



wwPDB X-ray Structure Validation Summary Report

Mar 31, 2014 – 05:29 PM BST

PDB ID : 2Y9A
Title : STRUCTURE OF THE SPLICEOSOMAL U4 SNRNP CORE DOMAIN
Authors : Leung, A.K.W.; Nagai, K.; Li, J.
Deposited on : 2011-02-13
Resolution : 3.60 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

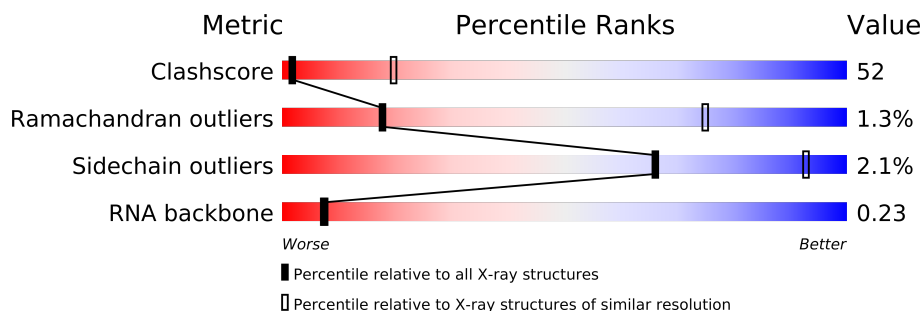
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23004

1 Overall quality at a glance

The reported resolution of this entry is 3.60 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))
Clashscore	79885	1155 (3.80-3.40)
Ramachandran outliers	78287	1109 (3.80-3.40)
Sidechain outliers	78261	1108 (3.80-3.40)
RNA backbone	1838	1012 (4.40-2.76)


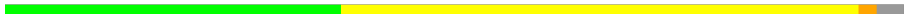
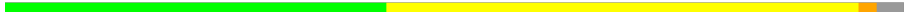

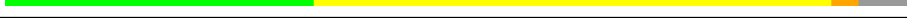



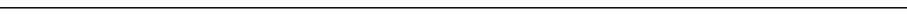
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	95	
1	H	95	
1	O	95	
2	B	119	
2	I	119	
2	P	119	
3	C	118	
3	J	118	
3	Q	118	
4	D	126	
4	K	126	
4	R	126	
5	E	92	
5	L	92	
5	S	92	

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Mol	Chain	Length	Quality of chain
6	F	86	
6	M	86	
6	T	86	
7	G	76	
7	N	76	
7	U	76	
8	V	68	
8	X	68	
8	Y	68	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 18920 atoms, of which 0 are hydrogen and 0 are deuterium.

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 SMALL NUCLEAR RIBONUCLEOPROTEIN-ASSOCIATE DPROTEINS B AND B'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	90	Total	C	N	O	S	0	0	0
			724	455	133	129	7			
1	H	91	Total	C	N	O	S	0	0	0
			733	461	135	130	7			
1	O	89	Total	C	N	O	S	0	0	0
			718	452	132	127	7			

- Molecule 2 is a protein called SMALL NUCLEAR RIBONUCLEOPROTEIN SM D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	S	0	0	1
			759	482	135	138	4			
2	I	96	Total	C	N	O	S	0	0	1
			751	477	134	137	3			
2	P	95	Total	C	N	O	S	0	0	1
			746	474	133	136	3			

- Molecule 3 is a protein called SMALL NUCLEAR RIBONUCLEOPROTEIN SM D2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	105	Total	C	N	O	S	0	0	0
			845	529	157	154	5			
3	J	107	Total	C	N	O	S	0	0	0
			859	538	159	157	5			
3	Q	90	Total	C	N	O	S	0	0	1
			709	446	135	123	5			

- Molecule 4 is a protein called SMALL NUCLEAR RIBONUCLEOPROTEIN SM D3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	89	Total	C	N	O	S	0	0	1
			696	433	126	130	7			
4	K	89	Total	C	N	O	S	0	0	1
			696	433	126	130	7			
4	R	89	Total	C	N	O	S	0	0	1
			696	433	126	130	7			

- Molecule 5 is a protein called SMALL NUCLEAR RIBONUCLEOPROTEIN E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	86	Total	C	N	O	S	0	0	0
			707	446	127	129	5			
5	L	76	Total	C	N	O	S	0	0	0
			629	397	112	116	4			
5	S	78	Total	C	N	O	S	0	0	0
			645	407	115	119	4			

- Molecule 6 is a protein called SMALL NUCLEAR RIBONUCLEOPROTEIN F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	83	Total	C	N	O	S	0	0	0
			657	416	107	128	6			
6	M	83	Total	C	N	O	S	0	0	0
			657	416	107	128	6			
6	T	83	Total	C	N	O	S	0	0	0
			657	416	107	128	6			

- Molecule 7 is a protein called SMALL NUCLEAR RIBONUCLEOPROTEIN G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	73	Total	C	N	O	S	0	0	0
			568	358	102	102	6			
7	N	71	Total	C	N	O	S	0	0	1
			541	342	97	96	6			
7	U	73	Total	C	N	O	S	0	0	0
			568	358	102	102	6			

- Molecule 8 is a RNA chain called HOMO SAPIENS U4A SNRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	V	68	Total	C	N	O	P	0	0	0
			1453	650	263	473	67			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	X	68	Total	C	N	O	P	0	0	0
			1453	650	263	473	67			
8	Y	68	Total	C	N	O	P	0	0	0
			1453	650	263	473	67			

There are 93 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	.	-	U	DELETION	GB 36174
V	.	-	G	DELETION	GB 36174
V	.	-	C	DELETION	GB 36174
V	.	-	A	DELETION	GB 36174
V	.	-	A	DELETION	GB 36174
V	.	-	U	DELETION	GB 36174
V	.	-	A	DELETION	GB 36174
V	.	-	U	DELETION	GB 36174
V	813	G	-	INSERTION	GB 36174
V	814	A	-	INSERTION	GB 36174
V	815	A	-	INSERTION	GB 36174
V	816	A	-	INSERTION	GB 36174
V	.	-	U	DELETION	GB 36174
V	.	-	A	DELETION	GB 36174
V	.	-	C	DELETION	GB 36174
V	.	-	G	DELETION	GB 36174
V	846	U	-	INSERTION	GB 36174
V	847	A	-	INSERTION	GB 36174
V	848	U	-	INSERTION	GB 36174
V	849	G	-	INSERTION	GB 36174
V	850	G	-	INSERTION	GB 36174
V	851	G	-	INSERTION	GB 36174
V	852	U	-	INSERTION	GB 36174
V	853	A	-	INSERTION	GB 36174
V	854	A	-	INSERTION	GB 36174
V	855	C	-	INSERTION	GB 36174
V	856	C	-	INSERTION	GB 36174
V	857	U	-	INSERTION	GB 36174
V	858	A	-	INSERTION	GB 36174
V	859	A	-	INSERTION	GB 36174
V	860	G	-	INSERTION	GB 36174
X	.	-	U	DELETION	GB 36174
X	.	-	G	DELETION	GB 36174
X	.	-	C	DELETION	GB 36174

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Chain	Residue	Modelled	Actual	Comment	Reference
X	.	-	A	DELETION	GB 36174
X	.	-	A	DELETION	GB 36174
X	.	-	U	DELETION	GB 36174
X	.	-	A	DELETION	GB 36174
X	.	-	U	DELETION	GB 36174
X	813	G	-	INSERTION	GB 36174
X	814	A	-	INSERTION	GB 36174
X	815	A	-	INSERTION	GB 36174
X	816	A	-	INSERTION	GB 36174
X	.	-	U	DELETION	GB 36174
X	.	-	A	DELETION	GB 36174
X	.	-	C	DELETION	GB 36174
X	.	-	G	DELETION	GB 36174
X	846	U	-	INSERTION	GB 36174
X	847	A	-	INSERTION	GB 36174
X	848	U	-	INSERTION	GB 36174
X	849	G	-	INSERTION	GB 36174
X	850	G	-	INSERTION	GB 36174
X	851	G	-	INSERTION	GB 36174
X	852	U	-	INSERTION	GB 36174
X	853	A	-	INSERTION	GB 36174
X	854	A	-	INSERTION	GB 36174
X	855	C	-	INSERTION	GB 36174
X	856	C	-	INSERTION	GB 36174
X	857	U	-	INSERTION	GB 36174
X	858	A	-	INSERTION	GB 36174
X	859	A	-	INSERTION	GB 36174
X	860	G	-	INSERTION	GB 36174
Y	.	-	U	DELETION	GB 36174
Y	.	-	G	DELETION	GB 36174
Y	.	-	C	DELETION	GB 36174
Y	.	-	A	DELETION	GB 36174
Y	.	-	A	DELETION	GB 36174
Y	.	-	U	DELETION	GB 36174
Y	.	-	A	DELETION	GB 36174
Y	.	-	U	DELETION	GB 36174
Y	813	G	-	INSERTION	GB 36174
Y	814	A	-	INSERTION	GB 36174
Y	815	A	-	INSERTION	GB 36174
Y	816	A	-	INSERTION	GB 36174
Y	.	-	U	DELETION	GB 36174
Y	.	-	A	DELETION	GB 36174

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	.	-	C	DELETION	GB 36174
Y	.	-	G	DELETION	GB 36174
Y	846	U	-	INSERTION	GB 36174
Y	847	A	-	INSERTION	GB 36174
Y	848	U	-	INSERTION	GB 36174
Y	849	G	-	INSERTION	GB 36174
Y	850	G	-	INSERTION	GB 36174
Y	851	G	-	INSERTION	GB 36174
Y	852	U	-	INSERTION	GB 36174
Y	853	A	-	INSERTION	GB 36174
Y	854	A	-	INSERTION	GB 36174
Y	855	C	-	INSERTION	GB 36174
Y	856	C	-	INSERTION	GB 36174
Y	857	U	-	INSERTION	GB 36174
Y	858	A	-	INSERTION	GB 36174
Y	859	A	-	INSERTION	GB 36174
Y	860	G	-	INSERTION	GB 36174

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

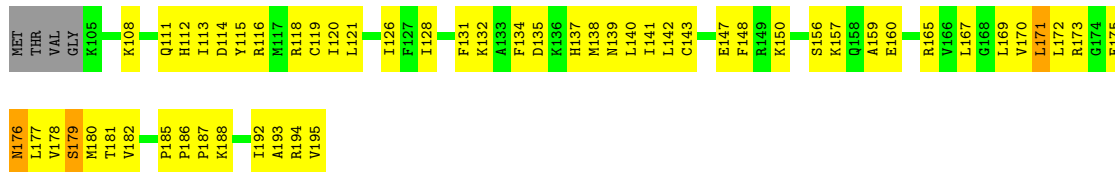
- Molecule 1: SMALL NUCLEAR RIBONUCLEOPROTEIN-ASSOCIATEDPROTEINS B AND B'

Chain A: 



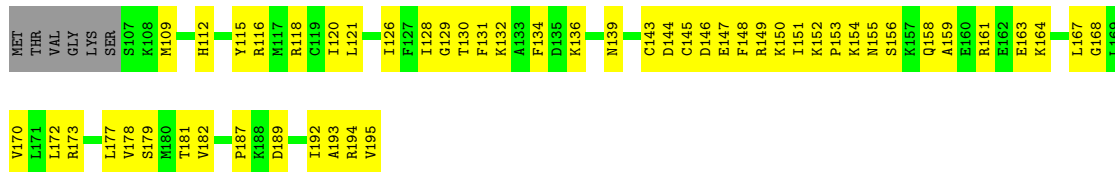
- Molecule 1: SMALL NUCLEAR RIBONUCLEOPROTEIN-ASSOCIATEDPROTEINS B AND B'

Chain H: 



- Molecule 1: SMALL NUCLEAR RIBONUCLEOPROTEIN-ASSOCIATEDPROTEINS B AND B'

Chain O: 



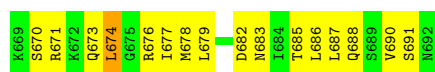
- Molecule 2: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D1

Chain B: 



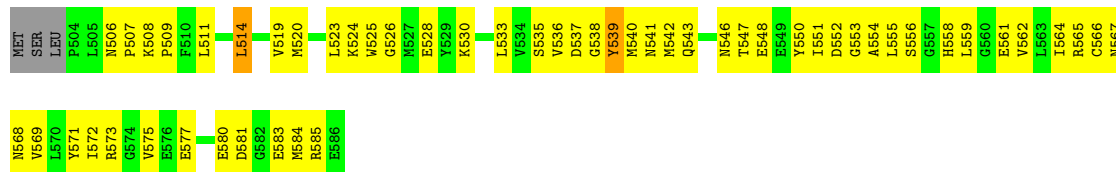


WORLD WIDE
PDB
PROTEIN DATA BANK



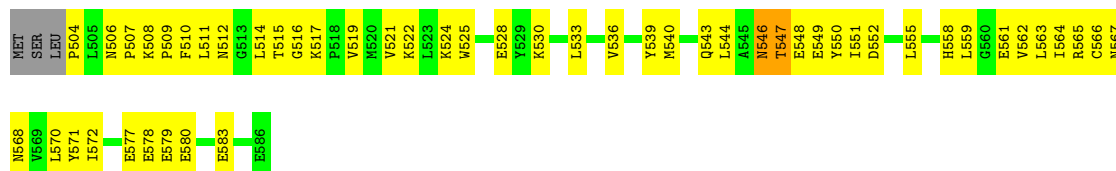
• Molecule 6: SMALL NUCLEAR RIBONUCLEOPROTEIN F

Chain F:



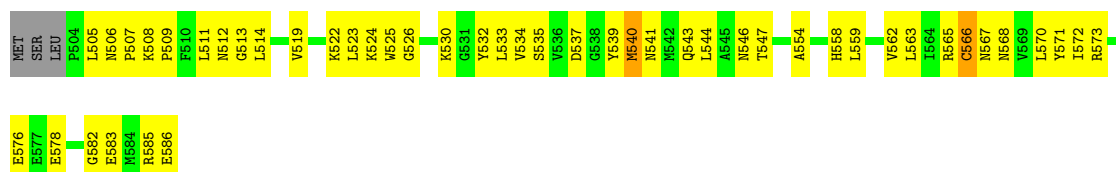
• Molecule 6: SMALL NUCLEAR RIBONUCLEOPROTEIN F

Chain M:



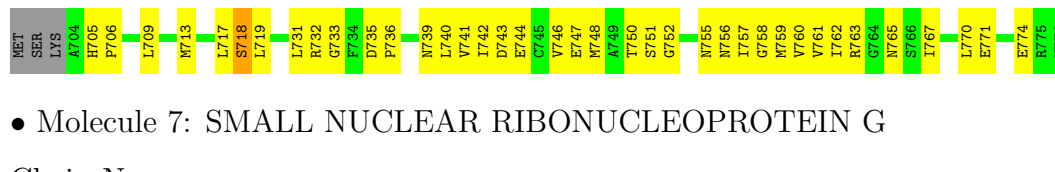
• Molecule 6: SMALL NUCLEAR RIBONUCLEOPROTEIN F

Chain T:



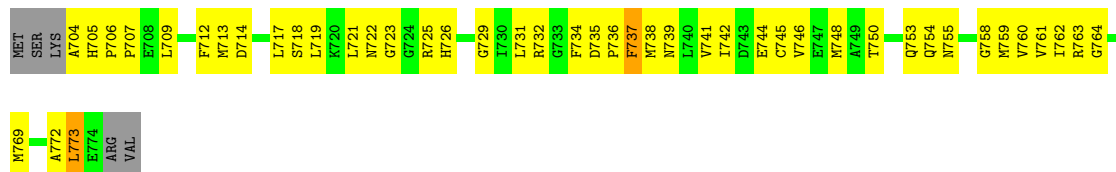
• Molecule 7: SMALL NUCLEAR RIBONUCLEOPROTEIN G

Chain G:



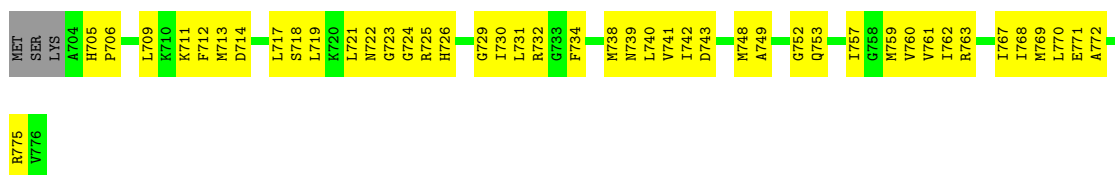
• Molecule 7: SMALL NUCLEAR RIBONUCLEOPROTEIN G

Chain N:



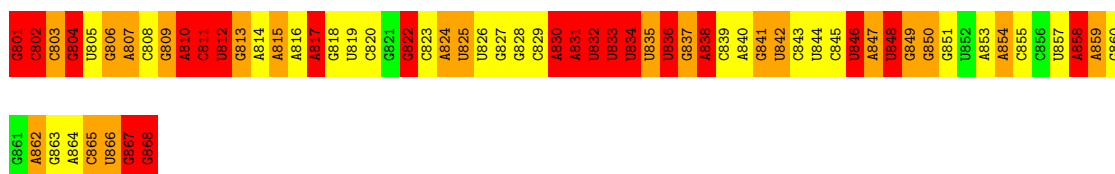
• Molecule 7: SMALL NUCLEAR RIBONUCLEOPROTEIN G

Chain U:



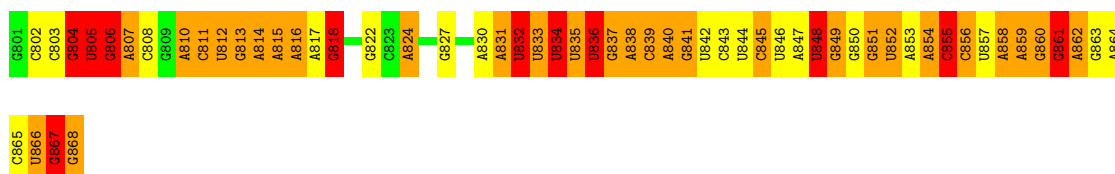
• Molecule 8: HOMO SAPIENS U4A SNRNA

Chain V:



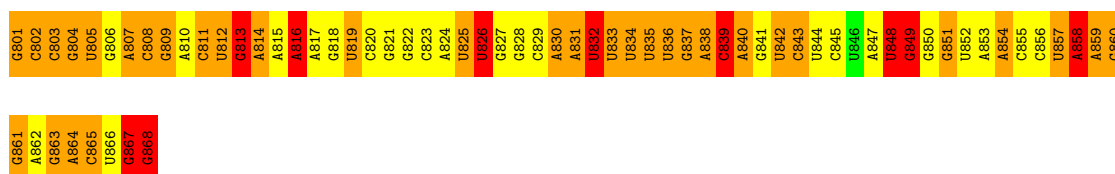
• Molecule 8: HOMO SAPIENS U4A SNRNA

Chain X:



• Molecule 8: HOMO SAPIENS U4A SNRNA

Chain Y:



4 Data and refinement statistics

EDS was not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	248.01Å 248.01Å 251.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	66.17 – 3.60	Depositor
% Data completeness (in resolution range)	82.9 (66.17-3.60)	Depositor
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.277 , 0.321	Depositor
Wilson B-factor (Å ²)	85.4	Xtriage
Anisotropy	0.027	Xtriage
Estimated twinning fraction	0.250 for H, K, L 0.252 for -H, H+K, -L 0.253 for K, H, -L 0.246 for -H, -K, L 0.428 for -h,-k,l 0.408 for h,-h-k,-l 0.298 for -k,-h,-l	Xtriage
Reported twinning fraction	0.250 for H, K, L 0.252 for -H, H+K, -L 0.253 for K, H, -L 0.246 for -H, -K, L	Depositor
L-test for twinning	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.16$	Xtriage
Outliers	0 of 94197 reflections	Xtriage
Total number of atoms	18920	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.65	0/734	0.75	0/978
1	H	0.65	0/743	0.72	0/989
1	O	0.61	0/728	0.72	0/970
2	B	0.63	1/768 (0.1%)	0.77	0/1036
2	I	0.64	0/760	0.76	0/1026
2	P	0.69	1/755 (0.1%)	0.81	1/1019 (0.1%)
3	C	0.66	0/855	0.80	1/1141 (0.1%)
3	J	0.70	0/870	0.77	0/1163
3	Q	0.69	0/718	0.77	0/962
4	D	0.63	0/704	0.72	0/946
4	K	0.68	2/704 (0.3%)	0.67	0/946
4	R	0.64	1/704 (0.1%)	0.70	0/946
5	E	0.60	0/715	0.75	0/957
5	L	0.59	0/637	0.74	0/853
5	S	0.68	0/653	0.77	1/876 (0.1%)
6	F	0.68	0/669	0.69	0/899
6	M	0.71	0/669	0.68	0/899
6	T	0.65	0/669	0.72	0/899
7	G	0.63	0/575	0.66	0/768
7	N	0.66	0/548	0.70	0/734
7	U	0.60	0/575	0.74	0/768
8	V	1.27	4/1626 (0.2%)	1.88	55/2534 (2.2%)
8	X	1.40	6/1626 (0.4%)	1.93	52/2534 (2.1%)
8	Y	1.32	8/1626 (0.5%)	1.91	52/2534 (2.1%)
All	All	0.87	23/19631 (0.1%)	1.19	162/27377 (0.6%)

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Y	822	G	C3'-O3'	7.17	1.52	1.42
8	Y	865	C	C1'-N1	7.03	1.59	1.48
8	X	832	U	C1'-N1	6.37	1.58	1.48
8	V	809	G	P-O5'	6.17	1.66	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Y	863	G	N1-C2	5.91	1.42	1.37

The worst 5 of 162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	X	804	G	C5-C6-O6	-10.74	122.16	128.60
8	Y	864	A	N1-C6-N6	10.30	124.78	118.60
8	Y	865	C	O4'-C1'-N1	9.55	115.84	108.20
8	X	804	G	N3-C4-N9	9.38	131.63	126.00
8	Y	812	U	O4'-C1'-N1	9.27	115.61	108.20

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	724	0	755	86	0
1	H	733	0	768	69	0
1	O	718	0	750	68	0
2	B	759	0	816	109	0
2	I	751	0	807	151	0
2	P	746	0	802	135	0
3	C	845	0	892	155	0
3	J	859	0	906	170	0
3	Q	709	0	764	145	0
4	D	696	0	714	41	0
4	K	696	0	714	75	0
4	R	696	0	714	53	0
5	E	707	0	731	86	0
5	L	629	0	643	68	0
5	S	645	0	659	91	0
6	F	657	0	645	118	0
6	M	657	0	645	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	T	657	0	645	110	0
7	G	568	0	590	47	0
7	N	541	0	562	83	0
7	U	568	0	590	81	0
8	V	1453	0	733	124	0
8	X	1453	0	733	96	0
8	Y	1453	0	733	93	0
All	All	18920	0	17311	1865	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 52.

The worst 5 of 1865 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:P:210:LEU:CD1	2:P:274:LEU:HD13	1.43	1.47
2:P:210:LEU:HD13	2:P:274:LEU:CD1	1.55	1.37
5:S:683:ASN:ND2	6:T:570:LEU:HD22	1.39	1.35
5:S:674:LEU:HD13	6:T:573:ARG:CD	1.54	1.35
6:T:547:THR:HG21	6:T:562:VAL:CG2	1.57	1.34

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	88/95 (93%)	81 (92%)	5 (6%)	2 (2%)	10 63
1	H	89/95 (94%)	80 (90%)	9 (10%)	0	100 100
1	O	87/95 (92%)	81 (93%)	6 (7%)	0	100 100
2	B	95/119 (80%)	85 (90%)	7 (7%)	3 (3%)	6 55
2	I	94/119 (79%)	82 (87%)	10 (11%)	2 (2%)	11 65
2	P	93/119 (78%)	83 (89%)	9 (10%)	1 (1%)	21 78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	103/118 (87%)	89 (86%)	11 (11%)	3 (3%)	7	58
3	J	105/118 (89%)	97 (92%)	7 (7%)	1 (1%)	22	80
3	Q	88/118 (75%)	77 (88%)	10 (11%)	1 (1%)	21	78
4	D	87/126 (69%)	77 (88%)	10 (12%)	0	100	100
4	K	87/126 (69%)	81 (93%)	5 (6%)	1 (1%)	21	78
4	R	87/126 (69%)	84 (97%)	2 (2%)	1 (1%)	21	78
5	E	84/92 (91%)	77 (92%)	6 (7%)	1 (1%)	19	77
5	L	74/92 (80%)	67 (90%)	6 (8%)	1 (1%)	16	72
5	S	76/92 (83%)	67 (88%)	8 (10%)	1 (1%)	18	75
6	F	81/86 (94%)	73 (90%)	7 (9%)	1 (1%)	19	77
6	M	81/86 (94%)	76 (94%)	4 (5%)	1 (1%)	19	77
6	T	81/86 (94%)	76 (94%)	4 (5%)	1 (1%)	19	77
7	G	71/76 (93%)	66 (93%)	5 (7%)	0	100	100
7	N	69/76 (91%)	63 (91%)	5 (7%)	1 (1%)	16	72
7	U	71/76 (93%)	64 (90%)	6 (8%)	1 (1%)	16	72
All	All	1791/2136 (84%)	1626 (91%)	142 (8%)	23 (1%)	18	75

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	284	GLU
3	J	412	ASN
7	N	773	LEU
1	A	149	ARG
2	B	221	ASN

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	81/85 (95%)	80 (99%)	1 (1%)	82	96
1	H	82/85 (96%)	79 (96%)	3 (4%)	45	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	80/85 (94%)	78 (98%)	2 (2%)	60	91
2	B	89/101 (88%)	87 (98%)	2 (2%)	64	92
2	I	88/101 (87%)	86 (98%)	2 (2%)	63	92
2	P	88/101 (87%)	86 (98%)	2 (2%)	63	92
3	C	97/110 (88%)	95 (98%)	2 (2%)	66	93
3	J	99/110 (90%)	95 (96%)	4 (4%)	42	85
3	Q	83/110 (76%)	81 (98%)	2 (2%)	61	92
4	D	78/101 (77%)	78 (100%)	0	100	100
4	K	78/101 (77%)	77 (99%)	1 (1%)	80	96
4	R	78/101 (77%)	77 (99%)	1 (1%)	80	96
5	E	80/84 (95%)	79 (99%)	1 (1%)	80	96
5	L	71/84 (84%)	70 (99%)	1 (1%)	78	96
5	S	73/84 (87%)	72 (99%)	1 (1%)	78	96
6	F	71/74 (96%)	70 (99%)	1 (1%)	78	96
6	M	71/74 (96%)	70 (99%)	1 (1%)	78	96
6	T	71/74 (96%)	69 (97%)	2 (3%)	56	90
7	G	63/66 (96%)	60 (95%)	3 (5%)	35	82
7	N	60/66 (91%)	59 (98%)	1 (2%)	73	95
7	U	63/66 (96%)	62 (98%)	1 (2%)	75	95
All	All	1644/1863 (88%)	1610 (98%)	34 (2%)	66	93

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	343	LEU
4	K	41	CYS
6	T	544	LEU
3	J	410	LEU
6	F	514	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
4	K	16	HIS

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Mol	Chain	Res	Type
4	K	88	ASN
5	S	683	ASN
4	K	57	GLN
5	L	640	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	V	68/68 (100%)	32 (47%)	8 (11%)
8	X	67/68 (98%)	28 (41%)	6 (8%)
8	Y	67/68 (98%)	35 (52%)	5 (7%)
All	All	202/204 (99%)	95 (47%)	19 (9%)

5 of 95 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	V	802	C
8	V	804	G
8	V	806	G
8	V	807	A
8	V	808	C

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	X	803	C
8	X	830	A
8	Y	816	A
8	V	867	G
8	Y	836	U

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 ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.