



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 08:29 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 Full wwPDB X-ray Structure Validation 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.

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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  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

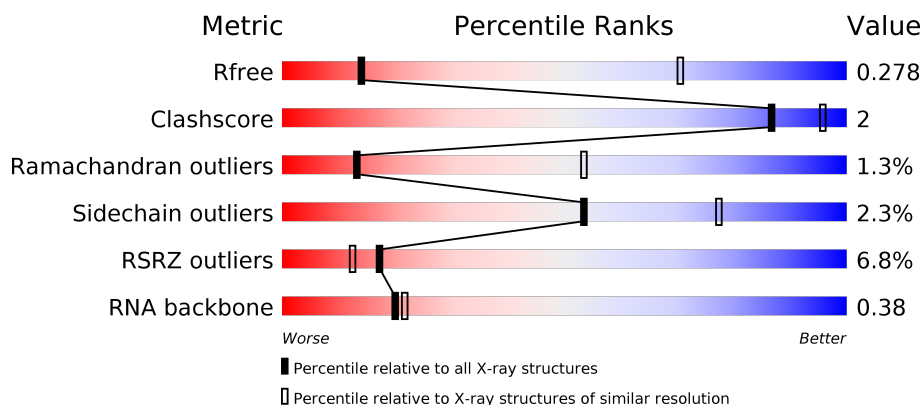
# 1 Overall quality at a glance

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))
$R_{free}$	111664	1145 (4.20-3.60)
Clashscore	122126	1225 (4.20-3.60)
Ramachandran outliers	120053	1184 (4.20-3.60)
Sidechain outliers	120020	1175 (4.20-3.60)
RSRZ outliers	108989	1046 (4.20-3.60)
RNA backbone	2636	1085 (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  $\geq 3$ , 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	<div> <div>6%</div> <div>88%</div> <div>9%</div> <div>..</div> </div>
1	B	245	<div> <div>2%</div> <div>94%</div> <div>..</div> </div>
1	C	245	<div> <div>2%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	D	245	<div> <div>24%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	E	245	<div><div></div><div>5%</div><div>89%</div><div>9%</div><div></div></div>
1	F	245	<div><div></div><div>2%</div><div>93%</div><div>6%</div><div></div></div>
1	G	245	<div><div></div><div>2%</div><div>91%</div><div>8%</div><div></div></div>
1	H	245	<div><div></div><div>21%</div><div>85%</div><div>14%</div><div></div></div>
1	I	245	<div><div></div><div>3%</div><div>92%</div><div>7%</div><div></div></div>
1	J	245	<div><div></div><div>2%</div><div>93%</div><div>6%</div><div></div></div>
2	K	35	<div><div></div><div>3%</div><div>57%</div><div>34%</div><div>9%</div><div></div></div>
2	L	35	<div><div></div><div>57%</div><div>31%</div><div>11%</div><div></div></div>

## 2 Entry composition

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
1	A	242	Total	C	N	O	S	0	0	0
			1894	1197	340	345	12			
1	B	244	Total	C	N	O	S	0	0	0
			1910	1205	343	350	12			
1	C	244	Total	C	N	O	S	0	0	0
			1910	1205	343	350	12			
1	D	244	Total	C	N	O	S	0	0	0
			1910	1205	343	350	12			
1	E	244	Total	C	N	O	S	0	0	0
			1910	1205	343	350	12			
1	F	244	Total	C	N	O	S	0	0	0
			1910	1205	343	350	12			
1	G	244	Total	C	N	O	S	0	0	0
			1910	1205	343	350	12			
1	H	244	Total	C	N	O	S	0	0	0
			1910	1205	343	350	12			
1	I	244	Total	C	N	O	S	0	0	0
			1910	1205	343	350	12			
1	J	244	Total	C	N	O	S	0	0	0
			1910	1205	343	350	12			

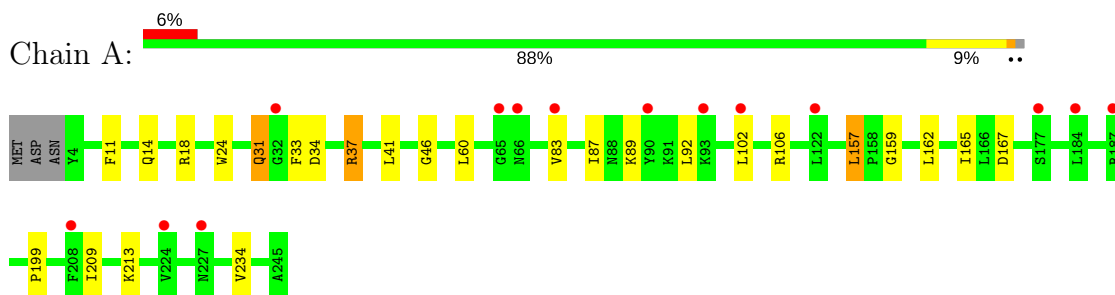
- Molecule 2 is a RNA chain called 35-mer poly(U) RNA.

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

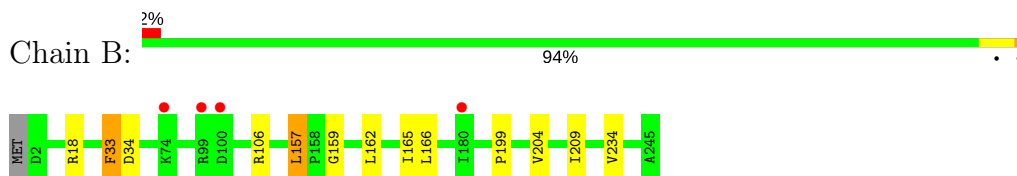
### 3 Residue-property plots [i](#)

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.

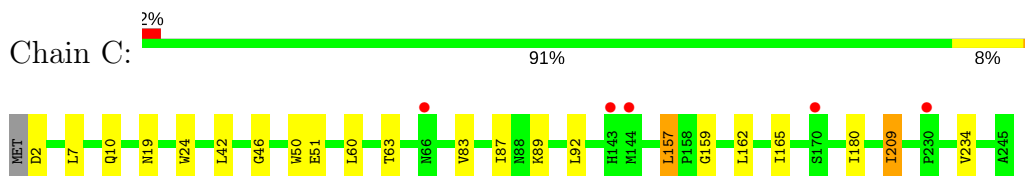
- Molecule 1: Nucleocapsid protein



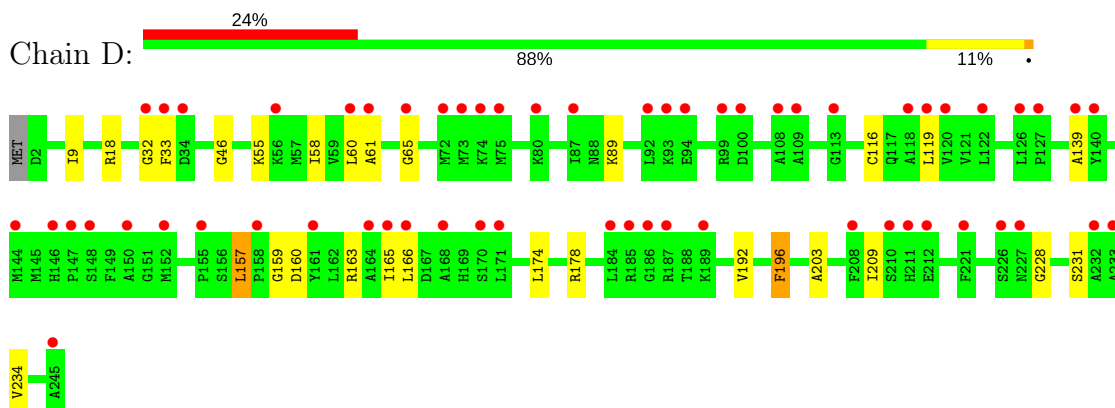
- Molecule 1: Nucleocapsid protein



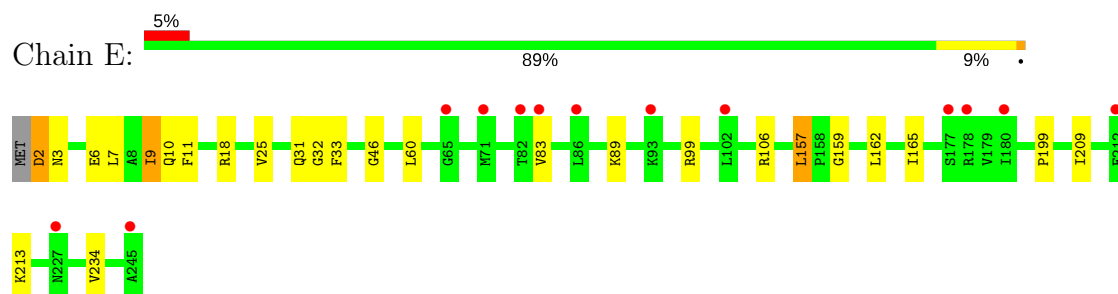
- Molecule 1: Nucleocapsid protein



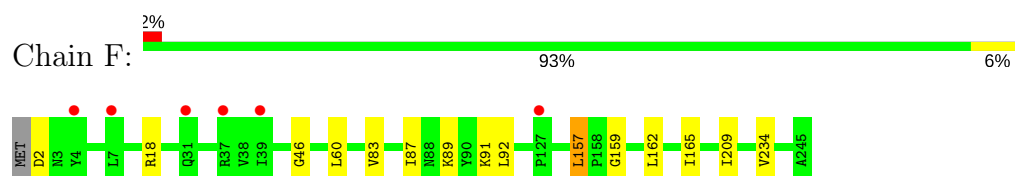
- Molecule 1: Nucleocapsid protein



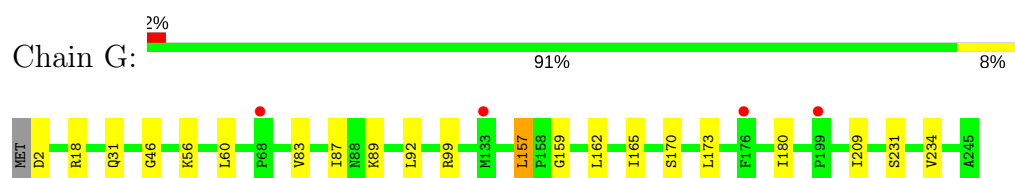
## ● Molecule 1: Nucleocapsid protein



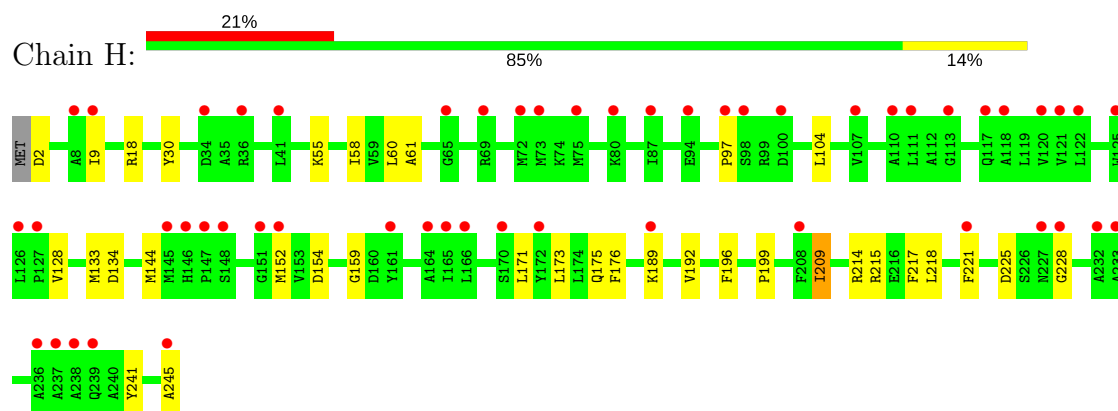
## ● Molecule 1: Nucleocapsid protein



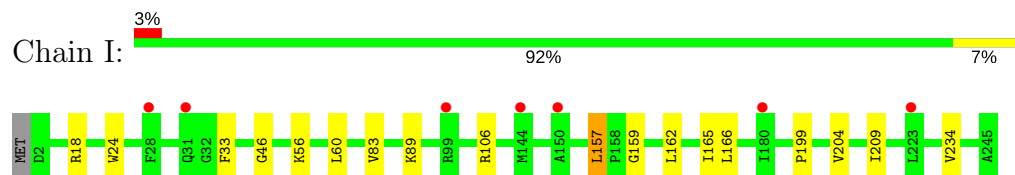
## ● Molecule 1: Nucleocapsid protein



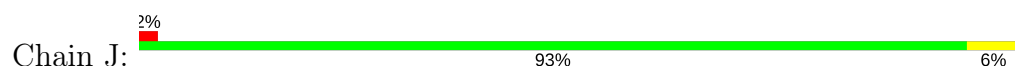
## ● Molecule 1: Nucleocapsid protein

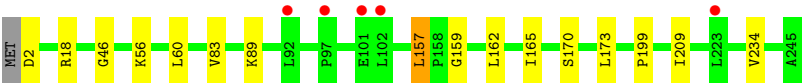


## ● Molecule 1: Nucleocapsid protein

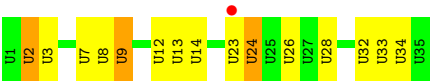


## ● Molecule 1: Nucleocapsid protein

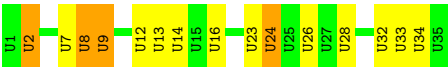




• Molecule 2: 35-mer poly(U) RNA



• Molecule 2: 35-mer poly(U) RNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 94.0 (41.60-3.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.21	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 3.88Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.10.0, BUSTER 2.10	Depositor
R, $R_{free}$	0.228 , 0.248 0.261 , 0.278	Depositor DCC
$R_{free}$ test set	1459 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	125.0	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.280 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	20484	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage'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.*

<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](#)

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

All (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
2	L	9	U	C1'-N1	5.54	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.

All (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
1:G:170:SER:HA	1:G:173:LEU:HD12	1.87	0.56
1:J:165:ILE:HD13	1:J:234:VAL:HG11	1.88	0.56
1:E:165:ILE:HD13	1:E:234:VAL:HG11	1.87	0.56
1:H:171:LEU:HD13	1:H:241:TYR:HA	1.89	0.55
1:H:55:LYS:HA	1:H:58:ILE:HD12	1.89	0.54
1:G:165:ILE:HD13	1:G:234:VAL:HG11	1.87	0.54
1:B:165:ILE:HD13	1:B:234:VAL:HG11	1.89	0.54
1:A:11:PHE:HA	1:A:14:GLN:HE21	1.73	0.54
1:C:180:ILE:HD12	2:L:32:U:H2'	1.90	0.54
1:D:116:CYS:HA	1:D:119:LEU:HD12	1.90	0.54
1:I:165:ILE:HD13	1:I:234:VAL:HG11	1.90	0.54
1:H:154:ASP:HA	1:H:214:ARG:HD3	1.89	0.53
1:E:33:PHE:CD1	1:E:106:ARG:HG2	2.42	0.52
1:A:199:PRO:HB3	2:K:2:U:H5'	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ILE:HG23	1:E:9:ILE:HD11	1.92	0.52
1:F:165:ILE:HD13	1:F:234:VAL:HG11	1.91	0.52
1:E:33:PHE:HD1	1:E:106:ARG:HG2	1.76	0.51
1:J:170:SER:HA	1:J:173:LEU:HD12	1.93	0.51
1:C:165:ILE:HD13	1:C:234:VAL:HG11	1.93	0.50
1:C:24:TRP:CE2	1:I:56:LYS:HG2	2.47	0.50
1:D:192:VAL:HG12	1:D:196:PHE:HD2	1.78	0.49
1:C:51:GLU:HA	1:E:11:PHE:HE1	1.76	0.49
1:G:31:GLN:HG3	1:G:99:ARG:HG3	1.95	0.49
1:D:157:LEU:HD22	1:D:165:ILE:HD11	1.95	0.48
1:A:34:ASP:HB2	1:A:37:ARG:HB2	1.96	0.48
1:H:199:PRO:HB3	2:L:9:U:H5'	1.96	0.48
1:E:213:LYS:HD3	1:H:9:ILE:HD13	1.97	0.47
1:E:32:GLY:O	1:E:106:ARG:NH2	2.48	0.47
1:E:199:PRO:HB3	2:L:2:U:H5'	1.96	0.47
1:H:215:ARG:HA	1:H:218:LEU:HD12	1.97	0.46
1:G:180:ILE:HD12	2:K:32:U:H2'	1.98	0.46
1:H:61:ALA:HB2	1:H:104:LEU:HB3	1.98	0.46
1:I:24:TRP:CE2	1:J:56:LYS:HG2	2.51	0.46
1:A:33:PHE:CE1	1:A:106:ARG:HG2	2.52	0.45
1:D:163:ARG:HA	1:D:166:LEU:HD12	1.98	0.45
1:I:33:PHE:HD1	1:I:106:ARG:HG2	1.80	0.45
1:B:33:PHE:HD1	1:B:106:ARG:HG2	1.82	0.45
1:E:2:ASP:N	1:F:91:LYS:HZ2	2.14	0.45
1:G:157:LEU:HB3	1:G:162:LEU:HB2	1.99	0.44
1:C:60:LEU:HD21	1:C:83:VAL:HG22	1.99	0.44
1:F:46:GLY:HA2	1:F:89:LYS:HE2	1.99	0.44
1:H:192:VAL:HG12	1:H:196:PHE:HE2	1.82	0.44
1:J:46:GLY:HA2	1:J:89:LYS:HE2	2.00	0.44
1:G:46:GLY:HA2	1:G:89:LYS:HE2	2.00	0.44
1:G:60:LEU:HD21	1:G:83:VAL:HG22	1.99	0.44
1:A:157:LEU:HB3	1:A:162:LEU:HB2	2.00	0.44
1:C:63:THR:HG21	1:E:25:VAL:HG23	2.00	0.44
1:C:157:LEU:HB3	1:C:162:LEU:HB2	2.00	0.44
1:D:174:LEU:HD11	1:D:178:ARG:HH21	1.82	0.43
1:E:157:LEU:HB3	1:E:162:LEU:HB2	2.00	0.43
1:A:213:LYS:HD3	1:D:9:ILE:CD1	2.48	0.43
1:H:128:VAL:HG21	1:H:175:GLN:HG3	1.99	0.43
1:C:46:GLY:HA2	1:C:89:LYS:HE2	2.01	0.43
1:A:46:GLY:HA2	1:A:89:LYS:HE2	2.00	0.43
1:E:3:ASN:HD22	1:E:6:GLU:CD	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:173:LEU:HA	1:H:176:PHE:HB3	2.01	0.43
1:H:189:LYS:HD3	1:H:245:ALA:HA	2.00	0.43
1:B:157:LEU:HB3	1:B:162:LEU:HB2	2.01	0.43
1:F:157:LEU:HB3	1:F:162:LEU:HB2	2.00	0.43
1:F:60:LEU:HD21	1:F:83:VAL:HG22	2.00	0.43
1:E:46:GLY:HA2	1:E:89:LYS:HE2	2.01	0.42
1:D:46:GLY:HA2	1:D:89:LYS:HE2	2.01	0.42
1:A:41:LEU:HB3	1:A:102:LEU:HD11	2.02	0.42
1:D:192:VAL:HG12	1:D:196:PHE:CD2	2.55	0.42
1:D:61:ALA:HA	1:D:65:GLY:O	2.19	0.42
1:I:46:GLY:HA2	1:I:89:LYS:HE2	2.01	0.42
1:D:203:ALA:HA	2:K:9:U:C4	2.55	0.42
1:J:157:LEU:HB3	1:J:162:LEU:HB2	2.01	0.42
1:B:166:LEU:HD21	1:B:204:VAL:HG21	2.02	0.42
1:E:60:LEU:HD21	1:E:83:VAL:HG22	2.02	0.42
1:A:60:LEU:HD21	1:A:83:VAL:HG22	2.02	0.42
1:E:213:LYS:HD3	1:H:9:ILE:CD1	2.50	0.42
1:I:166:LEU:HD21	1:I:204:VAL:HG21	2.02	0.41
1:J:199:PRO:HB3	2:L:16:U:O4'	2.20	0.41
1:C:50:TRP:CE2	1:C:51:GLU:HG3	2.56	0.41
1:I:157:LEU:HB3	1:I:162:LEU:HB2	2.02	0.41
1:A:24:TRP:CE2	1:G:56:LYS:HG2	2.56	0.41
1:A:87:ILE:HA	1:A:92:LEU:HB2	2.02	0.41
1:J:60:LEU:HD21	1:J:83:VAL:HG22	2.02	0.41
1:D:55:LYS:HA	1:D:58:ILE:HD12	2.01	0.41
1:C:87:ILE:HA	1:C:92:LEU:HB2	2.03	0.41
1:G:87:ILE:HA	1:G:92:LEU:HB2	2.03	0.40
1:F:87:ILE:HA	1:F:92:LEU:HB2	2.02	0.40
1:H:199:PRO:HG3	2:L:8:U:H4'	2.03	0.40
1:I:60:LEU:HD21	1:I:83:VAL:HG22	2.04	0.40
1:D:160:ASP:HA	1:D:163:ARG:HD2	2.04	0.40
1:D:231:SER:HB3	1:D:234:VAL:HG23	2.03	0.40

There are no symmetry-related clashes.

## 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	240/245 (98%)	222 (92%)	15 (6%)	3 (1%)	13	53
1	B	242/245 (99%)	225 (93%)	13 (5%)	4 (2%)	10	48
1	C	242/245 (99%)	226 (93%)	14 (6%)	2 (1%)	21	62
1	D	242/245 (99%)	220 (91%)	16 (7%)	6 (2%)	6	41
1	E	242/245 (99%)	226 (93%)	14 (6%)	2 (1%)	21	62
1	F	242/245 (99%)	227 (94%)	13 (5%)	2 (1%)	21	62
1	G	242/245 (99%)	227 (94%)	13 (5%)	2 (1%)	21	62
1	H	242/245 (99%)	219 (90%)	17 (7%)	6 (2%)	6	41
1	I	242/245 (99%)	226 (93%)	14 (6%)	2 (1%)	21	62
1	J	242/245 (99%)	227 (94%)	13 (5%)	2 (1%)	21	62
All	All	2418/2450 (99%)	2245 (93%)	142 (6%)	31 (1%)	13	53

All (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
1	D	159	GLY
1	E	159	GLY
1	F	159	GLY
1	G	159	GLY
1	I	159	GLY
1	J	159	GLY
1	H	228	GLY
1	A	209	ILE
1	B	33	PHE
1	B	34	ASP
1	B	209	ILE
1	C	209	ILE
1	E	209	ILE
1	F	209	ILE
1	G	209	ILE

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Mol	Chain	Res	Type
1	I	209	ILE
1	J	209	ILE
1	D	33	PHE
1	D	209	ILE
1	D	139	ALA
1	D	228	GLY
1	H	209	ILE
1	H	225	ASP
1	H	159	GLY
1	D	32	GLY
1	H	97	PRO

### 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	195/198 (98%)	190 (97%)	5 (3%)	49	75
1	B	197/198 (100%)	195 (99%)	2 (1%)	78	89
1	C	197/198 (100%)	191 (97%)	6 (3%)	44	71
1	D	197/198 (100%)	193 (98%)	4 (2%)	58	80
1	E	197/198 (100%)	191 (97%)	6 (3%)	44	71
1	F	197/198 (100%)	194 (98%)	3 (2%)	67	85
1	G	197/198 (100%)	193 (98%)	4 (2%)	58	80
1	H	197/198 (100%)	187 (95%)	10 (5%)	26	60
1	I	197/198 (100%)	195 (99%)	2 (1%)	78	89
1	J	197/198 (100%)	194 (98%)	3 (2%)	67	85
All	All	1968/1980 (99%)	1923 (98%)	45 (2%)	53	77

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	31	GLN

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Mol	Chain	Res	Type
1	A	37	ARG
1	A	157	LEU
1	A	167	ASP
1	B	18	ARG
1	B	157	LEU
1	C	2	ASP
1	C	7	LEU
1	C	10	GLN
1	C	19	ASN
1	C	42	LEU
1	C	157	LEU
1	D	18	ARG
1	D	60	LEU
1	D	157	LEU
1	D	196	PHE
1	E	2	ASP
1	E	7	LEU
1	E	9	ILE
1	E	10	GLN
1	E	18	ARG
1	E	157	LEU
1	F	2	ASP
1	F	18	ARG
1	F	157	LEU
1	G	2	ASP
1	G	18	ARG
1	G	157	LEU
1	G	231	SER
1	H	2	ASP
1	H	18	ARG
1	H	60	LEU
1	H	133	MET
1	H	134	ASP
1	H	144	MET
1	H	152	MET
1	H	209	ILE
1	H	217	PHE
1	H	221	PHE
1	I	18	ARG
1	I	157	LEU
1	J	2	ASP
1	J	18	ARG

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Mol	Chain	Res	Type
1	J	157	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	175	GLN
1	B	175	GLN
1	C	88	ASN
1	C	175	GLN
1	D	211	HIS
1	E	3	ASN
1	E	5	GLN
1	E	175	GLN
1	F	175	GLN
1	G	88	ASN
1	G	175	GLN
1	I	143	HIS
1	I	175	GLN
1	J	175	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	K	34/35 (97%)	9 (26%)	3 (8%)
2	L	34/35 (97%)	8 (23%)	3 (8%)
All	All	68/70 (97%)	17 (25%)	6 (8%)

All (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
2	K	24	U
2	K	28	U
2	K	33	U
2	K	34	U

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Mol	Chain	Res	Type
2	L	7	U
2	L	8	U
2	L	13	U
2	L	14	U
2	L	24	U
2	L	28	U
2	L	33	U
2	L	34	U

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	K	12	U
2	K	26	U
2	K	33	U
2	L	12	U
2	L	26	U
2	L	33	U

## 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, 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	242/245 (98%)	0.34	14 (5%) 23 17	10, 53, 124, 161	0
1	B	244/245 (99%)	0.20	4 (1%) 72 61	4, 22, 67, 91	0
1	C	244/245 (99%)	0.19	5 (2%) 65 54	6, 22, 70, 114	0
1	D	244/245 (99%)	1.08	59 (24%) 0 0	23, 120, 216, 266	0
1	E	244/245 (99%)	0.30	13 (5%) 26 21	18, 50, 122, 203	0
1	F	244/245 (99%)	0.23	6 (2%) 57 46	6, 36, 104, 149	0
1	G	244/245 (99%)	0.21	4 (1%) 72 61	4, 17, 77, 129	0
1	H	244/245 (99%)	0.93	52 (21%) 1 1	23, 113, 187, 216	0
1	I	244/245 (99%)	0.21	7 (2%) 51 39	4, 19, 76, 121	0
1	J	244/245 (99%)	0.24	5 (2%) 65 54	4, 36, 110, 185	0
2	K	35/35 (100%)	0.33	1 (2%) 51 39	31, 37, 44, 44	0
2	L	35/35 (100%)	0.24	0 100 100	31, 37, 44, 44	0
All	All	2508/2520 (99%)	0.39	170 (6%) 17 12	4, 40, 150, 266	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	34	ASP	10.3
1	H	227	ASN	9.1
1	H	165	ILE	8.5
1	D	164	ALA	7.7
1	H	34	ASP	7.6
1	D	165	ILE	6.9
1	H	164	ALA	6.2
1	D	33	PHE	6.0
1	D	227	ASN	5.6
1	H	245	ALA	5.6
1	D	185	ARG	5.1

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Mol	Chain	Res	Type	RSRZ
1	H	221	PHE	4.7
1	D	212	GLU	4.7
1	C	66	ASN	4.4
1	H	228	GLY	4.4
1	D	187	ARG	4.3
1	J	102	LEU	4.2
1	D	146	HIS	4.1
1	D	226	SER	4.1
1	D	166	LEU	4.0
1	H	73	MET	4.0
1	D	100	ASP	4.0
1	H	208	PHE	3.9
1	H	238	ALA	3.9
1	A	102	LEU	3.9
1	E	65	GLY	3.9
1	B	100	ASP	3.8
1	D	211	HIS	3.8
1	H	172	TYR	3.8
1	H	117	GLN	3.6
1	D	65	GLY	3.6
1	D	170	SER	3.6
1	H	161	TYR	3.6
1	D	127	PRO	3.5
1	H	147	PRO	3.5
1	H	75	MET	3.5
1	D	161	TYR	3.5
1	E	177	SER	3.5
1	H	152	MET	3.4
1	D	75	MET	3.4
1	D	122	LEU	3.4
1	H	125	TRP	3.4
1	D	126	LEU	3.4
1	E	245	ALA	3.4
1	H	121	VAL	3.3
1	H	189	LYS	3.3
1	D	99	ARG	3.3
1	D	158	PRO	3.3
1	E	83	VAL	3.3
1	A	65	GLY	3.3
1	D	73	MET	3.2
1	H	118	ALA	3.2
1	D	184	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	113	GLY	3.2
1	D	155	PRO	3.1
1	E	71	MET	3.1
1	H	145	MET	3.1
1	D	208	PHE	3.1
1	H	170	SER	3.1
1	H	65	GLY	3.1
1	D	74	LYS	3.1
1	I	28	PHE	3.1
1	H	122	LEU	3.0
1	D	189	LYS	3.0
1	B	180	ILE	3.0
1	H	166	LEU	3.0
1	G	133	MET	3.0
1	J	92	LEU	3.0
1	H	232	ALA	2.9
1	D	152	MET	2.9
1	H	126	LEU	2.9
1	D	233	ALA	2.9
1	A	177	SER	2.9
1	D	108	ALA	2.9
1	H	107	VAL	2.9
1	D	139	ALA	2.9
1	H	233	ALA	2.9
1	D	120	VAL	2.9
1	A	208	PHE	2.9
1	D	221	PHE	2.8
1	H	148	SER	2.8
1	J	101	GLU	2.8
1	H	41	LEU	2.8
1	D	93	LYS	2.7
1	B	99	ARG	2.7
1	H	72	MET	2.7
1	H	94	GLU	2.7
1	D	210	SER	2.7
1	C	144	MET	2.7
1	D	56	LYS	2.7
1	I	180	ILE	2.7
1	H	127	PRO	2.7
1	A	66	ASN	2.6
1	A	93	LYS	2.6
1	A	122	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	184	LEU	2.6
1	D	171	LEU	2.6
1	D	186	GLY	2.6
1	D	232	ALA	2.6
1	D	72	MET	2.6
1	E	227	ASN	2.6
1	C	170	SER	2.5
1	H	110	ALA	2.5
1	D	61	ALA	2.5
1	I	99	ARG	2.5
1	E	178	ARG	2.5
1	I	31	GLN	2.5
1	J	223	LEU	2.5
1	A	90	TYR	2.5
1	H	146	HIS	2.5
1	D	92	LEU	2.5
1	D	144	MET	2.4
1	F	39	ILE	2.4
1	C	230	PRO	2.4
1	E	82	THR	2.4
1	J	97	PRO	2.4
1	H	98	SER	2.4
1	H	111	LEU	2.4
1	D	80	LYS	2.4
1	G	199	PRO	2.4
2	K	23	U	2.4
1	A	32	GLY	2.4
1	F	7	LEU	2.4
1	H	113	GLY	2.3
1	G	68	PRO	2.3
1	A	227	ASN	2.3
1	H	87	ILE	2.3
1	D	148	SER	2.3
1	H	237	ALA	2.3
1	F	31	GLN	2.3
1	F	37	ARG	2.3
1	H	9	ILE	2.3
1	D	245	ALA	2.3
1	I	150	ALA	2.3
1	D	119	LEU	2.2
1	D	140	TYR	2.2
1	E	212	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	32	GLY	2.2
1	D	109	ALA	2.2
1	D	147	PRO	2.2
1	H	100	ASP	2.2
1	H	120	VAL	2.2
1	A	83	VAL	2.2
1	I	144	MET	2.2
1	E	102	LEU	2.2
1	H	239	GLN	2.2
1	F	4	TYR	2.1
1	H	69	ARG	2.1
1	E	93	LYS	2.1
1	F	127	PRO	2.1
1	H	97	PRO	2.1
1	H	80	LYS	2.1
1	D	94	GLU	2.1
1	C	143	HIS	2.1
1	D	87	ILE	2.1
1	H	36	ARG	2.1
1	D	168	ALA	2.1
1	D	150	ALA	2.1
1	A	224	VAL	2.1
1	H	151	GLY	2.1
1	H	8	ALA	2.1
1	I	223	LEU	2.1
1	D	60	LEU	2.0
1	E	180	ILE	2.0
1	B	74	LYS	2.0
1	A	187	ARG	2.0
1	H	236	ALA	2.0
1	D	118	ALA	2.0
1	E	86	LEU	2.0
1	G	176	PHE	2.0

## 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.