



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 05:21 PM BST

PDB ID : 4V5U
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>

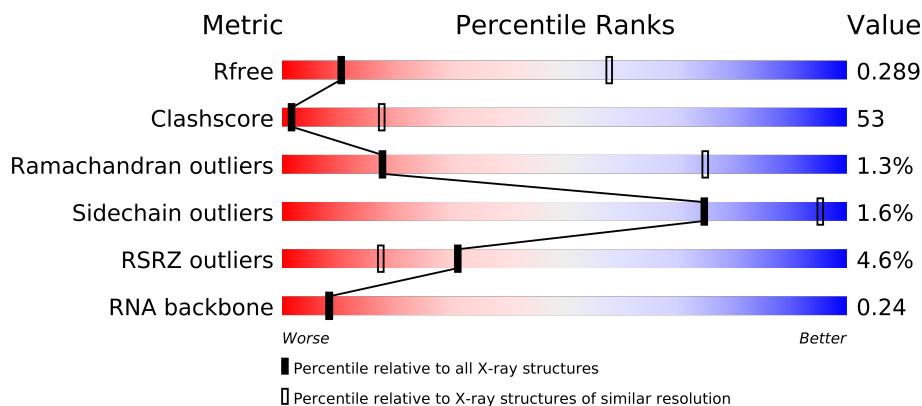
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
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) : stable23397

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	AA	95	
1	AH	95	
1	AO	95	
1	BA	95	
1	BH	95	
1	BO	95	
1	CA	95	
1	CH	95	
1	CO	95	
1	DA	95	
1	DH	95	

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Mol	Chain	Length	Quality of chain
1	DO	95	
2	AB	119	
2	AI	119	
2	AP	119	
2	BB	119	
2	BI	119	
2	BP	119	
2	CB	119	
2	CI	119	
2	CP	119	
2	DB	119	
2	DI	119	
2	DP	119	
3	AC	118	
3	AJ	118	
3	AQ	118	
3	BC	118	
3	BJ	118	
3	BQ	118	
3	CC	118	
3	CJ	118	
3	CQ	118	
3	DC	118	
3	DJ	118	
3	DQ	118	
4	AD	126	
4	AK	126	
4	AR	126	
4	BD	126	
4	BK	126	
4	BR	126	
4	CD	126	
4	CK	126	
4	CR	126	
4	DD	126	
4	DK	126	
4	DR	126	
5	AE	92	
5	AL	92	
5	AS	92	
5	BE	92	
5	BL	92	

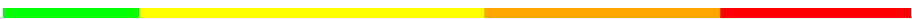
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Mol	Chain	Length	Quality of chain
5	BS	92	
5	CE	92	
5	CL	92	
5	CS	92	
5	DE	92	
5	DL	92	
5	DS	92	
6	AF	86	
6	AM	86	
6	AT	86	
6	BF	86	
6	BM	86	
6	BT	86	
6	CF	86	
6	CM	86	
6	CT	86	
6	DF	86	
6	DM	86	
6	DT	86	
7	AG	76	
7	AN	76	
7	AU	76	
7	BG	76	
7	BN	76	
7	BU	76	
7	CG	76	
7	CN	76	
7	CU	76	
7	DG	76	
7	DN	76	
7	DU	76	
8	AV	68	
8	AX	68	
8	AY	68	
8	BV	68	
8	BX	68	
8	BY	68	
8	CV	68	
8	CX	68	
8	CY	68	
8	DV	68	
8	DX	68	

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Mol	Chain	Length	Quality of chain
8	DY	68	 A horizontal bar chart representing the quality of the protein chain. The bar is divided into four segments of different colors: green (approximately 15% of the length), yellow (approximately 45% of the length), orange (approximately 25% of the length), and red (approximately 15% of the length). The green segment indicates good quality, while the red segment indicates poor quality.

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 75557 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	AA	90	Total	C	N	O	S	0	0	0
			724	455	133	129	7			
1	AH	91	Total	C	N	O	S	0	0	0
			733	461	135	130	7			
1	AO	89	Total	C	N	O	S	0	0	0
			718	452	132	127	7			
1	BA	91	Total	C	N	O	S	0	0	0
			733	461	135	130	7			
1	BH	95	Total	C	N	O	S	0	0	0
			759	477	139	135	8			
1	BO	90	Total	C	N	O	S	0	0	0
			724	455	133	129	7			
1	CA	90	Total	C	N	O	S	0	0	0
			724	455	133	129	7			
1	CH	91	Total	C	N	O	S	0	0	0
			733	461	135	130	7			
1	CO	91	Total	C	N	O	S	0	0	0
			733	461	135	130	7			
1	DA	90	Total	C	N	O	S	0	0	0
			724	455	133	129	7			
1	DH	95	Total	C	N	O	S	0	0	0
			759	477	139	135	8			
1	DO	91	Total	C	N	O	S	0	0	0
			733	461	135	130	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	97	Total	C	N	O	S	0	0	1
			759	482	135	138	4			
2	AI	96	Total	C	N	O	S	0	0	1
			751	477	134	137	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AP	95	Total	C	N	O	S	0	0	1
			746	474	133	136	3			
2	BB	96	Total	C	N	O	S	0	0	1
			751	477	134	137	3			
2	BI	96	Total	C	N	O	S	0	0	1
			751	477	134	137	3			
2	BP	96	Total	C	N	O	S	0	0	1
			754	479	134	137	4			
2	CB	97	Total	C	N	O	S	0	0	1
			759	482	135	138	4			
2	CI	96	Total	C	N	O	S	0	0	1
			751	477	134	137	3			
2	CP	95	Total	C	N	O	S	0	0	1
			746	474	133	136	3			
2	DB	96	Total	C	N	O	S	0	0	1
			754	479	134	137	4			
2	DI	94	Total	C	N	O	S	0	0	1
			737	468	131	135	3			
2	DP	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	AC	105	Total	C	N	O	S	0	0	0
			845	529	157	154	5			
3	AJ	107	Total	C	N	O	S	0	0	0
			859	538	159	157	5			
3	AQ	90	Total	C	N	O	S	0	0	1
			709	446	135	123	5			
3	BC	105	Total	C	N	O	S	0	0	0
			845	529	157	154	5			
3	BJ	106	Total	C	N	O	S	0	0	0
			852	534	158	155	5			
3	BQ	90	Total	C	N	O	S	0	0	1
			709	446	135	123	5			
3	CC	105	Total	C	N	O	S	0	0	0
			845	529	157	154	5			
3	CJ	107	Total	C	N	O	S	0	0	0
			859	538	159	157	5			
3	CQ	92	Total	C	N	O	S	0	0	1
			728	459	138	126	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	DC	105	Total	C	N	O	S	0	0	0
			845	529	157	154	5			
3	DJ	106	Total	C	N	O	S	0	0	0
			852	534	158	155	5			
3	DQ	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	AD	89	Total	C	N	O	S	0	0	1
			696	433	126	130	7			
4	AK	89	Total	C	N	O	S	0	0	1
			696	433	126	130	7			
4	AR	89	Total	C	N	O	S	0	0	1
			696	433	126	130	7			
4	BD	89	Total	C	N	O	S	0	0	1
			696	433	126	130	7			
4	BK	89	Total	C	N	O	S	0	0	1
			696	433	126	130	7			
4	BR	89	Total	C	N	O	S	0	0	1
			696	433	126	130	7			
4	CD	89	Total	C	N	O	S	0	0	1
			696	433	126	130	7			
4	CK	90	Total	C	N	O	S	0	0	1
			700	435	127	131	7			
4	CR	89	Total	C	N	O	S	0	0	1
			696	433	126	130	7			
4	DD	89	Total	C	N	O	S	0	0	1
			696	433	126	130	7			
4	DK	89	Total	C	N	O	S	0	0	1
			696	433	126	130	7			
4	DR	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	AE	86	Total	C	N	O	S	0	0	0
			707	446	127	129	5			
5	AL	76	Total	C	N	O	S	0	0	0
			629	397	112	116	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AS	78	Total	C	N	O	S	0	0	0
			645	407	115	119	4			
5	BE	75	Total	C	N	O	S	0	0	0
			622	392	111	115	4			
5	BL	75	Total	C	N	O	S	0	0	0
			622	392	111	115	4			
5	BS	82	Total	C	N	O	S	0	0	0
			678	428	121	124	5			
5	CE	84	Total	C	N	O	S	0	0	0
			694	439	124	126	5			
5	CL	75	Total	C	N	O	S	0	0	0
			622	392	111	115	4			
5	CS	78	Total	C	N	O	S	0	0	0
			645	407	115	119	4			
5	DE	76	Total	C	N	O	S	0	0	0
			629	397	112	116	4			
5	DL	75	Total	C	N	O	S	0	0	0
			622	392	111	115	4			
5	DS	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	AF	83	Total	C	N	O	S	0	0	0
			657	416	107	128	6			
6	AM	83	Total	C	N	O	S	0	0	0
			657	416	107	128	6			
6	AT	83	Total	C	N	O	S	0	0	0
			657	416	107	128	6			
6	BF	83	Total	C	N	O	S	0	0	1
			648	411	107	124	6			
6	BM	83	Total	C	N	O	S	0	0	0
			657	416	107	128	6			
6	BT	83	Total	C	N	O	S	0	0	0
			657	416	107	128	6			
6	CF	82	Total	C	N	O	S	0	0	1
			637	405	103	123	6			
6	CM	83	Total	C	N	O	S	0	0	0
			657	416	107	128	6			
6	CT	83	Total	C	N	O	S	0	0	0
			657	416	107	128	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	DF	83	Total	C	N	O	S	0	0	0
			657	416	107	128	6			
6	DM	83	Total	C	N	O	S	0	0	0
			657	416	107	128	6			
6	DT	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	AG	73	Total	C	N	O	S	0	0	0
			568	358	102	102	6			
7	AN	71	Total	C	N	O	S	0	0	1
			541	342	97	96	6			
7	AU	73	Total	C	N	O	S	0	0	0
			568	358	102	102	6			
7	BG	73	Total	C	N	O	S	0	0	0
			568	358	102	102	6			
7	BN	74	Total	C	N	O	S	0	0	0
			577	364	104	103	6			
7	BU	70	Total	C	N	O	S	0	0	1
			533	336	96	95	6			
7	CG	73	Total	C	N	O	S	0	0	0
			568	358	102	102	6			
7	CN	70	Total	C	N	O	S	0	0	1
			533	336	96	95	6			
7	CU	73	Total	C	N	O	S	0	0	0
			568	358	102	102	6			
7	DG	73	Total	C	N	O	S	0	0	0
			566	356	102	102	6			
7	DN	73	Total	C	N	O	S	0	0	0
			568	358	102	102	6			
7	DU	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	AV	68	Total	C	N	O	P	0	0	0
			1453	650	263	473	67			
8	AX	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	AY	68	Total 1453	C 650	N 263	O 473	P 67	0	0	0
8	BV	68	Total 1453	C 650	N 263	O 473	P 67	0	0	0
8	BX	68	Total 1453	C 650	N 263	O 473	P 67	0	0	0
8	BY	68	Total 1453	C 650	N 263	O 473	P 67	0	0	0
8	CV	68	Total 1453	C 650	N 263	O 473	P 67	0	0	0
8	CX	68	Total 1453	C 650	N 263	O 473	P 67	0	0	0
8	CY	68	Total 1453	C 650	N 263	O 473	P 67	0	0	0
8	DV	68	Total 1453	C 650	N 263	O 473	P 67	0	0	0
8	DX	68	Total 1453	C 650	N 263	O 473	P 67	0	0	0
8	DY	68	Total 1453	C 650	N 263	O 473	P 67	0	0	0

There are 372 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AV	?	-	U	DELETION	GB 36174
AV	?	-	G	DELETION	GB 36174
AV	?	-	C	DELETION	GB 36174
AV	?	-	A	DELETION	GB 36174
AV	?	-	A	DELETION	GB 36174
AV	?	-	U	DELETION	GB 36174
AV	?	-	A	DELETION	GB 36174
AV	?	-	U	DELETION	GB 36174
AV	813	G	-	INSERTION	GB 36174
AV	814	A	-	INSERTION	GB 36174
AV	815	A	-	INSERTION	GB 36174
AV	816	A	-	INSERTION	GB 36174
AV	?	-	U	DELETION	GB 36174
AV	?	-	A	DELETION	GB 36174
AV	?	-	C	DELETION	GB 36174
AV	?	-	G	DELETION	GB 36174
AV	846	U	-	INSERTION	GB 36174
AV	847	A	-	INSERTION	GB 36174
AV	848	U	-	INSERTION	GB 36174

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

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

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

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

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

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

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

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

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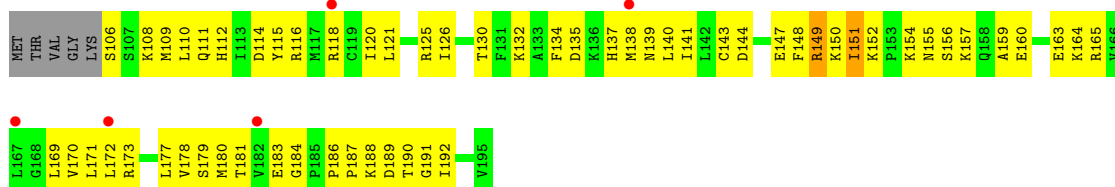
Chain	Residue	Modelled	Actual	Comment	Reference
DY	?	-	C	DELETION	GB 36174
DY	?	-	G	DELETION	GB 36174
DY	846	U	-	INSERTION	GB 36174
DY	847	A	-	INSERTION	GB 36174
DY	848	U	-	INSERTION	GB 36174
DY	849	G	-	INSERTION	GB 36174
DY	850	G	-	INSERTION	GB 36174
DY	851	G	-	INSERTION	GB 36174
DY	852	U	-	INSERTION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

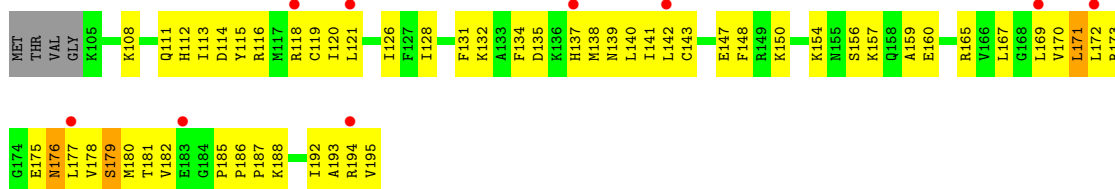
- Molecule 1: SMALL NUCLEAR RIBONUCLEOPROTEIN-ASSOCIATED PROTEINS B AND B'

Chain AA: 



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

Chain AH: 



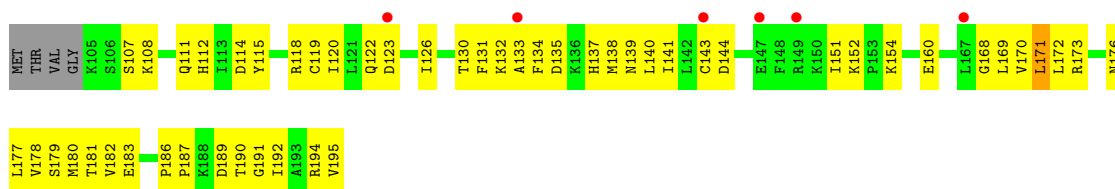
- Molecule 1: SMALL NUCLEAR RIBONUCLEOPROTEIN-ASSOCIATED PROTEINS B AND B'

Chain AO: 



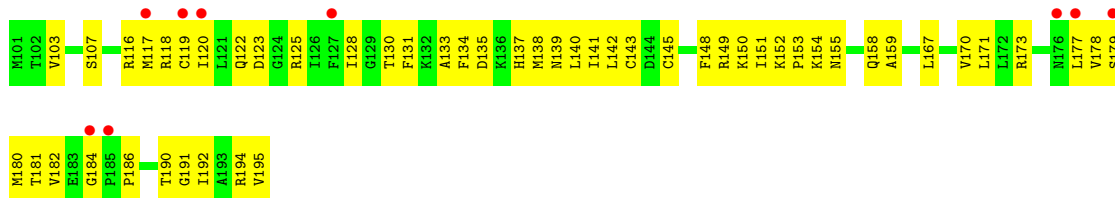
- Molecule 1: SMALL NUCLEAR RIBONUCLEOPROTEIN-ASSOCIATED PROTEINS B AND B'

Chain BA: 



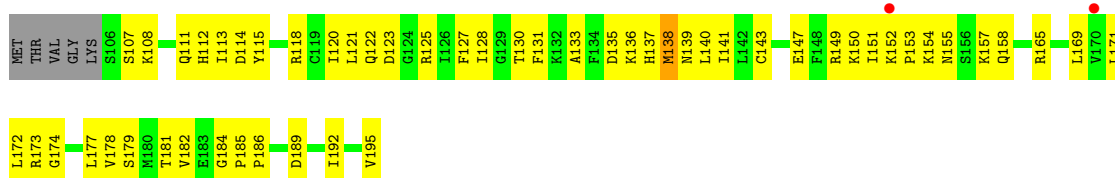
- Molecule 1: SMALL NUCLEAR RIBONUCLEOPROTEIN-ASSOCIATED PROTEINS B AND B'

Chain BH:



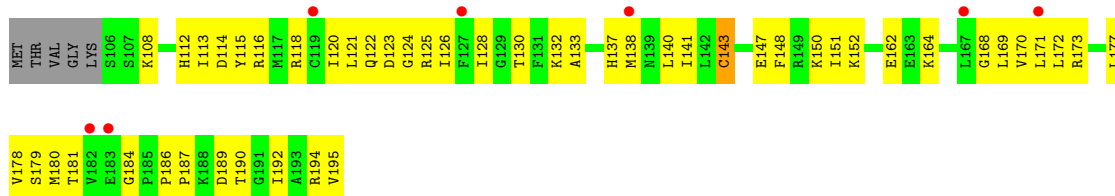
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Chain BO:



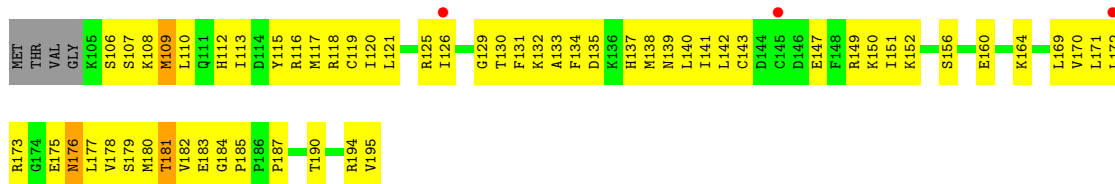
- Molecule 1: SMALL NUCLEAR RIBONUCLEOPROTEIN-ASSOCIATED PROTEINS B AND B'

Chain CA:



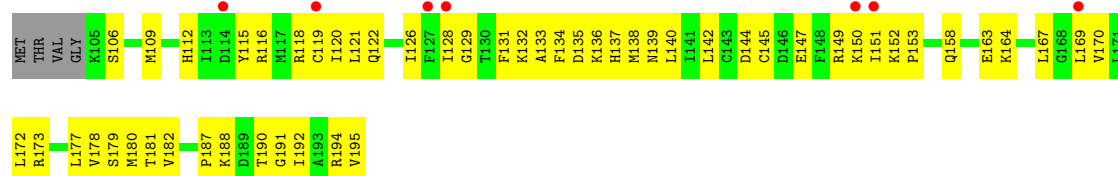
- Molecule 1: SMALL NUCLEAR RIBONUCLEOPROTEIN-ASSOCIATED PROTEINS B AND B'

Chain CH:



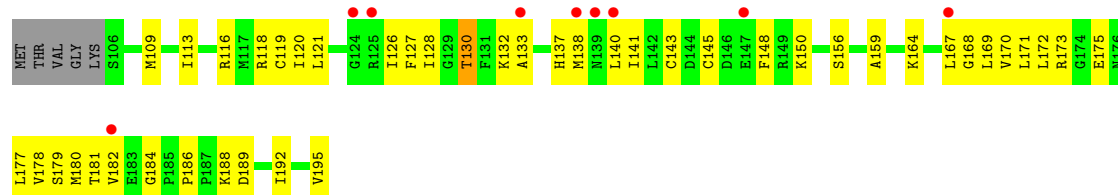
- Molecule 1: SMALL NUCLEAR RIBONUCLEOPROTEIN-ASSOCIATED PROTEINS B AND B'

Chain CO:



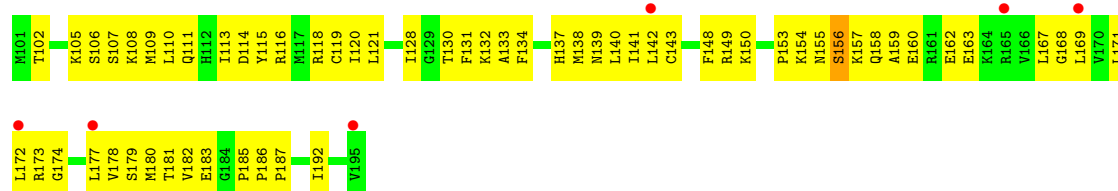
- Molecule 1: SMALL NUCLEAR RIBONUCLEOPROTEIN-ASSOCIATED PROTEINS B AND B'

Chain DA:



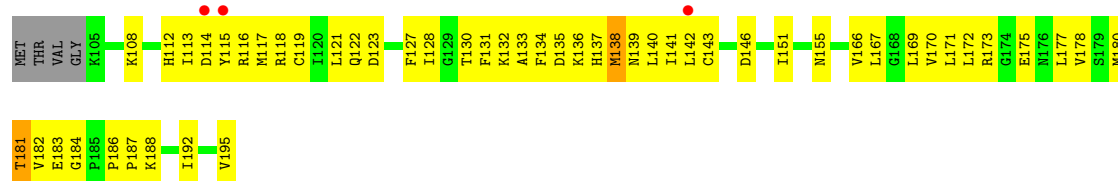
- Molecule 1: SMALL NUCLEAR RIBONUCLEOPROTEIN-ASSOCIATED PROTEINS B AND B'

Chain DH:



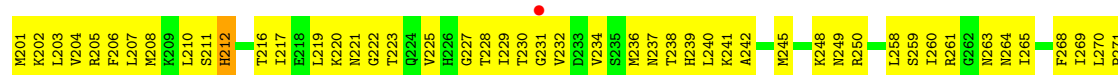
- Molecule 1: SMALL NUCLEAR RIBONUCLEOPROTEIN-ASSOCIATED PROTEINS B AND B'

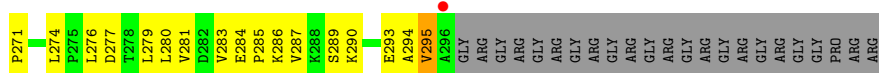
Chain DO:



- Molecule 2: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D1

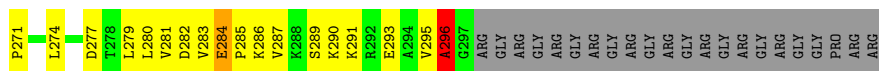
Chain AB:





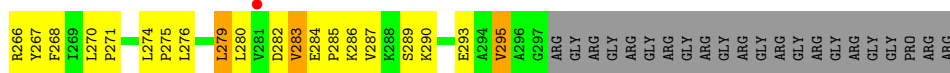
• Molecule 2: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D1

Chain CB:



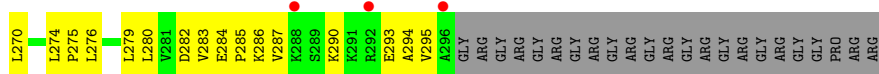
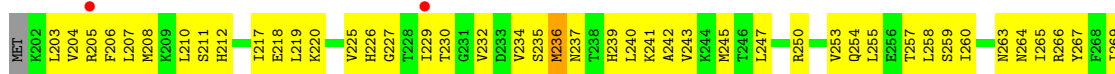
• Molecule 2: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D1

Chain CI:



• Molecule 2: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D1

Chain CP:



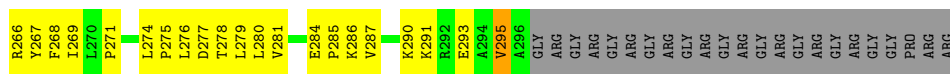
• Molecule 2: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D1

Chain DB:

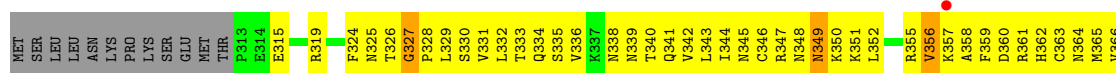


• Molecule 2: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D1

Chain DI:

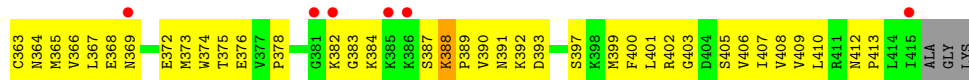


Chain BJ:



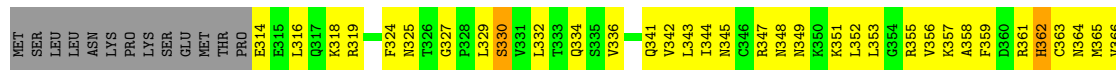
- Molecule 3: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D2

Chain BQ:



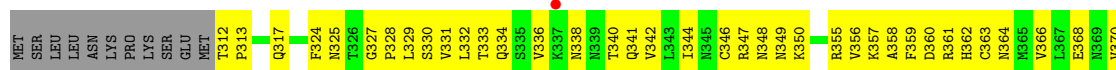
- Molecule 3: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D2

Chain CC:



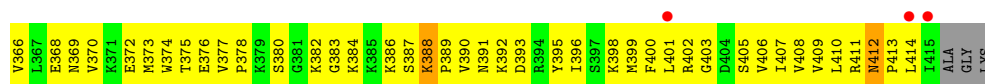
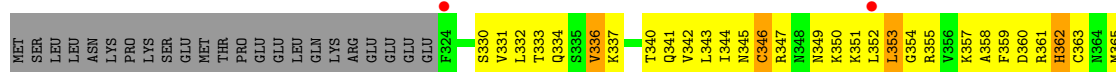
- Molecule 3: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D2

Chain CJ:



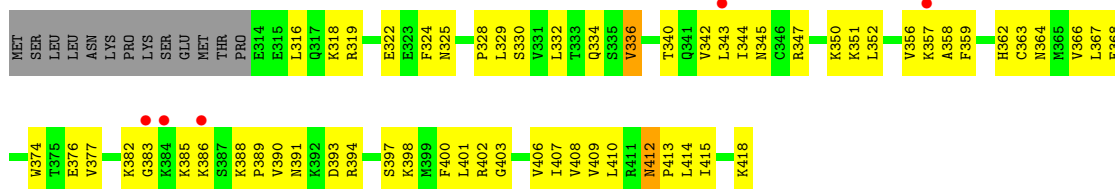
- Molecule 3: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D2

Chain CQ:



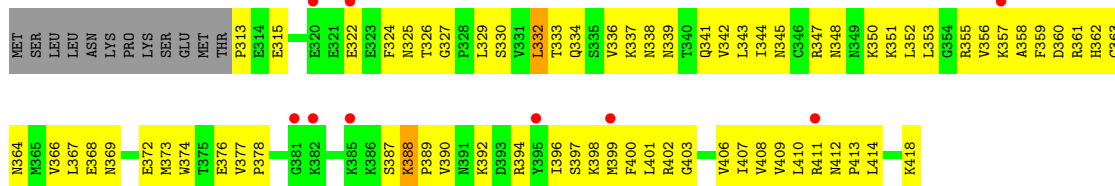
- Molecule 3: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D2

Chain DC:



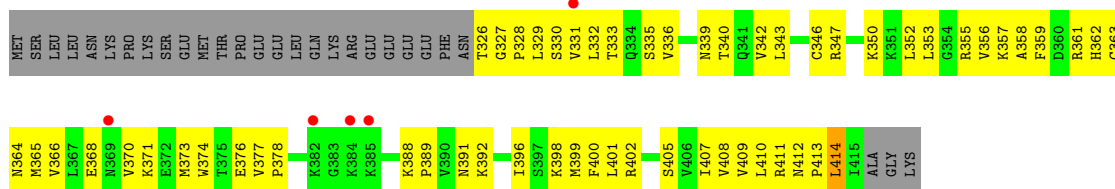
• Molecule 3: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D2

Chain DJ:



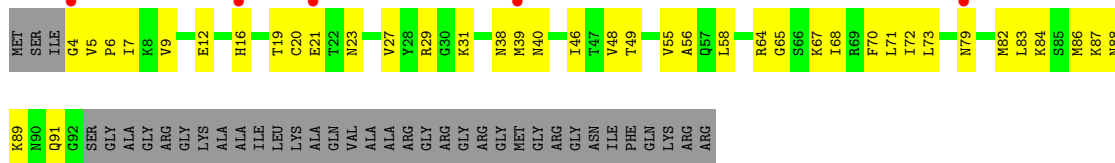
• Molecule 3: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D2

Chain DQ:



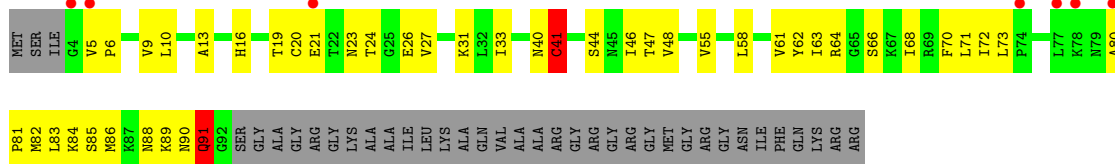
• Molecule 4: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D3

Chain AD:



• Molecule 4: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D3

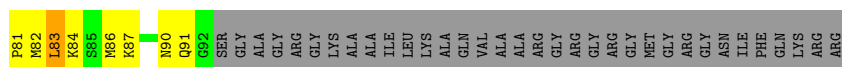
Chain AK:



• Molecule 4: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D3

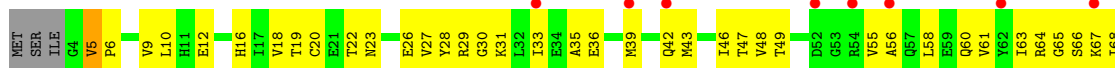
Chain AR:





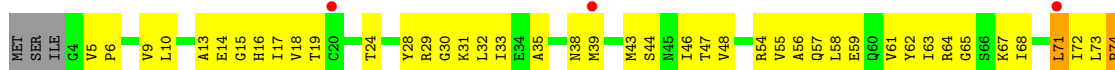
• Molecule 4: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D3

Chain BD:



• Molecule 4: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D3

Chain BK:



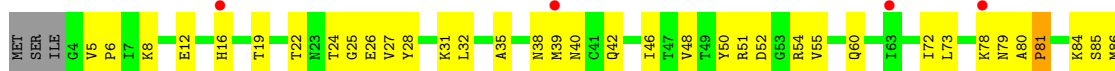
• Molecule 4: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D3

Chain BR:



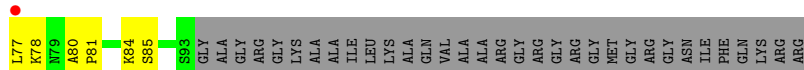
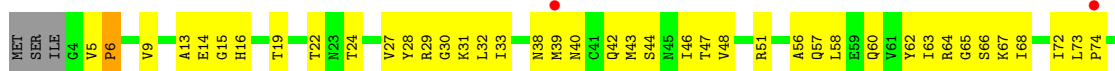
• Molecule 4: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D3

Chain CD:



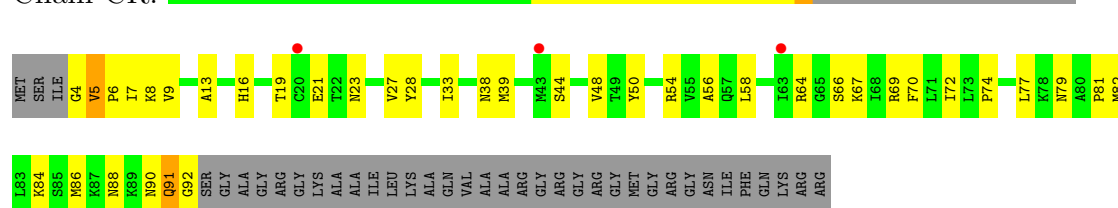
• Molecule 4: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D3

Chain CK:



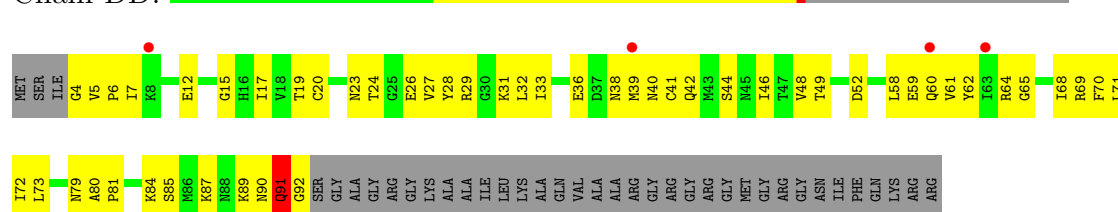
- Molecule 4: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D3

Chain CR:



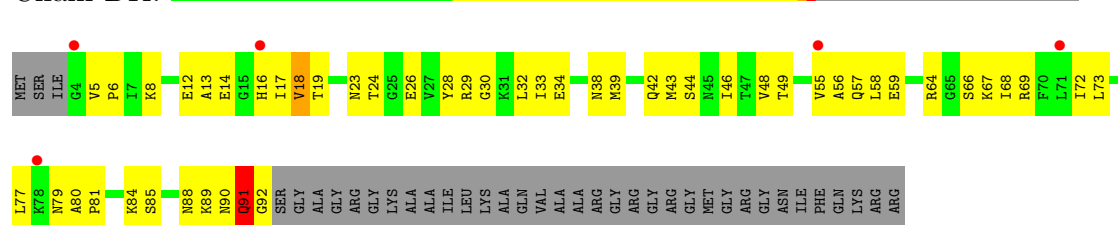
- Molecule 4: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D3

Chain DD:



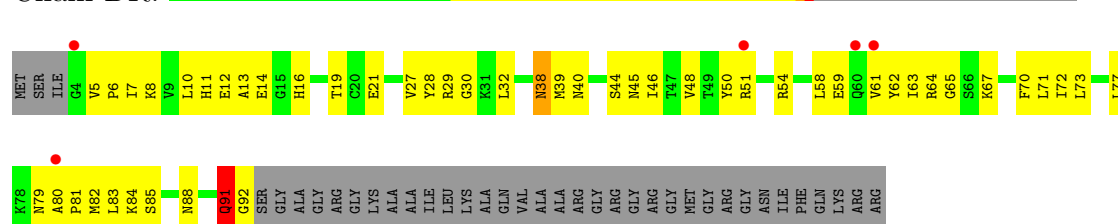
- Molecule 4: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D3

Chain DK:



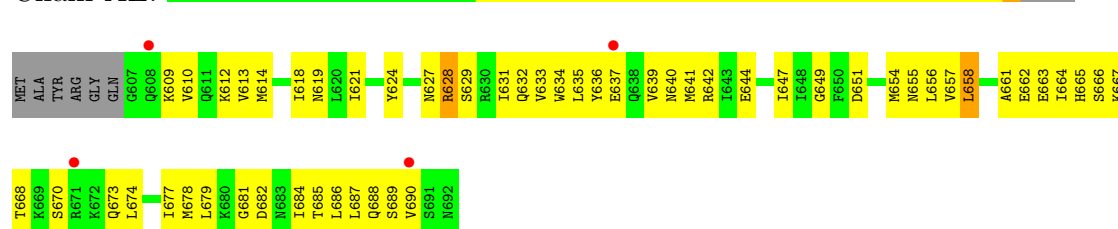
- Molecule 4: SMALL NUCLEAR RIBONUCLEOPROTEIN SM D3

Chain DR:



- Molecule 5: SMALL NUCLEAR RIBONUCLEOPROTEIN E

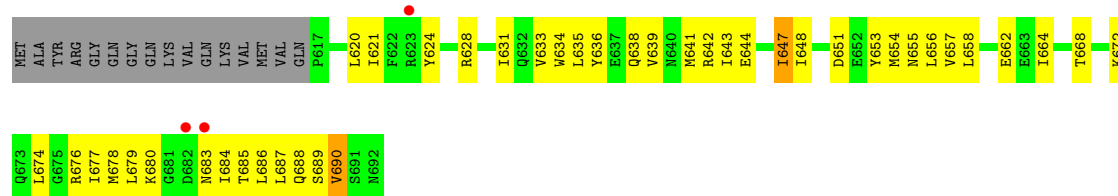
Chain AE:



- Molecule 5: SMALL NUCLEAR RIBONUCLEOPROTEIN E

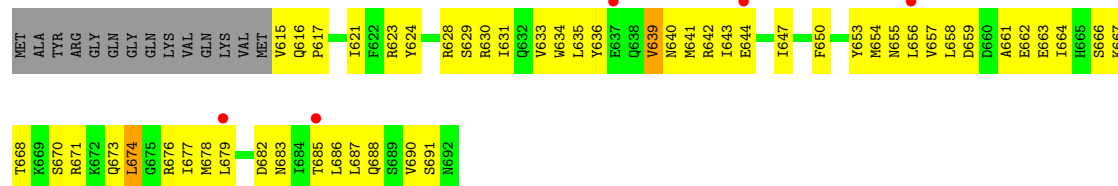
Chain AL:





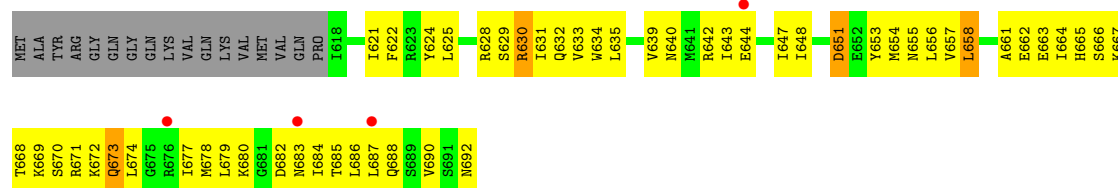
• Molecule 5: SMALL NUCLEAR RIBONUCLEOPROTEIN E

Chain AS: 



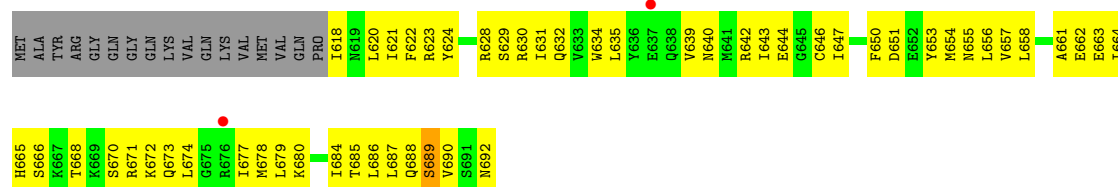
• Molecule 5: SMALL NUCLEAR RIBONUCLEOPROTEIN E

Chain BE: 



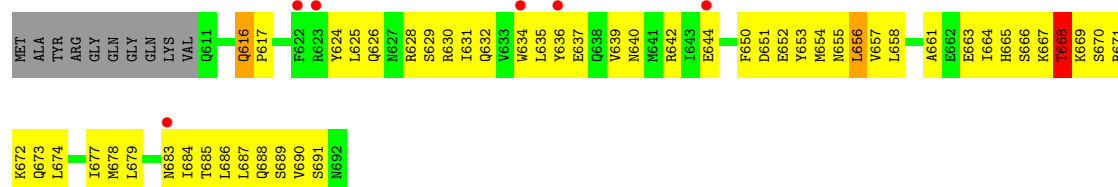
• Molecule 5: SMALL NUCLEAR RIBONUCLEOPROTEIN E

Chain BL: 



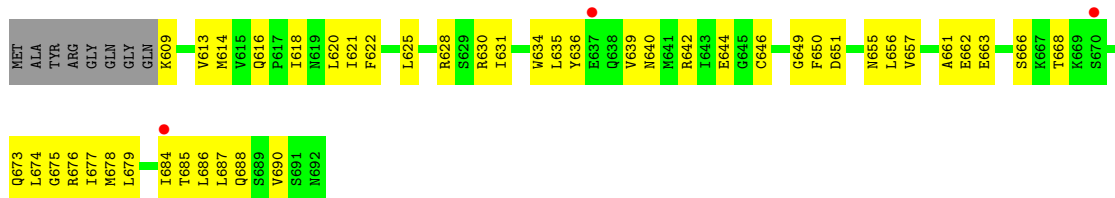
• Molecule 5: SMALL NUCLEAR RIBONUCLEOPROTEIN E

Chain BS: 



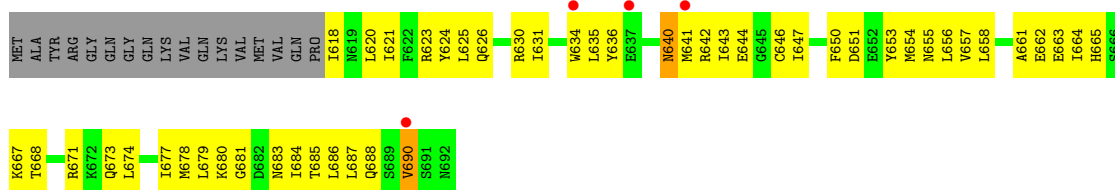
• Molecule 5: SMALL NUCLEAR RIBONUCLEOPROTEIN E

Chain CE: 



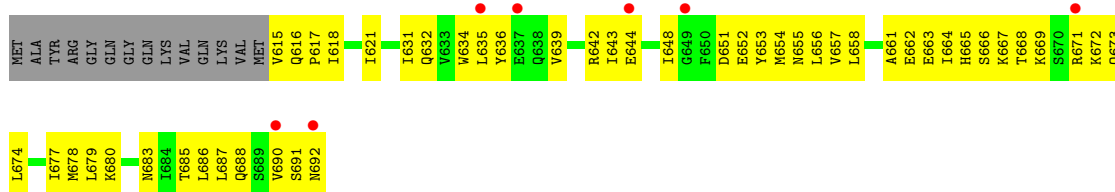
• Molecule 5: SMALL NUCLEAR RIBONUCLEOPROTEIN E

Chain CL:



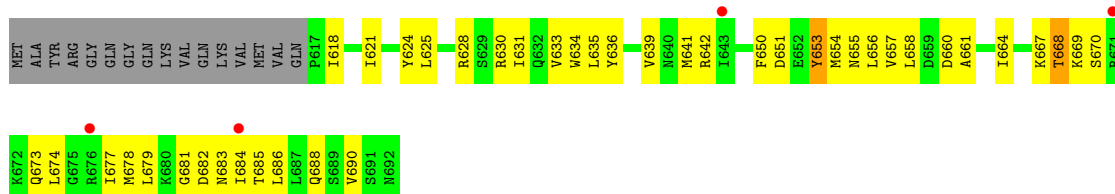
• Molecule 5: SMALL NUCLEAR RIBONUCLEOPROTEIN E

Chain CS:



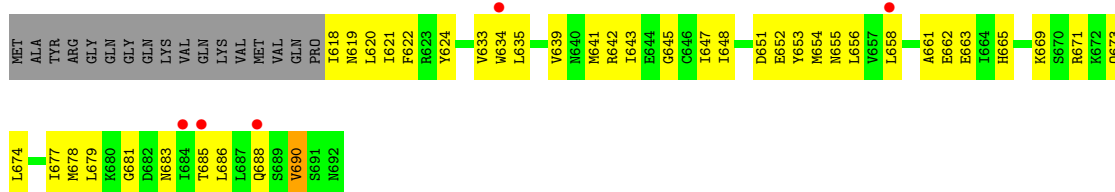
• Molecule 5: SMALL NUCLEAR RIBONUCLEOPROTEIN E

Chain DE:



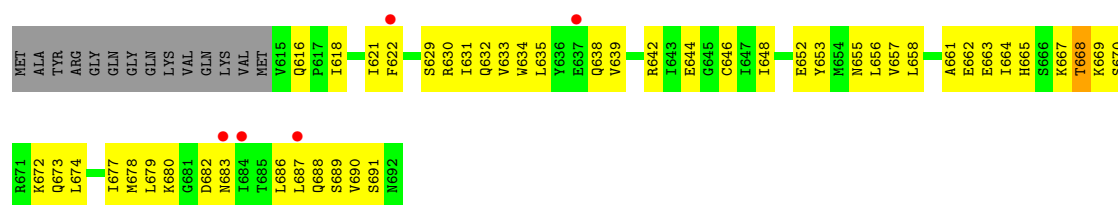
• Molecule 5: SMALL NUCLEAR RIBONUCLEOPROTEIN E

Chain DL:



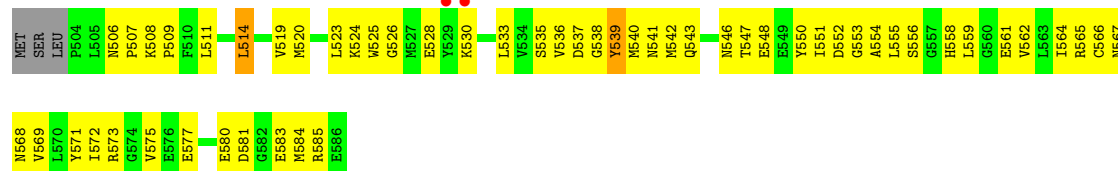
• Molecule 5: SMALL NUCLEAR RIBONUCLEOPROTEIN E

Chain DS:



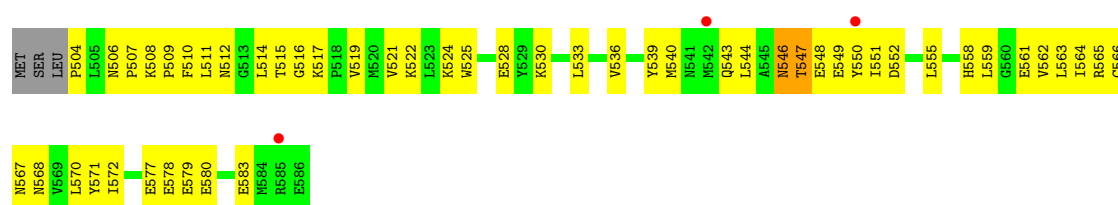
• Molecule 6: SMALL NUCLEAR RIBONUCLEOPROTEIN F

Chain AF:



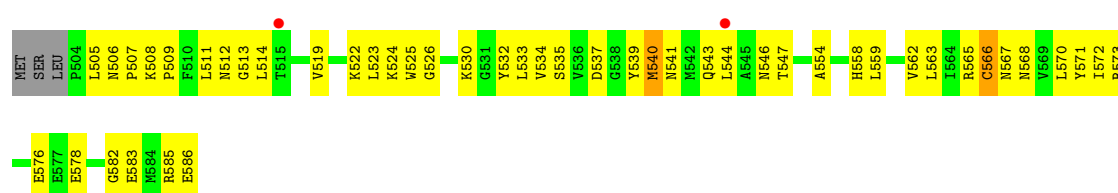
• Molecule 6: SMALL NUCLEAR RIBONUCLEOPROTEIN F

Chain AM:



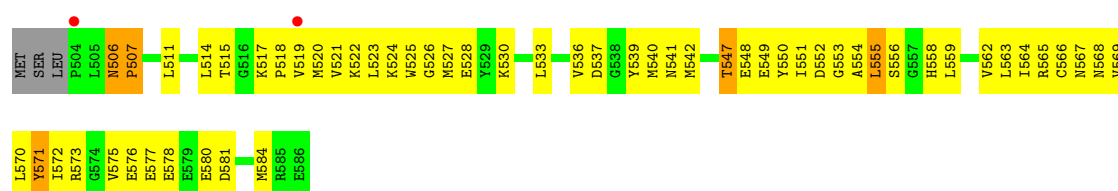
• Molecule 6: SMALL NUCLEAR RIBONUCLEOPROTEIN F

Chain AT:



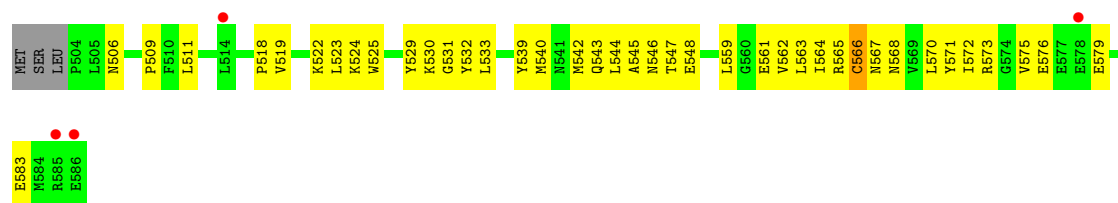
• Molecule 6: SMALL NUCLEAR RIBONUCLEOPROTEIN F

Chain BF:



• Molecule 6: SMALL NUCLEAR RIBONUCLEOPROTEIN F

Chain BM:



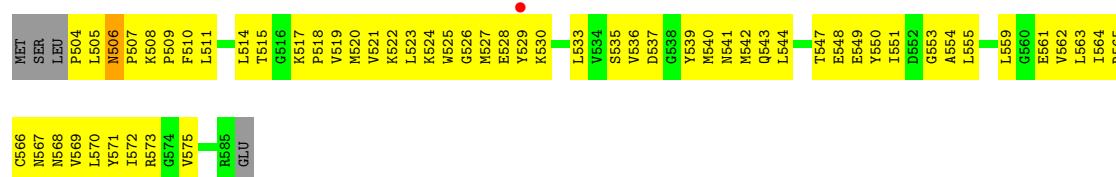
• Molecule 6: SMALL NUCLEAR RIBONUCLEOPROTEIN F

Chain BT:



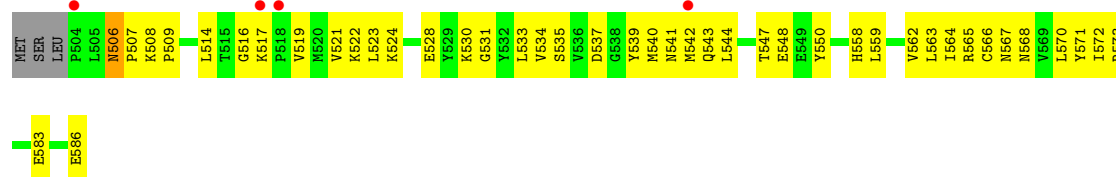
• Molecule 6: SMALL NUCLEAR RIBONUCLEOPROTEIN F

Chain CF:



• Molecule 6: SMALL NUCLEAR RIBONUCLEOPROTEIN F

Chain CM:



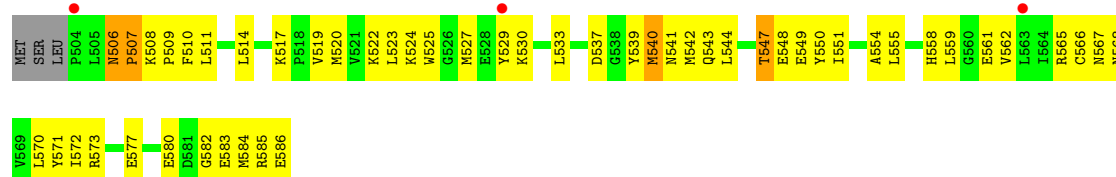
• Molecule 6: SMALL NUCLEAR RIBONUCLEOPROTEIN F

Chain CT:



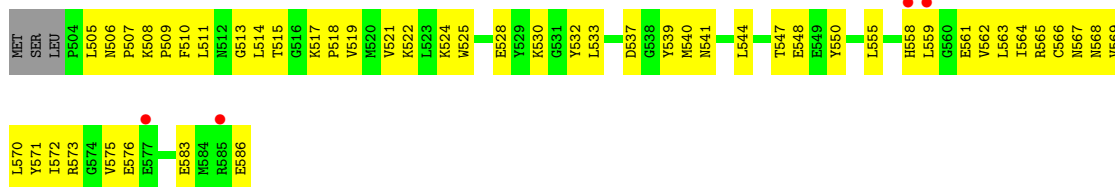
• Molecule 6: SMALL NUCLEAR RIBONUCLEOPROTEIN F

Chain DF:



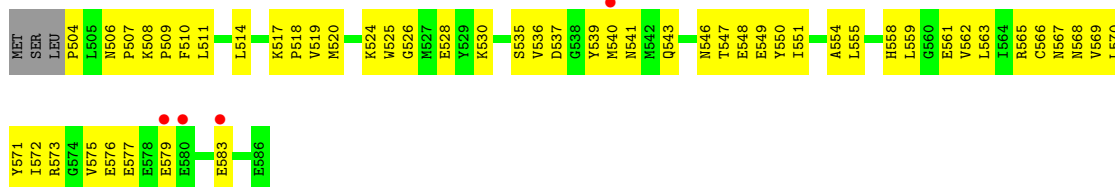
- Molecule 6: SMALL NUCLEAR RIBONUCLEOPROTEIN F

Chain DM:



- Molecule 6: SMALL NUCLEAR RIBONUCLEOPROTEIN F

Chain DT:



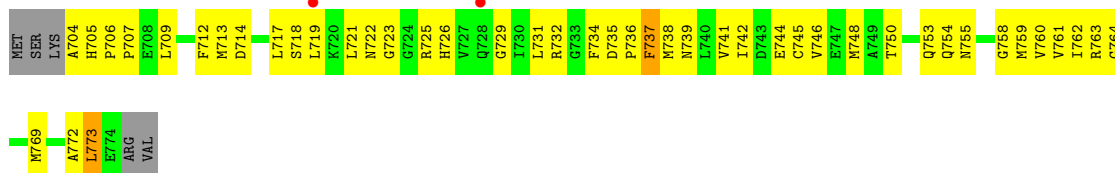
- Molecule 7: SMALL NUCLEAR RIBONUCLEOPROTEIN G

Chain AG:



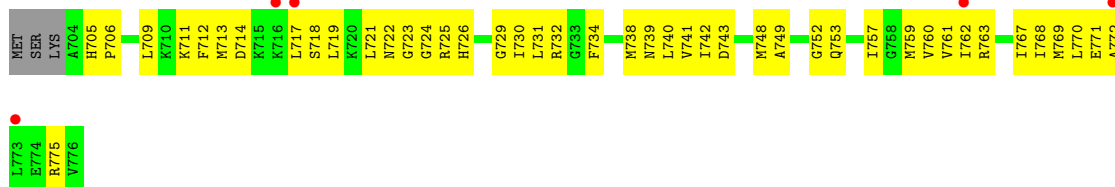
- Molecule 7: SMALL NUCLEAR RIBONUCLEOPROTEIN G

Chain AN:



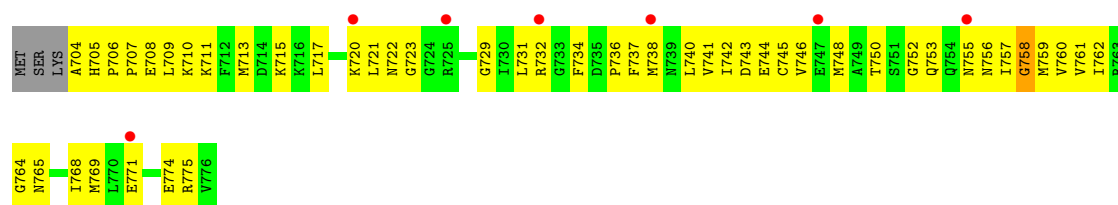
- Molecule 7: SMALL NUCLEAR RIBONUCLEOPROTEIN G

Chain AU:



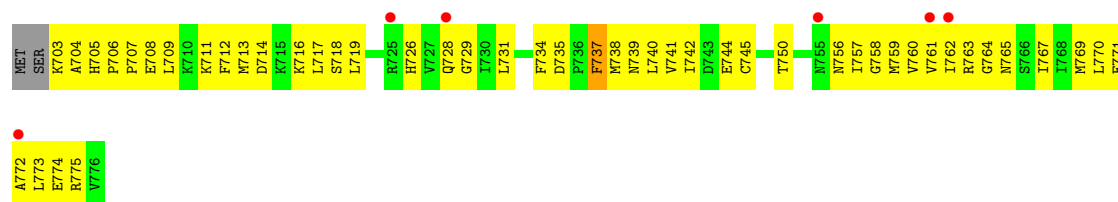
- Molecule 7: SMALL NUCLEAR RIBONUCLEOPROTEIN G

Chain BG:



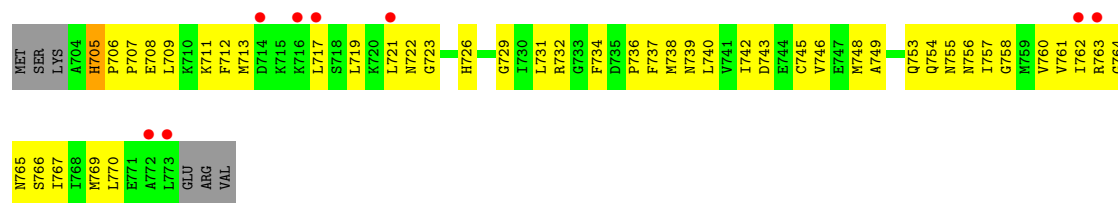
• Molecule 7: SMALL NUCLEAR RIBONUCLEOPROTEIN G

Chain BN:



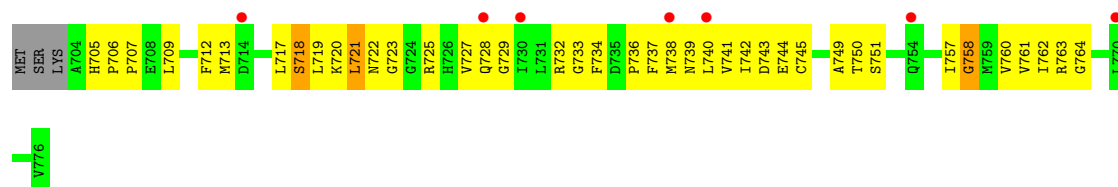
• Molecule 7: SMALL NUCLEAR RIBONUCLEOPROTEIN G

Chain BU:



• Molecule 7: SMALL NUCLEAR RIBONUCLEOPROTEIN G

Chain CG:



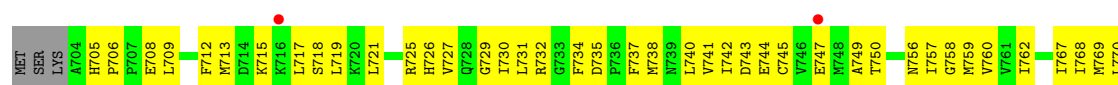
• Molecule 7: SMALL NUCLEAR RIBONUCLEOPROTEIN G

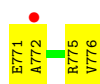
Chain CN:



• Molecule 7: SMALL NUCLEAR RIBONUCLEOPROTEIN G

Chain CU:





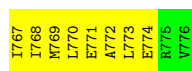
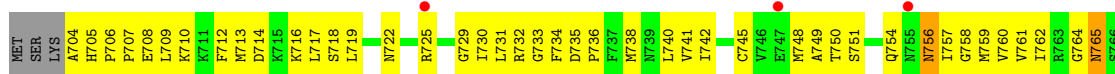
• Molecule 7: SMALL NUCLEAR RIBONUCLEOPROTEIN G

Chain DG:



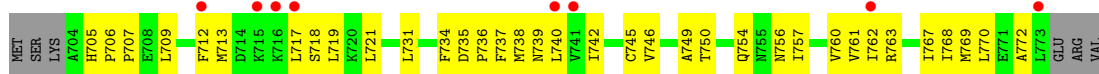
• Molecule 7: SMALL NUCLEAR RIBONUCLEOPROTEIN G

Chain DN:



• Molecule 7: SMALL NUCLEAR RIBONUCLEOPROTEIN G

Chain DU:



• Molecule 8: HOMO SAPIENS U4A SNRNA

Chain AV:



• Molecule 8: HOMO SAPIENS U4A SNRNA

Chain AX:



• Molecule 8: HOMO SAPIENS U4A SNRNA

Chain AY:

G801 G802 G803 G804 G805 G806 G807 G808 G809 G810 G811 G812 G813 G814 G815 G816 G817 G818 G819 G820 G821 G822 G823 G824 G825 G826 G827 G828 G829 G830 G831 G832 G833 G834 G835 G836 G837 G838 G839 G840 G841 G842 G843 G844 G845 G846 G847 G848 G849 G850 G851 G852 G853 G854 G855 G856 G857 G858 G859 G860

G861 G862 G863 G864 G865 G866 G867 G868

• Molecule 8: HOMO SAPIENS U4A SNRNA

Chain BV:

G801 G802 G803 G804 G805 G806 G807 G808 G809 G810 G811 G812 G813 G814 G815 G816 G817 G818 G819 G820 G821 G822 G823 G824 G825 G826 G827 G828 G829 G830 G831 G832 G833 G834 G835 G836 G837 G838 G839 G840 G841 G842 G843 G844 G845 G846 G847 G848 G849 G850 G851 G852 G853 G854 G855 G856 G857 G858 G859 G860

G861 G862 G863 G864 G865 G866 G867 G868

• Molecule 8: HOMO SAPIENS U4A SNRNA

Chain BX:

G801 G802 G803 G804 G805 G806 G807 G808 G809 G810 G811 G812 G813 G814 G815 G816 G817 G818 G819 G820 G821 G822 G823 G824 G825 G826 G827 G828 G829 G830 G831 G832 G833 G834 G835 G836 G837 G838 G839 G840 G841 G842 G843 G844 G845 G846 G847 G848 G849 G850 G851 G852 G853 G854 G855 G856 G857 G858 G859 G860

G862 G863 G864 G865 G866 G867 G868

• Molecule 8: HOMO SAPIENS U4A SNRNA

Chain BY:

G801 G802 G803 G804 G805 G806 G807 G808 G809 G810 G811 G812 G813 G814 G815 G816 G817 G818 G819 G820 G821 G822 G823 G824 G825 G826 G827 G828 G829 G830 G831 G832 G833 G834 G835 G836 G837 G838 G839 G840 G841 G842 G843 G844 G845 G846 G847 G848 G849 G850 G851 G852 G853 G854 G855 G856 G857 G858 G859 G860

G861 G862 G863 G864 G865 G866 G867 G868

• Molecule 8: HOMO SAPIENS U4A SNRNA

Chain CV:

G801 G802 G803 G804 G805 G806 G807 G808 G809 G810 G811 G812 G813 G814 G815 G816 G817 G818 G819 G820 G821 G822 G823 G824 G825 G826 G827 G828 G829 G830 G831 G832 G833 G834 G835 G836 G837 G838 G839 G840 G841 G842 G843 G844 G845 G846 G847 G848 G849 G850 G851 G852 G853 G854 G855 G856 G857 G858 G859 G860 G861

G863 G864 G865 G866 G867 G868

• Molecule 8: HOMO SAPIENS U4A SNRNA

Chain CX:

G801 G802 G803 G804 G805 G806 G807 G808 G809 G810 G811 G812 G813 G814 G815 G816 G817 G818 G819 G820 G821 G822 G823 G824 G825 G826 G827 G828 G829 G830 G831 G832 G833 G834 G835 G836 G837 G838 G839 G840 G841 G842 G843 G844 G845 G846 G847 G848 G849 G850 G851 G852 G853 G854 G855 G856 G857 G858 G859 G860

G861
A862
G863
A864
C865
U866
G867
G868

• Molecule 8: HOMO SAPIENS U4A SNRNA

Chain CY:

G801
C802
G803
C804
G805
G806
A807
C808
G809
A810
C811
U812
G813
A814
A815
A816
A817
G818
U819
C820
G821
C822
C823
A824
U825
U826
G827
G828
C829
A830
U831
U832
U833
U834
U835
U836
G837
A838
C839
A840
G841
U842
C843
U846
A847
U848
G849
G850
G851
U852
A853
A854
C855
C856
U857
A858
G859
A860
A862

G863
A864
C865
U866
G867
G868

• Molecule 8: HOMO SAPIENS U4A SNRNA

Chain DV:

G801
C802
G803
C804
G805
G806
A807
C808
C811
U812
G813
A814
A815
A816
U819
C820
G821
C822
C823
A824
U825
U826
G827
G828
C829
A830
A831
U832
U833
U834
U835
U836
G837
A838
C839
U842
C843
U844
C845
U846
A847
U848
G849
G850
G851
U852
A853
A854
C855
C856
U857
A858
A859
G860
A861
A862
G863

A864
C865
U866
G867
G868

• Molecule 8: HOMO SAPIENS U4A SNRNA

Chain DX:

G801
C802
G803
C804
U805
G806
A807
C808
G809
A810
C811
U812
G813
A814
A815
A816
A817
G818
C819
G820
C821
C822
U825
U826
G827
G828
C829
A830
A831
U832
U833
U834
U835
U836
G837
A838
C839
A840
G841
U842
C843
U844
C845
U846
A847
U848
G849
G850
G851
U852
A853
A854
C855
C856
U857
A858
A859
G860
A861
A862
G863

A862
G863
A864
C865
U866
G867
G868

• Molecule 8: HOMO SAPIENS U4A SNRNA

Chain DY:

G801
C802
G803
C804
U805
G806
A807
C808
G809
A810
C811
U812
G813
A814
A815
A816
A817
G818
C819
G820
C821
C822
C823
A824
U825
U826
G827
G828
C829
A830
A831
U832
U833
U834
U835
U836
G837
A838
C839
A840
G841
U842
U846
A847
U848
G849
G850
G851
U852
A853
A854
U857
A858
A859
G860
A861
A862
G863

A864
C865
U866
G867
G868

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 – 3.48	Depositor EDS
% Data completeness (in resolution range)	82.9 (66.17-3.60) 42.3 (66.15-3.48)	Depositor EDS
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 0.290 , 0.289	Depositor DCC
R_{free} test set	4696 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	85.4	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , -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 0.428 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
F_o, F_c correlation	0.79	EDS
Total number of atoms	75557	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 10.49% 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	AA	0.65	0/734	0.75	0/978
1	AH	0.65	0/743	0.72	0/989
1	AO	0.61	0/728	0.72	0/970
1	BA	0.61	0/743	0.72	0/989
1	BH	0.66	0/769	0.79	0/1024
1	BO	0.67	0/734	0.70	0/978
1	CA	0.60	0/734	0.75	0/978
1	CH	0.64	0/743	0.72	0/989
1	CO	0.52	0/743	0.68	0/989
1	DA	0.63	0/734	0.69	0/978
1	DH	0.64	0/769	0.76	0/1024
1	DO	0.63	0/743	0.76	0/989
2	AB	0.63	1/768 (0.1%)	0.77	0/1036
2	AI	0.64	0/760	0.76	0/1026
2	AP	0.69	1/755 (0.1%)	0.81	1/1019 (0.1%)
2	BB	0.67	0/760	0.83	0/1026
2	BI	0.65	1/760 (0.1%)	0.77	0/1026
2	BP	0.62	0/763	0.74	0/1029
2	CB	0.63	1/768 (0.1%)	0.73	0/1036
2	CI	0.67	0/760	0.78	0/1026
2	CP	0.59	0/755	0.74	0/1019
2	DB	0.67	0/763	0.77	0/1029
2	DI	0.64	0/746	0.77	0/1008
2	DP	0.67	0/755	0.78	0/1019
3	AC	0.66	0/855	0.80	1/1141 (0.1%)
3	AJ	0.70	0/870	0.77	0/1163
3	AQ	0.69	0/718	0.77	0/962
3	BC	0.70	0/855	0.75	0/1141
3	BJ	0.64	0/863	0.76	0/1152
3	BQ	0.64	0/718	0.77	0/962
3	CC	0.65	0/855	0.76	0/1141
3	CJ	0.66	0/870	0.78	0/1163
3	CQ	0.70	0/738	0.77	0/989
3	DC	0.66	0/855	0.75	0/1141

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	DJ	0.68	0/863	0.77	0/1152
3	DQ	0.65	0/718	0.85	1/962 (0.1%)
4	AD	0.63	0/704	0.72	0/946
4	AK	0.68	2/704 (0.3%)	0.67	0/946
4	AR	0.64	1/704 (0.1%)	0.70	0/946
4	BD	0.70	1/704 (0.1%)	0.70	0/946
4	BK	0.70	0/704	0.70	0/946
4	BR	0.67	1/704 (0.1%)	0.70	0/946
4	CD	0.67	0/704	0.70	0/946
4	CK	0.65	0/708	0.67	0/951
4	CR	0.65	0/704	0.69	0/946
4	DD	0.68	1/704 (0.1%)	0.73	0/946
4	DK	0.67	1/704 (0.1%)	0.73	0/946
4	DR	0.64	1/704 (0.1%)	0.71	0/946
5	AE	0.60	0/715	0.75	0/957
5	AL	0.59	0/637	0.74	0/853
5	AS	0.68	0/653	0.77	1/876 (0.1%)
5	BE	0.63	0/629	0.77	1/842 (0.1%)
5	BL	0.64	0/629	0.75	0/842
5	BS	0.63	0/686	0.73	0/919
5	CE	0.59	0/702	0.70	0/940
5	CL	0.63	0/629	0.72	0/842
5	CS	0.65	0/653	0.73	0/876
5	DE	0.64	0/637	0.75	0/853
5	DL	0.58	0/629	0.71	0/842
5	DS	0.59	0/653	0.63	0/876
6	AF	0.68	0/669	0.69	0/899
6	AM	0.71	0/669	0.68	0/899
6	AT	0.65	0/669	0.72	0/899
6	BF	0.64	0/660	0.71	0/889
6	BM	0.69	0/669	0.72	0/899
6	BT	0.65	0/669	0.66	0/899
6	CF	0.68	0/649	0.74	0/875
6	CM	0.70	0/669	0.68	0/899
6	CT	0.70	1/669 (0.1%)	0.69	0/899
6	DF	0.69	0/669	0.71	0/899
6	DM	0.65	0/669	0.75	0/899
6	DT	0.62	0/669	0.71	0/899
7	AG	0.63	0/575	0.66	0/768
7	AN	0.66	0/548	0.70	0/734
7	AU	0.60	0/575	0.74	0/768
7	BG	0.58	0/575	0.73	0/768
7	BN	0.63	0/584	0.76	0/779

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	BU	0.65	0/540	0.69	0/723
7	CG	0.67	0/575	0.72	0/768
7	CN	0.63	0/540	0.71	0/723
7	CU	0.59	0/575	0.72	0/768
7	DG	0.60	0/573	0.74	0/765
7	DN	0.58	0/575	0.74	0/768
7	DU	0.68	0/540	0.74	0/723
8	AV	1.27	4/1626 (0.2%)	1.88	55/2534 (2.2%)
8	AX	1.40	6/1626 (0.4%)	1.93	52/2534 (2.1%)
8	AY	1.32	8/1626 (0.5%)	1.91	52/2534 (2.1%)
8	BV	1.41	4/1626 (0.2%)	2.08	77/2534 (3.0%)
8	BX	1.37	3/1626 (0.2%)	1.92	48/2534 (1.9%)
8	BY	1.42	5/1626 (0.3%)	2.01	72/2534 (2.8%)
8	CV	1.41	9/1626 (0.6%)	1.98	63/2534 (2.5%)
8	CX	1.30	5/1626 (0.3%)	1.91	56/2534 (2.2%)
8	CY	1.39	7/1626 (0.4%)	1.90	55/2534 (2.2%)
8	DV	1.45	9/1626 (0.6%)	1.86	48/2534 (1.9%)
8	DX	1.35	6/1626 (0.4%)	2.03	75/2534 (3.0%)
8	DY	1.40	7/1626 (0.4%)	1.99	64/2534 (2.5%)
All	All	0.89	86/78398 (0.1%)	1.20	722/109335 (0.7%)

The worst 5 of 86 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	DX	839	C	C3'-O3'	7.55	1.52	1.42
8	DY	832	U	C1'-N1	7.51	1.60	1.48
8	AY	822	G	C3'-O3'	7.17	1.52	1.42
8	AY	865	C	C1'-N1	7.03	1.59	1.48
8	BV	826	U	C1'-N1	7.01	1.59	1.48

The worst 5 of 722 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	BV	826	U	O4'-C1'-N1	12.31	118.05	108.20
8	DV	850	G	N3-C2-N2	10.99	127.59	119.90
8	AX	804	G	C5-C6-O6	-10.74	122.16	128.60
8	AY	864	A	N1-C6-N6	10.30	124.78	118.60
8	BY	848	U	O4'-C1'-N1	10.10	116.28	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	AA	724	0	755	91	0
1	AH	733	0	768	75	0
1	AO	718	0	750	71	0
1	BA	733	0	768	78	0
1	BH	759	0	796	77	0
1	BO	724	0	755	86	0
1	CA	724	0	755	77	1
1	CH	733	0	768	88	0
1	CO	733	0	768	97	0
1	DA	724	0	755	72	0
1	DH	759	0	796	97	0
1	DO	733	0	768	91	1
2	AB	759	0	816	123	0
2	AI	751	0	807	151	0
2	AP	746	0	802	135	1
2	BB	751	0	807	134	0
2	BI	751	0	807	127	0
2	BP	754	0	811	169	1
2	CB	759	0	816	128	1
2	CI	751	0	807	135	0
2	CP	746	0	802	115	0
2	DB	754	0	811	132	1
2	DI	737	0	789	127	0
2	DP	746	0	802	135	0
3	AC	845	0	892	155	0
3	AJ	859	0	906	170	0
3	AQ	709	0	764	145	0
3	BC	845	0	892	139	0
3	BJ	852	0	900	156	0
3	BQ	709	0	764	139	0
3	CC	845	0	892	147	0
3	CJ	859	0	906	131	1
3	CQ	728	0	779	112	1
3	DC	845	0	892	126	0
3	DJ	852	0	900	184	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	DQ	709	0	764	138	0
4	AD	696	0	714	41	0
4	AK	696	0	714	75	0
4	AR	696	0	714	53	0
4	BD	696	0	714	63	0
4	BK	696	0	714	98	0
4	BR	696	0	714	56	0
4	CD	696	0	714	43	0
4	CK	700	0	717	64	0
4	CR	696	0	714	59	0
4	DD	696	0	714	60	0
4	DK	696	0	714	71	0
4	DR	696	0	714	84	0
5	AE	707	0	731	90	0
5	AL	629	0	643	68	0
5	AS	645	0	659	91	0
5	BE	622	0	635	114	0
5	BL	622	0	635	102	0
5	BS	678	0	698	102	0
5	CE	694	0	720	87	0
5	CL	622	0	635	84	0
5	CS	645	0	659	83	0
5	DE	629	0	643	75	0
5	DL	622	0	635	85	0
5	DS	645	0	659	104	0
6	AF	657	0	645	118	0
6	AM	657	0	645	100	0
6	AT	657	0	645	110	0
6	BF	648	0	639	143	0
6	BM	657	0	645	124	0
6	BT	657	0	645	92	0
6	CF	637	0	626	112	1
6	CM	657	0	645	94	0
6	CT	657	0	645	95	0
6	DF	657	0	645	99	0
6	DM	657	0	645	125	0
6	DT	657	0	645	85	0
7	AG	568	0	590	47	0
7	AN	541	0	562	83	0
7	AU	568	0	590	81	0
7	BG	568	0	590	81	0
7	BN	577	0	603	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	BU	533	0	551	69	0
7	CG	568	0	590	89	0
7	CN	533	0	551	65	0
7	CU	568	0	590	70	0
7	DG	566	0	583	78	0
7	DN	568	0	590	86	0
7	DU	533	0	551	77	0
8	AV	1453	0	733	147	0
8	AX	1453	0	733	103	2
8	AY	1453	0	733	96	0
8	BV	1453	0	733	127	0
8	BX	1453	0	733	118	1
8	BY	1453	0	733	128	2
8	CV	1453	0	733	114	1
8	CX	1453	0	733	116	0
8	CY	1453	0	733	108	0
8	DV	1453	0	733	52	0
8	DX	1453	0	733	108	0
8	DY	1453	0	733	59	1
All	All	75557	0	69105	7691	8

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 53.

The worst 5 of 7691 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:DF:547:THR:HG21	6:DF:562:VAL:CG2	1.43	1.48
3:CC:353:LEU:HD23	3:CC:371:LYS:NZ	1.24	1.47
2:AP:210:LEU:CD1	2:AP:274:LEU:HD13	1.43	1.47
3:DJ:407:ILE:HG23	6:DM:568:ASN:ND2	1.24	1.44
2:CP:207:LEU:CD1	2:CP:236:MET:SD	2.07	1.42

The worst 5 of 8 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:CF:553:GLY:O	3:CQ:393:ASP:OD1[2_664]	1.70	0.50
8:BX:866:U:O4'	3:CJ:386:LYS:NZ[2_665]	1.96	0.24
8:BY:815:A:O2'	8:DY:857:U:O2'[2_765]	2.07	0.13
8:AX:813:G:O3'	1:CA:152:LYS:NZ[2_655]	2.08	0.12
2:AP:212:HIS:ND1	2:BP:212:HIS:ND1[2_655]	2.13	0.07

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	AA	88/95 (93%)	81 (92%)	5 (6%)	2 (2%)	10	63
1	AH	89/95 (94%)	80 (90%)	9 (10%)	0	100	100
1	AO	87/95 (92%)	81 (93%)	6 (7%)	0	100	100
1	BA	89/95 (94%)	80 (90%)	9 (10%)	0	100	100
1	BH	93/95 (98%)	84 (90%)	9 (10%)	0	100	100
1	BO	88/95 (93%)	81 (92%)	6 (7%)	1 (1%)	21	78
1	CA	88/95 (93%)	81 (92%)	7 (8%)	0	100	100
1	CH	89/95 (94%)	83 (93%)	6 (7%)	0	100	100
1	CO	89/95 (94%)	82 (92%)	7 (8%)	0	100	100
1	DA	88/95 (93%)	84 (96%)	4 (4%)	0	100	100
1	DH	93/95 (98%)	85 (91%)	8 (9%)	0	100	100
1	DO	89/95 (94%)	79 (89%)	8 (9%)	2 (2%)	10	64
2	AB	95/119 (80%)	85 (90%)	7 (7%)	3 (3%)	6	55
2	AI	94/119 (79%)	82 (87%)	10 (11%)	2 (2%)	11	65
2	AP	93/119 (78%)	83 (89%)	9 (10%)	1 (1%)	21	78
2	BB	94/119 (79%)	79 (84%)	11 (12%)	4 (4%)	4	46
2	BI	94/119 (79%)	78 (83%)	13 (14%)	3 (3%)	6	55
2	BP	94/119 (79%)	87 (93%)	6 (6%)	1 (1%)	21	78
2	CB	95/119 (80%)	86 (90%)	7 (7%)	2 (2%)	11	65
2	CI	94/119 (79%)	83 (88%)	8 (8%)	3 (3%)	6	55
2	CP	93/119 (78%)	83 (89%)	9 (10%)	1 (1%)	21	78
2	DB	94/119 (79%)	93 (99%)	1 (1%)	0	100	100
2	DI	92/119 (77%)	87 (95%)	4 (4%)	1 (1%)	21	78
2	DP	93/119 (78%)	82 (88%)	11 (12%)	0	100	100
3	AC	103/118 (87%)	89 (86%)	11 (11%)	3 (3%)	7	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AJ	105/118 (89%)	97 (92%)	7 (7%)	1 (1%)	22	80
3	AQ	88/118 (75%)	77 (88%)	10 (11%)	1 (1%)	21	78
3	BC	103/118 (87%)	89 (86%)	13 (13%)	1 (1%)	22	80
3	BJ	104/118 (88%)	93 (89%)	9 (9%)	2 (2%)	12	67
3	BQ	88/118 (75%)	82 (93%)	3 (3%)	3 (3%)	6	54
3	CC	103/118 (87%)	88 (85%)	12 (12%)	3 (3%)	7	58
3	CJ	105/118 (89%)	91 (87%)	13 (12%)	1 (1%)	22	80
3	CQ	90/118 (76%)	78 (87%)	8 (9%)	4 (4%)	4	45
3	DC	103/118 (87%)	92 (89%)	9 (9%)	2 (2%)	12	67
3	DJ	104/118 (88%)	95 (91%)	7 (7%)	2 (2%)	12	67
3	DQ	88/118 (75%)	81 (92%)	7 (8%)	0	100	100
4	AD	87/126 (69%)	77 (88%)	10 (12%)	0	100	100
4	AK	87/126 (69%)	81 (93%)	5 (6%)	1 (1%)	21	78
4	AR	87/126 (69%)	84 (97%)	2 (2%)	1 (1%)	21	78
4	BD	87/126 (69%)	81 (93%)	5 (6%)	1 (1%)	21	78
4	BK	87/126 (69%)	80 (92%)	6 (7%)	1 (1%)	21	78
4	BR	87/126 (69%)	81 (93%)	4 (5%)	2 (2%)	10	63
4	CD	87/126 (69%)	81 (93%)	5 (6%)	1 (1%)	21	78
4	CK	88/126 (70%)	76 (86%)	11 (12%)	1 (1%)	21	78
4	CR	87/126 (69%)	78 (90%)	7 (8%)	2 (2%)	10	63
4	DD	87/126 (69%)	79 (91%)	7 (8%)	1 (1%)	21	78
4	DK	87/126 (69%)	83 (95%)	3 (3%)	1 (1%)	21	78
4	DR	87/126 (69%)	83 (95%)	3 (3%)	1 (1%)	21	78
5	AE	84/92 (91%)	77 (92%)	6 (7%)	1 (1%)	19	77
5	AL	74/92 (80%)	67 (90%)	6 (8%)	1 (1%)	16	72
5	AS	76/92 (83%)	67 (88%)	8 (10%)	1 (1%)	18	75
5	BE	73/92 (79%)	67 (92%)	6 (8%)	0	100	100
5	BL	73/92 (79%)	66 (90%)	7 (10%)	0	100	100
5	BS	80/92 (87%)	73 (91%)	5 (6%)	2 (2%)	9	61
5	CE	82/92 (89%)	74 (90%)	8 (10%)	0	100	100
5	CL	73/92 (79%)	67 (92%)	5 (7%)	1 (1%)	16	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	CS	76/92 (83%)	67 (88%)	9 (12%)	0	100	100
5	DE	74/92 (80%)	65 (88%)	7 (10%)	2 (3%)	8	59
5	DL	73/92 (79%)	66 (90%)	6 (8%)	1 (1%)	16	72
5	DS	76/92 (83%)	69 (91%)	6 (8%)	1 (1%)	18	75
6	AF	81/86 (94%)	73 (90%)	7 (9%)	1 (1%)	19	77
6	AM	81/86 (94%)	76 (94%)	4 (5%)	1 (1%)	19	77
6	AT	81/86 (94%)	76 (94%)	4 (5%)	1 (1%)	19	77
6	BF	81/86 (94%)	72 (89%)	7 (9%)	2 (2%)	9	61
6	BM	81/86 (94%)	76 (94%)	4 (5%)	1 (1%)	19	77
6	BT	81/86 (94%)	72 (89%)	7 (9%)	2 (2%)	9	61
6	CF	80/86 (93%)	73 (91%)	7 (9%)	0	100	100
6	CM	81/86 (94%)	74 (91%)	6 (7%)	1 (1%)	19	77
6	CT	81/86 (94%)	72 (89%)	8 (10%)	1 (1%)	19	77
6	DF	81/86 (94%)	70 (86%)	8 (10%)	3 (4%)	5	51
6	DM	81/86 (94%)	77 (95%)	4 (5%)	0	100	100
6	DT	81/86 (94%)	75 (93%)	5 (6%)	1 (1%)	19	77
7	AG	71/76 (93%)	66 (93%)	5 (7%)	0	100	100
7	AN	69/76 (91%)	63 (91%)	5 (7%)	1 (1%)	16	72
7	AU	71/76 (93%)	64 (90%)	6 (8%)	1 (1%)	16	72
7	BG	71/76 (93%)	67 (94%)	2 (3%)	2 (3%)	8	59
7	BN	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
7	BU	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	72
7	CG	71/76 (93%)	61 (86%)	9 (13%)	1 (1%)	16	72
7	CN	68/76 (90%)	67 (98%)	0	1 (2%)	15	72
7	CU	71/76 (93%)	62 (87%)	9 (13%)	0	100	100
7	DG	71/76 (93%)	65 (92%)	5 (7%)	1 (1%)	16	72
7	DN	71/76 (93%)	63 (89%)	8 (11%)	0	100	100
7	DU	68/76 (90%)	64 (94%)	4 (6%)	0	100	100
All	All	7151/8544 (84%)	6492 (91%)	565 (8%)	94 (1%)	18	75

5 of 94 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AI	284	GLU
3	AJ	412	ASN
7	AN	773	LEU
6	BF	506	ASN
2	BP	295	VAL

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	81/85 (95%)	80 (99%)	1 (1%)	82	96
1	AH	82/85 (96%)	79 (96%)	3 (4%)	45	86
1	AO	80/85 (94%)	78 (98%)	2 (2%)	60	91
1	BA	82/85 (96%)	81 (99%)	1 (1%)	82	96
1	BH	85/85 (100%)	85 (100%)	0	100	100
1	BO	81/85 (95%)	80 (99%)	1 (1%)	82	96
1	CA	81/85 (95%)	80 (99%)	1 (1%)	82	96
1	CH	82/85 (96%)	79 (96%)	3 (4%)	45	86
1	CO	82/85 (96%)	82 (100%)	0	100	100
1	DA	81/85 (95%)	80 (99%)	1 (1%)	82	96
1	DH	85/85 (100%)	84 (99%)	1 (1%)	82	96
1	DO	82/85 (96%)	81 (99%)	1 (1%)	82	96
2	AB	89/101 (88%)	87 (98%)	2 (2%)	64	92
2	AI	88/101 (87%)	86 (98%)	2 (2%)	63	92
2	AP	88/101 (87%)	86 (98%)	2 (2%)	63	92
2	BB	88/101 (87%)	87 (99%)	1 (1%)	84	96
2	BI	88/101 (87%)	86 (98%)	2 (2%)	63	92
2	BP	89/101 (88%)	87 (98%)	2 (2%)	64	92
2	CB	89/101 (88%)	89 (100%)	0	100	100
2	CI	88/101 (87%)	85 (97%)	3 (3%)	49	88
2	CP	88/101 (87%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	DB	89/101 (88%)	88 (99%)	1 (1%)	84	96
2	DI	87/101 (86%)	87 (100%)	0	100	100
2	DP	88/101 (87%)	85 (97%)	3 (3%)	49	88
3	AC	97/110 (88%)	95 (98%)	2 (2%)	66	93
3	AJ	99/110 (90%)	95 (96%)	4 (4%)	42	85
3	AQ	83/110 (76%)	81 (98%)	2 (2%)	61	92
3	BC	97/110 (88%)	93 (96%)	4 (4%)	41	85
3	BJ	98/110 (89%)	95 (97%)	3 (3%)	52	90
3	BQ	83/110 (76%)	82 (99%)	1 (1%)	82	96
3	CC	97/110 (88%)	95 (98%)	2 (2%)	66	93
3	CJ	99/110 (90%)	97 (98%)	2 (2%)	68	93
3	CQ	85/110 (77%)	80 (94%)	5 (6%)	28	76
3	DC	97/110 (88%)	96 (99%)	1 (1%)	85	97
3	DJ	98/110 (89%)	97 (99%)	1 (1%)	85	97
3	DQ	83/110 (76%)	83 (100%)	0	100	100
4	AD	78/101 (77%)	78 (100%)	0	100	100
4	AK	78/101 (77%)	77 (99%)	1 (1%)	80	96
4	AR	78/101 (77%)	77 (99%)	1 (1%)	80	96
4	BD	78/101 (77%)	78 (100%)	0	100	100
4	BK	78/101 (77%)	76 (97%)	2 (3%)	59	91
4	BR	78/101 (77%)	77 (99%)	1 (1%)	80	96
4	CD	78/101 (77%)	77 (99%)	1 (1%)	80	96
4	CK	78/101 (77%)	78 (100%)	0	100	100
4	CR	78/101 (77%)	78 (100%)	0	100	100
4	DD	78/101 (77%)	77 (99%)	1 (1%)	80	96
4	DK	78/101 (77%)	77 (99%)	1 (1%)	80	96
4	DR	78/101 (77%)	77 (99%)	1 (1%)	80	96
5	AE	80/84 (95%)	79 (99%)	1 (1%)	80	96
5	AL	71/84 (84%)	70 (99%)	1 (1%)	78	96
5	AS	73/84 (87%)	72 (99%)	1 (1%)	78	96
5	BE	70/84 (83%)	66 (94%)	4 (6%)	29	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	BL	70/84 (83%)	69 (99%)	1 (1%)	78	96
5	BS	77/84 (92%)	75 (97%)	2 (3%)	59	91
5	CE	79/84 (94%)	79 (100%)	0	100	100
5	CL	70/84 (83%)	68 (97%)	2 (3%)	55	90
5	CS	73/84 (87%)	73 (100%)	0	100	100
5	DE	71/84 (84%)	71 (100%)	0	100	100
5	DL	70/84 (83%)	70 (100%)	0	100	100
5	DS	73/84 (87%)	73 (100%)	0	100	100
6	AF	71/74 (96%)	70 (99%)	1 (1%)	78	96
6	AM	71/74 (96%)	70 (99%)	1 (1%)	78	96
6	AT	71/74 (96%)	69 (97%)	2 (3%)	56	90
6	BF	70/74 (95%)	67 (96%)	3 (4%)	40	84
6	BM	71/74 (96%)	70 (99%)	1 (1%)	78	96
6	BT	71/74 (96%)	71 (100%)	0	100	100
6	CF	69/74 (93%)	67 (97%)	2 (3%)	55	90
6	CM	71/74 (96%)	71 (100%)	0	100	100
6	CT	71/74 (96%)	71 (100%)	0	100	100
6	DF	71/74 (96%)	70 (99%)	1 (1%)	78	96
6	DM	71/74 (96%)	70 (99%)	1 (1%)	78	96
6	DT	71/74 (96%)	71 (100%)	0	100	100
7	AG	63/66 (96%)	60 (95%)	3 (5%)	35	82
7	AN	60/66 (91%)	59 (98%)	1 (2%)	73	95
7	AU	63/66 (96%)	62 (98%)	1 (2%)	75	95
7	BG	63/66 (96%)	63 (100%)	0	100	100
7	BN	64/66 (97%)	63 (98%)	1 (2%)	75	95
7	BU	59/66 (89%)	59 (100%)	0	100	100
7	CG	63/66 (96%)	60 (95%)	3 (5%)	35	82
7	CN	59/66 (89%)	58 (98%)	1 (2%)	73	95
7	CU	63/66 (96%)	62 (98%)	1 (2%)	75	95
7	DG	62/66 (94%)	61 (98%)	1 (2%)	75	95
7	DN	63/66 (96%)	61 (97%)	2 (3%)	51	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	DU	59/66 (89%)	59 (100%)	0	100	100
All	All	6562/7452 (88%)	6455 (98%)	107 (2%)	75	95

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	BI	280	LEU
2	BP	234	VAL
4	DK	18	VAL
3	BJ	349	ASN
5	BL	689	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 193 such sidechains are listed below:

Mol	Chain	Res	Type
4	BR	16	HIS
5	CE	640	ASN
2	DP	264	ASN
4	BR	60	GLN
3	CC	345	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	AV	68/68 (100%)	32 (47%)	8 (11%)
8	AX	67/68 (98%)	28 (41%)	6 (8%)
8	AY	67/68 (98%)	35 (52%)	5 (7%)
8	BV	67/68 (98%)	33 (49%)	6 (8%)
8	BX	67/68 (98%)	35 (52%)	2 (2%)
8	BY	67/68 (98%)	39 (58%)	3 (4%)
8	CV	67/68 (98%)	29 (43%)	6 (8%)
8	CX	67/68 (98%)	34 (50%)	5 (7%)
8	CY	67/68 (98%)	34 (50%)	8 (11%)
8	DV	67/68 (98%)	25 (37%)	5 (7%)
8	DX	67/68 (98%)	31 (46%)	7 (10%)
8	DY	67/68 (98%)	33 (49%)	6 (8%)
All	All	805/816 (98%)	388 (48%)	67 (8%)

5 of 388 RNA backbone outliers are listed below:

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

5 of 67 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	CV	811	C
8	CX	828	G
8	DY	811	C
8	CV	814	A
8	CV	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 ⓘ

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	AA	90/95 (94%)	0.37	5 (5%) 24 13	73, 93, 108, 121	0
1	AH	91/95 (95%)	0.42	9 (9%) 8 6	68, 97, 111, 135	0
1	AO	89/95 (93%)	0.31	3 (3%) 43 24	72, 99, 113, 139	0
1	BA	91/95 (95%)	0.41	6 (6%) 18 10	73, 95, 109, 132	0
1	BH	95/95 (100%)	0.37	9 (9%) 8 6	72, 98, 109, 114	0
1	BO	90/95 (94%)	0.34	2 (2%) 59 34	58, 95, 107, 128	0
1	CA	90/95 (94%)	0.46	7 (7%) 13 8	80, 96, 111, 125	0
1	CH	91/95 (95%)	0.32	3 (3%) 44 25	63, 95, 116, 121	0
1	CO	91/95 (95%)	0.48	7 (7%) 13 8	75, 100, 116, 133	0
1	DA	90/95 (94%)	0.53	9 (10%) 8 6	62, 95, 108, 120	0
1	DH	95/95 (100%)	0.29	6 (6%) 19 11	65, 97, 111, 116	0
1	DO	91/95 (95%)	0.23	3 (3%) 44 25	69, 96, 110, 118	0
2	AB	97/119 (81%)	0.26	3 (3%) 47 26	67, 90, 116, 137	0
2	AI	96/119 (80%)	0.33	6 (6%) 19 11	63, 94, 108, 114	0
2	AP	95/119 (79%)	0.11	1 (1%) 77 50	69, 91, 106, 116	0
2	BB	96/119 (80%)	0.25	3 (3%) 47 26	71, 92, 106, 112	0
2	BI	96/119 (80%)	0.19	2 (2%) 60 35	61, 94, 107, 120	0
2	BP	96/119 (80%)	0.20	3 (3%) 47 26	67, 92, 105, 115	0
2	CB	97/119 (81%)	0.20	5 (5%) 26 14	64, 91, 109, 129	0
2	CI	96/119 (80%)	0.14	1 (1%) 79 53	67, 91, 107, 126	0
2	CP	95/119 (79%)	0.23	5 (5%) 25 14	70, 91, 110, 119	0
2	DB	96/119 (80%)	0.23	3 (3%) 47 26	68, 91, 103, 111	0
2	DI	94/119 (78%)	0.35	3 (3%) 45 25	64, 92, 102, 123	0
2	DP	95/119 (79%)	0.27	5 (5%) 25 14	75, 91, 104, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	AC	105/118 (88%)	0.30	2 (1%) 64 37	57, 94, 116, 126	0
3	AJ	107/118 (90%)	0.42	10 (9%) 9 7	71, 92, 114, 124	0
3	AQ	90/118 (76%)	0.19	2 (2%) 59 34	64, 91, 104, 115	0
3	BC	105/118 (88%)	0.36	4 (3%) 38 22	62, 93, 106, 113	0
3	BJ	106/118 (89%)	0.24	5 (4%) 30 17	64, 92, 107, 117	0
3	BQ	90/118 (76%)	0.36	6 (6%) 17 10	62, 91, 105, 117	0
3	CC	105/118 (88%)	0.10	3 (2%) 49 28	60, 94, 106, 121	0
3	CJ	107/118 (90%)	0.26	7 (6%) 18 11	67, 92, 110, 121	0
3	CQ	92/118 (77%)	0.40	5 (5%) 25 13	68, 91, 106, 114	0
3	DC	105/118 (88%)	0.27	5 (4%) 29 16	73, 91, 107, 112	0
3	DJ	106/118 (89%)	0.34	9 (8%) 11 7	67, 92, 107, 124	0
3	DQ	90/118 (76%)	0.29	5 (5%) 24 13	65, 87, 105, 119	0
4	AD	89/126 (70%)	0.35	5 (5%) 24 13	76, 96, 111, 118	0
4	AK	89/126 (70%)	0.37	7 (7%) 13 8	86, 101, 118, 126	0
4	AR	89/126 (70%)	0.45	7 (7%) 13 8	80, 99, 110, 115	0
4	BD	89/126 (70%)	0.48	8 (8%) 10 7	83, 96, 111, 125	0
4	BK	89/126 (70%)	0.32	4 (4%) 32 18	81, 98, 112, 127	0
4	BR	89/126 (70%)	0.49	7 (7%) 13 8	70, 96, 109, 120	0
4	CD	89/126 (70%)	0.34	4 (4%) 32 18	74, 95, 112, 127	0
4	CK	90/126 (71%)	0.17	3 (3%) 44 25	73, 97, 114, 123	0
4	CR	89/126 (70%)	0.35	3 (3%) 43 24	66, 97, 106, 112	0
4	DD	89/126 (70%)	0.27	4 (4%) 32 18	70, 94, 107, 124	0
4	DK	89/126 (70%)	0.29	5 (5%) 24 13	76, 96, 106, 115	0
4	DR	89/126 (70%)	0.45	5 (5%) 24 13	72, 96, 106, 120	0
5	AE	86/92 (93%)	0.36	4 (4%) 30 17	68, 95, 111, 124	0
5	AL	76/92 (82%)	0.47	3 (3%) 37 21	81, 99, 114, 134	0
5	AS	78/92 (84%)	0.47	5 (6%) 19 11	82, 98, 117, 121	0
5	BE	75/92 (81%)	0.40	4 (5%) 25 14	76, 96, 115, 121	0
5	BL	75/92 (81%)	0.42	2 (2%) 52 29	75, 97, 114, 117	0
5	BS	82/92 (89%)	0.45	6 (7%) 15 9	68, 94, 103, 113	0
5	CE	84/92 (91%)	0.33	3 (3%) 41 23	71, 95, 107, 118	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
5	CL	75/92 (81%)	0.45	4 (5%)	25 14	68, 95, 109, 125	0
5	CS	78/92 (84%)	0.62	7 (8%)	10 7	78, 97, 110, 118	0
5	DE	76/92 (82%)	0.44	4 (5%)	25 14	70, 95, 114, 120	0
5	DL	75/92 (81%)	0.64	5 (6%)	17 10	72, 93, 106, 113	0
5	DS	78/92 (84%)	0.37	5 (6%)	19 11	72, 96, 112, 124	0
6	AF	83/86 (96%)	0.42	2 (2%)	56 32	71, 92, 103, 115	0
6	AM	83/86 (96%)	0.21	3 (3%)	41 23	60, 90, 109, 130	0
6	AT	83/86 (96%)	0.29	2 (2%)	56 32	65, 90, 107, 125	0
6	BF	83/86 (96%)	0.23	2 (2%)	56 32	74, 93, 104, 121	0
6	BM	83/86 (96%)	0.26	4 (4%)	29 16	74, 93, 106, 117	0
6	BT	83/86 (96%)	0.23	2 (2%)	56 32	58, 88, 102, 110	0
6	CF	82/86 (95%)	0.15	1 (1%)	75 49	68, 91, 100, 105	0
6	CM	83/86 (96%)	0.28	4 (4%)	29 16	71, 91, 115, 124	0
6	CT	83/86 (96%)	0.14	0	100 100	58, 89, 104, 113	0
6	DF	83/86 (96%)	0.22	3 (3%)	41 23	67, 90, 103, 110	0
6	DM	83/86 (96%)	0.21	4 (4%)	29 16	60, 91, 108, 123	0
6	DT	83/86 (96%)	0.40	4 (4%)	29 16	66, 88, 112, 120	0
7	AG	73/76 (96%)	0.39	4 (5%)	24 13	73, 97, 112, 133	0
7	AN	71/76 (93%)	0.20	2 (2%)	50 29	78, 95, 108, 119	0
7	AU	73/76 (96%)	0.42	5 (6%)	17 10	86, 99, 121, 129	0
7	BG	73/76 (96%)	0.63	7 (9%)	8 6	80, 98, 113, 127	0
7	BN	74/76 (97%)	0.31	6 (8%)	12 8	65, 97, 106, 111	0
7	BU	70/76 (92%)	0.47	8 (11%)	6 5	68, 97, 111, 118	0
7	CG	73/76 (96%)	0.60	7 (9%)	8 6	74, 97, 105, 110	0
7	CN	70/76 (92%)	0.22	1 (1%)	72 45	81, 96, 103, 110	0
7	CU	73/76 (96%)	0.34	3 (4%)	35 20	81, 97, 114, 119	0
7	DG	73/76 (96%)	0.18	2 (2%)	52 29	73, 98, 112, 120	0
7	DN	73/76 (96%)	0.46	3 (4%)	35 20	75, 96, 105, 107	0
7	DU	70/76 (92%)	0.54	8 (11%)	6 5	76, 98, 108, 117	0
8	AV	68/68 (100%)	-0.18	0	100 100	56, 83, 108, 117	0
8	AX	68/68 (100%)	-0.20	1 (1%)	70 43	54, 83, 107, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
8	AY	68/68 (100%)	-0.18	0	100	100	54, 85, 106, 113	0
8	BV	68/68 (100%)	-0.14	0	100	100	55, 80, 107, 111	0
8	BX	68/68 (100%)	-0.15	0	100	100	58, 82, 100, 117	0
8	BY	68/68 (100%)	-0.22	0	100	100	48, 79, 104, 115	0
8	CV	68/68 (100%)	-0.08	1 (1%)	70	43	55, 83, 102, 111	0
8	CX	68/68 (100%)	-0.15	0	100	100	61, 85, 94, 99	0
8	CY	68/68 (100%)	-0.10	0	100	100	61, 82, 97, 121	0
8	DV	68/68 (100%)	-0.17	0	100	100	57, 79, 97, 106	0
8	DX	68/68 (100%)	-0.10	0	100	100	50, 79, 94, 110	0
8	DY	68/68 (100%)	-0.19	0	100	100	53, 82, 101, 110	0
All	All	8135/9360 (86%)	0.28	375 (4%)	31	17	48, 94, 110, 139	0

The worst 5 of 375 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	CQ	415	ILE	8.8
7	DN	747	GLU	7.0
5	CL	637	GLU	6.6
1	DA	133	ALA	6.5
6	DT	583	GLU	6.2

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.