W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 02:00 PM EDT

PDB ID	:	1A9N
Title	:	CRYSTAL STRUCTURE OF THE SPLICEOSOMAL U2B"-U2A' PROTEIN COMPLEX BOUND TO A FRAGMENT OF U2 SMALL NUCLEAR RNA
Authors	:	Price, S.R.; Evans, P.R.; Nagai, K.
Deposited on	:	1998-04-08
Resolution	:	2.38 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

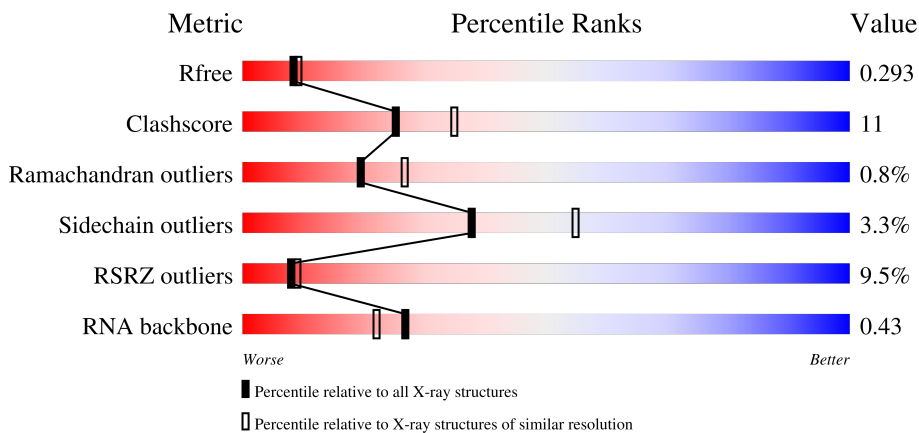|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.38 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.
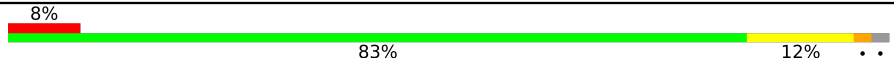
Metric	Percentile Ranks	Value
Rfree		0.293
Clashscore		11
Ramachandran outliers		0.8%
Sidechain outliers		3.3%
RSRZ outliers		9.5%
RNA backbone		0.43

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)
RNA backbone	3102	1017 (2.76-2.00)

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 of 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	Q	24	25% 38% 17% 21%
1	R	24	4% / 17% 25% 33% 25%
2	A	176	5% / 64% 24% ·· 8%
2	C	176	3% / 69% 27% ··

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	B	96	8% 83% 12%
3	D	96	32% 73% 24%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 5188 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 (5'-R(*CP*CP*UP*GP*GP*UP*AP*UP*UP*GP* CP*AP*GP*UP*AP*CP*CP*UP*CP*CP*AP*GP* GP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	24	Total	C	N	O	P	0	0	0
			503	226	85	169	23			
1	R	24	Total	C	N	O	P	0	0	0
			503	226	85	169	23			

- Molecule 2 is a protein called U2A'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	162	Total	C	N	O	S	0	0	0
			1292	825	222	242	3			
2	C	174	Total	C	N	O	S	0	0	0
			1373	874	239	257	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	ASP	CYS	engineered mutation	UNP P09661
A	119	CYS	SER	engineered mutation	UNP P09661
C	89	ASP	CYS	engineered mutation	UNP P09661
C	119	CYS	SER	engineered mutation	UNP P09661
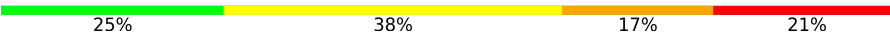
- Molecule 3 is a protein called SPLICEOSOMAL U2B".

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	94	Total	C	N	O	S	0	0	0
			761	488	135	133	5			
3	D	93	Total	C	N	O	S	0	0	0
			756	486	134	131	5			

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.
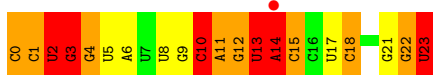
• Molecule 1: RNA (5'-R(*CP*CP*UP*GP*GP*UP*AP*UP*UP*GP*CP*AP*GP*UP*AP*CP *CP*UP*CP*CP*AP*GP* GP*U)-3')
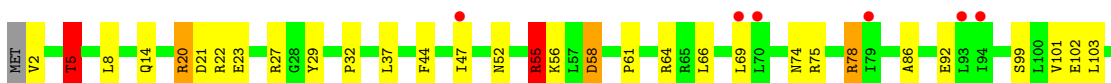
Chain Q:
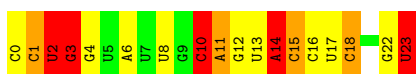
• Molecule 1: RNA (5'-R(*CP*CP*UP*GP*GP*UP*AP*UP*UP*GP*CP*AP*GP*UP*AP*CP *CP*UP*CP*CP*AP*GP* GP*U)-3')

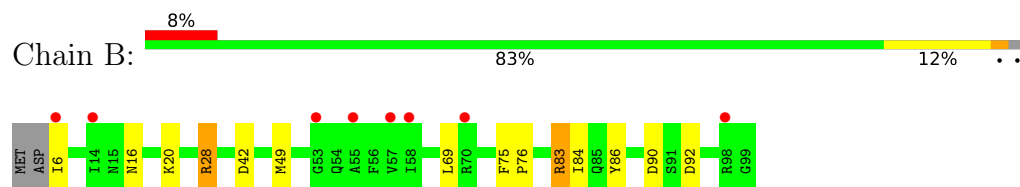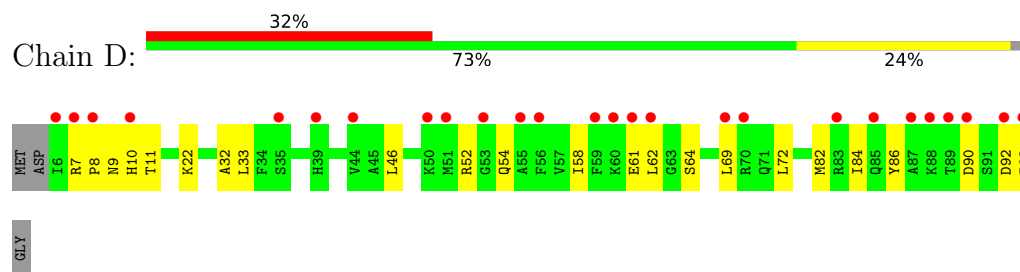Chain R:

• Molecule 2: U2A'

Chain A:

• Molecule 2: U2A'

Chain C:

• Molecule 3: SPLICEOSOMAL U2B"

Chain B:

• Molecule 3: SPLICEOSOMAL U2B"

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	98.37Å 128.24Å 66.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.38 25.39 – 2.39	Depositor EDS
% Data completeness (in resolution range)	95.8 (15.00-2.38) 94.8 (25.39-2.39)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.282 , 0.328 0.254 , 0.293	Depositor DCC
R_{free} test set	1650 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	45.8	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 41.8	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5188	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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 (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	Q	1.03	0/560	2.27	38/870 (4.4%)
1	R	1.03	0/560	2.39	45/870 (5.2%)
2	A	0.59	0/1309	1.64	18/1774 (1.0%)
2	C	0.56	0/1390	1.64	21/1882 (1.1%)
3	B	0.56	0/775	1.35	6/1035 (0.6%)
3	D	0.43	0/770	1.13	1/1030 (0.1%)
All	All	0.68	0/5364	1.74	129/7461 (1.7%)

There are no bond length outliers.

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	55	ARG	NE-CZ-NH1	-21.64	109.48	120.30
2	A	55	ARG	NE-CZ-NH1	15.05	127.82	120.30
2	A	55	ARG	CD-NE-CZ	13.80	142.92	123.60
2	C	27	ARG	NE-CZ-NH2	-13.73	113.43	120.30
2	C	55	ARG	NH1-CZ-NH2	12.97	133.66	119.40
1	Q	13	U	C5-C4-O4	11.87	133.02	125.90
2	A	55	ARG	NE-CZ-NH2	-11.52	114.54	120.30
2	A	75	ARG	NE-CZ-NH1	-11.28	114.66	120.30
1	R	15	C	P-O3'-C3'	10.43	132.22	119.70
1	Q	10	C	N1-C2-O2	-10.15	112.81	118.90
1	R	3	G	N1-C6-O6	-9.29	114.33	119.90
1	Q	8	U	N3-C2-O2	-8.88	115.98	122.20
3	B	83	ARG	CD-NE-CZ	8.87	136.02	123.60
3	B	28	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	R	10	C	P-O3'-C3'	8.75	130.19	119.70
1	R	23	U	C5-C6-N1	-8.56	118.42	122.70
1	Q	10	C	C5'-C4'-O4'	-8.33	99.10	109.10
1	R	23	U	C2-N3-C4	-8.31	122.01	127.00
1	Q	15	C	P-O3'-C3'	8.23	129.58	119.70
1	R	22	G	O4'-C1'-N9	-8.12	101.71	108.20
1	Q	12	G	O4'-C1'-N9	7.97	114.58	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	13	U	N3-C4-O4	-7.97	113.82	119.40
2	C	155	ARG	NE-CZ-NH2	7.65	124.12	120.30
2	A	107	ASP	CB-CG-OD1	7.61	125.15	118.30
2	C	132	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	Q	10	C	P-O3'-C3'	7.52	128.73	119.70
1	Q	10	C	N3-C2-O2	7.51	127.16	121.90
1	Q	13	U	N1-C2-O2	7.48	128.04	122.80
1	R	14	A	P-O5'-C5'	-7.43	109.02	120.90
2	C	65	ARG	CD-NE-CZ	7.41	133.97	123.60
2	A	27	ARG	NE-CZ-NH2	-7.38	116.61	120.30
2	C	27	ARG	NH1-CZ-NH2	7.28	127.41	119.40
1	R	4	G	C5-C6-O6	7.20	132.92	128.60
1	R	3	G	C5-C6-O6	7.17	132.90	128.60
2	A	20	ARG	CD-NE-CZ	7.11	133.55	123.60
1	Q	14	A	P-O5'-C5'	-7.09	109.55	120.90
1	Q	13	U	N3-C2-O2	-7.03	117.28	122.20
2	C	55	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	R	3	G	N9-C4-C5	6.87	108.15	105.40
1	R	23	U	N3-C4-O4	-6.77	114.66	119.40
2	A	23	GLU	OE1-CD-OE2	-6.77	115.18	123.30
1	Q	1	C	P-O3'-C3'	6.71	127.75	119.70
3	B	92	ASP	CB-CG-OD1	6.71	124.34	118.30
1	R	10	C	O4'-C1'-N1	6.65	113.52	108.20
1	Q	12	G	C8-N9-C4	-6.63	103.75	106.40
2	C	55	ARG	CG-CD-NE	-6.62	97.89	111.80
1	R	3	G	C8-N9-C4	-6.51	103.80	106.40
2	C	132	ARG	CD-NE-CZ	6.42	132.59	123.60
1	Q	3	G	C5-C6-O6	-6.42	124.75	128.60
1	R	2	U	O5'-C5'-C4'	-6.40	99.55	111.70
1	R	4	G	N3-C4-N9	-6.38	122.17	126.00
1	Q	0	C	N3-C4-C5	-6.35	119.36	121.90
1	R	23	U	C5-C4-O4	6.32	129.69	125.90
2	A	5	THR	N-CA-CB	-6.32	98.30	110.30
1	Q	3	G	N1-C6-O6	6.28	123.67	119.90
1	Q	12	G	N9-C4-C5	6.27	107.91	105.40
1	Q	8	U	N1-C2-O2	6.23	127.16	122.80
1	Q	11	A	O4'-C1'-N9	-6.23	103.22	108.20
2	C	21	ASP	CB-CG-OD1	6.18	123.87	118.30
1	R	5	U	O4'-C1'-N1	6.18	113.14	108.20
1	Q	12	G	N3-C4-C5	-6.10	125.55	128.60
1	R	6	A	OP1-P-OP2	-6.09	110.46	119.60
2	A	132	ARG	CD-NE-CZ	6.03	132.04	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	132	ARG	NH1-CZ-NH2	-6.01	112.78	119.40
1	R	23	U	C4-C5-C6	5.99	123.29	119.70
3	B	28	ARG	CD-NE-CZ	5.98	131.97	123.60
1	R	14	A	C1'-O4'-C4'	-5.97	105.12	109.90
2	A	21	ASP	CB-CG-OD1	5.96	123.67	118.30
1	R	8	U	P-O3'-C3'	5.96	126.85	119.70
2	C	131	TYR	CB-CG-CD1	5.93	124.56	121.00
1	R	4	G	P-O3'-C3'	5.89	126.77	119.70
1	R	3	G	O5'-C5'-C4'	-5.86	100.56	111.70
2	A	27	ARG	CB-CA-C	-5.85	98.69	110.40
1	Q	10	C	C5-C4-N4	-5.85	116.10	120.20
1	R	23	U	N1-C2-N3	5.84	118.40	114.90
1	Q	14	A	C5'-C4'-C3'	-5.82	106.69	116.00
1	Q	18	C	P-O3'-C3'	5.80	126.67	119.70
2	A	78	ARG	NE-CZ-NH2	-5.76	117.42	120.30
2	A	64	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	C	22	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	Q	2	U	P-O3'-C3'	-5.74	112.81	119.70
1	Q	13	U	O3'-P-O5'	-5.74	93.10	104.00
1	R	10	C	OP1-P-O3'	5.73	117.81	105.20
2	C	122	ARG	NE-CZ-NH2	-5.66	117.47	120.30
2	C	132	ARG	NE-CZ-NH2	5.65	123.13	120.30
1	R	9	G	N3-C2-N2	5.64	123.85	119.90
2	A	75	ARG	NH1-CZ-NH2	5.63	125.60	119.40
2	C	122	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	Q	23	U	C5-C6-N1	-5.62	119.89	122.70
3	D	92	ASP	CB-CG-OD1	5.62	123.36	118.30
1	R	23	U	O4'-C1'-N1	5.60	112.68	108.20
2	C	14	GLN	CA-CB-CG	5.57	125.66	113.40
2	A	58	ASP	N-CA-CB	-5.57	100.58	110.60
1	R	18	C	N3-C2-O2	5.56	125.79	121.90
1	R	4	G	C6-N1-C2	5.55	128.43	125.10
1	Q	12	G	C6-N1-C2	-5.50	121.80	125.10
1	R	13	U	N1-C1'-C2'	5.47	121.11	114.00
2	C	55	ARG	CD-NE-CZ	5.47	131.26	123.60
1	R	8	U	N3-C2-O2	-5.45	118.39	122.20
1	R	0	C	O4'-C1'-N1	-5.44	103.85	108.20
1	R	12	G	N1-C2-N2	-5.44	111.31	116.20
2	C	2	VAL	CA-C-O	5.41	131.47	120.10
1	R	12	G	C5-N7-C8	-5.39	101.61	104.30
1	Q	23	U	N1-C2-O2	-5.38	119.04	122.80
1	Q	2	U	OP2-P-O3'	5.37	117.01	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	21	G	C4'-C3'-C2'	-5.35	97.25	102.60
2	A	47	ILE	N-CA-CB	5.35	123.09	110.80
1	Q	16	C	N3-C4-C5	-5.34	119.76	121.90
1	R	0	C	C5-C6-N1	-5.33	118.34	121.00
3	B	42	ASP	CB-CG-OD2	-5.32	113.51	118.30
3	B	42	ASP	CB-CG-OD1	5.28	123.05	118.30
1	R	2	U	C5-C4-O4	5.28	129.07	125.90
1	R	11	A	P-O3'-C3'	5.27	126.03	119.70
1	R	10	C	C4'-C3'-C2'	-5.26	97.34	102.60
1	R	4	G	N3-C4-C5	5.19	131.19	128.60
1	R	12	G	O4'-C1'-N9	5.18	112.35	108.20
1	R	13	U	O4'-C1'-N1	-5.17	104.07	108.20
1	Q	6	A	C4'-C3'-C2'	-5.16	97.44	102.60
1	Q	2	U	C4'-C3'-C2'	5.16	107.76	102.60
1	Q	3	G	P-O5'-C5'	-5.15	112.66	120.90
1	R	1	C	P-O3'-C3'	5.14	125.87	119.70
1	Q	6	A	P-O5'-C5'	-5.13	112.69	120.90
1	Q	16	C	O4'-C1'-C2'	-5.12	100.68	105.80
1	R	8	U	OP1-P-OP2	-5.11	111.93	119.60
1	Q	22	G	OP1-P-OP2	-5.10	111.95	119.60
1	Q	8	U	C2-N3-C4	-5.07	123.96	127.00
1	R	5	U	OP1-P-OP2	-5.06	112.02	119.60
2	A	99	SER	N-CA-CB	-5.05	102.92	110.50
2	C	22	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	503	0	259	16	0
1	R	503	0	259	23	0
2	A	1292	0	1319	30	0
2	C	1373	0	1402	29	0
3	B	761	0	783	6	0

Continued on next page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	756	0	780	13	0
All	All	5188	0	4802	107	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 11.

All (107) 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:Q:2:U:H6	1:Q:2:U:H5"	1.10	1.14
1:R:14:A:H5"	1:R:14:A:H8	1.18	1.06
1:R:14:A:H5"	1:R:14:A:C8	1.94	1.01
1:R:2:U:H5"	1:R:2:U:H6	1.22	1.00
1:Q:14:A:C8	1:Q:14:A:H5"	1.98	0.99
1:R:2:U:H6	1:R:2:U:C5'	1.74	0.98
1:R:14:A:C8	1:R:14:A:C5'	2.50	0.95
1:Q:2:U:H5"	1:Q:2:U:C6	2.02	0.95
2:A:78:ARG:HH21	2:C:78:ARG:HE	1.12	0.93
1:Q:14:A:H5"	1:Q:14:A:H8	1.37	0.90
1:R:2:U:C5'	1:R:2:U:C6	2.58	0.86
1:Q:2:U:H6	1:Q:2:U:C5'	1.88	0.86
2:A:55:ARG:HD3	2:C:99:SER:HA	1.59	0.84
1:Q:23:U:H6	1:Q:23:U:H5"	1.45	0.81
3:D:69:LEU:HD12	3:D:84:ILE:HG22	1.68	0.75
2:A:78:ARG:NH2	2:C:78:ARG:HE	1.83	0.74
3:B:69:LEU:HD12	3:B:84:ILE:HG22	1.70	0.73
1:R:2:U:H5"	1:R:2:U:C6	2.15	0.71
1:Q:23:U:H6	1:Q:23:U:C5'	2.05	0.70
1:R:23:U:C5'	1:R:23:U:H6	2.05	0.68
1:Q:14:A:C8	1:Q:14:A:C5'	2.75	0.67
1:Q:2:U:C6	1:Q:2:U:C5'	2.72	0.67
2:A:5:THR:HG22	2:A:8:LEU:H	1.60	0.65
1:Q:10:C:H5'	1:Q:10:C:H6	1.63	0.64
2:A:78:ARG:HH21	2:C:78:ARG:NE	1.93	0.64
1:R:22:G:H2'	1:R:23:U:H5"	1.80	0.63
2:A:123:ASN:O	2:A:126:THR:HB	1.99	0.62
1:R:1:C:H2'	1:R:2:U:H5"	1.81	0.61
2:C:171:ALA:O	2:C:174:ILE:HG22	2.01	0.61
1:Q:3:G:H5"	1:Q:3:G:H8	1.65	0.61
2:C:5:THR:HG22	2:C:8:LEU:HB2	1.83	0.59
1:R:10:C:H6	1:R:10:C:H5'	1.68	0.58

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:14:A:C8	1:R:14:A:H5'	2.37	0.58
2:A:133:LEU:HD12	2:A:158:ALA:HB2	1.84	0.58
1:Q:23:U:C5'	1:Q:23:U:C6	2.87	0.57
2:A:78:ARG:NH2	2:C:78:ARG:NE	2.52	0.57
3:D:93:ILE:HD12	3:D:93:ILE:H	1.69	0.57
2:C:20:ARG:HH11	2:C:20:ARG:HG2	1.68	0.57
2:A:2:VAL:HG11	2:A:29:TYR:O	2.05	0.57
2:C:76:ILE:HG12	2:C:98:ASN:OD1	2.05	0.57
2:C:5:THR:CG2	2:C:8:LEU:H	2.17	0.56
2:A:101:VAL:HG23	2:A:102:GLU:HG3	1.86	0.56
3:D:9:ASN:OD1	3:D:10:HIS:N	2.39	0.56
2:A:14:GLN:HG2	2:A:22:ARG:NH2	2.21	0.55
1:Q:10:C:H5'	1:Q:10:C:C6	2.44	0.52
1:R:13:U:C2	3:D:46:LEU:HG	2.45	0.52
1:R:2:U:C6	1:R:2:U:H5'	2.43	0.52
2:A:5:THR:CG2	2:A:8:LEU:H	2.23	0.52
1:R:10:C:H5'	1:R:10:C:C6	2.46	0.51
1:R:23:U:H6	1:R:23:U:H5'	1.76	0.50
2:A:20:ARG:HG2	2:A:20:ARG:HH11	1.74	0.50
2:C:3:LYS:HG2	2:C:35:GLU:OE2	2.12	0.49
3:D:33:LEU:HD21	3:D:72:LEU:HD13	1.92	0.49
2:A:107:ASP:OD1	2:A:134:TYR:OH	2.27	0.49
2:C:90:LEU:HD23	2:C:112:LEU:HD13	1.93	0.49
2:A:102:GLU:HG2	2:A:128:LYS:HZ1	1.78	0.49
1:R:17:U:H2'	1:R:18:C:C6	2.48	0.49
1:R:3:G:H2'	1:R:4:G:O4'	2.13	0.49
2:C:123:ASN:O	2:C:126:THR:HB	2.13	0.48
2:A:66:LEU:HD21	2:A:69:LEU:HG	1.94	0.48
2:A:92:GLU:OE1	3:B:28:ARG:NE	2.39	0.48
1:R:23:U:C5'	1:R:23:U:C6	2.92	0.48
2:C:5:THR:HG22	2:C:8:LEU:H	1.78	0.48
2:A:2:VAL:HG13	2:A:2:VAL:O	2.13	0.48
1:R:0:C:H5"	3:D:22:LYS:HD3	1.96	0.47
2:A:153:LYS:O	2:A:157:GLU:HG3	2.14	0.47
2:C:129:LYS:O	2:C:130:HIS:HB2	2.15	0.47
1:R:23:U:H6	1:R:23:U:H5"	1.78	0.47
2:C:2:VAL:HG13	2:C:2:VAL:O	2.14	0.46
3:D:11:THR:OG1	3:D:58:ILE:HG12	2.16	0.46
2:A:14:GLN:HG3	2:A:44:PHE:HE1	1.80	0.46
3:D:8:PRO:HA	3:D:86:TYR:CE1	2.51	0.46
2:A:61:PRO:O	2:A:86:ALA:HB1	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:56:LYS:HG2	2:A:58:ASP:HB2	1.97	0.45
2:C:133:LEU:HD12	2:C:158:ALA:HB2	1.97	0.45
2:C:159:GLU:O	2:C:163:LYS:HB2	2.17	0.45
2:A:120:ILE:HG22	2:A:120:ILE:O	2.16	0.45
2:C:101:VAL:HG23	2:C:102:GLU:HG3	1.99	0.44
2:C:71:VAL:O	2:C:71:VAL:HG12	2.18	0.44
2:C:92:GLU:OE2	3:D:32:ALA:HB2	2.17	0.44
2:C:23:GLU:HA	2:C:46:ALA:O	2.18	0.43
2:A:161:MET:O	2:A:162:PHE:HB2	2.19	0.43
2:C:79:ILE:HD13	2:C:109:LEU:HD21	2.00	0.43
1:Q:3:G:H2'	1:Q:4:G:O4'	2.19	0.43
2:A:37:LEU:HB2	2:A:61:PRO:HD3	2.00	0.43
3:B:69:LEU:HD12	3:B:84:ILE:CG2	2.46	0.42
3:B:75:PHE:HA	3:B:76:PRO:HD3	1.83	0.42
3:D:61:GLU:O	3:D:64:SER:HB2	2.19	0.42
2:A:78:ARG:NH1	2:C:105:ASP:OD2	2.52	0.42
1:R:22:G:C2'	1:R:23:U:H5"	2.47	0.42
2:C:37:LEU:HB2	2:C:61:PRO:HD3	2.01	0.41
1:Q:1:C:H2'	1:Q:2:U:H5"	2.01	0.41
1:Q:17:U:H2'	1:Q:18:C:O4'	2.21	0.41
2:C:47:ILE:HG13	2:C:66:LEU:CD1	2.51	0.41
2:A:52:ASN:HB2	2:A:74:ASN:OD1	2.20	0.41
3:B:6:ILE:HG22	3:B:86:TYR:HB2	2.02	0.41
2:C:14:GLN:HG2	2:C:22:ARG:NH2	2.36	0.41
2:C:161:MET:O	2:C:162:PHE:HB2	2.20	0.41
3:B:16:ASN:HB2	3:B:83:ARG:HH21	1.86	0.41
3:D:8:PRO:HA	3:D:86:TYR:CZ	2.57	0.40
3:D:52:ARG:O	3:D:54:GLN:NE2	2.52	0.40
2:A:37:LEU:HB2	2:A:61:PRO:CD	2.51	0.40
2:A:140:PRO:O	2:A:155:ARG:NH1	2.48	0.40
1:R:3:G:H8	1:R:3:G:H5"	1.85	0.40
2:A:103:LEU:HD23	2:A:125:VAL:HG22	2.04	0.40
2:C:103:LEU:HD23	2:C:125:VAL:HG23	2.03	0.40
3:D:62:LEU:O	3:D:62:LEU:HD12	2.21	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	
2	A	160/176 (91%)	146 (91%)	12 (8%)	2 (1%)	12	15
2	C	172/176 (98%)	158 (92%)	12 (7%)	2 (1%)	13	17
3	B	92/96 (96%)	90 (98%)	2 (2%)	0	100	100
3	D	91/96 (95%)	87 (96%)	4 (4%)	0	100	100
All	All	515/544 (95%)	481 (93%)	30 (6%)	4 (1%)	19	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	160	LYS
2	A	32	PRO
2	C	163	LYS
2	C	32	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	
2	A	141/156 (90%)	137 (97%)	4 (3%)	43	61
2	C	147/156 (94%)	142 (97%)	5 (3%)	37	53
3	B	82/85 (96%)	79 (96%)	3 (4%)	34	50
3	D	82/85 (96%)	79 (96%)	3 (4%)	34	50
All	All	452/482 (94%)	437 (97%)	15 (3%)	38	55

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	5	THR
2	A	55	ARG
2	A	114	SER
2	A	126	THR
2	C	5	THR
2	C	77	CYS
2	C	78	ARG
2	C	111	SER
2	C	114	SER
3	B	20	LYS
3	B	49	MET
3	B	90	ASP
3	D	7	ARG
3	D	82	MET
3	D	90	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	130	HIS
2	C	14	GLN
2	C	130	HIS
3	B	10	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Q	23/24 (95%)	7 (30%)	3 (13%)
1	R	23/24 (95%)	8 (34%)	4 (17%)
All	All	46/48 (95%)	15 (32%)	7 (15%)

All (15) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Q	2	U
1	Q	3	G
1	Q	10	C
1	Q	11	A
1	Q	14	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Q	15	C
1	Q	23	U
1	R	2	U
1	R	3	G
1	R	10	C
1	R	11	A
1	R	13	U
1	R	14	A
1	R	15	C
1	R	23	U

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	Q	2	U
1	Q	10	C
1	Q	14	A
1	R	2	U
1	R	10	C
1	R	12	G
1	R	14	A

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 monosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	Q	24/24 (100%)	-0.02	0	100	100	44, 62, 73, 81	0
1	R	24/24 (100%)	0.46	1 (4%)	36	39	57, 67, 74, 80	0
2	A	162/176 (92%)	0.33	8 (4%)	29	32	29, 46, 68, 102	0
2	C	174/176 (98%)	0.48	6 (3%)	45	48	32, 51, 79, 95	0
3	B	94/96 (97%)	0.63	8 (8%)	10	12	33, 44, 75, 110	0
3	D	93/96 (96%)	1.74	31 (33%)	0	0	47, 65, 92, 122	0
All	All	571/592 (96%)	0.64	54 (9%)	8	9	29, 51, 82, 122	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	6	ILE	15.1
3	D	97	MET	7.9
3	D	98	ARG	6.8
3	D	7	ARG	5.7
3	D	10	HIS	5.3
3	B	6	ILE	5.1
3	D	93	ILE	4.8
3	D	70	ARG	4.6
3	D	88	LYS	4.5
2	C	69	LEU	4.2
2	C	20	ARG	4.0
3	D	60	LYS	4.0
2	A	162	PHE	3.7
3	D	56	PHE	3.7
3	D	8	PRO	3.3
3	B	57	VAL	3.2
3	D	69	LEU	3.2
2	A	159	GLU	3.1
3	D	96	LYS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	D	92	ASP	3.0
3	D	62	LEU	2.9
3	D	95	SER	2.8
3	D	59	PHE	2.7
2	A	93	LEU	2.7
3	D	89	THR	2.7
2	A	69	LEU	2.7
3	D	87	ALA	2.6
3	B	53	GLY	2.5
3	B	70	ARG	2.5
2	A	94	ILE	2.5
3	D	44	VAL	2.4
2	A	70	LEU	2.4
3	B	58	ILE	2.4
3	B	98	ARG	2.4
3	D	90	ASP	2.4
3	D	94	ILE	2.4
3	D	83	ARG	2.4
3	D	61	GLU	2.4
3	D	39	HIS	2.3
3	D	35	SER	2.3
2	C	47	ILE	2.3
2	C	175	ALA	2.3
2	C	93	LEU	2.3
3	D	50	LYS	2.3
2	C	166	ARG	2.2
3	B	14	ILE	2.2
3	D	53	GLY	2.2
3	D	51	MET	2.2
3	D	55	ALA	2.1
2	A	47	ILE	2.1
2	A	79	ILE	2.0
1	R	14	A	2.0
3	D	85	GLN	2.0
3	B	55	ALA	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.