



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:12 PM UTC

PDB ID : 1A9N / pdb_00001a9n
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)

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

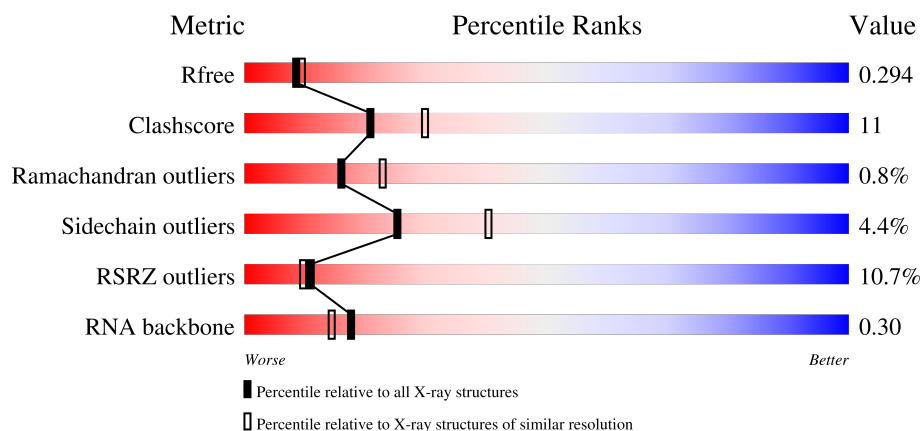
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)
RNA backbone	3983	1016 (2.66-2.10)

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 $\leq 5\%$. 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	Q	24	
1	R	24	
2	A	176	
2	C	176	

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Mol	Chain	Length	Quality of chain
3	B	96	6% 75% 19%
3	D	96	25% 68% 28%

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

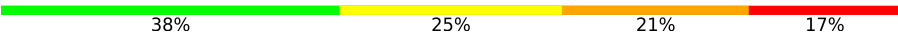
- Molecule 3 is a protein called SPLICEOSOMAL U2B''.

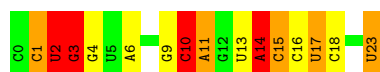
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	94	Total	C	N	O	S	0	0	0
			761	488	135	133	5			
3	D	93	Total	C	N	O	S	0	0	0
			756	486	134	131	5			

3 Residue-property plots [i](#)

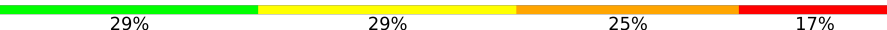
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 



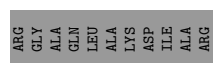
- Molecule 1: RNA (5'-R(*CP*CP*UP*GP*GP*UP*AP*UP*UP*GP*CP*AP*GP*UP*AP*CP*CP*UP*CP*CP*AP*GP*GP*U)-3')

Chain R: 



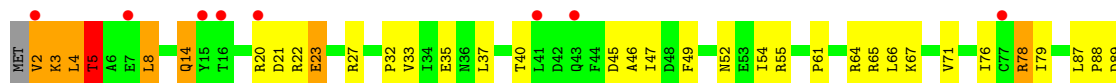
- Molecule 2: U2A'

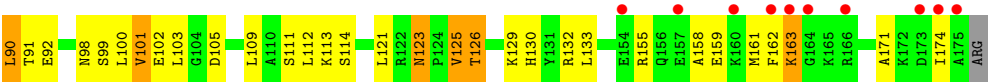
Chain A: 



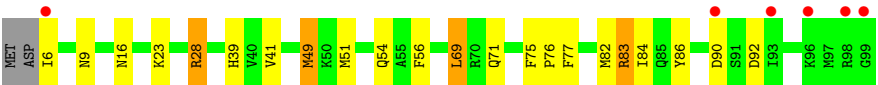
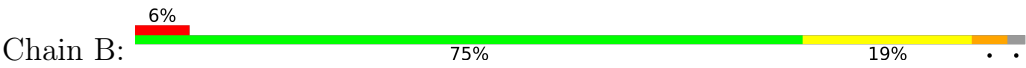
- Molecule 2: U2A'

Chain C: 

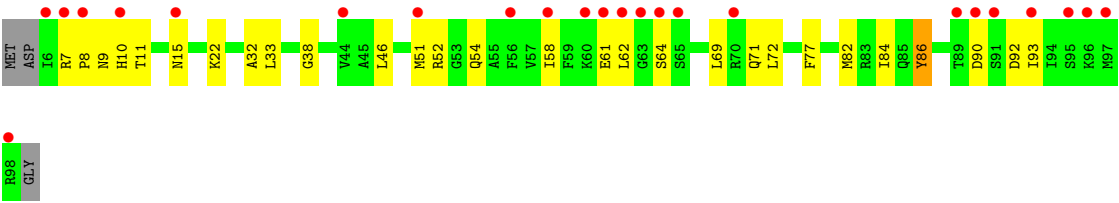




● Molecule 3: SPLICEOSOMAL U2B''



● Molecule 3: SPLICEOSOMAL U2B''



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 15.00 – 2.39	Depositor EDS
% Data completeness (in resolution range)	95.8 (15.00-2.38) 94.4 (15.00-2.39)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.282 , 0.328 0.254 , 0.294	Depositor DCC
R_{free} test set	1650 reflections (4.85%)	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)	0.32 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

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	Q	0.69	0/560	1.60	18/870 (2.1%)
1	R	0.69	0/560	1.73	16/870 (1.8%)
2	A	0.81	0/1309	2.06	59/1774 (3.3%)
2	C	0.75	0/1390	1.92	40/1882 (2.1%)
3	B	0.77	0/775	1.71	12/1035 (1.2%)
3	D	0.53	0/770	1.46	7/1030 (0.7%)
All	All	0.73	0/5364	1.81	152/7461 (2.0%)

There are no bond length outliers.

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	55	ARG	CD-NE-CZ	13.23	142.92	124.40
2	C	55	ARG	NE-CZ-NH1	-12.02	109.48	121.50
2	A	49	PHE	CA-CB-CG	11.50	125.30	113.80
2	C	55	ARG	NH1-CZ-NH2	11.05	133.66	119.30
2	C	49	PHE	CA-CB-CG	11.04	124.84	113.80
2	A	58	ASP	CA-CB-CG	8.91	121.51	112.60
2	A	5	THR	N-CA-CB	-8.50	98.30	111.05
3	B	83	ARG	CD-NE-CZ	8.30	136.02	124.40
3	D	77	PHE	CA-CB-CG	8.15	121.95	113.80
1	R	15	C	P-O3'-C3'	8.01	132.22	120.20
1	R	2	U	O5'-C5'-C4'	-7.97	99.55	111.50
2	A	47	ILE	N-CA-CB	7.93	123.09	111.52
2	A	99	SER	N-CA-C	7.93	122.72	112.26
1	R	14	A	P-O5'-C5'	-7.92	109.02	120.90
2	A	16	THR	CA-C-O	-7.89	111.91	120.36
2	A	117	TYR	CA-C-O	7.58	128.35	120.40
1	Q	14	A	P-O5'-C5'	-7.57	109.55	120.90
1	R	3	G	O5'-C5'-C4'	-7.29	100.56	111.50
1	Q	13	U	O3'-P-O5'	-7.27	93.10	104.00
2	A	71	VAL	CA-C-N	7.16	131.56	120.75
2	A	71	VAL	C-N-CA	7.16	131.56	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	21	ASP	CA-CB-CG	7.15	119.75	112.60
2	A	72	ASN	OD1-CG-ND2	7.04	129.64	122.60
1	Q	16	C	C3'-C2'-O2'	-7.00	104.10	114.60
1	R	1	C	C2'-C3'-O3'	-6.92	103.32	113.70
2	A	4	LEU	N-CA-C	-6.92	97.95	108.67
2	A	107	ASP	CA-CB-CG	6.89	119.49	112.60
2	A	121	LEU	CA-C-O	6.87	128.86	121.44
2	A	75	ARG	NE-CZ-NH1	-6.84	114.66	121.50
2	C	65	ARG	CD-NE-CZ	6.84	133.97	124.40
2	C	4	LEU	N-CA-C	-6.80	98.94	109.76
3	B	56	PHE	CA-C-O	-6.80	112.84	120.32
2	A	58	ASP	N-CA-CB	-6.75	100.58	111.24
2	C	125	VAL	CA-C-N	6.71	129.58	120.38
2	C	125	VAL	C-N-CA	6.71	129.58	120.38
2	C	121	LEU	CA-C-N	6.67	131.61	122.34
2	C	121	LEU	C-N-CA	6.67	131.61	122.34
1	Q	10	C	C5'-C4'-O4'	-6.67	99.10	109.10
1	R	10	C	P-O3'-C3'	6.66	130.19	120.20
2	A	20	ARG	CD-NE-CZ	6.54	133.55	124.40
2	C	55	ARG	CG-CD-NE	-6.41	97.89	112.00
2	C	27	ARG	NE-CZ-NH2	-6.41	113.43	119.20
3	D	92	ASP	CA-CB-CG	6.33	118.93	112.60
2	A	55	ARG	NE-CZ-NH1	6.32	127.82	121.50
2	A	87	LEU	CA-C-N	6.32	126.24	119.28
2	A	87	LEU	C-N-CA	6.32	126.24	119.28
2	A	40	THR	CA-C-N	6.29	131.52	122.40
2	A	40	THR	C-N-CA	6.29	131.52	122.40
2	C	2	VAL	CA-C-O	6.27	131.47	120.80
1	Q	15	C	P-O3'-C3'	6.25	129.58	120.20
2	C	27	ARG	NH1-CZ-NH2	6.24	127.41	119.30
1	Q	14	A	C5'-C4'-C3'	-6.21	106.69	116.00
2	C	21	ASP	CA-CB-CG	6.14	118.74	112.60
2	A	73	ASN	N-CA-C	6.13	119.81	111.17
2	C	52	ASN	CA-C-O	-6.12	113.33	121.47
2	A	52	ASN	CA-CB-CG	6.08	118.68	112.60
1	R	0	C	C2'-C3'-O3'	-6.08	104.59	113.70
2	C	121	LEU	CA-C-O	6.03	127.95	121.44
2	A	75	ARG	N-CA-CB	-6.02	102.60	111.51
3	B	92	ASP	CA-CB-CG	6.02	118.62	112.60
2	A	123	ASN	OD1-CG-ND2	5.99	128.59	122.60
3	D	71	GLN	N-CA-C	5.98	118.76	111.82
1	R	20	A	C2'-C3'-O3'	-5.94	104.80	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	79	ILE	CA-C-N	5.92	125.72	120.10
2	A	79	ILE	C-N-CA	5.92	125.72	120.10
2	C	3	LYS	N-CA-C	-5.91	102.31	110.35
2	C	40	THR	CA-C-O	5.90	126.17	119.27
2	A	27	ARG	CB-CA-C	-5.90	98.69	109.54
2	C	27	ARG	N-CA-C	5.90	118.31	110.53
3	B	49	MET	N-CA-C	-5.89	104.77	111.07
1	R	20	A	C1'-C2'-O2'	5.88	117.21	108.40
2	A	118	LEU	CA-C-N	-5.87	114.50	122.77
2	A	118	LEU	C-N-CA	-5.87	114.50	122.77
2	C	132	ARG	CD-NE-CZ	5.85	132.59	124.40
1	Q	9	G	O3'-P-O5'	-5.83	95.26	104.00
2	A	113	LYS	N-CA-C	5.82	118.38	111.33
2	A	50	SER	CA-C-O	5.80	127.70	121.55
2	C	5	THR	N-CA-CB	-5.79	102.22	111.43
2	C	14	GLN	CA-CB-CG	5.78	125.66	114.10
2	C	87	LEU	CA-C-N	5.78	125.63	119.28
2	C	87	LEU	C-N-CA	5.78	125.63	119.28
2	A	149	LYS	CB-CA-C	-5.70	101.95	110.16
2	C	33	VAL	N-CA-C	5.70	116.33	108.12
1	Q	10	C	P-O3'-C3'	5.68	128.73	120.20
2	A	27	ARG	CA-C-N	5.67	128.68	120.11
2	A	27	ARG	C-N-CA	5.67	128.68	120.11
1	R	14	A	O5'-C5'-C4'	-5.64	103.04	111.50
2	A	71	VAL	O-C-N	-5.59	115.59	122.57
1	Q	11	A	N9-C1'-C2'	5.57	120.35	112.00
1	Q	14	A	O4'-C1'-C2'	-5.56	102.04	107.60
2	A	34	ILE	CA-C-O	-5.53	114.22	120.74
2	C	123	ASN	CA-CB-CG	5.51	118.11	112.60
3	D	15	ASN	CA-CB-CG	5.51	118.11	112.60
1	Q	3	G	P-O5'-C5'	-5.50	112.66	120.90
2	C	155	ARG	NE-CZ-NH2	5.47	124.12	119.20
1	Q	6	A	P-O5'-C5'	-5.47	112.69	120.90
2	A	159	GLU	N-CA-C	-5.47	104.96	111.69
2	A	132	ARG	CD-NE-CZ	5.46	132.04	124.40
2	A	16	THR	O-C-N	5.42	129.40	123.22
2	A	32	PRO	CA-C-N	5.42	130.52	122.99
2	A	32	PRO	C-N-CA	5.42	130.52	122.99
3	B	28	ARG	CD-NE-CZ	5.41	131.97	124.40
2	C	101	VAL	CB-CA-C	-5.40	105.00	110.88
2	A	40	THR	N-CA-C	-5.38	106.22	112.89
2	C	100	LEU	CB-CA-C	5.36	118.31	110.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	14	A	O4'-C1'-C2'	-5.36	102.25	107.60
1	R	21	G	C4'-C3'-C2'	-5.35	97.25	102.60
2	C	40	THR	N-CA-C	-5.34	106.61	113.23
2	A	125	VAL	CA-C-N	5.32	127.94	120.28
2	A	125	VAL	C-N-CA	5.32	127.94	120.28
3	B	9	ASN	N-CA-CB	-5.31	101.66	111.53
1	R	3	G	C4'-C3'-O3'	-5.29	105.07	113.00
2	A	88	PRO	CB-CA-C	-5.29	103.97	112.21
2	C	113	LYS	N-CA-C	5.28	117.78	111.71
3	B	23	LYS	N-CA-C	5.27	117.44	111.11
2	A	146	ASP	CA-C-N	5.27	130.04	122.40
2	A	146	ASP	C-N-CA	5.27	130.04	122.40
1	R	2	U	N1-C1'-C2'	5.26	119.89	112.00
1	R	10	C	C4'-C3'-C2'	-5.26	97.34	102.60
2	A	33	VAL	N-CA-CB	-5.26	103.84	111.52
1	R	4	G	C2'-C3'-O3'	-5.25	105.83	113.70
2	C	91	THR	CA-C-O	5.24	124.59	118.77
2	C	90	LEU	CA-C-O	-5.22	115.16	120.80
1	Q	17	U	C2'-C3'-O3'	-5.21	105.89	113.70
2	A	55	ARG	NE-CZ-NH2	-5.18	114.54	119.20
3	D	86	TYR	N-CA-C	-5.17	102.82	110.48
3	B	54	GLN	N-CA-C	5.17	117.53	109.52
3	B	39	HIS	CA-CB-CG	-5.17	108.64	113.80
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
2	C	88	PRO	N-CA-C	5.15	120.60	113.65
3	B	51	MET	N-CA-C	5.15	119.56	113.28
2	C	54	ILE	CA-C-N	5.13	131.28	122.09
2	C	54	ILE	C-N-CA	5.13	131.28	122.09
3	D	38	GLY	CA-C-O	-5.13	116.52	121.75
1	Q	16	C	O4'-C1'-C2'	-5.12	100.68	105.80
3	B	71	GLN	OE1-CD-NE2	5.11	127.71	122.60
2	A	83	LEU	N-CA-C	5.11	117.51	111.33
2	C	23	GLU	N-CA-C	5.08	117.68	109.40
3	B	41	VAL	O-C-N	5.07	127.05	121.83
2	A	28	GLY	N-CA-C	5.06	120.87	113.48
1	Q	6	A	N9-C1'-C2'	5.06	119.59	112.00
3	D	51	MET	N-CA-C	5.05	119.44	113.28
2	A	90	LEU	CA-C-O	-5.04	113.31	120.51
1	Q	1	C	P-O3'-C3'	5.04	127.75	120.20
2	C	67	LYS	O-C-N	-5.04	116.21	122.25
2	C	45	ASP	CA-C-O	5.03	125.49	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	99	SER	N-CA-CB	-5.03	102.92	111.17
2	C	132	ARG	NH1-CZ-NH2	-5.01	112.78	119.30
2	A	81	GLU	N-CA-C	5.00	118.53	112.23
2	A	139	VAL	CA-C-N	5.00	124.66	119.56
2	A	139	VAL	C-N-CA	5.00	124.66	119.56

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	32	0
2	C	1373	0	1402	30	0
3	B	761	0	783	7	0
3	D	756	0	780	13	0
All	All	5188	0	4802	111	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 (111) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:A:102:GLU:HG2	2:A:128:LYS:HZ1	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:C:89:ASP:O	2:C:90:LEU:C	2.62	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:160:LYS:O	2:A:161:MET:C	2.63	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
3:B:77:PHE:CG	3:B:82:MET:HE3	2.55	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
2:A:56:LYS:HE2	2:A:58:ASP:CG	2.44	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%)	9	12
2	C	172/176 (98%)	158 (92%)	12 (7%)	2 (1%)	10	14
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%)	16	23

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%)	135 (96%)	6 (4%)	26	41
2	C	147/156 (94%)	139 (95%)	8 (5%)	20	32
3	B	82/85 (96%)	79 (96%)	3 (4%)	30	47
3	D	82/85 (96%)	79 (96%)	3 (4%)	30	47
All	All	452/482 (94%)	432 (96%)	20 (4%)	25	40

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	5	THR
2	A	71	VAL
2	A	79	ILE
2	A	101	VAL
2	A	114	SER
2	A	126	THR
2	C	4	LEU
2	C	5	THR
2	C	8	LEU
2	C	64	ARG
2	C	78	ARG
2	C	111	SER
2	C	114	SER
2	C	126	THR
3	B	49	MET
3	B	69	LEU

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Mol	Chain	Res	Type
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 (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	14	GLN
3	B	10	HIS
3	D	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%)	9 (39%)	4 (17%)
All	All	46/48 (95%)	16 (34%)	7 (15%)

All (16) 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
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	12	G
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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, 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%)	0.35	0	100	100	44, 62, 73, 81	0
1	R	24/24 (100%)	0.79	0	100	100	57, 67, 74, 80	0
2	A	162/176 (92%)	0.50	13 (8%)	18	17	29, 46, 68, 102	0
2	C	174/176 (98%)	0.81	18 (10%)	12	10	32, 51, 79, 95	0
3	B	94/96 (97%)	0.48	6 (6%)	25	24	33, 44, 75, 110	0
3	D	93/96 (96%)	1.39	24 (25%)	1	1	47, 65, 92, 122	0
All	All	571/592 (96%)	0.74	61 (10%)	11	10	29, 51, 82, 122	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	175	ALA	5.1
3	B	98	ARG	4.4
3	D	6	ILE	4.3
3	D	97	MET	4.2
2	A	160	LYS	4.0
2	C	174	ILE	3.9
3	D	62	LEU	3.8
2	A	5	THR	3.7
2	C	162	PHE	3.6
3	D	90	ASP	3.5
3	B	96	LYS	3.4
2	A	162	PHE	3.4
2	C	163	LYS	3.4
2	C	166	ARG	3.4
2	A	2	VAL	3.3
3	B	6	ILE	3.2
2	C	43	GLN	3.1
3	D	44	VAL	3.1
3	D	96	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
3	D	60	LYS	3.0
3	D	10	HIS	3.0
2	C	16	THR	3.0
3	D	93	ILE	2.9
2	C	77	CYS	2.9
2	C	7	GLU	2.9
2	A	161	MET	2.8
3	D	98	ARG	2.8
3	D	8	PRO	2.8
3	B	99	GLY	2.7
2	A	7	GLU	2.7
3	B	90	ASP	2.6
2	A	15	TYR	2.6
2	C	164	GLY	2.6
2	C	15	TYR	2.6
2	C	160	LYS	2.6
2	C	173	ASP	2.5
2	C	2	VAL	2.5
3	D	7	ARG	2.5
2	A	102	GLU	2.4
3	D	56	PHE	2.4
3	D	63	GLY	2.4
3	D	15	ASN	2.3
2	A	159	GLU	2.3
3	D	61	GLU	2.3
2	A	85	GLN	2.3
3	D	89	THR	2.2
2	C	41	LEU	2.2
2	A	153	LYS	2.2
3	D	70	ARG	2.1
3	B	93	ILE	2.1
3	D	64	SER	2.1
3	D	51	MET	2.1
3	D	95	SER	2.1
2	A	163	LYS	2.1
2	A	152	LEU	2.1
2	C	154	GLU	2.0
2	C	157	GLU	2.0
3	D	65	SER	2.0
3	D	91	SER	2.0
2	C	20	ARG	2.0
3	D	58	ILE	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 oligosaccharides 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.