1:Y:687:PHE:CD2	2.41	0.56
1:V:662:LEU:HD21	1:V:679:SER:HB2	1.87	0.55
1:U:644:ARG:HH21	1:U:664:ALA:HB1	1.71	0.55
1:T:686:THR:HG22	1:T:688:GLU:H	1.72	0.55
1:Q:656:THR:HG22	1:Q:657:PRO:O	2.07	0.55
1:S:639:LYS:HG2	1:S:645:GLU:HG2	1.89	0.54
1:P:687:PHE:HA	1:P:690:ARG:HD2	1.90	0.54
1:Q:634:TRP:CD1	1:Q:635:PRO:HD2	2.42	0.54
1:R:681:ASP:O	1:R:685:MET:HG3	2.07	0.54
1:T:658:PRO:HD2	1:T:661:LEU:HD12	1.89	0.54
1:P:692:ASN:OD1	1:P:696:ASN:ND2	2.41	0.54
1:V:633:ASP:CG	1:V:634:TRP:H	2.14	0.54
1:Z:644:ARG:NH2	1:Z:668:GLU:OE1	2.32	0.54
1:U:671:SER:OG	1:U:674:SER:HB2	2.08	0.54
1:R:682:TRP:O	1:R:690:ARG:NH2	2.41	0.54
1:U:651:ASP:HB3	1:U:658:PRO:HG3	1.89	0.53
1:T:676:THR:HG23	1:S:687:PHE:CD2	2.43	0.53
1:Q:644:ARG:HH12	1:Q:697:LEU:HG	1.73	0.53
1:Q:644:ARG:NH1	1:Q:697:LEU:O	2.42	0.53
1:Q:635:PRO:HB2	1:Q:647:MET:HE2	1.90	0.53
1:X:676:THR:HG23	1:W:687:PHE:CD2	2.44	0.52
1:S:658:PRO:HD2	1:S:661:LEU:HD12	1.92	0.52
1:Q:686:THR:HB	1:Q:689:GLU:HG2	1.92	0.52
1:V:676:THR:HG23	1:U:687:PHE:CD2	2.44	0.52
1:Y:658:PRO:HD2	1:Y:661:LEU:HD12	1.91	0.52
1:Z:675:ALA:HB3	1:Y:653:LEU:HD13	1.92	0.51
1:Z:658:PRO:HD2	1:Z:661:LEU:HD12	1.92	0.51
1:Q:686:THR:CG2	1:R:680:ASP:HA	2.35	0.51
1:A:686:THR:HG23	1:A:689:GLU:HB2	1.93	0.51
1:Y:656:THR:CB	1:X:684:GLU:HA	2.33	0.51
1:W:672:PRO:O	1:W:676:THR:HG23	2.11	0.51
1:Z:665:LEU:HD23	1:Z:669:TYR:HD2	1.77	0.50
1:V:657:PRO:HB3	1:V:682:TRP:CE3	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:681:ASP:O	1:O:685:MET:HG3	2.12	0.50
1:P:657:PRO:HB3	1:P:682:TRP:CE3	2.47	0.50
1:U:659:GLN:HA	1:U:662:LEU:HD12	1.92	0.50
1:Q:662:LEU:HD21	1:Q:679:SER:HB2	1.93	0.50
1:V:659:GLN:HG2	1:U:655:ARG:HB2	1.94	0.50
1:X:661:LEU:HD22	1:X:697:LEU:HD23	1.93	0.50
1:X:656:THR:CB	1:W:684:GLU:HA	2.39	0.49
1:V:684:GLU:HG2	1:W:656:THR:HG22	1.94	0.49
1:U:658:PRO:HD2	1:U:661:LEU:HD12	1.95	0.49
1:R:686:THR:CG2	1:R:689:GLU:CB	2.85	0.49
1:V:653:LEU:HD13	1:W:666:VAL:HG21	1.94	0.49
1:X:633:ASP:N	1:X:633:ASP:OD1	2.44	0.49
1:V:688:GLU:N	1:W:680:ASP:OD1	2.41	0.49
1:W:693:VAL:HG13	1:W:697:LEU:HD12	1.95	0.48
1:V:652:LEU:HA	1:V:682:TRP:HZ2	1.78	0.48
1:Y:639:LYS:HD3	1:Y:645:GLU:HB3	1.94	0.48
1:Z:679:SER:HB3	1:Y:687:PHE:HB2	1.94	0.48
1:O:656:THR:CB	1:A:684:GLU:HA	2.41	0.48
1:Q:657:PRO:HB3	1:Q:682:TRP:CE3	2.47	0.48
1:a:651:ASP:HB3	1:a:658:PRO:HG3	1.93	0.48
1:P:646:PHE:CZ	1:P:694:ALA:HB1	2.48	0.48
1:Z:683:PRO:O	1:a:656:THR:HG21	2.14	0.48
1:T:656:THR:HG22	1:T:657:PRO:O	2.13	0.48
1:X:658:PRO:HD2	1:X:661:LEU:HD12	1.96	0.48
1:O:657:PRO:HB3	1:O:682:TRP:CE3	2.49	0.47
1:V:651:ASP:HB3	1:V:658:PRO:HG3	1.96	0.47
1:R:658:PRO:HD2	1:R:661:LEU:HD12	1.96	0.47
1:O:685:MET:HE3	1:O:689:GLU:HG3	1.94	0.47
1:T:684:GLU:HA	1:U:656:THR:CB	2.43	0.47
1:V:680:ASP:CG	1:U:688:GLU:HG2	2.39	0.47
1:O:637:ARG:NH2	1:O:645:GLU:OE1	2.47	0.47
1:A:657:PRO:HB3	1:A:682:TRP:CE3	2.49	0.47
1:U:673:LEU:HA	1:U:676:THR:CG2	2.45	0.47
1:a:657:PRO:HB3	1:a:682:TRP:CE3	2.50	0.47
1:Q:682:TRP:O	1:Q:690:ARG:NH2	2.48	0.46
1:S:656:THR:HG22	1:S:657:PRO:O	2.15	0.46
1:S:685:MET:HE2	1:S:689:GLU:HB3	1.98	0.46
1:R:647:MET:HE3	1:R:647:MET:HB2	1.84	0.46
1:U:673:LEU:HA	1:U:676:THR:HG23	1.96	0.46
1:O:656:THR:CG2	1:A:684:GLU:HA	2.46	0.46
1:A:673:LEU:HD21	1:A:677:GLU:OE2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:672:PRO:HB2	1:U:649:PRO:CG	2.47	0.45
1:V:665:LEU:HD22	1:V:674:SER:HB3	1.98	0.45
1:Z:684:GLU:HA	1:a:656:THR:HB	1.98	0.45
1:a:657:PRO:HG2	1:a:662:LEU:HD11	1.99	0.45
1:U:657:PRO:HB3	1:U:682:TRP:CE3	2.51	0.45
1:Y:682:TRP:O	1:Y:690:ARG:NH2	2.49	0.45
1:S:676:THR:HG23	1:R:687:PHE:CD2	2.52	0.45
1:R:672:PRO:O	1:R:676:THR:HG23	2.15	0.45
1:T:644:ARG:HH12	1:T:697:LEU:HG	1.82	0.45
1:O:637:ARG:HD2	1:O:647:MET:HG2	1.99	0.45
1:O:656:THR:HG21	1:A:683:PRO:O	2.17	0.45
1:V:649:PRO:HG2	1:W:672:PRO:HB2	1.98	0.45
1:V:672:PRO:HB2	1:U:649:PRO:HG2	1.98	0.44
1:V:681:ASP:O	1:V:685:MET:HG3	2.17	0.44
1:U:681:ASP:O	1:U:685:MET:HG3	2.17	0.44
1:a:656:THR:HG22	1:a:657:PRO:O	2.16	0.44
1:P:683:PRO:O	1:Q:656:THR:HG21	2.17	0.44
1:Y:657:PRO:HB3	1:Y:682:TRP:CE3	2.52	0.44
1:T:657:PRO:HB3	1:T:682:TRP:CE3	2.52	0.44
1:P:658:PRO:HD2	1:P:661:LEU:HD12	1.98	0.44
1:V:687:PHE:CD2	1:W:676:THR:HB	2.53	0.44
1:Y:676:THR:CG2	1:X:687:PHE:CD2	2.84	0.44
1:P:676:THR:HG23	1:O:687:PHE:CD2	2.53	0.44
1:W:652:LEU:O	1:W:690:ARG:NH1	2.51	0.44
1:Q:657:PRO:HD3	1:Q:682:TRP:CB	2.48	0.44
1:S:657:PRO:HB3	1:S:682:TRP:CE3	2.53	0.43
1:W:648:PHE:HA	1:W:649:PRO:HA	1.83	0.43
1:Q:684:GLU:HA	1:R:656:THR:CG2	2.48	0.43
1:X:633:ASP:OD1	1:X:635:PRO:HD3	2.18	0.43
1:W:657:PRO:HB3	1:W:682:TRP:CE3	2.54	0.43
1:O:672:PRO:HB2	1:A:649:PRO:HG2	2.00	0.43
1:V:653:LEU:HD13	1:W:666:VAL:CG2	2.48	0.43
1:T:649:PRO:HG2	1:U:672:PRO:HB2	2.00	0.43
1:T:687:PHE:CD2	1:U:676:THR:HB	2.53	0.43
1:S:659:GLN:HA	1:S:662:LEU:HD12	2.00	0.43
1:A:682:TRP:O	1:A:690:ARG:NH2	2.52	0.43
1:V:657:PRO:HD3	1:V:682:TRP:CB	2.49	0.43
1:V:659:GLN:HA	1:V:662:LEU:HD12	2.01	0.43
1:R:691:LYS:HG3	1:R:695:PHE:CD2	2.54	0.43
1:Z:684:GLU:HA	1:a:656:THR:CB	2.48	0.43
1:Y:665:LEU:HG	1:Y:697:LEU:HD21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:656:THR:HG22	1:V:657:PRO:O	2.18	0.42
1:V:672:PRO:HG3	1:U:635:PRO:HD3	2.01	0.42
1:Z:680:ASP:HA	1:Y:686:THR:CG2	2.49	0.42
1:A:673:LEU:HA	1:A:676:THR:HB	2.00	0.42
1:Y:657:PRO:HD3	1:Y:682:TRP:CB	2.49	0.42
1:S:680:ASP:CG	1:R:688:GLU:HG2	2.44	0.42
1:a:681:ASP:O	1:a:685:MET:HG3	2.20	0.42
1:V:634:TRP:CD1	1:V:635:PRO:HD2	2.55	0.42
1:O:657:PRO:HG2	1:O:662:LEU:HD11	2.00	0.42
1:Z:656:THR:HG23	1:Z:657:PRO:O	2.20	0.42
1:O:679:SER:HB3	1:A:687:PHE:HB2	2.01	0.42
1:Y:637:ARG:HG2	1:Y:647:MET:SD	2.60	0.42
1:S:657:PRO:HD3	1:S:682:TRP:CB	2.50	0.42
1:S:666:VAL:HG11	1:R:650:THR:HG23	2.02	0.42
1:Q:655:ARG:HA	1:R:659:GLN:NE2	2.35	0.42
1:R:637:ARG:HA	1:R:647:MET:HA	2.01	0.42
1:V:652:LEU:O	1:V:690:ARG:HD3	2.19	0.42
1:Z:639:LYS:HB2	1:Z:645:GLU:HG2	2.02	0.42
1:T:641:ASN:ND2	1:T:695:PHE:O	2.51	0.42
1:P:637:ARG:HG3	1:P:647:MET:HE3	2.02	0.42
1:a:657:PRO:HD3	1:a:682:TRP:CB	2.50	0.42
1:a:672:PRO:O	1:a:676:THR:HG23	2.20	0.42
1:P:684:GLU:HA	1:Q:656:THR:HB	2.01	0.41
1:R:657:PRO:HB3	1:R:682:TRP:CE3	2.55	0.41
1:U:678:LEU:O	1:U:682:TRP:HB2	2.20	0.41
1:T:657:PRO:HD3	1:T:682:TRP:CB	2.50	0.41
1:P:649:PRO:CG	1:Q:672:PRO:HB2	2.50	0.41
1:W:657:PRO:HG3	1:W:679:SER:HA	2.02	0.41
1:Z:656:THR:HG22	1:Y:684:GLU:HG2	2.01	0.41
1:Y:656:THR:HG23	1:Y:657:PRO:O	2.20	0.41
1:Z:665:LEU:HG	1:Z:697:LEU:HD21	2.02	0.41
1:Y:680:ASP:HA	1:X:686:THR:HB	2.02	0.41
1:Q:656:THR:HG23	1:Q:657:PRO:HD2	2.01	0.41
1:T:633:ASP:CB	1:T:635:PRO:HD2	2.49	0.41
1:T:653:LEU:CD1	1:U:672:PRO:O	2.69	0.41
1:S:675:ALA:HB3	1:R:653:LEU:HD13	2.03	0.41
1:V:634:TRP:CG	1:V:635:PRO:HD2	2.55	0.41
1:S:686:THR:HG23	1:S:689:GLU:H	1.85	0.41
1:X:657:PRO:HD3	1:X:682:TRP:HB3	2.03	0.41
1:W:639:LYS:HB2	1:W:645:GLU:HG2	2.02	0.41
1:R:665:LEU:HD22	1:R:674:SER:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:LEU:O	1:A:673:LEU:HG	2.19	0.41
1:W:691:LYS:O	1:W:695:PHE:HD1	2.04	0.41
1:Q:648:PHE:CE1	1:Q:691:LYS:HD3	2.56	0.40
1:O:657:PRO:HA	1:O:682:TRP:CE2	2.55	0.40
1:Z:634:TRP:HA	1:Z:635:PRO:HD3	1.90	0.40
1:Z:685:MET:HE2	1:Z:689:GLU:HB3	2.03	0.40
1:V:680:ASP:HA	1:U:686:THR:CG2	2.51	0.40
1:Q:683:PRO:O	1:R:656:THR:HG21	2.22	0.40

All (2) 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:U:677:GLU:OE1	1:A:671:SER:OG[2_454]	2.05	0.15
1:a:655:ARG:NH1	4:D:616:UNK:O[3_455]	2.15	0.05

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	O	63/130 (48%)	60 (95%)	3 (5%)	0	100	100
1	P	63/130 (48%)	61 (97%)	2 (3%)	0	100	100
1	Q	63/130 (48%)	59 (94%)	4 (6%)	0	100	100
1	R	61/130 (47%)	58 (95%)	3 (5%)	0	100	100
1	S	62/130 (48%)	58 (94%)	4 (6%)	0	100	100
1	T	64/130 (49%)	58 (91%)	6 (9%)	0	100	100
1	U	67/130 (52%)	62 (92%)	5 (8%)	0	100	100
1	V	64/130 (49%)	60 (94%)	4 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	64/130 (49%)	62 (97%)	2 (3%)	0	100	100
1	X	63/130 (48%)	59 (94%)	4 (6%)	0	100	100
1	Y	63/130 (48%)	58 (92%)	5 (8%)	0	100	100
1	Z	62/130 (48%)	59 (95%)	3 (5%)	0	100	100
1	a	68/130 (52%)	63 (93%)	5 (7%)	0	100	100
All	All	891/1820 (49%)	837 (94%)	54 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	62/114 (54%)	62 (100%)	0	100	100
1	O	61/114 (54%)	61 (100%)	0	100	100
1	P	61/114 (54%)	61 (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	60/114 (53%)	60 (100%)	0	100	100
1	T	62/114 (54%)	62 (100%)	0	100	100
1	U	65/114 (57%)	65 (100%)	0	100	100
1	V	62/114 (54%)	62 (100%)	0	100	100
1	W	62/114 (54%)	62 (100%)	0	100	100
1	X	61/114 (54%)	61 (100%)	0	100	100
1	Y	61/114 (54%)	61 (100%)	0	100	100
1	Z	60/114 (53%)	60 (100%)	0	100	100
1	a	60/114 (53%)	60 (100%)	0	100	100
All	All	857/1596 (54%)	857 (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. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	V	659	GLN
1	V	696	ASN
1	Z	659	GLN
1	Y	659	GLN
1	P	667	ASN
1	P	696	ASN
1	S	667	ASN
1	S	696	ASN
1	W	667	ASN
1	U	659	GLN
1	U	667	ASN
1	a	659	GLN

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 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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	620:UNK	C	621:UNK	N	1.60

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	66/130 (50%)	-1.26	0 100 100	96, 155, 230, 270	0
1	O	65/130 (50%)	-1.00	0 100 100	120, 187, 241, 288	0
1	P	65/130 (50%)	-1.21	0 100 100	99, 166, 238, 268	0
1	Q	65/130 (50%)	-1.15	0 100 100	92, 184, 237, 244	0
1	R	63/130 (48%)	-1.14	0 100 100	108, 166, 211, 226	0
1	S	64/130 (49%)	-1.21	0 100 100	108, 167, 217, 261	0
1	T	66/130 (50%)	-1.15	0 100 100	84, 177, 230, 260	0
1	U	69/130 (53%)	-1.13	0 100 100	94, 151, 261, 342	0
1	V	66/130 (50%)	-1.08	0 100 100	128, 184, 237, 392	0
1	W	66/130 (50%)	-1.11	0 100 100	109, 173, 228, 275	0
1	X	65/130 (50%)	-1.17	0 100 100	116, 180, 245, 278	0
1	Y	65/130 (50%)	-1.18	0 100 100	121, 176, 220, 250	0
1	Z	64/130 (49%)	-1.19	0 100 100	107, 166, 232, 252	0
1	a	70/130 (53%)	-1.14	0 100 100	100, 170, 243, 270	0
2	C	0/5	-	-	-	-
3	B	0/33	-	-	-	-
4	D	0/34	-	-	-	-
All	All	919/1892 (48%)	-1.15	0 100 100	84, 173, 240, 392	0

There are no RSRZ outliers to report.

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.