



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:10 am GMT

PDB ID : 4CSF
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

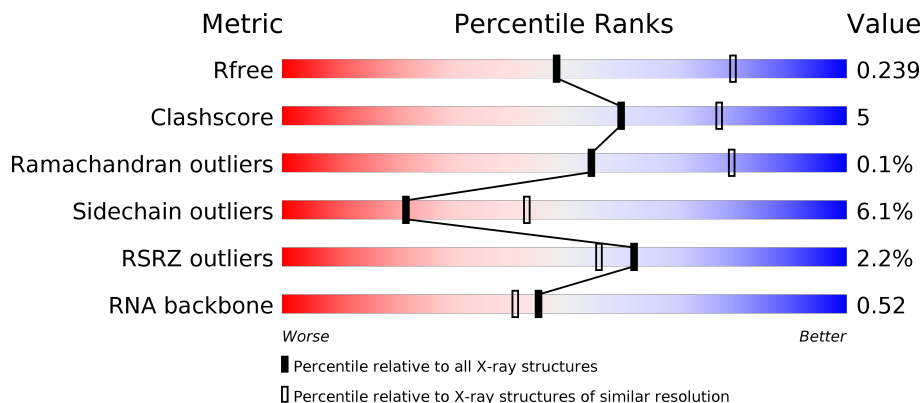
1 Overall quality at a glance

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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)
RNA backbone	2435	1140 (3.00-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>85%</div> <div>13%</div> <div>..</div> </div>
1	B	253	<div> <div>2%</div> <div>81%</div> <div>15%</div> <div>..</div> </div>
1	D	253	<div> <div>4%</div> <div>82%</div> <div>13%</div> <div>..</div> </div>
1	F	253	<div> <div>6%</div> <div>82%</div> <div>14%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	253	
1	H	253	
1	I	253	
1	J	253	
1	K	253	
1	L	253	
1	M	253	
1	N	253	
1	O	253	
1	P	253	
1	Q	253	
1	R	253	
1	S	253	
1	T	253	
1	U	253	
1	V	253	
1	W	253	
2	C	253	
2	X	253	
3	E	253	
4	a	9	
4	c	9	
4	e	9	
4	g	9	
4	i	9	

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Mol	Chain	Length	Quality of chain	
4	k	9		
4	m	9		
4	o	9		
4	q	9		
4	s	9		
4	u	9		
4	w	9		

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
1	A	249	Total	C	N	O	S	0	0	0
			1907	1210	333	353	11			
1	B	249	Total	C	N	O	S	0	0	0
			1907	1210	333	353	11			
1	D	249	Total	C	N	O	S	0	0	0
			1907	1210	333	353	11			
1	F	249	Total	C	N	O	S	0	0	0
			1904	1209	332	352	11			
1	G	249	Total	C	N	O	S	0	0	0
			1907	1210	333	353	11			
1	H	249	Total	C	N	O	S	0	0	0
			1907	1210	333	353	11			
1	I	249	Total	C	N	O	S	0	0	0
			1907	1210	333	353	11			
1	J	249	Total	C	N	O	S	0	0	0
			1904	1209	332	352	11			
1	K	251	Total	C	N	O	S	0	0	0
			1921	1218	335	357	11			
1	L	250	Total	C	N	O	S	0	0	0
			1919	1216	334	358	11			
1	M	248	Total	C	N	O	S	0	0	0
			1899	1206	331	351	11			
1	N	249	Total	C	N	O	S	0	0	0
			1907	1210	333	353	11			
1	O	248	Total	C	N	O	S	0	0	0
			1899	1206	331	351	11			
1	P	249	Total	C	N	O	S	0	0	0
			1907	1210	333	353	11			
1	Q	249	Total	C	N	O	S	0	0	0
			1906	1210	333	352	11			
1	R	248	Total	C	N	O	S	0	0	0
			1902	1207	332	352	11			

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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 183	C 83	N 25	O 67	P 8	0	0	0
4	e	9	Total 183	C 83	N 25	O 67	P 8	0	0	0
4	g	9	Total 183	C 83	N 25	O 67	P 8	0	0	0
4	i	9	Total 183	C 83	N 25	O 67	P 8	0	0	0
4	k	9	Total 183	C 83	N 25	O 67	P 8	0	0	0
4	m	9	Total 183	C 83	N 25	O 67	P 8	0	0	0
4	o	9	Total 183	C 83	N 25	O 67	P 8	0	0	0
4	q	9	Total 183	C 83	N 25	O 67	P 8	0	0	0
4	s	9	Total 183	C 83	N 25	O 67	P 8	0	0	0
4	u	9	Total 183	C 83	N 25	O 67	P 8	0	0	0
4	w	9	Total 183	C 83	N 25	O 67	P 8	0	0	0

- Molecule 5 is water.

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

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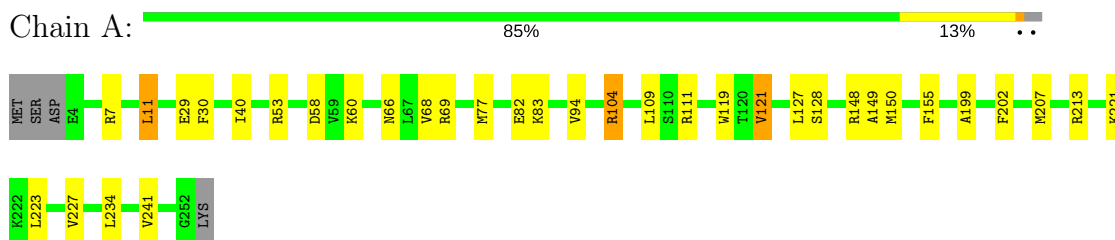
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	56	Total 56	O 56	0	0
5	J	26	Total 26	O 26	0	0
5	K	46	Total 46	O 46	0	0
5	L	56	Total 56	O 56	0	0
5	M	56	Total 56	O 56	0	0
5	N	55	Total 55	O 55	0	0
5	O	80	Total 80	O 80	0	0
5	P	83	Total 83	O 83	0	0
5	Q	86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

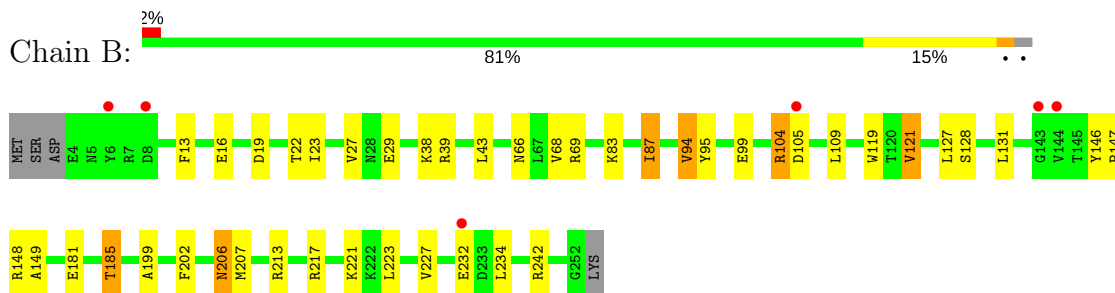
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

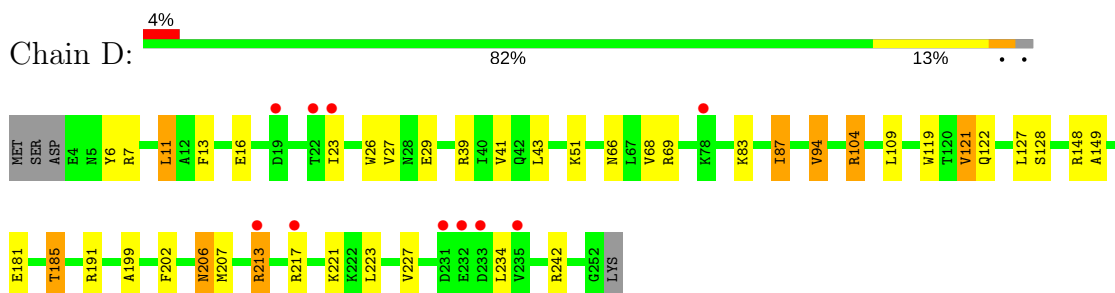
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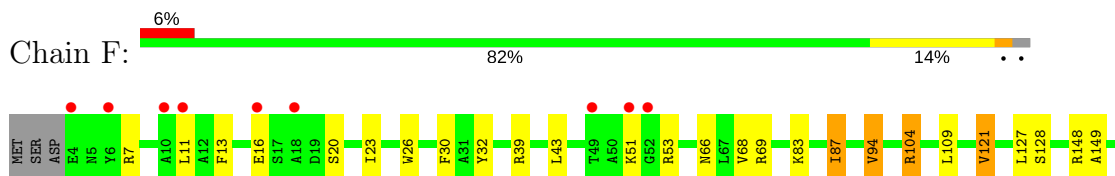
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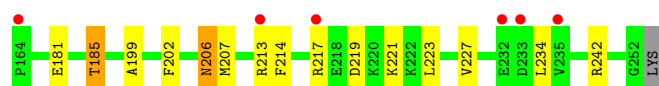


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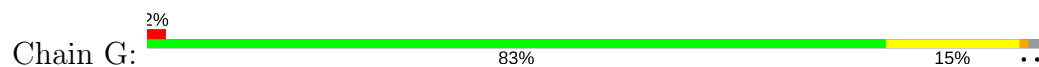


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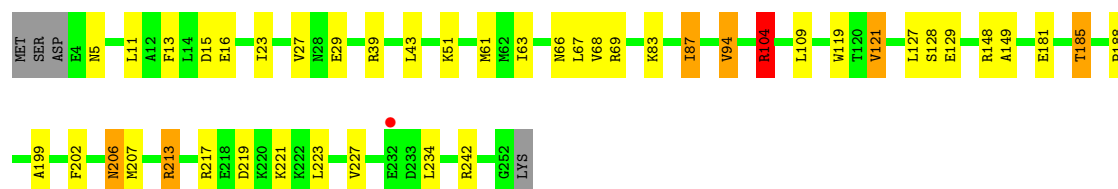
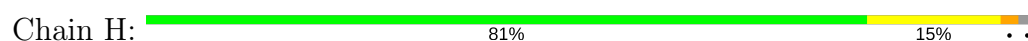




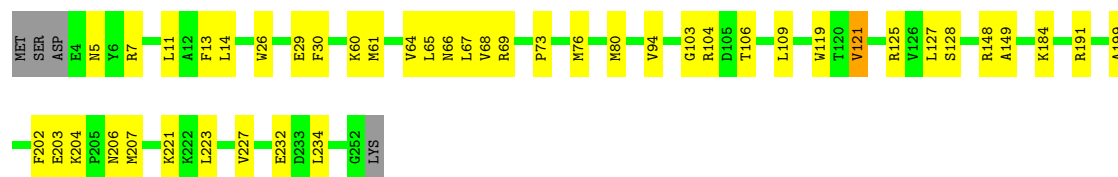
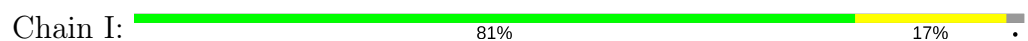
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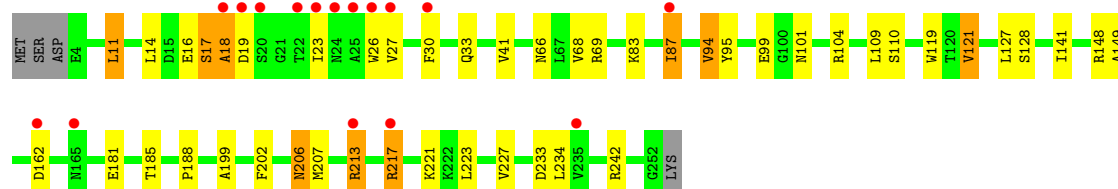
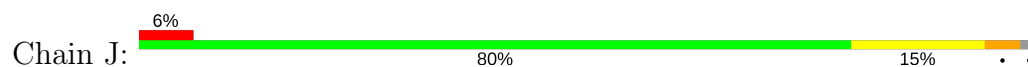
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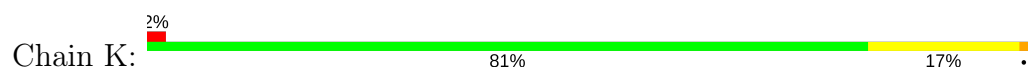
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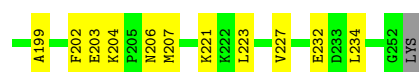


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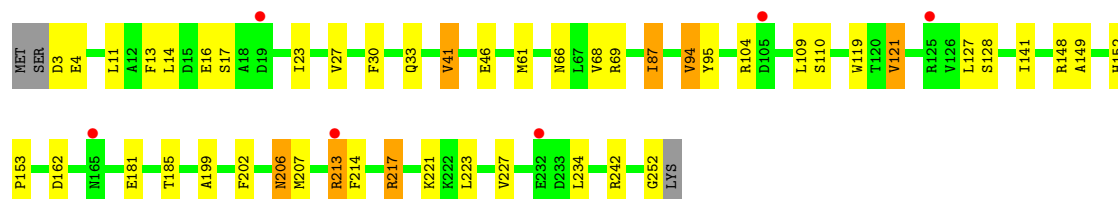
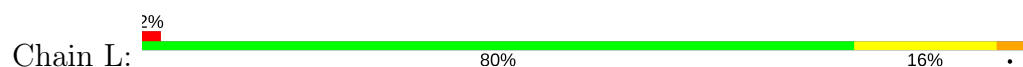


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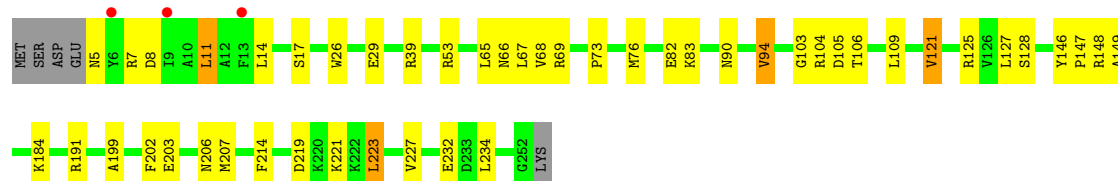
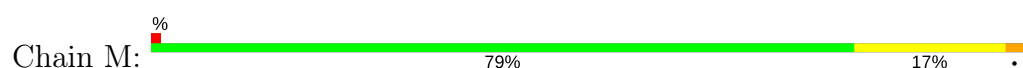




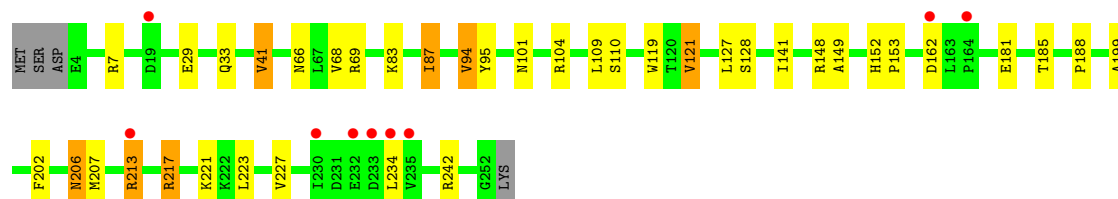
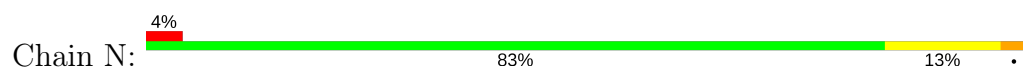
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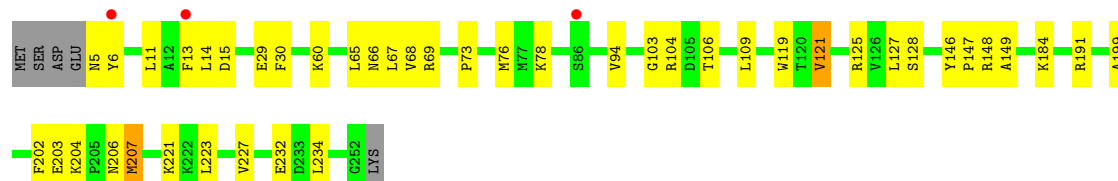
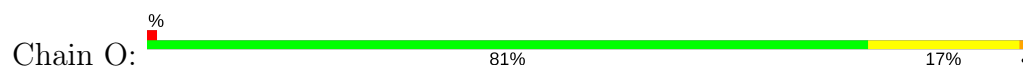
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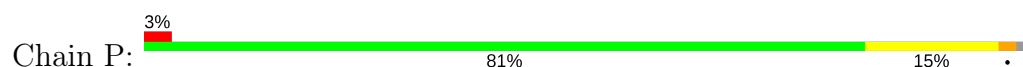
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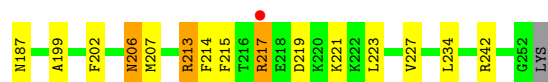


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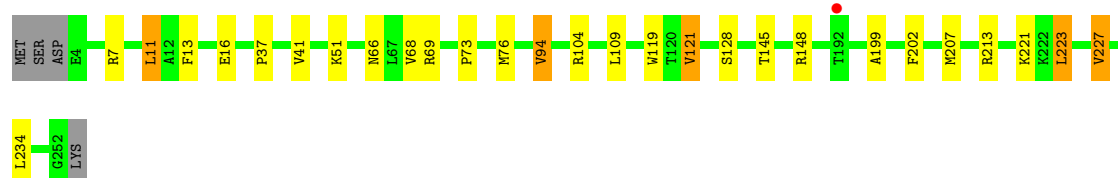
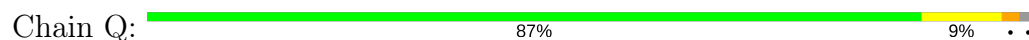


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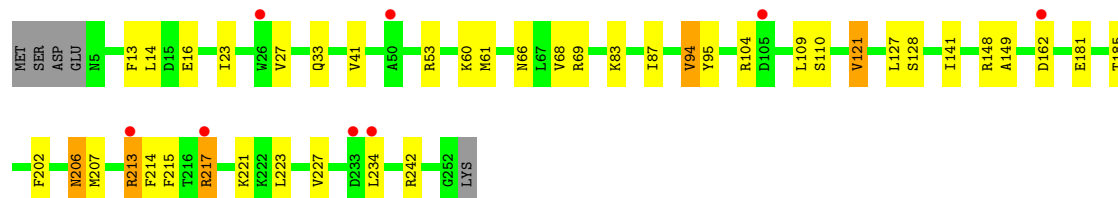
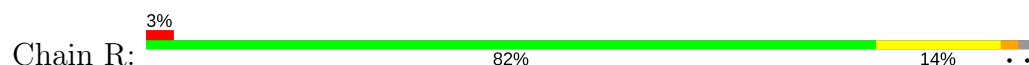




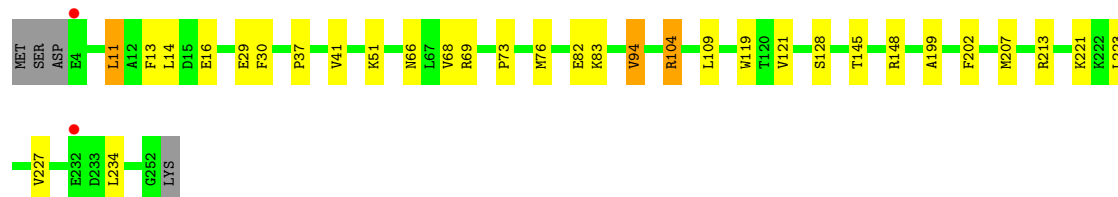
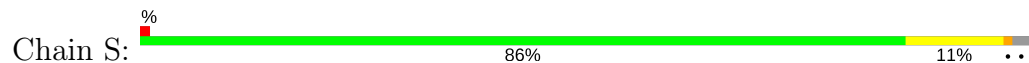
• Molecule 1: NUCLEOPROTEIN



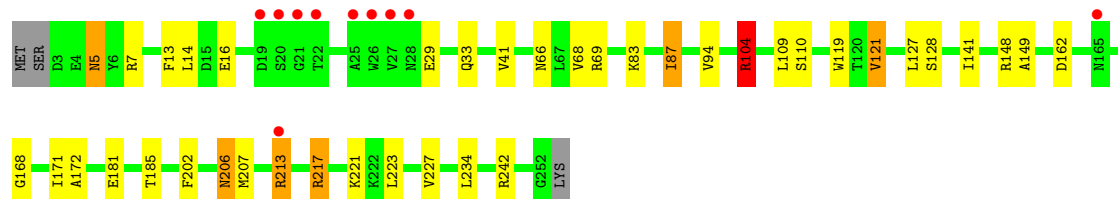
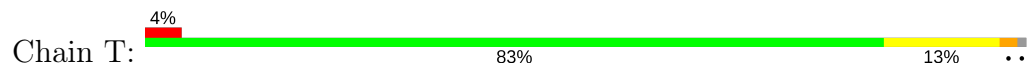
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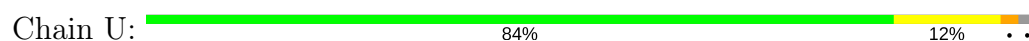
• Molecule 1: NUCLEOPROTEIN



• Molecule 1: NUCLEOPROTEIN

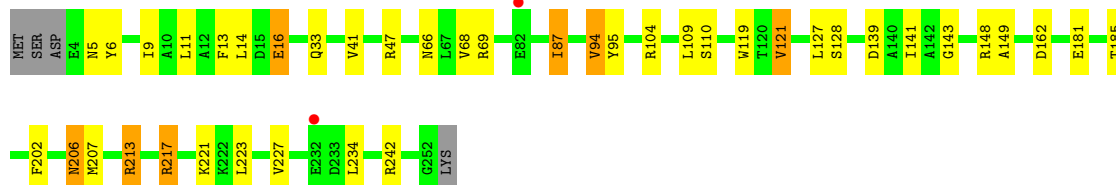
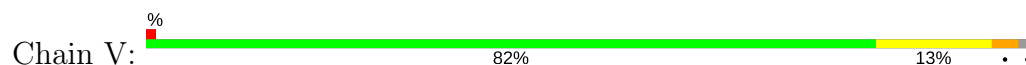


• Molecule 1: NUCLEOPROTEIN

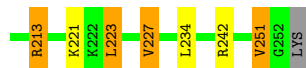
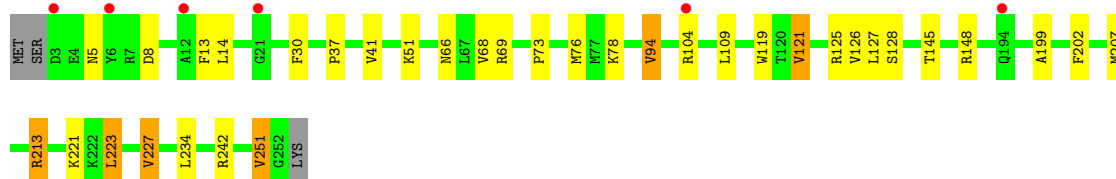
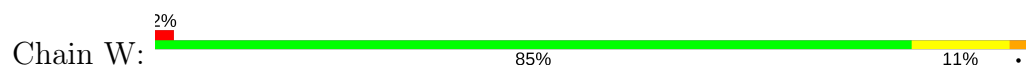




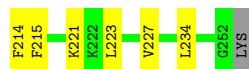
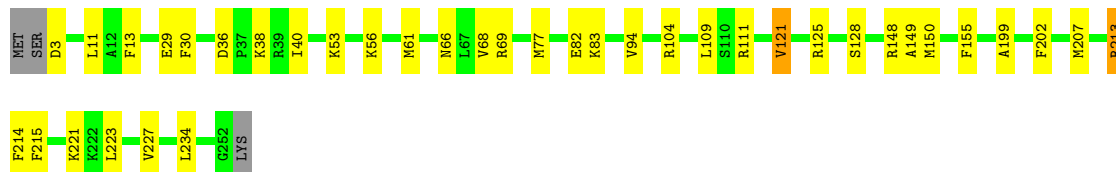
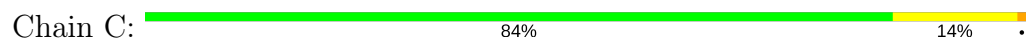
• Molecule 1: NUCLEOPROTEIN



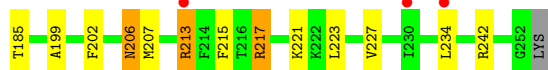
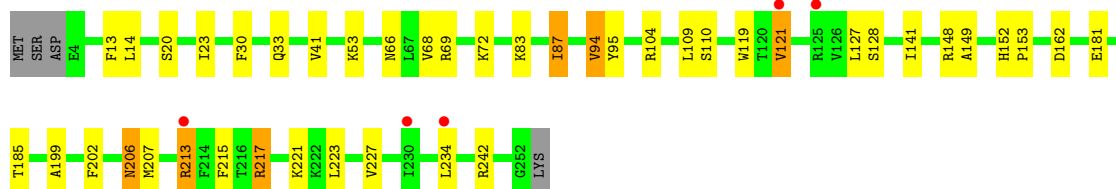
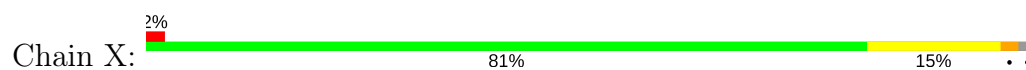
• Molecule 1: NUCLEOPROTEIN



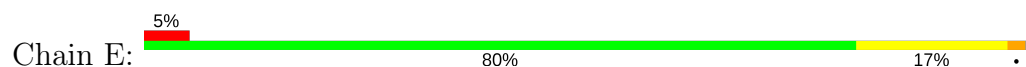
• Molecule 2: NUCLEOPROTEIN

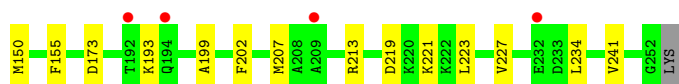


• Molecule 2: NUCLEOPROTEIN



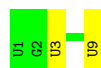
• Molecule 3: NUCLEOPROTEIN





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

Chain a: 78% 22%



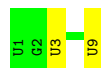
- Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain c: 78% 22%



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

Chain e: 78% 22%



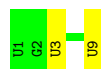
- Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain g: 89% 11%



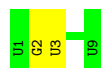
- Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain i: 78% 22%



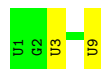
- Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain k: 78% 22%




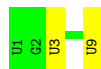
- Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain m: 78% 22%




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

Chain o:  78% 22%




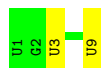
- Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain q:  89% 11%




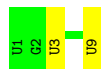
- Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain s:  78% 22%




- 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 34.48 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.7 (34.47-2.60) 93.0 (34.48-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.203 , 0.240 0.201 , 0.239	Depositor DCC
R_{free} test set	11463 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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 ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.29	0/1939	0.58	3/2617 (0.1%)
1	B	0.29	0/1939	0.48	0/2617
1	D	0.28	0/1939	0.48	1/2617 (0.0%)
1	F	0.28	0/1936	0.45	0/2613
1	G	0.29	0/1939	0.58	3/2617 (0.1%)
1	H	0.31	0/1939	0.49	2/2617 (0.1%)
1	I	0.28	0/1939	0.45	0/2617
1	J	0.29	0/1936	0.44	0/2613
1	K	0.28	0/1953	0.45	0/2636
1	L	0.29	0/1951	0.47	0/2633
1	M	0.28	0/1931	0.45	0/2606
1	N	0.28	0/1939	0.44	0/2617
1	O	0.28	0/1931	0.45	0/2606
1	P	0.31	0/1939	0.81	3/2617 (0.1%)
1	Q	0.30	0/1938	0.46	0/2616
1	R	0.28	0/1934	0.44	0/2610
1	S	0.28	0/1939	0.45	0/2617
1	T	0.30	0/1948	0.73	3/2629 (0.1%)
1	U	0.30	0/1927	0.46	0/2601
1	V	0.29	0/1939	0.44	0/2617
1	W	0.29	0/1948	0.49	1/2629 (0.0%)
2	C	0.30	0/1946	0.58	3/2626 (0.1%)
2	X	0.28	0/1934	0.44	0/2610
3	E	0.28	0/1936	0.58	3/2613 (0.1%)
4	a	0.40	0/202	0.86	0/312
4	c	0.37	0/202	0.89	0/312
4	e	0.30	0/202	0.77	0/312
4	g	0.38	0/202	0.83	0/312
4	i	0.40	0/202	0.82	0/312
4	k	0.37	0/202	0.79	0/312
4	m	0.38	0/202	0.86	0/312
4	o	0.39	0/202	0.74	0/312
4	q	0.41	0/202	0.87	0/312
4	s	0.36	0/202	0.82	0/312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	u	0.47	0/202	0.93	0/312
4	w	0.41	0/202	0.88	0/312
All	All	0.29	0/48963	0.54	22/66555 (0.0%)

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	217	ARG	NE-CZ-NH1	24.27	132.44	120.30
1	P	217	ARG	NE-CZ-NH2	-22.98	108.81	120.30
1	T	104	ARG	NE-CZ-NH1	20.51	130.55	120.30
1	T	104	ARG	NE-CZ-NH2	-20.06	110.27	120.30
2	C	104	ARG	NE-CZ-NH2	-12.87	113.87	120.30

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	19	0
1	B	1907	0	1955	28	0
1	D	1907	0	1955	27	0
1	F	1904	0	1951	31	0
1	G	1907	0	1955	22	0
1	H	1907	0	1955	27	0
1	I	1907	0	1955	45	0
1	J	1904	0	1951	48	1
1	K	1921	0	1963	27	0
1	L	1919	0	1963	34	0
1	M	1899	0	1949	28	0
1	N	1907	0	1955	25	0
1	O	1899	0	1949	27	0
1	P	1907	0	1955	28	0
1	Q	1906	0	1952	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	1902	0	1953	21	1
1	S	1907	0	1955	20	0
1	T	1916	0	1961	26	0
1	U	1895	0	1946	20	0
1	V	1907	0	1955	21	0
1	W	1916	0	1961	23	0
2	C	1914	0	1961	29	0
2	X	1902	0	1951	27	0
3	E	1904	0	1949	35	0
4	a	183	0	95	0	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	0	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	2	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	2	0
5	H	68	0	0	4	0
5	I	56	0	0	1	0
5	J	26	0	0	1	0
5	K	46	0	0	0	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	502	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 5.

The worst 5 of 502 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 ⓘ

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	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%)	22	44
1	K	249/253 (98%)	239 (96%)	9 (4%)	1 (0%)	38	63
1	L	248/253 (98%)	241 (97%)	6 (2%)	1 (0%)	38	63
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%)	38	63
All	All	5929/6072 (98%)	5759 (97%)	165 (3%)	5 (0%)	55	79

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 ⓘ

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%)	191 (95%)	10 (5%)	28	53
1	B	201/206 (98%)	188 (94%)	13 (6%)	20	39
1	D	201/206 (98%)	187 (93%)	14 (7%)	18	35
1	F	200/206 (97%)	186 (93%)	14 (7%)	18	35
1	G	201/206 (98%)	191 (95%)	10 (5%)	28	53
1	H	201/206 (98%)	187 (93%)	14 (7%)	18	35
1	I	201/206 (98%)	191 (95%)	10 (5%)	28	53
1	J	200/206 (97%)	185 (92%)	15 (8%)	16	31
1	K	202/206 (98%)	190 (94%)	12 (6%)	23	45
1	L	203/206 (98%)	189 (93%)	14 (7%)	18	36
1	M	200/206 (97%)	189 (94%)	11 (6%)	25	49
1	N	201/206 (98%)	188 (94%)	13 (6%)	20	39
1	O	200/206 (97%)	190 (95%)	10 (5%)	28	53
1	P	201/206 (98%)	186 (92%)	15 (8%)	16	31
1	Q	200/206 (97%)	191 (96%)	9 (4%)	32	59
1	R	201/206 (98%)	187 (93%)	14 (7%)	18	35
1	S	201/206 (98%)	191 (95%)	10 (5%)	28	53
1	T	202/206 (98%)	186 (92%)	16 (8%)	14	28
1	U	200/206 (97%)	190 (95%)	10 (5%)	28	53
1	V	201/206 (98%)	184 (92%)	17 (8%)	12	24
1	W	202/206 (98%)	192 (95%)	10 (5%)	28	53
2	C	202/206 (98%)	194 (96%)	8 (4%)	36	64
2	X	200/206 (97%)	186 (93%)	14 (7%)	18	35
3	E	200/206 (97%)	191 (96%)	9 (4%)	32	59
All	All	4822/4944 (98%)	4530 (94%)	292 (6%)	22	43

5 of 292 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	94	VAL
1	N	217	ARG
1	W	94	VAL
1	L	127	LEU
1	M	121	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	101	ASN
1	G	33	GLN
1	H	101	ASN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	249/253 (98%)	-0.04	0 100 100	34, 48, 77, 112	0
1	B	249/253 (98%)	-0.07	6 (2%) 59 52	30, 44, 76, 103	0
1	D	249/253 (98%)	0.30	10 (4%) 39 31	37, 68, 96, 126	0
1	F	249/253 (98%)	0.32	15 (6%) 23 17	42, 66, 97, 122	0
1	G	249/253 (98%)	0.00	4 (1%) 72 67	29, 45, 70, 102	0
1	H	249/253 (98%)	-0.05	1 (0%) 92 91	31, 49, 72, 98	0
1	I	249/253 (98%)	-0.19	0 100 100	34, 50, 70, 92	0
1	J	249/253 (98%)	0.40	16 (6%) 20 15	39, 62, 96, 126	0
1	K	251/253 (99%)	0.18	4 (1%) 72 67	37, 56, 79, 122	0
1	L	250/253 (98%)	0.11	6 (2%) 59 52	27, 46, 78, 100	0
1	M	248/253 (98%)	0.07	3 (1%) 79 75	35, 51, 75, 105	0
1	N	249/253 (98%)	0.04	9 (3%) 43 35	38, 55, 82, 103	0
1	O	248/253 (98%)	0.09	3 (1%) 79 75	33, 50, 77, 101	0
1	P	249/253 (98%)	-0.03	8 (3%) 48 40	26, 42, 77, 100	0
1	Q	249/253 (98%)	-0.03	1 (0%) 92 91	27, 44, 67, 87	0
1	R	248/253 (98%)	0.16	8 (3%) 48 40	38, 58, 85, 109	0
1	S	249/253 (98%)	-0.04	2 (0%) 86 83	36, 51, 74, 101	0
1	T	250/253 (98%)	0.01	10 (4%) 39 31	28, 45, 83, 117	0
1	U	247/253 (97%)	-0.24	0 100 100	24, 39, 62, 74	0
1	V	249/253 (98%)	0.04	2 (0%) 86 83	32, 52, 80, 105	0
1	W	250/253 (98%)	0.07	6 (2%) 59 52	31, 49, 74, 110	0
2	C	250/253 (98%)	-0.14	0 100 100	26, 44, 68, 124	0
2	X	249/253 (98%)	0.13	5 (2%) 65 59	34, 53, 82, 104	0
3	E	249/253 (98%)	0.49	12 (4%) 31 24	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%)	-0.67	0	100	100	42, 48, 58, 63	0
4	c	9/9 (100%)	-0.61	0	100	100	38, 42, 64, 76	0
4	e	9/9 (100%)	-0.60	0	100	100	55, 61, 78, 82	0
4	g	9/9 (100%)	-0.76	0	100	100	34, 43, 56, 69	0
4	i	9/9 (100%)	-0.78	0	100	100	38, 46, 56, 80	0
4	k	9/9 (100%)	-0.82	0	100	100	44, 51, 68, 73	0
4	m	9/9 (100%)	-0.79	0	100	100	44, 49, 64, 67	0
4	o	9/9 (100%)	-0.48	0	100	100	39, 48, 55, 62	0
4	q	9/9 (100%)	-0.76	0	100	100	35, 41, 61, 69	0
4	s	9/9 (100%)	-0.64	0	100	100	47, 50, 61, 63	0
4	u	9/9 (100%)	-0.84	0	100	100	33, 36, 50, 57	0
4	w	9/9 (100%)	-0.48	0	100	100	38, 46, 59, 78	0
All	All	6085/6180 (98%)	0.05	131 (2%)	62	56	24, 51, 83, 134	0

The worst 5 of 131 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	23	ILE	6.5
1	J	22	THR	5.9
1	P	20	SER	5.6
1	J	213	ARG	5.3
1	J	26	TRP	5.3

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 carbohydrates 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.