Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:20 am BST

PDB ID	:	4J1G
Title	:	Leanyer orthobunyavirus nucleoprotein-ssRNA complex
Authors	:	Niu, F.; Shaw, N.; Wang, Y.; Jiao, L.; Ding, W.; Li, X.; Zhu, P.; Upur, H.; Ouyang, S.; Cheng, G.; Liu, Z.J.
Deposited on	:	2013-02-01
Resolution	:	2.79 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*
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:

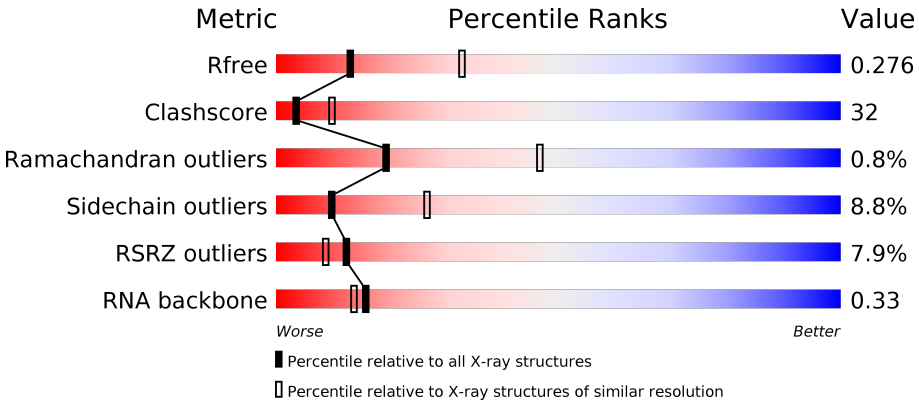
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)
RNA backbone	3102	1092 (3.06-2.50)

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 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 <=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	235	6% 53% 38% 5%
1	B	235	5% 60% 31% 5%
1	C	235	6% 64% 29%
1	D	235	16% 48% 42% 7%

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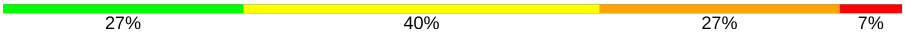
Mol	Chain	Length	Quality of chain
2	E	45	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8155 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1807	1166	308	326	7			
1	D	227	Total	C	N	O	S	0	0	0
			1799	1160	307	325	7			
1	C	228	Total	C	N	O	S	0	0	0
			1807	1166	308	326	7			
1	B	227	Total	C	N	O	S	0	0	0
			1799	1160	307	325	7			

- Molecule 2 is a RNA chain called RNA (45-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	45	Total	C	N	O	P	0	0	0
			881	396	88	353	44			

- Molecule 3 is water.

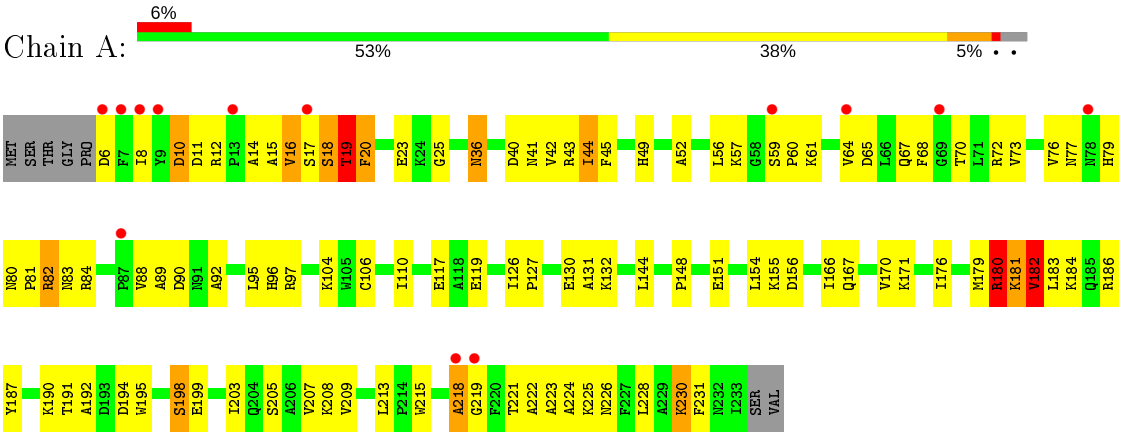
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		
3	D	11	Total	O	0	0
			11	11		
3	C	13	Total	O	0	0
			13	13		
3	B	10	Total	O	0	0
			10	10		
3	E	14	Total	O	0	0
			14	14		

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.

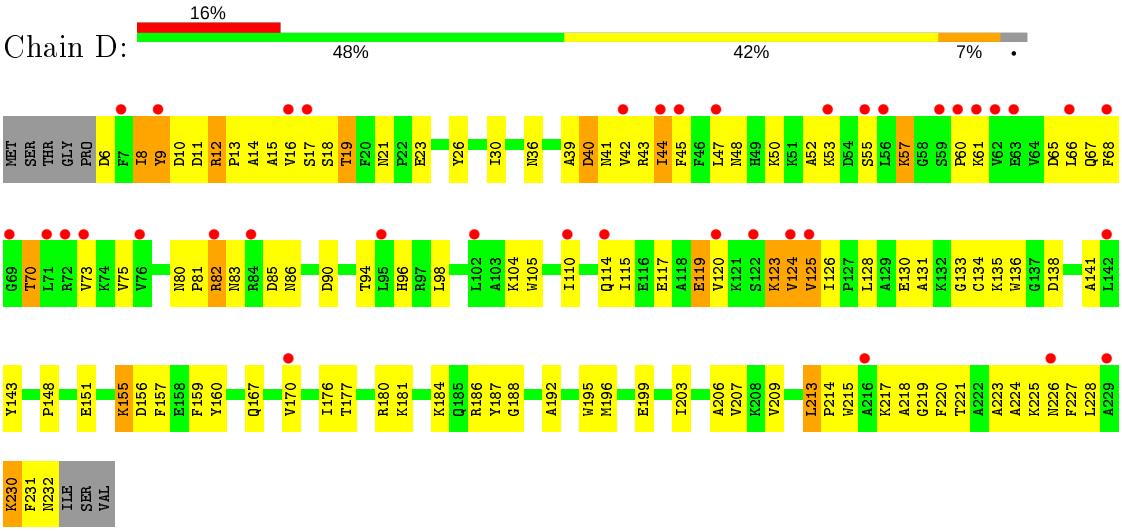
- Molecule 1: Nucleocapsid

Chain A:



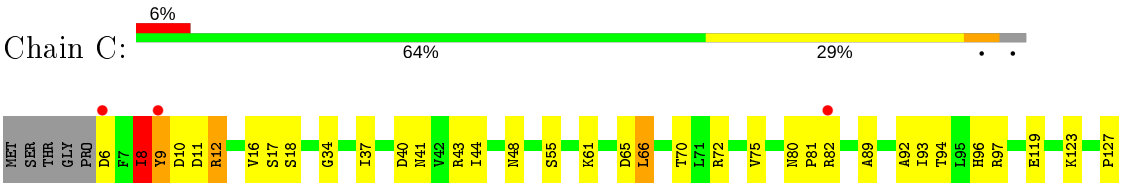
- Molecule 1: Nucleocapsid

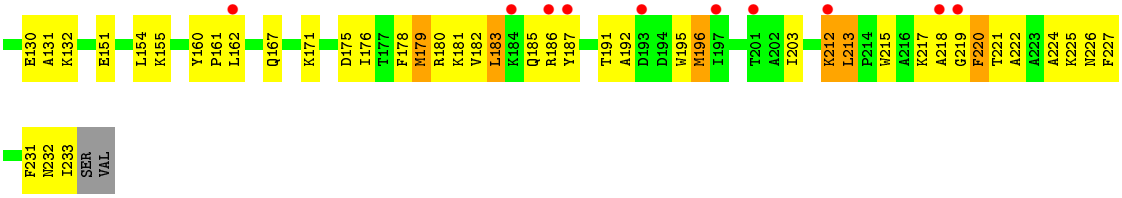
Chain D:



- Molecule 1: Nucleocapsid

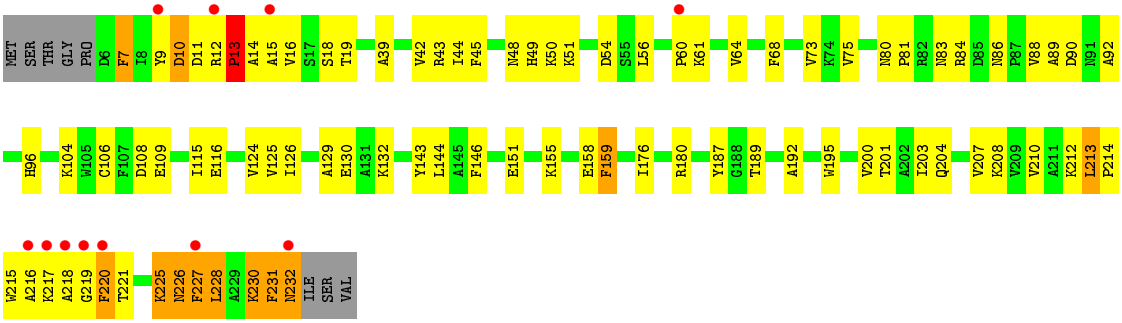
Chain C:





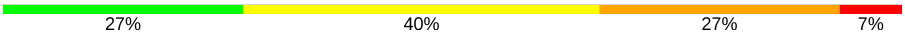
- Molecule 1: Nucleocapsid

Chain B:



- Molecule 2: RNA (45-MER)

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	49.84Å 73.83Å 79.88Å 69.74° 89.66° 75.44°	Depositor
Resolution (Å)	48.05 – 2.79 48.05 – 2.79	Depositor EDS
% Data completeness (in resolution range)	93.2 (48.05-2.79) 88.5 (48.05-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.47 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.233 , 0.274 0.236 , 0.276	Depositor DCC
R_{free} test set	2000 reflections (8.35%)	wwPDB-VP
Wilson B-factor (Å^2)	73.4	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 61.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8155	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.43	0/1849	0.62	0/2499
1	B	0.40	1/1841 (0.1%)	0.59	1/2488 (0.0%)
1	C	0.44	0/1849	0.63	1/2499 (0.0%)
1	D	0.38	0/1841	0.62	1/2488 (0.0%)
2	E	0.74	2/968 (0.2%)	1.22	12/1495 (0.8%)
All	All	0.46	3/8348 (0.0%)	0.72	15/11469 (0.1%)

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
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	25	U	C2-N3	-5.69	1.33	1.37
2	E	25	U	N3-C4	-5.20	1.33	1.38
1	B	13	PRO	N-CD	5.18	1.55	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	38	U	O5'-P-OP1	-14.35	92.78	105.70
2	E	37	U	OP1-P-O3'	9.67	126.47	105.20
2	E	25	U	O4'-C1'-N1	-8.53	101.37	108.20
2	E	1	U	C3'-C2'-O2'	-7.70	90.96	113.30
2	E	1	U	N1-C2-O2	6.69	127.48	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	24	U	P-O3'-C3'	-5.99	112.52	119.70
2	E	1	U	C1'-C2'-O2'	-5.95	92.74	110.60
2	E	26	U	OP1-P-OP2	5.95	128.53	119.60
2	E	1	U	N3-C2-O2	-5.79	118.15	122.20
2	E	26	U	O4'-C4'-C3'	-5.61	98.39	104.00
1	B	13	PRO	CA-N-CD	-5.31	104.06	111.50
1	C	8	ILE	N-CA-C	-5.26	96.81	111.00
2	E	26	U	C5'-C4'-O4'	-5.20	102.86	109.10
2	E	1	U	C2-N1-C1'	5.10	123.82	117.70
1	D	213	LEU	CA-CB-CG	5.09	127.02	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	218	ALA	Peptide
1	B	215	TRP	Peptide
1	C	8	ILE	Peptide

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	A	1807	0	1811	129	0
1	B	1799	0	1800	86	0
1	C	1807	0	1811	109	0
1	D	1799	0	1800	184	0
2	E	881	0	441	88	0
3	A	14	0	0	10	0
3	B	10	0	0	7	0
3	C	13	0	0	17	0
3	D	11	0	0	22	0
3	E	14	0	0	17	0
All	All	8155	0	7663	503	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 32.

All (503) 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:A:18:SER:CB	2:E:45:U:OP2	1.74	1.33
1:A:15:ALA:N	3:A:311:HOH:O	1.73	1.21
1:D:12:ARG:HH22	1:C:43:ARG:CZ	1.61	1.13
1:D:12:ARG:HB2	1:C:44:ILE:CG1	1.78	1.12
1:A:12:ARG:HB2	1:D:44:ILE:HG22	1.30	1.11
1:D:12:ARG:NE	1:D:13:PRO:O	1.83	1.09
1:A:18:SER:HB2	2:E:45:U:OP2	1.54	1.07
1:A:18:SER:HB3	2:E:45:U:OP2	1.54	1.06
1:D:220:PHE:HB3	1:D:224:ALA:HB3	1.41	1.02
1:A:12:ARG:HB2	1:D:44:ILE:CG2	1.91	1.00
1:D:40:ASP:OD2	3:D:309:HOH:O	1.81	0.98
1:A:16:VAL:HG23	2:E:43:U:O2	1.64	0.97
1:D:12:ARG:HH22	1:C:43:ARG:NE	1.62	0.97
1:D:43:ARG:HD3	1:D:124:VAL:HA	1.46	0.97
1:D:43:ARG:HG3	1:D:123:LYS:O	1.65	0.96
1:B:60:PRO:HA	1:B:80:ASN:HD22	1.30	0.96
1:D:12:ARG:HB2	1:C:44:ILE:HG13	1.46	0.95
1:A:8:ILE:O	3:A:305:HOH:O	1.85	0.94
1:A:119:GLU:OE2	3:A:308:HOH:O	1.84	0.94
1:D:196:MET:SD	3:C:305:HOH:O	2.25	0.93
1:B:228:LEU:HD12	1:B:228:LEU:H	1.33	0.92
1:D:12:ARG:NH1	1:D:14:ALA:HA	1.84	0.92
2:E:4:U:OP2	3:E:107:HOH:O	1.89	0.90
1:D:70:THR:CG2	3:D:309:HOH:O	2.19	0.89
1:A:20:PHE:HD2	2:E:1:U:C5'	1.86	0.88
1:D:43:ARG:CD	1:D:124:VAL:HG23	2.03	0.88
1:D:12:ARG:HE	1:D:13:PRO:C	1.76	0.88
1:D:8:ILE:HD13	1:C:55:SER:HB3	1.56	0.87
1:A:167:GLN:OE1	1:A:171:LYS:NZ	2.07	0.87
1:C:92:ALA:CA	3:C:306:HOH:O	2.23	0.87
1:C:92:ALA:HA	3:C:306:HOH:O	1.74	0.87
1:D:15:ALA:O	1:D:16:VAL:CG2	2.23	0.86
2:E:24:U:N3	3:E:104:HOH:O	2.08	0.86
1:A:230:LYS:HD2	1:A:230:LYS:O	1.75	0.86
1:A:65:ASP:OD2	1:A:72:ARG:NH1	2.07	0.85
1:A:83:ASN:HA	3:A:306:HOH:O	1.77	0.84
1:C:16:VAL:O	3:C:302:HOH:O	1.96	0.84
1:D:119:GLU:O	1:D:123:LYS:HG3	1.78	0.83
1:D:12:ARG:CZ	1:D:13:PRO:O	2.27	0.83
1:D:12:ARG:HB2	1:C:44:ILE:HG12	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:VAL:O	3:D:304:HOH:O	1.96	0.82
1:D:12:ARG:NH2	1:C:43:ARG:NE	2.28	0.82
1:C:212:LYS:O	1:C:213:LEU:HD12	1.80	0.82
1:A:230:LYS:HD2	1:A:230:LYS:C	1.89	0.81
1:D:209:VAL:HG21	3:D:303:HOH:O	1.80	0.81
1:D:41:ASN:HD21	1:D:70:THR:HG23	1.46	0.81
1:D:12:ARG:CB	1:C:44:ILE:HG13	2.11	0.81
1:D:43:ARG:HD3	1:D:124:VAL:HG23	1.63	0.79
1:D:192:ALA:HB3	3:D:305:HOH:O	1.82	0.79
1:D:125:VAL:HA	1:D:143:TYR:OH	1.83	0.79
1:A:230:LYS:CD	1:A:230:LYS:O	2.30	0.79
1:D:138:ASP:OD2	3:D:307:HOH:O	1.99	0.79
1:C:186:ARG:CZ	1:C:191:THR:HG22	2.12	0.79
1:A:181:LYS:O	1:A:184:LYS:N	2.13	0.78
1:A:6:ASP:HA	1:D:65:ASP:HB3	1.63	0.78
1:A:61:LYS:HB3	1:A:64:VAL:HG22	1.65	0.78
1:D:181:LYS:NZ	2:E:36:U:OP2	2.15	0.78
1:B:132:LYS:NZ	1:B:218:ALA:HB2	1.99	0.78
1:A:64:VAL:HG23	1:A:77:ASN:HB2	1.65	0.78
1:D:126:ILE:N	1:D:143:TYR:OH	2.17	0.78
1:C:10:ASP:OD1	1:B:48:ASN:HB3	1.84	0.78
1:D:12:ARG:NH2	1:C:43:ARG:CZ	2.45	0.77
1:D:213:LEU:HD22	1:D:215:TRP:HE3	1.50	0.77
1:C:93:ILE:N	3:C:306:HOH:O	1.99	0.77
1:D:43:ARG:NE	1:D:43:ARG:HA	1.98	0.76
2:E:37:U:OP1	3:E:101:HOH:O	2.03	0.76
1:D:220:PHE:HB3	1:D:224:ALA:CB	2.15	0.75
1:D:119:GLU:O	1:D:123:LYS:CG	2.34	0.75
1:A:225:LYS:HZ2	1:A:225:LYS:HB3	1.52	0.75
1:A:16:VAL:HG21	2:E:43:U:H1'	1.68	0.75
1:C:222:ALA:HB1	1:C:226:ASN:ND2	2.02	0.74
1:A:67:GLN:HB3	1:B:9:TYR:HB3	1.70	0.74
1:A:167:GLN:HB3	1:A:171:LYS:HZ1	1.51	0.74
2:E:10:U:OP2	3:E:105:HOH:O	2.06	0.74
1:D:12:ARG:HH11	1:D:14:ALA:HA	1.51	0.74
1:C:155:LYS:CB	3:C:307:HOH:O	2.34	0.73
1:D:218:ALA:N	1:D:219:GLY:HA2	2.02	0.73
1:C:167:GLN:HB3	1:C:171:LYS:HZ3	1.52	0.73
1:C:16:VAL:HG12	1:C:17:SER:H	1.52	0.73
1:B:228:LEU:N	1:B:228:LEU:HD12	2.03	0.73
2:E:25:U:C2	3:E:104:HOH:O	2.41	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:ALA:O	1:D:16:VAL:HG23	1.88	0.73
1:A:20:PHE:HD2	2:E:1:U:O5'	1.72	0.73
1:C:167:GLN:OE1	1:C:171:LYS:NZ	2.22	0.72
1:D:10:ASP:HB3	1:C:48:ASN:HD22	1.54	0.72
1:A:181:LYS:O	1:A:183:LEU:N	2.23	0.72
1:D:12:ARG:NH1	1:D:13:PRO:O	2.22	0.72
3:A:304:HOH:O	1:D:43:ARG:HB3	1.89	0.72
1:A:20:PHE:CD2	2:E:1:U:O5'	2.42	0.72
1:B:19:THR:OG1	1:B:90:ASP:OD2	2.06	0.72
1:A:127:PRO:HB2	2:E:8:U:H1'	1.72	0.71
1:A:176:ILE:HD11	1:D:228:LEU:HD23	1.72	0.71
2:E:24:U:C4	2:E:25:U:C5	2.79	0.71
1:B:180:ARG:NH2	2:E:15:U:O4	2.24	0.71
1:C:65:ASP:OD2	1:C:72:ARG:NH2	2.23	0.71
2:E:25:U:C4	3:E:104:HOH:O	2.43	0.70
1:A:180:ARG:O	1:A:181:LYS:C	2.30	0.70
1:C:41:ASN:ND2	1:C:70:THR:OG1	2.21	0.70
1:D:12:ARG:HG3	1:C:44:ILE:HG13	1.73	0.70
1:D:180:ARG:NH1	2:E:37:U:O4	2.25	0.70
1:C:12:ARG:HD3	1:B:43:ARG:NH2	2.06	0.70
1:A:16:VAL:CG2	2:E:43:U:O2	2.38	0.70
1:C:155:LYS:HD3	1:C:187:TYR:CE1	2.27	0.70
1:B:180:ARG:NH2	2:E:14:U:O4	2.19	0.70
1:D:12:ARG:HH11	1:D:14:ALA:CA	2.04	0.69
1:D:18:SER:HB2	2:E:33:U:H1'	1.74	0.69
1:A:167:GLN:HE21	1:A:207:VAL:HG13	1.57	0.69
1:B:88:VAL:O	3:B:302:HOH:O	2.10	0.69
1:B:96:HIS:NE2	1:B:151:GLU:OE2	2.22	0.69
1:B:50:LYS:N	3:B:303:HOH:O	1.84	0.69
1:D:120:VAL:O	1:D:124:VAL:N	2.25	0.69
1:C:16:VAL:N	3:C:302:HOH:O	2.17	0.69
1:D:228:LEU:O	1:D:232:ASN:ND2	2.25	0.69
1:C:231:PHE:O	3:C:301:HOH:O	2.11	0.68
1:B:214:PRO:O	1:B:216:ALA:HB3	1.93	0.68
1:A:20:PHE:HD2	2:E:1:U:H5"	1.56	0.68
2:E:35:U:O4	3:E:114:HOH:O	2.07	0.68
1:A:223:ALA:O	1:A:226:ASN:HB3	1.93	0.68
1:B:226:ASN:O	1:B:228:LEU:HD12	1.91	0.68
1:D:124:VAL:CG1	1:D:136:TRP:CZ2	2.77	0.68
1:B:125:VAL:O	3:B:301:HOH:O	2.12	0.68
1:D:43:ARG:HD2	1:D:124:VAL:HG23	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:SER:HB2	2:E:11:U:O2'	1.93	0.68
1:D:15:ALA:O	1:D:16:VAL:HG22	1.92	0.68
1:C:155:LYS:HB3	3:C:307:HOH:O	1.94	0.67
1:C:131:ALA:HA	1:C:218:ALA:CB	2.25	0.67
1:A:49:HIS:HE1	1:A:148:PRO:HG2	1.58	0.67
1:B:217:LYS:HG2	1:B:218:ALA:N	2.10	0.67
1:D:160:TYR:CE1	3:D:303:HOH:O	2.47	0.67
1:A:194:ASP:OD1	1:A:198:SER:OG	2.13	0.66
1:A:230:LYS:CE	1:A:230:LYS:O	2.44	0.66
1:D:12:ARG:CG	1:C:44:ILE:HG13	2.24	0.66
1:D:11:ASP:C	1:D:11:ASP:OD1	2.34	0.66
1:C:11:ASP:OD1	1:C:12:ARG:N	2.27	0.66
2:E:36:U:C2'	2:E:37:U:H5'	2.25	0.66
1:A:43:ARG:NH1	1:B:12:ARG:HG3	2.11	0.66
1:D:96:HIS:NE2	1:D:151:GLU:OE2	2.29	0.65
1:D:12:ARG:CZ	1:D:14:ALA:HA	2.27	0.65
1:A:225:LYS:HB3	1:A:225:LYS:NZ	2.09	0.65
1:C:179:MET:O	1:C:183:LEU:HD12	1.96	0.65
1:B:226:ASN:O	1:B:228:LEU:CD1	2.44	0.64
1:D:155:LYS:H	1:D:155:LYS:HE3	1.62	0.64
1:D:209:VAL:CG2	3:D:303:HOH:O	2.42	0.64
1:D:41:ASN:ND2	1:D:70:THR:HG23	2.12	0.64
1:A:10:ASP:HB3	3:A:305:HOH:O	1.97	0.64
1:A:25:GLY:O	3:A:303:HOH:O	2.14	0.64
1:B:132:LYS:HZ1	1:B:218:ALA:HB2	1.62	0.64
1:C:167:GLN:HB3	1:C:171:LYS:NZ	2.12	0.64
1:D:206:ALA:HA	3:D:303:HOH:O	1.98	0.64
2:E:37:U:O2'	2:E:38:U:O5'	2.15	0.64
1:A:10:ASP:OD1	1:D:48:ASN:ND2	2.31	0.63
1:A:49:HIS:CE1	1:A:148:PRO:HG2	2.32	0.63
1:D:15:ALA:C	1:D:16:VAL:HG23	2.19	0.63
2:E:25:U:H2'	2:E:26:U:O2	1.97	0.63
1:A:181:LYS:O	1:A:182:VAL:C	2.34	0.63
2:E:25:U:N3	3:E:104:HOH:O	2.31	0.63
1:D:45:PHE:HD1	1:D:68:PHE:CZ	2.17	0.63
1:D:16:VAL:HG12	1:D:17:SER:O	1.99	0.62
1:A:186:ARG:NH2	1:A:192:ALA:H	1.97	0.62
1:A:16:VAL:CG2	2:E:43:U:H1'	2.29	0.62
1:C:131:ALA:CB	1:C:218:ALA:HB2	2.29	0.62
1:B:60:PRO:HA	1:B:80:ASN:ND2	2.11	0.61
1:D:57:LYS:NZ	1:D:81:PRO:HD3	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ARG:HG2	2:E:1:U:O2	1.99	0.61
1:A:131:ALA:HA	1:A:218:ALA:HB3	1.81	0.61
1:C:131:ALA:HA	1:C:218:ALA:HB2	1.82	0.61
2:E:36:U:O2'	2:E:37:U:H5'	2.01	0.61
1:D:124:VAL:HG13	1:D:136:TRP:HE1	1.66	0.60
1:A:167:GLN:HB3	1:A:171:LYS:NZ	2.15	0.60
1:D:16:VAL:HG12	1:D:17:SER:N	2.16	0.60
1:A:12:ARG:NH1	3:A:304:HOH:O	1.90	0.60
1:D:10:ASP:HB3	1:C:48:ASN:ND2	2.16	0.60
1:D:124:VAL:HG11	1:D:136:TRP:HZ2	1.67	0.60
2:E:24:U:C5	2:E:25:U:C5	2.89	0.60
2:E:25:U:C2	2:E:26:U:O2	2.54	0.60
1:A:44:ILE:HG13	1:A:45:PHE:N	2.17	0.60
1:A:15:ALA:O	1:A:16:VAL:HG23	2.02	0.60
2:E:22:U:N3	3:E:102:HOH:O	2.02	0.60
1:C:89:ALA:N	3:C:304:HOH:O	1.96	0.60
2:E:34:U:O2	3:E:109:HOH:O	2.14	0.60
1:D:124:VAL:CG1	1:D:136:TRP:HZ2	2.15	0.59
1:D:155:LYS:HE2	1:D:187:TYR:HA	1.84	0.59
1:D:135:LYS:C	3:D:307:HOH:O	2.40	0.59
2:E:44:U:HO2'	2:E:45:U:P	2.25	0.59
1:D:80:ASN:OD1	1:D:81:PRO:HD2	2.02	0.59
1:D:213:LEU:HD22	1:D:215:TRP:CE3	2.36	0.59
1:A:12:ARG:CB	1:D:44:ILE:CG2	2.75	0.59
1:C:196:MET:HE2	1:B:226:ASN:HD22	1.68	0.59
1:D:160:TYR:HE1	3:D:303:HOH:O	1.82	0.59
1:D:217:LYS:C	1:D:219:GLY:HA2	2.22	0.59
1:A:18:SER:OG	2:E:45:U:OP2	2.20	0.59
1:C:132:LYS:HD2	1:C:215:TRP:CE2	2.38	0.59
1:D:43:ARG:HD3	1:D:124:VAL:CA	2.27	0.59
1:C:196:MET:HG3	1:C:196:MET:O	2.02	0.58
1:B:84:ARG:NE	2:E:15:U:O2'	2.29	0.58
1:D:43:ARG:CG	1:D:123:LYS:O	2.47	0.58
2:E:25:U:C5	3:E:104:HOH:O	2.56	0.58
2:E:25:U:C2	2:E:26:U:C2	2.91	0.58
1:C:96:HIS:NE2	1:C:151:GLU:OE2	2.32	0.58
1:B:217:LYS:CG	1:B:218:ALA:N	2.66	0.57
1:A:96:HIS:NE2	1:A:151:GLU:OE2	2.28	0.57
1:D:12:ARG:NH1	1:D:14:ALA:CA	2.62	0.57
2:E:44:U:O2	2:E:44:U:H5"	2.03	0.57
1:D:141:ALA:HB1	1:D:157:PHE:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:THR:HG23	1:A:194:ASP:H	1.68	0.57
1:B:210:VAL:O	1:B:213:LEU:HB2	2.05	0.57
1:A:56:LEU:HB2	1:A:77:ASN:OD1	2.05	0.56
1:B:208:LYS:O	1:B:212:LYS:HG2	2.05	0.56
1:A:12:ARG:HD2	1:D:44:ILE:HG23	1.86	0.56
1:A:14:ALA:O	1:A:15:ALA:HB2	2.05	0.56
1:D:135:LYS:HB2	3:D:307:HOH:O	2.04	0.56
1:D:12:ARG:CB	1:C:44:ILE:CG1	2.66	0.56
1:A:49:HIS:CD2	1:A:95:LEU:HD21	2.41	0.56
1:A:16:VAL:HG12	1:A:16:VAL:O	2.05	0.56
1:A:186:ARG:HG2	2:E:1:U:C2	2.41	0.56
1:C:16:VAL:HG12	1:C:17:SER:N	2.21	0.56
1:D:135:LYS:CA	3:D:307:HOH:O	2.53	0.56
1:D:124:VAL:HG11	1:D:136:TRP:CZ2	2.41	0.55
1:C:82:ARG:NH1	1:B:54:ASP:HB3	2.22	0.55
1:A:88:VAL:HG21	2:E:3:U:H5'	1.89	0.55
1:C:220:PHE:CD1	1:C:220:PHE:N	2.73	0.55
3:A:304:HOH:O	1:D:43:ARG:CB	2.51	0.55
1:D:160:TYR:HE1	1:D:206:ALA:HA	1.72	0.55
1:B:109:GLU:HG3	1:B:116:GLU:HB3	1.89	0.54
1:D:227:PHE:O	1:D:230:LYS:HG3	2.06	0.54
1:D:12:ARG:NH2	1:C:43:ARG:CD	2.70	0.54
1:D:135:LYS:O	3:D:307:HOH:O	2.18	0.54
1:A:40:ASP:O	1:A:44:ILE:HG23	2.06	0.54
1:D:213:LEU:HG	1:D:214:PRO:HD2	1.89	0.54
1:D:43:ARG:HD3	1:D:124:VAL:CG2	2.33	0.54
2:E:36:U:H2'	2:E:37:U:H5'	1.89	0.54
1:C:131:ALA:CA	1:C:218:ALA:HB2	2.38	0.54
2:E:33:U:O2'	2:E:35:U:O2	2.15	0.54
1:A:11:ASP:OD1	1:A:12:ARG:N	2.37	0.54
1:B:83:ASN:HD22	1:B:86:ASN:HD21	1.55	0.54
1:D:125:VAL:CA	1:D:143:TYR:OH	2.53	0.54
1:D:186:ARG:CZ	2:E:34:U:C5	2.91	0.54
1:D:41:ASN:HA	1:D:44:ILE:CG1	2.38	0.53
1:D:65:ASP:OD1	1:D:66:LEU:N	2.41	0.53
1:A:222:ALA:HA	1:A:223:ALA:C	2.27	0.53
1:C:222:ALA:HB1	1:C:226:ASN:HD22	1.73	0.53
1:D:57:LYS:HZ1	1:D:81:PRO:HD3	1.73	0.53
1:B:88:VAL:HG21	2:E:14:U:H4'	1.90	0.53
1:A:57:LYS:HD2	1:A:81:PRO:HD3	1.89	0.53
1:A:76:VAL:HG11	1:A:88:VAL:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:25:U:O2	2:E:26:U:C2	2.62	0.53
1:D:21:ASN:HD22	2:E:34:U:H3	1.57	0.53
1:B:43:ARG:HG3	1:B:124:VAL:HA	1.91	0.53
1:C:155:LYS:N	3:C:307:HOH:O	1.94	0.53
1:D:119:GLU:O	1:D:123:LYS:HG2	2.08	0.53
1:D:12:ARG:HB2	1:C:44:ILE:CD1	2.38	0.52
1:D:73:VAL:HG12	1:D:75:VAL:HG12	1.92	0.52
2:E:24:U:C4	3:E:104:HOH:O	2.49	0.52
1:A:110:ILE:HG23	1:A:117:GLU:HG3	1.91	0.52
1:B:216:ALA:N	1:B:217:LYS:HA	2.23	0.52
2:E:25:U:C6	3:E:104:HOH:O	2.63	0.52
2:E:25:U:N3	2:E:26:U:N3	2.58	0.52
1:B:45:PHE:HA	1:B:68:PHE:CD2	2.45	0.52
1:C:227:PHE:CB	3:C:305:HOH:O	2.56	0.52
1:C:233:ILE:O	3:C:303:HOH:O	2.19	0.52
1:A:56:LEU:HD12	1:A:57:LYS:N	2.24	0.52
1:A:203:ILE:O	1:A:207:VAL:HG23	2.09	0.52
1:D:138:ASP:CG	3:D:307:HOH:O	2.46	0.52
1:D:70:THR:HG23	3:D:309:HOH:O	2.00	0.52
1:A:20:PHE:CD2	2:E:1:U:H5"	2.42	0.52
1:A:52:ALA:O	1:A:56:LEU:HG	2.09	0.51
1:D:159:PHE:CE2	1:D:199:GLU:HG2	2.45	0.51
2:E:24:U:C5	2:E:25:U:H5	2.28	0.51
1:D:124:VAL:O	1:D:136:TRP:NE1	2.40	0.51
1:A:59:SER:O	1:A:80:ASN:ND2	2.44	0.51
1:D:199:GLU:HA	3:D:310:HOH:O	2.10	0.51
1:C:227:PHE:HB2	3:C:305:HOH:O	2.11	0.51
1:B:104:LYS:NZ	1:B:108:ASP:OD1	2.43	0.51
1:C:131:ALA:HB1	1:C:218:ALA:HB2	1.92	0.51
1:C:65:ASP:OD1	1:C:66:LEU:N	2.43	0.51
1:D:9:TYR:HD1	1:D:9:TYR:H	1.57	0.51
1:A:155:LYS:HA	1:A:187:TYR:CE1	2.46	0.51
1:B:86:ASN:N	3:B:306:HOH:O	2.44	0.51
1:D:70:THR:HG21	3:D:309:HOH:O	1.98	0.51
1:D:177:THR:HG22	1:C:217:LYS:HD3	1.92	0.50
1:C:222:ALA:CB	1:C:226:ASN:ND2	2.73	0.50
1:D:83:ASN:OD1	1:D:86:ASN:ND2	2.45	0.50
1:A:199:GLU:O	1:A:203:ILE:HG12	2.12	0.50
1:B:204:GLN:O	1:B:208:LYS:HG2	2.12	0.50
1:B:60:PRO:CA	1:B:80:ASN:HD22	2.16	0.50
1:D:218:ALA:N	1:D:219:GLY:CA	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ASP:N	1:B:10:ASP:OD1	2.45	0.50
1:C:66:LEU:HD21	1:C:75:VAL:HG11	1.93	0.50
1:C:130:GLU:HG3	2:E:31:U:H1'	1.94	0.50
1:C:10:ASP:OD1	1:B:48:ASN:CB	2.58	0.49
1:A:20:PHE:CD2	2:E:1:U:C5'	2.79	0.49
1:A:104:LYS:NZ	1:A:156:ASP:OD2	2.45	0.49
1:A:186:ARG:CD	1:A:191:THR:HA	2.41	0.49
1:B:15:ALA:O	2:E:10:U:O2	2.30	0.49
1:D:73:VAL:HG11	1:D:98:LEU:HD22	1.94	0.49
2:E:25:U:O2	2:E:26:U:O2	2.30	0.49
1:D:11:ASP:O	1:D:11:ASP:OD1	2.30	0.49
1:A:131:ALA:HB2	2:E:8:U:H4'	1.93	0.49
1:A:36:ASN:OD1	1:A:36:ASN:N	2.45	0.49
1:A:132:LYS:HD2	1:A:215:TRP:CE2	2.48	0.49
1:C:192:ALA:HA	1:C:195:TRP:NE1	2.27	0.49
1:B:226:ASN:N	1:B:226:ASN:ND2	2.60	0.49
1:D:124:VAL:HG13	1:D:136:TRP:NE1	2.27	0.49
1:D:9:TYR:CD1	1:D:9:TYR:N	2.73	0.49
1:A:221:THR:O	1:A:224:ALA:N	2.45	0.49
1:B:132:LYS:HZ3	1:B:218:ALA:HB2	1.77	0.49
1:A:19:THR:HB	1:A:90:ASP:OD2	2.13	0.49
1:C:40:ASP:O	1:C:44:ILE:HD12	2.13	0.49
1:D:43:ARG:HE	1:D:43:ARG:HA	1.72	0.49
1:D:26:TYR:O	1:D:30:ILE:HG12	2.14	0.48
1:A:18:SER:OG	1:A:18:SER:O	2.29	0.48
1:A:18:SER:HB2	2:E:44:U:O2'	2.13	0.48
1:D:221:THR:O	1:D:224:ALA:N	2.36	0.48
2:E:44:U:O2'	2:E:45:U:OP2	2.24	0.48
1:A:89:ALA:HB3	1:A:92:ALA:HB2	1.94	0.48
1:B:49:HIS:N	3:B:303:HOH:O	2.46	0.48
1:A:20:PHE:CE1	1:A:97:ARG:CZ	2.95	0.48
1:D:213:LEU:HD23	1:D:215:TRP:H	1.77	0.48
1:A:167:GLN:NE2	1:A:207:VAL:HG13	2.27	0.48
1:C:221:THR:HG22	1:C:222:ALA:N	2.28	0.48
1:C:224:ALA:HA	3:C:305:HOH:O	2.13	0.48
1:D:104:LYS:HE2	1:D:156:ASP:OD2	2.14	0.48
1:A:41:ASN:OD1	1:A:70:THR:OG1	2.23	0.48
1:A:42:VAL:HG11	1:A:106:CYS:SG	2.53	0.48
1:D:19:THR:OG1	1:D:90:ASP:OD2	2.31	0.48
1:A:130:GLU:HG3	2:E:9:U:H1'	1.96	0.48
1:C:196:MET:CE	1:B:226:ASN:ND2	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ILE:HD11	1:A:68:PHE:HA	1.96	0.47
1:D:12:ARG:HH21	1:C:43:ARG:HD3	1.78	0.47
1:D:126:ILE:O	1:D:130:GLU:HG2	2.14	0.47
1:D:226:ASN:O	1:D:230:LYS:HE3	2.14	0.47
1:B:126:ILE:O	1:B:130:GLU:HG2	2.14	0.47
1:B:226:ASN:HB2	1:B:228:LEU:HG	1.96	0.47
1:D:192:ALA:HA	1:D:195:TRP:NE1	2.29	0.47
2:E:26:U:O4'	2:E:26:U:O2	2.29	0.47
1:B:126:ILE:HD11	1:B:144:LEU:HD23	1.97	0.47
1:B:228:LEU:HD21	1:B:231:PHE:CD2	2.50	0.47
1:D:160:TYR:OH	3:D:303:HOH:O	2.19	0.47
1:A:181:LYS:C	1:A:183:LEU:N	2.68	0.47
1:B:228:LEU:HD22	1:B:230:LYS:C	2.34	0.47
1:D:114:GLN:HA	1:D:117:GLU:HB3	1.97	0.47
1:D:217:LYS:HZ3	1:D:225:LYS:HE2	1.78	0.47
1:D:227:PHE:CE2	1:D:231:PHE:HE2	2.32	0.47
1:D:39:ALA:CB	1:D:123:LYS:HD2	2.44	0.47
1:A:56:LEU:HD11	1:A:79:HIS:CG	2.50	0.47
1:A:205:SER:O	1:A:209:VAL:HG23	2.15	0.47
2:E:14:U:C4	3:E:103:HOH:O	2.62	0.47
1:C:222:ALA:HA	1:C:225:LYS:H	1.79	0.47
1:D:8:ILE:CD1	1:C:55:SER:HB3	2.35	0.47
1:D:19:THR:O	1:D:19:THR:OG1	2.29	0.47
1:D:66:LEU:HD23	1:D:67:GLN:N	2.30	0.47
1:B:192:ALA:HA	1:B:195:TRP:NE1	2.30	0.47
1:D:135:LYS:N	3:D:307:HOH:O	2.43	0.47
1:D:15:ALA:C	1:D:16:VAL:CG2	2.76	0.46
1:C:92:ALA:CB	3:C:306:HOH:O	2.58	0.46
1:A:127:PRO:CB	2:E:8:U:H1'	2.44	0.46
1:D:12:ARG:NH2	1:C:43:ARG:HD3	2.31	0.46
1:D:155:LYS:CE	1:D:188:GLY:H	2.28	0.46
1:D:221:THR:O	1:D:223:ALA:N	2.49	0.46
1:C:41:ASN:HD21	1:C:70:THR:HG1	1.56	0.46
1:D:124:VAL:CG1	1:D:136:TRP:HE1	2.28	0.46
1:C:222:ALA:HB2	1:C:225:LYS:HB3	1.98	0.46
1:B:130:GLU:OE2	1:B:143:TYR:OH	2.19	0.46
1:B:228:LEU:H	1:B:228:LEU:CD1	2.04	0.46
1:D:50:LYS:O	1:D:53:LYS:HB3	2.16	0.46
1:A:132:LYS:HD2	1:A:215:TRP:CD2	2.50	0.46
1:C:65:ASP:CG	1:C:72:ARG:HH21	2.16	0.46
1:A:179:MET:O	1:A:180:ARG:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ALA:HA	1:A:195:TRP:NE1	2.31	0.46
1:A:60:PRO:HA	1:A:82:ARG:HH21	1.81	0.46
1:C:8:ILE:HG22	1:C:9:TYR:H	1.80	0.46
1:A:218:ALA:N	1:A:219:GLY:HA3	2.31	0.45
1:C:11:ASP:HA	1:B:44:ILE:HD13	1.97	0.45
1:A:18:SER:HB2	2:E:44:U:HO2'	1.81	0.45
1:B:227:PHE:O	1:B:227:PHE:CG	2.69	0.45
1:D:45:PHE:O	1:D:48:ASN:N	2.49	0.45
1:B:13:PRO:O	1:B:13:PRO:HD2	2.17	0.45
1:B:39:ALA:O	1:B:43:ARG:HB2	2.16	0.45
1:C:175:ASP:O	1:C:178:PHE:HD2	1.98	0.45
1:D:180:ARG:HD3	1:C:219:GLY:CA	2.46	0.45
1:C:127:PRO:HB2	2:E:30:U:H1'	1.98	0.45
2:E:4:U:H2'	2:E:5:U:C6	2.51	0.45
2:E:38:U:H5"	2:E:39:U:OP2	2.16	0.45
1:A:20:PHE:O	2:E:1:U:H5"	2.17	0.45
1:C:179:MET:HB3	1:C:183:LEU:HD12	1.98	0.45
1:C:220:PHE:HB2	1:C:224:ALA:CB	2.47	0.45
1:D:42:VAL:HG21	1:D:105:TRP:CE3	2.52	0.45
2:E:1:U:O2	2:E:1:U:H2'	2.16	0.45
1:A:90:ASP:HB3	3:A:314:HOH:O	2.16	0.45
1:B:225:LYS:C	1:B:226:ASN:HD22	2.20	0.45
1:D:167:GLN:HA	1:D:170:VAL:HG12	1.98	0.45
1:C:162:LEU:HD23	1:C:203:ILE:HD12	1.99	0.45
1:C:218:ALA:O	2:E:32:U:OP1	2.35	0.45
1:D:186:ARG:NH1	2:E:34:U:C4	2.85	0.45
1:B:213:LEU:HG	1:B:214:PRO:HD2	1.98	0.45
1:B:89:ALA:HB3	1:B:92:ALA:HB2	1.99	0.45
1:C:179:MET:CB	1:C:183:LEU:HD12	2.46	0.45
1:B:12:ARG:HH11	1:B:14:ALA:HB2	1.81	0.45
1:C:160:TYR:N	1:C:161:PRO:HD2	2.32	0.45
1:D:124:VAL:CG1	1:D:136:TRP:NE1	2.80	0.45
1:D:159:PHE:HE2	1:D:199:GLU:HG2	1.81	0.45
1:C:92:ALA:HB1	3:C:306:HOH:O	2.15	0.44
1:D:52:ALA:HA	1:D:55:SER:HB2	1.99	0.44
1:A:166:ILE:O	1:A:170:VAL:HG23	2.17	0.44
1:B:227:PHE:O	1:B:227:PHE:CD2	2.70	0.44
1:C:220:PHE:H	1:C:220:PHE:HD1	1.66	0.44
1:A:84:ARG:HE	2:E:4:U:H1'	1.82	0.44
1:A:190:LYS:HZ3	1:A:198:SER:HB2	1.82	0.44
1:C:6:ASP:OD1	1:B:61:LYS:NZ	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:33:U:C2	2:E:35:U:O2	2.70	0.44
1:C:66:LEU:HD11	1:C:75:VAL:HB	2.00	0.44
1:D:177:THR:HG22	1:C:217:LYS:CD	2.48	0.44
1:B:219:GLY:O	1:B:220:PHE:HD1	2.01	0.44
1:D:155:LYS:N	1:D:155:LYS:HE3	2.28	0.44
1:C:127:PRO:CB	2:E:30:U:H1'	2.48	0.44
1:C:89:ALA:HB3	1:C:92:ALA:HB2	2.00	0.44
1:A:221:THR:O	1:A:224:ALA:HB3	2.18	0.43
1:A:44:ILE:CD1	1:B:10:ASP:O	2.66	0.43
1:A:61:LYS:HD2	1:A:61:LYS:HA	1.84	0.43
1:D:47:LEU:HA	1:D:47:LEU:HD23	1.84	0.43
1:D:9:TYR:CD1	1:D:9:TYR:O	2.70	0.43
2:E:13:U:C4	2:E:14:U:C4	3.06	0.43
1:A:56:LEU:CD1	1:A:79:HIS:HB2	2.48	0.43
1:C:181:LYS:O	1:C:185:GLN:HG2	2.17	0.43
1:A:230:LYS:HD2	1:A:230:LYS:HA	1.32	0.43
1:B:155:LYS:HA	1:B:187:TYR:CE1	2.53	0.43
1:B:80:ASN:OD1	1:B:81:PRO:HD2	2.19	0.43
1:C:179:MET:HA	1:C:182:VAL:HG13	2.01	0.43
1:C:186:ARG:CD	1:C:191:THR:HA	2.49	0.43
1:A:225:LYS:NZ	1:A:225:LYS:CB	2.73	0.43
1:D:40:ASP:O	1:D:44:ILE:HG12	2.18	0.43
1:C:183:LEU:HD13	1:B:220:PHE:HZ	1.84	0.43
1:D:110:ILE:HD13	1:D:117:GLU:HA	2.00	0.43
1:D:12:ARG:HA	1:D:13:PRO:HD2	1.91	0.43
1:D:134:CYS:HB2	1:D:213:LEU:HD11	2.00	0.43
1:D:184:LYS:HD2	2:E:35:U:OP2	2.19	0.43
1:A:192:ALA:HA	1:A:195:TRP:CE2	2.54	0.43
1:B:180:ARG:NH2	3:E:103:HOH:O	2.51	0.43
1:B:189:THR:N	3:B:304:HOH:O	1.99	0.43
1:A:12:ARG:HD2	1:D:44:ILE:CG2	2.48	0.43
1:A:171:LYS:HE2	1:A:215:TRP:CE2	2.54	0.43
1:D:160:TYR:CZ	3:D:303:HOH:O	2.69	0.43
2:E:24:U:C2'	2:E:25:U:H5'	2.49	0.43
1:B:158:GLU:O	1:B:159:PHE:HB2	2.18	0.42
1:D:21:ASN:OD1	1:D:23:GLU:HB2	2.19	0.42
2:E:33:U:C2	2:E:35:U:C2	3.07	0.42
1:C:232:ASN:O	1:C:233:ILE:C	2.54	0.42
1:B:228:LEU:HD22	1:B:230:LYS:O	2.19	0.42
1:D:16:VAL:CG1	1:D:17:SER:N	2.81	0.42
1:A:194:ASP:O	1:A:198:SER:OG	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:VAL:CG1	1:D:136:TRP:CE2	3.03	0.42
1:A:59:SER:HA	1:A:60:PRO:HD3	1.93	0.42
1:A:6:ASP:O	1:D:65:ASP:HB3	2.20	0.42
1:B:225:LYS:C	1:B:226:ASN:ND2	2.73	0.42
1:C:18:SER:HB2	2:E:22:U:H1'	2.01	0.42
1:B:56:LEU:HD11	1:B:64:VAL:HG21	2.01	0.42
1:C:221:THR:CG2	1:C:222:ALA:N	2.82	0.42
1:D:41:ASN:HA	1:D:44:ILE:HG12	2.02	0.42
1:C:196:MET:CE	1:B:226:ASN:HD22	2.31	0.42
1:B:217:LYS:CG	1:B:218:ALA:H	2.32	0.42
1:D:36:ASN:O	1:D:41:ASN:ND2	2.53	0.42
1:D:60:PRO:HA	1:D:80:ASN:ND2	2.34	0.42
1:C:171:LYS:HE2	1:C:215:TRP:CD2	2.55	0.42
1:C:94:THR:HG23	1:C:97:ARG:H	1.84	0.42
1:D:94:THR:HB	3:E:101:HOH:O	2.20	0.41
1:C:196:MET:HE1	1:B:226:ASN:ND2	2.36	0.41
1:D:131:ALA:HB1	1:D:218:ALA:HA	2.02	0.41
1:B:129:ALA:HB2	1:B:146:PHE:HB2	2.03	0.41
1:B:200:VAL:N	3:B:308:HOH:O	2.53	0.41
1:D:115:ILE:H	1:D:115:ILE:HD12	1.84	0.41
1:D:130:GLU:O	1:D:133:GLY:N	2.48	0.41
1:D:176:ILE:HA	1:D:176:ILE:HD12	1.92	0.41
1:A:213:LEU:HA	1:A:213:LEU:HD12	1.94	0.41
2:E:18:U:N3	3:E:106:HOH:O	2.34	0.41
2:E:1:U:O5'	2:E:2:U:H5'	2.20	0.41
2:E:37:U:O2'	2:E:38:U:O4'	2.35	0.41
2:E:43:U:O5'	2:E:43:U:H6	2.04	0.41
1:A:65:ASP:O	1:B:7:PHE:HB2	2.20	0.41
1:B:231:PHE:HD1	1:B:232:ASN:N	2.19	0.41
1:C:34:GLY:HA2	1:C:37:ILE:HD12	2.02	0.41
1:D:180:ARG:HD3	1:C:219:GLY:HA3	2.02	0.41
1:D:213:LEU:HD23	1:D:215:TRP:N	2.36	0.41
1:A:126:ILE:HD11	1:A:144:LEU:HD23	2.03	0.41
1:A:43:ARG:HH11	1:B:12:ARG:HG3	1.83	0.41
1:B:225:LYS:HG3	1:B:225:LYS:O	2.20	0.41
1:D:203:ILE:O	1:D:207:VAL:HG23	2.21	0.41
2:E:24:U:C2	2:E:25:U:C6	3.09	0.41
1:A:208:LYS:HA	1:A:208:LYS:HD3	1.89	0.41
1:C:222:ALA:CB	1:C:226:ASN:HD22	2.34	0.41
1:D:192:ALA:N	3:D:305:HOH:O	2.53	0.41
1:A:8:ILE:HD11	1:D:61:LYS:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:SER:O	2:E:44:U:H6	2.03	0.41
1:D:128:LEU:HD12	1:D:148:PRO:HD3	2.03	0.41
1:B:203:ILE:O	1:B:207:VAL:HG23	2.21	0.40
1:A:80:ASN:HD21	1:A:82:ARG:NH2	2.19	0.40
1:B:83:ASN:ND2	1:B:86:ASN:HD21	2.19	0.40
1:C:80:ASN:CG	1:C:81:PRO:HD2	2.42	0.40
1:D:39:ALA:HB1	1:D:123:LYS:HD2	2.03	0.40
1:D:42:VAL:HG21	1:D:105:TRP:CZ3	2.56	0.40
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.86	0.40
1:B:42:VAL:HG11	1:B:106:CYS:SG	2.62	0.40
1:C:43:ARG:HD2	1:C:123:LYS:O	2.21	0.40
1:D:80:ASN:OD1	1:D:82:ARG:CZ	2.70	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
1	A	226/235 (96%)	210 (93%)	10 (4%)	6 (3%)	5 15
1	B	225/235 (96%)	217 (96%)	7 (3%)	1 (0%)	34 64
1	C	226/235 (96%)	216 (96%)	10 (4%)	0	100 100
1	D	225/235 (96%)	218 (97%)	7 (3%)	0	100 100
All	All	902/940 (96%)	861 (96%)	34 (4%)	7 (1%)	19 47

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	180	ARG
1	A	181	LYS

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Mol	Chain	Res	Type
1	B	13	PRO
1	A	20	PHE
1	A	19	THR
1	A	182	VAL

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	189/195 (97%)	175 (93%)	14 (7%)	13 34
1	B	188/195 (96%)	167 (89%)	21 (11%)	6 16
1	C	189/195 (97%)	175 (93%)	14 (7%)	13 34
1	D	188/195 (96%)	171 (91%)	17 (9%)	9 26
All	All	754/780 (97%)	688 (91%)	66 (9%)	10 27

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASP
1	A	18	SER
1	A	19	THR
1	A	23	GLU
1	A	36	ASN
1	A	44	ILE
1	A	73	VAL
1	A	82	ARG
1	A	154	LEU
1	A	180	ARG
1	A	182	VAL
1	A	198	SER
1	A	230	LYS
1	A	231	PHE
1	D	6	ASP
1	D	8	ILE
1	D	9	TYR

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Mol	Chain	Res	Type
1	D	12	ARG
1	D	19	THR
1	D	40	ASP
1	D	44	ILE
1	D	57	LYS
1	D	70	THR
1	D	82	ARG
1	D	85	ASP
1	D	119	GLU
1	D	123	LYS
1	D	124	VAL
1	D	125	VAL
1	D	155	LYS
1	D	230	LYS
1	C	9	TYR
1	C	12	ARG
1	C	61	LYS
1	C	66	LEU
1	C	119	GLU
1	C	154	LEU
1	C	176	ILE
1	C	179	MET
1	C	180	ARG
1	C	183	LEU
1	C	196	MET
1	C	212	LYS
1	C	213	LEU
1	C	220	PHE
1	B	7	PHE
1	B	10	ASP
1	B	11	ASP
1	B	16	VAL
1	B	51	LYS
1	B	73	VAL
1	B	75	VAL
1	B	115	ILE
1	B	159	PHE
1	B	176	ILE
1	B	201	THR
1	B	213	LEU
1	B	220	PHE
1	B	221	THR

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Mol	Chain	Res	Type
1	B	225	LYS
1	B	226	ASN
1	B	227	PHE
1	B	228	LEU
1	B	230	LYS
1	B	231	PHE
1	B	232	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	49	HIS
1	A	79	HIS
1	C	48	ASN
1	C	226	ASN
1	B	86	ASN
1	B	226	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	43/45 (95%)	15 (34%)	0

All (15) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	2	U
2	E	9	U
2	E	11	U
2	E	12	U
2	E	22	U
2	E	23	U
2	E	24	U
2	E	26	U
2	E	31	U
2	E	34	U
2	E	35	U
2	E	38	U
2	E	42	U

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Mol	Chain	Res	Type
2	E	43	U
2	E	44	U

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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^{th} 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	228/235 (97%)	0.37	13 (5%) 23 18	41, 77, 134, 171	0
1	B	227/235 (96%)	0.15	11 (4%) 30 24	33, 65, 119, 160	0
1	C	228/235 (97%)	0.27	13 (5%) 23 18	51, 81, 119, 162	0
1	D	227/235 (96%)	0.77	38 (16%) 1 1	56, 93, 144, 174	0
2	E	45/45 (100%)	-0.63	0 100 100	68, 92, 109, 116	0
All	All	955/985 (96%)	0.34	75 (7%) 12 9	33, 81, 136, 174	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	219	GLY	8.9
1	A	218	ALA	8.5
1	B	219	GLY	7.5
1	D	60	PRO	7.3
1	B	216	ALA	6.4
1	C	9	TYR	6.4
1	B	232	ASN	6.1
1	A	6	ASP	5.8
1	A	9	TYR	5.4
1	A	7	PHE	5.0
1	D	9	TYR	4.9
1	A	64	VAL	4.7
1	D	56	LEU	4.5
1	D	120	VAL	4.2
1	C	219	GLY	4.1
1	C	218	ALA	4.0
1	D	95	LEU	4.0
1	C	197	ILE	3.9
1	D	59	SER	3.8
1	B	9	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	82	ARG	3.6
1	B	218	ALA	3.4
1	D	68	PHE	3.4
1	D	142	LEU	3.3
1	D	125	VAL	3.3
1	D	124	VAL	3.2
1	D	44	ILE	3.2
1	D	72	ARG	3.2
1	D	61	LYS	3.2
1	D	7	PHE	3.0
1	D	66	LEU	2.9
1	B	227	PHE	2.8
1	D	110	ILE	2.8
1	D	62	VAL	2.8
1	D	16	VAL	2.8
1	D	53	LYS	2.8
1	D	69	GLY	2.7
1	A	17	SER	2.7
1	D	45	PHE	2.7
1	D	71	LEU	2.7
1	C	201	THR	2.7
1	B	15	ALA	2.7
1	C	6	ASP	2.6
1	D	47	LEU	2.6
1	C	212	LYS	2.6
1	D	122	SER	2.6
1	B	220	PHE	2.5
1	C	82	ARG	2.5
1	D	63	GLU	2.4
1	C	186	ARG	2.4
1	B	217	LYS	2.3
1	D	55	SER	2.3
1	A	78	ASN	2.3
1	D	42	VAL	2.3
1	A	13	PRO	2.3
1	D	73	VAL	2.3
1	B	12	ARG	2.3
1	A	59	SER	2.3
1	A	69	GLY	2.2
1	D	170	VAL	2.2
1	D	17	SER	2.2
1	D	76	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	102	LEU	2.2
1	D	84	ARG	2.2
1	D	229	ALA	2.1
1	C	184	LYS	2.1
1	D	114	GLN	2.1
1	D	226	ASN	2.1
1	C	193	ASP	2.1
1	C	162	LEU	2.1
1	B	60	PRO	2.1
1	A	8	ILE	2.0
1	C	187	TYR	2.0
1	A	87	PRO	2.0
1	D	216	ALA	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.