



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:40 pm GMT

PDB ID : 4H5O
Title : Crystal Structure of Rift Valley Fever Virus Nucleocapsid Protein Pentamer Bound to Single-stranded RNA
Authors : Raymond, D.D.; Smith, J.L.
Deposited on : 2012-09-18
Resolution : 3.90 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
Xtrriage (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) : trunk28620

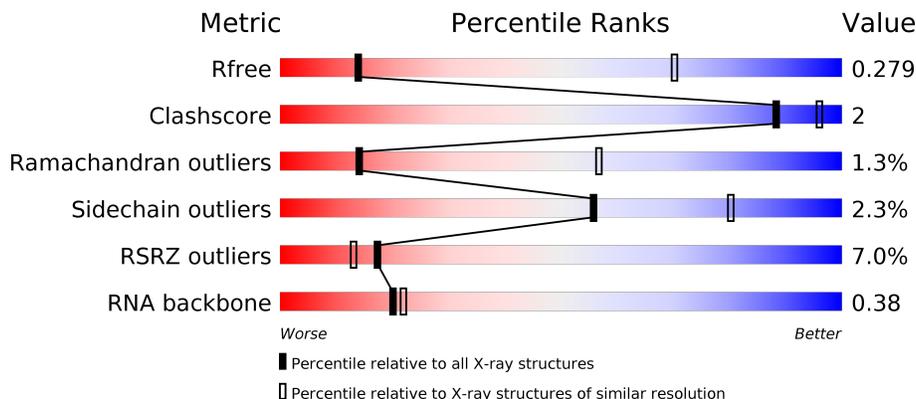
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1007 (4.20-3.60)
Clashscore	112137	1103 (4.20-3.60)
Ramachandran outliers	110173	1062 (4.20-3.60)
Sidechain outliers	110143	1053 (4.20-3.60)
RSRZ outliers	101464	1020 (4.20-3.60)
RNA backbone	2435	1018 (4.84-2.90)

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	245	 5% 88% 9% ..
1	B	245	 % 94% ..
1	C	245	 2% 91% 8% .
1	D	245	 25% 88% 11% .

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Mol	Chain	Length	Quality of chain
1	E	245	<p>6% 89% 9%</p>
1	F	245	<p>2% 93% 6%</p>
1	G	245	<p>2% 91% 8%</p>
1	H	245	<p>22% 85% 14%</p>
1	I	245	<p>3% 92% 7%</p>
1	J	245	<p>3% 93% 6%</p>
2	K	35	<p>3% 63% 29% 9%</p>
2	L	35	<p>63% 26% 11%</p>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 20484 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
			Total	C	N	O	S			
1	A	242	Total 1894	C 1197	N 340	O 345	S 12	0	0	0
1	B	244	Total 1910	C 1205	N 343	O 350	S 12	0	0	0
1	C	244	Total 1910	C 1205	N 343	O 350	S 12	0	0	0
1	D	244	Total 1910	C 1205	N 343	O 350	S 12	0	0	0
1	E	244	Total 1910	C 1205	N 343	O 350	S 12	0	0	0
1	F	244	Total 1910	C 1205	N 343	O 350	S 12	0	0	0
1	G	244	Total 1910	C 1205	N 343	O 350	S 12	0	0	0
1	H	244	Total 1910	C 1205	N 343	O 350	S 12	0	0	0
1	I	244	Total 1910	C 1205	N 343	O 350	S 12	0	0	0
1	J	244	Total 1910	C 1205	N 343	O 350	S 12	0	0	0

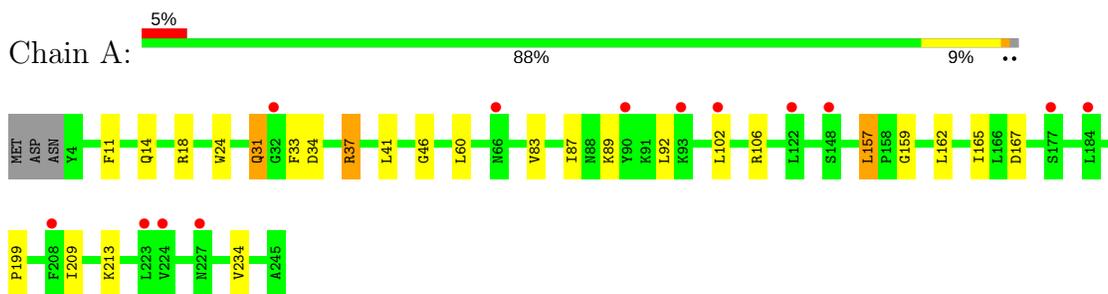
- Molecule 2 is a RNA chain called 35-mer poly(U) RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	K	35	Total 700	C 315	N 70	O 280	P 35	0	0	0
2	L	35	Total 700	C 315	N 70	O 280	P 35	0	0	0

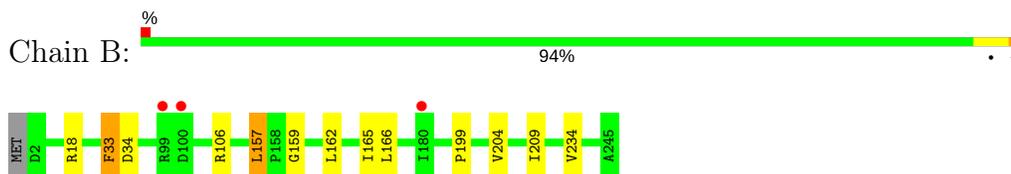
3 Residue-property plots [i](#)

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.

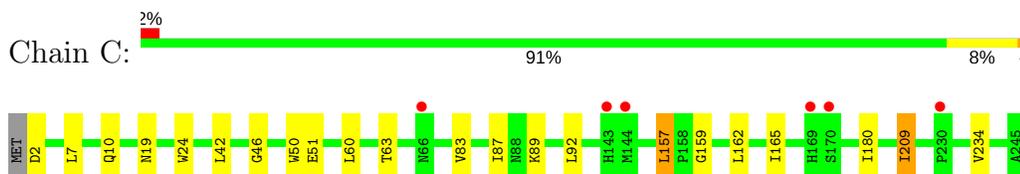
- Molecule 1: Nucleocapsid protein



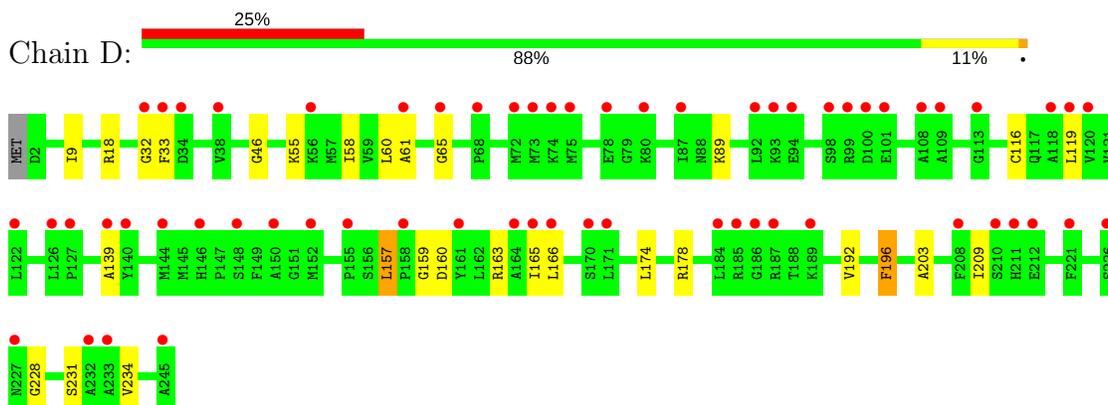
- Molecule 1: Nucleocapsid protein



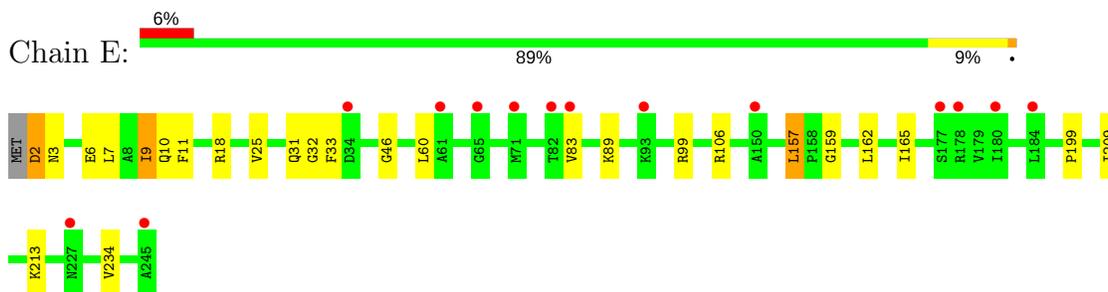
- Molecule 1: Nucleocapsid protein



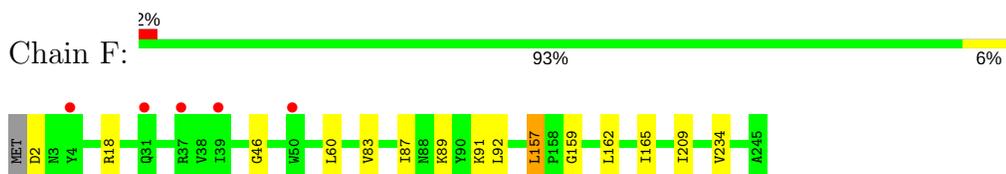
- Molecule 1: Nucleocapsid protein



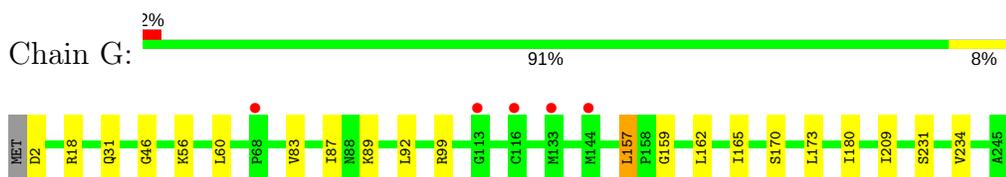
- Molecule 1: Nucleocapsid protein



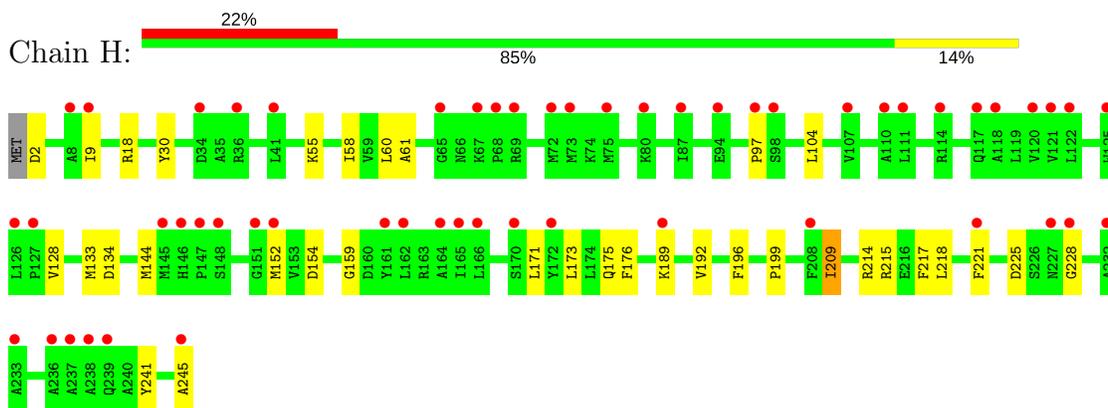
- Molecule 1: Nucleocapsid protein



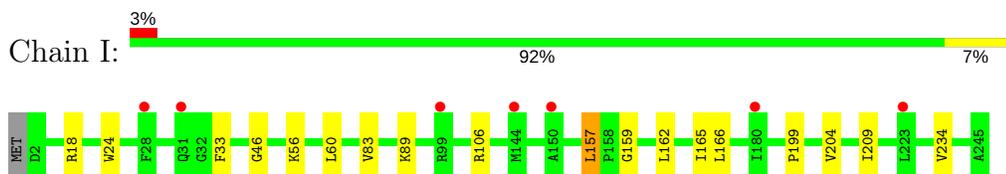
- Molecule 1: Nucleocapsid protein



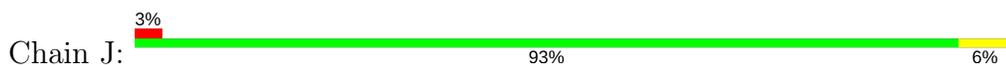
- Molecule 1: Nucleocapsid protein



- Molecule 1: Nucleocapsid protein

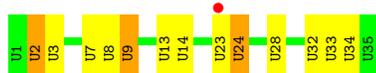


- Molecule 1: Nucleocapsid protein





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



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



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.81Å 93.59Å 124.78Å 101.70° 90.27° 114.18°	Depositor
Resolution (Å)	41.60 – 3.90 41.60 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (41.60-3.90) 86.9 (41.60-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 3.88Å)	Xtrriage
Refinement program	BUSTER 2.10	Depositor
R, R_{free}	0.228 , 0.248 0.261 , 0.279	Depositor DCC
R_{free} test set	1458 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	125.0	Xtrriage
Anisotropy	0.251	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	0.280 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	20484	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/1931	0.55	0/2604
1	B	0.38	0/1947	0.54	0/2626
1	C	0.38	0/1947	0.55	0/2626
1	D	0.41	0/1947	0.56	0/2626
1	E	0.38	0/1947	0.54	0/2626
1	F	0.37	0/1947	0.53	0/2626
1	G	0.38	0/1947	0.54	0/2626
1	H	0.42	0/1947	0.55	0/2626
1	I	0.39	0/1947	0.54	0/2626
1	J	0.38	0/1947	0.53	0/2626
2	K	1.31	3/769 (0.4%)	0.95	0/1186
2	L	1.30	3/769 (0.4%)	0.96	0/1186
All	All	0.52	6/20992 (0.0%)	0.59	0/28610

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	9	U	C1'-N1	6.02	1.57	1.48
2	K	2	U	C1'-N1	5.98	1.57	1.48
2	L	2	U	C1'-N1	5.80	1.57	1.48
2	L	24	U	C1'-N1	5.80	1.57	1.48
2	K	24	U	C1'-N1	5.74	1.57	1.48

There are no bond angle outliers.

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	1894	0	1915	13	0
1	B	1910	0	1925	5	0
1	C	1910	0	1925	11	0
1	D	1910	0	1925	14	0
1	E	1910	0	1925	16	0
1	F	1910	0	1925	6	0
1	G	1910	0	1925	9	0
1	H	1910	0	1925	13	0
1	I	1910	0	1925	9	0
1	J	1910	0	1925	7	0
2	K	700	0	351	4	0
2	L	700	0	351	6	0
All	All	20484	0	19942	92	0

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 92 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:199:PRO:HB3	2:L:23:U:H5'	1.46	0.97
1:B:199:PRO:HB3	2:K:23:U:H5'	1.63	0.79
1:E:31:GLN:HG2	1:E:99:ARG:HG3	1.81	0.63
1:A:213:LYS:HD3	1:D:9:ILE:HD13	1.86	0.58
1:A:165:ILE:HD13	1:A:234:VAL:HG11	1.85	0.57

There are no symmetry-related clashes.

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	240/245 (98%)	222 (92%)	15 (6%)	3 (1%)	14	57
1	B	242/245 (99%)	225 (93%)	13 (5%)	4 (2%)	11	52
1	C	242/245 (99%)	226 (93%)	14 (6%)	2 (1%)	22	65
1	D	242/245 (99%)	220 (91%)	16 (7%)	6 (2%)	6	44
1	E	242/245 (99%)	226 (93%)	14 (6%)	2 (1%)	22	65
1	F	242/245 (99%)	227 (94%)	13 (5%)	2 (1%)	22	65
1	G	242/245 (99%)	227 (94%)	13 (5%)	2 (1%)	22	65
1	H	242/245 (99%)	219 (90%)	17 (7%)	6 (2%)	6	44
1	I	242/245 (99%)	226 (93%)	14 (6%)	2 (1%)	22	65
1	J	242/245 (99%)	227 (94%)	13 (5%)	2 (1%)	22	65
All	All	2418/2450 (99%)	2245 (93%)	142 (6%)	31 (1%)	14	57

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	30	TYR
1	A	31	GLN
1	A	159	GLY
1	B	159	GLY
1	C	159	GLY

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	195/198 (98%)	190 (97%)	5 (3%)	51	78
1	B	197/198 (100%)	195 (99%)	2 (1%)	80	90
1	C	197/198 (100%)	191 (97%)	6 (3%)	46	75
1	D	197/198 (100%)	193 (98%)	4 (2%)	60	83
1	E	197/198 (100%)	191 (97%)	6 (3%)	46	75
1	F	197/198 (100%)	194 (98%)	3 (2%)	70	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	197/198 (100%)	193 (98%)	4 (2%)	60	83
1	H	197/198 (100%)	187 (95%)	10 (5%)	28	63
1	I	197/198 (100%)	195 (99%)	2 (1%)	80	90
1	J	197/198 (100%)	194 (98%)	3 (2%)	70	87
All	All	1968/1980 (99%)	1923 (98%)	45 (2%)	56	80

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	10	GLN
1	F	157	LEU
1	I	157	LEU
1	E	157	LEU
1	G	2	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	3	ASN
1	E	5	GLN
1	I	143	HIS
1	D	211	HIS
1	G	175	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	K	34/35 (97%)	9 (26%)	0
2	L	34/35 (97%)	8 (23%)	0
All	All	68/70 (97%)	17 (25%)	0

5 of 17 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	K	3	U
2	K	7	U
2	K	8	U
2	K	13	U
2	K	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](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	242/245 (98%)	0.35	13 (5%) 26 21	10, 53, 124, 161	0
1	B	244/245 (99%)	0.24	3 (1%) 79 70	4, 22, 67, 91	0
1	C	244/245 (99%)	0.20	6 (2%) 58 47	6, 22, 70, 114	0
1	D	244/245 (99%)	1.08	61 (25%) 1 1	23, 120, 216, 266	0
1	E	244/245 (99%)	0.31	14 (5%) 24 19	18, 50, 122, 203	0
1	F	244/245 (99%)	0.26	5 (2%) 65 56	6, 36, 104, 149	0
1	G	244/245 (99%)	0.21	5 (2%) 65 56	4, 17, 77, 129	0
1	H	244/245 (99%)	0.94	54 (22%) 1 2	23, 113, 187, 216	0
1	I	244/245 (99%)	0.24	7 (2%) 52 42	4, 19, 76, 121	0
1	J	244/245 (99%)	0.25	7 (2%) 52 42	4, 36, 110, 185	0
2	K	35/35 (100%)	0.36	1 (2%) 52 42	31, 37, 44, 44	0
2	L	35/35 (100%)	0.25	0 100 100	31, 37, 44, 44	0
All	All	2508/2520 (99%)	0.41	176 (7%) 17 13	4, 40, 150, 266	0

The worst 5 of 176 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	34	ASP	11.3
1	H	227	ASN	8.4
1	H	165	ILE	8.3
1	D	164	ALA	7.9
1	H	164	ALA	6.8

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.