



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:19 PM UTC

PDB ID : 4CSF / pdb_00004csf
Title : Structural insights into Toscana virus RNA encapsidation
Authors : Olal, D.; Daumke, O.
Deposited on : 2014-03-07
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (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

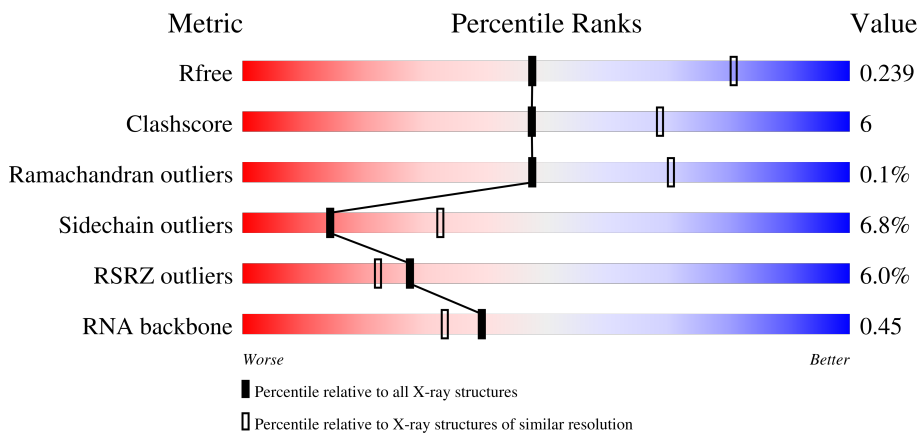
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

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	253	
1	B	253	
1	D	253	
1	F	253	





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Mol	Chain	Length	Quality of chain
1	G	253	4% 81% 16% ..
1	H	253	3% 79% 17% ..
1	I	253	2% 78% 19% ..
1	J	253	15% 78% 17% ..
1	K	253	6% 78% 20% ..
1	L	253	7% 79% 17% ..
1	M	253	5% 77% 19% ..
1	N	253	4% 82% 13% ..
1	O	253	4% 78% 19% ..
1	P	253	8% 81% 15% ..
1	Q	253	4% 85% 11% ..
1	R	253	6% 80% 16% ..
1	S	253	% 83% 13% ..
1	T	253	9% 82% 14% ..
1	U	253	% 82% 13% ..
1	V	253	7% 81% 15% ..
1	W	253	6% 82% 15% ..
2	C	253	2% 82% 15% ..
2	X	253	6% 80% 15% ..
3	E	253	9% 79% 17% ..
4	a	9	78% 11% 11%
4	c	9	78% 22%
4	e	9	78% 22%
4	g	9	89% 11%
4	i	9	78% 22%

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Mol	Chain	Length	Quality of chain
4	k	9	 78% 22%
4	m	9	 78% 22%
4	o	9	 78% 22%
4	q	9	 89% 11%
4	s	9	 78% 11% 11%
4	u	9	 78% 22%
4	w	9	 89% 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 49442 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	A	249	1907	1210	333	353	11	0	0	0
1	B	249	1907	1210	333	353	11	0	0	0
1	D	249	1907	1210	333	353	11	0	0	0
1	F	249	1904	1209	332	352	11	0	0	0
1	G	249	1907	1210	333	353	11	0	0	0
1	H	249	1907	1210	333	353	11	0	0	0
1	I	249	1907	1210	333	353	11	0	0	0
1	J	249	1904	1209	332	352	11	0	0	0
1	K	251	1921	1218	335	357	11	0	0	0
1	L	250	1919	1216	334	358	11	0	0	0
1	M	248	1899	1206	331	351	11	0	0	0
1	N	249	1907	1210	333	353	11	0	0	0
1	O	248	1899	1206	331	351	11	0	0	0
1	P	249	1907	1210	333	353	11	0	0	0
1	Q	249	1906	1210	333	352	11	0	0	0
1	R	248	1902	1207	332	352	11	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	249	Total	C	N	O	S	0	0	0
			1907	1210	333	353	11			
1	T	250	Total	C	N	O	S	0	0	0
			1916	1215	334	356	11			
1	U	247	Total	C	N	O	S	0	0	0
			1895	1204	330	350	11			
1	V	249	Total	C	N	O	S	0	0	0
			1907	1210	333	353	11			
1	W	250	Total	C	N	O	S	0	0	0
			1916	1215	334	356	11			

- Molecule 2 is a protein called NUCLEOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	250	Total	C	N	O	S	0	0	0
			1914	1215	332	356	11			
2	X	249	Total	C	N	O	S	0	0	0
			1902	1209	330	352	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	53	LYS	ARG	conflict	UNP P21701
X	53	LYS	ARG	conflict	UNP P21701

- Molecule 3 is a protein called NUCLEOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	249	Total	C	N	O	S	0	0	0
			1904	1209	331	353	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	33	GLU	GLN	conflict	UNP P21701

- Molecule 4 is a RNA chain called RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	a	9	Total	C	N	O	P	0	0	0
			183	83	25	67	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	c	9	Total	C	N	O	P	0	0	0
			183	83	25	67	8			
4	e	9	Total	C	N	O	P	0	0	0
			183	83	25	67	8			
4	g	9	Total	C	N	O	P	0	0	0
			183	83	25	67	8			
4	i	9	Total	C	N	O	P	0	0	0
			183	83	25	67	8			
4	k	9	Total	C	N	O	P	0	0	0
			183	83	25	67	8			
4	m	9	Total	C	N	O	P	0	0	0
			183	83	25	67	8			
4	o	9	Total	C	N	O	P	0	0	0
			183	83	25	67	8			
4	q	9	Total	C	N	O	P	0	0	0
			183	83	25	67	8			
4	s	9	Total	C	N	O	P	0	0	0
			183	83	25	67	8			
4	u	9	Total	C	N	O	P	0	0	0
			183	83	25	67	8			
4	w	9	Total	C	N	O	P	0	0	0
			183	83	25	67	8			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	80	Total	O	0	0
			80	80		
5	B	86	Total	O	0	0
			86	86		
5	C	103	Total	O	0	0
			103	103		
5	D	26	Total	O	0	0
			26	26		
5	E	38	Total	O	0	0
			38	38		
5	F	20	Total	O	0	0
			20	20		
5	G	73	Total	O	0	0
			73	73		
5	H	68	Total	O	0	0
			68	68		

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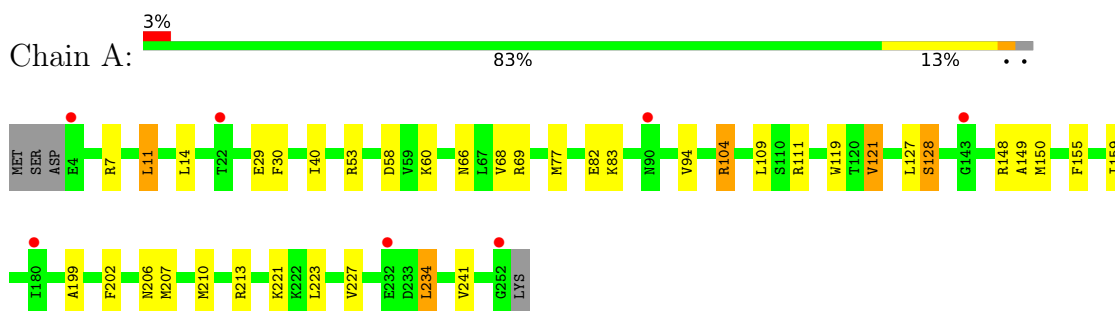
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	56	Total O 56 56	0	0
5	J	26	Total O 26 26	0	0
5	K	46	Total O 46 46	0	0
5	L	56	Total O 56 56	0	0
5	M	56	Total O 56 56	0	0
5	N	55	Total O 55 55	0	0
5	O	80	Total O 80 80	0	0
5	P	83	Total O 83 83	0	0
5	Q	86	Total O 86 86	0	0
5	R	31	Total O 31 31	0	0
5	S	67	Total O 67 67	0	0
5	T	87	Total O 87 87	0	0
5	U	84	Total O 84 84	0	0
5	V	65	Total O 65 65	0	0
5	W	62	Total O 62 62	0	0
5	X	41	Total O 41 41	0	0

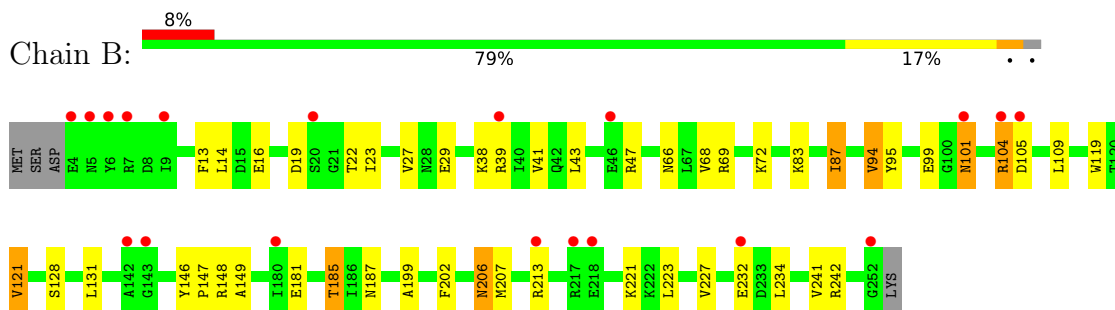
3 Residue-property plots [i](#)

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.

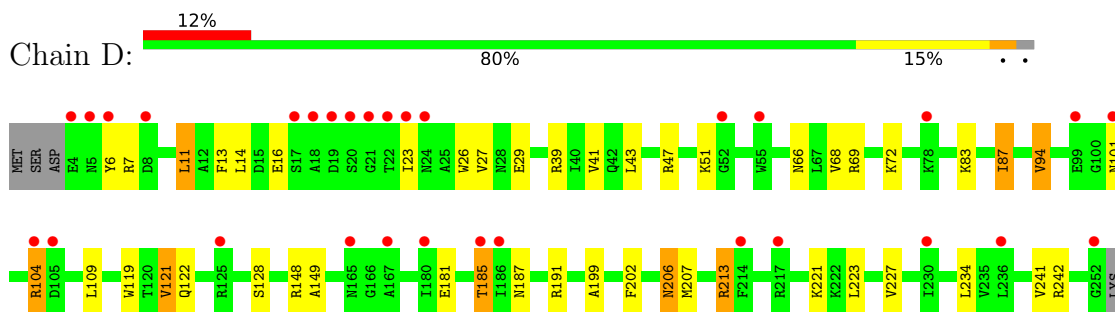
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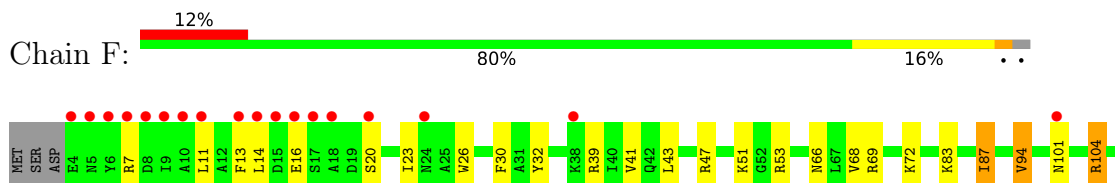
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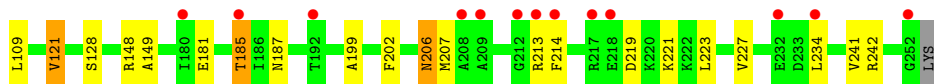


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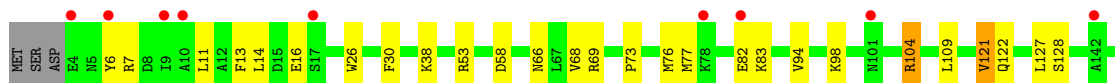
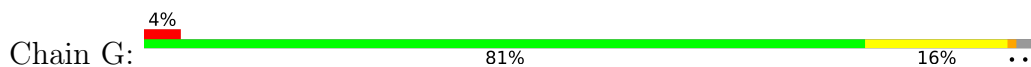


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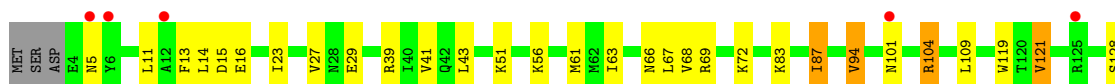
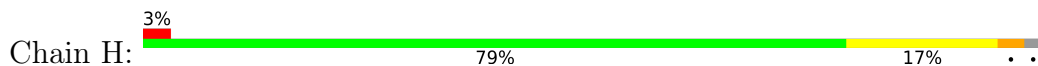




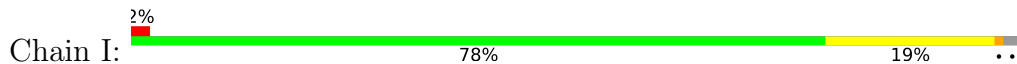
- Molecule 1: NUCLEOPROTEIN



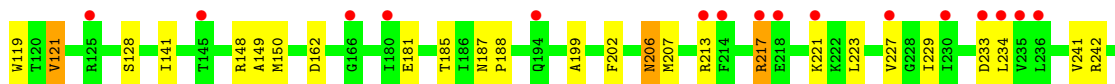
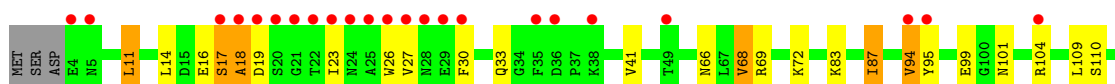
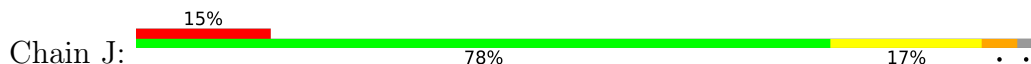
- Molecule 1: NUCLEOPROTEIN



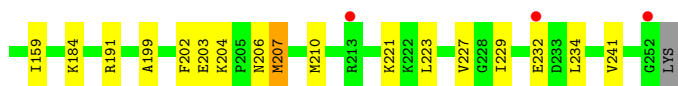
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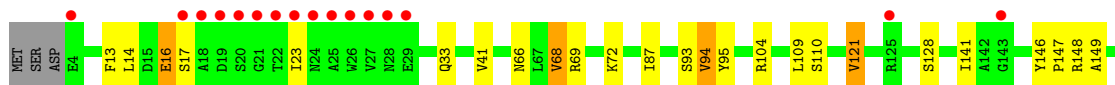
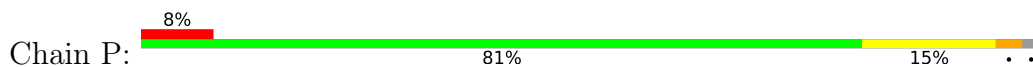
- Molecule 1: NUCLEOPROTEIN



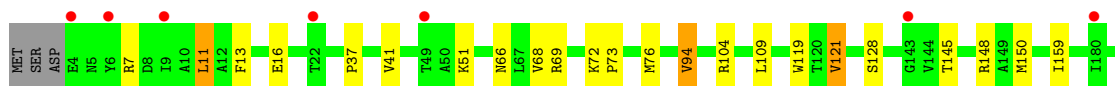
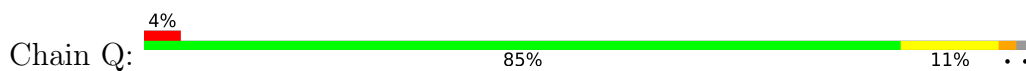
- Molecule 1: NUCLEOPROTEIN



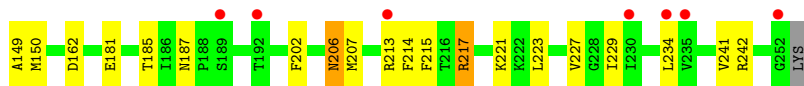
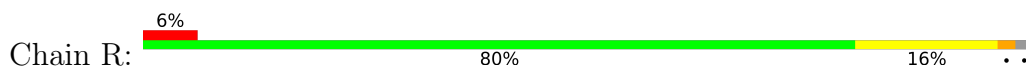
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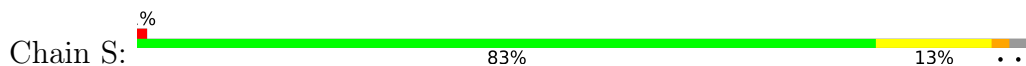
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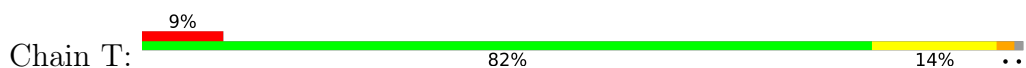
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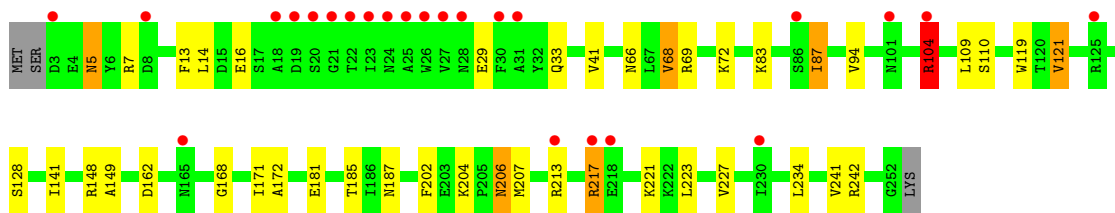


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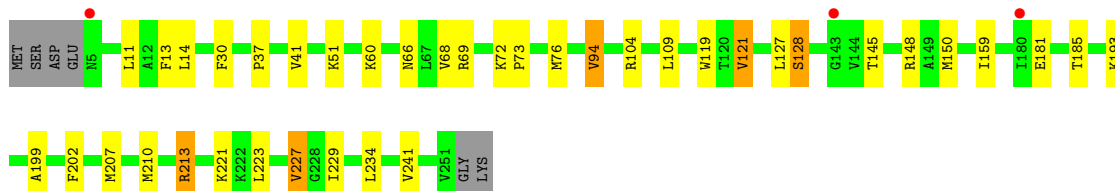
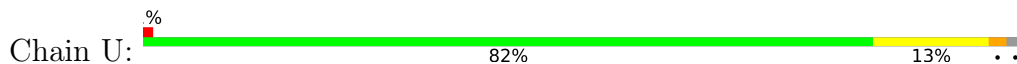


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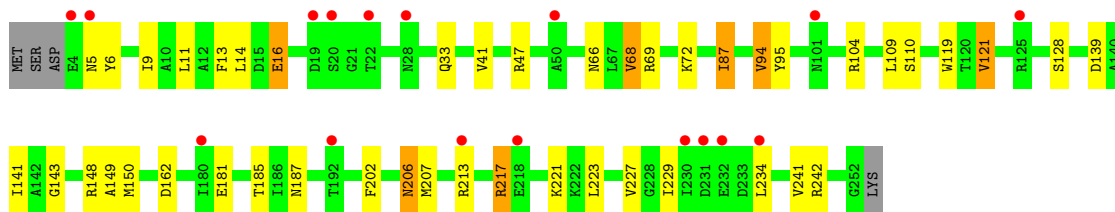
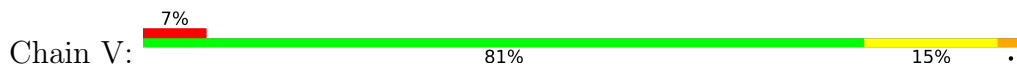




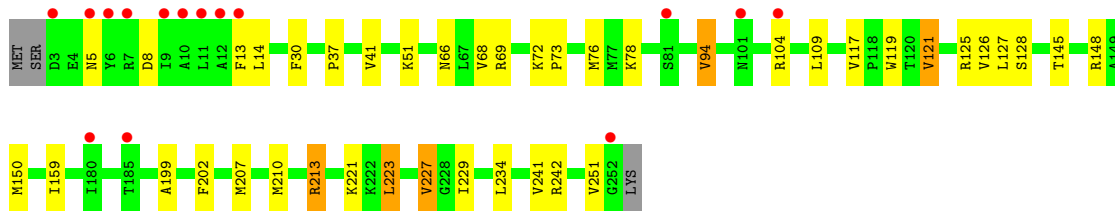
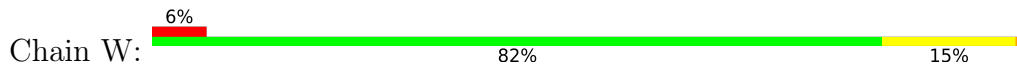
● Molecule 1: NUCLEOPROTEIN



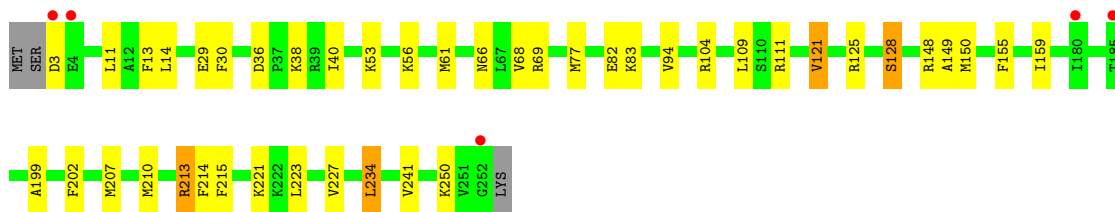
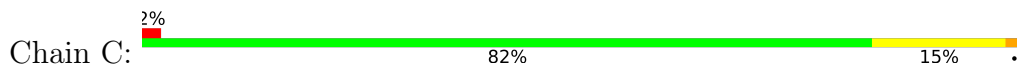
● Molecule 1: NUCLEOPROTEIN



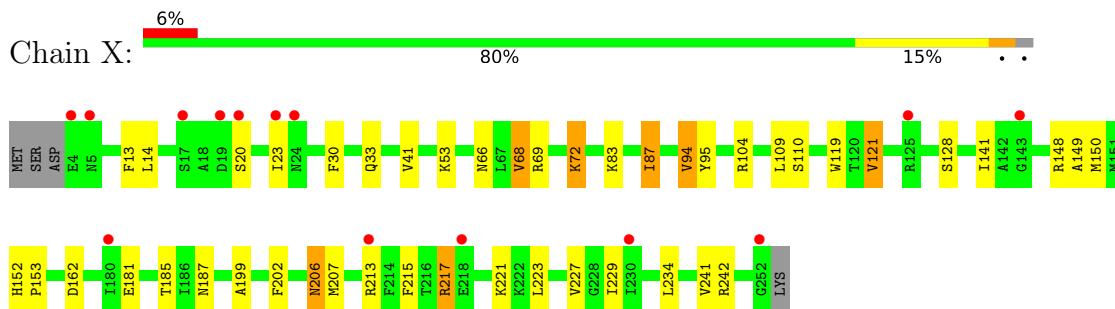
● Molecule 1: NUCLEOPROTEIN



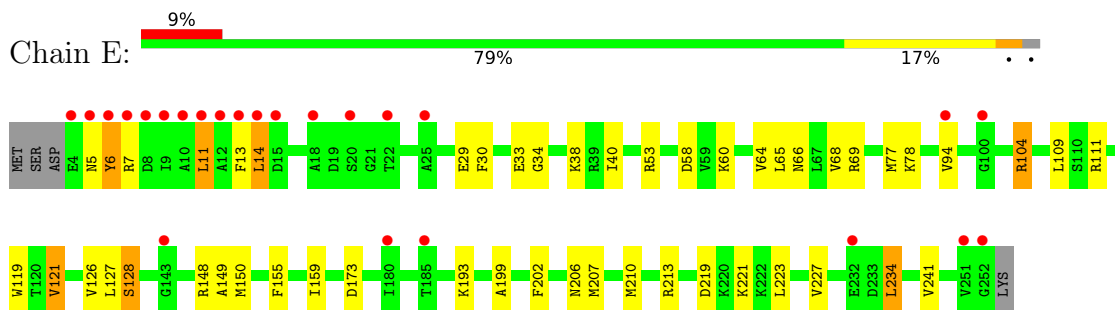
● Molecule 2: NUCLEOPROTEIN



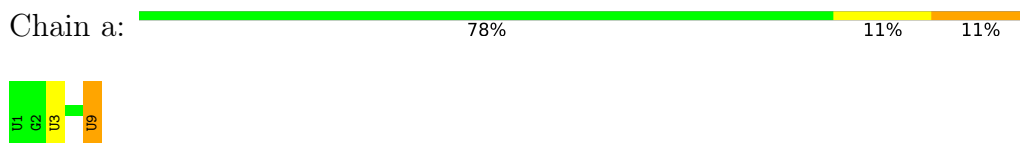
- Molecule 2: NUCLEOPROTEIN



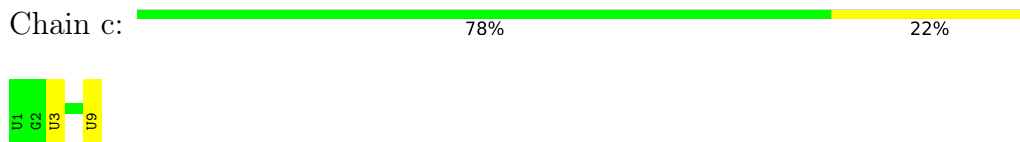
- Molecule 3: NUCLEOPROTEIN



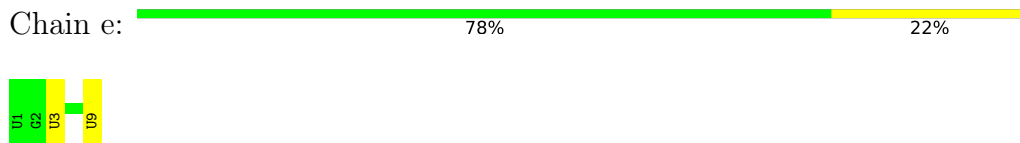
- Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')



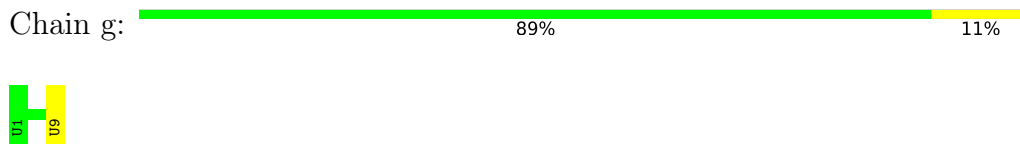
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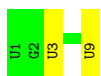


- Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')




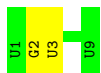
- Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain i:  78% 22%




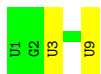
- Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain k:  78% 22%




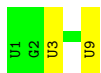
- Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain m:  78% 22%




- Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain o:  78% 22%




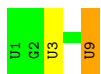
- Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain q:  89% 11%




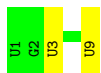
- Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain s:  78% 11% 11%




- Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain u:  78% 22%



- Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain w:  89% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	98.78Å 127.84Å 170.47Å 82.10° 79.75° 74.49°	Depositor
Resolution (Å)	34.47 – 2.60 34.47 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.7 (34.47-2.60) 94.7 (34.47-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.61Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.203 , 0.240 0.204 , 0.239	Depositor DCC
R_{free} test set	11465 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtrriage
Anisotropy	0.056	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	49442	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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	0.37	0/1939	0.79	3/2617 (0.1%)
1	B	0.37	0/1939	0.79	4/2617 (0.2%)
1	D	0.36	0/1939	0.80	5/2617 (0.2%)
1	F	0.35	0/1936	0.79	4/2613 (0.2%)
1	G	0.38	0/1939	0.80	3/2617 (0.1%)
1	H	0.38	0/1939	0.80	5/2617 (0.2%)
1	I	0.36	0/1939	0.78	2/2617 (0.1%)
1	J	0.35	0/1936	0.77	4/2613 (0.2%)
1	K	0.36	0/1953	0.78	2/2636 (0.1%)
1	L	0.36	0/1951	0.79	4/2633 (0.2%)
1	M	0.35	0/1931	0.78	2/2606 (0.1%)
1	N	0.36	0/1939	0.77	4/2617 (0.2%)
1	O	0.36	0/1931	0.78	2/2606 (0.1%)
1	P	0.39	0/1939	0.85	7/2617 (0.3%)
1	Q	0.39	0/1938	0.79	2/2616 (0.1%)
1	R	0.35	0/1934	0.77	4/2610 (0.2%)
1	S	0.37	0/1939	0.79	2/2617 (0.1%)
1	T	0.37	0/1948	0.83	7/2629 (0.3%)
1	U	0.38	0/1927	0.80	2/2601 (0.1%)
1	V	0.36	0/1939	0.77	4/2617 (0.2%)
1	W	0.37	0/1948	0.82	4/2629 (0.2%)
2	C	0.39	0/1946	0.78	3/2626 (0.1%)
2	X	0.36	0/1934	0.78	4/2610 (0.2%)
3	E	0.37	0/1936	0.81	2/2613 (0.1%)
4	a	0.21	0/202	0.39	0/312
4	c	0.22	0/202	0.37	0/312
4	e	0.16	0/202	0.35	0/312
4	g	0.21	0/202	0.35	0/312
4	i	0.21	0/202	0.41	0/312
4	k	0.19	0/202	0.37	0/312
4	m	0.20	0/202	0.37	0/312
4	o	0.21	0/202	0.36	0/312
4	q	0.23	0/202	0.39	0/312
4	s	0.20	0/202	0.38	0/312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	u	0.24	0/202	0.41	0/312
4	w	0.21	0/202	0.38	0/312
All	All	0.36	0/48963	0.77	85/66555 (0.1%)

There are no bond length outliers.

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	217	ARG	NE-CZ-NH2	-11.54	108.81	119.20
1	P	217	ARG	NE-CZ-NH1	10.94	132.44	121.50
1	T	104	ARG	NE-CZ-NH2	-9.92	110.27	119.20
1	T	104	ARG	NE-CZ-NH1	9.05	130.55	121.50
1	P	217	ARG	CD-NE-CZ	8.95	136.93	124.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1907	0	1955	21	0
1	B	1907	0	1955	29	0
1	D	1907	0	1955	27	0
1	F	1904	0	1951	31	0
1	G	1907	0	1955	25	0
1	H	1907	0	1955	28	0
1	I	1907	0	1955	48	0
1	J	1904	0	1951	51	1
1	K	1921	0	1963	31	0
1	L	1919	0	1963	34	0
1	M	1899	0	1949	30	0
1	N	1907	0	1955	25	0
1	O	1899	0	1949	29	0
1	P	1907	0	1955	28	0
1	Q	1906	0	1952	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	1902	0	1953	22	1
1	S	1907	0	1955	22	0
1	T	1916	0	1961	26	0
1	U	1895	0	1946	21	0
1	V	1907	0	1955	22	0
1	W	1916	0	1961	25	0
2	C	1914	0	1961	31	0
2	X	1902	0	1951	28	0
3	E	1904	0	1949	37	0
4	a	183	0	95	1	0
4	c	183	0	95	0	0
4	e	183	0	95	0	0
4	g	183	0	95	0	0
4	i	183	0	95	0	0
4	k	183	0	95	0	0
4	m	183	0	95	0	0
4	o	183	0	95	0	0
4	q	183	0	95	0	0
4	s	183	0	95	1	0
4	u	183	0	95	0	0
4	w	183	0	95	0	0
5	A	80	0	0	0	0
5	B	86	0	0	4	0
5	C	103	0	0	3	0
5	D	26	0	0	0	0
5	E	38	0	0	4	0
5	F	20	0	0	0	0
5	G	73	0	0	3	0
5	H	68	0	0	5	0
5	I	56	0	0	1	0
5	J	26	0	0	1	0
5	K	46	0	0	1	0
5	L	56	0	0	4	0
5	M	56	0	0	1	0
5	N	55	0	0	0	0
5	O	80	0	0	2	0
5	P	83	0	0	1	0
5	Q	86	0	0	0	0
5	R	31	0	0	0	0
5	S	67	0	0	1	0
5	T	87	0	0	4	0
5	U	84	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	V	65	0	0	4	0
5	W	62	0	0	2	0
5	X	41	0	0	1	0
All	All	49442	0	48050	537	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 537 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:I:61:MET:HG2	1:J:26:TRP:CE2	2.01	0.95
1:T:168:GLY:O	5:T:2059:HOH:O	1.92	0.87
1:L:3:ASP:N	5:L:2001:HOH:O	2.10	0.84
1:S:83:LYS:NZ	1:T:29:GLU:OE2	2.13	0.81
3:E:119:TRP:HB2	1:F:13:PHE:HB3	1.64	0.80

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:233:ASP:OD2	1:R:53:ARG:NH2[1_564]	2.17	0.03

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	247/253 (98%)	240 (97%)	7 (3%)	0	100 100
1	B	247/253 (98%)	238 (96%)	9 (4%)	0	100 100
1	D	247/253 (98%)	239 (97%)	8 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	247/253 (98%)	239 (97%)	8 (3%)	0	100	100
1	G	247/253 (98%)	239 (97%)	8 (3%)	0	100	100
1	H	247/253 (98%)	237 (96%)	10 (4%)	0	100	100
1	I	247/253 (98%)	239 (97%)	8 (3%)	0	100	100
1	J	247/253 (98%)	240 (97%)	5 (2%)	2 (1%)	16	34
1	K	249/253 (98%)	239 (96%)	9 (4%)	1 (0%)	30	51
1	L	248/253 (98%)	241 (97%)	6 (2%)	1 (0%)	30	51
1	M	246/253 (97%)	238 (97%)	8 (3%)	0	100	100
1	N	247/253 (98%)	241 (98%)	6 (2%)	0	100	100
1	O	246/253 (97%)	239 (97%)	7 (3%)	0	100	100
1	P	247/253 (98%)	240 (97%)	7 (3%)	0	100	100
1	Q	247/253 (98%)	242 (98%)	5 (2%)	0	100	100
1	R	246/253 (97%)	240 (98%)	6 (2%)	0	100	100
1	S	247/253 (98%)	243 (98%)	4 (2%)	0	100	100
1	T	248/253 (98%)	241 (97%)	7 (3%)	0	100	100
1	U	245/253 (97%)	241 (98%)	4 (2%)	0	100	100
1	V	247/253 (98%)	241 (98%)	6 (2%)	0	100	100
1	W	248/253 (98%)	243 (98%)	5 (2%)	0	100	100
2	C	248/253 (98%)	241 (97%)	7 (3%)	0	100	100
2	X	247/253 (98%)	240 (97%)	7 (3%)	0	100	100
3	E	247/253 (98%)	238 (96%)	8 (3%)	1 (0%)	30	51
All	All	5929/6072 (98%)	5759 (97%)	165 (3%)	5 (0%)	48	70

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	6	TYR
1	J	18	ALA
1	J	17	SER
1	L	4	GLU
1	K	3	ASP

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	201/206 (98%)	188 (94%)	13 (6%)	15	35
1	B	201/206 (98%)	185 (92%)	16 (8%)	11	25
1	D	201/206 (98%)	185 (92%)	16 (8%)	11	25
1	F	200/206 (97%)	183 (92%)	17 (8%)	10	22
1	G	201/206 (98%)	189 (94%)	12 (6%)	17	37
1	H	201/206 (98%)	185 (92%)	16 (8%)	11	25
1	I	201/206 (98%)	188 (94%)	13 (6%)	15	35
1	J	200/206 (97%)	185 (92%)	15 (8%)	12	28
1	K	202/206 (98%)	189 (94%)	13 (6%)	16	35
1	L	203/206 (98%)	190 (94%)	13 (6%)	16	35
1	M	200/206 (97%)	187 (94%)	13 (6%)	15	35
1	N	201/206 (98%)	188 (94%)	13 (6%)	15	35
1	O	200/206 (97%)	188 (94%)	12 (6%)	17	37
1	P	201/206 (98%)	186 (92%)	15 (8%)	12	28
1	Q	200/206 (97%)	190 (95%)	10 (5%)	22	46
1	R	201/206 (98%)	187 (93%)	14 (7%)	14	31
1	S	201/206 (98%)	189 (94%)	12 (6%)	17	37
1	T	202/206 (98%)	186 (92%)	16 (8%)	11	26
1	U	200/206 (97%)	188 (94%)	12 (6%)	17	37
1	V	201/206 (98%)	184 (92%)	17 (8%)	10	22
1	W	202/206 (98%)	191 (95%)	11 (5%)	20	42
2	C	202/206 (98%)	190 (94%)	12 (6%)	18	38
2	X	200/206 (97%)	186 (93%)	14 (7%)	14	31
3	E	200/206 (97%)	187 (94%)	13 (6%)	15	35
All	All	4822/4944 (98%)	4494 (93%)	328 (7%)	14	32

5 of 328 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	241	VAL
1	V	5	ASN
1	R	121	VAL
1	T	41	VAL
1	V	227	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	122	GLN
1	W	122	GLN
1	N	66	ASN
1	V	66	ASN
1	L	66	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	a	8/9 (88%)	2 (25%)	0
4	c	8/9 (88%)	2 (25%)	0
4	e	8/9 (88%)	2 (25%)	0
4	g	8/9 (88%)	1 (12%)	0
4	i	8/9 (88%)	2 (25%)	0
4	k	8/9 (88%)	2 (25%)	0
4	m	8/9 (88%)	2 (25%)	0
4	o	8/9 (88%)	2 (25%)	0
4	q	8/9 (88%)	1 (12%)	0
4	s	8/9 (88%)	2 (25%)	0
4	u	8/9 (88%)	2 (25%)	0
4	w	8/9 (88%)	1 (12%)	0
All	All	96/108 (88%)	21 (21%)	0

5 of 21 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	a	3	U
4	a	9	U
4	c	3	U
4	c	9	U
4	e	3	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	249/253 (98%)	0.21	7 (2%) 55 49	34, 48, 77, 112	0
1	B	249/253 (98%)	0.36	19 (7%) 20 16	30, 44, 76, 103	0
1	D	249/253 (98%)	1.02	30 (12%) 9 7	37, 68, 96, 126	0
1	F	249/253 (98%)	0.99	31 (12%) 8 6	42, 66, 97, 122	0
1	G	249/253 (98%)	0.33	11 (4%) 39 33	29, 45, 70, 102	0
1	H	249/253 (98%)	0.28	8 (3%) 50 44	31, 49, 72, 98	0
1	I	249/253 (98%)	0.23	5 (2%) 65 60	34, 50, 70, 92	0
1	J	249/253 (98%)	1.15	39 (15%) 5 4	39, 62, 96, 126	0
1	K	251/253 (99%)	0.60	16 (6%) 25 20	37, 56, 79, 122	0
1	L	250/253 (98%)	0.51	17 (6%) 23 19	27, 46, 78, 100	0
1	M	248/253 (98%)	0.48	12 (4%) 35 30	35, 51, 75, 105	0
1	N	249/253 (98%)	0.47	10 (4%) 42 37	38, 55, 82, 103	0
1	O	248/253 (98%)	0.39	11 (4%) 39 33	33, 50, 77, 101	0
1	P	249/253 (98%)	0.36	21 (8%) 17 13	26, 42, 77, 100	0
1	Q	249/253 (98%)	0.27	9 (3%) 46 40	27, 44, 67, 87	0
1	R	248/253 (98%)	0.71	15 (6%) 27 22	38, 58, 85, 109	0
1	S	249/253 (98%)	0.28	3 (1%) 76 73	36, 51, 74, 101	0
1	T	250/253 (98%)	0.43	24 (9%) 13 10	28, 45, 83, 117	0
1	U	247/253 (97%)	-0.04	3 (1%) 76 73	24, 39, 62, 74	0
1	V	249/253 (98%)	0.49	17 (6%) 23 19	32, 52, 80, 105	0
1	W	250/253 (98%)	0.43	15 (6%) 27 22	31, 49, 74, 110	0
2	C	250/253 (98%)	0.12	5 (2%) 65 60	26, 44, 68, 124	0
2	X	249/253 (98%)	0.39	14 (5%) 30 24	34, 53, 82, 104	0
3	E	249/253 (98%)	0.99	24 (9%) 13 10	47, 66, 99, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
4	a	9/9 (100%)	-0.33	0 100 100	42, 48, 58, 63	0
4	c	9/9 (100%)	-0.24	0 100 100	38, 42, 64, 76	0
4	e	9/9 (100%)	0.18	0 100 100	55, 61, 78, 82	0
4	g	9/9 (100%)	-0.33	0 100 100	34, 43, 56, 69	0
4	i	9/9 (100%)	-0.19	0 100 100	38, 46, 56, 80	0
4	k	9/9 (100%)	-0.21	0 100 100	44, 51, 68, 73	0
4	m	9/9 (100%)	-0.30	0 100 100	44, 49, 64, 67	0
4	o	9/9 (100%)	-0.29	0 100 100	39, 48, 55, 62	0
4	q	9/9 (100%)	-0.47	0 100 100	35, 41, 61, 69	0
4	s	9/9 (100%)	-0.22	0 100 100	46, 50, 61, 63	0
4	u	9/9 (100%)	-0.55	0 100 100	33, 36, 50, 57	0
4	w	9/9 (100%)	-0.28	0 100 100	38, 46, 59, 78	0
All	All	6085/6180 (98%)	0.46	366 (6%) 27 22	24, 51, 83, 134	0

The worst 5 of 366 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	23	ILE	8.8
1	J	26	TRP	7.9
1	J	22	THR	7.0
3	E	6	TYR	6.9
1	J	235	VAL	6.5

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.