



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:46 am GMT

PDB ID : 3JCR
EMDB ID: : EMD-6581
Title : 3D structure determination of the human*U4/U6.U5* tri-snRNP complex
Authors : Agafonov, D.E.; Kastner, B.; Dybkov, O.; Hofele, R.V.; Liu, W.T.; Urlaub, H.; Luhrmann, R.; Stark, H.
Deposited on : 2016-01-21
Resolution : 7.00 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

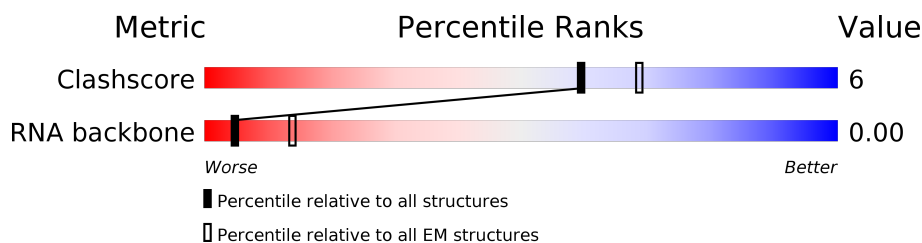
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY




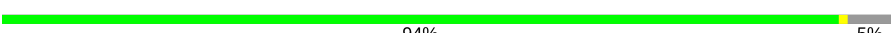






The reported resolution of this entry is 7.00 Å.

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.











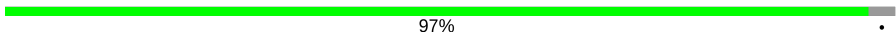
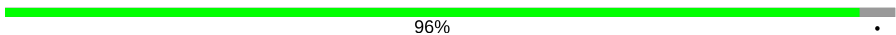
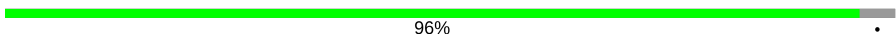





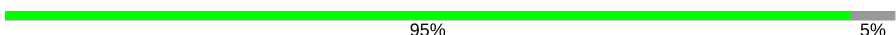








Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	G	941	 43% . 56%
2	D	357	 84% . 15%
3	C	2136	 88% 12%
4	E	142	 94% . 5%
5	A	2335	 94% . 5%
6	F	820	 52% . 47%
7	B	972	 86% 13%
8	O	240	 37% 63%
8	o	240	 37% 63%
9	P	119	 78% 22%

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Mol	Chain	Length	Quality of chain
9	p	119	
10	Q	118	
10	q	118	
11	R	126	
11	r	126	
12	S	92	
12	s	92	
13	T	86	
13	t	86	
14	U	76	
14	u	76	
15	8	96	
16	6	80	
17	5	91	
18	4	139	
19	3	102	
20	2	95	
21	7	103	
22	K	683	
23	L	521	
24	J	499	
25	I	128	
26	V	565	
27	M	145	
28	N	106	

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Mol	Chain	Length	Quality of chain
29	H	116	<div><div></div><div>54%</div><div>46%</div></div>

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 9403 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 hPrp6.

Mol	Chain	Residues	Atoms		AltConf	Trace
1	G	418	Total	C	0	418
			418	418		

- Molecule 2 is a protein called U5-40K.

Mol	Chain	Residues	Atoms		AltConf	Trace
2	D	302	Total	C	0	302
			302	302		

- Molecule 3 is a protein called hBrr2.

Mol	Chain	Residues	Atoms		AltConf	Trace
3	C	1885	Total	C	0	1885
			1885	1885		

- Molecule 4 is a protein called hDim1.

Mol	Chain	Residues	Atoms		AltConf	Trace
4	E	135	Total	C	0	135
			135	135		

- Molecule 5 is a protein called hPrp8.

Mol	Chain	Residues	Atoms		AltConf	Trace
5	A	2222	Total	C	0	2222
			2222	2222		

- Molecule 6 is a protein called hPrp28.

Mol	Chain	Residues	Atoms		AltConf	Trace
6	F	435	Total	C	0	435
			435	435		

- Molecule 7 is a protein called hSnu114.

Mol	Chain	Residues	Atoms	AltConf	Trace
7	B	844	Total C 844 844	0	844

- Molecule 8 is a protein called SmB.

Mol	Chain	Residues	Atoms	AltConf	Trace
8	O	89	Total C 89 89	0	89
8	o	89	Total C 89 89	0	89

- Molecule 9 is a protein called SmD1.

Mol	Chain	Residues	Atoms	AltConf	Trace
9	P	93	Total C 93 93	0	93
9	p	94	Total C 94 94	0	94

- Molecule 10 is a protein called SmD2.

Mol	Chain	Residues	Atoms	AltConf	Trace
10	Q	89	Total C 89 89	0	89
10	q	89	Total C 89 89	0	89

- Molecule 11 is a protein called SmD3.

Mol	Chain	Residues	Atoms	AltConf	Trace
11	R	88	Total C 88 88	0	88
11	r	88	Total C 88 88	0	88

- Molecule 12 is a protein called SmE.

Mol	Chain	Residues	Atoms	AltConf	Trace
12	S	78	Total C 78 78	0	78

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Mol	Chain	Residues	Atoms	AltConf	Trace
12	s	78	Total C 78 78	0	78

- Molecule 13 is a protein called SmF.

Mol	Chain	Residues	Atoms	AltConf	Trace
13	T	73	Total C 73 73	0	73
13	t	83	Total C 83 83	0	83

- Molecule 14 is a protein called SmG.

Mol	Chain	Residues	Atoms	AltConf	Trace
14	U	73	Total C 73 73	0	73
14	u	73	Total C 73 73	0	73

- Molecule 15 is a protein called LSm8.

Mol	Chain	Residues	Atoms	AltConf	Trace
15	8	70	Total C 70 70	0	70

- Molecule 16 is a protein called LSm6.

Mol	Chain	Residues	Atoms	AltConf	Trace
16	6	70	Total C 70 70	0	70

- Molecule 17 is a protein called LSm5.

Mol	Chain	Residues	Atoms	AltConf	Trace
17	5	76	Total C 76 76	0	76

- Molecule 18 is a protein called LSm4.

Mol	Chain	Residues	Atoms		AltConf	Trace
18	4	80	Total	C	0	80
			80	80		

- Molecule 19 is a protein called LSm3.

Mol	Chain	Residues	Atoms		AltConf	Trace
19	3	83	Total	C	0	83
			83	83		

- Molecule 20 is a protein called LSm2.

Mol	Chain	Residues	Atoms		AltConf	Trace
20	2	90	Total	C	0	90
			90	90		

- Molecule 21 is a protein called LSm7.

Mol	Chain	Residues	Atoms		AltConf	Trace
21	7	79	Total	C	0	79
			79	79		

- Molecule 22 is a protein called hPrp3.

Mol	Chain	Residues	Atoms		AltConf	Trace
22	K	131	Total	C	0	131
			131	131		

- Molecule 23 is a protein called hPrp4.

Mol	Chain	Residues	Atoms		AltConf	Trace
23	L	307	Total	C	0	307
			307	307		

- Molecule 24 is a protein called hPrp31.

Mol	Chain	Residues	Atoms		AltConf	Trace
24	J	239	Total	C	0	239
			239	239		

- Molecule 25 is a protein called hSnu13.

Mol	Chain	Residues	Atoms		AltConf	Trace
25	I	126	Total	C	0	126
			126	126		

- Molecule 26 is a protein called hSad1.

Mol	Chain	Residues	Atoms		AltConf	Trace
26	V	431	Total	C	0	431
			431	431		

- Molecule 27 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms		AltConf	Trace
27	M	103	Total	P	0	103
			103	103		

- Molecule 28 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms		AltConf	Trace
28	N	37	Total	P	0	37
			37	37		

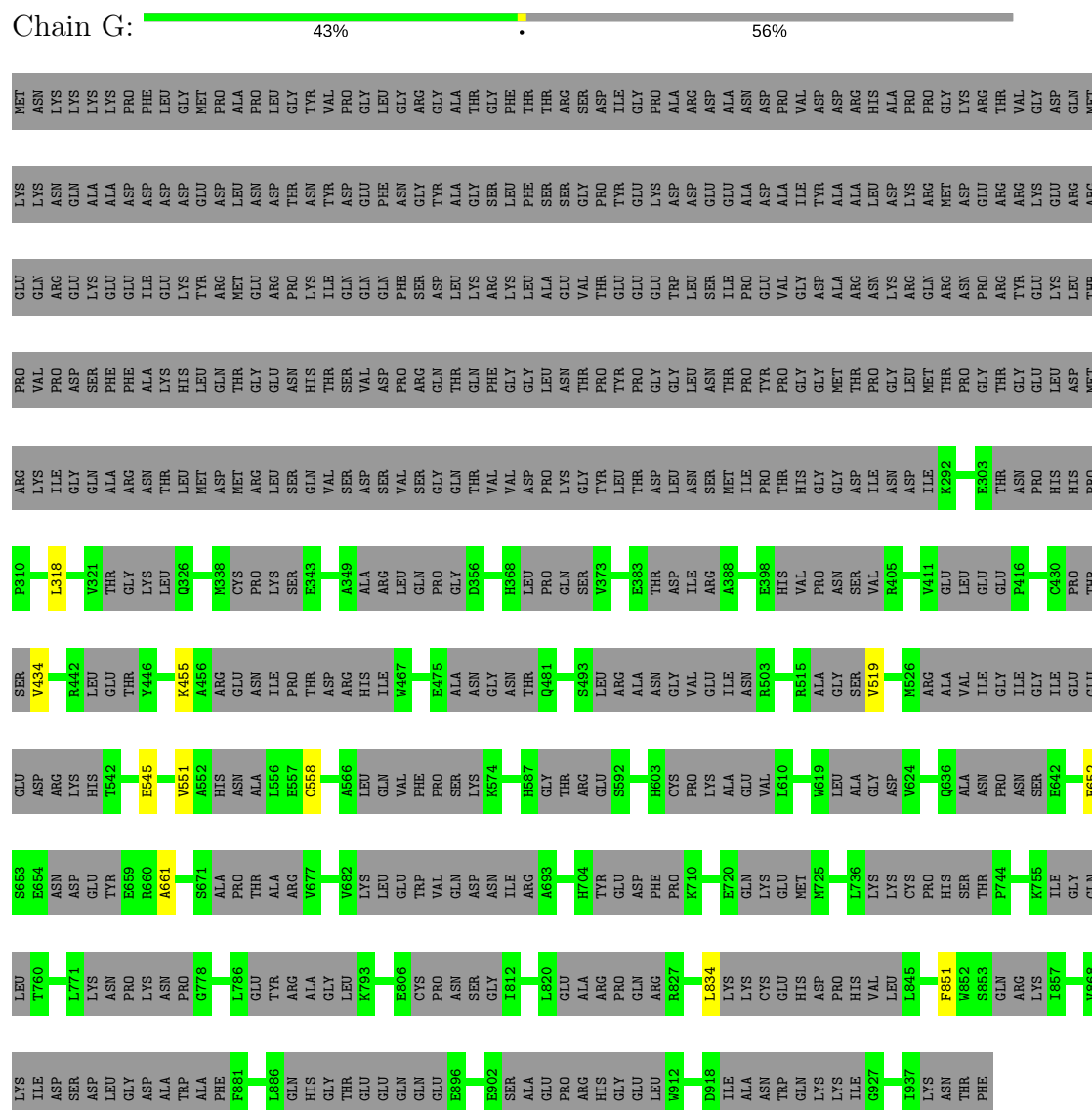
- Molecule 29 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms		AltConf	Trace
29	H	63	Total	P	0	63
			63	63		

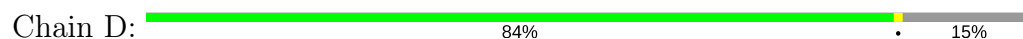
3 Residue-property plots

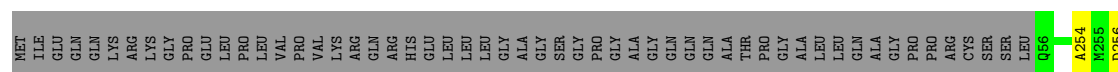
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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: hPrp6



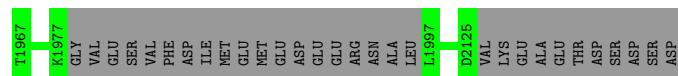
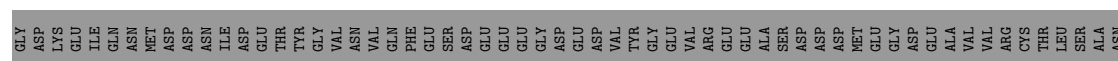
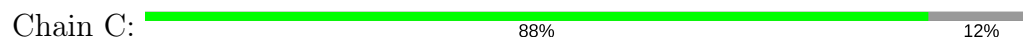
- Molecule 2: U5-40K





- Molecule 3: hBrr2

Chain C:



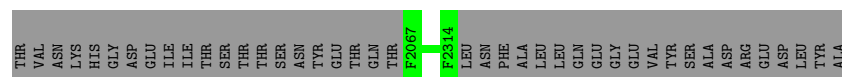
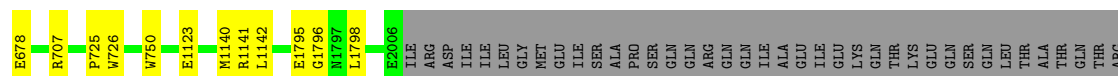
- Molecule 4: hDim1

Chain E:



- Molecule 5: hPrp8

Chain A:



- Molecule 6: hPrp28

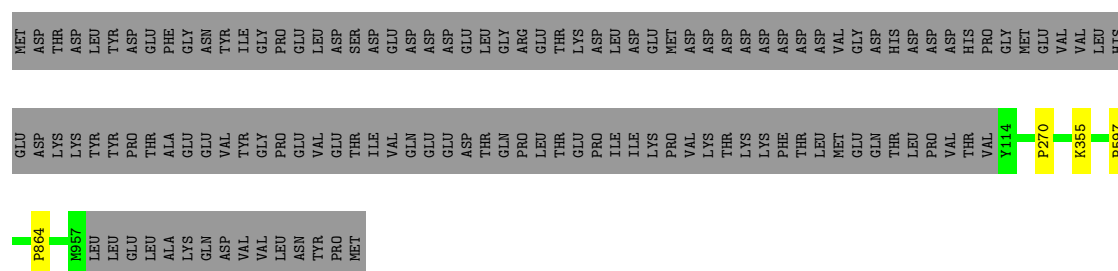
Chain F:





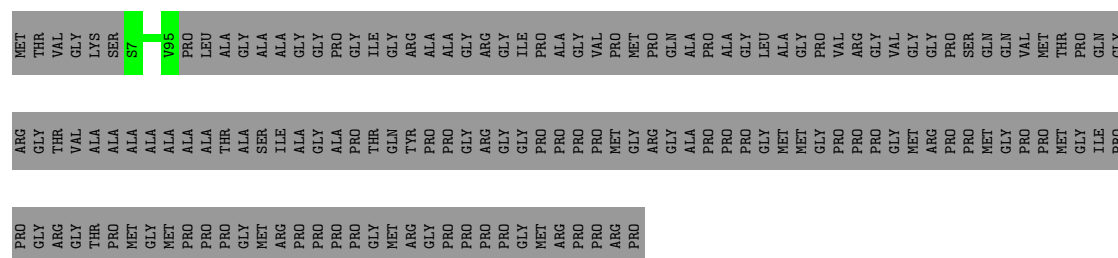
- Molecule 7: hSnu114

Chain B:  86% 13%



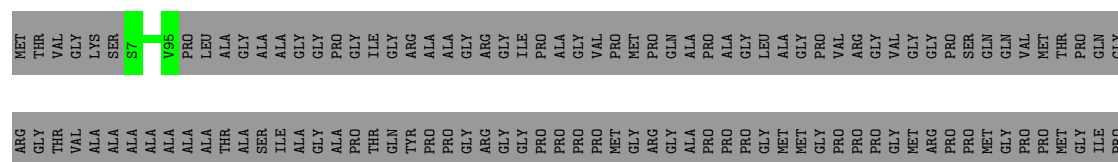
- Molecule 8: SmB

Chain O: 37% 63%



- Molecule 8: SmB

Chain o: 37% 63%



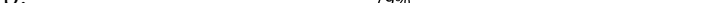
PRO	GLY	ARG	GLY	THR	PRO	MET	GLY	MET	PRO	PRO	PRO	GLY	MET	ARG	PRO	PRO	PRO	GLY	MET	ARG	GLY	PRO	PRO	PRO	GLY	MET	ARG	PRO	PRO	ARG	PRO
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 9: SmD1

Chain P: 78% 22%

MET	K2	S35	MET	N37	V95	ALA	GLY	ARG	GLY	ARG	GLY	ARG	GLY	ARG	GLY	GLY	ARG	GLY	GLY	ARG	GLY	GLY	PRO	ARG	ARG
-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 9: SmD1

Chain p:  79% 21%

[illegible]

- Molecule 10: SmD2

Chain Q: 75% 25%

MET	SER	LEU	LEU	ASN	LYS	PRO	LYS	SER	GLU	THR	PRO	GLU	GLU	LEU	GLN	LYS	ARG	GLU	GLU	GLU	PHE	ASN	T26	L114	ILE	ALA	GLY	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	-----	-----	-----	-----

- Molecule 10: SmD2

Chain q:  75% 25%

MET	SER	LEU	LEU	ASN	LYS	PRO	LYS	SER	GLU	MET	THR	PRO	GLU	GLU	LEU	GLN	LYS	ARG	GLU	GLU	GLU	PHE	ASN	T26	L114	ILE	ALA	GLY	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	-----	-----	-----	-----

- Molecule 11: SmD3

Chain R:  70% 30%

[illegible]

- Molecule 11: SmD3

Chain r:  70% 30%


MET	SER	ILE	G4	H	Q91	GLY	SER	GLY	ALA	GLY	ARG	GLY	LYS	ALA	ALA	ILE	LEU	LYS	ALA	GLN	VAL	ALA	ALA	ARG	GLY	ARG	GLY	GLY	GLY	MET	GLY	GLY	ASN	ILE	PHE	GLN	LYS	ARG	ARG
-----	-----	-----	----	---	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 12: SmE

Chain S: 85% 15%


MET
ALA
TYR
ARG
GLY
GLN
GLY
GLN
LYS
VAL
GLN
LYS
VAL
MET
V15
N92

- Molecule 12: SmE

Chain s:  85% 15%

MET ALA TYR ARG GLY GLN GLN VAL GLN VAL MET V15 N92

- Molecule 13: SmF

Chain T:  85% 15%

MET SER LEU P4 E76 GLU GLU GLU GLU ASP GLY GLU MET ARG GLU

- Molecule 13: SmF

Chain t:  97% .

MET SER LEU P4 E86

- Molecule 14: SmG

Chain U:  96% .

MET SER LYS A4 V76

- Molecule 14: SmG

Chain u:  96% .


MET SER LYS A4 V76

- Molecule 15: LSm8

Chain 8:  73% 27%


MET THR SER A4 I73 ASP GLU GLU THR ASP SER ALA LEU ASP LEU GLY ASN ILE ARG ALA LYS PRO PRO LEU ASN SER VAL ALA HIS

- Molecule 16: LSm6

Chain 6:  88% 13%

MET SER LEU ARG LYS GLN T7 Q76 LYS ARG ARG MET

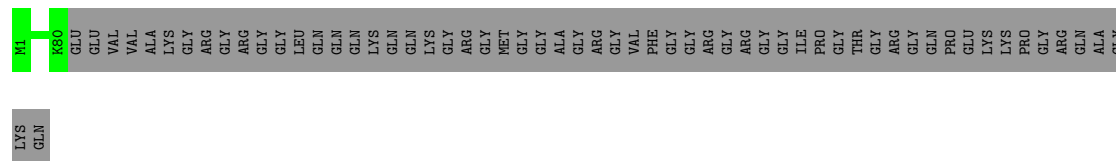
- Molecule 17: LSm5

Chain 5:  84% 16%


MET ALA ALA ASN ALA THR THR ASN PRO S10 Q85 GLY GLU GLY PRO GLU VAL

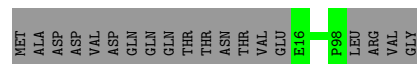
- Molecule 18: LS_m4

Chain 4: 58% 42%



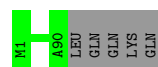
- Molecule 19: LSm3

Chain 3:  81% 19%



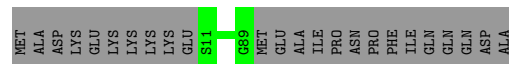
- Molecule 20: LSm2

Chain 2: 95% 5%



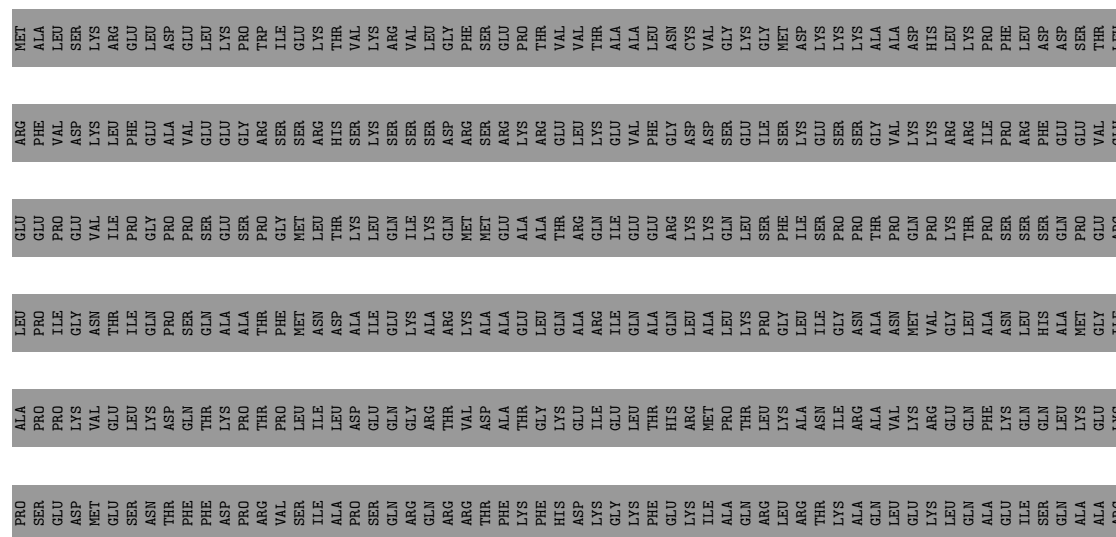
- Molecule 21: LSm7

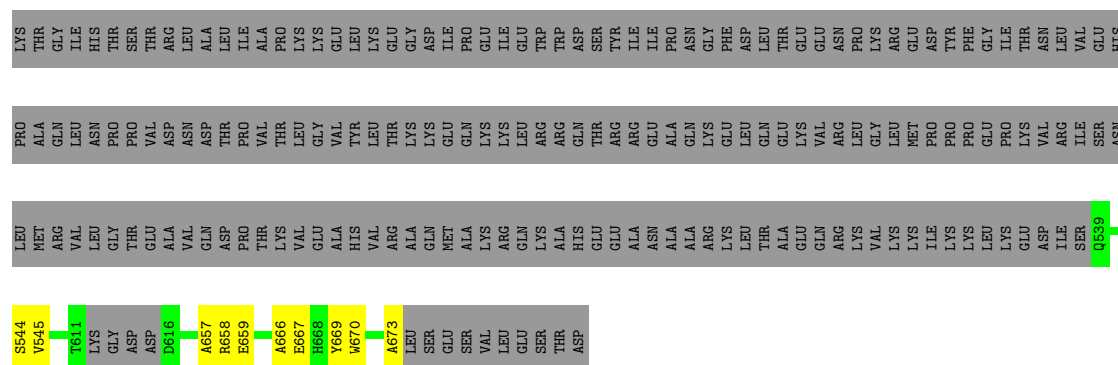
Chain 7: 77% 23%



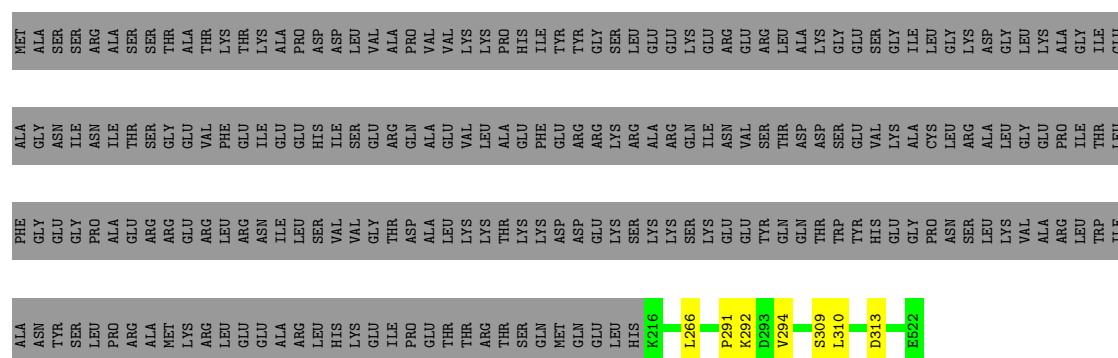
- Molecule 22: hPrp3

Chain K: 18% 81%

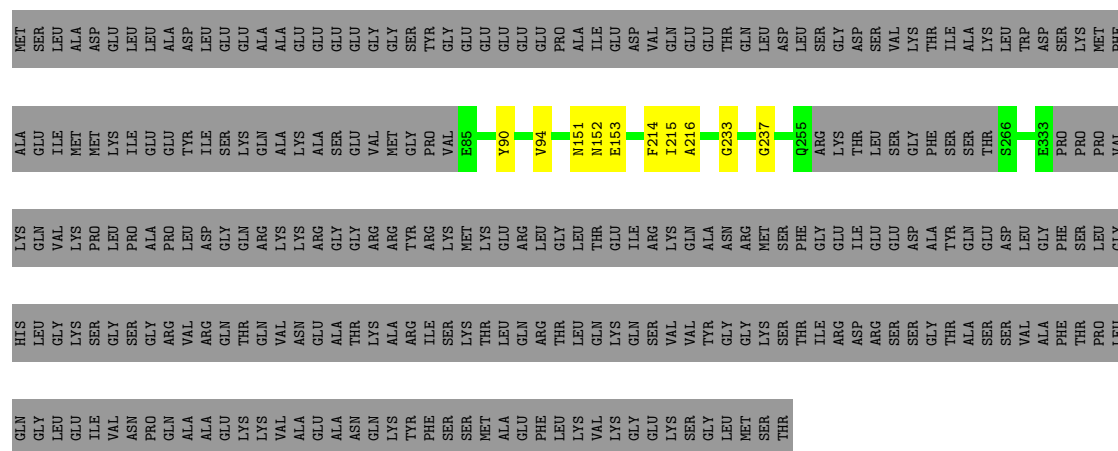




- Molecule 23: hPrp4



- Molecule 24: hPrp31

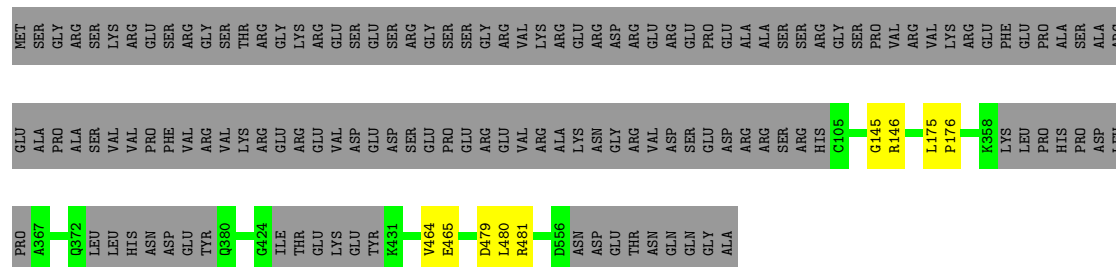


- Molecule 25: hSnu13



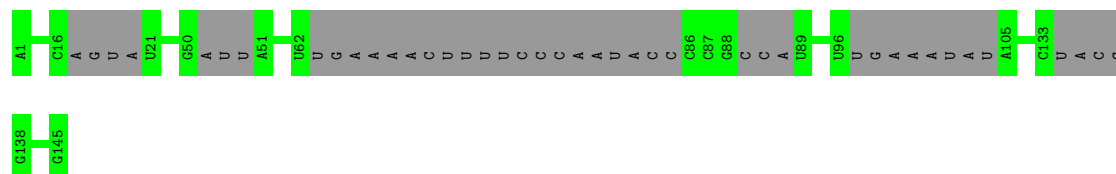
- Molecule 26: hSad1

Chain V:  75% . 24%



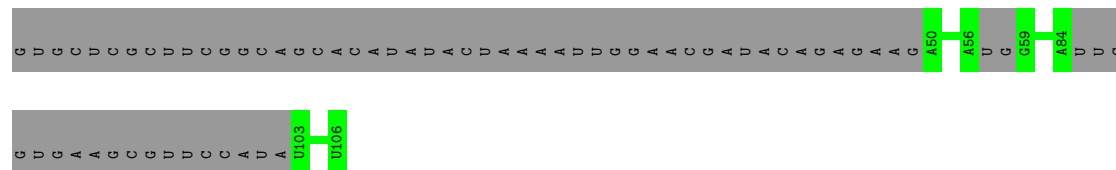
- Molecule 27: U4 snRNA

Chain M: 71% 29%



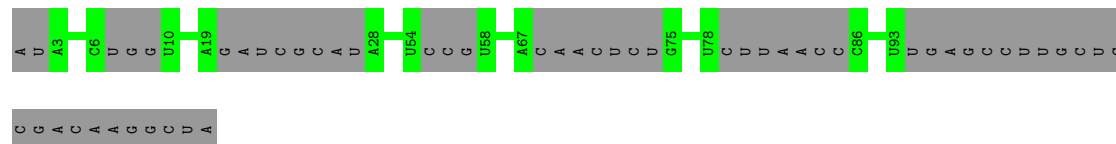
- Molecule 28: U6 snRNA

Chain N:  35% 65%



- Molecule 29: U5 snRNA

Chain H:  54% 46%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	141109	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5350	Depositor
Magnification	74000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	418	0	0	6	0
2	D	302	0	0	3	0
3	C	1885	0	0	1	0
4	E	135	0	0	1	0
5	A	2222	0	0	20	0
6	F	435	0	0	6	0
7	B	844	0	0	4	0
8	O	89	0	0	0	0
8	o	89	0	0	0	0
9	P	93	0	0	0	0
9	p	94	0	0	0	0
10	Q	89	0	0	0	0
10	q	89	0	0	0	0
11	R	88	0	0	0	0
11	r	88	0	0	0	0
12	S	78	0	0	0	0
12	s	78	0	0	0	0
13	T	73	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	t	83	0	0	0	0
14	U	73	0	0	0	0
14	u	73	0	0	0	0
15	8	70	0	0	0	0
16	6	70	0	0	0	0
17	5	76	0	0	0	0
18	4	80	0	0	0	0
19	3	83	0	0	0	0
20	2	90	0	0	0	0
21	7	79	0	0	0	0
22	K	131	0	0	10	0
23	L	307	0	0	10	0
24	J	239	0	0	7	0
25	I	126	0	0	2	0
26	V	431	0	0	6	0
27	M	103	0	0	0	0
28	N	37	0	0	0	0
29	H	63	0	0	0	0
All	All	9403	0	0	52	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (52) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:J:94:VAL:CA	24:J:233:GLY:CA	1.95	1.44
5:A:294:ASN:CA	5:A:1141:ARG:CA	1.96	1.43
4:E:95:GLY:CA	5:A:707:ARG:CA	1.95	1.42
22:K:669:TYR:CA	23:L:294:VAL:CA	1.98	1.39
24:J:215:ILE:CA	24:J:216:ALA:CA	2.03	1.36
24:J:153:GLU:CA	26:V:479:ASP:CA	2.11	1.28
5:A:295:GLU:CA	5:A:1142:LEU:CA	2.11	1.27
5:A:675:GLN:CA	5:A:676:ARG:CA	2.27	1.13
5:A:678:GLU:CA	5:A:750:TRP:CA	2.29	1.10
5:A:158:ARG:CA	6:F:372:ILE:CA	2.39	1.00
1:G:652:GLU:CA	1:G:661:ALA:CA	2.40	0.99
5:A:292:ASP:CA	5:A:1140:MET:CA	2.51	0.88
22:K:667:GLU:CA	23:L:310:LEU:CA	2.53	0.86
24:J:151:ASN:CA	26:V:481:ARG:CA	0.84	0.84
2:D:254:ALA:CA	5:A:30:LEU:CA	2.56	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:350:PHE:CA	7:B:270:PRO:CA	2.57	0.82
5:A:384:VAL:CA	7:B:355:LYS:CA	2.60	0.79
24:J:214:PHE:CA	24:J:216:ALA:CA	2.60	0.78
6:F:637:GLU:CA	6:F:638:ARG:CA	2.65	0.75
22:K:659:GLU:CA	23:L:313:ASP:CA	2.68	0.71
24:J:152:ASN:CA	26:V:480:LEU:CA	0.67	0.67
1:G:318:LEU:CA	5:A:1798:LEU:CA	2.73	0.66
1:G:434:VAL:CA	1:G:455:LYS:CA	2.74	0.65
22:K:673:ALA:CA	23:L:266:LEU:CA	2.76	0.63
5:A:293:TRP:CA	5:A:1141:ARG:CA	2.77	0.62
1:G:519:VAL:CA	1:G:551:VAL:CA	2.78	0.62
3:C:105:LYS:CA	3:C:110:ARG:CA	2.78	0.61
1:G:834:LEU:CA	1:G:851:PHE:CA	2.79	0.60
6:F:665:PRO:CA	6:F:666:PRO:CA	2.80	0.60
6:F:629:ILE:CA	6:F:630:GLY:CA	0.59	0.58
26:V:145:GLY:CA	26:V:146:ARG:CA	2.82	0.57
5:A:725:PRO:CA	5:A:726:TRP:CA	2.84	0.56
24:J:90:TYR:CA	24:J:237:GLY:CA	2.84	0.56
25:I:3:GLU:CA	25:I:4:ALA:CA	2.87	0.53
25:I:61:GLU:CA	25:I:62:PRO:CA	2.87	0.52
2:D:256:ASP:CA	5:A:29:LYS:CA	2.87	0.52
5:A:388:LEU:CA	5:A:389:LYS:CA	2.88	0.52
22:K:658:ARG:CA	23:L:313:ASP:CA	2.88	0.52
26:V:175:LEU:CA	26:V:176:PRO:CA	2.91	0.49
22:K:670:TRP:CA	23:L:310:LEU:CA	2.90	0.48
22:K:657:ALA:CA	23:L:313:ASP:CA	2.91	0.48
5:A:1795:GLU:CA	5:A:1796:GLY:CA	2.92	0.47
5:A:159:ARG:CA	6:F:372:ILE:CA	2.93	0.47
22:K:545:VAL:CA	23:L:291:PRO:CA	0.45	0.45
5:A:357:ASN:CA	7:B:864:PRO:CA	2.95	0.45
1:G:545:GLU:CA	1:G:558:CYS:CA	2.95	0.44
2:D:256:ASP:CA	5:A:30:LEU:CA	2.96	0.43
5:A:1123:GLU:CA	7:B:597:PRO:CA	2.97	0.43
22:K:666:ALA:CA	23:L:309:SER:CA	2.96	0.43
6:F:638:ARG:CA	6:F:639:VAL:CA	2.98	0.42
22:K:544:SER:CA	23:L:292:LYS:CA	2.98	0.42
26:V:464:VAL:CA	26:V:465:GLU:CA	2.98	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	M	0/145	-	-
28	N	0/106	-	-
29	H	0/116	-	-
All	All	0/367	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.