



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 12:39 am BST

PDB ID : 4JNG  
Title : Schmallenberg virus nucleoprotein-RNA complex  
Authors : Dong, H.H.; Li, P.; Bottcher, B.; Elliott, R.M.; Dong, C.J.  
Deposited on : 2013-03-15  
Resolution : 2.12 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.

---

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 : 2.11  
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) : 2.11

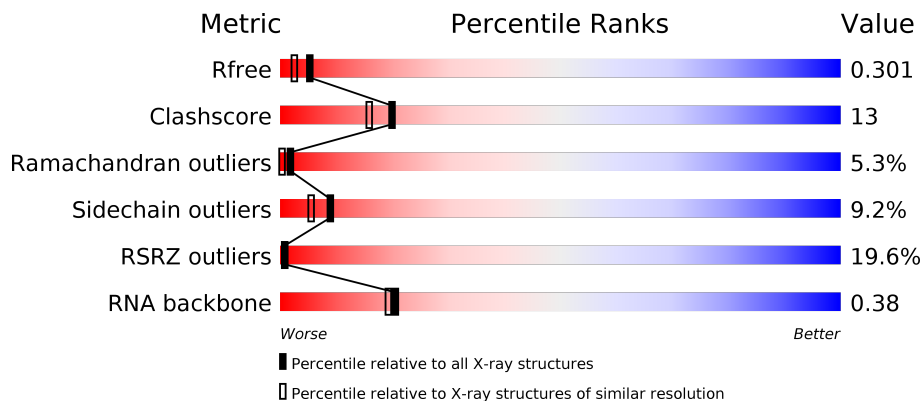
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.12 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.



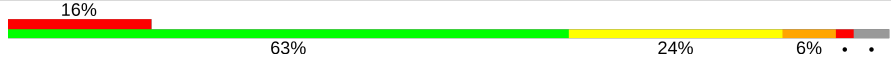
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)
RNA backbone	3102	1013 (2.58-1.66)

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 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	L	42	
2	A	233	
2	B	233	
2	C	233	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	D	233	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the left labeled '16%', a green segment labeled '63%', a yellow segment labeled '24%', and a small grey segment on the far right labeled '6%'. There are two small black dots to the right of the grey segment.</p>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8038 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 RNA chain called RNA (42-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	L	42	840	378	84	336	42	0	0	0

- Molecule 2 is a protein called Nucleocapsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	226	1796	1168	301	315	12	0	0	0
2	B	214	1689	1097	284	296	12	0	0	0
2	C	224	1781	1160	298	311	12	0	0	0
2	D	223	1769	1146	298	313	12	0	0	0

- Molecule 3 is water.

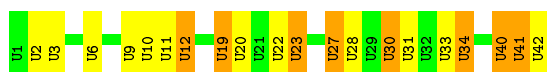
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	33	Total 33	O 33	0	0
3	A	97	Total 97	O 97	0	0
3	B	17	Total 17	O 17	0	0
3	C	16	Total 16	O 16	0	0

### 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.

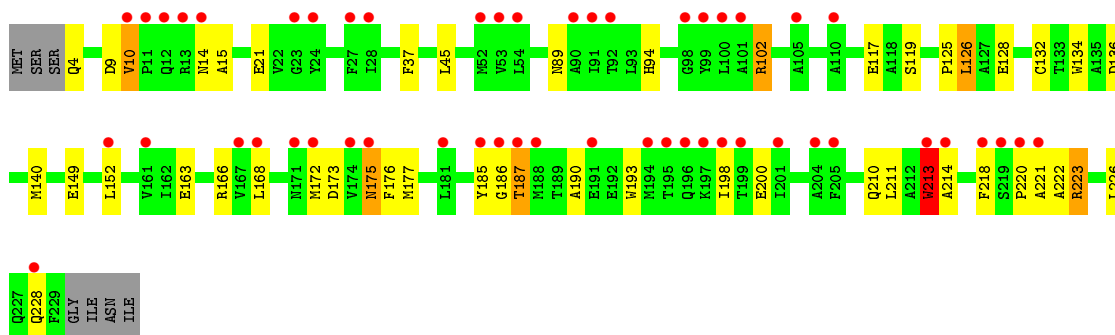
- Molecule 1: RNA (42-MER)

Chain L: 



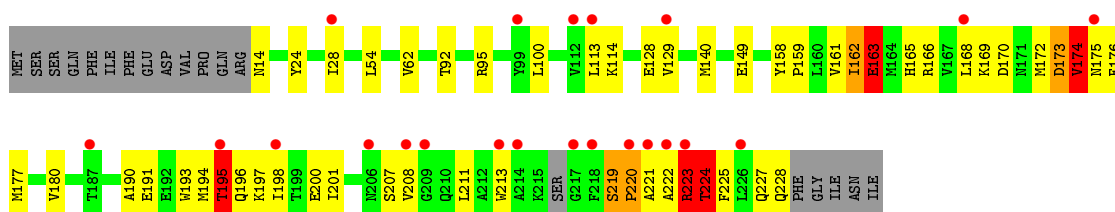
- Molecule 2: Nucleocapsid protein

Chain A: 



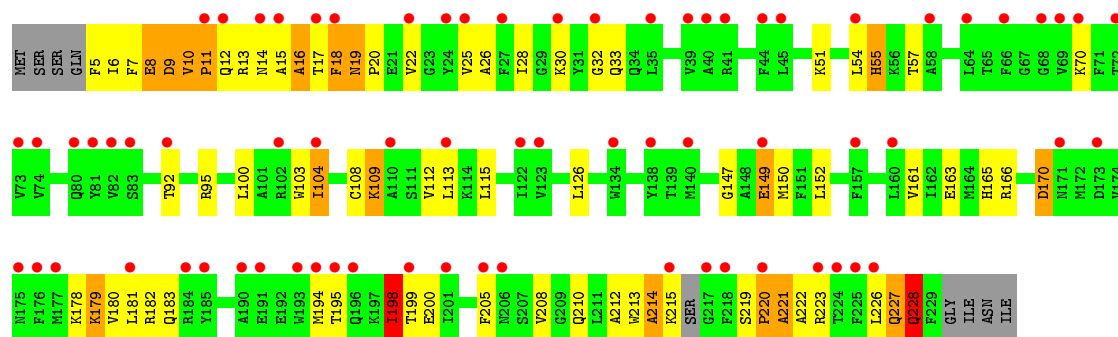
- Molecule 2: Nucleocapsid protein

Chain B: 

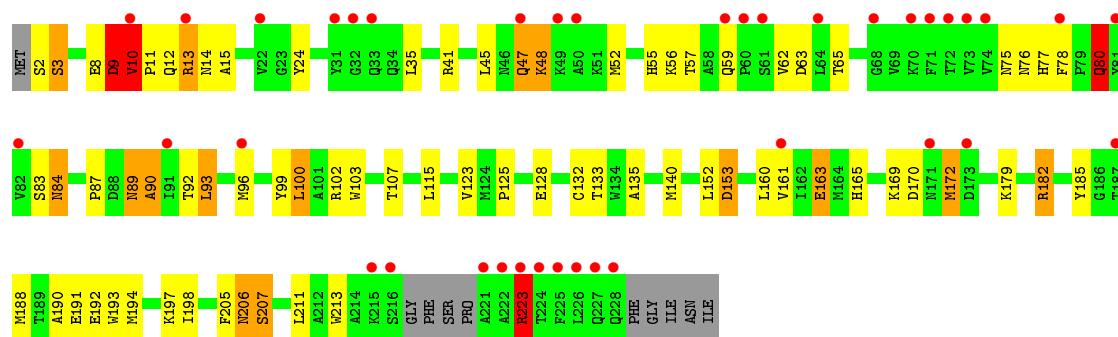


- Molecule 2: Nucleocapsid protein

Chain C: 



- Molecule 2: Nucleocapsid protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.35Å 85.96Å 77.33Å 90.00° 102.02° 90.00°	Depositor
Resolution (Å)	37.40 – 2.12 37.37 – 2.12	Depositor EDS
% Data completeness (in resolution range)	97.7 (37.40-2.12) 97.7 (37.37-2.12)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.12Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.264 , 0.283 0.280 , 0.301	Depositor DCC
$R_{free}$ test set	2755 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.6	Xtrriage
Anisotropy	0.653	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.023 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8038	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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	L	0.32	0/923	0.70	0/1424
2	A	0.36	0/1844	0.64	0/2497
2	B	0.36	0/1732	0.65	1/2344 (0.0%)
2	C	0.33	0/1828	0.61	0/2474
2	D	0.35	0/1813	0.68	3/2453 (0.1%)
All	All	0.35	0/8140	0.65	4/11192 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	223	ARG	NE-CZ-NH1	6.02	123.31	120.30
2	D	206	ASN	N-CA-C	5.78	126.60	111.00
2	D	206	ASN	C-N-CA	5.23	134.77	121.70
2	D	10	VAL	C-N-CD	-5.11	109.36	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	224	THR	Peptide



## 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	L	840	0	421	29	0
2	A	1796	0	1781	34	0
2	B	1689	0	1682	47	0
2	C	1781	0	1767	53	0
2	D	1769	0	1757	60	0
3	A	97	0	0	3	0
3	B	17	0	0	0	0
3	C	16	0	0	0	0
3	L	33	0	0	0	0
All	All	8038	0	7408	192	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 13.

All (192) 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)
2:B:220:PRO:HB2	2:B:221:ALA:HA	1.28	1.15
2:C:12:GLN:HB3	2:C:13:ARG:HA	1.11	1.10
2:A:9:ASP:HA	2:A:10:VAL:HG22	1.36	1.07
1:L:12:U:H5'	1:L:12:U:H6	1.24	1.03
2:B:162:ILE:O	2:B:163:GLU:HB2	1.55	1.01
1:L:27:U:O2	2:A:172:MET:HE1	1.62	1.00
2:C:12:GLN:CB	2:C:13:ARG:HA	1.92	0.99
2:C:12:GLN:HB3	2:C:13:ARG:CA	1.95	0.96
2:D:8:GLU:HB2	2:D:9:ASP:HB2	1.47	0.95
2:D:9:ASP:N	2:D:10:VAL:HB	1.83	0.94
2:D:161:VAL:HG21	2:D:205:PHE:HA	1.48	0.93
2:B:194:MET:HB2	2:C:223:ARG:HD3	1.50	0.91
2:D:12:GLN:HA	2:D:13:ARG:CG	2.01	0.90
1:L:12:U:H5'	1:L:12:U:C6	2.07	0.88
1:L:12:U:C5'	1:L:12:U:H6	1.86	0.88
2:D:12:GLN:HA	2:D:13:ARG:CB	2.05	0.86
2:C:220:PRO:HA	2:C:222:ALA:N	1.95	0.81
2:B:24:TYR:CZ	2:B:28:ILE:HD11	2.17	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:220:PRO:HA	2:C:221:ALA:C	2.04	0.78
2:B:223:ARG:HH11	2:B:223:ARG:HG3	1.49	0.78
2:D:12:GLN:HA	2:D:13:ARG:HB2	1.67	0.77
2:D:188:MET:HG2	2:D:192:GLU:HB2	1.68	0.76
2:A:220:PRO:HA	2:A:222:ALA:H	1.50	0.76
2:B:220:PRO:HB2	2:B:221:ALA:CA	2.14	0.75
1:L:23:U:H6	1:L:23:U:H5'	1.51	0.75
2:C:7:PHE:HA	2:C:8:GLU:HB2	1.68	0.74
2:D:8:GLU:CB	2:D:9:ASP:HB2	2.17	0.74
2:D:99:TYR:O	2:D:100:LEU:HB2	1.89	0.73
2:D:96:MET:O	2:D:99:TYR:O	2.06	0.72
2:C:20:PRO:HB3	2:C:150:MET:HG2	1.70	0.71
1:L:23:U:H6	1:L:23:U:C5'	2.03	0.71
2:A:9:ASP:HA	2:A:10:VAL:CG2	2.18	0.70
1:L:27:U:O2	2:A:172:MET:CE	2.40	0.68
2:B:194:MET:HB2	2:C:223:ARG:CD	2.23	0.68
3:A:301:HOH:O	2:B:92:THR:HG21	1.92	0.68
1:L:23:U:C6	1:L:23:U:C5'	2.78	0.66
2:B:219:SER:HB3	2:B:220:PRO:HD3	1.78	0.66
2:B:113:LEU:O	2:B:114:LYS:HB2	1.95	0.66
2:D:133:THR:HG22	2:D:135:ALA:H	1.62	0.65
2:A:220:PRO:HA	2:A:222:ALA:N	2.12	0.65
2:B:220:PRO:CB	2:B:221:ALA:HA	2.14	0.65
2:C:8:GLU:O	2:C:9:ASP:HB2	1.96	0.65
2:D:12:GLN:HA	2:D:13:ARG:HG2	1.78	0.65
2:D:59:GLN:HG2	2:D:62:VAL:HG22	1.79	0.65
2:A:213:TRP:CD1	2:A:214:ALA:HA	2.33	0.64
1:L:2:U:H2'	1:L:3:U:C6	2.33	0.64
1:L:30:U:H5'	2:A:125:PRO:HB3	1.81	0.63
2:A:223:ARG:HG3	2:D:194:MET:HG2	1.81	0.63
1:L:31:U:O2	2:D:13:ARG:HB3	1.99	0.62
1:L:31:U:O2	2:D:13:ARG:CB	2.47	0.62
2:C:20:PRO:HB3	2:C:150:MET:CG	2.30	0.61
2:D:9:ASP:CA	2:D:10:VAL:HB	2.30	0.61
2:C:7:PHE:HB2	2:D:65:THR:O	2.00	0.60
2:C:13:ARG:HD2	2:D:123:VAL:HG21	1.83	0.60
2:D:75:ASN:HD21	2:D:77:HIS:HB2	1.67	0.60
2:C:100:LEU:O	2:C:103:TRP:O	2.19	0.60
1:L:12:U:C5'	1:L:12:U:C6	2.75	0.60
2:D:165:HIS:O	2:D:169:LYS:HG2	2.02	0.59
2:D:89:ASN:O	2:D:90:ALA:CB	2.48	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:92:THR:O	2:D:93:LEU:HB2	2.03	0.59
2:C:103:TRP:O	2:C:104:ILE:HB	2.03	0.58
1:L:31:U:C2	2:D:13:ARG:HB3	2.37	0.58
2:D:161:VAL:CG2	2:D:205:PHE:HA	2.30	0.58
2:C:7:PHE:CA	2:C:8:GLU:HB2	2.34	0.58
2:A:21:GLU:OE1	2:A:102:ARG:NH2	2.36	0.57
2:B:166:ARG:NH1	2:B:172:MET:SD	2.77	0.57
2:B:54:LEU:CD2	2:B:62:VAL:HG21	2.35	0.57
2:A:223:ARG:HH21	2:D:160:LEU:HD21	1.70	0.56
1:L:10:U:O4'	2:B:14:ASN:HB3	2.06	0.55
2:D:12:GLN:CA	2:D:13:ARG:HG2	2.36	0.54
2:C:112:VAL:HG12	2:C:113:LEU:H	1.72	0.54
2:C:54:LEU:O	2:C:55:HIS:HB2	2.06	0.54
2:A:128:GLU:HA	2:A:128:GLU:OE1	2.06	0.54
2:C:161:VAL:HG11	2:C:205:PHE:HA	1.90	0.54
2:D:99:TYR:O	2:D:100:LEU:CB	2.57	0.53
2:A:226:LEU:HD23	2:D:198:ILE:HD11	1.90	0.53
2:A:223:ARG:NH2	2:D:160:LEU:HD21	2.23	0.53
2:B:173:ASP:O	2:B:174:VAL:HG12	2.09	0.53
2:B:201:ILE:HG21	2:C:223:ARG:HH12	1.74	0.53
2:D:48:LYS:O	2:D:52:MET:HG2	2.09	0.53
2:A:190:ALA:HA	2:A:193:TRP:NE1	2.24	0.52
2:B:128:GLU:O	2:B:129:VAL:HB	2.09	0.52
2:B:158:TYR:O	2:B:162:ILE:HG12	2.09	0.52
2:B:92:THR:HG22	2:B:95:ARG:HG3	1.90	0.52
2:B:225:PHE:CD1	2:B:228:GLN:O	2.64	0.51
1:L:40:U:H1'	2:D:125:PRO:HB2	1.92	0.51
2:D:83:SER:O	2:D:84:ASN:HB2	2.11	0.51
2:B:162:ILE:CG2	2:B:208:VAL:HG21	2.41	0.50
2:B:54:LEU:HD21	2:B:62:VAL:HG21	1.93	0.50
2:D:55:HIS:HD2	2:D:56:LYS:HG2	1.76	0.50
2:A:89:ASN:ND2	3:A:331:HOH:O	2.44	0.50
2:B:223:ARG:HG3	2:B:224:THR:N	2.26	0.50
2:C:108:CYS:O	2:C:109:LYS:HB3	2.11	0.50
2:A:175:ASN:O	2:A:176:PHE:HB2	2.10	0.50
1:L:31:U:O2	2:D:13:ARG:HB2	2.12	0.50
2:D:140:MET:CE	2:D:211:LEU:HD22	2.42	0.50
3:A:334:HOH:O	2:B:14:ASN:ND2	2.43	0.49
2:B:168:LEU:HD11	2:C:228:GLN:HB2	1.94	0.49
2:C:15:ALA:O	2:C:16:ALA:HB2	2.12	0.49
2:A:213:TRP:CB	2:A:214:ALA:HA	2.42	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:5:PHE:CD2	2:C:6:ILE:HD13	2.48	0.49
2:C:161:VAL:CG1	2:C:205:PHE:HA	2.43	0.49
2:C:165:HIS:CE1	2:C:208:VAL:HG23	2.46	0.49
2:C:180:VAL:HA	2:C:183:GLN:HG2	1.94	0.49
2:C:194:MET:O	2:C:194:MET:HG3	2.12	0.49
2:D:103:TRP:O	2:D:107:THR:HG23	2.13	0.49
2:A:140:MET:CE	2:A:211:LEU:HD22	2.42	0.49
2:D:12:GLN:H	2:D:13:ARG:HG2	1.77	0.49
1:L:19:U:H2'	1:L:20:U:O4'	2.13	0.48
1:L:3:U:O4	2:C:179:LYS:NZ	2.41	0.48
2:A:94:HIS:HE1	2:A:149:GLU:OE2	1.96	0.48
2:B:162:ILE:O	2:B:163:GLU:CB	2.40	0.48
2:C:165:HIS:CE1	2:C:208:VAL:CG2	2.97	0.48
2:D:169:LYS:HE2	2:D:213:TRP:CD2	2.49	0.48
2:D:47:GLN:O	2:D:48:LYS:CB	2.61	0.48
2:C:22:VAL:O	2:C:25:VAL:HG12	2.14	0.47
2:D:153:ASP:HA	2:D:185:TYR:CE1	2.49	0.47
2:D:190:ALA:HA	2:D:193:TRP:NE1	2.29	0.47
2:C:178:LYS:O	2:C:182:ARG:HG3	2.14	0.47
1:L:23:U:H5'	1:L:23:U:C6	2.50	0.47
2:A:213:TRP:HD1	2:A:214:ALA:HA	1.76	0.47
2:C:112:VAL:HG12	2:C:113:LEU:N	2.30	0.47
2:C:112:VAL:O	2:C:113:LEU:HB2	2.15	0.47
2:B:140:MET:HE2	2:B:211:LEU:HD11	1.97	0.46
2:A:220:PRO:HB3	2:A:223:ARG:N	2.30	0.46
2:C:103:TRP:O	2:C:104:ILE:CB	2.63	0.46
2:A:168:LEU:HD21	2:B:227:GLN:HB3	1.98	0.46
2:C:161:VAL:HG12	2:C:208:VAL:HG21	1.98	0.46
2:C:8:GLU:O	2:C:9:ASP:CB	2.61	0.46
2:A:173:ASP:OD2	2:A:175:ASN:HB2	2.16	0.46
2:B:162:ILE:HG22	2:B:208:VAL:HG21	1.97	0.46
2:C:10:VAL:HG11	2:D:41:ARG:HE	1.79	0.46
2:B:92:THR:HG23	2:B:95:ARG:H	1.81	0.46
2:C:10:VAL:HG23	2:C:11:PRO:N	2.30	0.46
2:C:213:TRP:O	2:C:214:ALA:HB2	2.16	0.46
2:A:132:CYS:O	2:A:136:ASP:OD2	2.34	0.45
2:C:147:GLY:N	2:C:149:GLU:OE2	2.46	0.45
2:D:89:ASN:O	2:D:90:ALA:HB3	2.16	0.45
2:C:20:PRO:CB	2:C:150:MET:HG2	2.43	0.45
2:C:166:ARG:O	2:C:170:ASP:O	2.33	0.45
2:D:132:CYS:HB2	2:D:211:LEU:HD21	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:30:U:C5'	2:A:125:PRO:HB3	2.47	0.45
2:B:220:PRO:HA	2:B:222:ALA:H	1.82	0.45
2:C:10:VAL:CG1	2:D:41:ARG:HE	2.30	0.45
2:B:169:LYS:HD2	2:B:213:TRP:HE3	1.82	0.45
2:B:219:SER:CB	2:B:220:PRO:HD3	2.47	0.45
2:B:223:ARG:NH1	2:B:223:ARG:HG3	2.27	0.44
2:C:26:ALA:O	2:C:30:LYS:HG2	2.17	0.44
2:D:12:GLN:N	2:D:13:ARG:HG2	2.31	0.44
2:B:191:GLU:O	2:B:195:THR:OG1	2.35	0.44
1:L:28:U:C2	2:A:166:ARG:NH1	2.86	0.44
2:B:223:ARG:CG	2:B:223:ARG:HH11	2.24	0.44
2:C:212:ALA:HB1	2:C:215:LYS:HD3	1.99	0.44
1:L:41:U:O2'	2:D:128:GLU:HB3	2.18	0.44
2:B:190:ALA:HA	2:B:193:TRP:NE1	2.33	0.44
2:C:219:SER:HA	2:C:221:ALA:HB3	2.00	0.44
2:D:9:ASP:HB3	2:D:10:VAL:HG23	1.99	0.44
2:D:2:SER:O	2:D:3:SER:CB	2.65	0.44
2:C:7:PHE:HA	2:C:8:GLU:CB	2.34	0.44
2:B:174:VAL:HG13	2:B:175:ASN:N	2.33	0.43
2:D:206:ASN:N	2:D:207:SER:HB3	2.33	0.43
2:B:113:LEU:O	2:B:114:LYS:CB	2.66	0.43
2:C:103:TRP:CE3	2:C:104:ILE:HG13	2.53	0.43
2:D:223:ARG:HG2	2:D:223:ARG:O	2.19	0.43
2:C:227:GLN:HB3	2:C:228:GLN:HG3	2.00	0.42
1:L:30:U:C4	2:A:45:LEU:HD22	2.55	0.42
2:C:198:ILE:HG13	2:C:199:THR:H	1.84	0.42
2:C:51:LYS:O	2:C:54:LEU:O	2.37	0.42
2:B:190:ALA:O	2:B:191:GLU:C	2.55	0.42
1:L:28:U:O2	2:A:166:ARG:NH1	2.53	0.42
1:L:34:U:OP1	2:D:179:LYS:NZ	2.46	0.42
2:A:37:PHE:HE2	2:A:117:GLU:HG3	1.85	0.41
2:A:132:CYS:HA	2:A:211:LEU:HD11	2.02	0.41
2:B:159:PRO:O	2:B:162:ILE:O	2.37	0.41
2:B:149:GLU:HB2	2:B:180:VAL:HG23	2.02	0.41
2:A:119:SER:HA	2:A:134:TRP:CE2	2.55	0.41
2:C:92:THR:HG22	2:C:95:ARG:HG3	2.02	0.41
2:D:9:ASP:H	2:D:10:VAL:HB	1.77	0.41
2:B:174:VAL:O	2:B:176:PHE:N	2.47	0.41
2:A:185:TYR:O	2:A:187:THR:N	2.53	0.41
2:B:24:TYR:CE2	2:B:28:ILE:HD11	2.53	0.41
2:B:197:LYS:HD2	2:B:200:GLU:CG	2.51	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:34:U:OP2	2:D:182:ARG:HD2	2.21	0.41
2:D:78:PHE:O	2:D:80:GLN:N	2.42	0.41
2:D:24:TYR:CZ	2:D:102:ARG:HG3	2.56	0.41
2:D:163:GLU:HG2	2:D:172:MET:HE1	2.03	0.41
2:D:87:PRO:HB2	2:D:89:ASN:O	2.21	0.41
2:D:89:ASN:N	2:D:89:ASN:OD1	2.54	0.40
1:L:9:U:O2	2:B:14:ASN:ND2	2.54	0.40
2:B:165:HIS:CE1	2:B:208:VAL:HG13	2.55	0.40
1:L:12:U:C4'	1:L:12:U:C6	3.04	0.40
2:A:175:ASN:C	2:A:177:MET:H	2.25	0.40

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	
2	A	224/233 (96%)	198 (88%)	19 (8%)	7 (3%)	4	1
2	B	210/233 (90%)	181 (86%)	21 (10%)	8 (4%)	3	1
2	C	220/233 (94%)	184 (84%)	19 (9%)	17 (8%)	1	0
2	D	219/233 (94%)	190 (87%)	15 (7%)	14 (6%)	1	0
All	All	873/932 (94%)	753 (86%)	74 (8%)	46 (5%)	2	0

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	126	LEU
2	A	213	TRP
2	A	221	ALA
2	B	163	GLU
2	B	174	VAL

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	207	SER
2	B	219	SER
2	C	9	ASP
2	C	11	PRO
2	C	16	ALA
2	C	17	THR
2	C	18	PHE
2	C	33	GLN
2	C	55	HIS
2	C	214	ALA
2	C	220	PRO
2	C	221	ALA
2	D	3	SER
2	D	10	VAL
2	D	11	PRO
2	D	13	ARG
2	D	48	LYS
2	D	90	ALA
2	D	207	SER
2	D	223	ARG
2	A	186	GLY
2	B	224	THR
2	C	228	GLN
2	D	9	ASP
2	D	84	ASN
2	D	93	LEU
2	D	100	LEU
2	A	15	ALA
2	A	175	ASN
2	B	173	ASP
2	B	195	THR
2	C	8	GLU
2	C	195	THR
2	D	15	ALA
2	B	220	PRO
2	C	19	ASN
2	C	104	ILE
2	D	80	GLN
2	A	10	VAL
2	C	32	GLY
2	C	198	ILE

### 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	
2	A	187/193 (97%)	173 (92%)	14 (8%)	13	10
2	B	175/193 (91%)	164 (94%)	11 (6%)	18	14
2	C	185/193 (96%)	163 (88%)	22 (12%)	5	2
2	D	185/193 (96%)	165 (89%)	20 (11%)	6	3
All	All	732/772 (95%)	665 (91%)	67 (9%)	9	5

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	4	GLN
2	A	14	ASN
2	A	102	ARG
2	A	126	LEU
2	A	152	LEU
2	A	163	GLU
2	A	187	THR
2	A	198	ILE
2	A	200	GLU
2	A	210	GLN
2	A	213	TRP
2	A	218	PHE
2	A	223	ARG
2	A	228	GLN
2	B	100	LEU
2	B	161	VAL
2	B	162	ILE
2	B	163	GLU
2	B	170	ASP
2	B	174	VAL
2	B	177	MET
2	B	195	THR
2	B	196	GLN
2	B	198	ILE

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	223	ARG
2	C	10	VAL
2	C	14	ASN
2	C	18	PHE
2	C	19	ASN
2	C	28	ILE
2	C	57	THR
2	C	70	LYS
2	C	109	LYS
2	C	115	LEU
2	C	126	LEU
2	C	149	GLU
2	C	152	LEU
2	C	163	GLU
2	C	170	ASP
2	C	179	LYS
2	C	181	LEU
2	C	198	ILE
2	C	200	GLU
2	C	210	GLN
2	C	226	LEU
2	C	227	GLN
2	C	228	GLN
2	D	9	ASP
2	D	14	ASN
2	D	35	LEU
2	D	45	LEU
2	D	47	GLN
2	D	57	THR
2	D	63	ASP
2	D	76	ASN
2	D	80	GLN
2	D	89	ASN
2	D	115	LEU
2	D	152	LEU
2	D	153	ASP
2	D	163	GLU
2	D	170	ASP
2	D	172	MET
2	D	182	ARG
2	D	191	GLU
2	D	197	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	223	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	12	GLN
2	A	89	ASN
2	A	94	HIS
2	A	210	GLN
2	A	227	GLN
2	B	14	ASN
2	B	59	GLN
2	B	94	HIS
2	B	206	ASN
2	C	33	GLN
2	C	34	GLN
2	C	47	GLN
2	C	210	GLN
2	D	47	GLN
2	D	55	HIS
2	D	75	ASN
2	D	76	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L	41/42 (97%)	11 (26%)	6 (14%)

All (11) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L	6	U
1	L	11	U
1	L	12	U
1	L	19	U
1	L	22	U
1	L	23	U
1	L	27	U
1	L	30	U
1	L	34	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	L	41	U
1	L	42	U

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L	11	U
1	L	12	U
1	L	22	U
1	L	23	U
1	L	33	U
1	L	40	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 [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	L	42/42 (100%)	-0.54	0 100 100	5, 18, 32, 54	0
2	A	226/233 (96%)	1.31	51 (22%) 0 0	5, 10, 40, 49	0
2	B	214/233 (91%)	1.04	22 (10%) 6 8	5, 13, 42, 67	0
2	C	224/233 (96%)	1.73	71 (31%) 0 0	10, 28, 49, 78	0
2	D	223/233 (95%)	1.16	38 (17%) 1 1	5, 16, 41, 52	0
All	All	929/974 (95%)	1.23	182 (19%) 1 1	5, 17, 43, 78	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	221	ALA	15.1
2	C	218	PHE	9.3
2	C	191	GLU	8.6
2	B	213	TRP	8.5
2	A	167	VAL	6.6
2	D	60	PRO	6.4
2	C	69	VAL	6.3
2	C	176	PHE	6.1
2	B	220	PRO	5.9
2	C	199	THR	5.9
2	C	181	LEU	5.8
2	C	40	ALA	5.8
2	A	171	ASN	5.8
2	A	168	LEU	5.5
2	B	217	GLY	5.4
2	B	208	VAL	5.2
2	A	174	VAL	5.2
2	C	215	LYS	5.2
2	B	222	ALA	5.2
2	A	213	TRP	5.0

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	C	193	TRP	4.9
2	B	113	LEU	4.8
2	A	186	GLY	4.8
2	B	168	LEU	4.8
2	C	54	LEU	4.7
2	C	225	PHE	4.7
2	D	78	PHE	4.7
2	A	199	THR	4.6
2	D	68	GLY	4.6
2	A	10	VAL	4.6
2	A	201	ILE	4.4
2	C	184	ARG	4.4
2	C	195	THR	4.4
2	D	215	LYS	4.3
2	C	206	ASN	4.3
2	B	187	THR	4.3
2	C	14	ASN	4.3
2	D	226	LEU	4.3
2	B	112	VAL	4.3
2	D	73	VAL	4.2
2	D	225	PHE	4.1
2	C	113	LEU	4.0
2	C	224	THR	4.0
2	C	160	LEU	4.0
2	C	32	GLY	4.0
2	D	81	TYR	3.9
2	C	15	ALA	3.8
2	C	17	THR	3.8
2	C	223	ARG	3.7
2	A	185	TYR	3.6
2	D	173	ASP	3.6
2	D	71	PHE	3.6
2	C	171	ASN	3.6
2	C	217	GLY	3.6
2	C	140	MET	3.5
2	C	74	VAL	3.4
2	C	45	LEU	3.4
2	C	226	LEU	3.4
2	C	82	VAL	3.3
2	D	32	GLY	3.3
2	C	190	ALA	3.3
2	C	72	THR	3.3

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	64	LEU	3.3
2	C	30	LYS	3.3
2	C	68	GLY	3.2
2	A	14	ASN	3.2
2	A	218	PHE	3.2
2	B	218	PHE	3.2
2	A	198	ILE	3.2
2	C	201	ILE	3.1
2	A	228	GLN	3.1
2	D	216	SER	3.1
2	C	104	ILE	3.1
2	C	35	LEU	3.1
2	A	195	THR	3.1
2	D	171	ASN	3.1
2	B	226	LEU	3.0
2	C	122	ILE	3.0
2	C	80	GLN	3.0
2	C	83	SER	3.0
2	A	13	ARG	3.0
2	C	64	LEU	3.0
2	C	134	TRP	3.0
2	A	172	MET	3.0
2	C	175	ASN	2.9
2	B	198	ILE	2.9
2	A	12	GLN	2.9
2	B	223	ARG	2.9
2	C	73	VAL	2.8
2	D	10	VAL	2.8
2	A	110	ALA	2.8
2	C	70	LYS	2.8
2	C	123	VAL	2.8
2	D	221	ALA	2.8
2	D	13	ARG	2.8
2	D	33	GLN	2.8
2	C	58	ALA	2.8
2	B	206	ASN	2.8
2	A	52	MET	2.7
2	C	81	TYR	2.7
2	D	22	VAL	2.7
2	C	66	PHE	2.7
2	A	90	ALA	2.7
2	C	27	PHE	2.7

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	C	39	VAL	2.7
2	C	157	PHE	2.7
2	D	70	LYS	2.7
2	C	18	PHE	2.6
2	C	102	ARG	2.6
2	B	209	GLY	2.6
2	C	194	MET	2.5
2	C	25	VAL	2.5
2	C	11	PRO	2.5
2	A	205	PHE	2.5
2	A	204	ALA	2.5
2	A	187	THR	2.4
2	C	177	MET	2.4
2	D	82	VAL	2.4
2	A	175	ASN	2.4
2	A	191	GLU	2.4
2	C	110	ALA	2.4
2	C	205	PHE	2.4
2	A	197	LYS	2.4
2	A	220	PRO	2.4
2	A	92	THR	2.4
2	C	173	ASP	2.4
2	A	214	ALA	2.4
2	A	219	SER	2.4
2	B	99	TYR	2.4
2	C	196	GLN	2.4
2	D	227	GLN	2.4
2	C	44	PHE	2.4
2	D	224	THR	2.3
2	D	91	ILE	2.3
2	D	228	GLN	2.3
2	D	50	ALA	2.3
2	B	28	ILE	2.3
2	A	152	LEU	2.3
2	A	181	LEU	2.3
2	A	194	MET	2.3
2	D	161	VAL	2.3
2	B	129	VAL	2.3
2	C	41	ARG	2.3
2	A	28	ILE	2.2
2	A	105	ALA	2.2
2	B	195	THR	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	A	99	TYR	2.2
2	C	24	TYR	2.2
2	A	221	ALA	2.2
2	A	100	LEU	2.2
2	C	220	PRO	2.2
2	A	53	VAL	2.2
2	A	98	GLY	2.2
2	A	11	PRO	2.2
2	A	27	PHE	2.2
2	D	61	SER	2.2
2	C	22	VAL	2.1
2	C	149	GLU	2.1
2	A	196	GLN	2.1
2	C	185	TYR	2.1
2	A	188	MET	2.1
2	D	49	LYS	2.1
2	A	91	ILE	2.1
2	D	223	ARG	2.1
2	C	12	GLN	2.1
2	A	24	TYR	2.1
2	B	214	ALA	2.1
2	D	31	TYR	2.1
2	B	175	ASN	2.1
2	D	74	VAL	2.1
2	A	101	ALA	2.1
2	D	187	THR	2.1
2	D	222	ALA	2.1
2	D	96	MET	2.1
2	D	47	GLN	2.1
2	D	72	THR	2.1
2	C	138	TYR	2.1
2	A	54	LEU	2.0
2	D	59	GLN	2.0
2	C	92	THR	2.0
2	A	161	VAL	2.0
2	A	23	GLY	2.0

## 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 [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.