



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Aug 27, 2017 – 08:09 AM EDT

PDB ID : 5O9Z  
EMDB ID: : EMD-3766  
Title : Cryo-EM structure of a pre-catalytic human spliceosome primed for activation (B complex)  
Authors : Bertram, K.; Kastner, B.  
Deposited on : unknown  
Resolution : 4.50 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](mailto: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.

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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) : rb-20029824

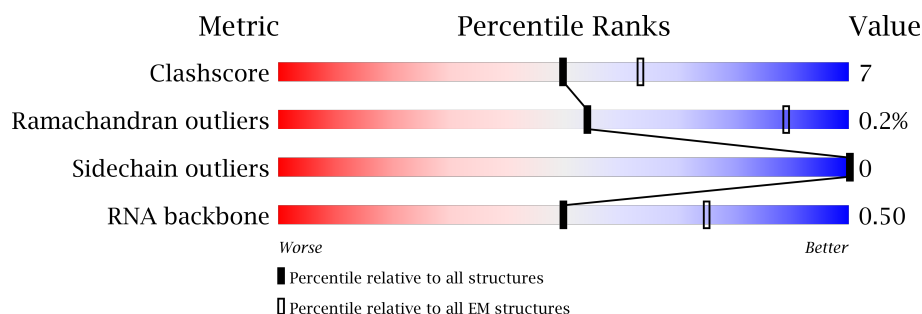
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.50 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.




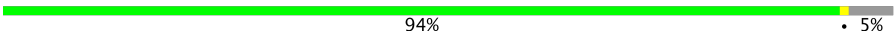




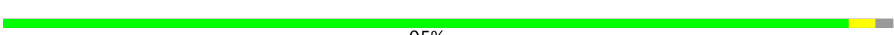




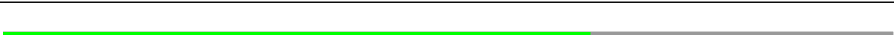

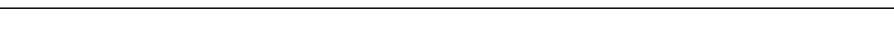
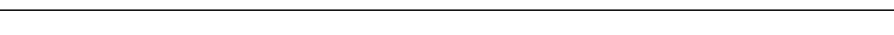
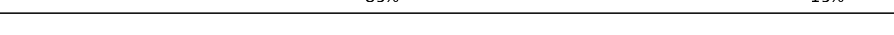

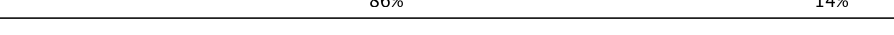


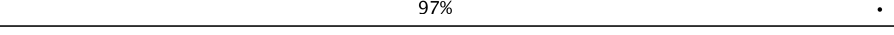

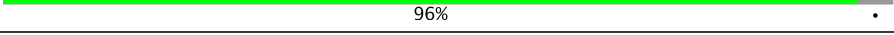


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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  $\geq 3$ , 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	A	2335	89% 5% 6%
2	B	972	81% 6% 13%
3	C	2136	75% 21%
4	D	357	85% 15%
5	E	683	28% 68%
6	F	521	72% 9% 19%
7	G	941	79% 6% 15%
8	H	499	77% 5% 17%







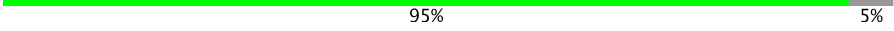






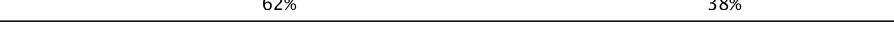
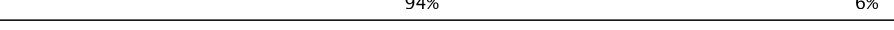






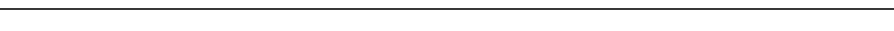


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Mol	Chain	Length	Quality of chain
9	I	312	
10	J	142	
11	K	439	
12	L	513	
13	M	177	
14	N	199	
15	O	128	
16	P	800	
17	Q	376	
18	R	557	
19	S	118	
19	a	118	
19	h	118	
20	T	86	
20	b	86	
20	i	86	
21	U	92	
21	c	92	
21	j	92	
22	V	76	
22	d	76	
22	k	76	
23	W	126	
23	e	126	
23	l	126	

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Mol	Chain	Length	Quality of chain
24	X	240	
24	f	240	
24	m	240	
25	Z	119	
25	g	119	
25	n	119	
26	o	95	
27	p	102	
28	q	139	
29	r	91	
30	s	80	
31	t	103	
32	u	96	
33	v	1304	
34	w	1217	
35	x	86	
36	y	110	
37	z	256	
38	1	225	
39	Y	324	
40	2	188	
41	4	145	
42	5	116	
43	6	106	

## 2 Entry composition

There are 43 unique types of molecules in this entry. The entry contains 59243 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 Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	2190	Total	C	N	O	0	0
			11100	6725	2190	2185		

- Molecule 2 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	844	Total	C	N	O	0	0
			4264	2577	844	843		

- Molecule 3 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	1693	Total	C	N	O	0	0
			8538	5154	1693	1691		

- Molecule 4 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

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

- Molecule 5 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	219	Total	C	N	O	0	0
			1101	663	219	219		

- Molecule 6 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	420	Total	C	N	O	0	0
			2100	1260	420	420		

- Molecule 7 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	804	Total	C	N	O	0	0
			4057	2449	804	804		

- Molecule 8 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	413	Total	C	N	O	0	0
			2068	1243	413	412		

- Molecule 9 is a protein called Pre-mRNA-splicing factor 38A.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	176	Total	C	N	O	0	0
			883	531	176	176		

- Molecule 10 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	135	Total	C	N	O	0	0
			677	408	135	134		

- Molecule 11 is a protein called Microfibrillar-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	45	Total	C	N	O	0	0
			225	135	45	45		

- Molecule 12 is a protein called WD40 repeat-containing protein SMU1.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	459	Total	C	N	O	0	0
			2288	1370	459	459		

- Molecule 13 is a protein called Peptidyl-prolyl cis-trans isomerase H.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	169	Total	C	N	O	0	0
			844	506	169	169		

- Molecule 14 is a protein called Zinc finger matrin-type protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	56	Total	C	N	O	0	0
			277	165	56	56		

- Molecule 15 is a protein called NHP2-like protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	126	Total	C	N	O	0	0
			636	385	126	125		

- Molecule 16 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	91	Total	C	N	O	0	0
			458	276	91	91		

- Molecule 17 is a protein called WW domain-binding protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	75	Total	C	N	O	0	0
			378	228	75	75		

- Molecule 18 is a protein called Protein Red.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	16	Total	C	N	O	0	0
			79	47	16	16		

- Molecule 19 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	a	78	Total	C	N	O	0	0
			393	237	78	78		
19	h	74	Total	C	N	O	0	0
			371	223	74	74		
19	S	87	Total	C			0	87
			87	87				

- Molecule 20 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	b	73	Total	C	N	O	0	0
			364	218	73	73		

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Mol	Chain	Residues	Atoms				AltConf	Trace
20	i	71	Total	C	N	O	0	0
			354	212	71	71		
20	T	74	Total	C			0	74
			74	74				

- Molecule 21 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	c	78	Total	C	N	O	0	0
			388	232	78	78		
21	j	78	Total	C	N	O	0	0
			388	232	78	78		
21	U	79	Total	C			0	79
			79	79				

- Molecule 22 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	d	69	Total	C	N	O	0	0
			344	206	69	69		
22	k	73	Total	C	N	O	0	0
			364	218	73	73		
22	V	74	Total	C			0	74
			74	74				

- Molecule 23 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	e	78	Total	C	N	O	0	0
			390	234	78	78		
23	l	71	Total	C	N	O	0	0
			353	211	71	71		
23	W	80	Total	C			0	80
			80	80				

- Molecule 24 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	f	64	Total	C	N	O	0	0
			319	191	64	64		

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Mol	Chain	Residues	Atoms				AltConf	Trace
24	m	64	Total	C	N	O	0	0
			316	188	64	64		
24	X	71	Total	C			0	71
			71	71				

- Molecule 25 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	g	93	Total	C	N	O	0	0
			469	283	93	93		
25	n	82	Total	C	N	O	0	0
			412	248	82	82		
25	Z	82	Total	C			0	82
			82	82				

- Molecule 26 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms		AltConf	Trace
26	o	90	Total	C	0	90
			90	90		

- Molecule 27 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms		AltConf	Trace
27	p	73	Total	C	0	73
			73	73		

- Molecule 28 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms		AltConf	Trace
28	q	80	Total	C	0	80
			80	80		

- Molecule 29 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms		AltConf	Trace
29	r	76	Total	C	0	76
			76	76		

- Molecule 30 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms		AltConf	Trace
30	s	69	Total	C	0	69
			69	69		

- Molecule 31 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms		AltConf	Trace
31	t	79	Total	C	0	79
			79	79		

- Molecule 32 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms		AltConf	Trace
32	u	62	Total	C	0	62
			62	62		

- Molecule 33 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms		AltConf	Trace
33	v	806	Total	C	0	806
			806	806		

- Molecule 34 is a protein called Splicing factor 3B subunit 3 (SF3B3).

Mol	Chain	Residues	Atoms		AltConf	Trace
34	w	1140	Total	C	0	1140
			1140	1140		

- Molecule 35 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms		AltConf	Trace
35	x	54	Total	C	0	54
			54	54		

- Molecule 36 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms		AltConf	Trace
36	y	89	Total	C	0	89
			89	89		

- Molecule 37 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms		AltConf	Trace
37	z	162	Total	C	0	162
			162	162		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	89	ASP	CYS	conflict	UNP P09661
z	119	CYS	SER	conflict	UNP P09661
z	151A	PHE	-	insertion	UNP P09661

- Molecule 38 is a protein called U2 small nuclear ribonucleoprotein B”.

Mol	Chain	Residues	Atoms		AltConf	Trace
38	1	94	Total	C	0	94
			94	94		

- Molecule 39 is a RNA chain called MINX pre-mRNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	Y	46	Total	C	N	O	P	
			972	435	167	324	46	0

- Molecule 40 is a RNA chain called Human gene for small nuclear RNA U2 (snRNA U2).

Mol	Chain	Residues	Atoms				AltConf	Trace
40	2	100	Total	C	N	O	P	
			2123	947	367	709	100	0

- Molecule 41 is a RNA chain called Homo sapiens U4A snRNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	4	137	Total	C	N	O	P	
			2904	1298	501	968	137	0

- Molecule 42 is a RNA chain called Homo sapiens U5 A small nuclear RNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	5	114	Total	C	N	O	P	
			2397	1074	399	810	114	0

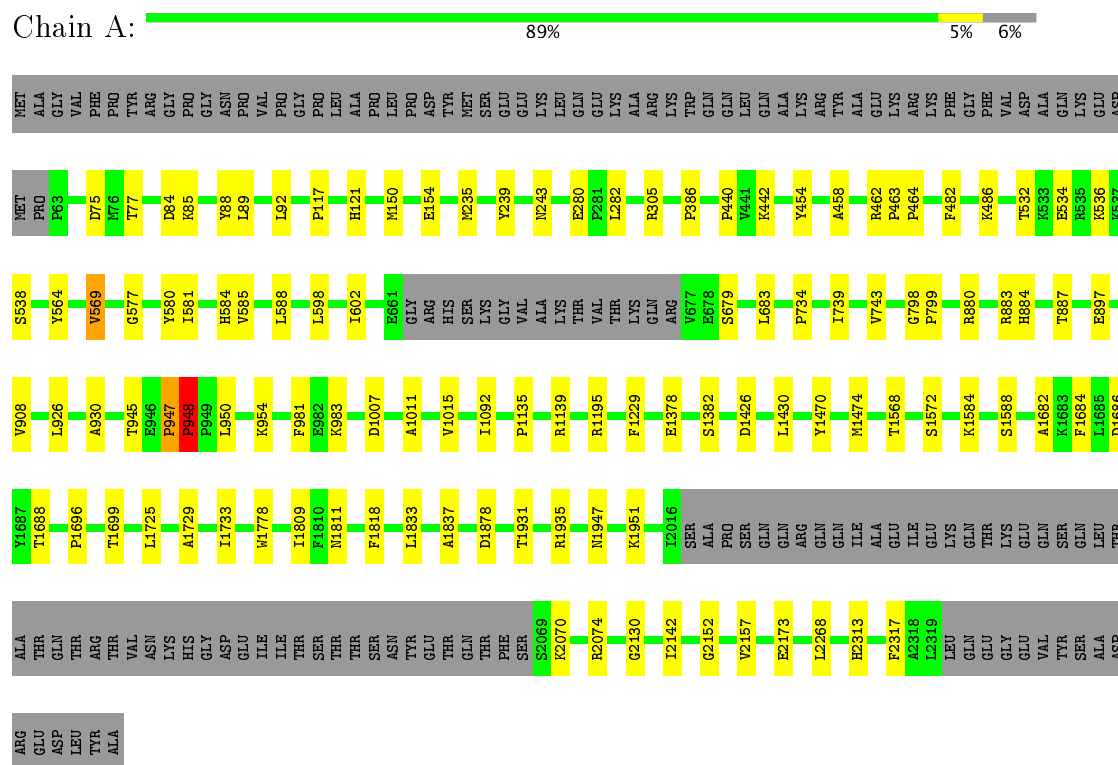
- Molecule 43 is a RNA chain called Homo sapiens RNA, U6 small nuclear 1 (RNU6-1), small nuclear RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	6	90	Total	C	N	O	P	0	0
			1926	861	353	622	90		

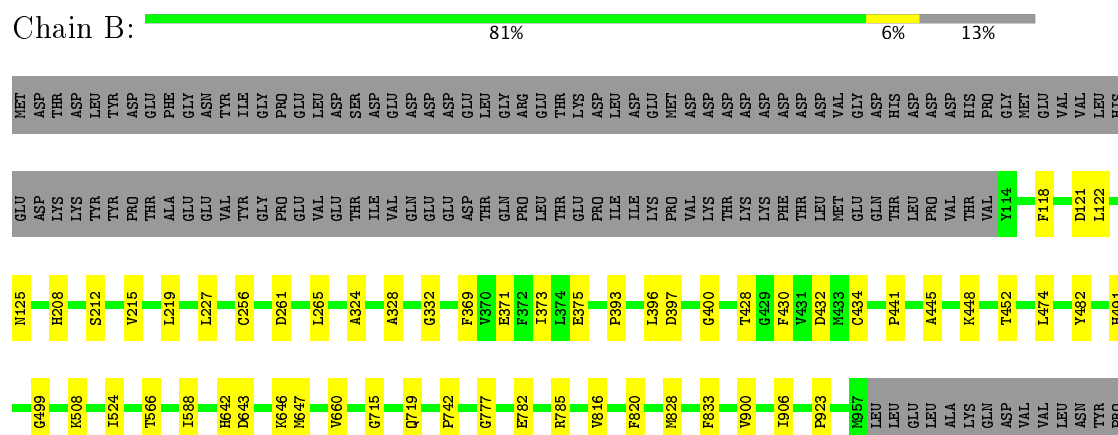
### 3 Residue-property plots

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.

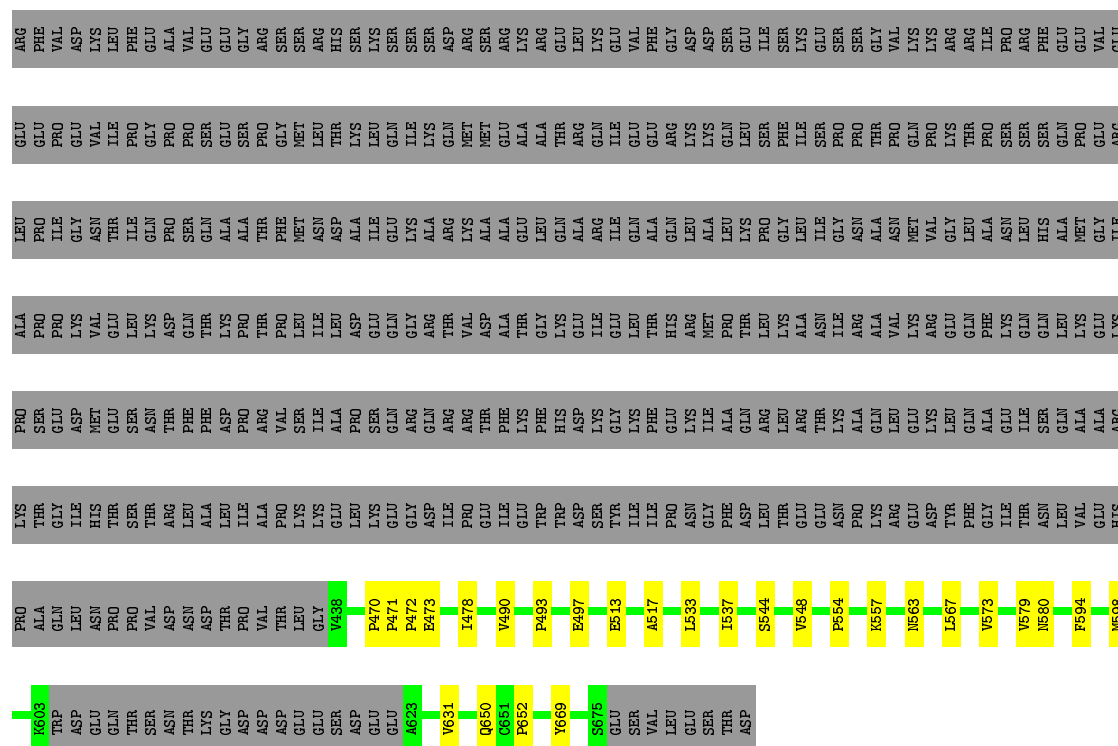
- Molecule 1: Pre-mRNA-processing-splicing factor 8



- Molecule 2: 116 kDa U5 small nuclear ribonucleoprotein component

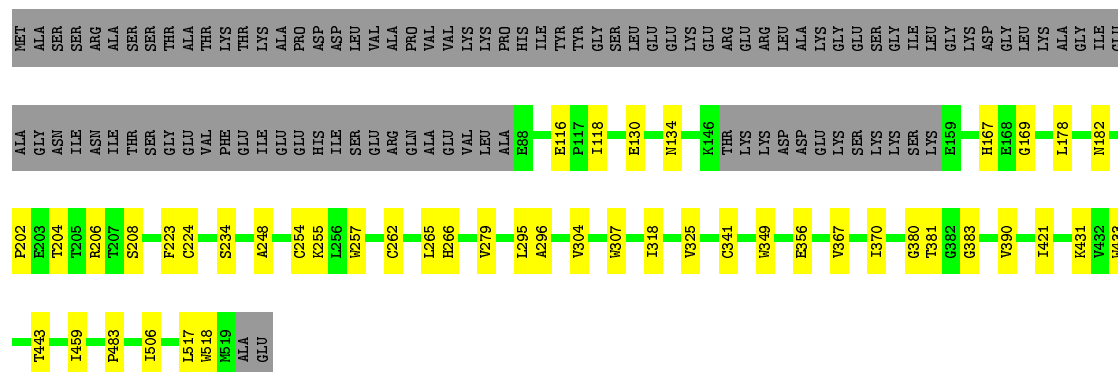


MET	ALA	LEU	SER	LYS	ARG	GLU	LEU	ASP	GLY	LEU	LYS	PRO	TRP	ILE	GLY	LYS	THR	VAL	ARG	VAL	LEU	GLY	PHE	SER	GLU	PRO	THR	VAL	VAL	ALA	ALA	ASN	CYS	VAL	GLY	LYS	GLY	GLY	MET	LYS	LYS	LYS	ALA	ALA	ASP	HIS	LEU	LEU	PRO	PHE	ASP	ASP	SER	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



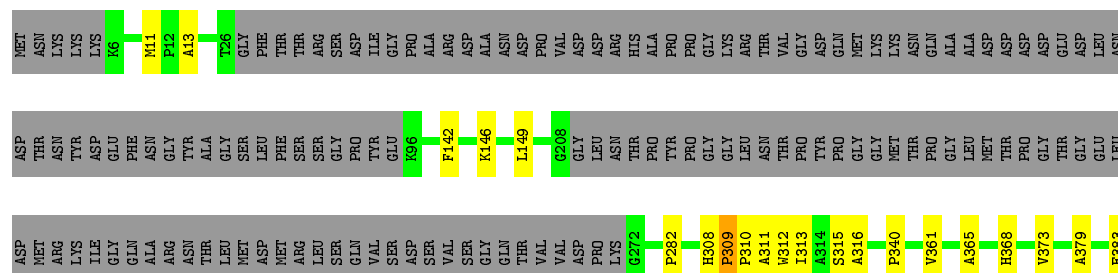
• Molecule 6: U4/U6 small nuclear ribonucleoprotein Prp4

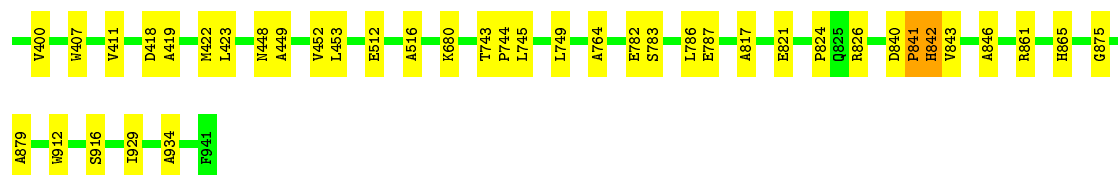
Chain F: 72% 9% 19%



• Molecule 7: Pre-mRNA-processing factor 6

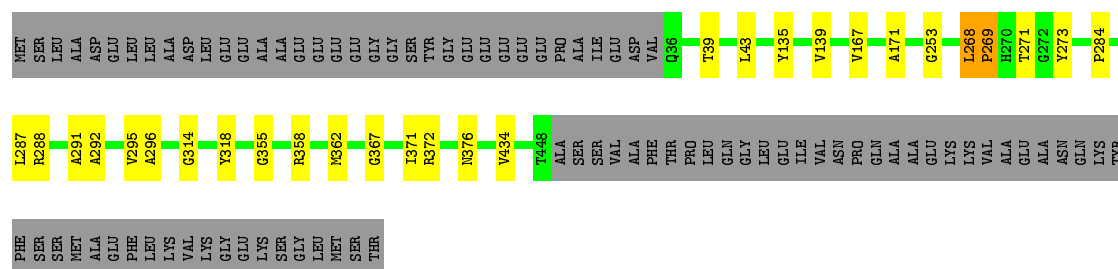
Chain G: 79% 6% 15%





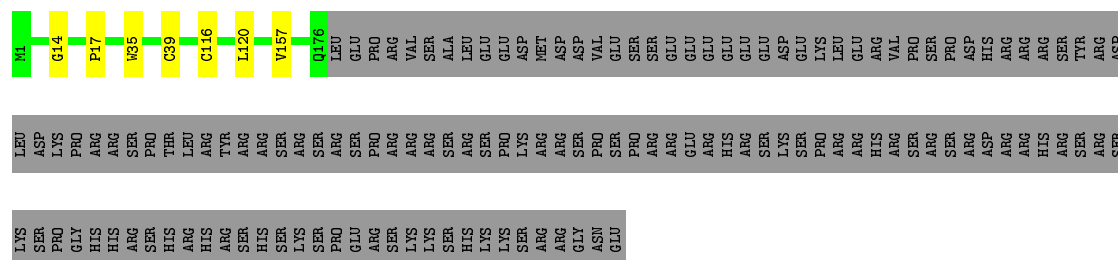
- Molecule 8: U4/U6 small nuclear ribonucleoprotein Prp31

Chain H: 77% 5% 17%



- Molecule 9: Pre-mRNA-splicing factor 38A

Chain I: 54% 44%



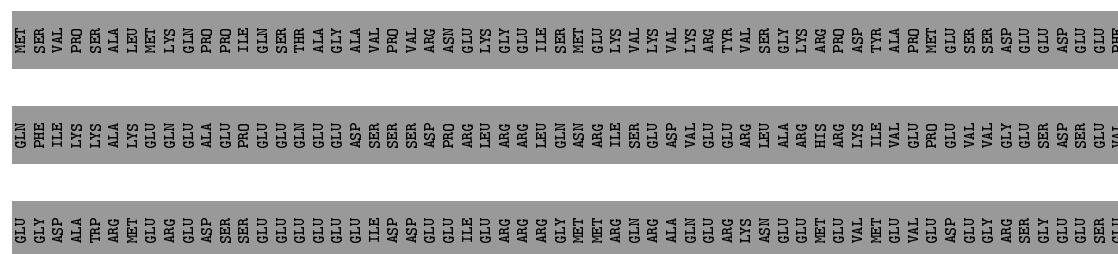
- Molecule 10: Thioredoxin-like protein 4A

Chain J: 94% 5%

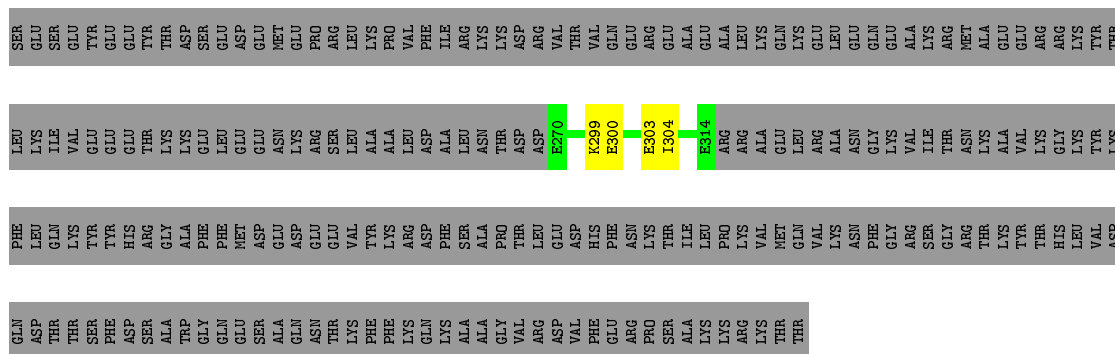


- Molecule 11: Microfibrillar-associated protein 1

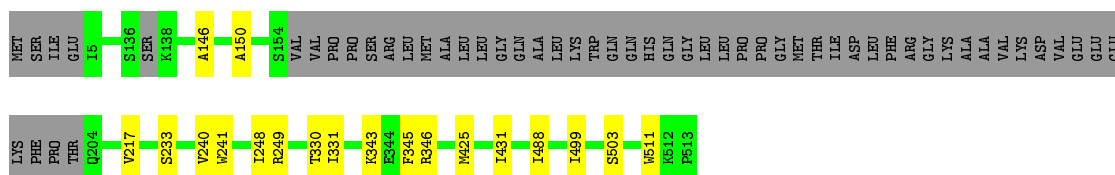
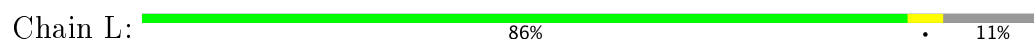
Chain K: 9% 90%







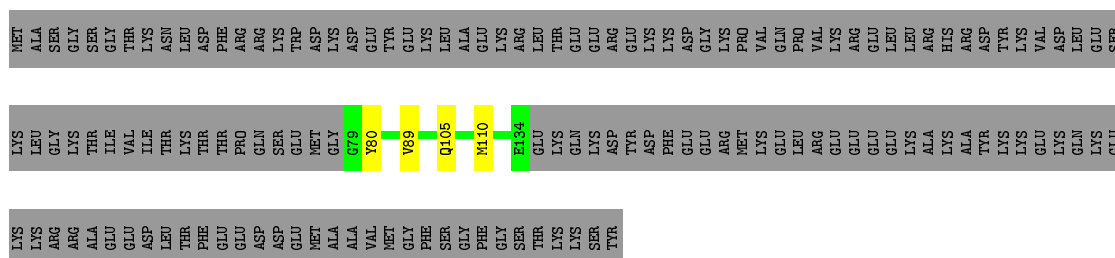
- Molecule 12: WD40 repeat-containing protein SMU1



- Molecule 13: Peptidyl-prolyl cis-trans isomerase H



- Molecule 14: Zinc finger matrin-type protein 2



- Molecule 15: NHP2-like protein 1



- Molecule 16: U4/U6.U5 tri-snRNP-associated protein 1



[illegible]

- Molecule 17: WW domain-binding protein 4

Chain Q:  19% . 80%

[illegible]

ARG GLN ARG GLY ASP ASP GLN

- Molecule 18: Protein Red

Chain R:  97%

ARG	ASN	GLN	ARG	ALA	THR	LYS	SER	PRO	MET
PRO	ASN	LEU	GLU	ASP	THR	GLU	THR	ARG	PRO
LYS	ASN	GLY	GLU	MET	LEU	LYS	THR	GLU	GLY
TYR	GLU	ASP	LYS	ASN	ILE	GLU	ALA	TYR	GLU
	ALA	PHE	LYS	ILE	ARG	GLU	ASN	GLU	ASN
	LEU	PHE	LYS	PHE	SER	GLU	TYR	GLU	SER
	PRO	GLY	ARG	GLU	LYS	GLU	ARG	ASP	GLU
	LYS	MET	HIS	ASP	ALA	LEU	ALA	GLU	PRO
	ALA	SER	TYR	ILE	ASP	MET	VAL	ASP	SER
	ALA	ASN	TYR	GLY	CYS	GLY	GLY	PRO	ALA
	PHE	SER	PHE	ASP	PRO	LYS	THR	ALA	ASN
	GLN	TYR	GLU	TYR	THR	PRO	THR	ARG	PRO
	TYR	ALA	LYS	VAL	MET	GLN	ALA	ARG	LEU
	GLY	GLU	PRO	PRO	GLU	LYS	GLU	ARG	ALA
	ILE	CYS	LYS	SER	ALA	GLU	ALA	ARG	PRO
	LYS	TYR	VAL	THR	GLN	THR	LYS	ASP	ASP
	MET	PRO	ASP	THR	THR	LYS	LYS	LYS	GLY
	SER	ALA	ASP	LYS	THR	LYS	SER	LYS	HIS
	GLU	THR	GLU	THR	LEU	ASP	ALA	SER	ASP
	GLY	THR	GLU	PRO	THR	GLU	ALA	TYR	VAL
	ARG	ASP	MET	ASP	THR	PRO	ALA	VAL	ASP
	LYS	ASP	ASP	ASP	ASN	PRO	LYS	ASP	ALA
	THR	MET	VAL	LYS	ILE	ASN	ARG	LYS	PRO
	ARG	ALA	ASP	GLU	ILE	ASN	ARG	LYS	HIS
	ARG	VAL	LYS	ARG	VAL	LYS	GLN	ARG	THR
	PHE	ASP	GLY	GLU	ILE	ILE	ILE	GLN	PHE
	LYS	SER	PRO	ARG	SER	E2Q7	ILE	GLN	HIS
	GLU	ASP	GLU	TYR	LYS	E2Q2	GLU	GLU	GLN
	THR	GLU	SER	ARG	LEU	SER	GLU	ILE	SER
	ASN	GLU	THR	GLU	THR	SER	SER	GLU	LYS
	ASP	VAL	LYS	ARG	GLN	LYS	LYS	ARG	LEU
	LYS	ASP	GLU	GLU	ILE	ALA	PHE	GLU	THR
	ALA	TYR	LEU	ARG	LEU	TYR	GLU	ARG	ASN
	GLU	SER	ILE	ASP	SER	GLU	GLY	GLU	GLU
	LEU	LYS	LYS	ARG	TYR	ARG	GLY	LEU	ASP
	ASP	MET	SER	GLU	LEU	ASN	ASP	ALA	PHE
	ARG	ASP	ILE	ARG	ARG	GLU	MET	ARG	ARG
	GLN	GLN	ASN	ASP	GLN	LEU	GLU	LYS	LYS
	TRP	GLY	GLU	ARG	GLN	PHE	HIS	TYR	LEU
	LYS	ASN	LYS	ASP	THR	LEU	THR	ARG	ASP
	LYS	LYS	PHE	ARG	ARG	PRO	HIS	ASP	MET
	ILE	LYS	ALA	ASP	ASN	GLY	LEU	ARG	THR
	SER	GLY	GLY	ARG	LYS	ARG	VAL	ALA	PRO
	ALA	PRO	SER	GLU	LYS	MET	LYS	LYS	ARG
	ILE	LEU	ALA	ARG	LEU	ALA	GLY	GLU	ALA
	ILE	GLY	GLY	GLU	LYS	VAL	LEU	ARG	PRO
	GLU	ARG	TRP	ARG	LYS	VAL	ASP	ARG	PRO
	LYS	TRP	GLU	GLU	LYS	VAL	PHE	ASP	THR
	ARG	PHE	GLY	GLU	LYS	VAL	GLY	ASP	SER
	LYS	LYS	GLY	GLU	LYS	VAL	LEU	GLN	LYS
	ASN	THR	THR	GLU	LYS	GLU	LYS	ASP	PRO
	ALA	GLU	LYS	GLU	GLU	TYR	VAL	SER	LYS
	ASP	GLU	TYR	ARG	GLU	ALA	ARG	GLU	THR
	GLY	TYR	PRO	GLU	LYS	ASP	ALA	GLU	GLU
	VAL	SER	GLU	ASP	PRO	THR	ILE	GLU	HIS
	VAL	TYR	LYS	GLU	PRO	ILE	SER	GLU	HIS
	LYS	MET	LYS	GLU	THR	PRO	SER	LEU	THR

- Molecule 19: Small nuclear ribonucleoprotein Sm D2

Chain a:  66% 34%

MET	SER	LEU	LEU	ASN	LYS	PRO	LYS	SER	GLU	GLN	ARG	GLU	GLU	GLU	PHE	ASN	T26	V77	PRO	LYS	SER	GLY	LYS	LYS	LYS	LYS	SER	LYS	P89	L114	L114	ALA	GLY	LYS
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- Molecule 19: Small nuclear ribonucleoprotein Sm D2

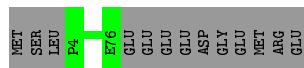
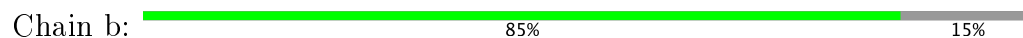
Chain h:  63% 37%

MET	SER	LEU	ASU	LVS	PRO	SER	GLU	MET	THR	PRO	GLU	GLU	LEU	GLN	LVS	ARG	GLU	GLU	GLU	GLU	PHE	ASN	T26	T75	GLU	VAL	PRO	LYS	SER	GLY	LVS	GLY	LVS	LVS	LVS	SER	LVS	PRO	VAL	N91	L114	IIE	ALA	GLY	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	-----	-----	-----	-----

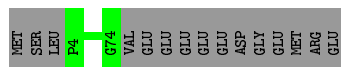
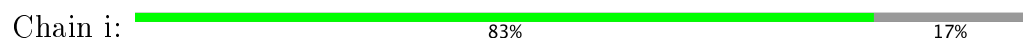
- Molecule 19: Small nuclear ribonucleoprotein Sm D2

Chain S:  74% 26%

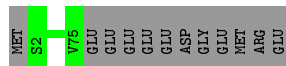
- Molecule 20: Small nuclear ribonucleoprotein F



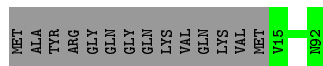
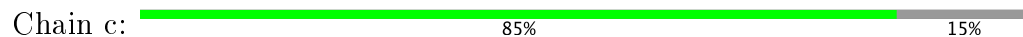
- Molecule 20: Small nuclear ribonucleoprotein F



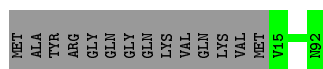
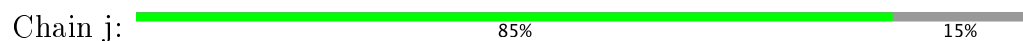
- Molecule 20: Small nuclear ribonucleoprotein F



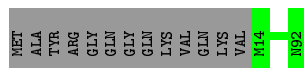
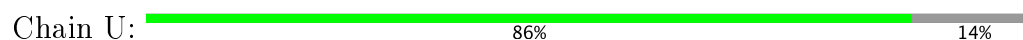
- Molecule 21: Small nuclear ribonucleoprotein E



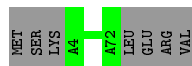
- Molecule 21: Small nuclear ribonucleoprotein E



- Molecule 21: Small nuclear ribonucleoprotein E



- Molecule 22: Small nuclear ribonucleoprotein G



- Molecule 22: Small nuclear ribonucleoprotein G

Chain k:  96%



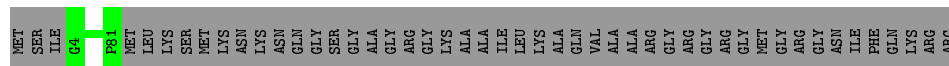
- Molecule 22: Small nuclear ribonucleoprotein G

Chain V:  97%



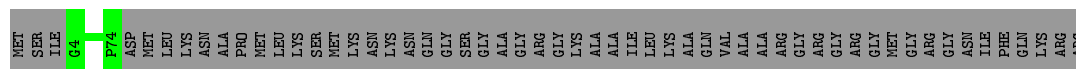
- Molecule 23: Small nuclear ribonucleoprotein Sm D3

Chain e:  62%



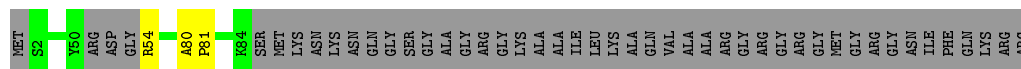
- Molecule 23: Small nuclear ribonucleoprotein Sm D3

Chain l:  56%



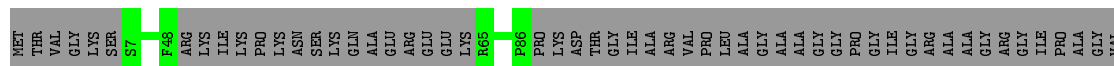
- Molecule 23: Small nuclear ribonucleoprotein Sm D3

Chain W:  61%



- Molecule 24: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain f:  27%



- Molecule 24: Small nuclear ribonucleoprotein-associated proteins B and B'

- Molecule 24: Small nuclear ribonucleoprotein-associated proteins B and B'

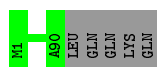
- Molecule 25: Small nuclear ribonucleoprotein Sm D1

- Molecule 25: Small nuclear ribonucleoprotein Sm D1

- Molecule 25: Small nuclear ribonucleoprotein Sm D1

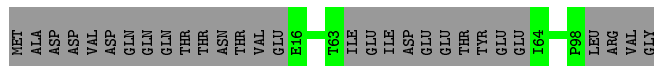
- Molecule 26: U6 snRNA-associated Sm-like protein LSm2



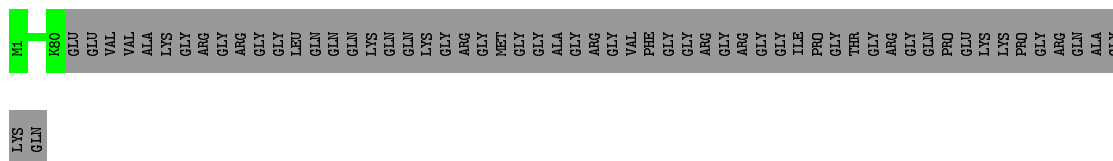
- Molecule 27: U6 snRNA-associated Sm-like protein LSm3

Chain p: 72% 28%



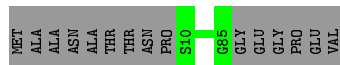
- Molecule 28: U6 snRNA-associated Sm-like protein LSm4

Chain q: 58% 42%



- Molecule 29: U6 snRNA-associated Sm-like protein LSm5

Chain r: 84% 16%



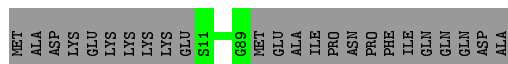
- Molecule 30: U6 snRNA-associated Sm-like protein LSm6

Chain s: 86% 14%



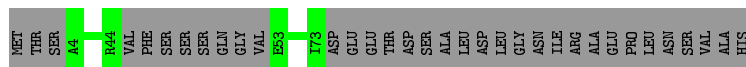
- Molecule 31: U6 snRNA-associated Sm-like protein LSm7

Chain t: 77% 23%



- Molecule 32: U6 snRNA-associated Sm-like protein LSm8

Chain u: 65% 35%

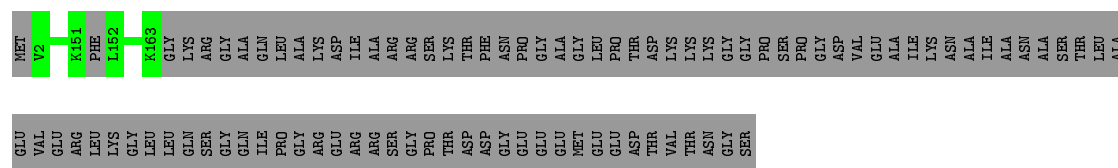


- Molecule 33: Splicing factor 3B subunit 1

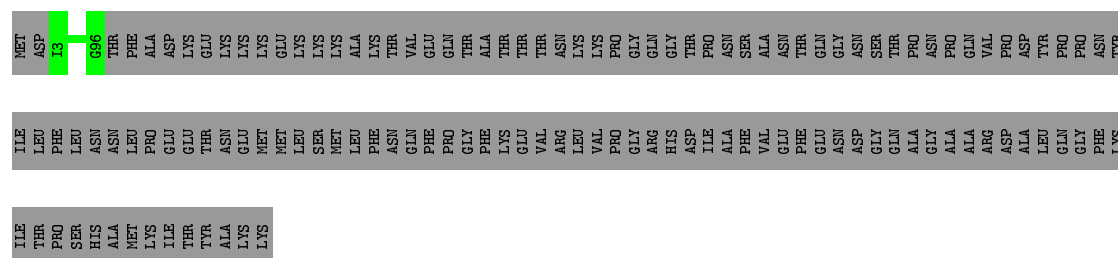
Chain v: 62% 38%



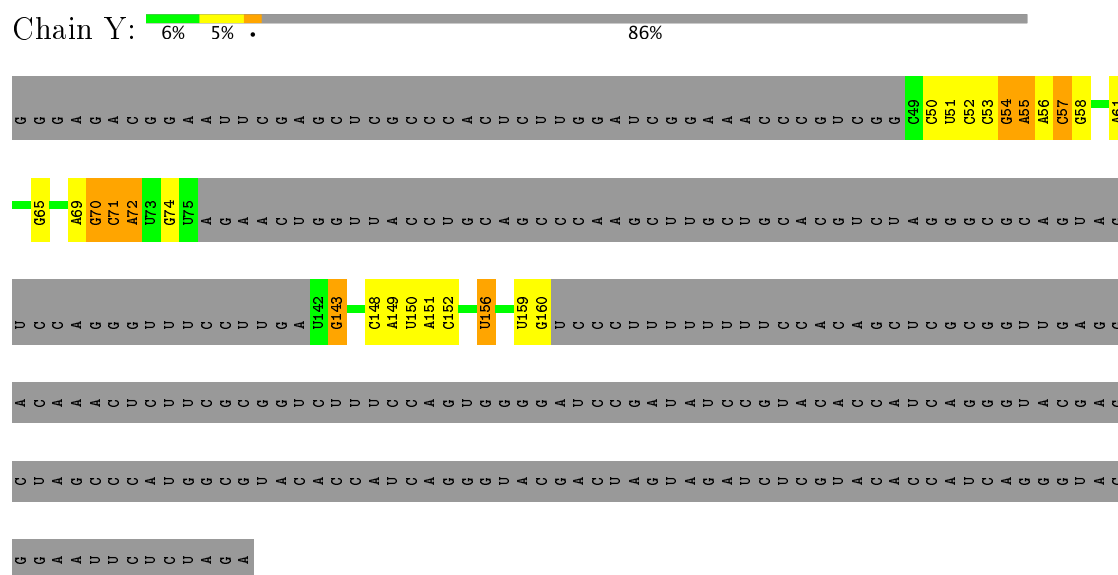




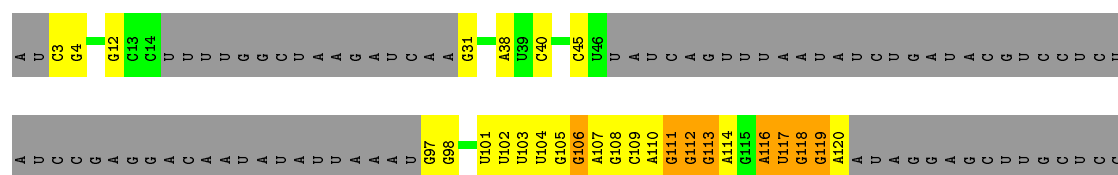
- Molecule 38: U2 small nuclear ribonucleoprotein B''



- Molecule 39: MINX pre-mRNA

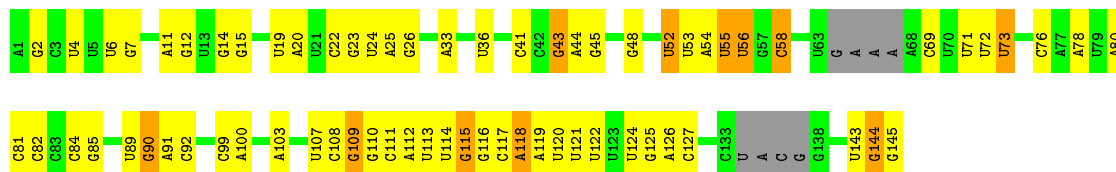


- Molecule 40: Human gene for small nuclear RNA U2 (snRNA U2)

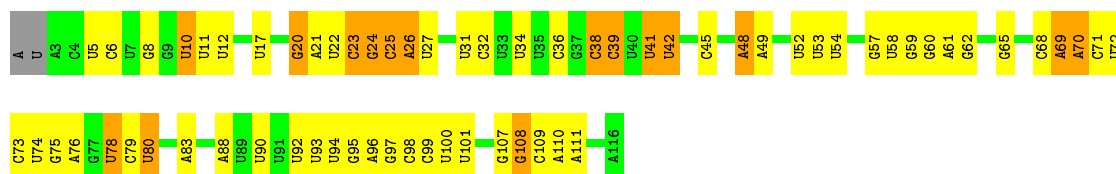




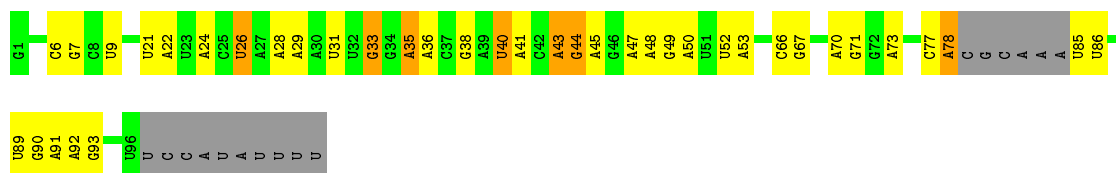
• Molecule 41: Homo sapiens U4A snRNA



• Molecule 42: Homo sapiens U5 A small nuclear RNA



• Molecule 43: Homo sapiens RNA, U6 small nuclear 1 (RNU6-1), small nuclear RNA



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	44629	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.5	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

## 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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.23	0/11222	0.41	0/15747
10	J	0.23	0/681	0.38	0/952
11	K	0.22	0/224	0.29	0/312
12	L	0.24	0/2295	0.44	0/3198
13	M	0.24	0/853	0.47	0/1188
14	N	0.22	0/276	0.43	0/383
15	O	0.22	0/641	0.39	0/898
16	P	0.22	0/459	0.36	0/640
17	Q	0.24	0/379	0.35	0/530
18	R	0.21	0/78	0.35	0/107
19	a	0.22	0/394	0.44	0/548
19	h	0.22	0/371	0.44	0/516
2	B	0.24	0/4312	0.43	0/6043
20	b	0.24	0/367	0.45	0/509
20	i	0.24	0/357	0.46	0/495
21	c	0.22	0/388	0.46	0/540
21	j	0.22	0/388	0.45	0/540
22	d	0.23	0/346	0.48	0/481
22	k	0.23	0/366	0.47	0/509
23	e	0.23	0/392	0.47	0/546
23	l	0.23	0/354	0.45	0/492
24	f	0.23	0/319	0.43	0/442
24	m	0.22	0/314	0.44	0/434
25	g	0.23	0/471	0.42	0/657
25	n	0.22	0/414	0.45	0/578
3	C	0.23	0/8613	0.41	0/12069
39	Y	0.44	4/1083 (0.4%)	0.75	0/1681
40	2	0.88	16/2366 (0.7%)	1.55	70/3677 (1.9%)
41	4	0.16	0/3240	0.71	0/5039
42	5	0.16	0/2672	0.76	0/4154
43	6	0.14	0/2155	0.70	0/3355
5	E	0.23	0/1107	0.42	0/1547
6	F	0.24	0/2115	0.45	0/2951
7	G	0.26	1/4089 (0.0%)	0.40	0/5728

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
8	H	0.49	1/2082 (0.0%)	0.40	0/2910
9	I	0.23	0/888	0.40	0/1241
All	All	0.30	22/57071 (0.0%)	0.58	70/81637 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
7	G	0	3
All	All	0	5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	268	LEU	C-N	19.79	1.71	1.34
40	2	150	U	C1'-N1	6.93	1.59	1.48
40	2	111	G	C1'-N9	-6.89	1.37	1.46
40	2	182	U	C1'-N1	6.86	1.59	1.48
40	2	142	U	C1'-N1	6.77	1.58	1.48
40	2	137	U	C1'-N1	6.76	1.58	1.48
40	2	148	C	C1'-N1	6.49	1.58	1.48
40	2	143	C	C1'-N1	6.35	1.58	1.48
7	G	400	VAL	C-N	6.35	1.46	1.34
40	2	141	C	C1'-N1	6.31	1.58	1.48
40	2	139	C	C1'-N1	6.31	1.58	1.48
40	2	97	G	C1'-N9	-6.30	1.38	1.46
39	Y	143	G	C1'-N9	-6.30	1.38	1.46
40	2	179	C	C1'-N1	6.29	1.58	1.48
40	2	151	C	C1'-N1	6.23	1.58	1.48
40	2	144	C	C1'-N1	6.23	1.58	1.48
40	2	138	C	C1'-N1	6.21	1.58	1.48
40	2	184	C	C1'-N1	6.21	1.58	1.48
40	2	110	A	C1'-N9	-5.70	1.38	1.46
39	Y	148	C	C1'-N1	5.48	1.56	1.48
39	Y	152	C	C1'-N1	5.38	1.56	1.48
39	Y	156	U	C1'-N1	5.25	1.56	1.48

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	2	167	U	C5-C4-O4	11.77	132.96	125.90
40	2	164	C	N1-C2-O2	-10.19	112.78	118.90
40	2	162	U	N3-C2-O2	-9.05	115.87	122.20
40	2	164	C	C5'-C4'-O4'	-8.38	99.04	109.10
40	2	169	C	P-O3'-C3'	8.20	129.53	119.70
40	2	167	U	N3-C4-O4	-8.02	113.78	119.40
40	2	166	G	O4'-C1'-N9	7.91	114.53	108.20
40	2	164	C	P-O3'-C3'	7.55	128.76	119.70
40	2	164	C	N3-C2-O2	7.50	127.15	121.90
40	2	167	U	N1-C2-O2	7.27	127.89	122.80
40	2	179	C	OP2-P-O3'	7.27	121.19	105.20
40	2	141	C	OP2-P-O3'	7.25	121.15	105.20
40	2	151	C	OP2-P-O3'	7.25	121.15	105.20
40	2	143	C	OP2-P-O3'	7.24	121.12	105.20
40	2	139	C	OP2-P-O3'	7.24	121.12	105.20
40	2	149	A	OP2-P-O3'	7.22	121.09	105.20
40	2	150	U	OP2-P-O3'	7.22	121.08	105.20
40	2	140	A	OP2-P-O3'	7.21	121.06	105.20
40	2	180	G	OP2-P-O3'	7.21	121.06	105.20
40	2	119	G	OP2-P-O3'	7.20	121.04	105.20
40	2	181	G	OP2-P-O3'	7.19	121.02	105.20
40	2	182	U	OP2-P-O3'	7.19	121.02	105.20
40	2	138	C	OP2-P-O3'	7.19	121.01	105.20
40	2	142	U	OP2-P-O3'	7.18	121.00	105.20
40	2	148	C	OP2-P-O3'	7.16	120.94	105.20
40	2	183	G	OP2-P-O3'	7.14	120.92	105.20
40	2	137	U	OP2-P-O3'	7.14	120.92	105.20
40	2	168	A	P-O5'-C5'	-7.14	109.48	120.90
40	2	167	U	N3-C2-O2	-7.04	117.27	122.20
40	2	106	G	O5'-P-OP1	6.92	119.00	110.70
40	2	119	G	O3'-P-O5'	-6.80	91.08	104.00
40	2	151	C	O3'-P-O5'	-6.80	91.08	104.00
40	2	181	G	O3'-P-O5'	-6.80	91.09	104.00
40	2	183	G	O3'-P-O5'	-6.79	91.10	104.00
40	2	142	U	O3'-P-O5'	-6.79	91.10	104.00
40	2	141	C	O3'-P-O5'	-6.78	91.11	104.00
40	2	150	U	O3'-P-O5'	-6.78	91.11	104.00
40	2	166	G	C8-N9-C4	-6.78	103.69	106.40
40	2	182	U	O3'-P-O5'	-6.78	91.12	104.00
40	2	180	G	O3'-P-O5'	-6.77	91.14	104.00
40	2	137	U	O3'-P-O5'	-6.77	91.14	104.00
40	2	139	C	O3'-P-O5'	-6.76	91.15	104.00
40	2	140	A	O3'-P-O5'	-6.76	91.16	104.00

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*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	2	179	C	O3'-P-O5'	-6.76	91.16	104.00
40	2	149	A	O3'-P-O5'	-6.75	91.17	104.00
40	2	138	C	O3'-P-O5'	-6.73	91.22	104.00
40	2	143	C	O3'-P-O5'	-6.72	91.22	104.00
40	2	148	C	O3'-P-O5'	-6.72	91.24	104.00
40	2	155	C	P-O3'-C3'	6.69	127.72	119.70
40	2	157	G	C5-C6-O6	-6.29	124.83	128.60
40	2	162	U	N1-C2-O2	6.28	127.20	122.80
40	2	157	G	N1-C6-O6	6.26	123.66	119.90
40	2	166	G	N9-C4-C5	6.24	107.90	105.40
40	2	165	A	O4'-C1'-N9	-6.16	103.27	108.20
40	2	166	G	N3-C4-C5	-5.95	125.63	128.60
40	2	172	C	P-O3'-C3'	5.87	126.75	119.70
40	2	167	U	O3'-P-O5'	-5.79	93.01	104.00
40	2	168	A	C5'-C4'-C3'	-5.79	106.75	116.00
40	2	164	C	C5-C4-N4	-5.72	116.19	120.20
40	2	156	U	P-O3'-C3'	-5.72	112.84	119.70
40	2	166	G	C6-N1-C2	-5.40	121.86	125.10
40	2	156	U	OP2-P-O3'	5.39	117.06	105.20
40	2	157	G	P-O5'-C5'	-5.22	112.55	120.90
40	2	160	A	C4'-C3'-C2'	-5.21	97.39	102.60
40	2	162	U	C2-N3-C4	-5.20	123.88	127.00
40	2	160	A	P-O5'-C5'	-5.15	112.66	120.90
40	2	170	C	N3-C4-C5	-5.14	119.84	121.90
40	2	156	U	C4'-C3'-C2'	5.12	107.72	102.60
40	2	170	C	O4'-C1'-C2'	-5.12	100.68	105.80
40	2	176	G	OP1-P-OP2	-5.11	111.93	119.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	462	ARG	Peptide
1	A	948	PRO	Peptide
7	G	308	HIS	Peptide
7	G	840	ASP	Peptide
7	G	841	PRO	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11100	0	5431	72	0
2	B	4264	0	2120	32	0
3	C	8538	0	4146	60	0
4	D	302	0	0	0	0
5	E	1101	0	543	15	0
6	F	2100	0	1038	24	0
7	G	4057	0	2089	37	0
8	H	2068	0	1019	20	0
9	I	883	0	414	4	0
10	J	677	0	316	1	0
11	K	225	0	98	2	0
12	L	2288	0	1076	10	0
13	M	844	0	426	3	0
14	N	277	0	114	2	0
15	O	636	0	322	2	0
16	P	458	0	225	1	0
17	Q	378	0	190	1	0
18	R	79	0	32	0	0
19	S	87	0	0	0	0
19	a	393	0	176	0	0
19	h	371	0	162	0	0
20	T	74	0	0	0	0
20	b	364	0	181	0	0
20	i	354	0	177	0	0
21	U	79	0	0	0	0
21	c	388	0	167	0	0
21	j	388	0	167	0	0
22	V	74	0	0	0	0
22	d	344	0	168	0	0
22	k	364	0	176	0	0
23	W	80	0	0	2	0
23	e	390	0	188	0	0
23	l	353	0	166	0	0
24	X	71	0	0	0	0
24	f	319	0	144	0	0
24	m	316	0	133	0	0
25	Z	82	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	g	469	0	214	0	0
25	n	412	0	185	0	0
26	o	90	0	0	0	0
27	p	73	0	0	0	0
28	q	80	0	0	0	0
29	r	76	0	0	0	0
30	s	69	0	0	0	0
31	t	79	0	0	0	0
32	u	62	0	0	0	0
33	v	806	0	0	0	0
34	w	1140	0	0	0	0
35	x	54	0	0	0	0
36	y	89	0	0	0	0
37	z	162	0	0	0	0
38	1	94	0	0	0	0
39	Y	972	0	495	31	0
40	2	2123	0	1076	178	0
41	4	2904	0	1470	44	0
42	5	2397	0	1216	40	0
43	6	1926	0	973	33	0
All	All	59243	0	27233	553	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 7.

All (553) 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)
40:2:153:A:H2	40:2:178:A:N1	1.00	1.46
1:A:2313:HIS:CB	3:C:1045:PRO:HB3	1.47	1.44
40:2:153:A:C2'	40:2:154:C:H5'	1.46	1.42
8:H:268:LEU:C	8:H:269:PRO:N	1.71	1.39
40:2:153:A:N1	40:2:178:A:N6	1.73	1.37
40:2:153:A:C2	40:2:178:A:N1	1.91	1.36
40:2:106:G:H21	40:2:107:A:N6	1.23	1.35
40:2:106:G:N2	40:2:107:A:C6	1.97	1.29
39:Y:149:A:N1	40:2:40:C:N4	1.78	1.29
40:2:153:A:O2'	40:2:154:C:C5'	1.79	1.29
40:2:108:G:H2'	40:2:109:C:C6	1.68	1.27
39:Y:143:G:O6	40:2:45:C:N4	1.71	1.21
40:2:153:A:C2	40:2:178:A:C6	2.31	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2:153:A:O2'	40:2:154:C:H5'	1.01	1.17
40:2:153:A:C2'	40:2:154:C:C5'	2.22	1.16
40:2:106:G:N2	40:2:107:A:N6	1.94	1.13
40:2:156:U:H5''	40:2:156:U:H6	1.10	1.10
40:2:154:C:O2	40:2:178:A:N6	1.85	1.09
1:A:2268:LEU:O	3:C:1264:PRO:HG2	1.53	1.08
39:Y:149:A:H61	40:2:40:C:N4	1.50	1.07
39:Y:149:A:N6	40:2:40:C:N4	2.03	1.07
1:A:2268:LEU:O	3:C:1264:PRO:CG	2.04	1.06
39:Y:149:A:C6	40:2:40:C:N4	2.19	1.06
40:2:105:G:H2'	40:2:106:G:H5''	1.37	1.05
40:2:153:A:H2'	40:2:154:C:C5'	1.81	1.05
39:Y:72:A:N6	43:6:33:G:H1	1.53	1.03
1:A:2074:ARG:CB	3:C:1047:PRO:HG2	1.86	1.03
40:2:153:A:H2	40:2:178:A:C6	1.74	1.01
1:A:2313:HIS:CB	3:C:1045:PRO:CB	2.37	1.01
40:2:153:A:C2	40:2:178:A:N6	2.28	1.00
40:2:168:A:C8	40:2:168:A:H5''	1.99	0.98
40:2:112:G:C2	40:2:113:G:C5	2.51	0.97
42:5:12:U:H3	42:5:65:G:H1	1.12	0.97
41:4:91:A:H2	41:4:110:G:N2	1.61	0.97
40:2:153:A:H2'	40:2:154:C:H5'	1.34	0.96
40:2:112:G:H2'	40:2:113:G:H8	1.29	0.96
41:4:4:U:H3	43:6:71:G:H1	0.98	0.94
40:2:156:U:H5''	40:2:156:U:C6	2.02	0.93
39:Y:149:A:N6	40:2:40:C:H42	1.62	0.93
39:Y:149:A:N1	40:2:40:C:C4	2.37	0.93
39:Y:65:G:H1	43:6:40:U:H3	0.99	0.92
40:2:118:G:H2'	40:2:119:G:H8	1.33	0.92
40:2:153:A:N1	40:2:178:A:C6	2.34	0.91
40:2:112:G:O2'	40:2:113:G:H5'	1.69	0.91
40:2:168:A:H5''	40:2:168:A:H8	1.37	0.90
39:Y:149:A:H61	40:2:40:C:H41	1.14	0.90
40:2:112:G:N3	40:2:113:G:C8	2.40	0.89
40:2:144:C:H2'	40:2:145:A:H5''	1.54	0.89
39:Y:58:G:H1	42:5:41:U:H3	0.92	0.89
40:2:112:G:C2	40:2:113:G:N7	2.42	0.87
40:2:144:C:H3'	40:2:145:A:H5'	1.56	0.86
7:G:312:TRP:O	7:G:316:ALA:HB3	1.75	0.86
39:Y:143:G:O6	40:2:45:C:C4	2.29	0.86
40:2:108:G:H2'	40:2:109:C:H6	1.35	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2:106:G:N2	40:2:107:A:N1	2.22	0.86
40:2:156:U:H6	40:2:156:U:C5'	1.89	0.86
39:Y:74:G:H1	43:6:31:U:H3	0.86	0.85
40:2:105:G:C2'	40:2:106:G:H5''	2.09	0.81
40:2:108:G:H2'	40:2:109:C:C5	2.14	0.81
41:4:91:A:H2	41:4:110:G:H22	0.83	0.81
41:4:108:C:O2'	41:4:109:G:H5'	1.81	0.81
40:2:112:G:C4	40:2:113:G:N7	2.49	0.80
40:2:112:G:N3	40:2:113:G:N7	2.30	0.80
42:5:17:U:H3	42:5:60:G:H1	0.83	0.80
40:2:101:U:H5''	40:2:102:U:H5'	1.64	0.80
7:G:842:HIS:O	7:G:846:ALA:HB2	1.83	0.80
40:2:154:C:C2	40:2:178:A:N6	2.47	0.79
40:2:178:A:O2'	40:2:179:C:H5'	1.85	0.77
39:Y:72:A:H61	43:6:33:G:H1	0.78	0.77
1:A:2070:LYS:O	3:C:1047:PRO:HG3	1.84	0.76
40:2:112:G:H2'	40:2:113:G:C8	2.18	0.76
39:Y:149:A:N1	40:2:40:C:N3	2.33	0.76
40:2:106:G:H4'	40:2:107:A:O4'	1.85	0.76
40:2:178:A:H2'	40:2:179:C:H6	1.49	0.75
40:2:144:C:H3'	40:2:145:A:C5'	2.17	0.75
1:A:464:PRO:HG2	42:5:20:G:H4'	1.69	0.75
1:A:75:ASP:HA	9:I:14:GLY:HA2	1.70	0.73
40:2:118:G:H2'	40:2:119:G:C8	2.23	0.72
2:B:441:PRO:O	2:B:445:ALA:HB2	1.88	0.72
7:G:361:VAL:O	7:G:365:ALA:HB2	1.89	0.72
40:2:153:A:HO2'	40:2:154:C:C5'	2.02	0.72
40:2:109:C:H6	40:2:109:C:O5'	1.73	0.71
39:Y:143:G:O6	40:2:45:C:N3	2.23	0.71
40:2:153:A:H2'	40:2:154:C:O5'	1.91	0.70
40:2:154:C:H1'	40:2:178:A:N1	2.05	0.70
8:H:288:ARG:O	8:H:292:ALA:HB2	1.91	0.70
7:G:842:HIS:O	7:G:846:ALA:CB	2.39	0.70
1:A:2313:HIS:CA	3:C:1045:PRO:HB3	2.19	0.70
40:2:12:G:H1	43:6:86:U:H3	1.39	0.69
40:2:177:A:H2	40:2:178:A:H62	1.39	0.68
40:2:150:U:H3	40:2:181:G:H1	1.41	0.68
7:G:312:TRP:O	7:G:316:ALA:CB	2.42	0.68
8:H:292:ALA:O	8:H:296:ALA:HB2	1.93	0.68
40:2:112:G:N1	40:2:113:G:C6	2.62	0.67
15:O:113:LYS:O	15:O:117:GLN:CB	2.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:111:SER:HA	13:M:140:VAL:HA	1.76	0.67
41:4:24:U:H3	41:4:48:G:H1	1.42	0.67
7:G:841:PRO:O	7:G:843:VAL:N	2.27	0.67
41:4:2:G:O6	43:6:73:A:N1	2.27	0.67
11:K:299:LYS:O	11:K:303:GLU:CB	2.43	0.67
39:Y:150:U:H6	39:Y:150:U:O5'	1.77	0.67
41:4:111:C:O5'	41:4:111:C:H6	1.78	0.67
40:2:168:A:C8	40:2:168:A:C5'	2.75	0.66
42:5:78:U:O2'	42:5:80:U:OP1	2.14	0.66
40:2:154:C:O2	40:2:178:A:C6	2.49	0.66
41:4:6:U:H2'	41:4:7:G:H8	1.61	0.65
42:5:58:U:H2'	42:5:59:G:H8	1.62	0.65
1:A:2152:GLY:HA3	1:A:2157:VAL:HA	1.79	0.65
41:4:117:C:O5'	41:4:117:C:H6	1.80	0.65
9:I:35:TRP:O	9:I:39:CYS:CB	2.45	0.65
40:2:144:C:C3'	40:2:145:A:C5'	2.75	0.65
40:2:153:A:C2'	40:2:154:C:O5'	2.43	0.65
6:F:349:TRP:HA	6:F:356:GLU:HA	1.78	0.65
40:2:156:U:C6	40:2:156:U:C5'	2.72	0.64
39:Y:149:A:C2	40:2:40:C:N3	2.65	0.64
3:C:1084:VAL:O	3:C:1088:ALA:HB2	1.97	0.64
3:C:1077:LEU:O	3:C:1081:MET:N	2.27	0.63
40:2:112:G:N1	40:2:113:G:C5	2.66	0.63
40:2:164:C:H6	40:2:164:C:H5'	1.63	0.63
2:B:371:GLU:O	2:B:375:GLU:CB	2.46	0.63
41:4:89:U:C2'	41:4:90:G:H5'	2.29	0.63
40:2:112:G:C2	40:2:113:G:C8	2.85	0.63
41:4:108:C:H2'	41:4:109:G:H8	1.63	0.62
1:A:2074:ARG:CB	3:C:1047:PRO:CG	2.73	0.62
7:G:311:ALA:O	7:G:315:SER:CB	2.47	0.62
41:4:89:U:O2'	41:4:90:G:H5'	1.99	0.62
3:C:1081:MET:O	3:C:1085:THR:CB	2.48	0.62
41:4:91:A:H8	41:4:91:A:O5'	1.82	0.62
7:G:407:TRP:O	7:G:411:VAL:CB	2.48	0.62
1:A:534:GLU:O	1:A:538:SER:CB	2.48	0.62
1:A:2317:PHE:CB	3:C:1043:ARG:CB	2.78	0.62
5:E:513:GLU:O	5:E:517:ALA:HB2	2.00	0.62
7:G:875:GLY:O	7:G:879:ALA:HB2	2.00	0.61
3:C:488:LEU:O	3:C:492:ALA:HB3	2.01	0.61
13:M:107:PRO:HG3	13:M:129:SER:HA	1.81	0.61
2:B:328:ALA:HA	2:B:332:GLY:HA3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:745:LEU:O	7:G:749:LEU:CB	2.47	0.61
1:A:239:TYR:O	1:A:243:ASN:CB	2.49	0.61
40:2:147:G:H2'	40:2:148:C:H6	1.66	0.61
42:5:12:U:O4	42:5:65:G:O6	2.19	0.61
40:2:146:C:O5'	40:2:147:G:H4'	2.01	0.61
40:2:146:C:OP2	40:2:147:G:H4'	2.01	0.60
40:2:157:G:H8	40:2:157:G:H5''	1.65	0.60
23:W:54:ARG:CA	40:2:151:C:O2	2.50	0.60
39:Y:151:A:O5'	39:Y:151:A:H8	1.84	0.60
3:C:1393:TRP:O	3:C:1397:PHE:CB	2.49	0.60
3:C:1080:ASP:O	3:C:1084:VAL:CB	2.50	0.60
7:G:861:ARG:O	7:G:865:HIS:CB	2.50	0.59
3:C:774:LEU:O	3:C:778:LEU:N	2.31	0.59
1:A:1007:ASP:O	1:A:1011:ALA:HB2	2.02	0.59
7:G:379:ALA:O	7:G:383:GLU:CB	2.50	0.59
40:2:176:G:H2'	40:2:177:A:O4'	2.02	0.59
13:M:29:ILE:HA	13:M:144:ILE:HA	1.83	0.59
16:P:198:ASP:HA	16:P:202:ALA:HB3	1.84	0.59
41:4:110:G:H8	41:4:110:G:O5'	1.86	0.58
3:C:1084:VAL:O	3:C:1088:ALA:CB	2.52	0.58
3:C:482:ASN:O	3:C:486:SER:N	2.36	0.58
40:2:118:G:O2'	40:2:119:G:H5'	2.04	0.58
40:2:114:A:O5'	40:2:114:A:H8	1.86	0.58
39:Y:143:G:C6	40:2:45:C:N3	2.71	0.58
41:4:33:A:H62	41:4:43:G:H21	1.49	0.58
2:B:441:PRO:O	2:B:445:ALA:CB	2.51	0.58
1:A:77:THR:HA	9:I:17:PRO:HD3	1.84	0.58
6:F:130:GLU:O	6:F:134:ASN:CB	2.52	0.58
40:2:146:C:H2'	40:2:148:C:OP1	2.03	0.58
7:G:783:SER:O	7:G:787:GLU:CB	2.52	0.58
2:B:208:HIS:O	2:B:212:SER:N	2.37	0.57
2:B:474:LEU:HA	2:B:499:GLY:HA3	1.85	0.57
40:2:112:G:C2'	40:2:113:G:H5'	2.33	0.57
40:2:108:G:C5	40:2:109:C:C4	2.91	0.57
40:2:152:G:H2'	40:2:153:A:H8	1.68	0.57
40:2:144:C:C2'	40:2:145:A:H5''	2.30	0.57
8:H:372:ARG:O	8:H:376:ASN:CB	2.52	0.57
1:A:85:LYS:O	1:A:89:LEU:CB	2.53	0.57
1:A:305:ARG:HA	2:B:923:PRO:HG3	1.85	0.57
41:4:108:C:C2'	41:4:109:G:H5'	2.34	0.57
39:Y:74:G:O6	43:6:31:U:O4	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:5:61:A:H2'	42:5:62:G:H8	1.69	0.56
2:B:428:THR:O	2:B:432:ASP:CB	2.53	0.56
40:2:146:C:P	40:2:147:G:H4'	2.45	0.56
40:2:183:G:H2'	40:2:184:C:H6	1.70	0.56
39:Y:57:C:N4	42:5:42:U:O4	2.36	0.56
1:A:1682:ALA:O	1:A:1686:ASP:CB	2.53	0.56
5:E:548:VAL:O	5:E:579:VAL:N	2.26	0.56
40:2:143:C:C2	40:2:144:C:C5	2.93	0.56
6:F:295:LEU:O	6:F:307:TRP:N	2.33	0.56
9:I:116:CYS:O	9:I:120:LEU:CB	2.53	0.56
11:K:300:GLU:O	11:K:304:ILE:CB	2.54	0.56
40:2:109:C:C6	40:2:109:C:O5'	2.57	0.56
40:2:137:U:H2'	40:2:138:C:H6	1.71	0.56
40:2:138:C:C2	40:2:139:C:C5	2.93	0.56
40:2:106:G:C2	40:2:107:A:C6	2.89	0.56
42:5:109:C:H2'	42:5:110:A:H8	1.70	0.56
42:5:69:A:O2'	42:5:70:A:N3	2.39	0.56
1:A:950:LEU:O	1:A:954:LYS:CB	2.52	0.56
40:2:105:G:N2	40:2:107:A:H5'	2.20	0.56
40:2:141:C:C2	40:2:142:U:C5	2.94	0.56
40:2:141:C:H2'	40:2:142:U:H6	1.71	0.56
41:4:111:C:H2'	41:4:112:A:H8	1.69	0.56
40:2:137:U:C2	40:2:138:C:C5	2.94	0.56
40:2:149:A:H2'	40:2:150:U:H6	1.70	0.56
3:C:485:GLN:O	3:C:489:TYR:CB	2.53	0.56
40:2:142:U:C2	40:2:143:C:C5	2.94	0.56
41:4:108:C:H2'	41:4:109:G:C8	2.41	0.56
39:Y:65:G:O6	43:6:40:U:O4	2.24	0.56
3:C:1395:GLU:O	3:C:1399:ASP:CB	2.54	0.56
6:F:202:PRO:O	6:F:206:ARG:CB	2.55	0.55
7:G:11:MET:O	7:G:13:ALA:N	2.38	0.55
40:2:140:A:C4	40:2:141:C:C5	2.95	0.55
40:2:150:U:C2	40:2:151:C:C5	2.94	0.55
40:2:147:G:H2'	40:2:148:C:C6	2.40	0.55
1:A:532:THR:O	1:A:536:LYS:CB	2.54	0.55
5:E:544:SER:HA	5:E:631:VAL:HA	1.87	0.55
40:2:143:C:H2'	40:2:144:C:H6	1.71	0.55
3:C:1332:GLN:O	3:C:1336:PHE:CB	2.54	0.55
42:5:109:C:H2'	42:5:110:A:C8	2.41	0.55
40:2:106:G:N2	40:2:107:A:H61	1.98	0.55
40:2:142:U:H2'	40:2:143:C:H6	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2:178:A:O2'	40:2:179:C:C5'	2.53	0.55
43:6:78:A:N1	43:6:85:U:OP1	2.39	0.55
7:G:419:ALA:O	7:G:423:LEU:CB	2.54	0.55
1:A:584:HIS:O	1:A:588:LEU:CB	2.55	0.55
40:2:118:G:O2'	40:2:119:G:C5'	2.55	0.55
40:2:140:A:H2'	40:2:141:C:H6	1.71	0.55
40:2:181:G:C4	40:2:182:U:C5	2.95	0.55
41:4:113:U:O5'	41:4:113:U:H6	1.90	0.55
40:2:138:C:H2'	40:2:139:C:H6	1.71	0.55
40:2:183:G:C4	40:2:184:C:C5	2.94	0.55
1:A:1725:LEU:O	1:A:1729:ALA:CB	2.55	0.55
2:B:588:ILE:HA	2:B:660:VAL:HA	1.89	0.55
1:A:2268:LEU:O	3:C:1264:PRO:HG3	2.04	0.54
42:5:17:U:O2	42:5:60:G:N2	2.28	0.54
1:A:947:PRO:HG2	1:A:948:PRO:HD2	1.90	0.54
12:L:330:THR:HA	12:L:346:ARG:HA	1.88	0.54
2:B:448:LYS:O	2:B:452:THR:CB	2.55	0.54
40:2:150:U:H2'	40:2:151:C:H6	1.71	0.54
39:Y:159:U:H3	40:2:31:G:H22	1.55	0.54
5:E:650:GLN:H	5:E:652:PRO:HD2	1.72	0.54
40:2:153:A:O2'	40:2:154:C:H5''	1.95	0.54
41:4:2:G:N1	43:6:73:A:C2	2.75	0.54
42:5:107:G:H3'	42:5:108:G:H8	1.73	0.54
40:2:181:G:H2'	40:2:182:U:H6	1.70	0.54
1:A:1729:ALA:O	1:A:1733:ILE:CB	2.56	0.54
3:C:489:TYR:O	3:C:493:LEU:CB	2.55	0.54
6:F:223:PHE:N	6:F:517:LEU:O	2.40	0.54
2:B:324:ALA:O	2:B:328:ALA:CB	2.56	0.54
40:2:146:C:OP2	40:2:147:G:C4'	2.56	0.54
40:2:149:A:C4	40:2:150:U:C5	2.95	0.54
40:2:164:C:C6	40:2:164:C:H5'	2.44	0.53
39:Y:58:G:N2	42:5:41:U:O2	2.28	0.53
40:2:178:A:H2'	40:2:179:C:C6	2.37	0.53
1:A:734:PRO:HB3	7:G:149:LEU:HA	1.89	0.53
2:B:482:TYR:O	2:B:491:HIS:N	2.40	0.53
1:A:235:MET:O	1:A:239:TYR:CB	2.56	0.53
1:A:1426:ASP:O	1:A:1430:LEU:CB	2.57	0.53
40:2:112:G:N2	40:2:113:G:C4	2.77	0.53
41:4:4:U:O2	43:6:71:G:N2	2.33	0.53
3:C:1563:VAL:O	3:C:1648:ARG:N	2.41	0.53
42:5:98:C:H2'	42:5:99:C:C6	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:PHE:O	2:B:122:LEU:CB	2.56	0.53
3:C:490:ARG:O	3:C:494:GLU:CB	2.57	0.53
1:A:84:ASP:O	1:A:88:TYR:CB	2.57	0.53
2:B:643:ASP:O	2:B:647:MET:CB	2.57	0.53
8:H:287:LEU:O	8:H:291:ALA:HB3	2.09	0.53
41:4:118:A:H8	41:4:118:A:OP2	1.92	0.53
3:C:1412:THR:O	3:C:1416:LEU:CB	2.57	0.53
1:A:1135:PRO:O	1:A:1139:ARG:N	2.41	0.52
2:B:742:PRO:HG2	2:B:785:ARG:HA	1.90	0.52
8:H:288:ARG:O	8:H:292:ALA:CB	2.56	0.52
7:G:361:VAL:O	7:G:365:ALA:CB	2.55	0.52
1:A:1725:LEU:O	1:A:1729:ALA:HB3	2.09	0.52
5:E:554:PRO:O	5:E:557:LYS:N	2.42	0.52
12:L:425:MET:HA	12:L:431:ILE:HA	1.92	0.52
41:4:2:G:H1	43:6:73:A:H2	1.56	0.52
43:6:52:U:O4	43:6:53:A:N6	2.42	0.52
7:G:875:GLY:O	7:G:879:ALA:CB	2.58	0.52
3:C:1224:LEU:HA	3:C:1236:HIS:HA	1.92	0.52
3:C:1033:GLU:O	3:C:1037:LEU:CB	2.58	0.51
8:H:167:VAL:O	8:H:171:ALA:CB	2.58	0.51
41:4:143:U:H2'	41:4:144:G:H5''	1.92	0.51
39:Y:69:A:O2'	43:6:35:A:N6	2.42	0.51
3:C:1389:VAL:O	3:C:1393:TRP:CB	2.57	0.51
40:2:152:G:H2'	40:2:153:A:C8	2.45	0.51
1:A:1931:THR:O	1:A:1935:ARG:CB	2.59	0.51
5:E:493:PRO:O	5:E:497:GLU:CB	2.59	0.51
7:G:418:ASP:O	7:G:422:MET:CB	2.58	0.51
8:H:355:GLY:H	41:4:58:C:H41	1.56	0.51
42:5:99:C:H2'	42:5:100:U:C6	2.46	0.51
1:A:1684:PHE:O	1:A:1688:THR:CB	2.59	0.51
2:B:430:PHE:O	2:B:434:CYS:CB	2.59	0.51
6:F:204:THR:O	6:F:208:SER:CB	2.59	0.51
8:H:292:ALA:O	8:H:296:ALA:CB	2.59	0.51
40:2:108:G:C2'	40:2:109:C:C6	2.65	0.51
42:5:48:A:H2'	42:5:49:A:H8	1.76	0.51
3:C:1221:PHE:HA	3:C:1272:SER:HA	1.93	0.51
3:C:1432:TRP:O	3:C:1436:SER:CB	2.59	0.51
6:F:224:CYS:HA	7:G:764:ALA:HB2	1.91	0.50
6:F:304:VAL:N	6:F:318:ILE:O	2.39	0.50
42:5:97:G:H2'	42:5:98:C:H6	1.77	0.50
2:B:393:PRO:O	2:B:397:ASP:CB	2.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1665:ASP:HA	3:C:1706:CYS:HA	1.93	0.50
5:E:573:VAL:N	5:E:580:ASN:O	2.41	0.50
15:O:56:MET:O	15:O:83:VAL:N	2.43	0.50
40:2:112:G:C4	40:2:113:G:C8	2.96	0.50
40:2:177:A:N3	40:2:178:A:N7	2.58	0.50
6:F:370:ILE:HA	6:F:381:THR:HA	1.92	0.50
41:4:52:U:O2'	41:4:56:U:OP2	2.22	0.50
1:A:1584:LYS:O	1:A:1588:SER:CB	2.59	0.50
1:A:564:TYR:O	1:A:569:VAL:N	2.45	0.50
7:G:142:PHE:O	7:G:146:LYS:CB	2.59	0.50
8:H:367:GLY:O	8:H:371:ILE:N	2.41	0.50
1:A:1378:GLU:O	1:A:1382:SER:CB	2.60	0.50
1:A:1833:LEU:O	1:A:1837:ALA:CB	2.60	0.50
10:J:25:VAL:N	10:J:55:PHE:O	2.40	0.50
1:A:880:ARG:O	1:A:884:HIS:CB	2.60	0.50
40:2:117:U:H2'	40:2:118:G:C8	2.47	0.49
1:A:150:MET:O	1:A:154:GLU:CB	2.60	0.49
7:G:782:GLU:O	7:G:786:LEU:CB	2.59	0.49
40:2:113:G:H2'	40:2:114:A:C8	2.47	0.49
41:4:111:C:H2'	41:4:112:A:C8	2.46	0.49
42:5:97:G:H2'	42:5:98:C:C6	2.47	0.49
42:5:17:U:O4	42:5:60:G:O6	2.31	0.49
42:5:25:C:H2'	42:5:26:A:C8	2.47	0.49
2:B:369:PHE:O	2:B:373:ILE:CB	2.60	0.49
2:B:777:GLY:N	2:B:782:GLU:O	2.46	0.49
5:E:554:PRO:HG3	43:6:78:A:H8	1.78	0.49
6:F:254:CYS:HA	6:F:266:HIS:HA	1.95	0.49
6:F:506:ILE:N	6:F:518:TRP:O	2.41	0.49
3:C:778:LEU:HA	3:C:782:PHE:O	2.13	0.49
3:C:872:SER:O	3:C:876:LEU:N	2.45	0.49
43:6:24:A:H4'	43:6:26:U:H1'	1.94	0.49
1:A:581:ILE:O	1:A:585:VAL:CB	2.61	0.49
1:A:2268:LEU:O	3:C:1264:PRO:CD	2.59	0.49
42:5:58:U:H2'	42:5:59:G:C8	2.46	0.48
39:Y:69:A:H62	43:6:35:A:H2'	1.77	0.48
40:2:116:A:H8	40:2:116:A:O5'	1.95	0.48
1:A:280:GLU:O	1:A:282:LEU:N	2.46	0.48
1:A:1007:ASP:O	1:A:1011:ALA:CB	2.60	0.48
7:G:841:PRO:C	7:G:843:VAL:H	2.17	0.48
2:B:508:LYS:N	2:B:566:THR:O	2.39	0.48
7:G:512:GLU:O	7:G:516:ALA:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:431:LYS:HA	6:F:443:THR:HA	1.94	0.48
7:G:449:ALA:O	7:G:453:LEU:CB	2.61	0.48
42:5:72:U:H2'	42:5:73:C:H6	1.78	0.48
1:A:2070:LYS:O	3:C:1047:PRO:CG	2.59	0.48
7:G:817:ALA:O	7:G:821:GLU:CB	2.61	0.48
1:A:883:ARG:O	1:A:887:THR:CB	2.62	0.48
41:4:110:G:H2'	41:4:111:C:C6	2.49	0.48
40:2:108:G:C2'	40:2:109:C:C5	2.92	0.48
41:4:2:G:C6	43:6:73:A:N1	2.82	0.48
1:A:121:HIS:HA	1:A:482:PHE:HA	1.96	0.48
6:F:178:LEU:O	6:F:182:ASN:CB	2.62	0.48
8:H:268:LEU:C	8:H:269:PRO:CA	2.75	0.48
1:A:1947:ASN:O	1:A:1951:LYS:CB	2.62	0.47
3:C:1037:LEU:O	3:C:1041:LEU:CB	2.62	0.47
3:C:612:ILE:N	3:C:647:ARG:O	2.47	0.47
40:2:143:C:H2'	40:2:144:C:C6	2.49	0.47
42:5:23:C:H3'	42:5:24:G:H4'	1.96	0.47
39:Y:151:A:H2	40:2:38:A:N1	2.12	0.47
3:C:1761:TYR:O	3:C:1765:THR:CB	2.62	0.47
3:C:725:VAL:N	3:C:811:SER:O	2.46	0.47
40:2:142:U:H2'	40:2:143:C:C6	2.49	0.47
1:A:1778:TRP:HA	1:A:1811:ASN:HA	1.96	0.47
2:B:816:VAL:O	2:B:820:PHE:CB	2.63	0.47
3:C:1088:ALA:O	3:C:1092:MET:CB	2.63	0.47
42:5:110:A:H2'	42:5:111:A:C8	2.49	0.47
42:5:98:C:H2'	42:5:99:C:H6	1.80	0.47
1:A:1568:THR:O	1:A:1572:SER:CB	2.62	0.47
3:C:1964:PRO:HA	3:C:2054:PRO:HG3	1.96	0.47
8:H:135:TYR:O	8:H:139:VAL:CB	2.62	0.47
41:4:109:G:H2'	41:4:110:G:C8	2.50	0.47
7:G:680:LYS:HA	7:G:934:ALA:HB1	1.97	0.47
3:C:1831:LEU:O	3:C:1835:SER:CB	2.62	0.47
1:A:117:PRO:HA	1:A:486:LYS:HA	1.96	0.47
2:B:261:ASP:O	2:B:265:LEU:CB	2.63	0.47
8:H:291:ALA:O	8:H:295:VAL:CB	2.63	0.47
40:2:117:U:H2'	40:2:118:G:H8	1.79	0.47
40:2:138:C:H2'	40:2:139:C:C6	2.50	0.46
41:4:11:A:H2'	41:4:12:G:C8	2.50	0.46
5:E:554:PRO:HG3	43:6:78:A:C8	2.50	0.46
1:A:1470:TYR:O	1:A:1474:MET:CB	2.63	0.46
3:C:525:ILE:HA	3:C:531:ILE:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2:154:C:H6	40:2:154:C:O5'	1.97	0.46
41:4:89:U:HO2'	41:4:90:G:H5'	1.81	0.46
3:C:1620:LEU:N	3:C:1645:VAL:O	2.48	0.46
7:G:309:PRO:HB2	7:G:310:PRO:HD3	1.97	0.46
40:2:137:U:H2'	40:2:138:C:C6	2.50	0.46
40:2:149:A:H2'	40:2:150:U:C6	2.50	0.46
6:F:325:VAL:HA	6:F:341:CYS:HA	1.97	0.46
7:G:309:PRO:O	7:G:313:ILE:CB	2.63	0.46
40:2:140:A:H2'	40:2:141:C:C6	2.50	0.46
40:2:150:U:H2'	40:2:151:C:C6	2.50	0.46
40:2:181:G:H2'	40:2:182:U:C6	2.50	0.46
1:A:1833:LEU:O	1:A:1837:ALA:HB3	2.14	0.46
8:H:253:GLY:HA3	8:H:273:TYR:H	1.81	0.46
1:A:88:TYR:O	1:A:92:LEU:CB	2.64	0.46
40:2:180:G:H2'	40:2:181:G:H8	1.81	0.46
2:B:833:PHE:N	2:B:900:VAL:O	2.41	0.46
6:F:167:HIS:C	6:F:169:GLY:H	2.19	0.46
43:6:40:U:H2'	43:6:41:A:C8	2.51	0.46
1:A:2130:GLY:HA3	1:A:2142:ILE:HA	1.98	0.46
14:N:105:GLN:O	14:N:110:MET:N	2.34	0.46
43:6:66:C:H2'	43:6:67:G:C8	2.50	0.46
2:B:508:LYS:HA	2:B:524:ILE:HA	1.98	0.46
5:E:563:ASN:O	5:E:567:LEU:N	2.48	0.46
8:H:167:VAL:O	8:H:171:ALA:HB3	2.16	0.46
40:2:112:G:C6	40:2:113:G:O6	2.69	0.46
40:2:112:G:N2	40:2:113:G:C5	2.82	0.46
7:G:512:GLU:O	7:G:516:ALA:CB	2.63	0.46
40:2:183:G:H2'	40:2:184:C:C6	2.50	0.45
42:5:61:A:H2'	42:5:62:G:C8	2.50	0.45
6:F:421:ILE:N	6:F:433:TRP:O	2.49	0.45
8:H:39:THR:O	8:H:43:LEU:CB	2.64	0.45
40:2:178:A:C2'	40:2:179:C:O5'	2.64	0.45
6:F:255:LYS:N	6:F:265:LEU:O	2.49	0.45
40:2:177:A:H2	40:2:178:A:N6	2.09	0.45
40:2:3:C:H2'	40:2:4:G:C8	2.51	0.45
1:A:463:PRO:O	42:5:24:G:N2	2.47	0.45
1:A:798:GLY:N	1:A:799:PRO:HD3	2.32	0.45
40:2:148:C:H2'	40:2:149:A:H8	1.82	0.45
40:2:151:C:H2'	40:2:152:G:H8	1.81	0.45
7:G:912:TRP:O	7:G:916:SER:CB	2.64	0.45
40:2:179:C:H2'	40:2:180:G:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:912:ASN:HA	3:C:978:ASN:HA	1.98	0.45
1:A:598:LEU:O	1:A:602:ILE:CB	2.64	0.45
17:Q:9:PRO:HB2	17:Q:22:ASP:HA	1.98	0.45
40:2:112:G:C2	40:2:113:G:C4	3.04	0.45
40:2:182:U:H2'	40:2:183:G:H8	1.81	0.45
42:5:10:U:H2'	42:5:11:U:C6	2.52	0.45
2:B:324:ALA:O	2:B:328:ALA:HB2	2.17	0.45
40:2:119:G:H2'	40:2:120:A:H8	1.82	0.45
6:F:234:SER:N	6:F:248:ALA:O	2.49	0.45
2:B:715:GLY:O	2:B:719:GLN:CB	2.64	0.44
40:2:116:A:C8	40:2:116:A:O5'	2.70	0.44
43:6:91:A:H2'	43:6:92:A:H8	1.82	0.44
3:C:2067:VAL:HA	3:C:2079:ILE:HA	2.00	0.44
40:2:141:C:H2'	40:2:142:U:C6	2.50	0.44
1:A:1809:ILE:O	1:A:1818:PHE:N	2.49	0.44
3:C:1522:PRO:HG2	12:L:343:LYS:HA	1.99	0.44
6:F:367:VAL:HA	6:F:383:GLY:HA2	2.00	0.44
7:G:340:PRO:HB2	7:G:368:HIS:O	2.18	0.44
41:4:115:G:H2'	41:4:116:G:C8	2.52	0.44
1:A:897:GLU:O	1:A:908:VAL:N	2.48	0.44
3:C:785:HIS:N	3:C:810:VAL:O	2.51	0.44
40:2:139:C:H2'	40:2:140:A:H8	1.81	0.44
43:6:89:U:H2'	43:6:90:G:C8	2.53	0.44
43:6:90:G:H2'	43:6:91:A:H8	1.82	0.44
43:6:91:A:H2'	43:6:92:A:C8	2.53	0.44
5:E:594:PHE:O	5:E:598:MET:CB	2.66	0.44
40:2:118:G:O6	40:2:140:A:N6	2.51	0.44
41:4:91:A:H2'	41:4:92:C:C6	2.53	0.44
41:4:118:A:C8	41:4:118:A:OP2	2.70	0.43
1:A:1878:ASP:HA	7:G:282:PRO:HA	1.99	0.43
40:2:117:U:C2'	40:2:118:G:H5'	2.48	0.43
2:B:215:VAL:O	2:B:219:LEU:CB	2.66	0.43
8:H:284:PRO:O	8:H:288:ARG:N	2.48	0.43
42:5:72:U:H2'	42:5:73:C:C6	2.53	0.43
8:H:355:GLY:N	41:4:58:C:H41	2.16	0.43
43:6:40:U:H2'	43:6:41:A:H8	1.83	0.43
39:Y:71:C:H2'	39:Y:72:A:H8	1.83	0.43
40:2:108:G:C4	40:2:109:C:C4	3.07	0.43
42:5:74:U:H2'	42:5:75:G:C8	2.52	0.43
3:C:1186:LEU:HA	3:C:1204:ILE:HA	2.00	0.43
39:Y:70:G:H22	43:6:36:A:H2	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:513:GLU:O	5:E:517:ALA:CB	2.64	0.43
8:H:358:ARG:O	8:H:362:MET:CB	2.66	0.43
12:L:499:ILE:N	12:L:511:TRP:O	2.43	0.43
42:5:31:U:H2'	42:5:32:C:C6	2.54	0.43
6:F:279:VAL:N	6:F:296:ALA:O	2.51	0.43
8:H:314:GLY:O	8:H:318:TYR:CB	2.67	0.43
1:A:440:PRO:HB2	1:A:442:LYS:H	1.83	0.43
40:2:144:C:C4	40:2:146:C:OP1	2.72	0.43
40:2:153:A:H2'	40:2:154:C:H6	1.84	0.43
40:2:157:G:C8	40:2:157:G:H5''	2.50	0.43
1:A:1195:ARG:O	1:A:1229:PHE:N	2.46	0.43
2:B:642:HIS:O	2:B:646:LYS:CB	2.67	0.43
40:2:178:A:H2'	40:2:179:C:O5'	2.18	0.43
43:6:89:U:H2'	43:6:90:G:H8	1.84	0.43
1:A:679:SER:O	1:A:683:LEU:CB	2.67	0.43
3:C:548:VAL:O	3:C:552:VAL:CB	2.67	0.43
3:C:783:ALA:HB3	3:C:809:LEU:HA	2.01	0.42
6:F:380:GLY:HA2	6:F:390:VAL:HA	2.00	0.42
12:L:488:ILE:H	12:L:503:SER:HA	1.84	0.42
40:2:108:G:C5	40:2:109:C:N4	2.87	0.42
40:2:112:G:HO2'	40:2:113:G:H5'	1.79	0.42
40:2:114:A:C8	40:2:114:A:O5'	2.70	0.42
40:2:118:G:C2'	40:2:119:G:O5'	2.67	0.42
2:B:396:LEU:O	2:B:400:GLY:N	2.51	0.42
12:L:146:ALA:O	12:L:150:ALA:CB	2.68	0.42
43:6:92:A:H2'	43:6:93:G:H8	1.83	0.42
1:A:580:TYR:O	1:A:584:HIS:CB	2.67	0.42
3:C:1390:TYR:O	3:C:1394:TYR:CB	2.67	0.42
3:C:488:LEU:O	3:C:492:ALA:CB	2.66	0.42
40:2:98:G:H5'	40:2:104:U:OP2	2.19	0.42
7:G:448:ASN:O	7:G:452:VAL:CB	2.68	0.42
12:L:331:ILE:N	12:L:345:PHE:O	2.44	0.42
23:W:80:ALA:CA	23:W:81:PRO:CA	2.98	0.42
40:2:155:C:H2'	40:2:156:U:H5''	2.02	0.42
1:A:926:LEU:O	1:A:930:ALA:CB	2.67	0.42
41:4:90:G:H2'	41:4:91:A:C8	2.55	0.42
3:C:1386:ALA:O	3:C:1390:TYR:CB	2.68	0.42
7:G:841:PRO:C	7:G:843:VAL:N	2.73	0.42
40:2:157:G:H2'	40:2:158:G:O4'	2.19	0.42
41:4:107:U:H2'	41:4:108:C:H6	1.85	0.42
2:B:227:LEU:O	2:B:256:CYS:N	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2:3:C:H2'	40:2:4:G:H8	1.84	0.42
12:L:241:TRP:HA	12:L:248:ILE:HA	2.01	0.42
41:4:14:G:H2'	41:4:15:G:C8	2.55	0.42
43:6:92:A:H2'	43:6:93:G:C8	2.54	0.42
2:B:828:MET:HA	2:B:906:ILE:HA	2.01	0.42
1:A:2130:GLY:O	1:A:2173:GLU:N	2.53	0.41
42:5:75:G:H2'	42:5:76:A:C8	2.55	0.41
1:A:981:PHE:C	1:A:983:LYS:H	2.23	0.41
42:5:31:U:H2'	42:5:32:C:H6	1.85	0.41
42:5:59:G:C2	42:5:60:G:C8	3.08	0.41
1:A:577:GLY:O	1:A:581:ILE:CB	2.68	0.41
3:C:1609:LEU:O	3:C:1613:LEU:CB	2.68	0.41
3:C:823:ALA:O	3:C:857:GLY:N	2.50	0.41
6:F:257:TRP:N	6:F:262:CYS:O	2.43	0.41
40:2:171:U:H2'	40:2:172:C:O4'	2.21	0.41
7:G:824:PRO:C	7:G:826:ARG:H	2.24	0.41
41:4:22:C:H2'	41:4:23:G:C8	2.56	0.41
42:5:71:C:H2'	42:5:72:U:C6	2.56	0.41
1:A:1696:PRO:HB2	1:A:1699:THR:O	2.21	0.41
3:C:1915:ILE:O	3:C:1919:ALA:CB	2.69	0.41
41:4:55:U:H2'	41:4:56:U:C6	2.56	0.41
14:N:80:TYR:O	14:N:89:VAL:N	2.47	0.41
42:5:38:C:N4	42:5:39:C:N3	2.68	0.41
42:5:5:U:H2'	42:5:6:C:C6	2.56	0.41
40:2:117:U:H6	40:2:117:U:H5'	1.85	0.41
3:C:1058:LYS:O	3:C:1062:LEU:CB	2.69	0.41
39:Y:54:G:O2'	39:Y:55:A:H5''	2.21	0.41
40:2:103:U:C3'	40:2:104:U:H5'	2.51	0.41
40:2:107:A:H2'	40:2:108:G:C8	2.56	0.41
41:4:72:U:O2'	41:4:73:U:H5''	2.21	0.41
42:5:100:U:H2'	42:5:101:U:C6	2.57	0.41
43:6:43:A:H3'	43:6:44:G:H8	1.86	0.41
2:B:121:ASP:O	2:B:125:ASN:CB	2.69	0.41
3:C:1431:LYS:O	3:C:1435:LEU:CB	2.69	0.41
6:F:116:GLU:O	6:F:118:ILE:N	2.52	0.40
7:G:743:THR:N	7:G:744:PRO:HD3	2.36	0.40
12:L:240:VAL:O	12:L:249:ARG:N	2.52	0.40
40:2:149:A:C6	40:2:150:U:C4	3.09	0.40
5:E:470:PRO:O	5:E:472:PRO:HD3	2.21	0.40
12:L:217:VAL:HA	12:L:233:SER:HA	2.04	0.40
43:6:66:C:H2'	43:6:67:G:H8	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2:183:G:C6	40:2:184:C:N4	2.89	0.40
41:4:14:G:H2'	41:4:15:G:H8	1.87	0.40
1:A:454:TYR:O	1:A:458:ALA:HB2	2.22	0.40
1:A:739:ILE:O	1:A:743:VAL:CB	2.69	0.40
5:E:471:PRO:O	5:E:473:GLU:N	2.54	0.40
41:4:110:G:C8	41:4:110:G:O5'	2.70	0.40
5:E:669:TYR:HA	6:F:483:PRO:HG3	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2184/2335 (94%)	1969 (90%)	208 (10%)	7 (0%)	44	81
2	B	842/972 (87%)	772 (92%)	70 (8%)	0	100	100
3	C	1689/2136 (79%)	1624 (96%)	63 (4%)	2 (0%)	55	89
5	E	215/683 (32%)	174 (81%)	37 (17%)	4 (2%)	9	49
6	F	416/521 (80%)	376 (90%)	39 (9%)	1 (0%)	51	85
7	G	798/941 (85%)	700 (88%)	94 (12%)	4 (0%)	32	74
8	H	411/499 (82%)	359 (87%)	49 (12%)	3 (1%)	25	68
9	I	174/312 (56%)	158 (91%)	15 (9%)	1 (1%)	28	71
10	J	133/142 (94%)	126 (95%)	7 (5%)	0	100	100
11	K	43/439 (10%)	42 (98%)	1 (2%)	0	100	100
12	L	451/513 (88%)	437 (97%)	14 (3%)	0	100	100
13	M	167/177 (94%)	158 (95%)	9 (5%)	0	100	100
14	N	54/199 (27%)	47 (87%)	7 (13%)	0	100	100
15	O	124/128 (97%)	119 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P	87/800 (11%)	79 (91%)	8 (9%)	0	100	100
17	Q	73/376 (19%)	70 (96%)	3 (4%)	0	100	100
18	R	14/557 (2%)	13 (93%)	1 (7%)	0	100	100
19	a	74/118 (63%)	71 (96%)	3 (4%)	0	100	100
19	h	70/118 (59%)	68 (97%)	2 (3%)	0	100	100
20	b	71/86 (83%)	70 (99%)	1 (1%)	0	100	100
20	i	69/86 (80%)	67 (97%)	2 (3%)	0	100	100
21	c	76/92 (83%)	70 (92%)	6 (8%)	0	100	100
21	j	76/92 (83%)	70 (92%)	6 (8%)	0	100	100
22	d	67/76 (88%)	63 (94%)	4 (6%)	0	100	100
22	k	71/76 (93%)	67 (94%)	4 (6%)	0	100	100
23	e	76/126 (60%)	73 (96%)	3 (4%)	0	100	100
23	l	69/126 (55%)	69 (100%)	0	0	100	100
24	f	60/240 (25%)	57 (95%)	3 (5%)	0	100	100
24	m	60/240 (25%)	57 (95%)	3 (5%)	0	100	100
25	g	89/119 (75%)	84 (94%)	5 (6%)	0	100	100
25	n	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
All	All	8883/13444 (66%)	8186 (92%)	675 (8%)	22 (0%)	54	85

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	957	VAL
7	G	842	HIS
7	G	373	VAL
8	H	434	VAL
1	A	1015	VAL
3	C	531	ILE
9	I	157	VAL
1	A	1092	ILE
5	E	478	ILE
5	E	490	VAL
1	A	569	VAL
1	A	945	THR
5	E	533	LEU
7	G	309	PRO

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Mol	Chain	Res	Type
7	G	929	ILE
1	A	948	PRO
8	H	271	THR
1	A	947	PRO
5	E	537	ILE
1	A	386	PRO
8	H	269	PRO
6	F	459	ILE

### 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 PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	125/2108 (6%)	125 (100%)	0	100	100
2	B	49/866 (6%)	49 (100%)	0	100	100
3	C	77/1908 (4%)	77 (100%)	0	100	100
5	E	8/599 (1%)	8 (100%)	0	100	100
6	F	17/441 (4%)	17 (100%)	0	100	100
7	G	35/792 (4%)	35 (100%)	0	100	100
8	H	15/424 (4%)	15 (100%)	0	100	100
9	I	6/293 (2%)	6 (100%)	0	100	100
10	J	5/130 (4%)	5 (100%)	0	100	100
12	L	11/450 (2%)	11 (100%)	0	100	100
13	M	10/148 (7%)	10 (100%)	0	100	100
15	O	6/111 (5%)	6 (100%)	0	100	100
16	P	3/681 (0%)	3 (100%)	0	100	100
17	Q	2/333 (1%)	2 (100%)	0	100	100
19	a	3/110 (3%)	3 (100%)	0	100	100
19	h	2/110 (2%)	2 (100%)	0	100	100
20	b	4/74 (5%)	4 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	i	4/74 (5%)	4 (100%)	0	100	100
21	c	1/84 (1%)	1 (100%)	0	100	100
21	j	1/84 (1%)	1 (100%)	0	100	100
22	d	3/66 (4%)	3 (100%)	0	100	100
22	k	3/66 (4%)	3 (100%)	0	100	100
23	e	3/101 (3%)	3 (100%)	0	100	100
23	l	2/101 (2%)	2 (100%)	0	100	100
24	f	2/177 (1%)	2 (100%)	0	100	100
25	g	4/101 (4%)	4 (100%)	0	100	100
25	n	3/101 (3%)	3 (100%)	0	100	100
All	All	404/10533 (4%)	404 (100%)	0	100	100

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
39	Y	44/324 (13%)	14 (31%)	0
40	2	96/188 (51%)	18 (18%)	3 (3%)
41	4	134/145 (92%)	41 (30%)	4 (2%)
42	5	113/116 (97%)	36 (31%)	2 (1%)
43	6	88/106 (83%)	22 (25%)	3 (3%)
All	All	475/879 (54%)	131 (27%)	12 (2%)

All (131) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
39	Y	50	C
39	Y	51	U
39	Y	52	C
39	Y	53	C
39	Y	54	G
39	Y	55	A
39	Y	56	A
39	Y	57	C

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Mol	Chain	Res	Type
39	Y	61	A
39	Y	70	G
39	Y	71	C
39	Y	72	A
39	Y	156	U
39	Y	160	G
40	2	111	G
40	2	112	G
40	2	113	G
40	2	116	A
40	2	117	U
40	2	118	G
40	2	145	A
40	2	146	C
40	2	147	G
40	2	154	C
40	2	156	U
40	2	157	G
40	2	164	C
40	2	165	A
40	2	168	A
40	2	169	C
40	2	177	A
40	2	178	A
41	4	19	U
41	4	20	A
41	4	25	A
41	4	26	G
41	4	36	U
41	4	41	C
41	4	44	A
41	4	45	G
41	4	52	U
41	4	53	U
41	4	54	A
41	4	55	U
41	4	56	U
41	4	58	C
41	4	69	C
41	4	71	U
41	4	73	U
41	4	76	C

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Mol	Chain	Res	Type
41	4	78	A
41	4	80	A
41	4	81	C
41	4	82	C
41	4	84	C
41	4	85	G
41	4	90	G
41	4	100	A
41	4	103	A
41	4	109	G
41	4	114	U
41	4	115	G
41	4	118	A
41	4	119	A
41	4	120	U
41	4	121	U
41	4	122	U
41	4	124	U
41	4	125	G
41	4	126	A
41	4	127	C
41	4	144	G
41	4	145	G
42	5	8	G
42	5	10	U
42	5	20	G
42	5	21	A
42	5	22	U
42	5	23	C
42	5	24	G
42	5	25	C
42	5	26	A
42	5	27	U
42	5	34	U
42	5	36	C
42	5	38	C
42	5	39	C
42	5	41	U
42	5	42	U
42	5	45	C
42	5	48	A
42	5	52	U

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Mol	Chain	Res	Type
42	5	53	U
42	5	54	U
42	5	57	G
42	5	68	C
42	5	69	A
42	5	70	A
42	5	79	C
42	5	80	U
42	5	83	A
42	5	88	A
42	5	90	U
42	5	92	U
42	5	93	U
42	5	94	U
42	5	95	G
42	5	96	A
42	5	108	G
43	6	6	C
43	6	7	G
43	6	9	U
43	6	21	U
43	6	22	A
43	6	26	U
43	6	28	A
43	6	29	A
43	6	33	G
43	6	35	A
43	6	38	G
43	6	40	U
43	6	43	A
43	6	44	G
43	6	45	A
43	6	47	A
43	6	48	A
43	6	49	G
43	6	50	A
43	6	70	A
43	6	77	C
43	6	78	A

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
40	2	156	U
40	2	164	C
40	2	168	A
41	4	43	G
41	4	55	U
41	4	99	C
41	4	114	U
42	5	78	U
42	5	94	U
43	6	28	A
43	6	49	G
43	6	77	C

## 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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	H	1
12	L	1
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	39:ASN	C	40:THR	N	8.39
1	C	1296:PRO	C	1297:PRO	N	3.45
1	H	268:LEU	C	269:PRO	N	1.71