



Full wwPDB EM Validation Report ⓘ

Nov 9, 2024 – 01:17 pm GMT

PDB ID : 5NRL
EMDB ID : EMD-3683
Title : Structure of a pre-catalytic spliceosome
Authors : Plaschka, C.; Lin, P.-C.; Nagai, K.
Deposited on : 2017-04-24
Resolution : 7.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

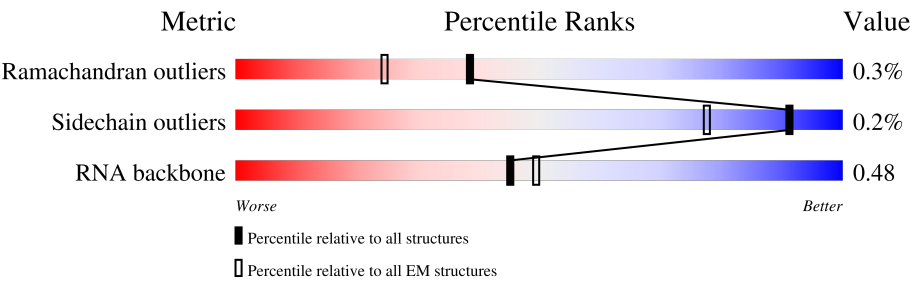
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.20 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	1175	<div><div>9%</div><div>5% 6% .</div><div>87%</div></div>
2	3	89	<div><div>31%</div><div>87%</div><div>13%</div></div>
3	4	160	<div><div>.</div><div>46%</div><div>24%</div><div>29%</div></div>
4	5	214	<div><div>7%</div><div>48%</div><div>31%</div><div>21%</div></div>
5	6	112	<div><div>.</div><div>53%</div><div>32%</div><div>15%</div></div>
6	7	115	<div><div>26%</div><div>57%</div><div>43%</div></div>
7	8	109	<div><div>20%</div><div>59%</div><div>41%</div></div>
8	A	2413	<div><div>5%</div><div>92%</div><div>8%</div></div>

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Mol	Chain	Length	Quality of chain
9	B	2163	
10	C	1008	
11	D	143	
12	E	587	
13	F	494	
14	G	469	
15	H	465	
16	I	95	
17	J	899	
18	K	126	
19	L	194	
20	M	242	
21	N	291	
22	O	971	
23	P	1361	
24	Q	435	
25	R	213	
26	S	107	
27	T	530	
28	U	266	
29	V	280	
30	W	238	
31	X	111	
32	Y	111	
33	Z	85	

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Mol	Chain	Length	Quality of chain
34	a	95	
35	b	196	
35	k	196	
35	s	196	
36	d	101	
36	n	101	
36	v	101	
37	e	94	
37	p	94	
37	w	94	
38	f	86	
38	q	86	
38	x	86	
39	g	77	
39	r	77	
39	y	77	
40	h	146	
40	l	146	
40	t	146	
41	i	110	
41	m	110	
41	u	110	
42	j	187	
43	o	93	
44	z	86	

2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 118701 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 RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	155	Total	C	N	O	P	0	0
			3275	1464	552	1104	155		

- Molecule 2 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	77	Total	C	N	O	S	0	0
			611	382	105	121	3		

- Molecule 3 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	114	Total	C	N	O	P	0	0
			2423	1084	419	806	114		

- Molecule 4 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	170	Total	C	N	O	P	0	0
			3615	1618	640	1188	169		

- Molecule 5 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	95	Total	C	N	O	P	0	0
			2019	904	355	665	95		

- Molecule 6 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	66	Total	C	N	O	S	0	0
			504	325	85	91	3		

- Molecule 7 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	64	Total	C	N	O	S	0	0
			498	320	86	90	2		

- Molecule 8 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	2216	Total	C	N	O	S	0	0
			18122	11661	3103	3294	64		

- Molecule 9 is a protein called Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	1699	Total	C	N	O	S	1	0
			13607	8720	2269	2564	54		

- Molecule 10 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	850	Total	C	N	O	S	0	0
			6784	4392	1129	1237	26		

- Molecule 11 is a protein called Spliceosomal protein DIB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	142	Total	C	N	O	S	0	0
			1164	736	202	215	11		

- Molecule 12 is a protein called 66 kDa U4/U6.U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	124	Total	C	N	O	S	0	0
			825	501	153	170	1		

- Molecule 13 is a protein called Pre-mRNA-processing factor 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	413	Total	C	N	O	S	0	0
			3238	2064	578	584	12		

- Molecule 14 is a protein called U4/U6 small nuclear ribonucleoprotein PRP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	372	Total	C	N	O	S	0	0
			2835	1786	523	512	14		

- Molecule 15 is a protein called U4/U6 small nuclear ribonucleoprotein PRP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	429	Total	C	N	O	S	0	0
			3396	2120	609	653	14		

- Molecule 16 is a RNA chain called Yeast UBC4 gene for ubiquitin-conjugating enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	29	Total	C	N	O	P	0	0
			600	271	95	205	29		

- Molecule 17 is a protein called Pre-mRNA-splicing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	800	Total	C	N	O	S	0	0
			6485	4151	1106	1201	27		

- Molecule 18 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	124	Total	C	N	O	S	0	0
			936	597	161	174	4		

- Molecule 19 is a protein called 23 kDa U4/U6.U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	109	Total	C	N	O	S	0	0
			882	570	150	159	3		

- Molecule 20 is a protein called Pre-mRNA-splicing factor 38.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	174	Total	C	N	O	S	0	0
			1407	915	236	249	7		

- Molecule 21 is a protein called Pre-mRNA-splicing factor SPP381.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	N	85	Total	C	N	O	0	0
			425	255	85	85		

- Molecule 22 is a protein called U2 snRNP component HSH155.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	833	Total	C	N	O	S	0	0
			6612	4258	1121	1192	41		

- Molecule 23 is a protein called Pre-mRNA-splicing factor RSE1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	1186	Total	C	N	O	S	0	0
			9437	6034	1589	1763	51		

- Molecule 24 is a protein called Cold sensitive U2 snRNA suppressor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	220	Total	C	N	O	S	0	0
			1786	1157	307	313	9		

- Molecule 25 is a protein called Protein HSH49.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	173	Total	C	N	O	S	0	0
			1429	930	239	258	2		

- Molecule 26 is a protein called Pre-mRNA-splicing factor RDS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S	103	Total	C	N	O	S	0	0
			814	503	154	143	14		

- Molecule 27 is a protein called Pre-mRNA-splicing factor PRP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	462	Total	C	N	O	S	0	0
			3915	2487	677	735	16		

- Molecule 28 is a protein called Pre-mRNA-splicing factor PRP11.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	196	Total	C	N	O	S	0	0
			1488	933	258	291	6		

- Molecule 29 is a protein called Pre-mRNA-splicing factor PRP21.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	127	Total	C	N	O	S	0	0
			1084	689	193	196	6		

- Molecule 30 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	170	Total	C	N	O	S	0	0
			1383	866	253	257	7		

- Molecule 31 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	X	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 32 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	84	Total	C	N	O	S	0	0
			683	439	119	122	3		

- Molecule 33 is a protein called RDS3 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	83	Total	C	N	O	S	0	0
			685	424	129	131	1		

- Molecule 34 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	90	Total	C	N	O	S	0	0
			735	469	124	139	3		

- Molecule 35 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	70	Total	C	N	O	S	0	0
			563	360	98	102	3		
35	k	70	Total	C	N	O	S	0	0
			563	360	98	102	3		
35	s	70	Total	C	N	O	S	0	0
			563	360	98	102	3		

- Molecule 36 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	83	Total	C	N	O	S	0	0
			641	408	111	120	2		
36	n	82	Total	C	N	O	S	0	0
			632	402	109	119	2		
36	v	82	Total	C	N	O	S	0	0
			632	402	109	119	2		

- Molecule 37 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	77	Total	C	N	O	S	0	0
			602	396	95	108	3		
37	p	77	Total	C	N	O	S	0	0
			602	396	95	108	3		
37	w	77	Total	C	N	O	S	0	0
			602	396	95	108	3		

- Molecule 38 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	72	Total	C	N	O	S	0	0
			578	371	101	105	1		
38	q	73	Total	C	N	O	S	0	0
			585	376	102	106	1		
38	x	73	Total	C	N	O	S	0	0
			585	376	102	106	1		

- Molecule 39 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	71	Total	C	N	O	S	0	0
			549	345	96	106	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
39	r	75	Total	C	N	O	S	0	0
			577	363	100	112	2		
39	y	75	Total	C	N	O	S	0	0
			577	363	100	112	2		

- Molecule 40 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	80	Total	C	N	O	S	0	0
			630	402	108	118	2		
40	l	99	Total	C	N	O	S	0	0
			751	475	137	137	2		
40	t	72	Total	C	N	O	S	0	0
			569	364	99	104	2		

- Molecule 41 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	92	Total	C	N	O	S	0	0
			752	481	136	131	4		
41	m	92	Total	C	N	O	S	0	0
			752	481	136	131	4		
41	u	92	Total	C	N	O	S	0	0
			752	481	136	131	4		

- Molecule 42 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	74	Total	C	N	O	S	0	0
			588	381	96	108	3		

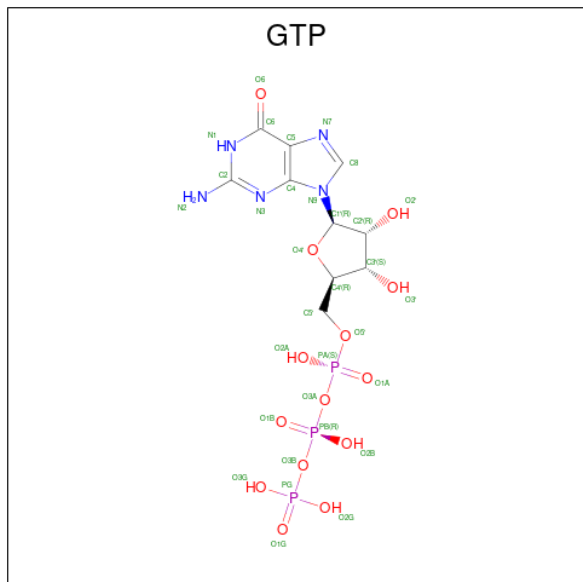
- Molecule 43 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	75	Total	C	N	O	S	0	0
			588	378	98	110	2		

- Molecule 44 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	z	74	Total	C	N	O	S	0	0
			577	364	95	116	2		

- Molecule 45 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
45	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

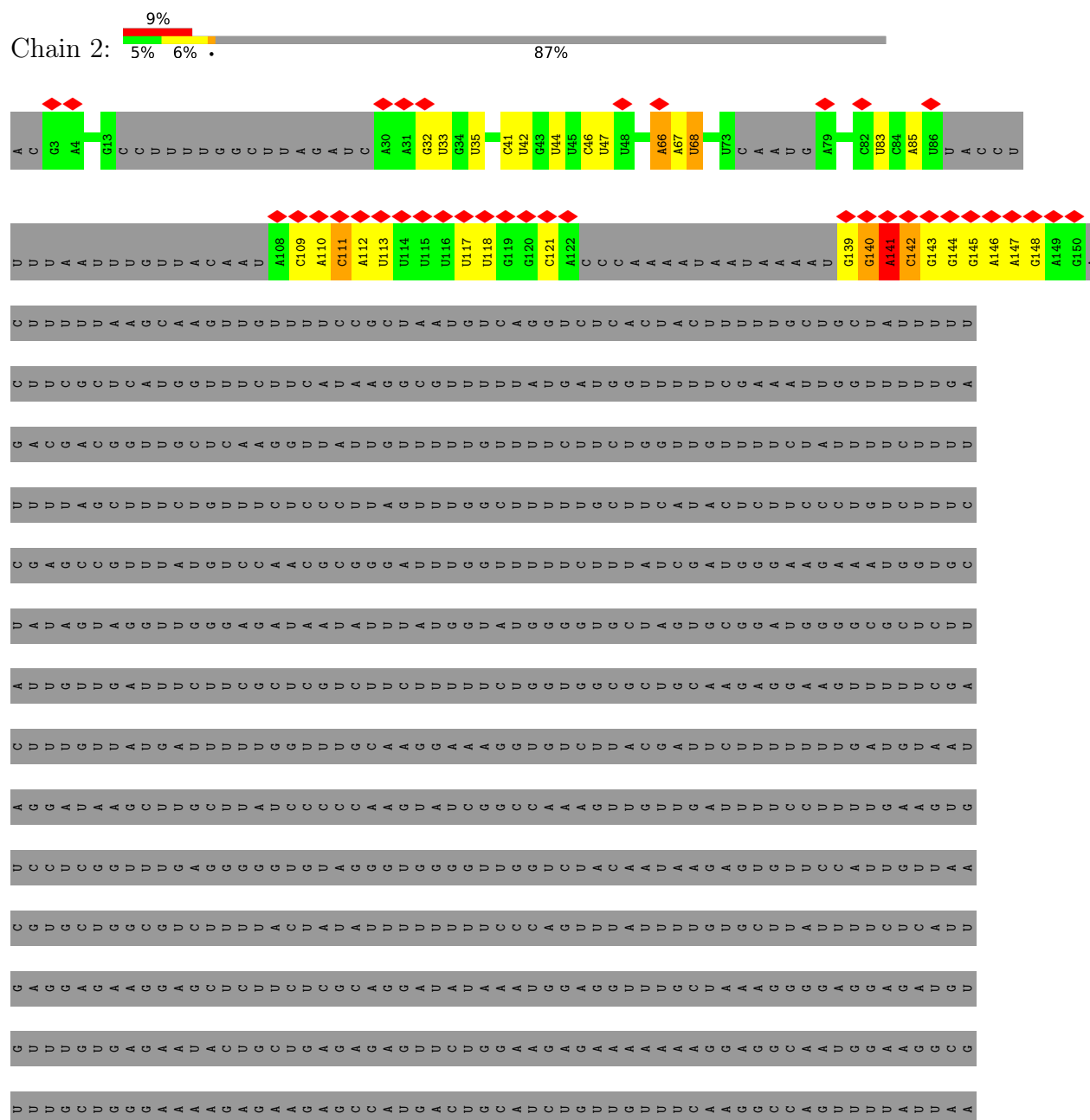
- Molecule 46 is ZINC ION (three-letter code: ZN) (formula: Zn).

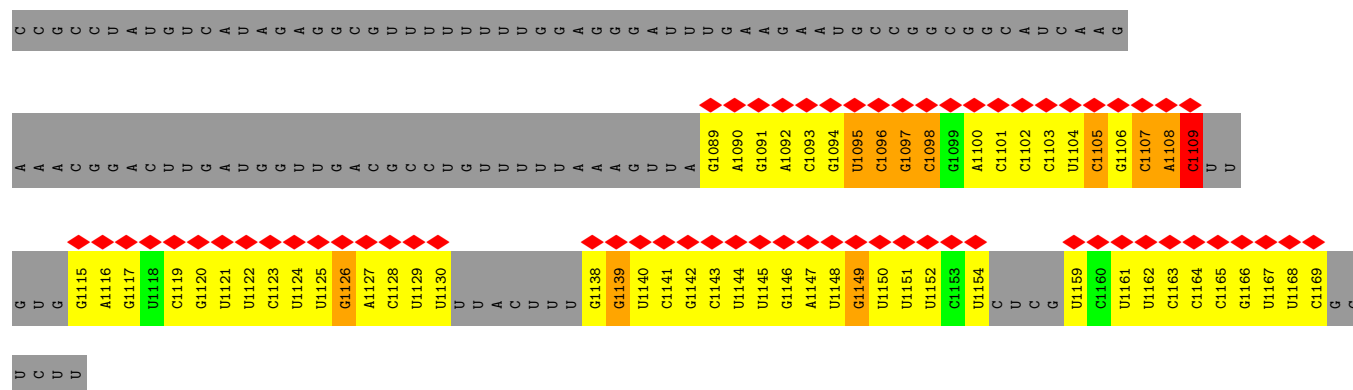
Mol	Chain	Residues	Atoms		AltConf
46	L	1	Total	Zn	0
			1	1	
46	S	3	Total	Zn	0
			3	3	
46	T	2	Total	Zn	0
			2	2	
46	U	1	Total	Zn	0
			1	1	

3 Residue-property plots

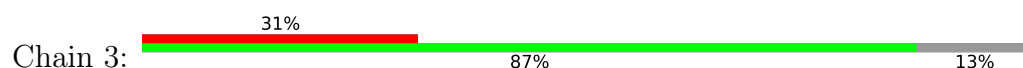
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: U2 snRNA

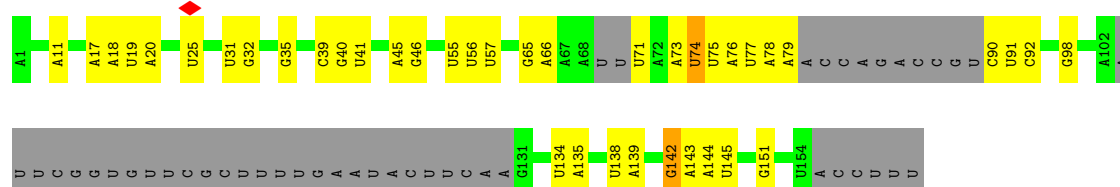




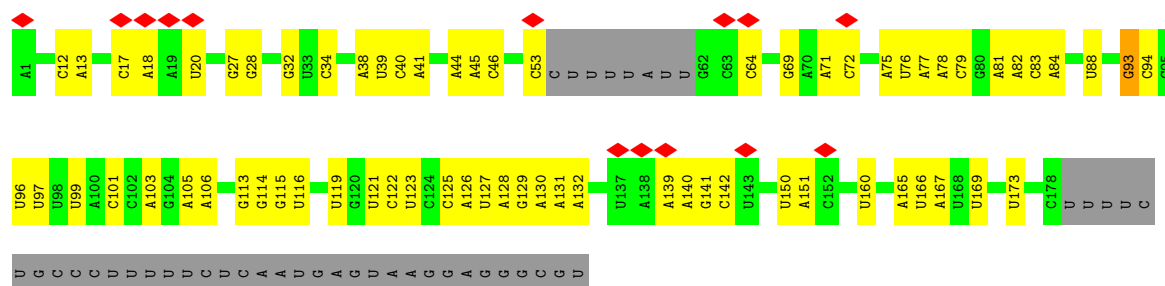
• Molecule 2: U6 snRNA-associated Sm-like protein LSm3



• Molecule 3: U4 snRNA

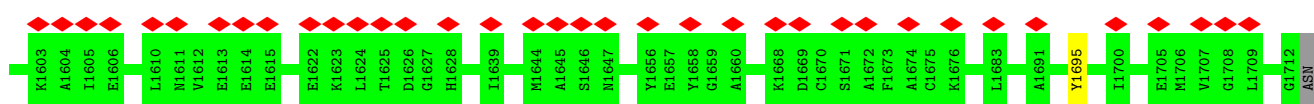


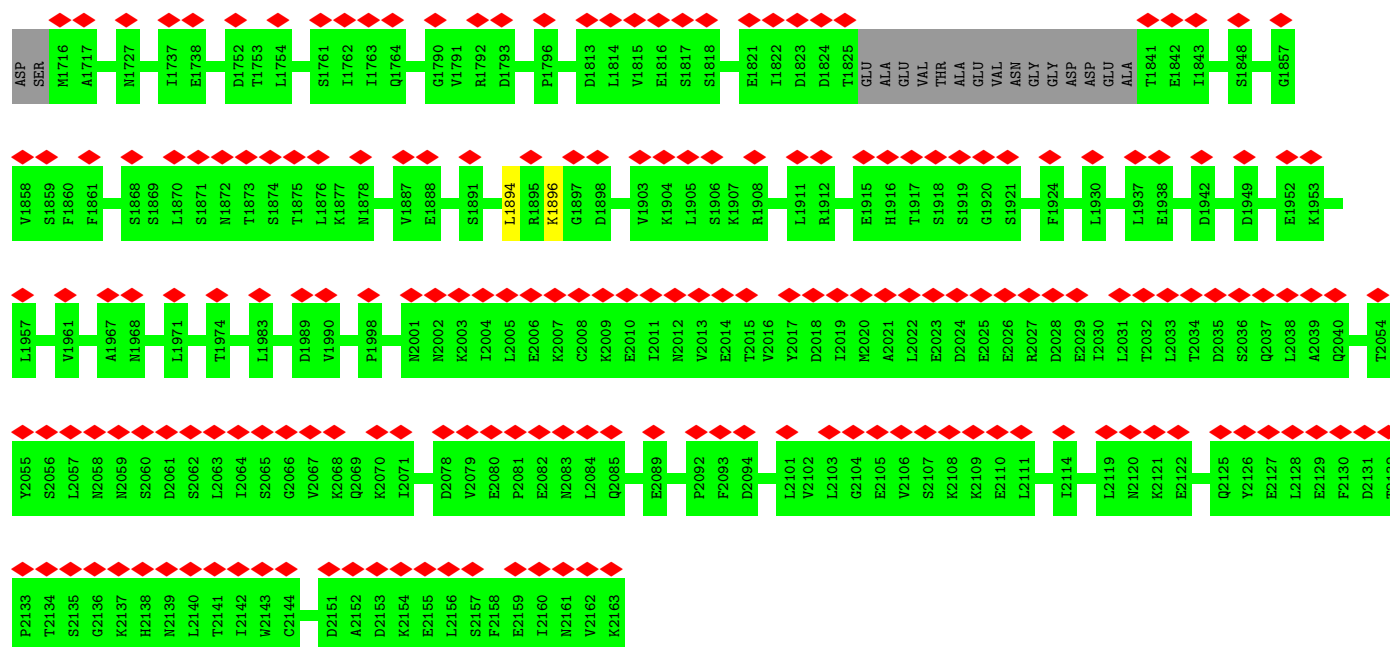
• Molecule 4: U5 snRNA



• Molecule 5: U6 snRNA

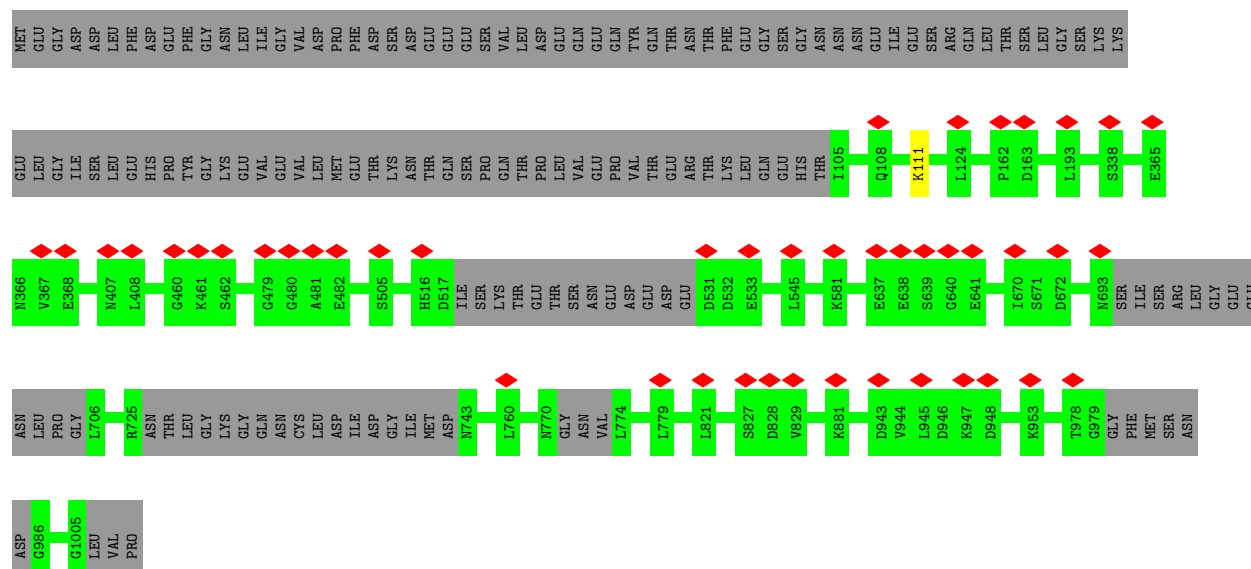






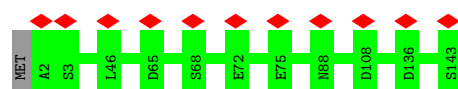
• Molecule 10: Pre-mRNA-splicing factor SNU114

Chain C: 84% 16%

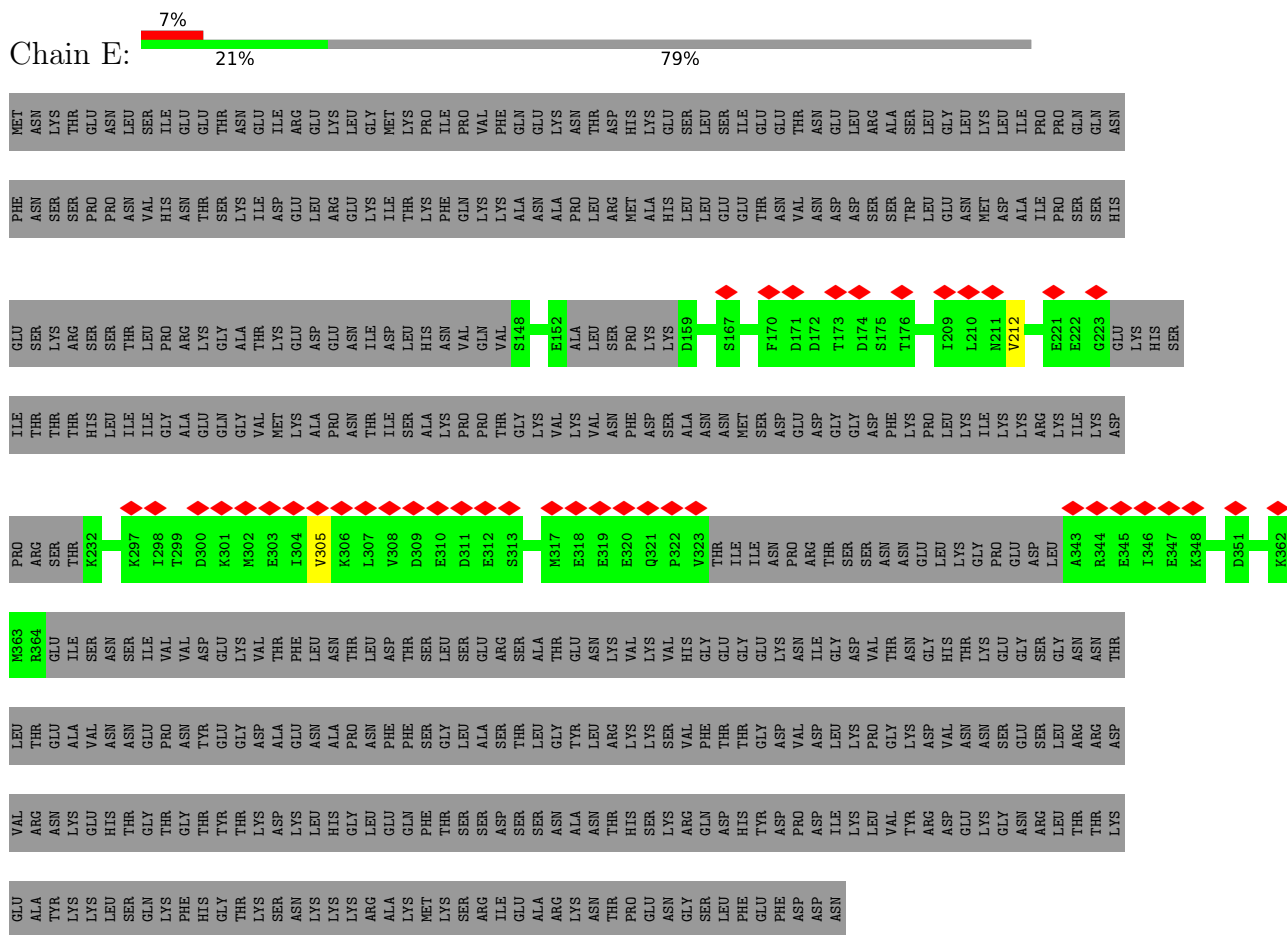


• Molecule 11: Spliceosomal protein DIB1

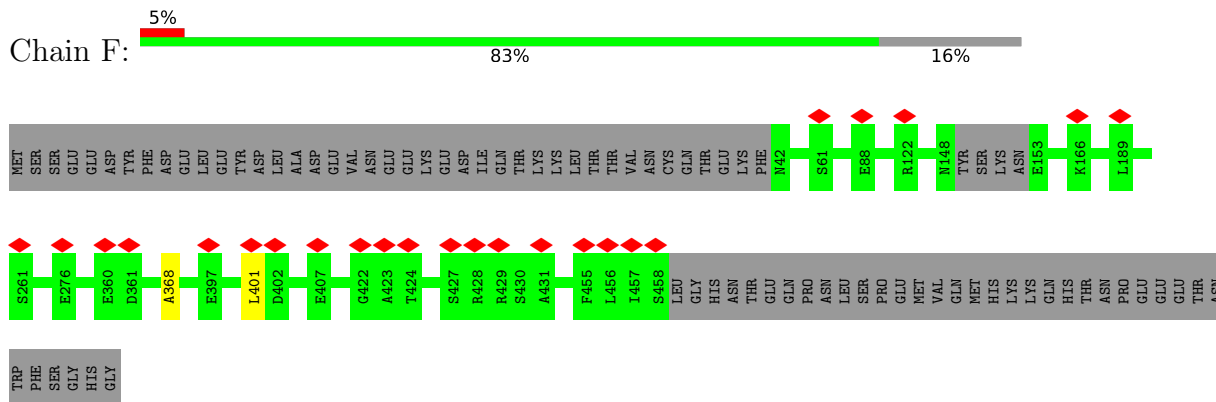
Chain D: 8% 99%



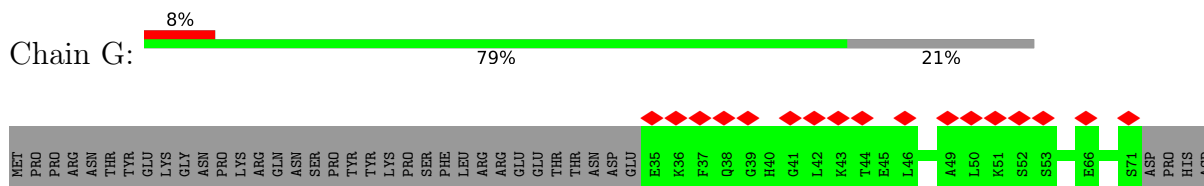
• Molecule 12: 66 kDa U4/U6.U5 small nuclear ribonucleoprotein component



- Molecule 13: Pre-mRNA-processing factor 31

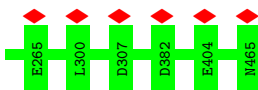
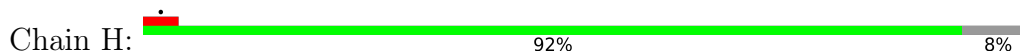


- Molecule 14: U4/U6 small nuclear ribonucleoprotein PRP3





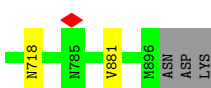
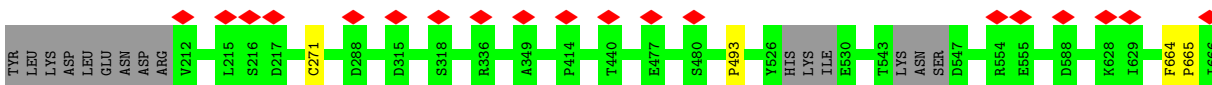
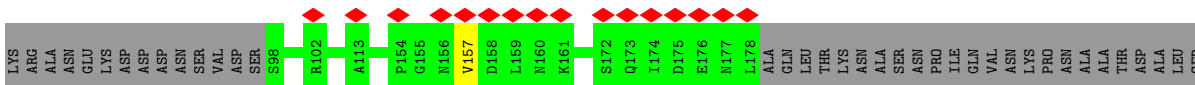
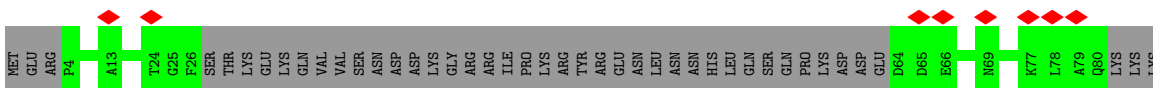
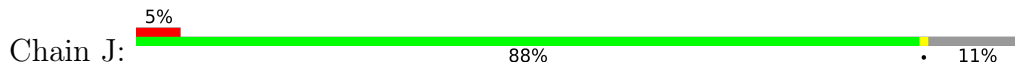
- Molecule 15: U4/U6 small nuclear ribonucleoprotein PRP4



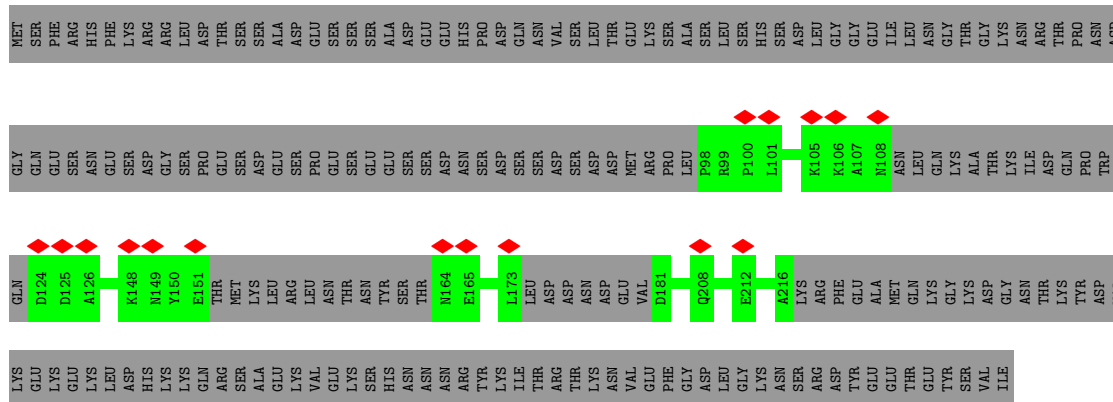
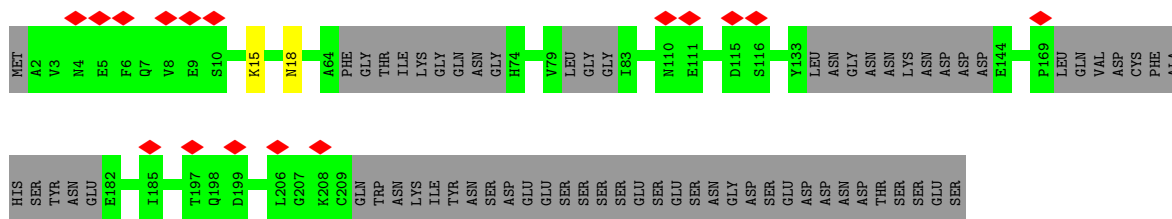
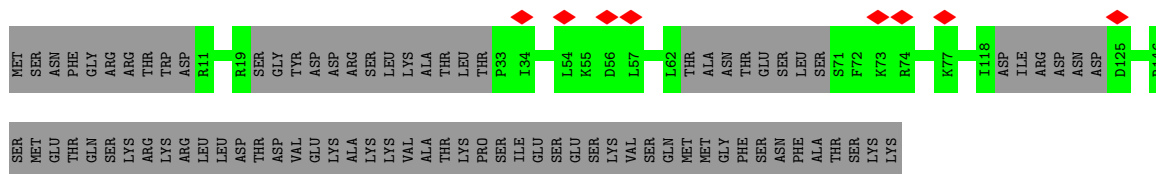
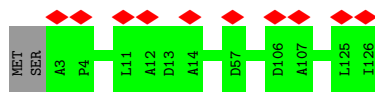
- Molecule 16: Yeast UBC4 gene for ubiquitin-conjugating enzyme



- Molecule 17: Pre-mRNA-splicing factor 6

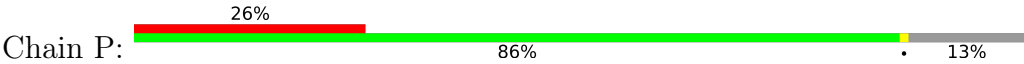


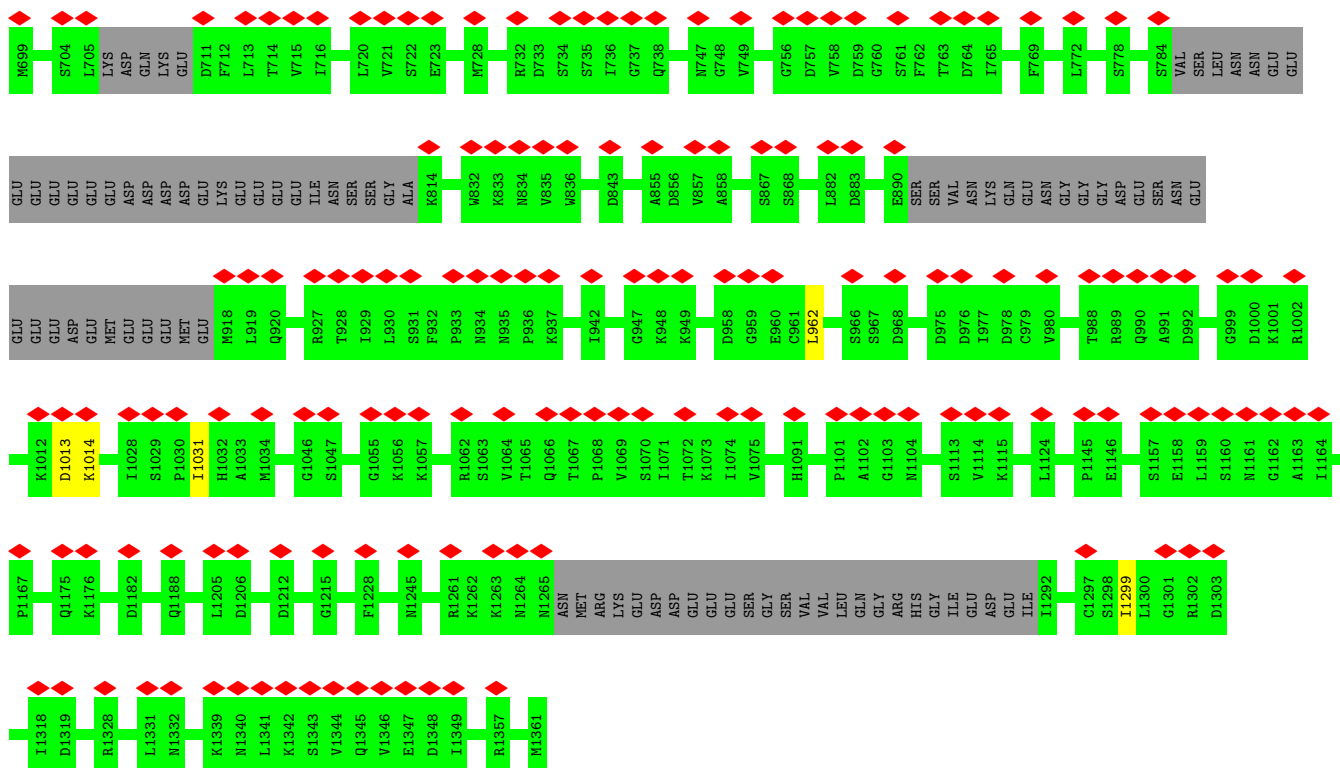
- Molecule 18: 13 kDa ribonucleoprotein-associated protein



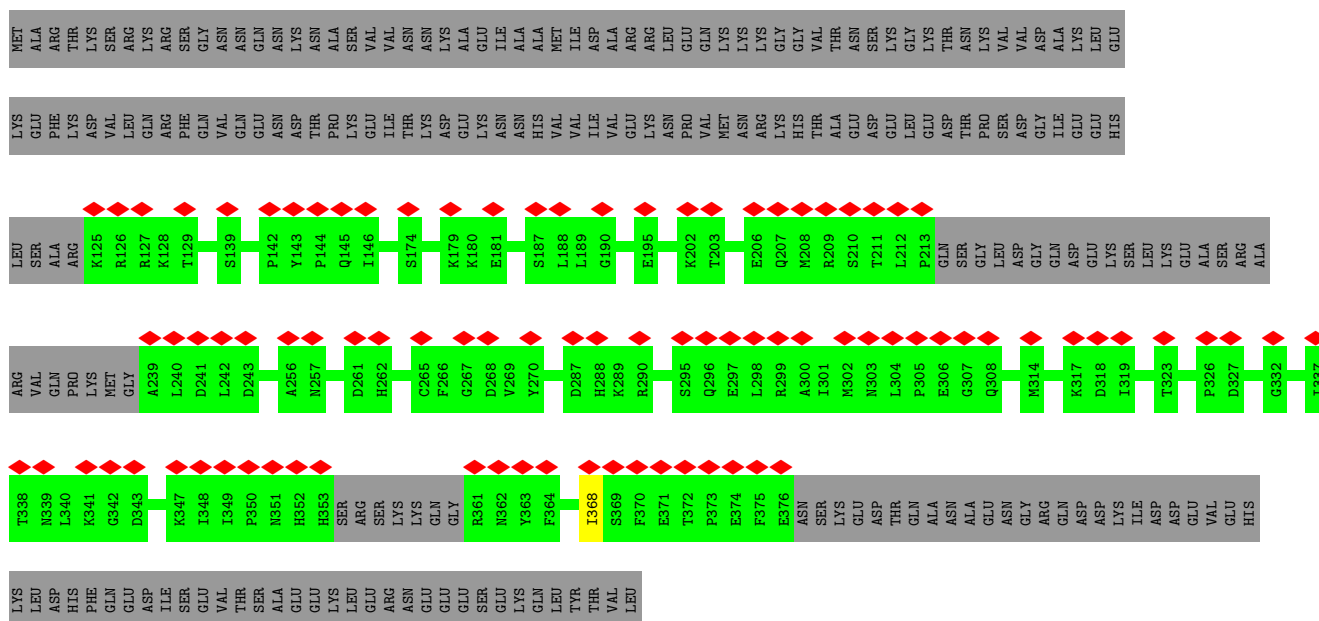


● Molecule 23: Pre-mRNA-splicing factor RSE1

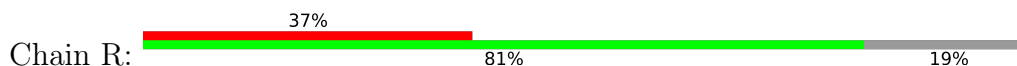


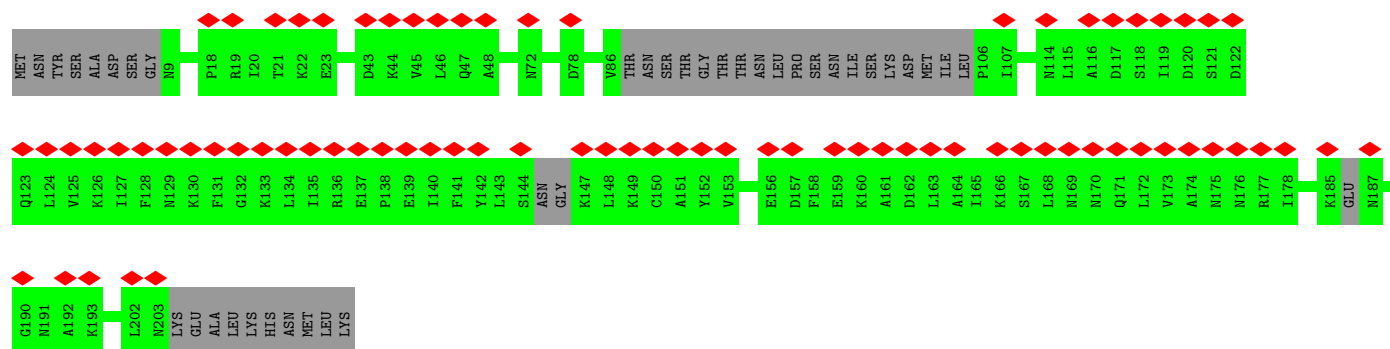


- Molecule 24: Cold sensitive U2 snRNA suppressor 1

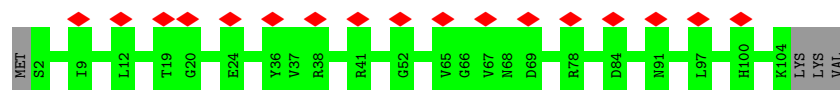


- Molecule 25: Protein HSH49

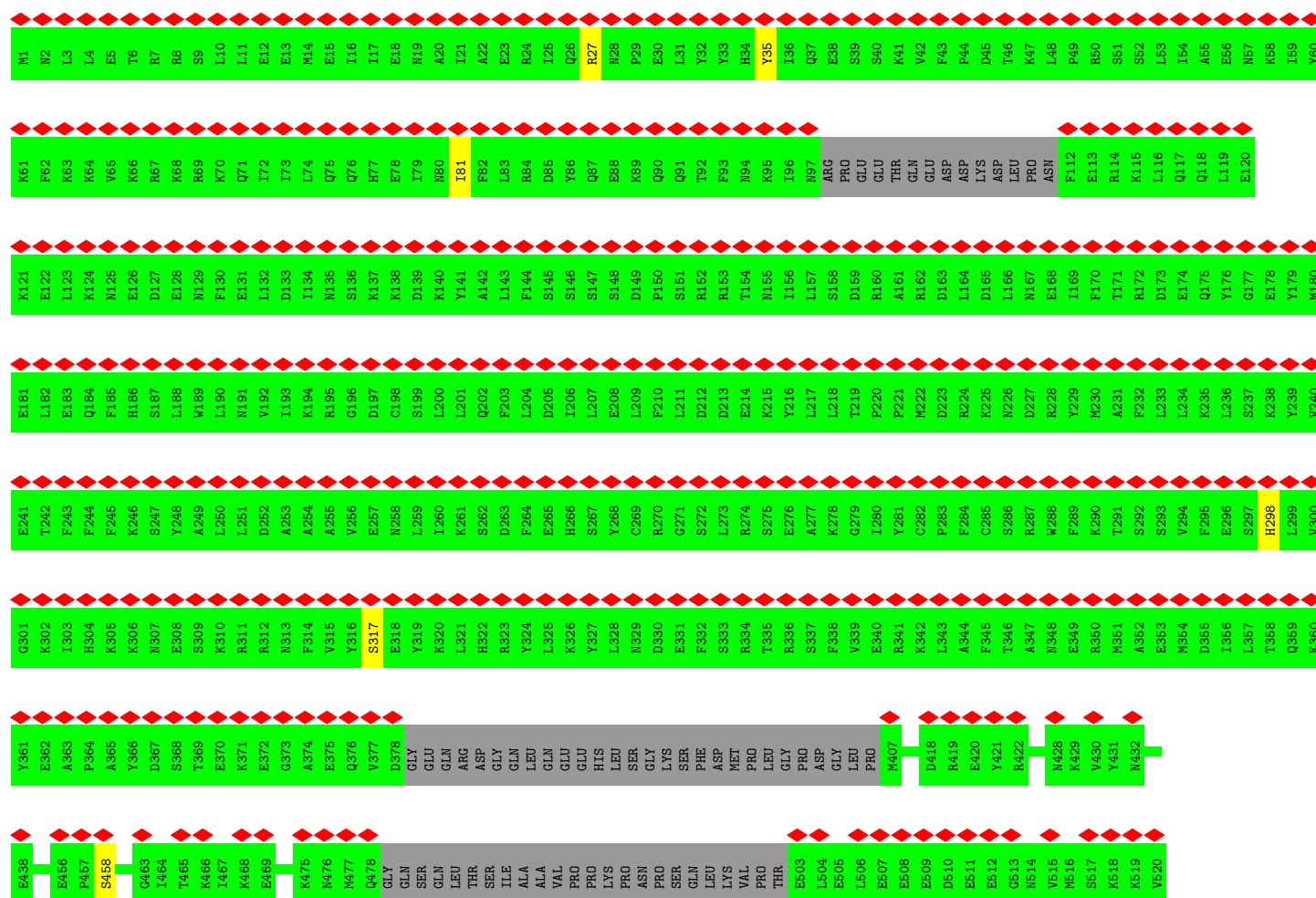
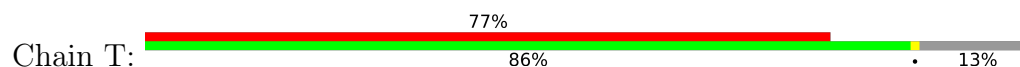


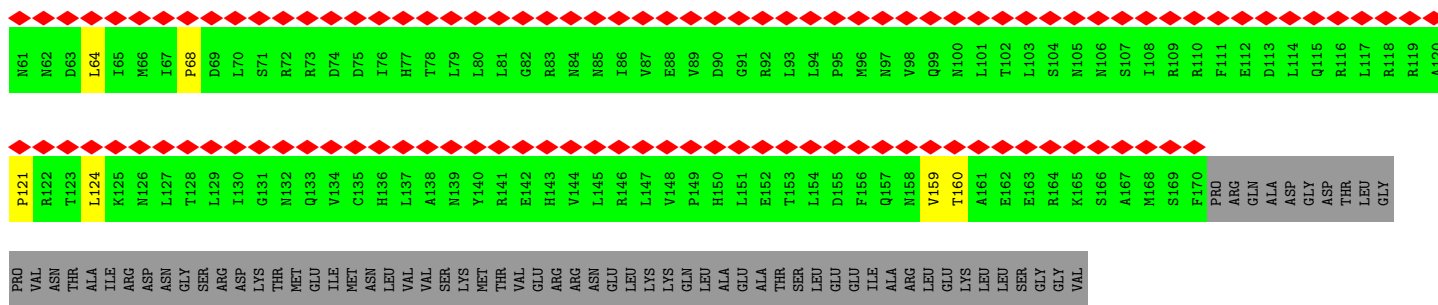


• Molecule 26: Pre-mRNA-splicing factor RDS3

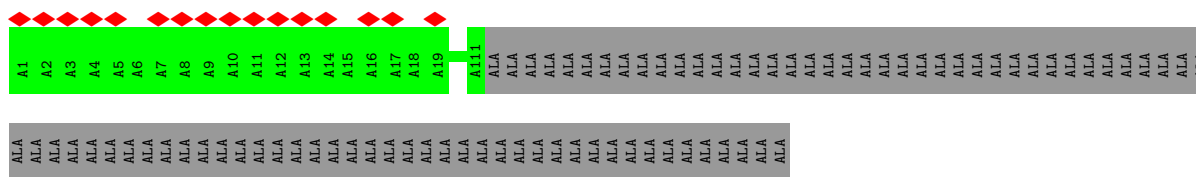


• Molecule 27: Pre-mRNA-splicing factor PRP9

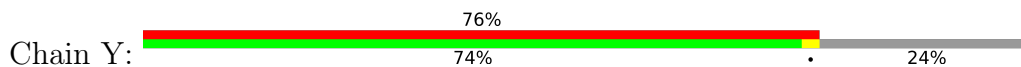




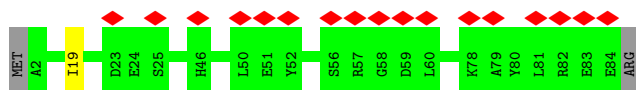
• Molecule 31: Unknown



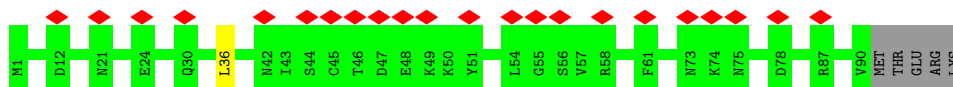
• Molecule 32: U2 small nuclear ribonucleoprotein B''



• Molecule 33: RDS3 complex subunit 10

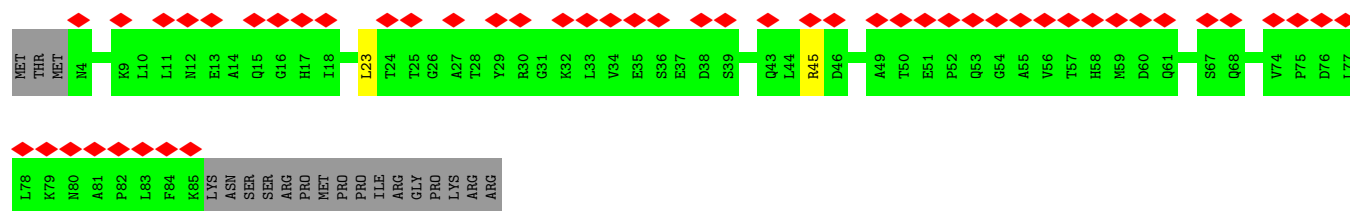


• Molecule 34: U6 snRNA-associated Sm-like protein LSm2

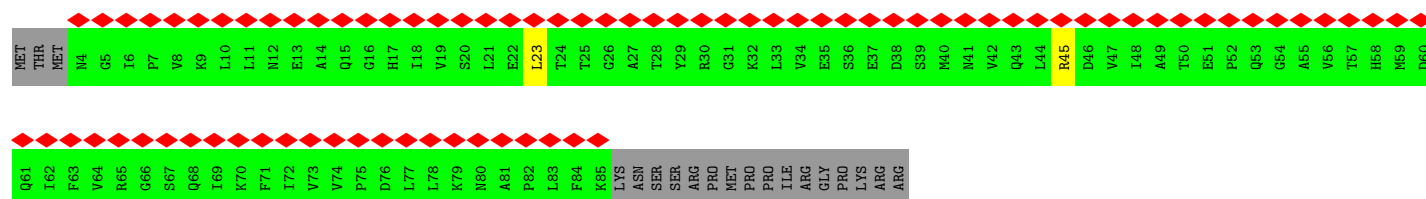
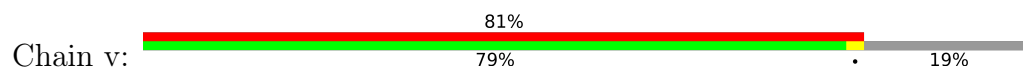


• Molecule 35: Small nuclear ribonucleoprotein-associated protein B

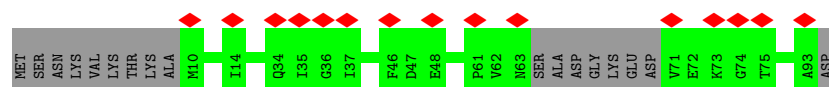
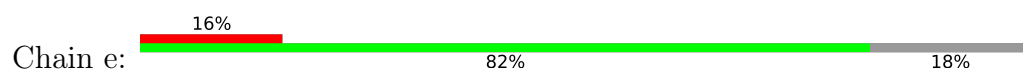




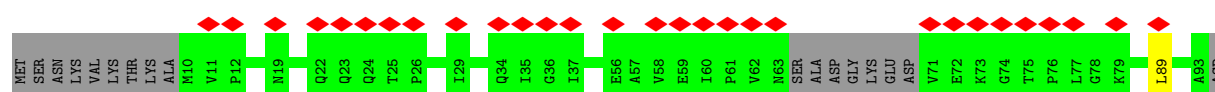
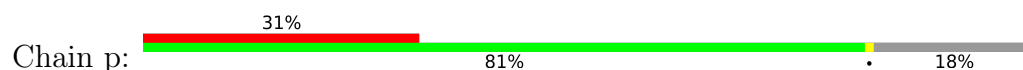
• Molecule 36: Small nuclear ribonucleoprotein Sm D3



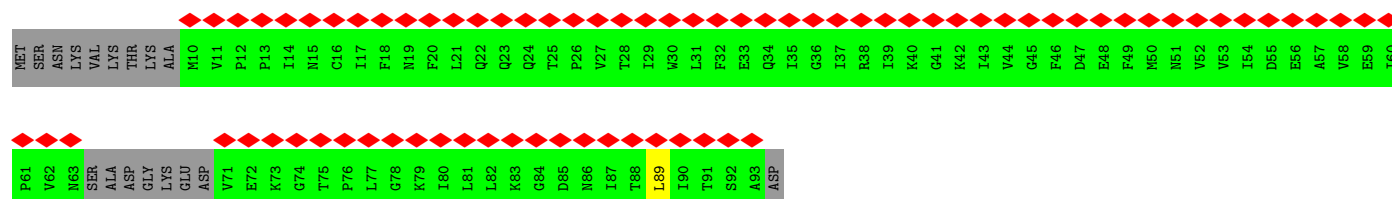
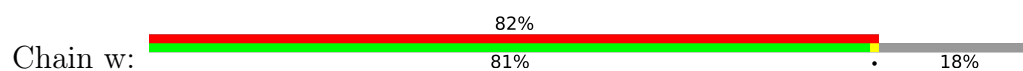
• Molecule 37: Small nuclear ribonucleoprotein E



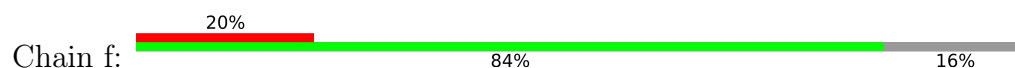
• Molecule 37: Small nuclear ribonucleoprotein E

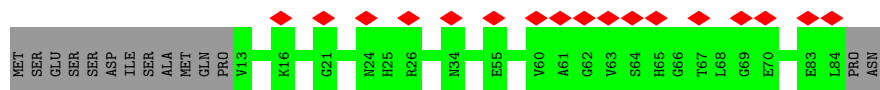


• Molecule 37: Small nuclear ribonucleoprotein E

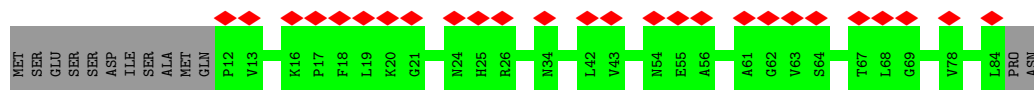
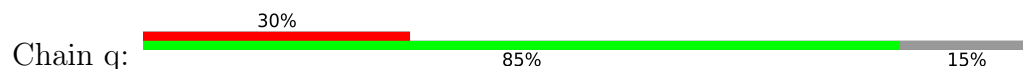


• Molecule 38: Small nuclear ribonucleoprotein F

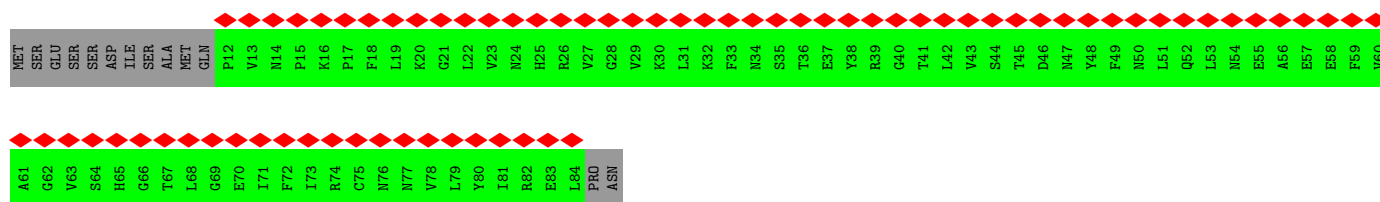
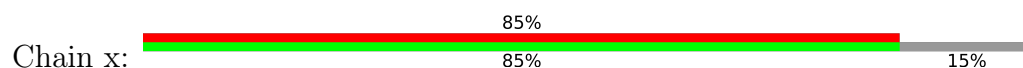




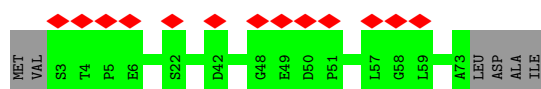
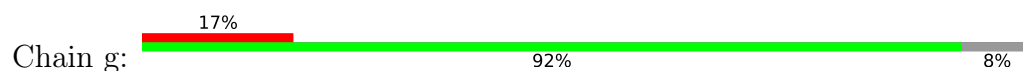
- Molecule 38: Small nuclear ribonucleoprotein F



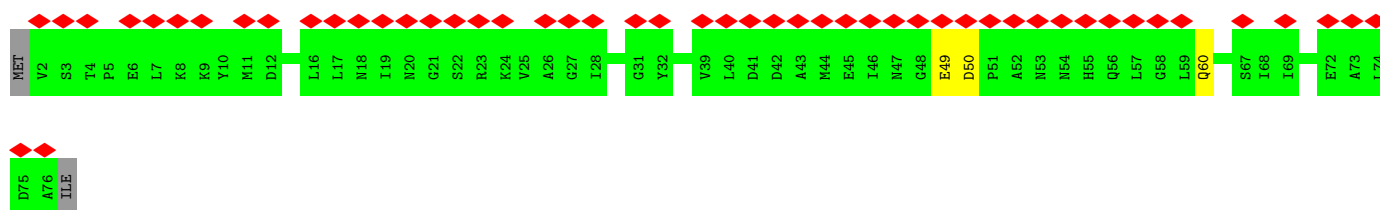
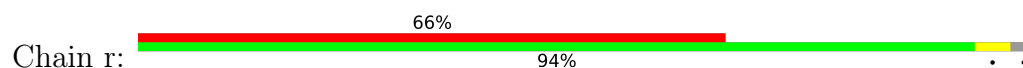
- Molecule 38: Small nuclear ribonucleoprotein F



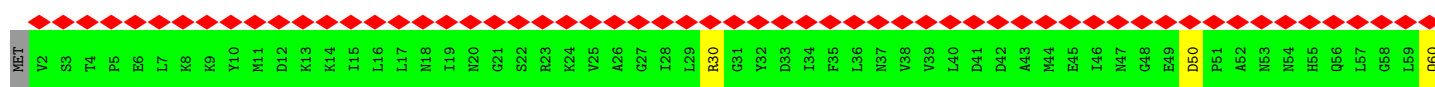
- Molecule 39: Small nuclear ribonucleoprotein G

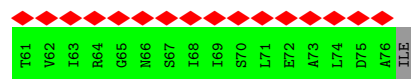


- Molecule 39: Small nuclear ribonucleoprotein G

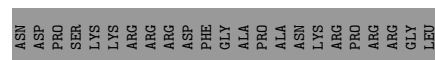
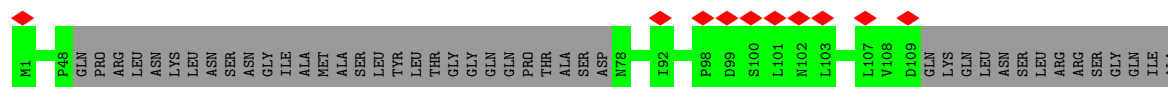


- Molecule 39: Small nuclear ribonucleoprotein G

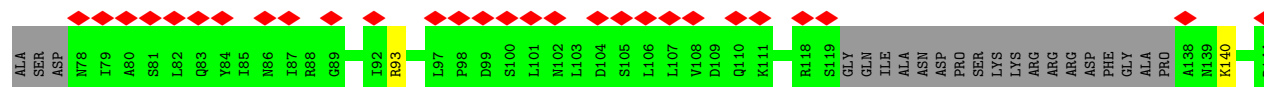
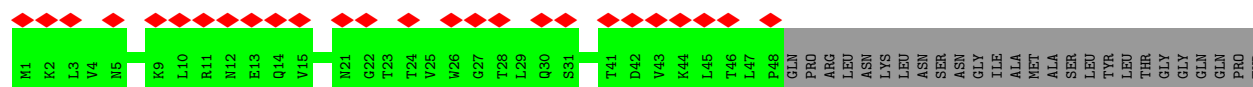
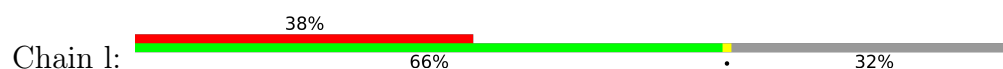




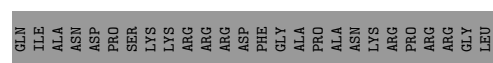
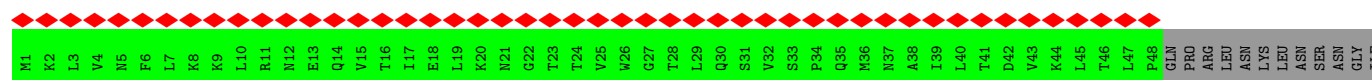
- Molecule 40: Small nuclear ribonucleoprotein Sm D1



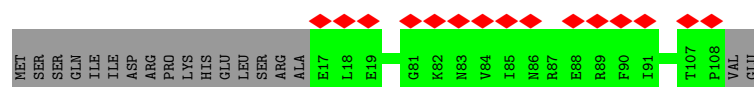
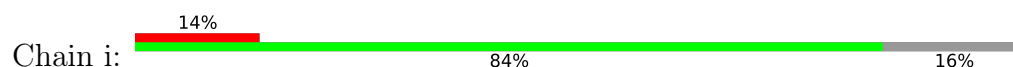
- Molecule 40: Small nuclear ribonucleoprotein Sm D1



- Molecule 40: Small nuclear ribonucleoprotein Sm D1



- Molecule 41: Small nuclear ribonucleoprotein Sm D2



- Molecule 41: Small nuclear ribonucleoprotein Sm D2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	9559	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 ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	350	Depositor
Maximum defocus (nm)	5300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.080	Depositor
Minimum map value	-0.019	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0258	Depositor
Map size (Å)	686.39996, 686.39996, 686.39996	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.43, 1.43, 1.43	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, GTP, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	1.35	52/3579 (1.5%)	1.69	123/5551 (2.2%)
2	3	0.25	0/617	0.45	0/836
3	4	0.45	4/2705 (0.1%)	0.95	10/4204 (0.2%)
4	5	0.42	1/4039 (0.0%)	0.90	6/6284 (0.1%)
5	6	0.24	0/2253	0.83	3/3497 (0.1%)
6	7	0.24	0/505	0.44	0/675
7	8	0.24	0/501	0.45	0/673
8	A	0.29	0/18580	0.46	1/25189 (0.0%)
9	B	0.40	1/13905 (0.0%)	0.62	6/18852 (0.0%)
10	C	0.32	0/6928	0.47	0/9377
11	D	0.28	0/1185	0.46	0/1596
12	E	0.24	0/822	0.40	0/1109
13	F	0.27	0/3292	0.45	1/4432 (0.0%)
14	G	0.29	0/2885	0.45	0/3882
15	H	0.27	0/3455	0.49	0/4663
16	I	0.28	0/665	0.82	0/1024
17	J	0.26	0/6613	0.43	0/8942
18	K	0.26	0/949	0.45	0/1292
19	L	0.25	0/899	0.44	0/1204
20	M	0.24	0/1430	0.44	0/1927
21	N	0.22	0/421	0.29	0/583
22	O	0.28	0/6745	0.45	0/9157
23	P	0.30	1/9623 (0.0%)	0.53	1/13041 (0.0%)
24	Q	0.27	0/1835	0.46	0/2480
25	R	0.26	0/1453	0.42	0/1954
26	S	0.29	0/827	0.46	0/1105
27	T	0.27	0/3992	0.41	0/5346
28	U	0.25	0/1511	0.41	1/2038 (0.0%)
29	V	0.24	0/1105	0.36	0/1475
30	W	0.42	0/1406	0.69	4/1905 (0.2%)
31	X	0.25	0/148	0.39	0/204
32	Y	0.30	0/692	0.54	0/923

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Z	0.28	0/694	0.47	0/929
34	a	0.26	0/745	0.51	1/1005 (0.1%)
35	b	0.29	0/567	0.47	0/762
35	k	0.41	0/567	0.61	0/762
35	s	0.40	0/567	0.63	0/762
36	d	0.30	0/650	0.50	0/879
36	n	0.41	0/641	0.65	2/868 (0.2%)
36	v	0.43	0/641	0.65	2/868 (0.2%)
37	e	0.26	0/612	0.44	0/830
37	p	0.39	0/612	0.59	1/830 (0.1%)
37	w	0.40	0/612	0.61	1/830 (0.1%)
38	f	0.27	0/589	0.46	0/796
38	q	0.39	0/597	0.62	0/807
38	x	0.42	0/597	0.63	0/807
39	g	0.25	0/554	0.53	0/746
39	r	0.32	0/582	0.63	0/785
39	y	0.26	0/582	0.49	0/785
40	h	0.25	0/635	0.48	0/861
40	l	0.38	0/756	0.70	1/1023 (0.1%)
40	t	0.41	0/574	0.68	1/777 (0.1%)
41	i	0.25	0/764	0.44	0/1026
41	m	0.38	0/764	0.57	0/1026
41	u	0.40	0/764	0.57	0/1026
42	j	0.25	0/594	0.42	0/802
43	o	0.24	0/595	0.41	0/806
44	z	0.24	0/584	0.43	0/787
All	All	0.39	59/122004 (0.0%)	0.62	165/167605 (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	2	0	2
8	A	0	2
9	B	0	4
17	J	0	2
20	M	0	2
23	P	0	2
27	T	0	1
30	W	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
39	r	0	1
All	All	0	17

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1149	G	O3'-P	24.35	1.90	1.61
1	2	143	G	O3'-P	18.92	1.83	1.61
4	5	105	A	O3'-P	18.04	1.82	1.61
1	2	1161	U	O3'-P	-15.56	1.42	1.61
1	2	143	G	C3'-O3'	15.28	1.63	1.42
1	2	1092	A	O3'-P	-14.79	1.43	1.61
1	2	1090	A	O3'-P	14.49	1.78	1.61
1	2	144	G	O3'-P	-14.29	1.44	1.61
1	2	1116	A	O3'-P	-11.58	1.47	1.61
1	2	1166	G	O3'-P	9.99	1.73	1.61
1	2	1149	G	C3'-O3'	9.99	1.56	1.42
1	2	1163	C	O5'-C5'	9.13	1.59	1.44
1	2	1116	A	C3'-O3'	-8.93	1.29	1.42
1	2	1127	A	O3'-P	-8.69	1.50	1.61
1	2	1167	U	O3'-P	8.63	1.71	1.61
1	2	1164	C	O3'-P	-8.23	1.51	1.61
1	2	1090	A	C3'-O3'	7.79	1.53	1.42
3	4	142	G	N7-C5	-7.73	1.34	1.39
1	2	1162	U	P-O5'	7.53	1.67	1.59
1	2	1163	C	P-O5'	7.49	1.67	1.59
1	2	1117	G	P-O5'	7.31	1.67	1.59
1	2	144	G	P-O5'	7.10	1.66	1.59
1	2	1096	C	O3'-P	6.96	1.69	1.61
1	2	1154	U	C1'-N1	6.95	1.59	1.48
1	2	1128	C	C5'-C4'	-6.95	1.43	1.51
1	2	1140	U	C1'-N1	6.88	1.59	1.48
1	2	1165	C	O3'-P	6.55	1.69	1.61
1	2	1095	U	O3'-P	6.54	1.69	1.61
1	2	145	G	P-O5'	-6.44	1.53	1.59
1	2	1169	C	C1'-N1	6.44	1.58	1.48
1	2	1150	U	O5'-C5'	6.37	1.54	1.44
1	2	1090	A	C4'-O4'	6.36	1.53	1.45
1	2	1117	G	C5'-C4'	6.25	1.58	1.51
1	2	1168	U	C5'-C4'	-6.22	1.43	1.51
1	2	1162	U	O3'-P	6.22	1.68	1.61
1	2	1165	C	O5'-C5'	6.05	1.54	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	73	A	C1'-N9	-6.04	1.38	1.46
23	P	188	SER	C-N	-6.03	1.22	1.34
1	2	1162	U	O5'-C5'	6.01	1.54	1.44
3	4	142	G	C2-N2	-6.01	1.28	1.34
1	2	1162	U	C2-N3	5.96	1.42	1.37
1	2	1151	U	O5'-C5'	-5.88	1.33	1.42
1	2	1163	C	O3'-P	5.81	1.68	1.61
1	2	68	U	C1'-N1	5.78	1.57	1.48
1	2	1161	U	C3'-O3'	-5.73	1.34	1.42
3	4	74	U	C1'-N1	5.72	1.57	1.48
1	2	1097	G	O3'-P	5.70	1.68	1.61
1	2	1162	U	C3'-C2'	-5.60	1.46	1.52
1	2	118	U	C1'-N1	5.59	1.57	1.48
1	2	144	G	C3'-O3'	-5.50	1.34	1.42
1	2	143	G	P-O5'	-5.46	1.54	1.59
1	2	121	C	C1'-N1	5.44	1.56	1.48
1	2	111	C	C1'-N1	5.38	1.56	1.48
1	2	109	C	C1'-N1	5.29	1.56	1.48
1	2	147	A	O3'-P	-5.24	1.54	1.61
1	2	1166	G	C5'-C4'	5.23	1.57	1.51
1	2	1090	A	O5'-C5'	5.16	1.52	1.44
1	2	85	A	C1'-N9	-5.09	1.39	1.46
9	B	1695	TYR	CE1-CZ	-5.02	1.32	1.38

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	144	G	C4'-C3'-O3'	-16.52	74.71	109.40
1	2	1093	C	P-O5'-C5'	14.80	144.59	120.90
1	2	1162	U	C5'-C4'-O4'	14.80	126.86	109.10
1	2	1147	A	C5'-C4'-C3'	-14.15	93.35	116.00
1	2	1092	A	C2'-C3'-O3'	14.11	140.53	109.50
1	2	143	G	C4'-C3'-O3'	13.61	140.22	113.00
1	2	1098	C	N1-C1'-C2'	-13.39	96.59	114.00
1	2	1151	U	C4'-C3'-O3'	-12.56	83.02	109.40
1	2	144	G	C2'-C3'-O3'	12.27	136.49	109.50
9	B	1213	ARG	NE-CZ-NH2	-12.11	114.25	120.30
1	2	143	G	P-O3'-C3'	11.89	133.97	119.70
1	2	1149	G	P-O3'-C3'	11.89	133.97	119.70
1	2	144	G	C5'-C4'-O4'	-11.80	94.94	109.10
1	2	1151	U	P-O5'-C5'	11.68	139.59	120.90
1	2	1117	G	C5'-C4'-O4'	11.40	122.78	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	145	G	C5'-C4'-C3'	-11.24	98.02	116.00
1	2	1109	C	C2-N1-C1'	11.21	131.14	118.80
1	2	1109	C	C6-N1-C1'	-11.15	107.42	120.80
1	2	1150	U	C5'-C4'-C3'	11.08	133.72	116.00
1	2	1117	G	C5'-C4'-C3'	-10.88	98.59	116.00
1	2	1163	C	C5'-C4'-O4'	10.55	121.76	109.10
1	2	141	A	N9-C1'-C2'	-10.47	100.38	114.00
1	2	144	G	C5'-C4'-C3'	10.44	132.71	116.00
1	2	1126	G	N9-C1'-C2'	-10.02	100.97	114.00
1	2	143	G	C5'-C4'-C3'	-9.89	100.17	116.00
1	2	1091	G	C5'-C4'-C3'	9.88	131.81	116.00
3	4	142	G	N1-C6-O6	-9.83	114.00	119.90
4	5	88	U	P-O3'-C3'	9.73	131.38	119.70
1	2	1139	G	N9-C1'-C2'	-9.71	101.31	112.00
1	2	1163	C	C5'-C4'-C3'	-9.72	100.45	116.00
1	2	1147	A	P-O5'-C5'	9.59	136.25	120.90
1	2	1090	A	P-O3'-C3'	9.52	131.12	119.70
1	2	1162	U	C5'-C4'-C3'	-9.20	101.28	116.00
1	2	1168	U	C4'-C3'-O3'	-8.97	90.56	109.40
1	2	1150	U	C4'-C3'-O3'	-8.96	90.59	109.40
1	2	142	C	N1-C1'-C2'	-8.85	102.27	112.00
3	4	142	G	C5-C6-O6	8.78	133.87	128.60
1	2	1152	U	P-O5'-C5'	8.70	134.82	120.90
1	2	1151	U	O4'-C1'-N1	8.64	115.11	108.20
1	2	1090	A	C4'-C3'-O3'	8.63	130.26	113.00
1	2	1148	U	C4'-C3'-O3'	-8.54	91.46	109.40
1	2	1092	A	P-O5'-C5'	8.52	134.54	120.90
1	2	145	G	P-O5'-C5'	8.31	134.20	120.90
1	2	1165	C	C5'-C4'-C3'	-8.27	102.77	116.00
1	2	1109	C	C4'-C3'-O3'	8.25	129.50	113.00
1	2	148	G	C5'-C4'-C3'	-8.24	102.81	116.00
3	4	142	G	N1-C2-N3	8.21	128.82	123.90
1	2	1150	U	C2'-C3'-O3'	8.14	127.41	109.50
1	2	1151	U	C5'-C4'-O4'	8.13	118.86	109.10
1	2	1090	A	C5'-C4'-O4'	8.09	118.81	109.10
1	2	1109	C	O4'-C1'-N1	8.05	114.64	108.20
1	2	144	G	O3'-P-O5'	-8.02	88.75	104.00
1	2	1149	G	O3'-P-O5'	8.01	119.22	104.00
1	2	1150	U	P-O5'-C5'	7.98	133.67	120.90
1	2	1168	U	P-O5'-C5'	-7.93	108.21	120.90
1	2	1167	U	C2'-C3'-O3'	7.88	126.84	109.50
1	2	1092	A	C4'-C3'-O3'	-7.83	92.96	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1165	C	C5'-C4'-O4'	7.79	118.44	109.10
1	2	1147	A	C4'-C3'-O3'	7.77	128.53	113.00
3	4	71	U	C2-N1-C1'	7.76	127.01	117.70
1	2	1107	C	N1-C1'-C2'	-7.75	103.47	112.00
1	2	1161	U	C5'-C4'-C3'	-7.74	103.61	116.00
1	2	1093	C	C5'-C4'-C3'	-7.71	103.66	116.00
1	2	1169	C	P-O5'-C5'	-7.65	108.66	120.90
1	2	1097	G	C3'-C2'-O2'	7.61	135.37	113.30
1	2	1165	C	C4'-C3'-O3'	7.53	128.06	113.00
5	6	24	A	OP2-P-O3'	-7.34	89.04	105.20
3	4	71	U	N1-C2-O2	7.32	127.92	122.80
1	2	1168	U	C2'-C3'-O3'	7.29	125.53	109.50
1	2	1128	C	C5'-C4'-O4'	7.28	117.84	109.10
5	6	24	A	P-O3'-C3'	7.26	128.41	119.70
1	2	1089	G	C4'-C3'-O3'	7.26	127.51	113.00
1	2	1115	G	O5'-P-OP1	-7.22	99.20	105.70
1	2	1149	G	C4'-C3'-O3'	7.22	127.45	113.00
1	2	1159	U	O5'-P-OP1	-7.22	99.20	105.70
30	W	50	LEU	CA-CB-CG	7.17	131.78	115.30
1	2	139	G	O5'-P-OP1	-7.16	99.26	105.70
1	2	139	G	O5'-P-OP2	-7.15	99.27	105.70
1	2	1089	G	O5'-P-OP2	-7.12	99.29	105.70
1	2	1159	U	O5'-P-OP2	-7.12	99.30	105.70
1	2	1089	G	O5'-P-OP1	-7.11	99.30	105.70
1	2	1115	G	C4'-C3'-O3'	7.04	127.08	113.00
1	2	1115	G	O5'-P-OP2	-7.04	99.37	105.70
8	A	265	ASN	C-N-CA	-6.72	104.89	121.70
1	2	1090	A	C5'-C4'-C3'	-6.71	105.26	116.00
4	5	105	A	P-O3'-C3'	-6.71	111.64	119.70
1	2	1096	C	C1'-C2'-O2'	-6.68	90.55	110.60
40	l	93	ARG	CG-CD-NE	-6.64	97.86	111.80
1	2	1129	U	C5'-C4'-O4'	6.61	117.03	109.10
1	2	148	G	C5'-C4'-O4'	6.56	116.98	109.10
36	n	45	ARG	NE-CZ-NH1	-6.56	117.02	120.30
3	4	142	G	C6-N1-C2	-6.55	121.17	125.10
40	t	93	ARG	CG-CD-NE	-6.49	98.17	111.80
1	2	140	G	N9-C1'-C2'	-6.47	104.88	112.00
34	a	36	LEU	CA-CB-CG	6.45	130.14	115.30
1	2	1166	G	O5'-C5'-C4'	6.37	123.81	111.70
1	2	145	G	O4'-C1'-N9	6.31	113.25	108.20
1	2	1166	G	C5'-C4'-C3'	6.31	126.09	116.00
5	6	24	A	OP1-P-O3'	6.30	119.07	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4	71	U	N3-C2-O2	-6.27	117.81	122.20
1	2	1092	A	N9-C1'-C2'	6.25	122.12	114.00
1	2	145	G	O5'-C5'-C4'	-6.23	99.87	111.70
36	v	45	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	2	1152	U	C5'-C4'-C3'	-6.14	106.17	116.00
1	2	1096	C	C4'-C3'-O3'	6.12	125.24	113.00
4	5	93	G	C5-C6-O6	6.10	132.26	128.60
37	w	89	LEU	CA-CB-CG	6.09	129.31	115.30
9	B	1213	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	2	1167	U	P-O3'-C3'	-6.05	112.44	119.70
1	2	143	G	O4'-C1'-N9	6.04	113.03	108.20
1	2	1151	U	O3'-P-O5'	-5.99	92.61	104.00
1	2	143	G	O3'-P-O5'	5.98	115.37	104.00
1	2	144	G	P-O3'-C3'	-5.96	112.55	119.70
1	2	1167	U	C5'-C4'-O4'	-5.90	102.02	109.10
1	2	1091	G	O5'-C5'-C4'	5.89	122.90	111.70
1	2	1108	A	C3'-C2'-C1'	5.89	106.21	101.50
1	2	1162	U	C4'-C3'-O3'	5.89	124.78	113.00
1	2	1150	U	N1-C1'-C2'	5.83	121.57	114.00
30	W	36	LEU	CA-CB-CG	5.83	128.70	115.30
28	U	136	PRO	N-CA-CB	5.77	110.22	103.30
1	2	1115	G	P-O3'-C3'	5.76	126.61	119.70
1	2	1148	U	C5'-C4'-O4'	5.75	116.01	109.10
1	2	1162	U	C2'-C3'-O3'	-5.75	96.86	109.50
3	4	142	G	C8-N9-C4	-5.72	104.11	106.40
1	2	141	A	C4'-C3'-O3'	5.69	124.38	113.00
37	p	89	LEU	CA-CB-CG	5.63	128.25	115.30
30	W	57	LEU	CA-CB-CG	5.63	128.24	115.30
4	5	93	G	N1-C6-O6	-5.61	116.53	119.90
1	2	1167	U	C5'-C4'-C3'	5.59	124.94	116.00
4	5	88	U	OP1-P-O3'	5.56	117.44	105.20
1	2	1097	G	C2'-C3'-O3'	-5.55	97.30	109.50
3	4	71	U	C6-N1-C1'	-5.54	113.44	121.20
1	2	1162	U	P-O3'-C3'	5.53	126.33	119.70
1	2	145	G	C3'-C2'-O2'	-5.49	97.37	113.30
1	2	1091	G	C4'-C3'-O3'	-5.49	97.88	109.40
1	2	145	G	C5'-C4'-O4'	5.48	115.68	109.10
9	B	789	LEU	CA-CB-CG	5.48	127.90	115.30
1	2	1105	C	C4'-C3'-O3'	-5.45	97.95	109.40
4	5	88	U	OP2-P-O3'	-5.45	93.21	105.20
1	2	1162	U	C4'-C3'-C2'	5.43	108.03	102.60
1	2	1151	U	N1-C1'-C2'	5.43	121.05	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1168	U	C4'-C3'-C2'	-5.41	97.19	102.60
36	n	23	LEU	CA-CB-CG	5.40	127.72	115.30
36	v	23	LEU	CA-CB-CG	5.39	127.70	115.30
1	2	1089	G	P-O3'-C3'	5.34	126.11	119.70
1	2	1168	U	O3'-P-O5'	-5.33	93.86	104.00
1	2	144	G	C1'-C2'-O2'	-5.32	94.63	110.60
1	2	1150	U	P-O3'-C3'	-5.28	113.37	119.70
3	4	90	C	C2-N3-C4	5.25	122.52	119.90
9	B	813	ARG	CG-CD-NE	5.20	122.72	111.80
1	2	1152	U	O4'-C4'-C3'	5.18	110.25	106.10
1	2	66	A	C4'-C3'-O3'	5.17	123.35	113.00
1	2	1163	C	C4'-C3'-O3'	5.15	123.30	113.00
1	2	1148	U	P-O5'-C5'	5.12	129.10	120.90
1	2	145	G	C4'-C3'-O3'	5.12	123.24	113.00
9	B	793	LEU	CA-CB-CG	5.12	127.07	115.30
23	P	962	LEU	CA-CB-CG	5.11	127.04	115.30
9	B	1894	LEU	CA-CB-CG	5.10	127.03	115.30
30	W	34	LEU	CB-CG-CD2	-5.08	102.36	111.00
13	F	401	LEU	CA-CB-CG	5.08	126.99	115.30
1	2	1169	C	O5'-C5'-C4'	-5.06	102.08	111.70
1	2	1147	A	O5'-C5'-C4'	5.04	121.28	111.70
1	2	146	A	C5'-C4'-C3'	-5.03	107.96	116.00
1	2	1161	U	C5'-C4'-O4'	5.02	115.13	109.10
1	2	145	G	P-O3'-C3'	5.02	125.72	119.70

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	1109	C	Sidechain
1	2	141	A	Sidechain
8	A	1190	ASN	Peptide
8	A	1481	GLU	Peptide
9	B	1369	GLY	Peptide
9	B	684	LEU	Peptide
9	B	685	ARG	Peptide
9	B	790	ASP	Peptide
17	J	271	CYS	Peptide
17	J	664	PHE	Peptide
20	M	15	LYS	Peptide
20	M	18	ASN	Peptide
23	P	1013	ASP	Peptide

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Mol	Chain	Res	Type	Group
23	P	1014	LYS	Peptide
27	T	458	SER	Peptide
30	W	16	VAL	Peptide
39	r	50	ASP	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
2	3	75/89 (84%)	74 (99%)	1 (1%)	0	100	100
6	7	62/115 (54%)	62 (100%)	0	0	100	100
7	8	62/109 (57%)	61 (98%)	1 (2%)	0	100	100
8	A	2202/2413 (91%)	2095 (95%)	105 (5%)	2 (0%)	48	83
9	B	1694/2163 (78%)	1631 (96%)	60 (4%)	3 (0%)	44	78
10	C	838/1008 (83%)	785 (94%)	52 (6%)	1 (0%)	48	83
11	D	140/143 (98%)	126 (90%)	14 (10%)	0	100	100
12	E	114/587 (19%)	103 (90%)	9 (8%)	2 (2%)	7	35
13	F	409/494 (83%)	387 (95%)	21 (5%)	1 (0%)	44	78
14	G	358/469 (76%)	335 (94%)	23 (6%)	0	100	100
15	H	425/465 (91%)	398 (94%)	27 (6%)	0	100	100
17	J	788/899 (88%)	722 (92%)	61 (8%)	5 (1%)	22	60
18	K	122/126 (97%)	121 (99%)	1 (1%)	0	100	100
19	L	101/194 (52%)	94 (93%)	7 (7%)	0	100	100
20	M	164/242 (68%)	141 (86%)	23 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	N	77/291 (26%)	76 (99%)	1 (1%)	0	100	100
22	O	829/971 (85%)	789 (95%)	40 (5%)	0	100	100
23	P	1170/1361 (86%)	1059 (90%)	104 (9%)	7 (1%)	22	60
24	Q	214/435 (49%)	202 (94%)	11 (5%)	1 (0%)	25	64
25	R	165/213 (78%)	162 (98%)	3 (2%)	0	100	100
26	S	101/107 (94%)	88 (87%)	13 (13%)	0	100	100
27	T	454/530 (86%)	416 (92%)	38 (8%)	0	100	100
28	U	188/266 (71%)	159 (85%)	28 (15%)	1 (0%)	25	64
29	V	123/280 (44%)	112 (91%)	11 (9%)	0	100	100
30	W	168/238 (71%)	129 (77%)	28 (17%)	11 (6%)	1	12
31	X	26/111 (23%)	26 (100%)	0	0	100	100
32	Y	82/111 (74%)	76 (93%)	5 (6%)	1 (1%)	11	44
33	Z	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	11	44
34	a	88/95 (93%)	81 (92%)	7 (8%)	0	100	100
35	b	66/196 (34%)	61 (92%)	5 (8%)	0	100	100
35	k	66/196 (34%)	62 (94%)	4 (6%)	0	100	100
35	s	66/196 (34%)	62 (94%)	4 (6%)	0	100	100
36	d	81/101 (80%)	79 (98%)	2 (2%)	0	100	100
36	n	80/101 (79%)	77 (96%)	3 (4%)	0	100	100
36	v	80/101 (79%)	77 (96%)	3 (4%)	0	100	100
37	e	73/94 (78%)	71 (97%)	2 (3%)	0	100	100
37	p	73/94 (78%)	72 (99%)	1 (1%)	0	100	100
37	w	73/94 (78%)	72 (99%)	1 (1%)	0	100	100
38	f	70/86 (81%)	67 (96%)	3 (4%)	0	100	100
38	q	71/86 (83%)	68 (96%)	3 (4%)	0	100	100
38	x	71/86 (83%)	69 (97%)	2 (3%)	0	100	100
39	g	69/77 (90%)	63 (91%)	6 (9%)	0	100	100
39	r	73/77 (95%)	66 (90%)	5 (7%)	2 (3%)	4	25
39	y	73/77 (95%)	64 (88%)	6 (8%)	3 (4%)	2	18
40	h	76/146 (52%)	75 (99%)	1 (1%)	0	100	100
40	l	93/146 (64%)	89 (96%)	3 (3%)	1 (1%)	12	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	t	68/146 (47%)	67 (98%)	1 (2%)	0	100	100
41	i	90/110 (82%)	90 (100%)	0	0	100	100
41	m	90/110 (82%)	89 (99%)	1 (1%)	0	100	100
41	u	90/110 (82%)	89 (99%)	1 (1%)	0	100	100
42	j	70/187 (37%)	67 (96%)	3 (4%)	0	100	100
43	o	71/93 (76%)	66 (93%)	5 (7%)	0	100	100
44	z	72/86 (84%)	70 (97%)	2 (3%)	0	100	100
All	All	13125/17406 (75%)	12318 (94%)	765 (6%)	42 (0%)	38	73

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	J	881	VAL
23	P	1299	ILE
24	Q	368	ILE
30	W	34	LEU
30	W	52	LYS
39	y	50	ASP
13	F	368	ALA
23	P	363	VAL
23	P	413	ILE
30	W	17	ASP
30	W	18	HIS
30	W	51	THR
30	W	68	PRO
30	W	121	PRO
30	W	124	LEU
32	Y	71	GLN
40	l	140	LYS
9	B	791	PRO
9	B	1896	LYS
10	C	111	LYS
30	W	29	VAL
39	r	60	GLN
8	A	2321	ILE
9	B	960	ILE
12	E	212	VAL
17	J	157	VAL
17	J	665	PRO
23	P	107	ALA

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Mol	Chain	Res	Type
30	W	12	PRO
33	Z	19	ILE
17	J	493	PRO
28	U	232	GLY
39	r	49	GLU
39	y	30	ARG
39	y	60	GLN
23	P	364	THR
23	P	486	PRO
30	W	159	VAL
17	J	718	ASN
8	A	1621	VAL
12	E	305	VAL
23	P	1031	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	
2	3	71/81 (88%)	71 (100%)	0	100	100
6	7	56/103 (54%)	56 (100%)	0	100	100
7	8	56/99 (57%)	56 (100%)	0	100	100
8	A	1982/2182 (91%)	1982 (100%)	0	100	100
9	B	1525/1955 (78%)	1523 (100%)	2 (0%)	92	95
10	C	761/910 (84%)	761 (100%)	0	100	100
11	D	131/132 (99%)	131 (100%)	0	100	100
12	E	60/534 (11%)	60 (100%)	0	100	100
13	F	354/445 (80%)	354 (100%)	0	100	100
14	G	267/436 (61%)	267 (100%)	0	100	100
15	H	377/410 (92%)	377 (100%)	0	100	100
17	J	708/813 (87%)	708 (100%)	0	100	100
18	K	102/104 (98%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	L	92/179 (51%)	92 (100%)	0	100	100
20	M	154/224 (69%)	154 (100%)	0	100	100
22	O	739/867 (85%)	738 (100%)	1 (0%)	92	95
23	P	1093/1244 (88%)	1093 (100%)	0	100	100
24	Q	192/391 (49%)	192 (100%)	0	100	100
25	R	154/189 (82%)	154 (100%)	0	100	100
26	S	93/97 (96%)	93 (100%)	0	100	100
27	T	429/492 (87%)	424 (99%)	5 (1%)	67	78
28	U	158/236 (67%)	157 (99%)	1 (1%)	84	88
29	V	118/259 (46%)	116 (98%)	2 (2%)	56	72
30	W	161/219 (74%)	151 (94%)	10 (6%)	15	36
32	Y	76/100 (76%)	75 (99%)	1 (1%)	65	77
33	Z	75/77 (97%)	75 (100%)	0	100	100
34	a	85/91 (93%)	85 (100%)	0	100	100
35	b	64/176 (36%)	64 (100%)	0	100	100
35	k	64/176 (36%)	64 (100%)	0	100	100
35	s	64/176 (36%)	64 (100%)	0	100	100
36	d	72/89 (81%)	72 (100%)	0	100	100
36	n	71/89 (80%)	71 (100%)	0	100	100
36	v	71/89 (80%)	71 (100%)	0	100	100
37	e	69/83 (83%)	69 (100%)	0	100	100
37	p	69/83 (83%)	69 (100%)	0	100	100
37	w	69/83 (83%)	69 (100%)	0	100	100
38	f	64/77 (83%)	64 (100%)	0	100	100
38	q	65/77 (84%)	65 (100%)	0	100	100
38	x	65/77 (84%)	65 (100%)	0	100	100
39	g	61/66 (92%)	61 (100%)	0	100	100
39	r	64/66 (97%)	64 (100%)	0	100	100
39	y	64/66 (97%)	64 (100%)	0	100	100
40	h	75/129 (58%)	75 (100%)	0	100	100
40	l	81/129 (63%)	81 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	t	67/129 (52%)	67 (100%)	0	100	100
41	i	85/103 (82%)	85 (100%)	0	100	100
41	m	85/103 (82%)	85 (100%)	0	100	100
41	u	85/103 (82%)	85 (100%)	0	100	100
42	j	64/172 (37%)	64 (100%)	0	100	100
43	o	66/84 (79%)	66 (100%)	0	100	100
44	z	66/75 (88%)	66 (100%)	0	100	100
All	All	11739/15369 (76%)	11717 (100%)	22 (0%)	91	94

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	B	491	PHE
9	B	1008	PHE
22	O	321	CYS
27	T	27	ARG
27	T	35	TYR
27	T	81	ILE
27	T	298	HIS
27	T	317	SER
28	U	246	ILE
29	V	129	HIS
29	V	158	ARG
30	W	4	THR
30	W	8	VAL
30	W	30	ILE
30	W	31	LEU
30	W	34	LEU
30	W	36	LEU
30	W	41	GLU
30	W	50	LEU
30	W	64	LEU
30	W	160	THR
32	Y	37	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (193) such sidechains are listed below:

Mol	Chain	Res	Type
2	3	31	GLN

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Mol	Chain	Res	Type
7	8	28	ASN
8	A	185	GLN
8	A	344	ASN
8	A	404	ASN
8	A	487	ASN
8	A	508	GLN
8	A	559	GLN
8	A	570	GLN
8	A	592	HIS
8	A	658	ASN
8	A	760	ASN
8	A	784	GLN
8	A	796	ASN
8	A	848	ASN
8	A	907	ASN
8	A	952	ASN
8	A	974	ASN
8	A	976	GLN
8	A	997	GLN
8	A	1030	GLN
8	A	1087	ASN
8	A	1128	GLN
8	A	1173	HIS
8	A	1218	GLN
8	A	1471	GLN
8	A	1522	ASN
8	A	1531	HIS
8	A	1532	HIS
8	A	1647	GLN
8	A	1667	GLN
8	A	1677	GLN
8	A	1883	ASN
8	A	1895	HIS
8	A	1947	HIS
8	A	2047	GLN
8	A	2144	GLN
8	A	2306	ASN
8	A	2338	GLN
9	B	516	ASN
9	B	568	GLN
9	B	621	ASN
9	B	676	ASN

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Mol	Chain	Res	Type
9	B	706	GLN
9	B	739	GLN
9	B	768	HIS
9	B	804	HIS
9	B	894	ASN
9	B	904	GLN
9	B	921	ASN
9	B	1103	GLN
9	B	1148	GLN
9	B	1281	GLN
9	B	1349	ASN
9	B	1418	HIS
9	B	1443	HIS
9	B	1611	ASN
9	B	1726	HIS
9	B	1931	GLN
9	B	1968	ASN
9	B	1996	GLN
9	B	2069	GLN
9	B	2139	ASN
10	C	183	GLN
10	C	220	ASN
10	C	251	GLN
10	C	290	HIS
10	C	309	ASN
10	C	423	HIS
10	C	471	HIS
10	C	511	GLN
10	C	554	HIS
10	C	693	ASN
10	C	869	HIS
11	D	101	ASN
11	D	104	ASN
11	D	138	ASN
13	F	113	HIS
13	F	136	GLN
13	F	171	GLN
13	F	244	HIS
13	F	270	HIS
13	F	418	GLN
13	F	443	HIS
14	G	145	HIS

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Mol	Chain	Res	Type
14	G	276	ASN
15	H	38	GLN
15	H	160	GLN
15	H	200	GLN
15	H	203	ASN
15	H	306	HIS
15	H	392	HIS
15	H	394	ASN
15	H	420	ASN
17	J	99	ASN
17	J	140	GLN
17	J	303	ASN
17	J	367	GLN
17	J	379	GLN
17	J	657	ASN
17	J	673	GLN
17	J	733	ASN
17	J	785	ASN
17	J	803	ASN
17	J	884	GLN
18	K	25	GLN
18	K	38	ASN
19	L	104	HIS
20	M	19	ASN
20	M	43	ASN
20	M	112	ASN
22	O	376	HIS
22	O	539	HIS
22	O	695	ASN
22	O	769	ASN
22	O	853	HIS
22	O	882	ASN
22	O	887	ASN
22	O	894	HIS
22	O	908	GLN
23	P	209	GLN
23	P	248	ASN
23	P	375	ASN
23	P	382	GLN
23	P	385	HIS
23	P	436	ASN
23	P	481	GLN

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Mol	Chain	Res	Type
23	P	504	HIS
23	P	546	ASN
23	P	590	HIS
23	P	609	HIS
23	P	738	GLN
23	P	920	GLN
23	P	944	ASN
23	P	945	HIS
23	P	950	GLN
23	P	1023	HIS
23	P	1117	HIS
23	P	1154	HIS
23	P	1203	HIS
23	P	1359	ASN
24	Q	145	GLN
24	Q	204	ASN
24	Q	288	HIS
25	R	31	GLN
25	R	47	GLN
25	R	50	GLN
25	R	170	ASN
27	T	34	HIS
27	T	91	GLN
27	T	167	ASN
27	T	202	GLN
27	T	415	HIS
27	T	440	HIS
30	W	55	HIS
30	W	85	ASN
30	W	99	GLN
30	W	133	GLN
30	W	157	GLN
30	W	158	ASN
32	Y	47	ASN
32	Y	90	ASN
33	Z	7	GLN
33	Z	37	ASN
33	Z	41	ASN
34	a	83	GLN
38	f	25	HIS
38	f	65	HIS
38	f	77	ASN

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Mol	Chain	Res	Type
39	g	53	ASN
39	g	54	ASN
39	g	56	GLN
39	g	60	GLN
41	i	28	HIS
42	j	14	GLN
42	j	16	GLN
35	k	33	GLN
40	l	30	GLN
41	m	52	HIS
36	n	4	ASN
43	o	77	ASN
38	q	76	ASN
38	q	77	ASN
39	r	20	ASN
39	r	54	ASN
35	s	33	GLN
40	t	30	GLN
41	u	51	ASN
41	u	52	HIS
36	v	4	ASN
38	x	77	ASN
39	y	20	ASN
39	y	54	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	147/1175 (12%)	47 (31%)	25 (17%)
16	I	26/95 (27%)	8 (30%)	2 (7%)
3	4	110/160 (68%)	33 (30%)	6 (5%)
4	5	166/214 (77%)	61 (36%)	8 (4%)
5	6	91/112 (81%)	33 (36%)	8 (8%)
All	All	540/1756 (30%)	182 (33%)	49 (9%)

All (182) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	33	U
1	2	41	C
1	2	46	C

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Mol	Chain	Res	Type
1	2	47	U
1	2	66	A
1	2	67	A
1	2	68	U
1	2	83	U
1	2	111	C
1	2	112	A
1	2	113	U
1	2	117	U
1	2	140	G
1	2	141	A
1	2	142	C
1	2	1094	G
1	2	1095	U
1	2	1096	C
1	2	1097	G
1	2	1098	C
1	2	1100	A
1	2	1101	C
1	2	1102	C
1	2	1103	C
1	2	1104	U
1	2	1105	C
1	2	1106	G
1	2	1107	C
1	2	1108	A
1	2	1109	C
1	2	1119	C
1	2	1120	G
1	2	1121	U
1	2	1122	U
1	2	1123	C
1	2	1124	U
1	2	1125	U
1	2	1126	G
1	2	1130	U
1	2	1139	G
1	2	1141	C
1	2	1142	G
1	2	1143	C
1	2	1144	U
1	2	1145	U

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Mol	Chain	Res	Type
1	2	1146	G
1	2	1149	G
3	4	11	A
3	4	18	A
3	4	19	U
3	4	20	A
3	4	25	U
3	4	31	U
3	4	32	G
3	4	35	G
3	4	40	G
3	4	41	U
3	4	45	A
3	4	46	G
3	4	55	U
3	4	56	U
3	4	57	U
3	4	65	G
3	4	66	A
3	4	74	U
3	4	75	U
3	4	76	A
3	4	77	U
3	4	78	A
3	4	79	A
3	4	92	C
3	4	98	G
3	4	134	U
3	4	135	A
3	4	138	U
3	4	139	A
3	4	143	A
3	4	144	A
3	4	145	U
3	4	151	G
4	5	12	C
4	5	13	A
4	5	18	A
4	5	20	U
4	5	27	G
4	5	28	G
4	5	32	G

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Mol	Chain	Res	Type
4	5	34	C
4	5	38	A
4	5	39	U
4	5	41	A
4	5	44	A
4	5	45	A
4	5	46	C
4	5	53	C
4	5	64	C
4	5	69	G
4	5	71	A
4	5	72	C
4	5	75	A
4	5	76	U
4	5	77	A
4	5	78	A
4	5	79	C
4	5	81	A
4	5	82	A
4	5	83	C
4	5	84	A
4	5	93	G
4	5	94	C
4	5	96	U
4	5	97	U
4	5	99	U
4	5	101	C
4	5	103	A
4	5	106	A
4	5	113	G
4	5	115	G
4	5	116	U
4	5	119	U
4	5	121	U
4	5	122	C
4	5	123	U
4	5	125	C
4	5	126	A
4	5	127	U
4	5	128	A
4	5	129	G
4	5	131	A

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Mol	Chain	Res	Type
4	5	132	A
4	5	139	A
4	5	140	A
4	5	141	G
4	5	142	C
4	5	151	A
4	5	160	U
4	5	165	A
4	5	166	U
4	5	167	A
4	5	169	U
4	5	173	U
5	6	2	U
5	6	17	U
5	6	19	C
5	6	25	C
5	6	26	A
5	6	27	U
5	6	28	U
5	6	31	G
5	6	33	C
5	6	37	U
5	6	38	U
5	6	39	G
5	6	41	A
5	6	42	A
5	6	44	A
5	6	45	A
5	6	46	U
5	6	47	A
5	6	48	C
5	6	49	A
5	6	51	A
5	6	56	A
5	6	63	G
5	6	75	A
5	6	76	A
5	6	83	A
5	6	84	C
5	6	85	C
5	6	86	G
5	6	87	U

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Mol	Chain	Res	Type
5	6	88	U
5	6	109	U
5	6	111	U
16	I	58	U
16	I	62	A
16	I	70	A
16	I	71	C
16	I	72	A
16	I	74	A
16	I	78	A
16	I	79	A

All (49) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	32	G
1	2	46	C
1	2	66	A
1	2	67	A
1	2	110	A
1	2	1095	U
1	2	1096	C
1	2	1097	G
1	2	1100	A
1	2	1101	C
1	2	1102	C
1	2	1105	C
1	2	1107	C
1	2	1119	C
1	2	1120	G
1	2	1121	U
1	2	1122	U
1	2	1123	C
1	2	1124	U
1	2	1125	U
1	2	1138	G
1	2	1141	C
1	2	1142	G
1	2	1144	U
1	2	1145	U
3	4	17	A
3	4	19	U

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Mol	Chain	Res	Type
3	4	39	C
3	4	91	U
3	4	134	U
3	4	142	G
4	5	17	C
4	5	40	C
4	5	82	A
4	5	83	C
4	5	114	G
4	5	128	A
4	5	130	A
4	5	150	U
5	6	26	A
5	6	27	U
5	6	38	U
5	6	43	C
5	6	45	A
5	6	55	G
5	6	83	A
5	6	84	C
16	I	77	C
16	I	78	A

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	PSU	2	35	16,1	18,21,22	1.07	1 (5%)	22,30,33	1.73	4 (18%)
1	PSU	2	44	16,1	18,21,22	1.03	1 (5%)	22,30,33	1.65	4 (18%)
1	PSU	2	42	16,1	18,21,22	1.08	1 (5%)	22,30,33	1.73	4 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2	35	16,1	-	0/7/25/26	0/2/2/2
1	PSU	2	44	16,1	-	0/7/25/26	0/2/2/2
1	PSU	2	42	16,1	-	0/7/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	42	PSU	C6-C5	3.46	1.39	1.35
1	2	35	PSU	C6-C5	3.35	1.39	1.35
1	2	44	PSU	C6-C5	3.22	1.39	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	42	PSU	C4-N3-C2	-4.57	119.75	126.34
1	2	35	PSU	C4-N3-C2	-4.49	119.87	126.34
1	2	42	PSU	N1-C2-N3	4.43	120.14	115.13
1	2	35	PSU	N1-C2-N3	4.37	120.08	115.13
1	2	44	PSU	N1-C2-N3	4.28	119.98	115.13
1	2	44	PSU	C4-N3-C2	-4.07	120.47	126.34
1	2	44	PSU	C6-N1-C2	-2.72	119.90	122.68
1	2	44	PSU	O2-C2-N1	-2.44	120.11	122.79
1	2	35	PSU	O2-C2-N1	-2.38	120.17	122.79
1	2	42	PSU	O2-C2-N1	-2.23	120.34	122.79
1	2	35	PSU	C6-N1-C2	-2.22	120.42	122.68
1	2	42	PSU	C6-N1-C2	-2.13	120.50	122.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	GTP	C	1101	-	26,34,34	1.19	2 (7%)	32,54,54	1.66	7 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	GTP	C	1101	-	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	C	1101	GTP	C5-C6	-4.24	1.38	1.47
45	C	1101	GTP	C2-N3	2.11	1.38	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	C	1101	GTP	PB-O3B-PG	-4.88	116.09	132.83
45	C	1101	GTP	PA-O3A-PB	-3.57	120.59	132.83
45	C	1101	GTP	C5-C6-N1	3.39	119.93	113.95
45	C	1101	GTP	C2-N1-C6	-2.98	119.61	125.10
45	C	1101	GTP	C8-N7-C5	2.94	108.60	102.99
45	C	1101	GTP	C3'-C2'-C1'	2.89	105.33	100.98
45	C	1101	GTP	O6-C6-C5	-2.16	120.16	124.37

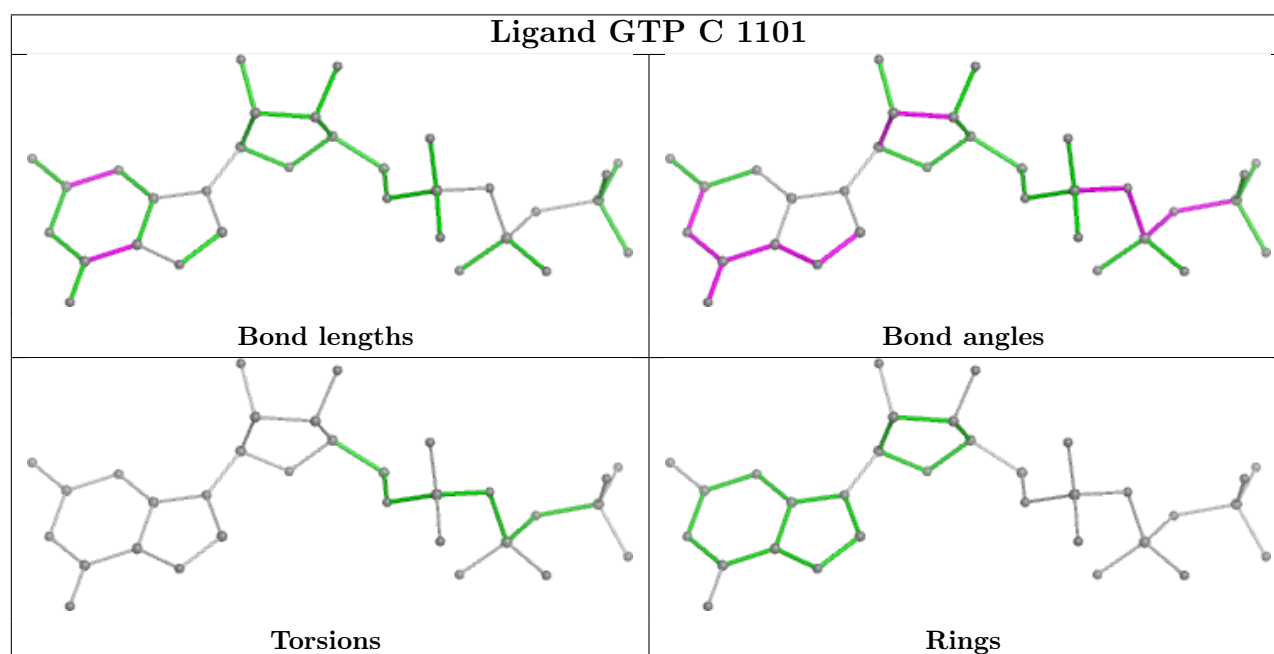
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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
4	5	3
1	2	3
12	E	1
31	X	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	236:SER	C	297:LYS	N	126.30
1	X	19:ALA	C	101:ALA	N	56.70
1	5	72:C	O3'	73:U	P	3.93
1	5	42:A	O3'	43:G	P	3.10
1	2	1149:G	O3'	1150:U	P	1.90
1	2	143:G	O3'	144:G	P	1.83
1	5	105:A	O3'	106:A	P	1.82
1	2	1090:A	O3'	1091:G	P	1.78

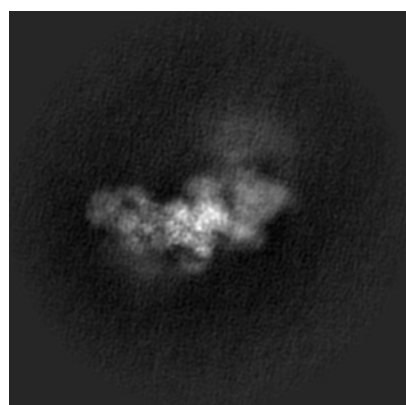
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3683. These allow visual inspection of the internal detail of the map and identification of artifacts.

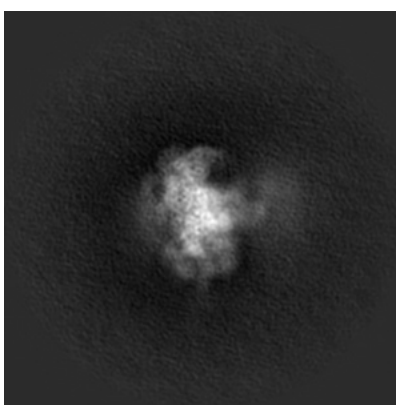
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

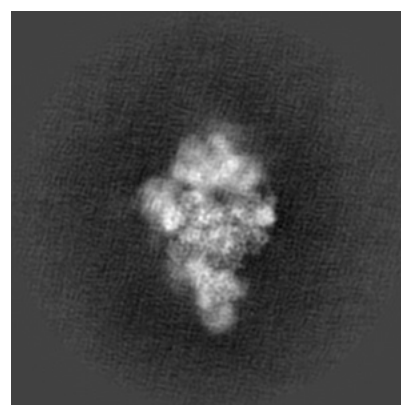
6.1.1 Primary map



X



Y

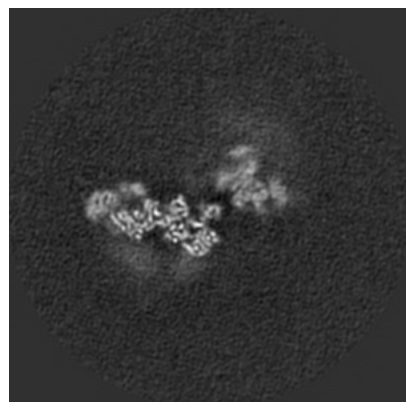


Z

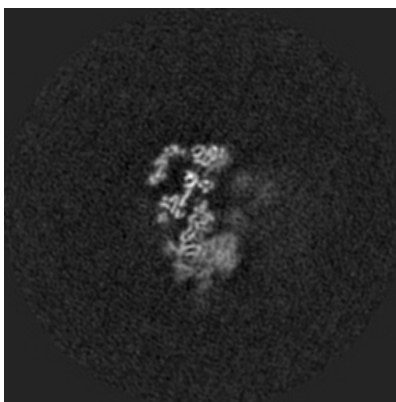
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

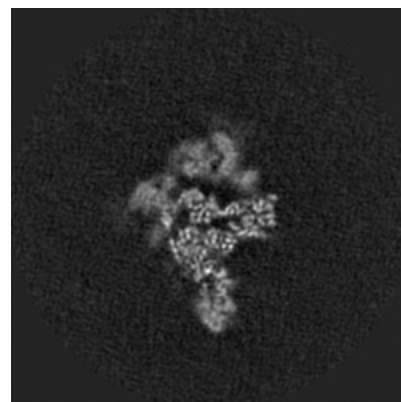
6.2.1 Primary map



X Index: 240



Y Index: 240

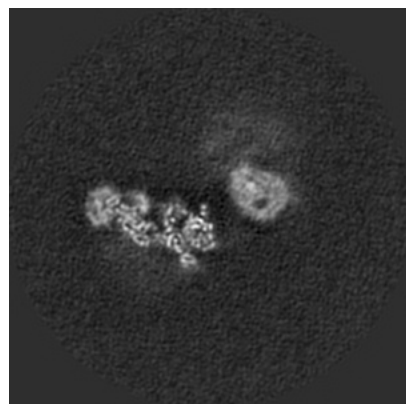


Z Index: 240

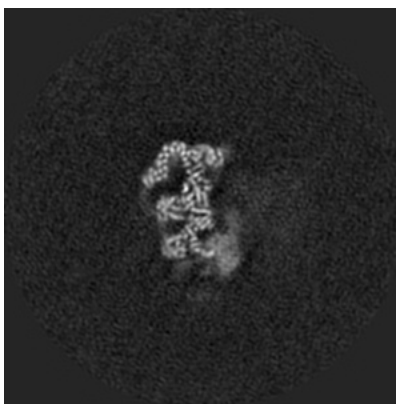
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

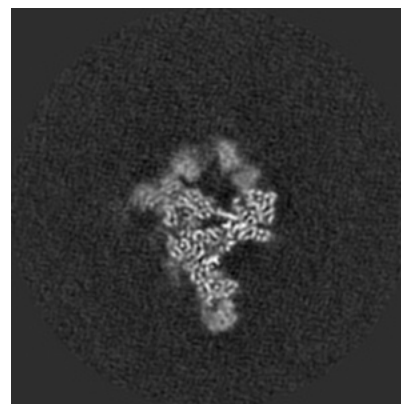
6.3.1 Primary map



X Index: 253



Y Index: 232

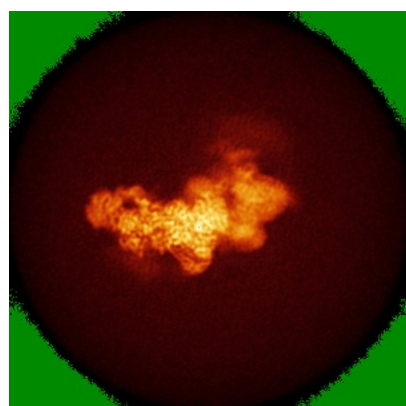


Z Index: 232

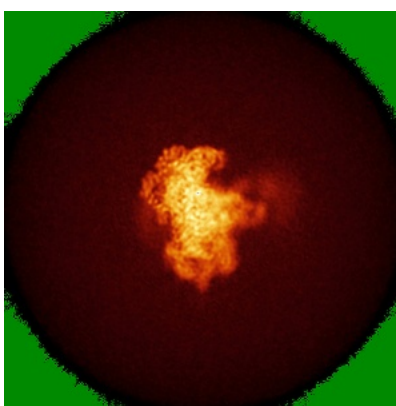
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

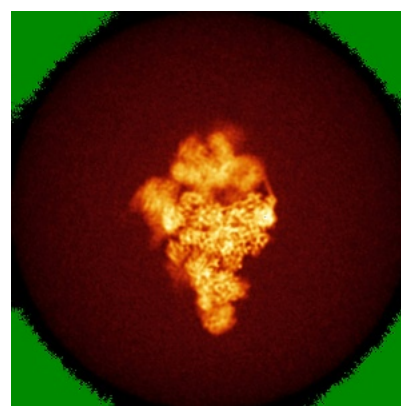
6.4.1 Primary map



X



Y

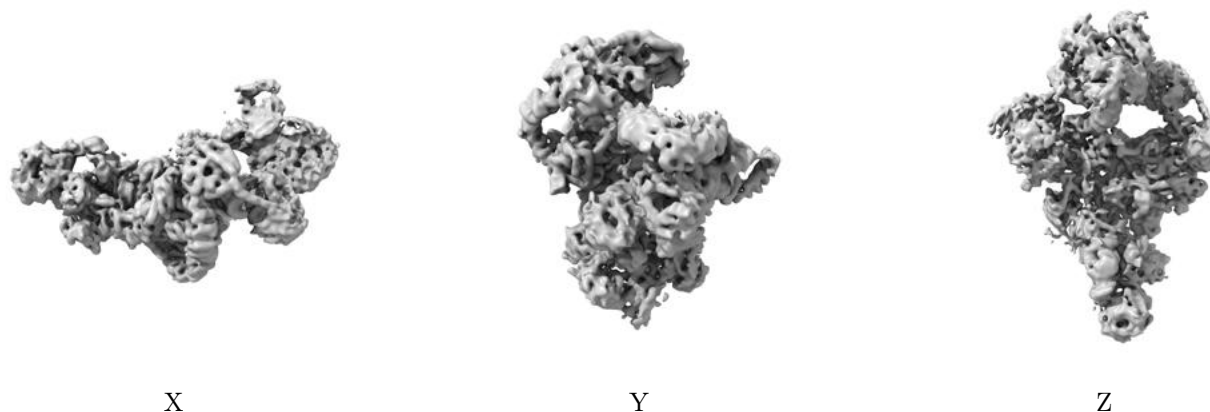


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0258. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

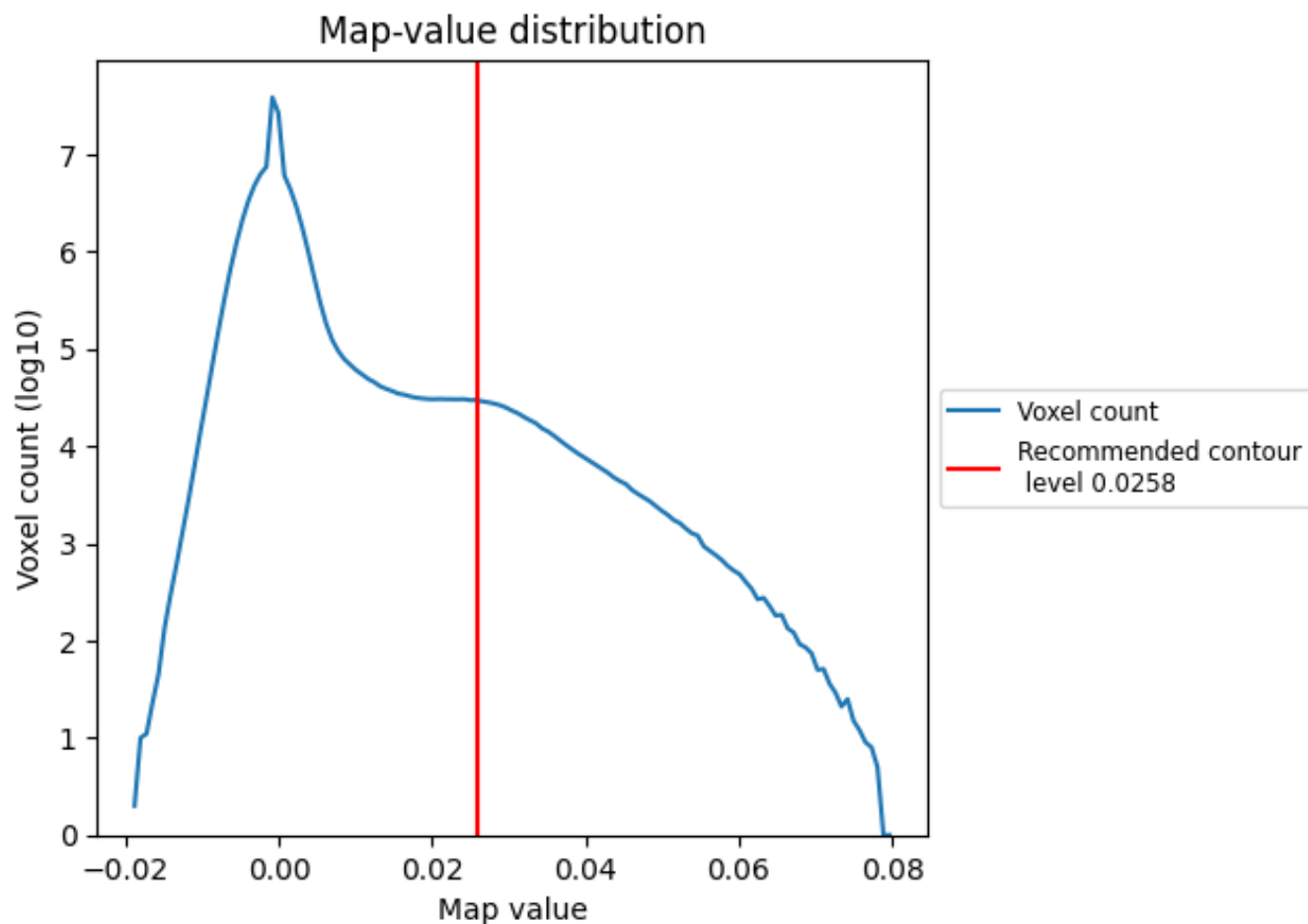
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

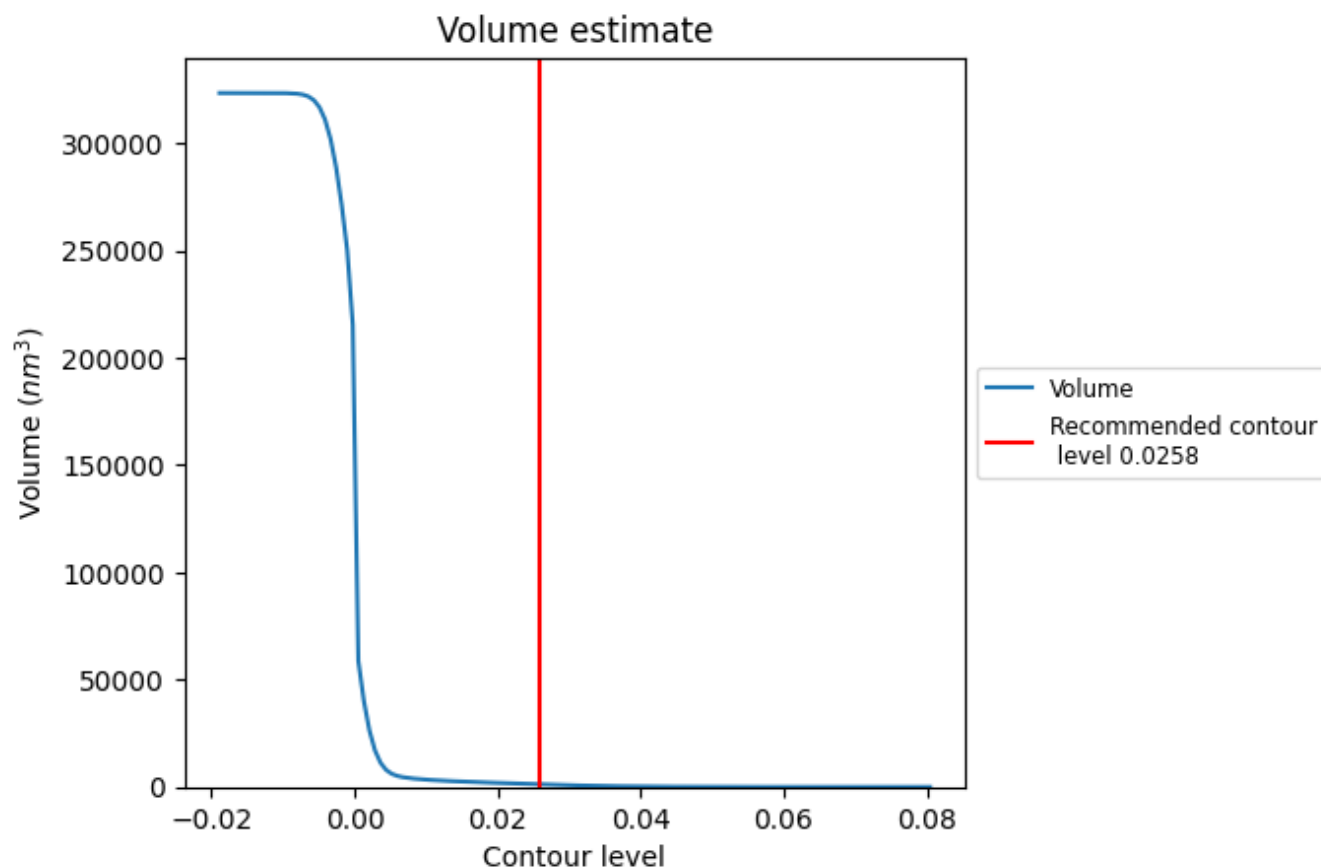
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

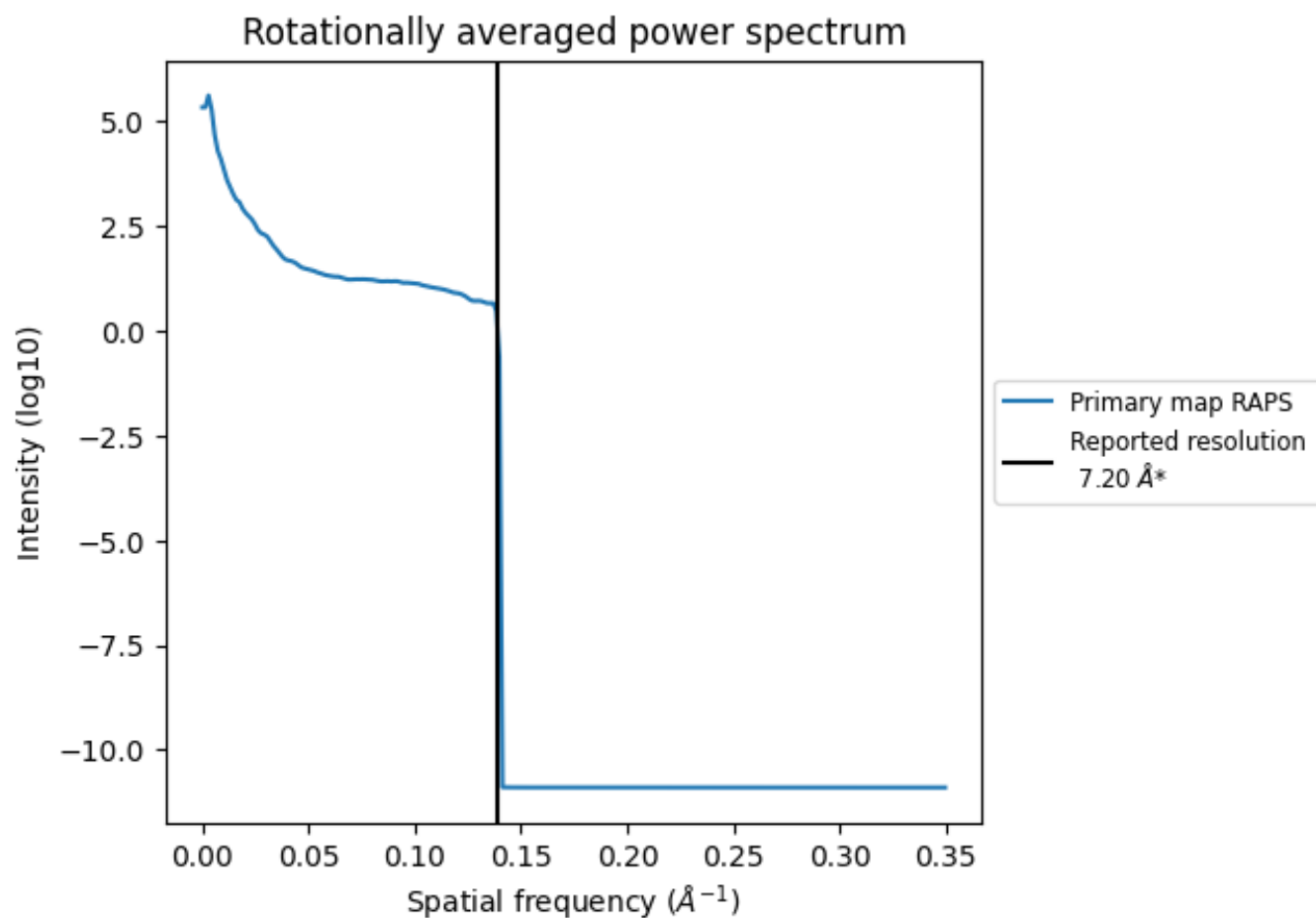
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1240 nm^3 ; this corresponds to an approximate mass of 1120 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.139 Å⁻¹

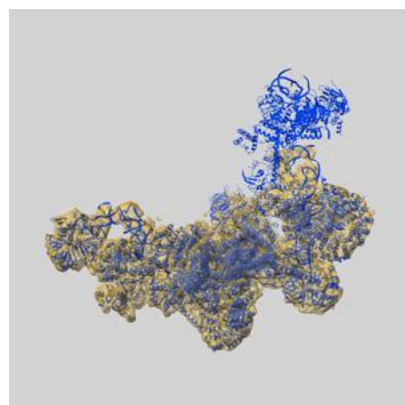
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

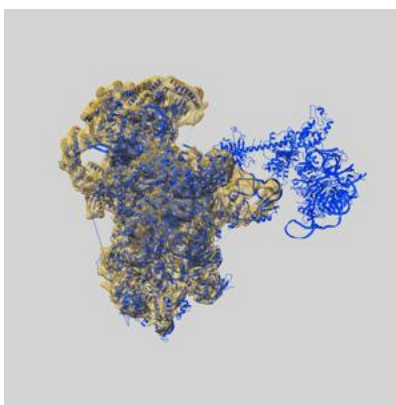
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3683 and PDB model 5NRL. Per-residue inclusion information can be found in section 3 on page 13.

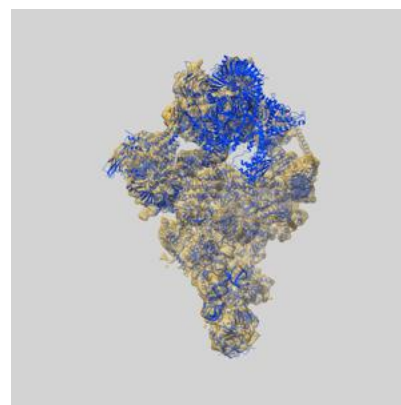
9.1 Map-model overlay [i](#)



X



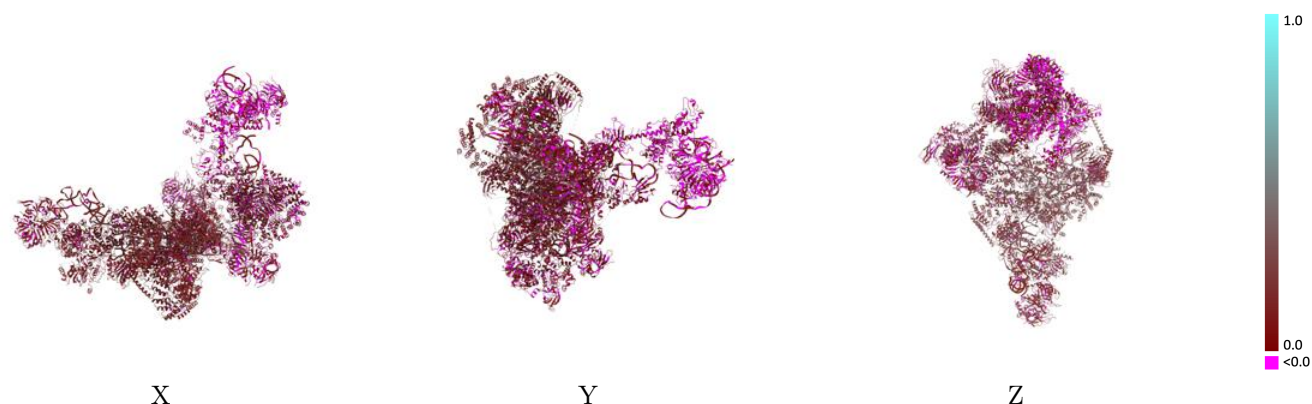
Y



Z

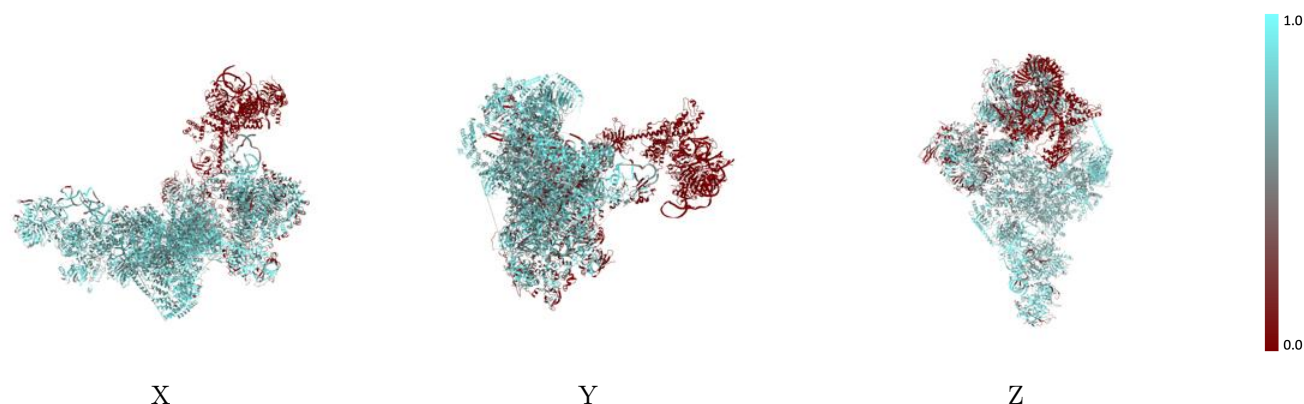
The images above show the 3D surface view of the map at the recommended contour level 0.0258 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



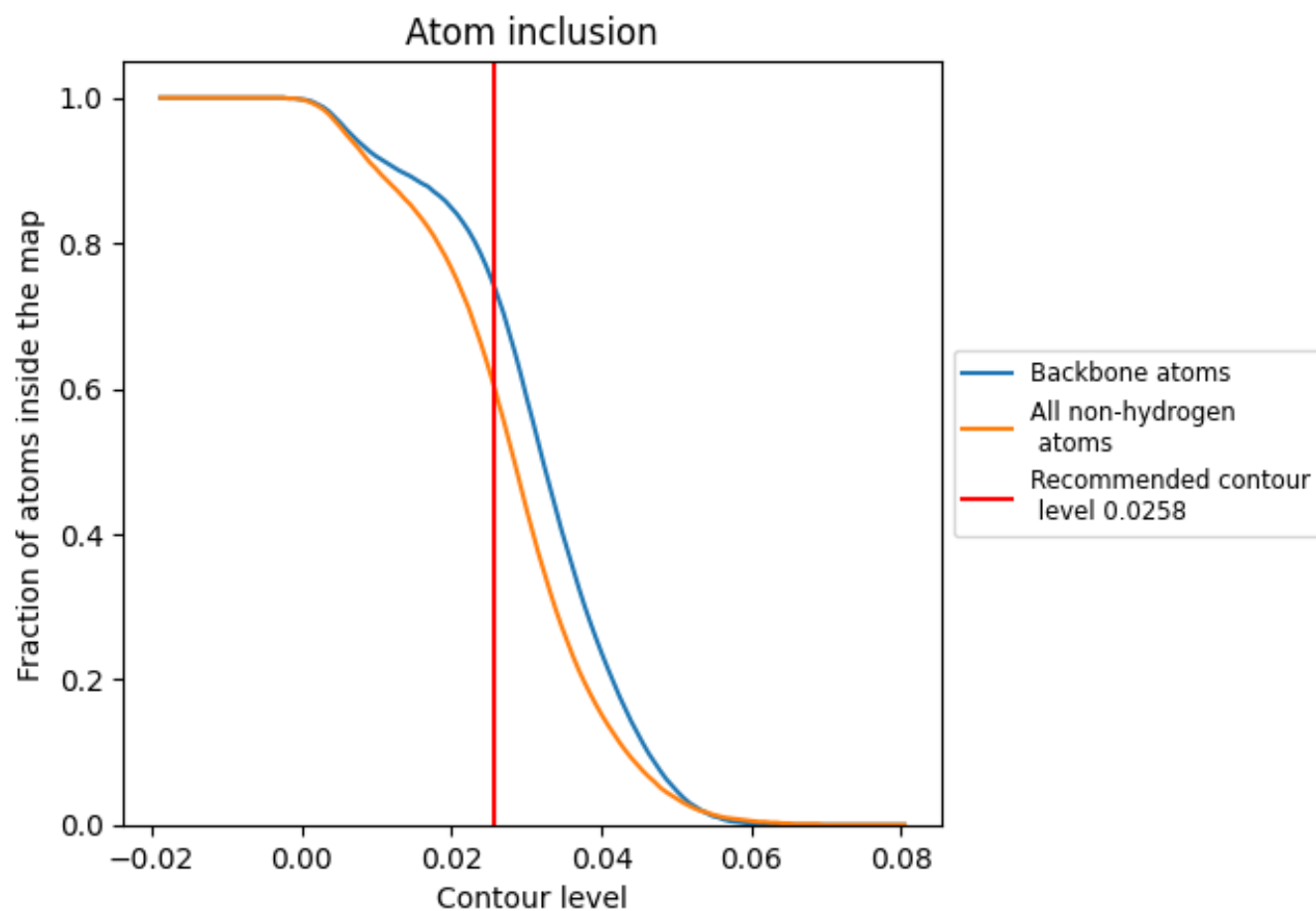
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0258).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

















































The table lists the average atom inclusion at the recommended contour level (0.0258) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5990	 0.1170
2	 0.2760	 0.0470
3	 0.5440	 0.0880
4	 0.9080	 0.1920
5	 0.8050	 0.1610
6	 0.8490	 0.1950
7	 0.5250	 0.0490
8	 0.5600	 0.0820
A	 0.7100	 0.1500
B	 0.6040	 0.1240
C	 0.7390	 0.1500
D	 0.6650	 0.1440
E	 0.5550	 0.1590
F	 0.7210	 0.1670
G	 0.7410	 0.1600
H	 0.7760	 0.1380
I	 0.7900	 0.1290
J	 0.7460	 0.1600
K	 0.6930	 0.1580
L	 0.7210	 0.1510
M	 0.7060	 0.1400
N	 0.7880	 0.2460
O	 0.6550	 0.1020
P	 0.6160	 0.0950
Q	 0.5210	 0.1160
R	 0.4630	 0.0960
S	 0.7310	 0.0980
T	 0.1060	 0.0240
U	 0.2500	 0.0420
V	 0.0000	 0.0440
W	 0.0000	 -0.0000
X	 0.5070	 0.2310
Y	 0.0000	 0.0080
Z	 0.6490	 0.1080
a	 0.6180	 0.0880



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Chain	Atom inclusion	Q-score
b	 0.6820	 0.1200
d	 0.6500	 0.1270
e	 0.6880	 0.1190
f	 0.6930	 0.1170
g	 0.6540	 0.1230
h	 0.7060	 0.1050
i	 0.7160	 0.1360
j	 0.5100	 0.0780
k	 0.4970	 0.0340
l	 0.3620	 0.0730
m	 0.4950	 0.0640
n	 0.3060	 0.0440
o	 0.6960	 0.0800
p	 0.5580	 0.0620
q	 0.5850	 0.0790
r	 0.3290	 0.0510
s	 0.0000	 0.0010
t	 0.0000	 0.0150
u	 0.0000	 -0.0040
v	 0.0000	 -0.0080
w	 0.0000	 0.0040
x	 0.0000	 -0.0260
y	 0.0000	 -0.0010
z	 0.5740	 0.0700