



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 29, 2023 – 11:53 AM EDT

PDB ID : 8FFR  
Title : Revised structure of the rabies virus nucleoprotein-RNA complex  
Authors : Leyrat, C.; Bourhis, J.M.; Albertini, A.A.V.; Wernimont, A.K.; Muziol, T.;  
Ravelli, R.B.G.; Weissenhorn, W.; Ruigrok, R.W.H.; Jamin, M.  
Deposited on : 2022-12-09  
Resolution : 3.49 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

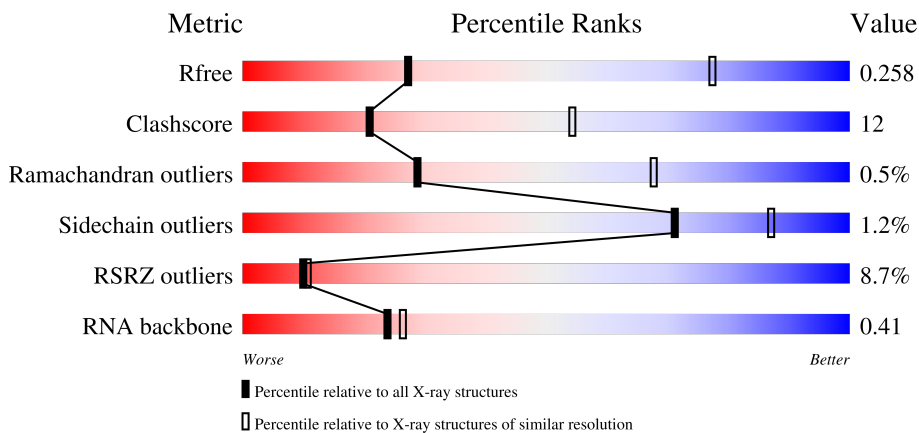
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.49 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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  $\geq 3$ , 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	450	 7% 69% 22% • 7%
1	B	450	 7% 68% 25% 7%
1	C	450	 11% 65% 27% • 7%
1	D	450	 6% 71% 21% • 7%

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Mol	Chain	Length	Quality of chain			
1	E	450	12%	64%	28%	7%
1	F	450	12%	70%	22%	7%
1	G	450	9%	65%	27%	7%
1	H	450	14%	66%	25%	7%
1	I	450	9%	68%	23%	7%
1	J	450	5%	71%	21%	7%
1	K	450	7%	66%	26%	7%
1	L	450	2%	69%	24%	7%
1	M	450	6%	64%	28%	7%
1	N	450	4%	68%	24%	7%
1	O	450	7%	73%	20%	7%
1	P	450	10%	71%	21%	7%
1	Q	450	15%	67%	25%	7%
1	R	450	6%	67%	25%	7%
1	S	450	10%	70%	22%	7%
1	T	450	4%	68%	24%	7%
1	U	450	6%	70%	22%	7%
1	V	450	12%	72%	21%	7%
2	W	99	20%	44%	28%	7%
3	X	99	15%	48%	28%	8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	X	101	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 77284 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	418	3322	2123	570	611	18	0	0	0
1	B	419	3331	2129	572	612	18	0	0	0
1	C	418	3322	2123	570	611	18	0	0	0
1	D	418	3322	2123	570	611	18	0	0	0
1	E	418	3322	2123	570	611	18	0	0	0
1	F	418	3322	2123	570	611	18	0	0	0
1	G	418	3322	2123	570	611	18	0	0	0
1	H	418	3322	2123	570	611	18	0	0	0
1	I	418	3322	2123	570	611	18	0	0	0
1	J	418	3322	2123	570	611	18	0	0	0
1	K	420	3339	2133	573	615	18	0	0	0
1	L	419	3331	2129	572	612	18	0	0	0
1	M	420	3339	2133	573	615	18	0	0	0
1	N	418	3322	2123	570	611	18	0	0	0
1	O	419	3331	2129	572	612	18	0	0	0
1	P	420	3339	2133	573	615	18	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	418	Total	C	N	O	S	0	0	0
			3322	2123	570	611	18			
1	R	418	Total	C	N	O	S	0	0	0
			3322	2123	570	611	18			
1	S	418	Total	C	N	O	S	0	0	0
			3322	2123	570	611	18			
1	T	418	Total	C	N	O	S	0	0	0
			3322	2123	570	611	18			
1	U	418	Total	C	N	O	S	0	0	0
			3322	2123	570	611	18			
1	V	419	Total	C	N	O	S	0	0	0
			3331	2129	572	612	18			

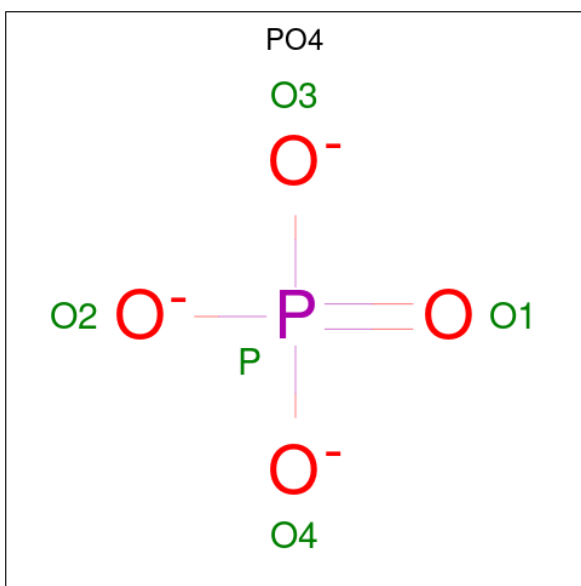
- Molecule 2 is a RNA chain called RNA (99-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	99	Total	C	N	O	P	0	0	0
			2059	932	379	650	98			

- Molecule 3 is a RNA chain called RNA (99-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	99	Total	C	N	O	P	0	0	0
			2044	925	365	656	98			

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

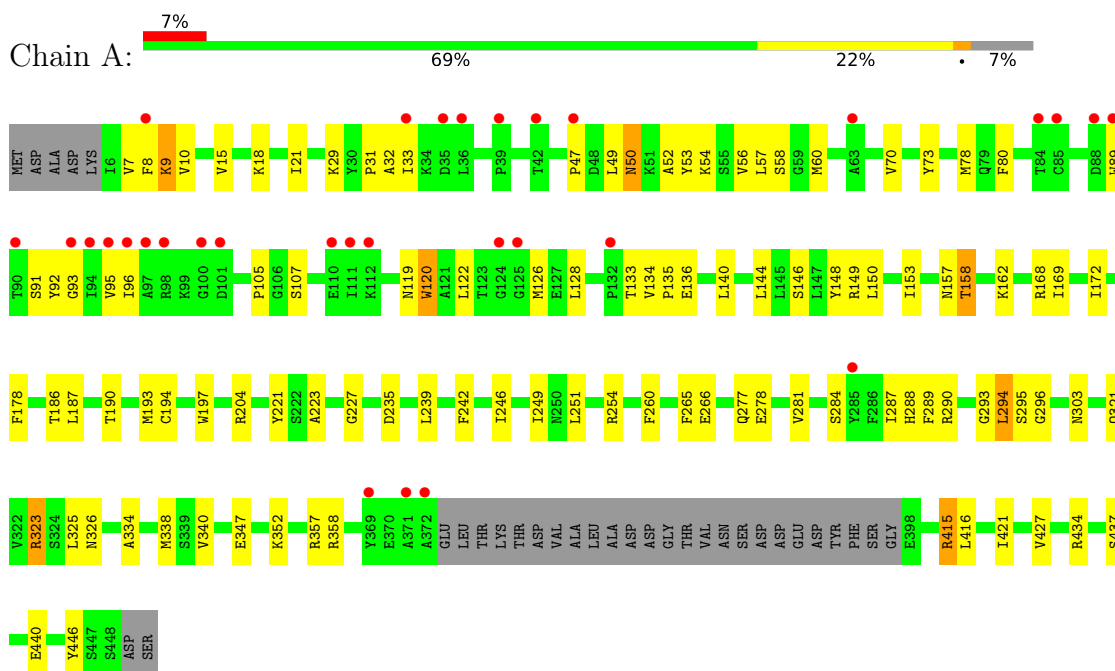


<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>			<b>ZeroOcc</b>	<b>AltConf</b>
4	W	1	Total	O	P	0	0
			5	4	1		
4	X	1	Total	O	P	0	0
			5	4	1		

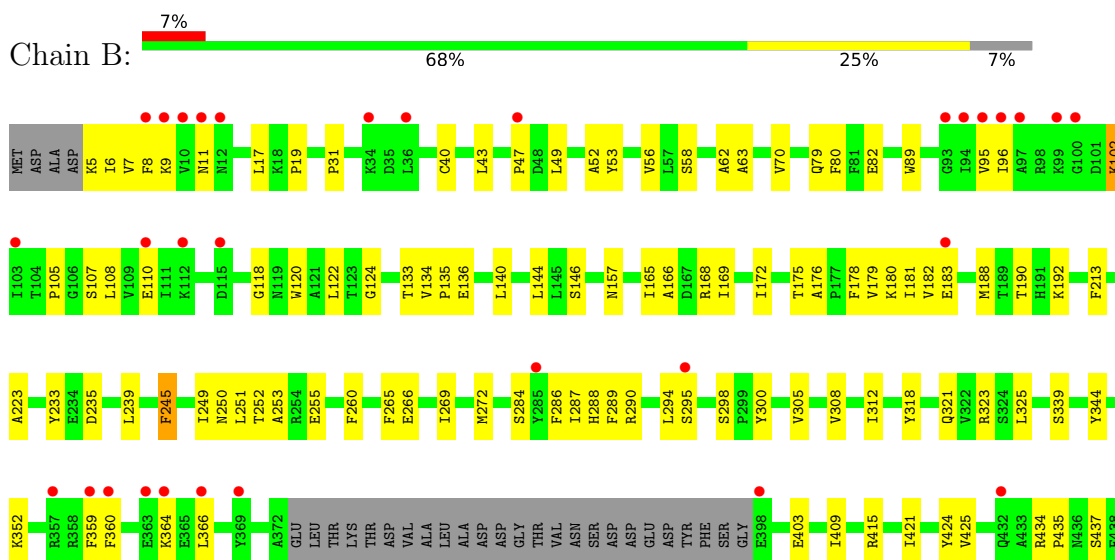
### 3 Residue-property plots [i](#)

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



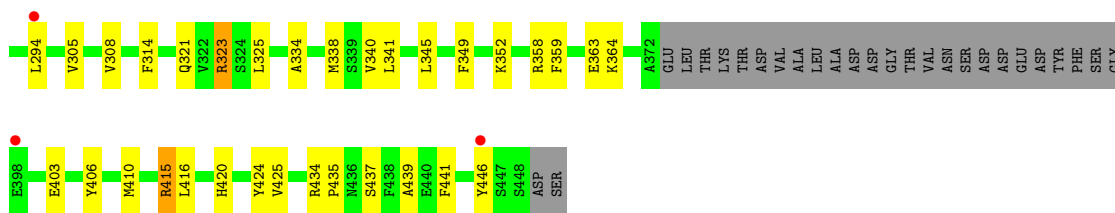
#### • Molecule 1: Nucleoprotein



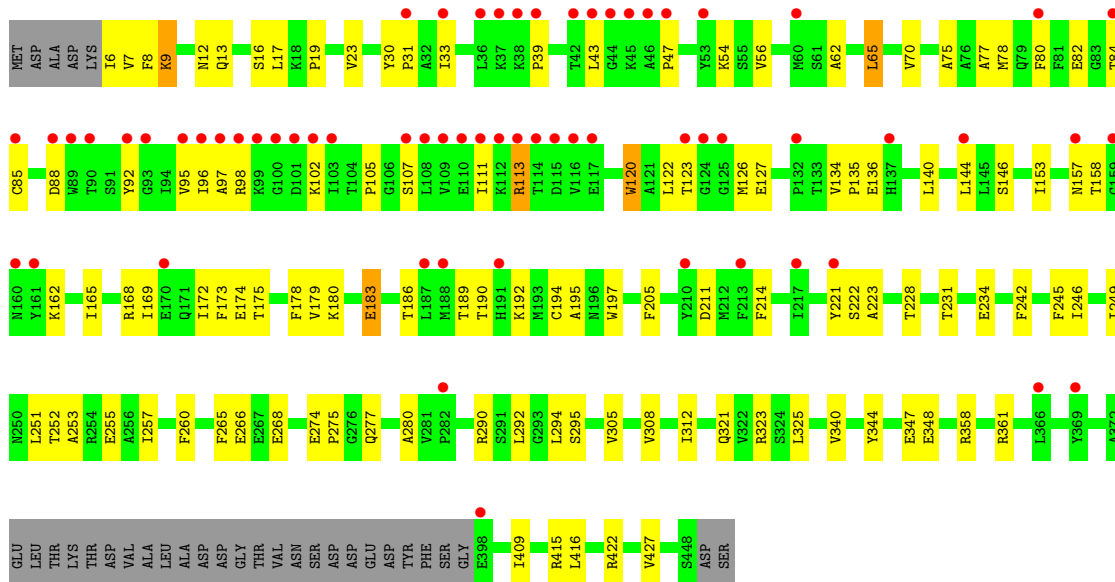




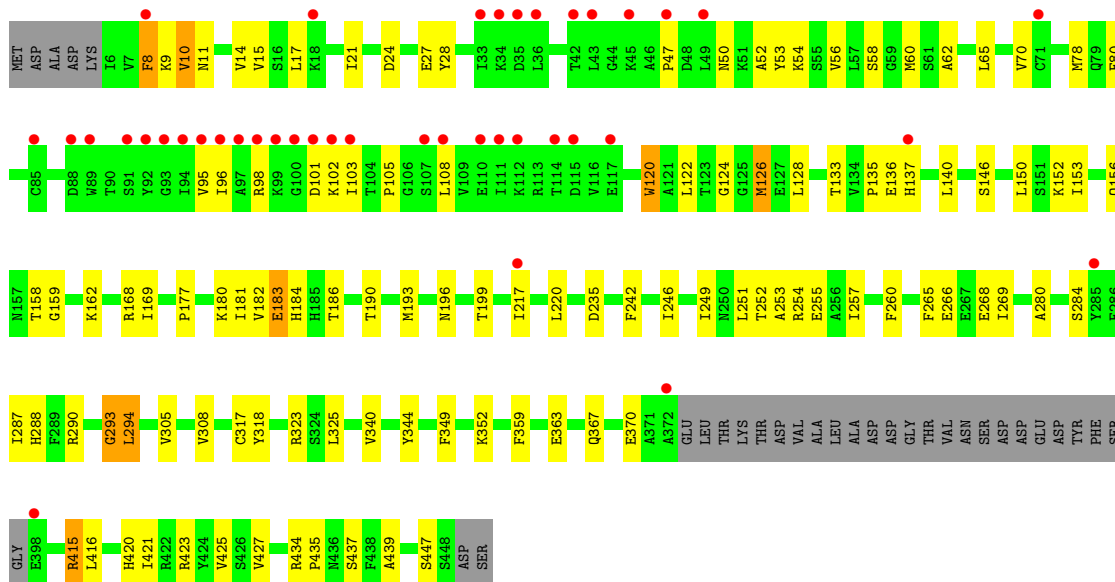




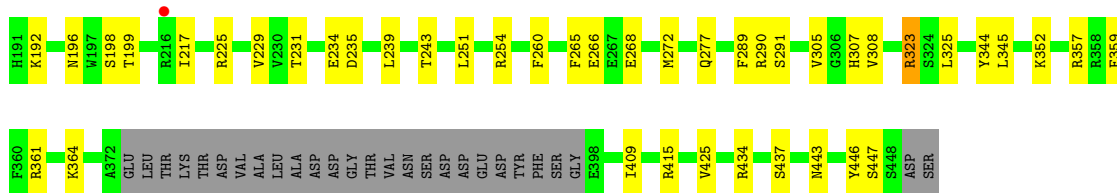
• Molecule 1: Nucleoprotein



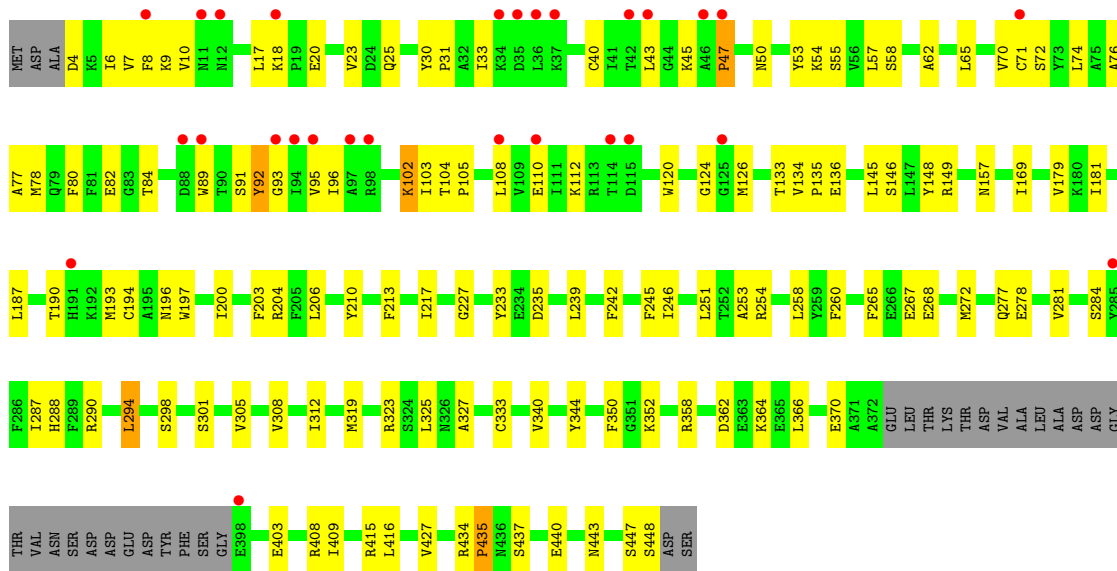
• Molecule 1: Nucleoprotein



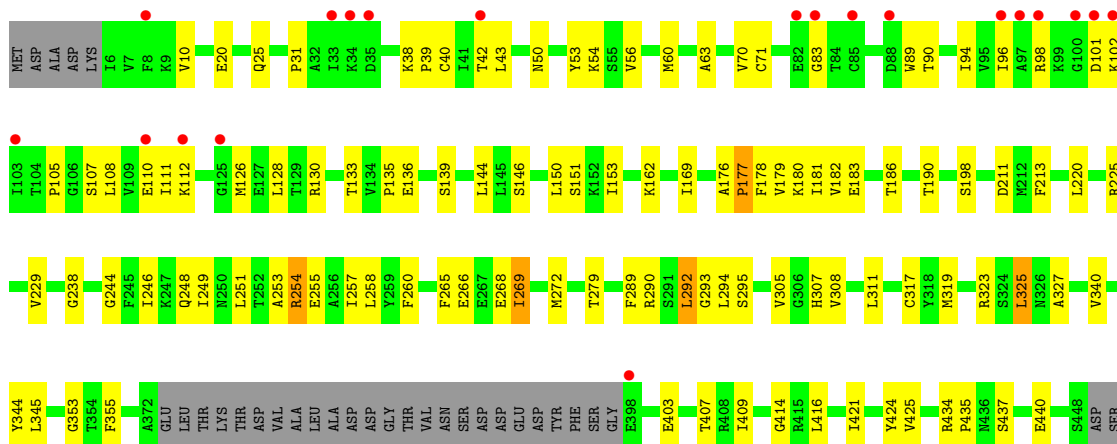




• Molecule 1: Nucleoprotein

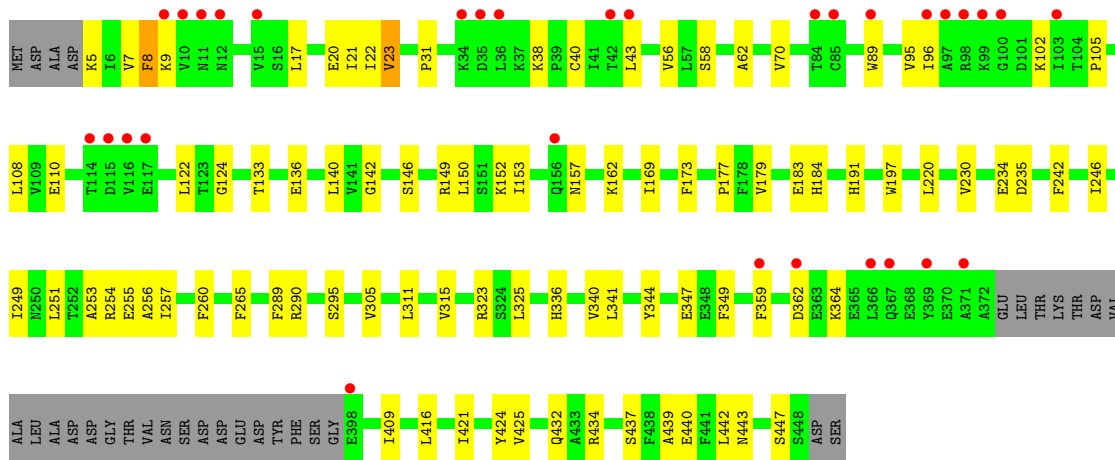


• Molecule 1: Nucleoprotein

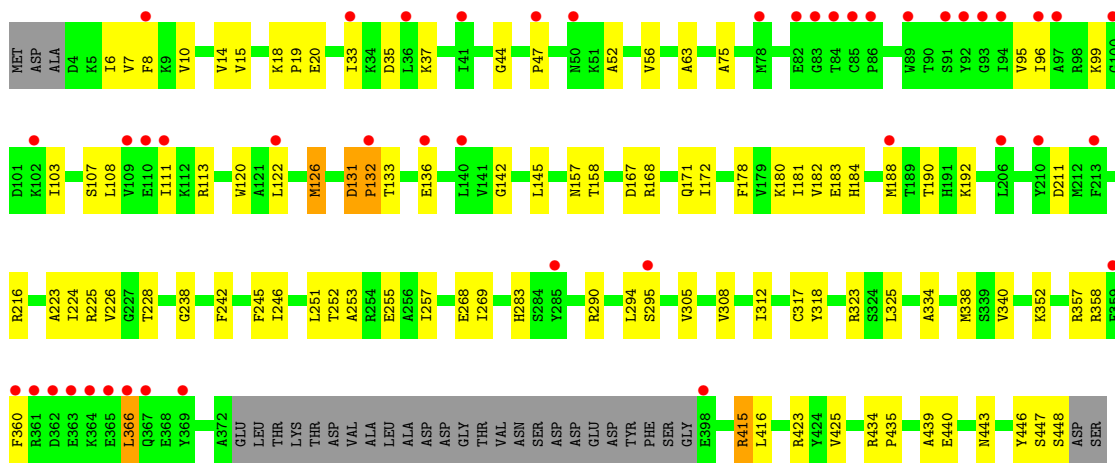


• Molecule 1: Nucleoprotein

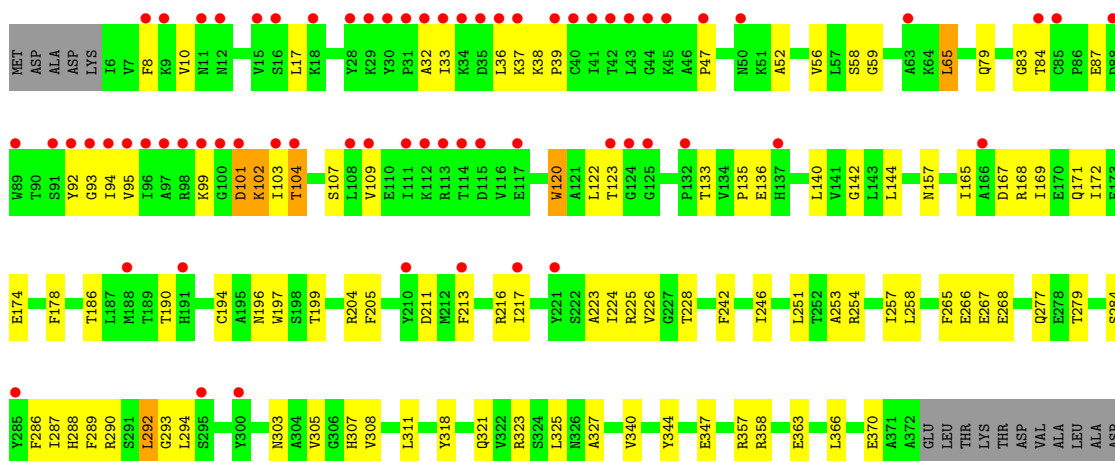




• Molecule 1: Nucleoprotein

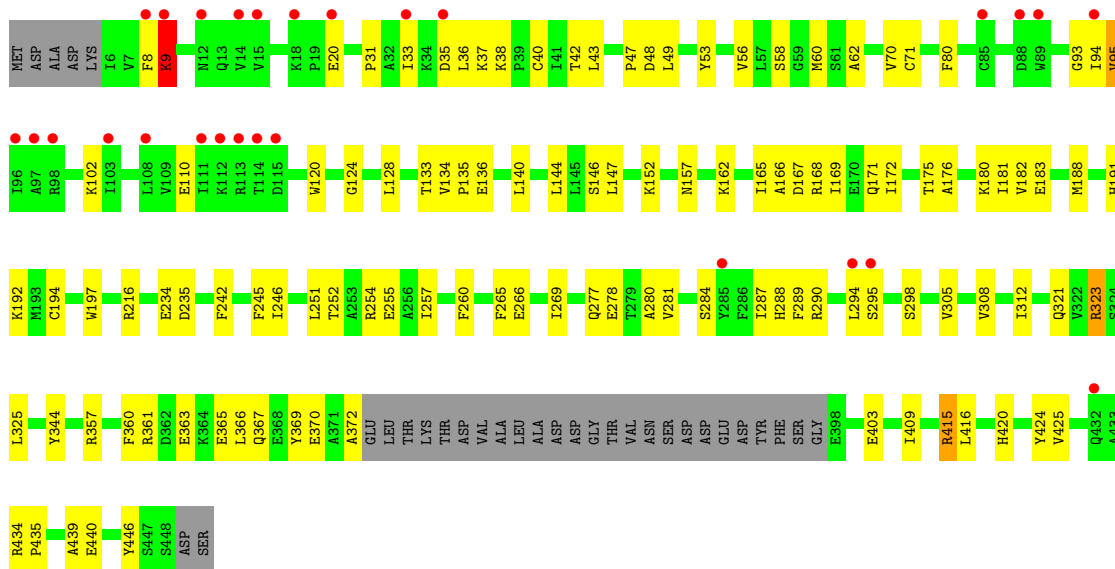


• Molecule 1: Nucleoprotein

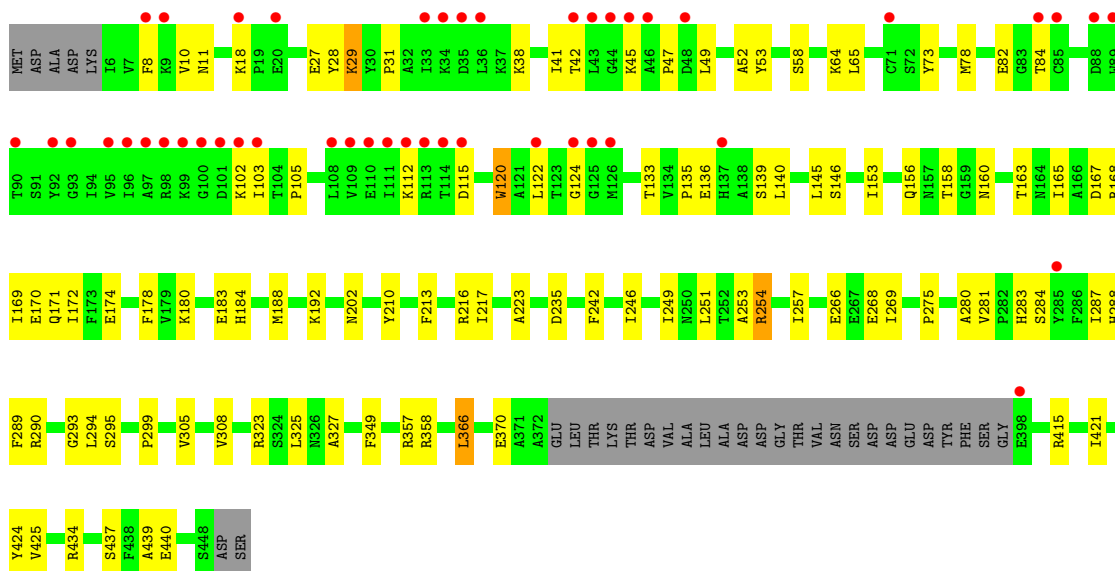




- Molecule 1: Nucleoprotein

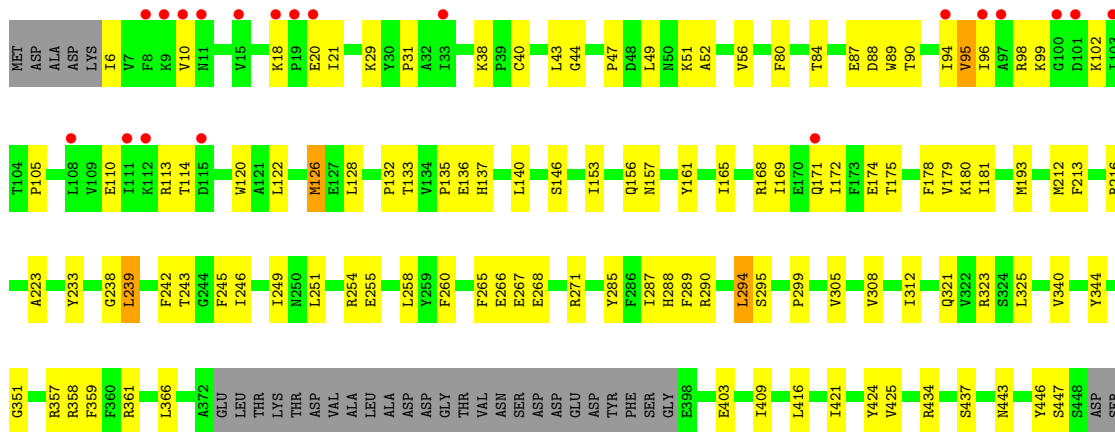


- Molecule 1: Nucleoprotein

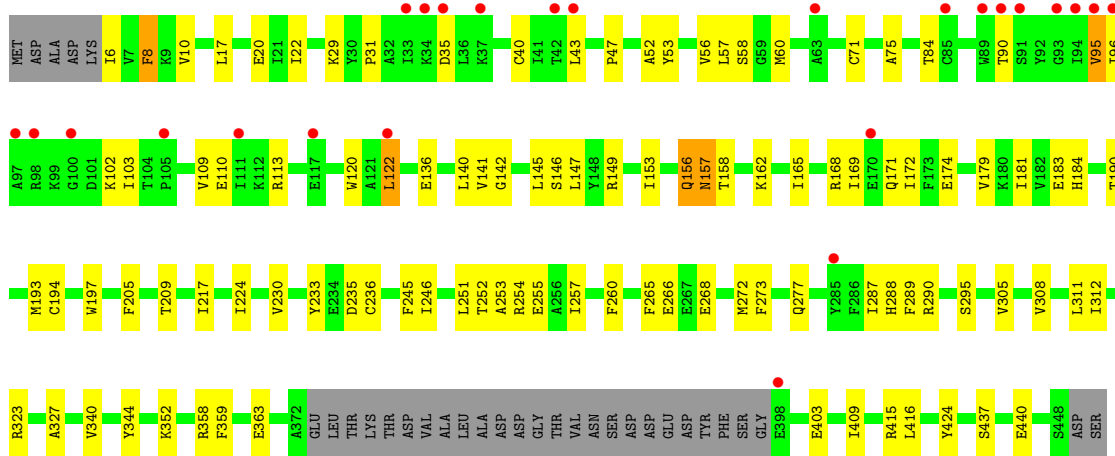


- Molecule 1: Nucleoprotein

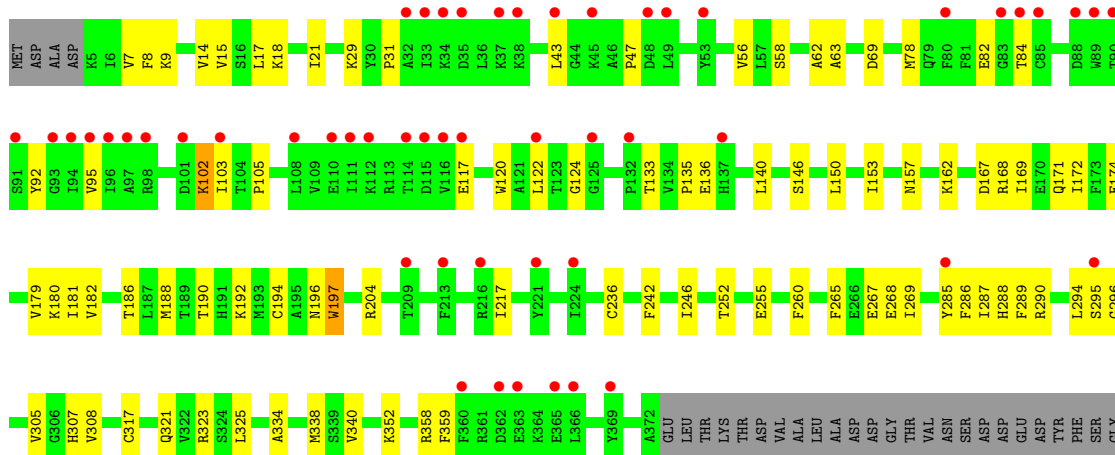
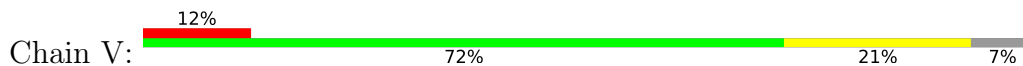




• Molecule 1: Nucleoprotein

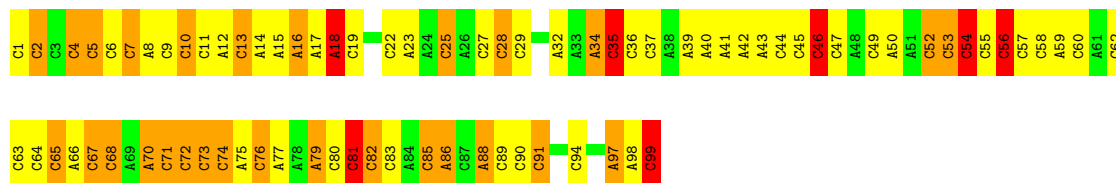


• Molecule 1: Nucleoprotein

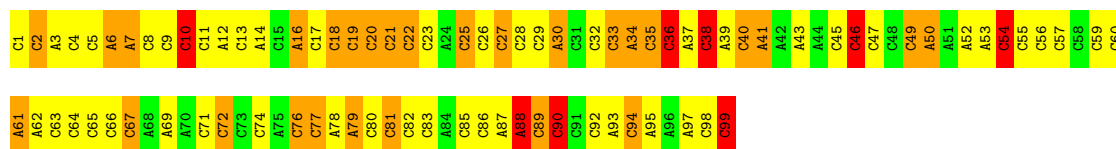
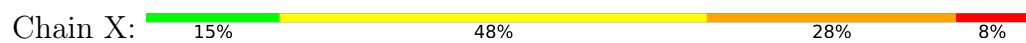




- Molecule 2: RNA (99-MER)



- Molecule 3: RNA (99-MER)





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	270.43Å 281.00Å 236.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.75 – 3.49 49.75 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.75-3.49) 99.3 (49.75-3.49)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 3.48Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487, BUSTER	Depositor
R, $R_{free}$	0.224 , 0.255 0.226 , 0.258	Depositor DCC
$R_{free}$ test set	11062 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	103.2	Xtrriage
Anisotropy	0.401	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 65.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	0.057 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	77284	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	103.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.62	3/3402 (0.1%)	0.73	1/4597 (0.0%)
1	B	0.63	6/3411 (0.2%)	0.76	1/4608 (0.0%)
1	C	0.57	3/3402 (0.1%)	0.69	0/4597
1	D	0.57	0/3402	0.73	3/4597 (0.1%)
1	E	0.60	6/3402 (0.2%)	0.72	0/4597
1	F	0.57	2/3402 (0.1%)	0.70	1/4597 (0.0%)
1	G	0.57	1/3402 (0.0%)	0.72	0/4597
1	H	0.59	4/3402 (0.1%)	0.70	1/4597 (0.0%)
1	I	0.61	5/3402 (0.1%)	0.70	1/4597 (0.0%)
1	J	0.62	3/3402 (0.1%)	0.78	3/4597 (0.1%)
1	K	0.63	1/3419 (0.0%)	0.78	2/4619 (0.0%)
1	L	0.66	2/3411 (0.1%)	0.84	4/4608 (0.1%)
1	M	0.65	3/3419 (0.1%)	0.82	2/4619 (0.0%)
1	N	0.61	0/3402	0.77	3/4597 (0.1%)
1	O	0.64	4/3411 (0.1%)	0.78	1/4608 (0.0%)
1	P	0.59	3/3419 (0.1%)	0.72	2/4619 (0.0%)
1	Q	0.64	9/3402 (0.3%)	0.70	2/4597 (0.0%)
1	R	0.60	5/3402 (0.1%)	0.75	2/4597 (0.0%)
1	S	0.56	0/3402	0.69	1/4597 (0.0%)
1	T	0.63	2/3402 (0.1%)	0.76	4/4597 (0.1%)
1	U	0.64	4/3402 (0.1%)	0.75	2/4597 (0.0%)
1	V	0.61	6/3411 (0.2%)	0.72	2/4608 (0.0%)
2	W	0.89	1/2297 (0.0%)	1.97	120/3563 (3.4%)
3	X	0.94	0/2275	2.11	147/3525 (4.2%)
All	All	0.63	73/79503 (0.1%)	0.89	305/108332 (0.3%)

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	95	VAL	CB-CG1	8.64	1.71	1.52
1	M	95	VAL	CB-CG1	8.00	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	95	VAL	CB-CG1	7.48	1.68	1.52
1	K	8	PHE	CB-CG	-7.41	1.38	1.51
1	Q	104	THR	C-N	7.37	1.48	1.34

The worst 5 of 305 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	73	C	C6-N1-C2	-18.30	112.98	120.30
2	W	53	C	C6-N1-C2	-14.76	114.40	120.30
3	X	28	C	C6-N1-C2	-13.73	114.81	120.30
3	X	25	C	C6-N1-C2	-13.67	114.83	120.30
2	W	35	C	C6-N1-C2	-13.54	114.88	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	3322	0	3277	86	0
1	B	3331	0	3290	98	0
1	C	3322	0	3277	93	0
1	D	3322	0	3277	82	0
1	E	3322	0	3277	104	0
1	F	3322	0	3277	87	0
1	G	3322	0	3277	104	0
1	H	3322	0	3277	100	0
1	I	3322	0	3277	98	0
1	J	3322	0	3277	88	0
1	K	3339	0	3294	128	0
1	L	3331	0	3290	95	0
1	M	3339	0	3294	104	1
1	N	3322	0	3277	89	0
1	O	3331	0	3290	77	0
1	P	3339	0	3294	73	0
1	Q	3322	0	3277	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	3322	0	3277	92	0
1	S	3322	0	3277	77	0
1	T	3322	0	3277	109	0
1	U	3322	0	3277	81	0
1	V	3331	0	3290	77	1
2	W	2059	0	1091	33	0
3	X	2044	0	1091	37	0
4	W	5	0	0	0	0
4	X	5	0	0	3	0
All	All	77284	0	74379	1846	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 12.

The worst 5 of 1846 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:K:96:ILE:HD11	1:K:108:LEU:HG	1.23	1.10
1:D:96:ILE:CD1	1:D:108:LEU:HA	1.84	1.07
1:C:134:VAL:HG23	1:C:135:PRO:HD3	1.38	1.05
1:D:96:ILE:HD11	1:D:108:LEU:HA	1.41	1.01
1:C:84:THR:HB	1:C:102:LYS:HG2	1.41	0.99

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:M:4:ASP:OD2	1:V:18:LYS:NZ[3_655]	2.14	0.06

## 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	414/450 (92%)	390 (94%)	20 (5%)	4 (1%)	15	54
1	B	415/450 (92%)	396 (95%)	19 (5%)	0	100	100
1	C	414/450 (92%)	393 (95%)	18 (4%)	3 (1%)	22	61
1	D	414/450 (92%)	396 (96%)	16 (4%)	2 (0%)	29	68
1	E	414/450 (92%)	391 (94%)	19 (5%)	4 (1%)	15	54
1	F	414/450 (92%)	404 (98%)	9 (2%)	1 (0%)	47	81
1	G	414/450 (92%)	393 (95%)	21 (5%)	0	100	100
1	H	414/450 (92%)	395 (95%)	16 (4%)	3 (1%)	22	61
1	I	414/450 (92%)	389 (94%)	20 (5%)	5 (1%)	13	50
1	J	414/450 (92%)	392 (95%)	19 (5%)	3 (1%)	22	61
1	K	416/450 (92%)	399 (96%)	16 (4%)	1 (0%)	47	81
1	L	415/450 (92%)	391 (94%)	20 (5%)	4 (1%)	15	54
1	M	416/450 (92%)	394 (95%)	18 (4%)	4 (1%)	15	54
1	N	414/450 (92%)	395 (95%)	18 (4%)	1 (0%)	47	81
1	O	415/450 (92%)	397 (96%)	18 (4%)	0	100	100
1	P	416/450 (92%)	389 (94%)	24 (6%)	3 (1%)	22	61
1	Q	414/450 (92%)	396 (96%)	16 (4%)	2 (0%)	29	68
1	R	414/450 (92%)	392 (95%)	22 (5%)	0	100	100
1	S	414/450 (92%)	391 (94%)	22 (5%)	1 (0%)	47	81
1	T	414/450 (92%)	393 (95%)	19 (5%)	2 (0%)	29	68
1	U	414/450 (92%)	398 (96%)	15 (4%)	1 (0%)	47	81
1	V	415/450 (92%)	399 (96%)	16 (4%)	0	100	100
All	All	9118/9900 (92%)	8673 (95%)	401 (4%)	44 (0%)	29	68

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	TYR
1	A	158	THR
1	A	294	LEU
1	C	294	LEU
1	D	158	THR

### 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	359/386 (93%)	351 (98%)	8 (2%)	52	78
1	B	360/386 (93%)	358 (99%)	2 (1%)	86	94
1	C	359/386 (93%)	354 (99%)	5 (1%)	67	85
1	D	359/386 (93%)	353 (98%)	6 (2%)	60	82
1	E	359/386 (93%)	350 (98%)	9 (2%)	47	75
1	F	359/386 (93%)	356 (99%)	3 (1%)	81	91
1	G	359/386 (93%)	354 (99%)	5 (1%)	67	85
1	H	359/386 (93%)	356 (99%)	3 (1%)	81	91
1	I	359/386 (93%)	356 (99%)	3 (1%)	81	91
1	J	359/386 (93%)	358 (100%)	1 (0%)	92	97
1	K	361/386 (94%)	357 (99%)	4 (1%)	73	88
1	L	360/386 (93%)	358 (99%)	2 (1%)	86	94
1	M	361/386 (94%)	357 (99%)	4 (1%)	73	88
1	N	359/386 (93%)	354 (99%)	5 (1%)	67	85
1	O	360/386 (93%)	357 (99%)	3 (1%)	81	91
1	P	361/386 (94%)	356 (99%)	5 (1%)	67	85
1	Q	359/386 (93%)	353 (98%)	6 (2%)	60	82
1	R	359/386 (93%)	353 (98%)	6 (2%)	60	82
1	S	359/386 (93%)	352 (98%)	7 (2%)	57	80
1	T	359/386 (93%)	356 (99%)	3 (1%)	81	91
1	U	359/386 (93%)	356 (99%)	3 (1%)	81	91
1	V	360/386 (93%)	358 (99%)	2 (1%)	86	94
All	All	7908/8492 (93%)	7813 (99%)	95 (1%)	71	87

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	323	ARG
1	Q	303	ASN
1	N	440	GLU
1	P	415	ARG
1	R	216	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	250	ASN
1	U	11	ASN
1	R	171	GLN
1	S	283	HIS
1	U	196	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	W	98/99 (98%)	27 (27%)	1 (1%)
3	X	98/99 (98%)	23 (23%)	0
All	All	196/198 (98%)	50 (25%)	1 (0%)

5 of 50 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	W	2	C
2	W	9	C
2	W	10	C
2	W	13	C
2	W	16	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	W	53	C

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PO4	X	101	-	4,4,4	0.98	0	6,6,6	1.12	1 (16%)
4	PO4	W	101	-	4,4,4	0.86	0	6,6,6	1.04	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	101	PO4	O4-P-O1	-2.03	103.47	110.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	101	PO4	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	418/450 (92%)	0.45	31 (7%) 14 14	73, 98, 121, 132	0
1	B	419/450 (93%)	0.39	31 (7%) 14 14	75, 95, 118, 135	0
1	C	418/450 (92%)	0.62	51 (12%) 4 5	78, 108, 138, 148	0
1	D	418/450 (92%)	0.37	26 (6%) 20 18	81, 98, 123, 143	0
1	E	418/450 (92%)	0.64	53 (12%) 3 4	85, 114, 138, 154	0
1	F	418/450 (92%)	0.69	53 (12%) 3 4	85, 119, 141, 149	0
1	G	418/450 (92%)	0.54	40 (9%) 8 8	85, 109, 131, 143	0
1	H	418/450 (92%)	0.77	64 (15%) 2 2	83, 121, 142, 152	0
1	I	418/450 (92%)	0.53	41 (9%) 7 8	81, 106, 127, 139	0
1	J	418/450 (92%)	0.32	22 (5%) 26 24	76, 93, 120, 138	0
1	K	420/450 (93%)	0.42	32 (7%) 13 14	74, 97, 118, 134	0
1	L	419/450 (93%)	0.21	10 (2%) 59 53	65, 85, 108, 127	0
1	M	420/450 (93%)	0.42	28 (6%) 17 16	65, 92, 117, 127	0
1	N	418/450 (92%)	0.32	20 (4%) 30 27	69, 92, 113, 129	0
1	O	419/450 (93%)	0.37	31 (7%) 14 14	72, 89, 113, 136	0
1	P	420/450 (93%)	0.55	45 (10%) 6 6	75, 107, 127, 135	0
1	Q	418/450 (92%)	0.82	69 (16%) 1 2	81, 122, 144, 152	0
1	R	418/450 (92%)	0.42	27 (6%) 18 17	79, 102, 124, 143	0
1	S	418/450 (92%)	0.58	46 (11%) 5 6	82, 114, 136, 149	0
1	T	418/450 (92%)	0.38	20 (4%) 30 27	76, 96, 122, 135	0
1	U	418/450 (92%)	0.33	25 (5%) 21 19	69, 101, 122, 137	0
1	V	419/450 (93%)	0.63	53 (12%) 3 5	81, 114, 136, 149	0
2	W	99/99 (100%)	0.30	0 100 100	84, 103, 121, 129	0
3	X	99/99 (100%)	0.29	0 100 100	78, 100, 120, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	9404/10098 (93%)	0.49	818 (8%) 10 11	65, 102, 133, 154	0

The worst 5 of 818 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	96	ILE	8.1
1	D	9	LYS	8.0
1	C	94	ILE	6.8
1	G	11	ASN	6.7
1	T	11	ASN	6.3

## 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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	PO4	W	101	5/5	0.96	0.17	97,104,108,116	0
4	PO4	X	101	5/5	0.97	0.17	70,77,88,106	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.