



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 10:47 PM GMT

PDB ID : 2Y9B
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>

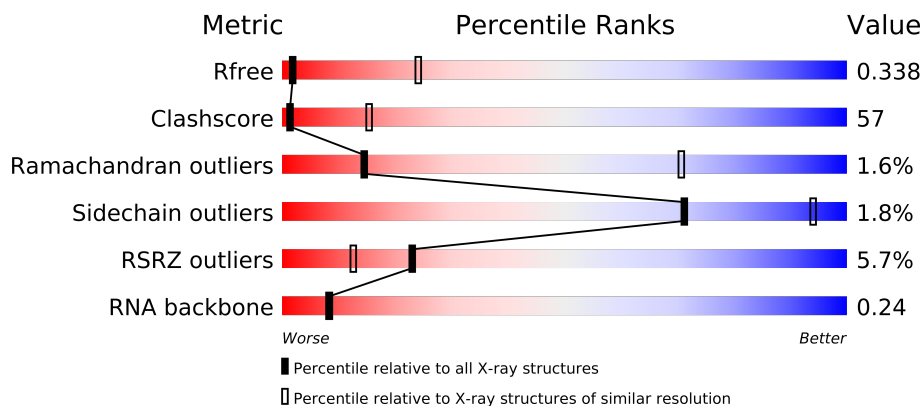
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

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))
R_{free}	66092	1020 (3.86-3.34)
Clashscore	79885	1155 (3.80-3.40)
Ramachandran outliers	78287	1109 (3.80-3.40)
Sidechain outliers	78261	1108 (3.80-3.40)
RSRZ outliers	66119	1000 (3.84-3.36)
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.

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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	R	126	
5	E	92	
5	L	92	
5	S	92	
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 18887 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	91	Total	C	N	O	S	0	0	0
			733	461	135	130	7			
1	H	95	Total	C	N	O	S	0	0	0
			759	477	139	135	8			
1	O	90	Total	C	N	O	S	0	0	0
			724	455	133	129	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	96	Total	C	N	O	S	0	0	1
			751	477	134	137	3			
2	I	96	Total	C	N	O	S	0	0	1
			751	477	134	137	3			
2	P	96	Total	C	N	O	S	0	0	1
			754	479	134	137	4			

- 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	106	Total	C	N	O	S	0	0	0
			852	534	158	155	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	75	Total	C	N	O	S	0	0	0
			622	392	111	115	4			
5	L	75	Total	C	N	O	S	0	0	0
			622	392	111	115	4			
5	S	82	Total	C	N	O	S	0	0	0
			678	428	121	124	5			

- 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	1
			648	411	107	124	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	74	Total	C	N	O	S	0	0	0
			577	364	104	103	6			
7	U	70	Total	C	N	O	S	0	0	1
			533	336	96	95	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			

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

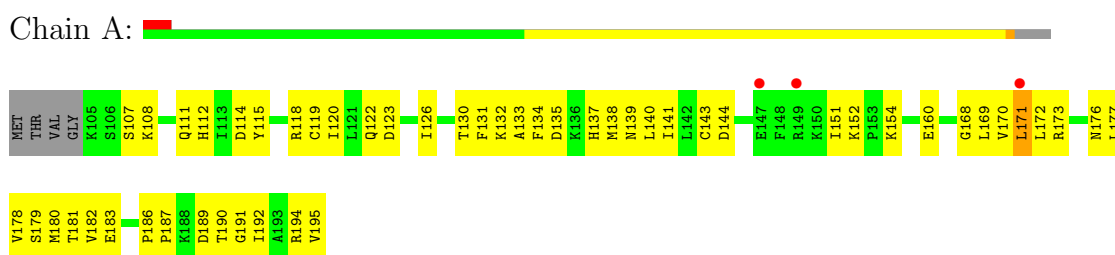
Continued from previous page...

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

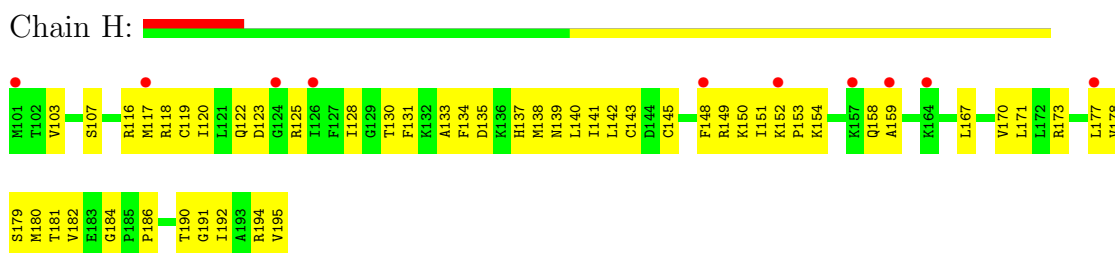
3 Residue-property plots

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.

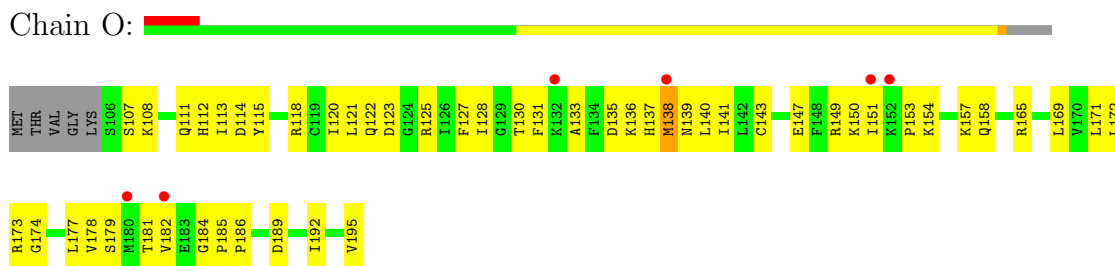
- Molecule 1: SMALL NUCLEAR RIBONUCLEOPROTEIN-ASSOCIATED PROTEINS B AND B'



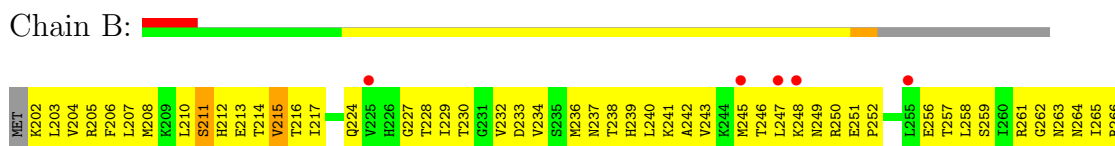
- Molecule 1: SMALL NUCLEAR RIBONUCLEOPROTEIN-ASSOCIATED PROTEINS B AND B'



- Molecule 1: SMALL NUCLEAR RIBONUCLEOPROTEIN-ASSOCIATED PROTEINS B AND B'



- Molecule 2: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D1





• Molecule 2: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D1

Chain I:



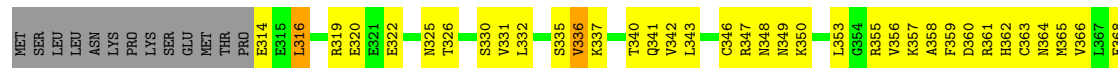
• Molecule 2: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D1

Chain P:



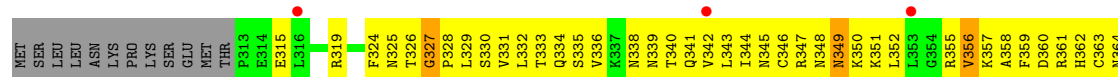
• Molecule 3: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D2

Chain C:



• Molecule 3: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D2

Chain J:



• Molecule 3: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D2

Chain Q:





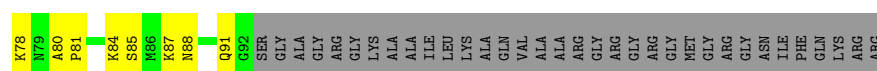
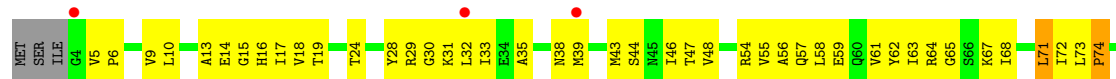
• Molecule 4: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D3

Chain D:



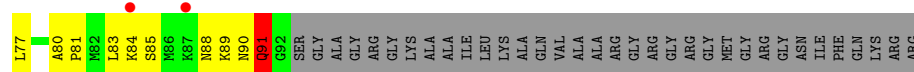
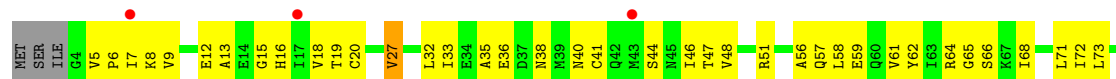
• Molecule 4: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D3

Chain K:



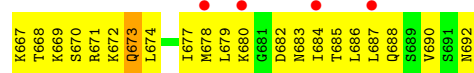
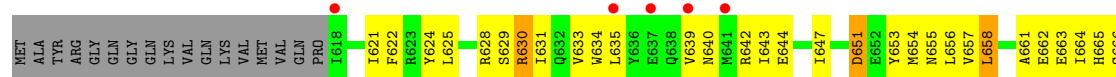
• Molecule 4: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D3

Chain R:



• Molecule 5: SMALL NUCLEAR RIBONUCLEOPROTEIN E

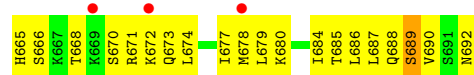
Chain E:



• Molecule 5: SMALL NUCLEAR RIBONUCLEOPROTEIN E

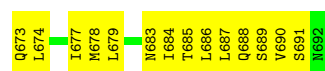
Chain L:





• Molecule 5: SMALL NUCLEAR RIBONUCLEOPROTEIN E

Chain S:



• Molecule 6: SMALL NUCLEAR RIBONUCLEOPROTEIN F

Chain F:



• Molecule 6: SMALL NUCLEAR RIBONUCLEOPROTEIN F

Chain M:



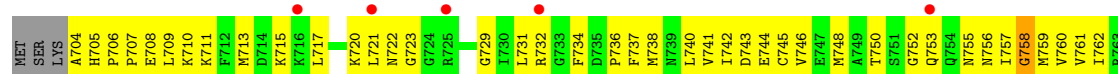
• Molecule 6: SMALL NUCLEAR RIBONUCLEOPROTEIN F

Chain T:



• Molecule 7: SMALL NUCLEAR RIBONUCLEOPROTEIN G

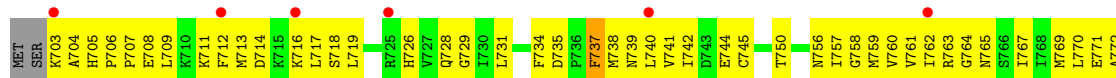
Chain G:





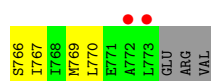
• Molecule 7: SMALL NUCLEAR RIBONUCLEOPROTEIN G

Chain N:



• Molecule 7: SMALL NUCLEAR RIBONUCLEOPROTEIN G

Chain U:



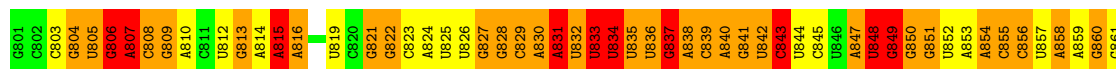
• Molecule 8: HOMO SAPIENS U4A SNRNA

Chain V:



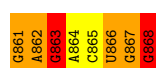
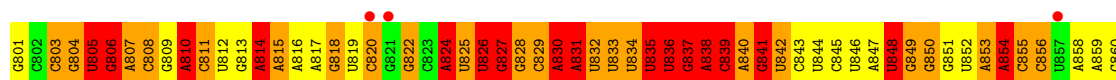
• Molecule 8: HOMO SAPIENS U4A SNRNA

Chain X:



• Molecule 8: HOMO SAPIENS U4A SNRNA

Chain Y:



4 Data and refinement statistics

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 66.15 – 3.47	Depositor EDS
% Data completeness (in resolution range)	82.9 (66.17-3.60) 60.8 (66.15-3.47)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.277 , 0.321 0.346 , 0.338	Depositor DCC
R_{free} test set	6801 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	78.5	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , -20.0	EDS
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 0.357 for -h,-k,l 0.339 for h,-h-k,-l 0.297 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	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.14$	Xtriage
Outliers	0 of 135989 reflections	Xtriage
F_o, F_c correlation	0.67	EDS
Total number of atoms	18887	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	A	0.61	0/743	0.72	0/989
1	H	0.66	0/769	0.79	0/1024
1	O	0.67	0/734	0.70	0/978
2	B	0.67	0/760	0.83	0/1026
2	I	0.65	1/760 (0.1%)	0.77	0/1026
2	P	0.62	0/763	0.74	0/1029
3	C	0.70	0/855	0.75	0/1141
3	J	0.64	0/863	0.76	0/1152
3	Q	0.64	0/718	0.77	0/962
4	D	0.70	1/704 (0.1%)	0.70	0/946
4	K	0.70	0/704	0.70	0/946
4	R	0.67	1/704 (0.1%)	0.70	0/946
5	E	0.63	0/629	0.77	1/842 (0.1%)
5	L	0.64	0/629	0.75	0/842
5	S	0.63	0/686	0.73	0/919
6	F	0.64	0/660	0.71	0/889
6	M	0.69	0/669	0.72	0/899
6	T	0.65	0/669	0.66	0/899
7	G	0.58	0/575	0.73	0/768
7	N	0.63	0/584	0.76	0/779
7	U	0.65	0/540	0.69	0/723
8	V	1.41	4/1626 (0.2%)	2.08	77/2534 (3.0%)
8	X	1.37	3/1626 (0.2%)	1.92	48/2534 (1.9%)
8	Y	1.42	5/1626 (0.3%)	2.01	72/2534 (2.8%)
All	All	0.90	15/19596 (0.1%)	1.23	198/27327 (0.7%)

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	V	826	U	C1'-N1	7.01	1.59	1.48
8	V	816	A	C3'-O3'	6.13	1.50	1.42
8	Y	831	A	C3'-O3'	6.12	1.50	1.42
4	R	91	GLN	C-N	-5.84	1.22	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Y	827	G	N1-C2	5.62	1.42	1.37

The worst 5 of 198 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	826	U	O4'-C1'-N1	12.31	118.05	108.20
8	Y	848	U	O4'-C1'-N1	10.10	116.28	108.20
8	Y	862	A	P-O3'-C3'	9.97	131.66	119.70
8	V	804	G	O4'-C1'-N9	9.88	116.11	108.20
8	V	858	A	P-O3'-C3'	9.87	131.54	119.70

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	733	0	768	79	0
1	H	759	0	796	76	0
1	O	724	0	755	81	0
2	B	751	0	807	121	0
2	I	751	0	807	126	0
2	P	754	0	811	169	0
3	C	845	0	892	139	0
3	J	852	0	900	156	0
3	Q	709	0	764	139	0
4	D	696	0	714	63	0
4	K	696	0	714	98	0
4	R	696	0	714	56	0
5	E	622	0	635	102	0
5	L	622	0	635	102	0
5	S	678	0	698	102	0
6	F	648	0	639	143	0
6	M	657	0	645	124	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	T	657	0	645	92	0
7	G	568	0	590	80	0
7	N	577	0	603	103	0
7	U	533	0	551	69	0
8	V	1453	0	733	125	0
8	X	1453	0	733	113	0
8	Y	1453	0	733	128	0
All	All	18887	0	17282	2059	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 57.

The worst 5 of 2059 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:688:GLN:OE1	7:G:757:ILE:HG21	1.18	1.33
4:K:47:THR:HG23	4:K:55:VAL:CG1	1.57	1.31
5:E:621:ILE:CD1	7:G:741:VAL:HG23	1.62	1.27
5:E:634:TRP:CZ2	5:E:642:ARG:HD2	1.70	1.26
5:E:621:ILE:HD12	7:G:741:VAL:CG2	1.70	1.20

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	89/95 (94%)	80 (90%)	9 (10%)	0	100	100
1	H	93/95 (98%)	84 (90%)	9 (10%)	0	100	100
1	O	88/95 (93%)	81 (92%)	6 (7%)	1 (1%)	21	78
2	B	94/119 (79%)	79 (84%)	11 (12%)	4 (4%)	4	46
2	I	94/119 (79%)	78 (83%)	13 (14%)	3 (3%)	6	55
2	P	94/119 (79%)	87 (93%)	6 (6%)	1 (1%)	21	78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	103/118 (87%)	89 (86%)	13 (13%)	1 (1%)	22	80
3	J	104/118 (88%)	93 (89%)	9 (9%)	2 (2%)	12	67
3	Q	88/118 (75%)	82 (93%)	3 (3%)	3 (3%)	6	54
4	D	87/126 (69%)	81 (93%)	5 (6%)	1 (1%)	21	78
4	K	87/126 (69%)	80 (92%)	6 (7%)	1 (1%)	21	78
4	R	87/126 (69%)	81 (93%)	4 (5%)	2 (2%)	10	63
5	E	73/92 (79%)	67 (92%)	6 (8%)	0	100	100
5	L	73/92 (79%)	66 (90%)	7 (10%)	0	100	100
5	S	80/92 (87%)	73 (91%)	5 (6%)	2 (2%)	9	61
6	F	81/86 (94%)	72 (89%)	7 (9%)	2 (2%)	9	61
6	M	81/86 (94%)	76 (94%)	4 (5%)	1 (1%)	19	77
6	T	81/86 (94%)	72 (89%)	7 (9%)	2 (2%)	9	61
7	G	71/76 (93%)	67 (94%)	2 (3%)	2 (3%)	8	59
7	N	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
7	U	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	72
All	All	1788/2136 (84%)	1622 (91%)	137 (8%)	29 (2%)	14	71

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	506	ASN
2	P	295	VAL
2	B	272	ASP
3	C	412	ASN
4	R	91	GLN

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	82/85 (96%)	81 (99%)	1 (1%)	82	96
1	H	85/85 (100%)	85 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	81/85 (95%)	80 (99%)	1 (1%)	82	96
2	B	88/101 (87%)	87 (99%)	1 (1%)	84	96
2	I	88/101 (87%)	86 (98%)	2 (2%)	63	92
2	P	89/101 (88%)	87 (98%)	2 (2%)	64	92
3	C	97/110 (88%)	93 (96%)	4 (4%)	41	85
3	J	98/110 (89%)	95 (97%)	3 (3%)	52	90
3	Q	83/110 (76%)	82 (99%)	1 (1%)	82	96
4	D	78/101 (77%)	78 (100%)	0	100	100
4	K	78/101 (77%)	76 (97%)	2 (3%)	59	91
4	R	78/101 (77%)	77 (99%)	1 (1%)	80	96
5	E	70/84 (83%)	66 (94%)	4 (6%)	29	77
5	L	70/84 (83%)	69 (99%)	1 (1%)	78	96
5	S	77/84 (92%)	75 (97%)	2 (3%)	59	91
6	F	70/74 (95%)	67 (96%)	3 (4%)	40	84
6	M	71/74 (96%)	70 (99%)	1 (1%)	78	96
6	T	71/74 (96%)	71 (100%)	0	100	100
7	G	63/66 (96%)	63 (100%)	0	100	100
7	N	64/66 (97%)	63 (98%)	1 (2%)	75	95
7	U	59/66 (89%)	59 (100%)	0	100	100
All	All	1640/1863 (88%)	1610 (98%)	30 (2%)	71	94

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	279	LEU
3	J	356	VAL
4	R	27	VAL
3	J	349	ASN
3	J	410	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
4	K	42	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L	640	ASN
6	T	543	GLN
4	K	57	GLN
4	K	91	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	V	67/68 (98%)	33 (49%)	6 (8%)
8	X	67/68 (98%)	35 (52%)	2 (2%)
8	Y	67/68 (98%)	39 (58%)	3 (4%)
All	All	201/204 (98%)	107 (53%)	11 (5%)

5 of 107 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	V	803	C
8	V	804	G
8	V	805	U
8	V	806	G
8	V	807	A

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	V	858	A
8	V	867	G
8	Y	830	A
8	V	836	U
8	X	837	G

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, 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	A	91/95 (95%)	0.46	3 (3%) 44 25	73, 95, 109, 132	0
1	H	95/95 (100%)	0.63	10 (10%) 7 6	72, 98, 109, 114	0
1	O	90/95 (94%)	0.53	6 (6%) 17 10	58, 95, 107, 128	0
2	B	96/119 (80%)	0.43	7 (7%) 15 9	71, 92, 106, 112	0
2	I	96/119 (80%)	0.49	4 (4%) 35 19	61, 94, 107, 120	0
2	P	96/119 (80%)	0.58	7 (7%) 15 9	67, 92, 105, 115	0
3	C	105/118 (88%)	0.40	1 (0%) 79 53	62, 93, 106, 113	0
3	J	106/118 (89%)	0.49	5 (4%) 30 17	64, 92, 107, 117	0
3	Q	90/118 (76%)	0.61	6 (6%) 17 10	62, 91, 105, 117	0
4	D	89/126 (70%)	0.63	7 (7%) 13 8	83, 96, 111, 125	0
4	K	89/126 (70%)	0.45	3 (3%) 43 24	81, 98, 112, 127	0
4	R	89/126 (70%)	0.53	5 (5%) 24 13	70, 96, 109, 120	0
5	E	75/92 (81%)	0.76	9 (12%) 5 5	76, 96, 115, 121	0
5	L	75/92 (81%)	0.69	5 (6%) 17 10	75, 97, 114, 117	0
5	S	82/92 (89%)	0.54	1 (1%) 75 49	68, 94, 103, 113	0
6	F	83/86 (96%)	0.60	5 (6%) 21 12	74, 93, 104, 121	0
6	M	83/86 (96%)	0.75	9 (10%) 6 6	74, 93, 106, 117	0
6	T	83/86 (96%)	0.62	2 (2%) 56 32	58, 88, 102, 110	0
7	G	73/76 (96%)	0.56	6 (8%) 12 8	80, 98, 113, 127	0
7	N	74/76 (97%)	0.48	6 (8%) 12 8	65, 97, 106, 111	0
7	U	70/76 (92%)	0.73	5 (7%) 16 9	68, 97, 111, 118	0
8	V	68/68 (100%)	0.27	0 100 100	55, 80, 107, 111	0
8	X	68/68 (100%)	0.34	0 100 100	58, 82, 100, 117	0
8	Y	68/68 (100%)	0.42	3 (4%) 33 18	48, 79, 104, 115	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	2034/2340 (86%)	0.54	115 (5%)	23	12	48, 94, 110, 132	0

The worst 5 of 115 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	753	GLN	6.3
4	D	54	ARG	5.8
1	H	148	PHE	5.7
7	U	773	LEU	5.2
7	N	725	ARG	4.7

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 carbohydrates 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.