



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:55 PM GMT

PDB ID : 4V9E
Title : Crystal Structure of Rift Valley Fever Virus Nucleocapsid Protein Hexamer Bound to Single-stranded RNA.
Authors : Raymond, D.D.; Smith, J.L.
Deposited on : 2012-09-19
Resolution : 3.40 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

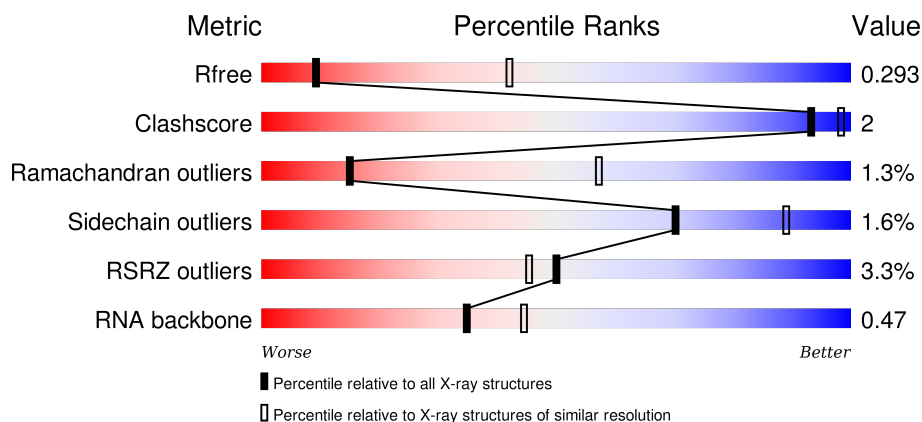
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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.






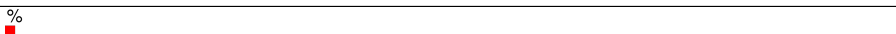
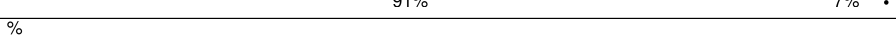
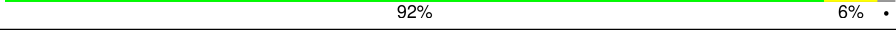



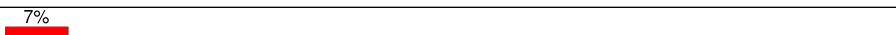
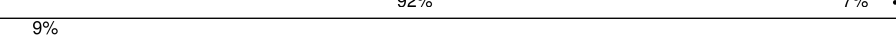
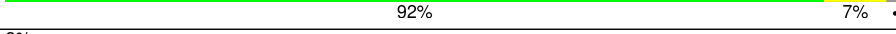



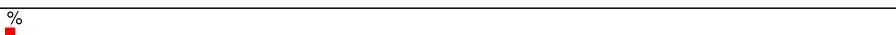






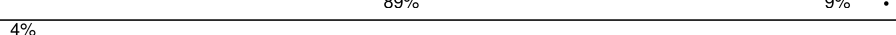


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)
RNA backbone	2183	1041 (4.00-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	AA	245	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div></div> </div> <div></div> </div>
1	AB	245	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div></div> </div> <div></div> </div>
1	AC	245	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div></div> </div> <div></div> </div>
1	AD	245	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div></div> </div> <div></div> </div>

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Mol	Chain	Length	Quality of chain
1	AE	245	 91% 7% .
1	AF	245	 88% 10% .
1	AG	245	 91% 7% .
1	AH	245	 91% 7% .
1	AI	245	 92% 6% .
1	AJ	245	 89% 9% .
1	AK	245	 89% 9% .
1	AL	245	 90% 9% .
1	AM	245	 92% 7% .
1	AN	245	 92% 7% .
1	AO	245	 92% 7% .
1	AP	245	 91% 8% .
1	AQ	245	 93% 6% .
1	AR	245	 91% 7% .
1	BA	245	 89% 9% ..
1	BB	245	 91% 7% ..
1	BC	245	 91% 7% .
1	BD	245	 90% 8% .
1	BE	245	 89% 9% .
1	BF	245	 89% 9% ..
1	BG	245	 91% 7% .
1	BH	245	 90% 8% .
1	BI	245	 90% 9% .
1	BJ	245	 89% 9% .
1	BK	245	 91% 7% .

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Mol	Chain	Length	Quality of chain
1	BL	245	
1	BM	245	
1	BN	245	
1	BO	245	
1	BP	245	
1	BQ	245	
1	BR	245	
2	Aa	36	
2	Ag	36	
2	Am	36	
2	Ba	36	
2	Bg	36	
2	Bm	36	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 72072 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 Nucleocapsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	AB	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	AC	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	AD	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	AE	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	AF	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	AG	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	AH	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	AI	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	AJ	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	AK	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	AL	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	AM	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	AN	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	AO	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	AP	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AQ	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	AR	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BA	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BB	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BC	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BD	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BE	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BF	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BG	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BH	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BI	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BJ	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BK	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BL	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BM	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BN	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BO	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BP	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BQ	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BR	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			

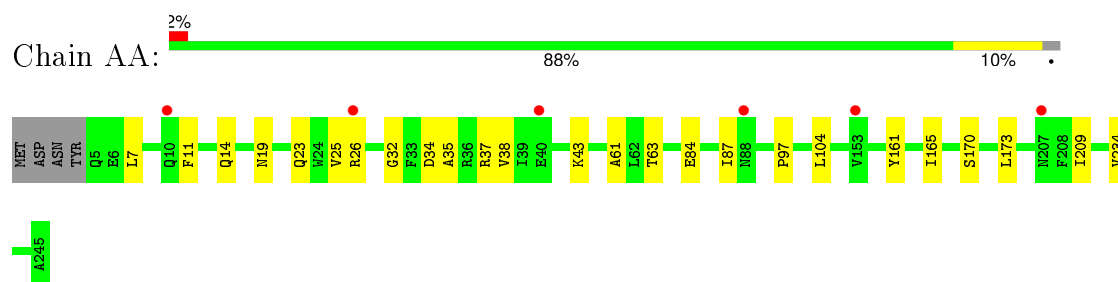
- Molecule 2 is a RNA chain called 35-mer poly(U) RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Aa	36	Total	C	N	O	P	0	0	0
			720	324	72	288	36			
2	Ag	36	Total	C	N	O	P	0	0	0
			720	324	72	288	36			
2	Am	36	Total	C	N	O	P	0	0	0
			720	324	72	288	36			
2	Ba	36	Total	C	N	O	P	0	0	0
			720	324	72	288	36			
2	Bg	36	Total	C	N	O	P	0	0	0
			720	324	72	288	36			
2	Bm	36	Total	C	N	O	P	0	0	0
			720	324	72	288	36			

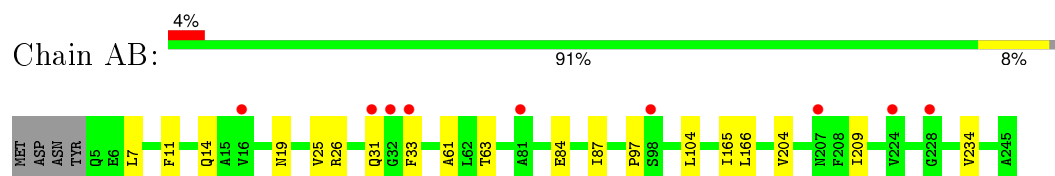
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

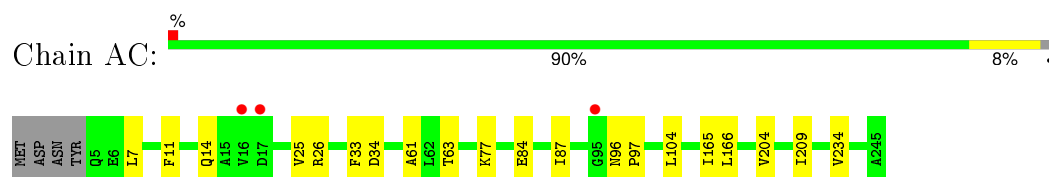
- Molecule 1: Nucleocapsid protein



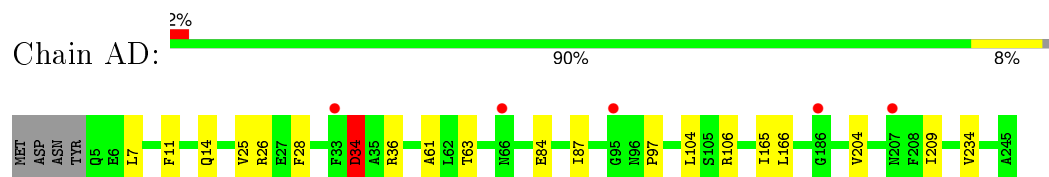
- Molecule 1: Nucleocapsid protein



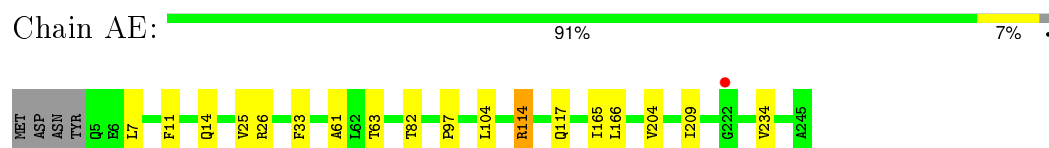
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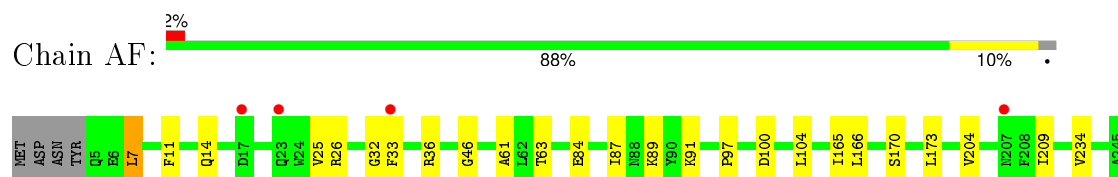
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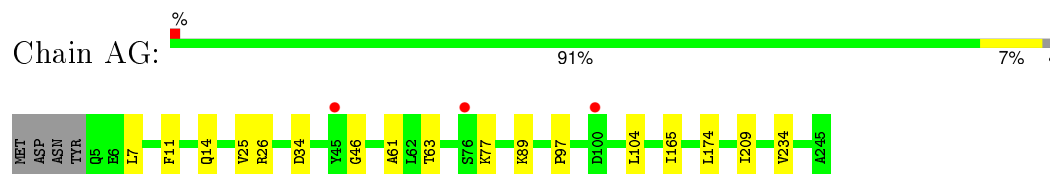
- Molecule 1: Nucleocapsid protein



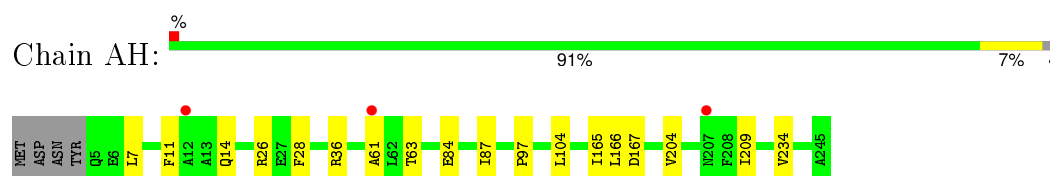
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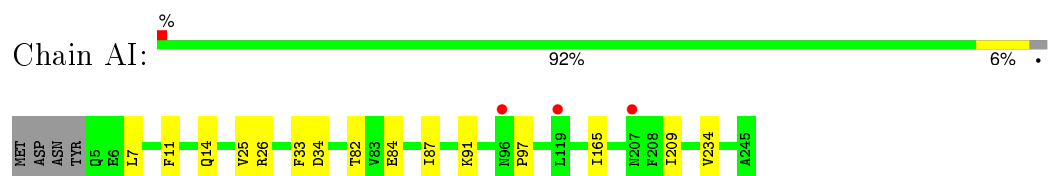
- Molecule 1: Nucleocapsid protein



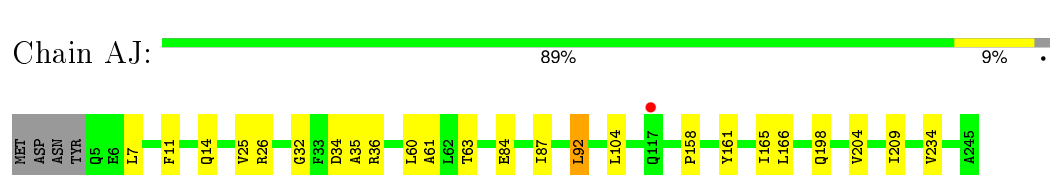
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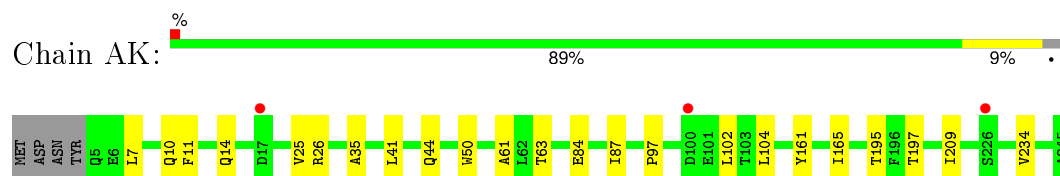
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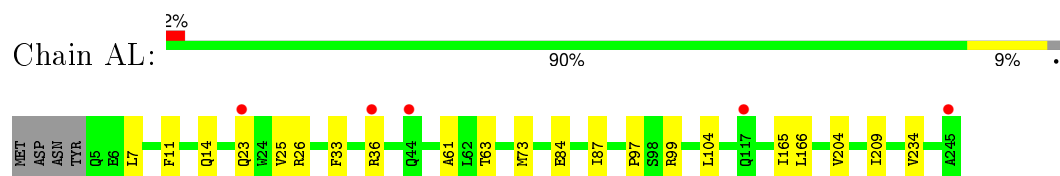
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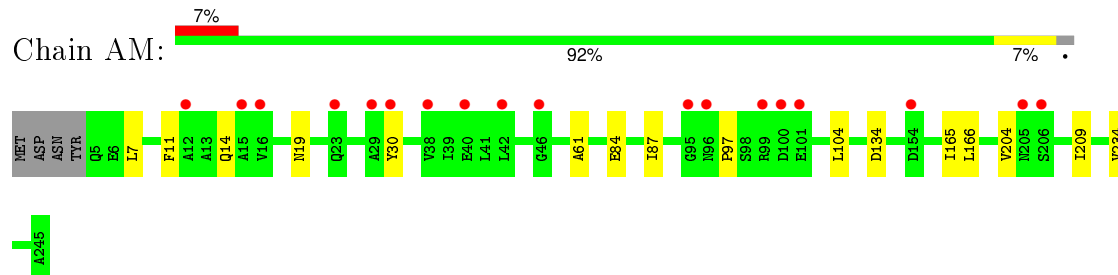
- Molecule 1: Nucleocapsid protein



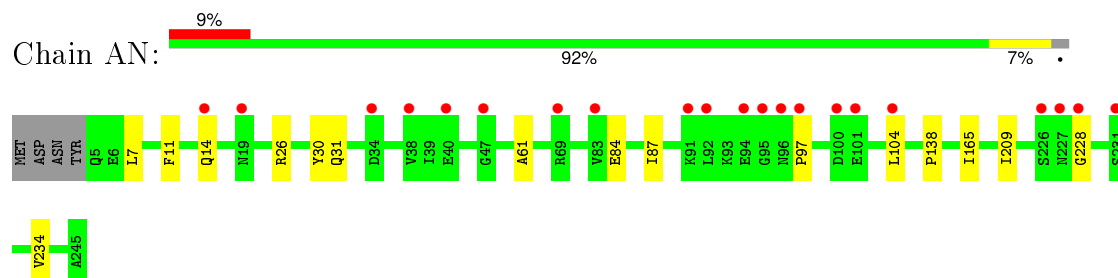
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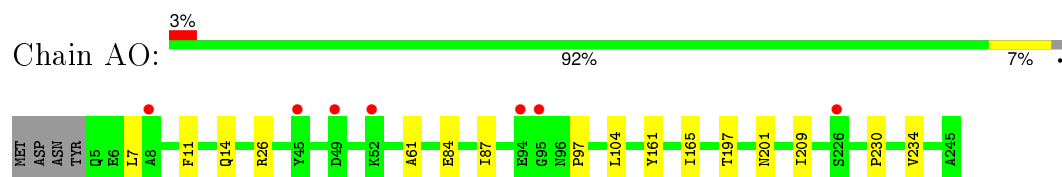
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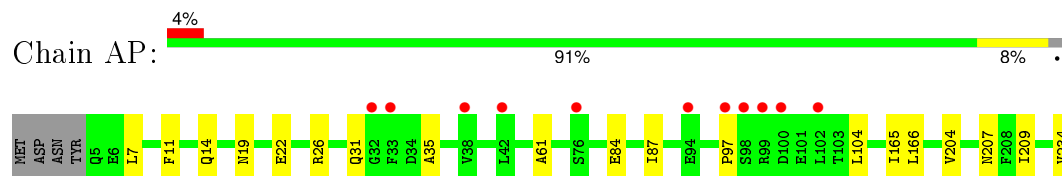
- Molecule 1: Nucleocapsid protein



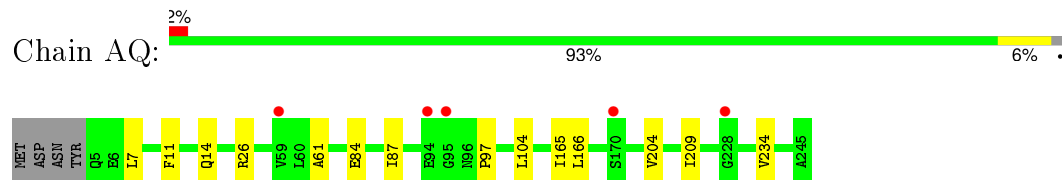
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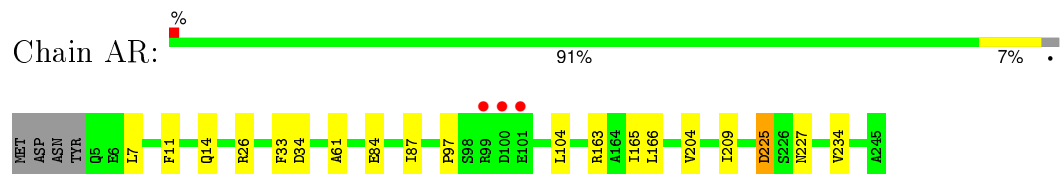
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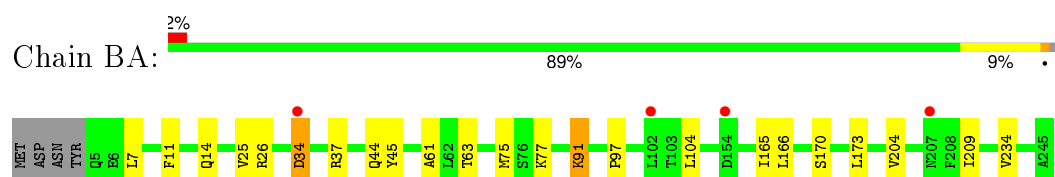
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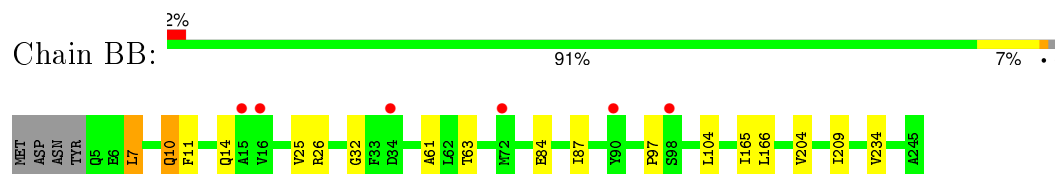
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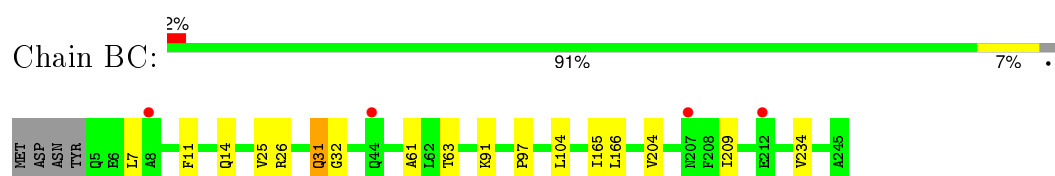
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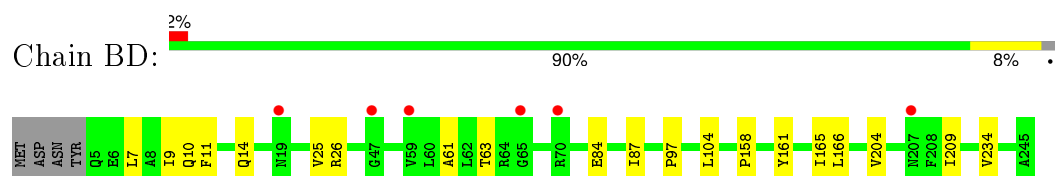
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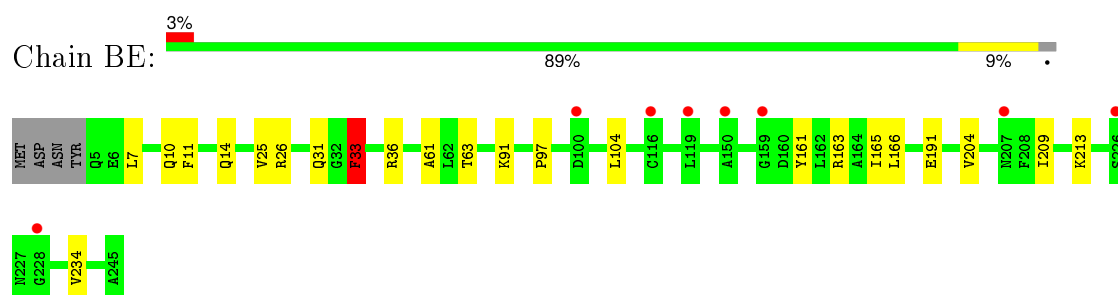
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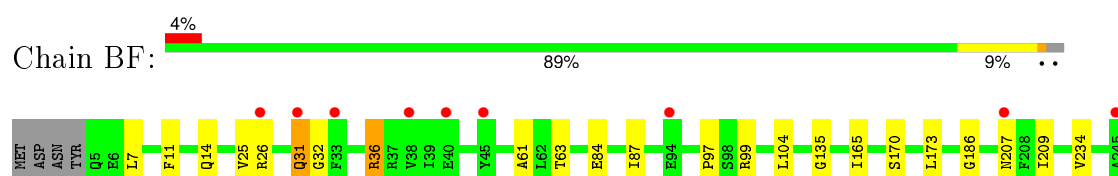
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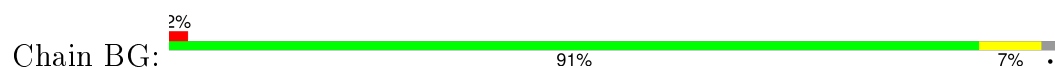
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- Molecule 1: Nucleocapsid protein

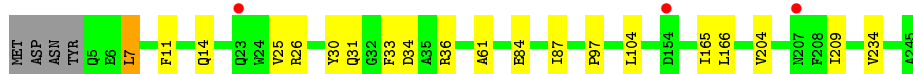
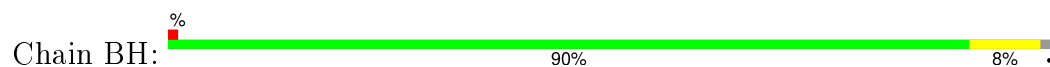


- Molecule 1: Nucleocapsid protein





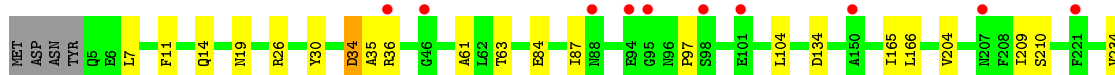
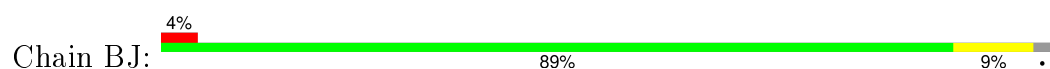
- Molecule 1: Nucleocapsid protein



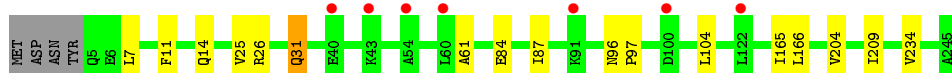
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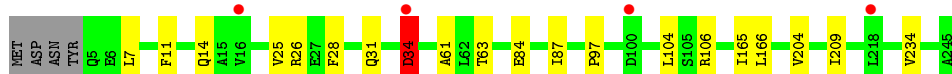
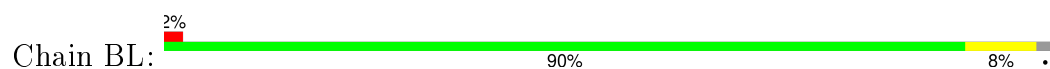
- Molecule 1: Nucleocapsid protein



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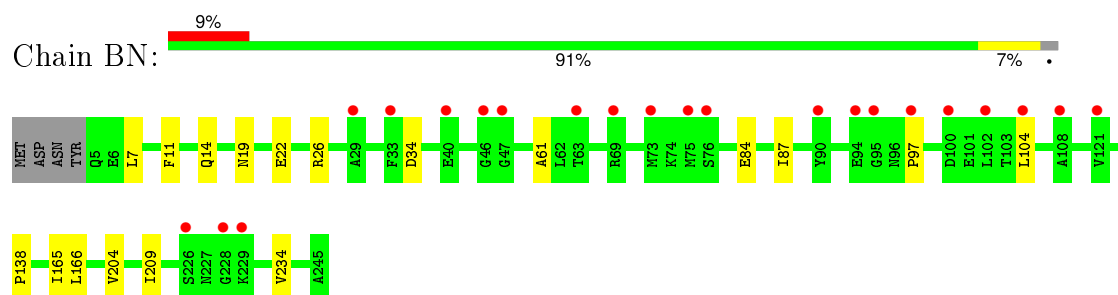


- Molecule 1: Nucleocapsid protein

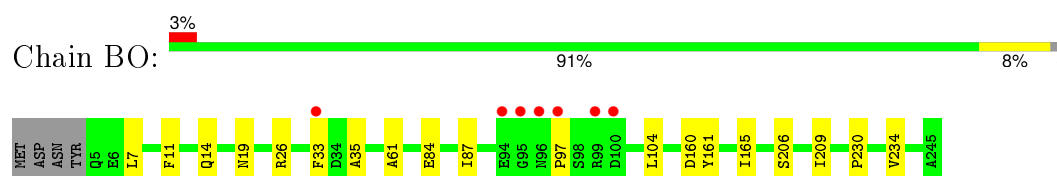




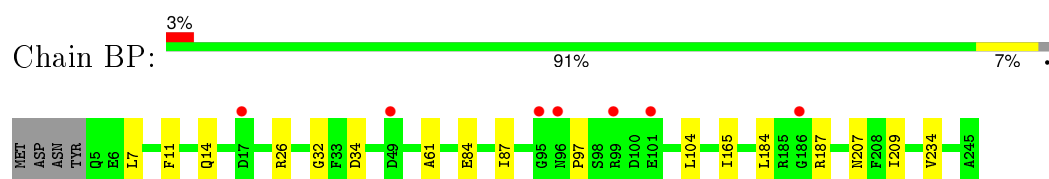
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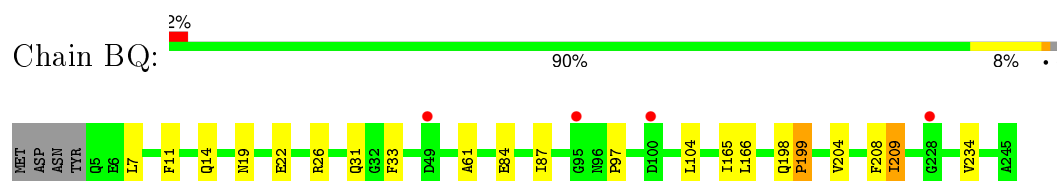
- Molecule 1: Nucleocapsid protein



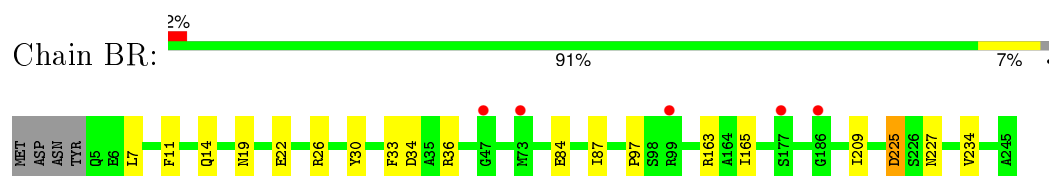
- Molecule 1: Nucleocapsid protein



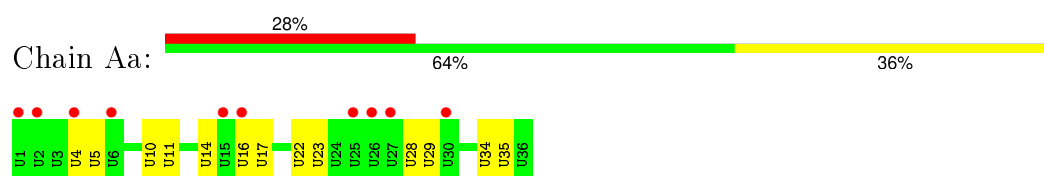
- Molecule 1: Nucleocapsid protein



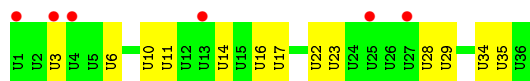
- Molecule 1: Nucleocapsid protein



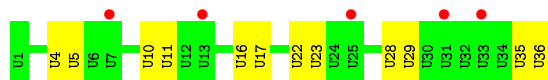
- Molecule 2: 35-mer poly(U) RNA



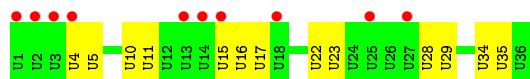
- Molecule 2: 35-mer poly(U) RNA



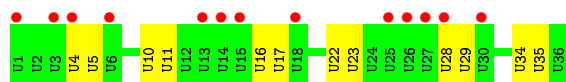
- Molecule 2: 35-mer poly(U) RNA



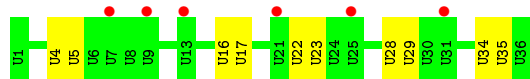
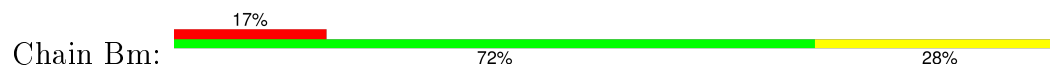
- Molecule 2: 35-mer poly(U) RNA



- Molecule 2: 35-mer poly(U) RNA



- Molecule 2: 35-mer poly(U) RNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	91.66Å 173.33Å 172.90Å 119.95° 99.34° 90.12°	Depositor
Resolution (Å)	57.42 – 3.40 57.42 – 3.40	Depositor EDS
% Data completeness (in resolution range)	94.7 (57.42-3.40) 76.0 (57.42-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.225 , 0.240 0.283 , 0.293	Depositor DCC
R_{free} test set	5930 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	58.7	Xtriage
Anisotropy	0.679	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.0	EDS
Estimated twinning fraction	0.316 for -h,k,-k-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 117932 reflections	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	72072	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.66 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.6968e-03.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	AA	0.40	0/1918	0.53	0/2586
1	AB	0.40	0/1918	0.53	0/2586
1	AC	0.40	0/1918	0.53	0/2586
1	AD	0.39	0/1918	0.54	0/2586
1	AE	0.40	0/1918	0.53	0/2586
1	AF	0.40	0/1918	0.53	0/2586
1	AG	0.40	0/1918	0.54	0/2586
1	AH	0.39	0/1918	0.53	0/2586
1	AI	0.40	0/1918	0.53	0/2586
1	AJ	0.40	0/1918	0.56	0/2586
1	AK	0.39	0/1918	0.53	0/2586
1	AL	0.40	0/1918	0.53	0/2586
1	AM	0.39	0/1918	0.53	0/2586
1	AN	0.40	0/1918	0.53	0/2586
1	AO	0.40	0/1918	0.53	0/2586
1	AP	0.40	0/1918	0.53	0/2586
1	AQ	0.40	0/1918	0.53	0/2586
1	AR	0.40	0/1918	0.53	0/2586
1	BA	0.40	0/1918	0.53	0/2586
1	BB	0.40	0/1918	0.53	0/2586
1	BC	0.40	0/1918	0.54	0/2586
1	BD	0.39	0/1918	0.55	0/2586
1	BE	0.40	0/1918	0.53	0/2586
1	BF	0.39	0/1918	0.53	0/2586
1	BG	0.40	0/1918	0.53	0/2586
1	BH	0.40	0/1918	0.54	0/2586
1	BI	0.40	0/1918	0.53	0/2586
1	BJ	0.40	0/1918	0.54	0/2586
1	BK	0.39	0/1918	0.52	0/2586
1	BL	0.39	0/1918	0.52	0/2586
1	BM	0.40	0/1918	0.53	0/2586
1	BN	0.39	0/1918	0.53	0/2586
1	BO	0.40	0/1918	0.54	0/2586
1	BP	0.40	0/1918	0.53	0/2586

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BQ	0.40	0/1918	0.53	0/2586
1	BR	0.40	0/1918	0.54	0/2586
2	Aa	1.10	0/786	0.92	0/1200
2	Ag	1.11	0/786	0.94	0/1200
2	Am	1.12	0/786	0.92	0/1200
2	Ba	1.11	0/786	0.93	0/1200
2	Bg	1.09	0/786	0.92	0/1200
2	Bm	1.11	0/786	0.92	0/1200
All	All	0.47	0/73764	0.57	0/100296

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	1882	0	1906	11	1
1	AB	1882	0	1906	7	0
1	AC	1882	0	1906	9	0
1	AD	1882	0	1906	9	0
1	AE	1882	0	1906	8	0
1	AF	1882	0	1906	11	0
1	AG	1882	0	1906	7	0
1	AH	1882	0	1906	7	0
1	AI	1882	0	1906	6	0
1	AJ	1882	0	1906	12	0
1	AK	1882	0	1906	9	1
1	AL	1882	0	1906	11	0
1	AM	1882	0	1906	6	0
1	AN	1882	0	1906	6	0
1	AO	1882	0	1906	6	0
1	AP	1882	0	1906	9	0
1	AQ	1882	0	1906	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AR	1882	0	1906	8	0
1	BA	1882	0	1906	12	0
1	BB	1882	0	1906	8	0
1	BC	1882	0	1906	8	0
1	BD	1882	0	1906	12	0
1	BE	1882	0	1906	11	1
1	BF	1882	0	1906	13	0
1	BG	1882	0	1906	9	0
1	BH	1882	0	1906	9	0
1	BI	1882	0	1906	12	1
1	BJ	1882	0	1906	8	0
1	BK	1882	0	1906	7	0
1	BL	1882	0	1906	10	0
1	BM	1882	0	1906	6	0
1	BN	1882	0	1906	8	0
1	BO	1882	0	1906	9	0
1	BP	1882	0	1906	6	0
1	BQ	1882	0	1906	8	0
1	BR	1882	0	1906	8	0
2	Aa	720	0	366	0	0
2	Ag	720	0	366	0	0
2	Am	720	0	366	0	0
2	Ba	720	0	366	0	0
2	Bg	720	0	366	0	0
2	Bm	720	0	366	0	0
All	All	72072	0	70812	257	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 257 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:BD:10:GLN:HB3	1:BI:19:ASN:HD21	1.35	0.91
1:BA:34:ASP:HB2	1:BA:37:ARG:HB3	1.63	0.81
1:AA:34:ASP:HB3	1:AA:37:ARG:HB3	1.66	0.77
1:BE:10:GLN:HE21	1:BP:207:ASN:HD22	1.35	0.75
1:AA:34:ASP:HB2	1:AA:38:VAL:HG23	1.68	0.74

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AK:161:TYR:OH	1:BI:161:TYR:OH[1_455]	1.89	0.31
1:AA:161:TYR:OH	1:BE:161:TYR:OH[1_455]	1.91	0.29

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	AA	239/245 (98%)	227 (95%)	8 (3%)	4 (2%)	11	51
1	AB	239/245 (98%)	227 (95%)	8 (3%)	4 (2%)	11	51
1	AC	239/245 (98%)	227 (95%)	8 (3%)	4 (2%)	11	51
1	AD	239/245 (98%)	225 (94%)	11 (5%)	3 (1%)	15	57
1	AE	239/245 (98%)	225 (94%)	12 (5%)	2 (1%)	24	67
1	AF	239/245 (98%)	227 (95%)	9 (4%)	3 (1%)	15	57
1	AG	239/245 (98%)	227 (95%)	9 (4%)	3 (1%)	15	57
1	AH	239/245 (98%)	227 (95%)	10 (4%)	2 (1%)	24	67
1	AI	239/245 (98%)	229 (96%)	7 (3%)	3 (1%)	15	57
1	AJ	239/245 (98%)	224 (94%)	12 (5%)	3 (1%)	15	57
1	AK	239/245 (98%)	229 (96%)	7 (3%)	3 (1%)	15	57
1	AL	239/245 (98%)	224 (94%)	12 (5%)	3 (1%)	15	57
1	AM	239/245 (98%)	229 (96%)	8 (3%)	2 (1%)	24	67
1	AN	239/245 (98%)	224 (94%)	11 (5%)	4 (2%)	11	51
1	AO	239/245 (98%)	227 (95%)	10 (4%)	2 (1%)	24	67
1	AP	239/245 (98%)	225 (94%)	10 (4%)	4 (2%)	11	51
1	AQ	239/245 (98%)	227 (95%)	10 (4%)	2 (1%)	24	67
1	AR	239/245 (98%)	226 (95%)	9 (4%)	4 (2%)	11	51
1	BA	239/245 (98%)	225 (94%)	12 (5%)	2 (1%)	24	67
1	BB	239/245 (98%)	226 (95%)	10 (4%)	3 (1%)	15	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BC	239/245 (98%)	223 (93%)	13 (5%)	3 (1%)	15	57
1	BD	239/245 (98%)	229 (96%)	8 (3%)	2 (1%)	24	67
1	BE	239/245 (98%)	222 (93%)	14 (6%)	3 (1%)	15	57
1	BF	239/245 (98%)	226 (95%)	9 (4%)	4 (2%)	11	51
1	BG	239/245 (98%)	227 (95%)	9 (4%)	3 (1%)	15	57
1	BH	239/245 (98%)	223 (93%)	11 (5%)	5 (2%)	9	47
1	BI	239/245 (98%)	226 (95%)	11 (5%)	2 (1%)	24	67
1	BJ	239/245 (98%)	224 (94%)	10 (4%)	5 (2%)	9	47
1	BK	239/245 (98%)	229 (96%)	7 (3%)	3 (1%)	15	57
1	BL	239/245 (98%)	226 (95%)	10 (4%)	3 (1%)	15	57
1	BM	239/245 (98%)	228 (95%)	8 (3%)	3 (1%)	15	57
1	BN	239/245 (98%)	226 (95%)	10 (4%)	3 (1%)	15	57
1	BO	239/245 (98%)	224 (94%)	13 (5%)	2 (1%)	24	67
1	BP	239/245 (98%)	224 (94%)	11 (5%)	4 (2%)	11	51
1	BQ	239/245 (98%)	224 (94%)	11 (5%)	4 (2%)	11	51
1	BR	239/245 (98%)	223 (93%)	13 (5%)	3 (1%)	15	57
All	All	8604/8820 (98%)	8131 (94%)	361 (4%)	112 (1%)	15	57

5 of 112 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AJ	35	ALA
1	BC	31	GLN
1	BH	34	ASP
1	BM	30	TYR
1	AA	32	GLY

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	AA	194/198 (98%)	191 (98%)	3 (2%)	72	90
1	AB	194/198 (98%)	191 (98%)	3 (2%)	72	90
1	AC	194/198 (98%)	192 (99%)	2 (1%)	82	93
1	AD	194/198 (98%)	190 (98%)	4 (2%)	61	86
1	AE	194/198 (98%)	190 (98%)	4 (2%)	61	86
1	AF	194/198 (98%)	189 (97%)	5 (3%)	54	84
1	AG	194/198 (98%)	191 (98%)	3 (2%)	72	90
1	AH	194/198 (98%)	190 (98%)	4 (2%)	61	86
1	AI	194/198 (98%)	191 (98%)	3 (2%)	72	90
1	AJ	194/198 (98%)	190 (98%)	4 (2%)	61	86
1	AK	194/198 (98%)	189 (97%)	5 (3%)	54	84
1	AL	194/198 (98%)	192 (99%)	2 (1%)	82	93
1	AM	194/198 (98%)	191 (98%)	3 (2%)	72	90
1	AN	194/198 (98%)	191 (98%)	3 (2%)	72	90
1	AO	194/198 (98%)	192 (99%)	2 (1%)	82	93
1	AP	194/198 (98%)	192 (99%)	2 (1%)	82	93
1	AQ	194/198 (98%)	192 (99%)	2 (1%)	82	93
1	AR	194/198 (98%)	191 (98%)	3 (2%)	72	90
1	BA	194/198 (98%)	189 (97%)	5 (3%)	54	84
1	BB	194/198 (98%)	191 (98%)	3 (2%)	72	90
1	BC	194/198 (98%)	192 (99%)	2 (1%)	82	93
1	BD	194/198 (98%)	192 (99%)	2 (1%)	82	93
1	BE	194/198 (98%)	189 (97%)	5 (3%)	54	84
1	BF	194/198 (98%)	191 (98%)	3 (2%)	72	90
1	BG	194/198 (98%)	191 (98%)	3 (2%)	72	90
1	BH	194/198 (98%)	191 (98%)	3 (2%)	72	90
1	BI	194/198 (98%)	192 (99%)	2 (1%)	82	93
1	BJ	194/198 (98%)	190 (98%)	4 (2%)	61	86
1	BK	194/198 (98%)	191 (98%)	3 (2%)	72	90
1	BL	194/198 (98%)	191 (98%)	3 (2%)	72	90
1	BM	194/198 (98%)	191 (98%)	3 (2%)	72	90
1	BN	194/198 (98%)	192 (99%)	2 (1%)	82	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BO	194/198 (98%)	191 (98%)	3 (2%)	72	90
1	BP	194/198 (98%)	192 (99%)	2 (1%)	82	93
1	BQ	194/198 (98%)	191 (98%)	3 (2%)	72	90
1	BR	194/198 (98%)	190 (98%)	4 (2%)	61	86
All	All	6984/7128 (98%)	6872 (98%)	112 (2%)	70	89

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AP	7	LEU
1	BB	7	LEU
1	BP	7	LEU
1	AQ	7	LEU
1	AR	225	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
1	AP	207	ASN
1	BB	205	ASN
1	BO	211	HIS
1	AP	211	HIS
1	BA	14	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Aa	30/36 (83%)	13 (43%)	0
2	Ag	30/36 (83%)	13 (43%)	0
2	Am	30/36 (83%)	12 (40%)	0
2	Ba	30/36 (83%)	13 (43%)	0
2	Bg	30/36 (83%)	12 (40%)	0
2	Bm	30/36 (83%)	10 (33%)	0
All	All	180/216 (83%)	73 (40%)	0

5 of 73 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	Aa	4	U
2	Aa	5	U
2	Aa	10	U
2	Aa	11	U
2	Aa	14	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	Ag	5
2	Ba	5
2	Bm	5
2	Bg	5
2	Aa	5
2	Am	5

The worst 5 of 30 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ag	12:U	O3'	13:U	P	7.07
1	Ba	12:U	O3'	13:U	P	6.29
1	Ag	6:U	O3'	7:U	P	6.03
1	Ag	24:U	O3'	25:U	P	5.86
1	Ba	24:U	O3'	25:U	P	5.80

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	AA	241/245 (98%)	0.25	6 (2%) 61 55	33, 69, 98, 112	0
1	AB	241/245 (98%)	0.39	9 (3%) 45 40	47, 80, 111, 142	0
1	AC	241/245 (98%)	0.15	3 (1%) 81 75	32, 62, 87, 109	0
1	AD	241/245 (98%)	0.17	5 (2%) 67 61	29, 66, 96, 113	0
1	AE	241/245 (98%)	0.18	1 (0%) 93 91	28, 58, 89, 103	0
1	AF	241/245 (98%)	0.23	4 (1%) 73 67	24, 62, 93, 116	0
1	AG	241/245 (98%)	0.11	3 (1%) 81 75	23, 57, 85, 109	0
1	AH	241/245 (98%)	0.08	3 (1%) 81 75	20, 62, 87, 103	0
1	AI	241/245 (98%)	0.10	3 (1%) 81 75	27, 59, 87, 98	0
1	AJ	241/245 (98%)	0.10	1 (0%) 93 91	24, 63, 90, 105	0
1	AK	241/245 (98%)	0.19	3 (1%) 81 75	35, 66, 88, 112	0
1	AL	241/245 (98%)	0.24	5 (2%) 67 61	33, 66, 93, 109	0
1	AM	241/245 (98%)	0.44	18 (7%) 17 17	34, 77, 118, 129	0
1	AN	241/245 (98%)	0.60	21 (8%) 13 12	33, 82, 138, 152	0
1	AO	241/245 (98%)	0.30	7 (2%) 55 50	33, 69, 98, 109	0
1	AP	241/245 (98%)	0.26	11 (4%) 36 32	22, 67, 100, 123	0
1	AQ	241/245 (98%)	0.10	5 (2%) 67 61	28, 63, 95, 112	0
1	AR	241/245 (98%)	0.14	3 (1%) 81 75	27, 65, 99, 114	0
1	BA	241/245 (98%)	0.21	4 (1%) 73 67	32, 65, 91, 108	0
1	BB	241/245 (98%)	0.23	6 (2%) 61 55	30, 65, 98, 111	0
1	BC	241/245 (98%)	0.24	4 (1%) 73 67	40, 65, 92, 105	0
1	BD	241/245 (98%)	0.33	6 (2%) 61 55	40, 69, 95, 107	0
1	BE	241/245 (98%)	0.33	8 (3%) 50 45	48, 71, 93, 108	0
1	BF	241/245 (98%)	0.29	9 (3%) 45 40	26, 72, 99, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	BG	241/245 (98%)	0.23	4 (1%) 73 67	22, 63, 95, 109	0
1	BH	241/245 (98%)	0.28	3 (1%) 81 75	30, 65, 96, 114	0
1	BI	241/245 (98%)	0.33	7 (2%) 55 50	35, 74, 101, 114	0
1	BJ	241/245 (98%)	0.45	10 (4%) 41 36	46, 81, 108, 144	0
1	BK	241/245 (98%)	0.35	7 (2%) 55 50	37, 68, 94, 115	0
1	BL	241/245 (98%)	0.33	4 (1%) 73 67	39, 70, 97, 112	0
1	BM	241/245 (98%)	0.52	16 (6%) 22 20	39, 78, 114, 124	0
1	BN	241/245 (98%)	0.66	22 (9%) 11 11	46, 86, 133, 146	0
1	BO	241/245 (98%)	0.31	7 (2%) 55 50	35, 70, 102, 121	0
1	BP	241/245 (98%)	0.31	7 (2%) 55 50	24, 70, 102, 123	0
1	BQ	241/245 (98%)	0.21	4 (1%) 73 67	37, 64, 98, 109	0
1	BR	241/245 (98%)	0.27	5 (2%) 67 61	28, 71, 101, 119	0
2	Aa	36/36 (100%)	1.42	10 (27%) 1 1	77, 88, 154, 155	0
2	Ag	36/36 (100%)	1.06	6 (16%) 2 2	71, 98, 151, 151	0
2	Am	36/36 (100%)	1.32	5 (13%) 4 4	105, 125, 146, 147	0
2	Ba	36/36 (100%)	1.43	10 (27%) 1 1	77, 96, 174, 175	0
2	Bg	36/36 (100%)	1.48	13 (36%) 0 1	84, 97, 152, 152	0
2	Bm	36/36 (100%)	1.29	6 (16%) 2 2	109, 126, 131, 133	0
All	All	8892/9036 (98%)	0.30	294 (3%) 50 45	20, 69, 106, 175	0

The worst 5 of 294 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BP	95	GLY	9.0
1	BM	95	GLY	8.0
1	BJ	95	GLY	7.4
1	AN	95	GLY	7.3
1	AP	32	GLY	6.5

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.