



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 08:54 pm GMT

PDB ID : 6ELZ
EMDB ID : EMD-3891
Title : State E (TAP-Flag-Ytm1 E80A) - Visualizing the assembly pathway of nuclear pre-60S ribosomes
Authors : Kater, L.; Cheng, J.; Barrio-Garcia, C.; Hurt, E.; Beckmann, R.
Deposited on : 2017-09-30
Resolution : 3.30 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:

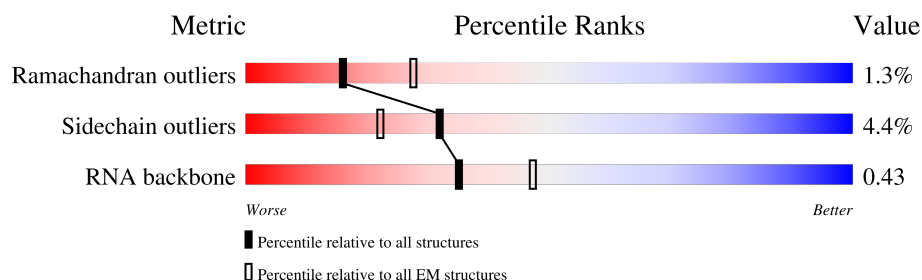
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 3.30 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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	1	3396	
2	2	158	
3	6	232	
4	L	199	
5	N	204	
6	Q	186	
7	R	189	
8	S	172	

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Mol	Chain	Length	Quality of chain
9	T	160	
10	U	121	
11	Z	136	
12	c	105	
13	d	113	
14	e	130	
15	f	107	
16	g	121	
17	i	100	
18	j	88	
19	k	78	
20	O	199	
21	V	137	
22	a	149	
23	P	184	
24	X	142	
25	Y	127	
26	h	120	
27	F	244	
28	B	387	
29	C	362	
30	H	191	
31	A	291	
32	K	376	
33	m	807	

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Mol	Chain	Length	Quality of chain
34	D	505	
35	W	236	
36	l	181	
37	b	647	
38	o	220	
39	n	605	
40	r	261	
41	s	520	
42	t	322	
43	y	245	
44	z	106	
45	p	460	
46	q	618	
47	u	199	
48	v	231	
49	w	841	
50	I	663	
51	J	427	
52	E	176	
53	G	256	
54	M	138	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 134887 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 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2457	Total	C	N	O	P	0	0
			52595	23485	9508	17146	2456		

- Molecule 2 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 3 is a RNA chain called Internal transcribed spacer 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	65	Total	C	N	O	P	0	0
			1370	614	228	463	65		

- Molecule 4 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	L	122	Total	C	N	O	0	0
			998	628	209	161		

- Molecule 5 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	186	Total	C	N	O	S	0	0
			1587	994	333	259	1		

- Molecule 6 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	134	Total	C	N	O	S	0	0
			1035	659	196	179	1		

- Molecule 7 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	R	120	Total	C	N	O	0	0
			964	610	194	160		

- Molecule 8 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	170	Total	C	N	O	S	0	0
			1432	922	265	242	3		

- Molecule 9 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	55	Total	C	N	O	S	0	0
			422	259	85	77	1		

- Molecule 10 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	U	98	Total	C	N	O	0	0
			778	505	127	146		

- Molecule 11 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	Z	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 12 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	c	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 13 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	d	107	Total	C	N	O	S	0	0
			873	553	165	154	1		

- Molecule 14 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	e	125	Total	C	N	O	S	0	0
			1009	641	203	164	1		

- Molecule 15 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	f	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 16 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	g	112	Total	C	N	O	S	0	0
			881	546	179	152	4		

- Molecule 17 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	i	83	Total	C	N	O	S	0	0
			658	408	135	113	2		

- Molecule 18 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	j	73	Total	C	N	O	S	0	0
			580	353	126	96	5		

- Molecule 19 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	k	77	Total	C	N	O	S	0	0
			612	391	115	106			

- Molecule 20 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 21 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	134	Total	C	N	O	S	0	0
			993	623	187	176	7		

- Molecule 22 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	81	Total	C	N	O		0	0
			626	408	108	110			

- Molecule 23 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	183	Total	C	N	O		0	0
			1442	896	287	259			

- Molecule 24 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	141	Total	C	N	O	S	0	0
			1100	705	196	197	2		

- Molecule 25 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	126	Total	C	N	O		0	0
			993	625	192	176			

- Molecule 26 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	h	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 27 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	F	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 28 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B	341	Total	C	N	O	S	0	0
			2702	1715	501	480	6		

- Molecule 29 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	C	359	Total	C	N	O	S	0	0
			2731	1720	518	490	3		

- Molecule 30 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	H	190	Total	C	N	O	S	0	0
			1510	957	273	276	4		

- Molecule 31 is a protein called Ribosome biogenesis protein BRX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	A	198	Total	C	N	O	S	0	0
			1623	1043	284	290	6		

- Molecule 32 is a protein called Proteasome-interacting protein CIC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	K	257	Total	C	N	O	S	0	0
			2073	1337	341	392	3		

- Molecule 33 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	m	645	Total	C	N	O	S	0	0
			5223	3322	907	979	15		

- Molecule 34 is a protein called ATP-dependent RNA helicase HAS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	D	194	Total	C	N	O	S	0	0
			1590	1030	268	287	5		

- Molecule 35 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	W	232	Total	C	N	O	S	0	0
			1870	1184	321	360	5		

- Molecule 36 is a protein called 60S ribosome subunit biogenesis protein NIP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	l	174	Total	C	N	O	S	0	0
			1377	887	242	241	7		

- Molecule 37 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	b	421	Total	C	N	O	S	0	0
			3410	2180	585	627	18		

- Molecule 38 is a protein called Ribosome biogenesis protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	133	Total	C	N	O	S	0	0
			1107	716	198	189	4		

- Molecule 39 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	411	Total	C	N	O	S	0	0
			3369	2179	585	592	13		

- Molecule 40 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	176	Total	C	N	O	S	0	0
			1438	906	279	248	5		

- Molecule 41 is a protein called Nuclear GTP-binding protein NUG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	36	Total	C	N	O	S	0	0
			301	184	69	46	2		

- Molecule 42 is a protein called Ribosome biogenesis protein RLP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	t	290	Total	C	N	O	S	0	0
			2328	1472	431	422	3		

- Molecule 43 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	y	225	Total	C	N	O	S	0	0
			1701	1056	295	343	7		

- Molecule 44 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	z	55	Total	C	N	O	0	0
			444	273	88	83		

- Molecule 45 is a protein called Ribosome biogenesis protein YTM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	p	298	Total	C	N	O	S	0	0
			2321	1448	410	457	6		

- Molecule 46 is a protein called 25S rRNA (cytosine(2870)-C(5))-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	q	317	Total	C	N	O	S	0	0
			2485	1591	429	455	10		

- Molecule 47 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	u	116	Total	C	N	O	S	0	0
			976	612	200	155	9		

- Molecule 48 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	v	130	Total	C	N	O	S	0	0
			1087	678	211	195	3		

- Molecule 49 is a protein called 27S pre-rRNA (guanosine(2922)-2'-O)-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	w	436	Total	C	N	O	S	0	0
			3511	2235	628	630	18		

- Molecule 50 is a protein called Nucleolar complex-associated protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	I	433	Total	C	N	O	S	0	1
			3470	2217	591	645	17		

- Molecule 51 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	J	145	Total	C	N	O	S	0	0
			1215	759	225	228	3		

- Molecule 52 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	E	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 53 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	G	184	Total	C	N	O	S	0	0
			1438	930	249	257	2		

- Molecule 54 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	M	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

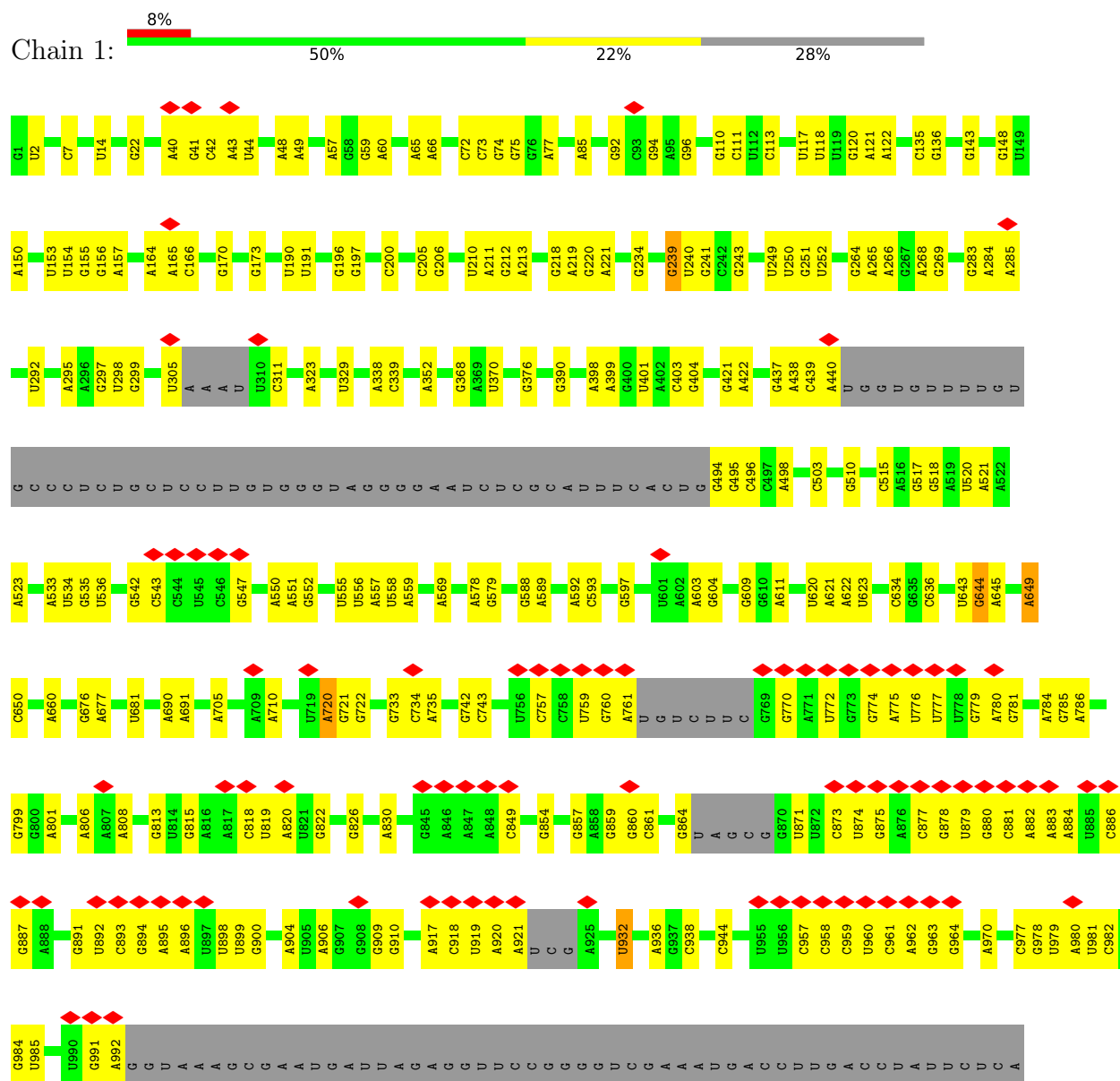
- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

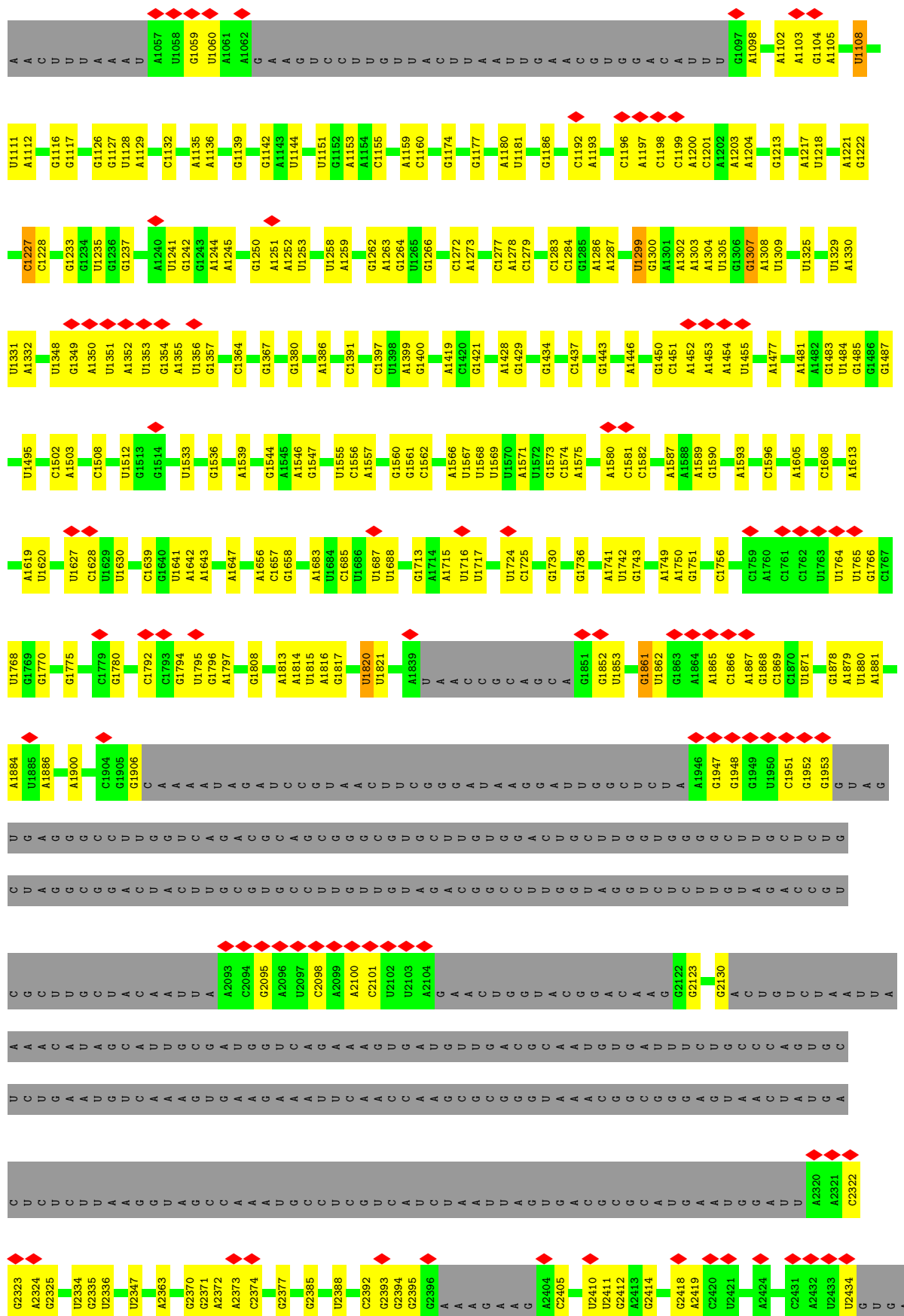
Mol	Chain	Residues	Atoms		AltConf
55	j	1	Total	Zn	0
			1	1	

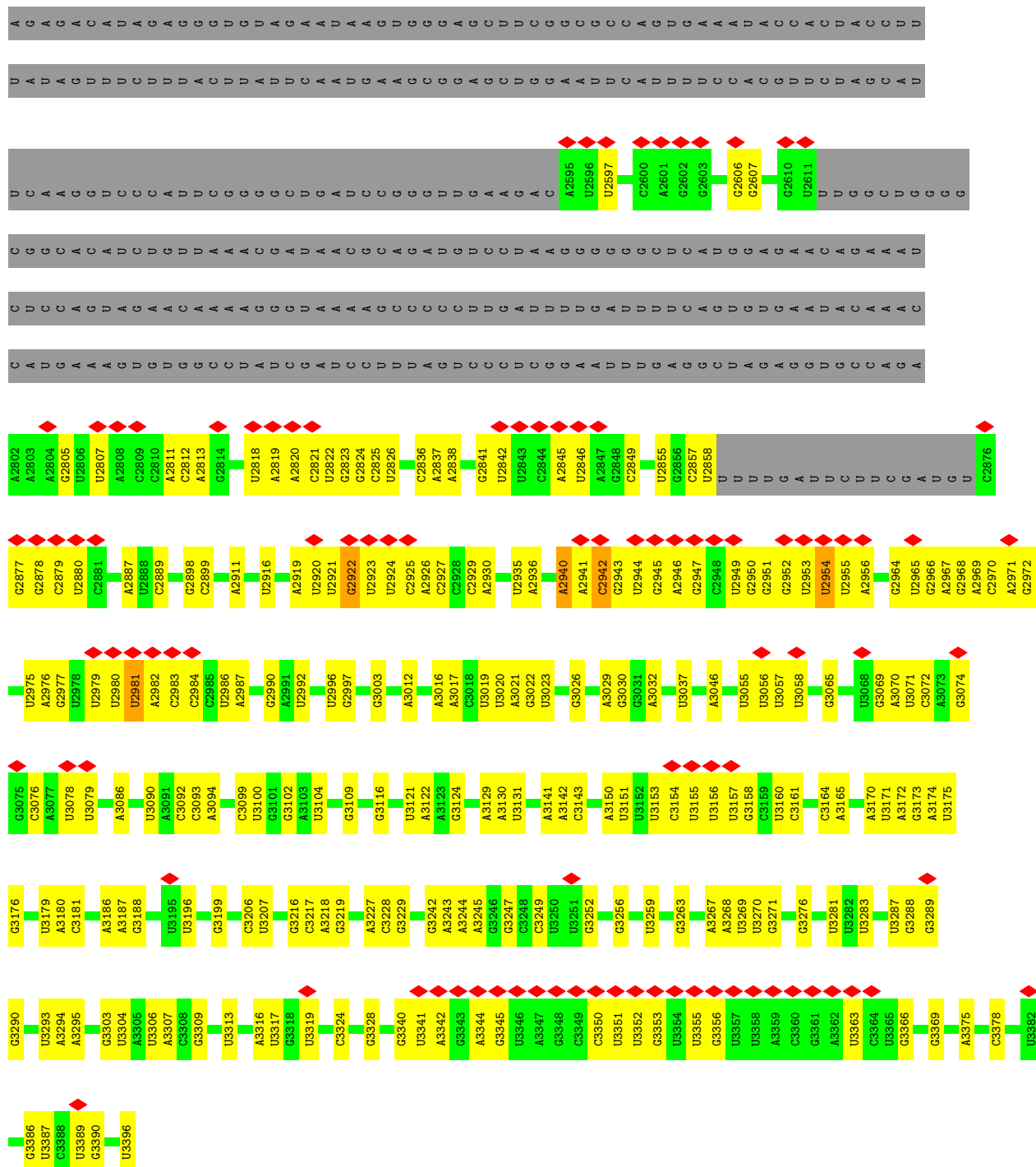
3 Residue-property plots

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: 25S ribosomal RNA

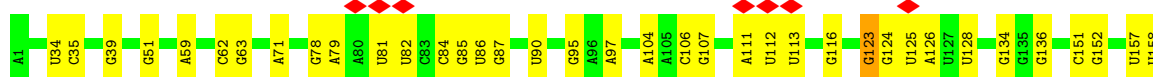




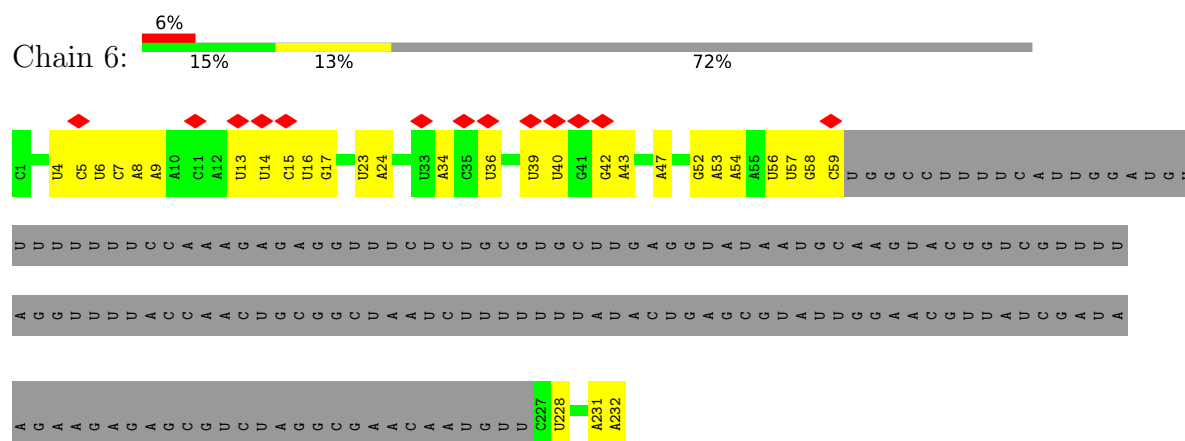


- Molecule 2: 5.8S ribosomal RNA

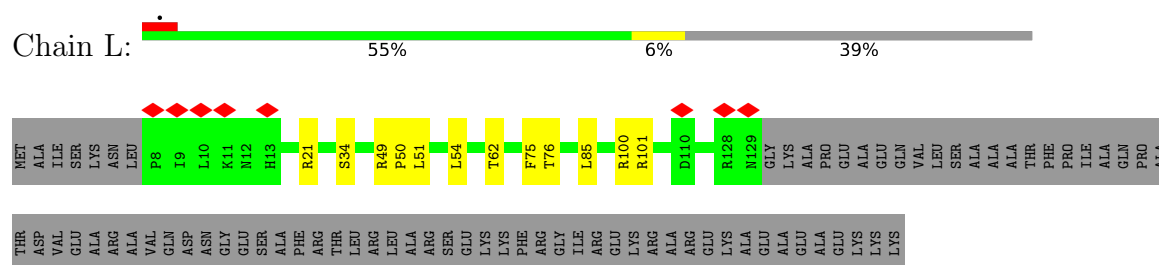
Chain 2: 77% 23%



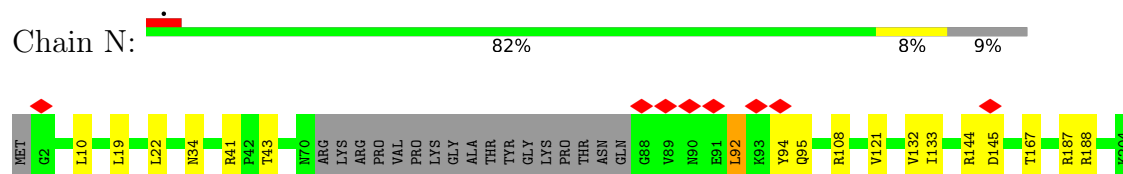
- Molecule 3: Internal transcribed spacer 2



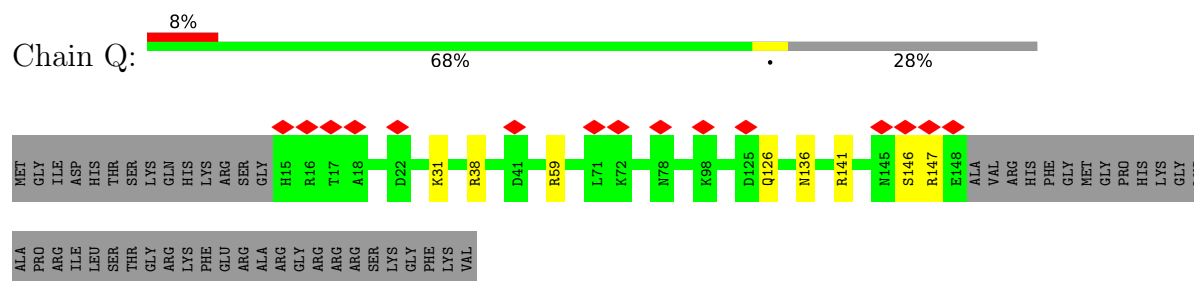
- Molecule 4: 60S ribosomal protein L13-A



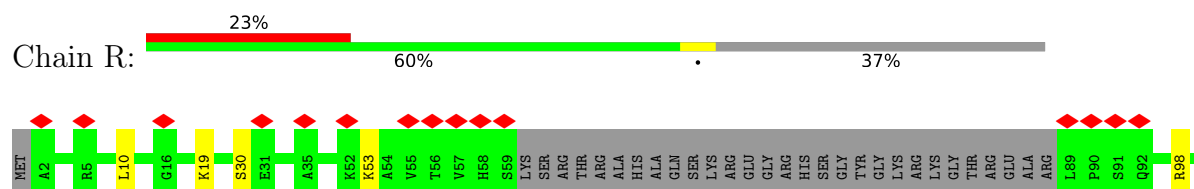
- Molecule 5: 60S ribosomal protein L15-A

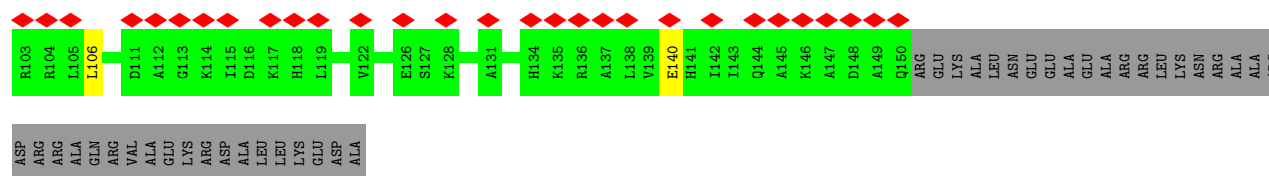


- Molecule 6: 60S ribosomal protein L18-A

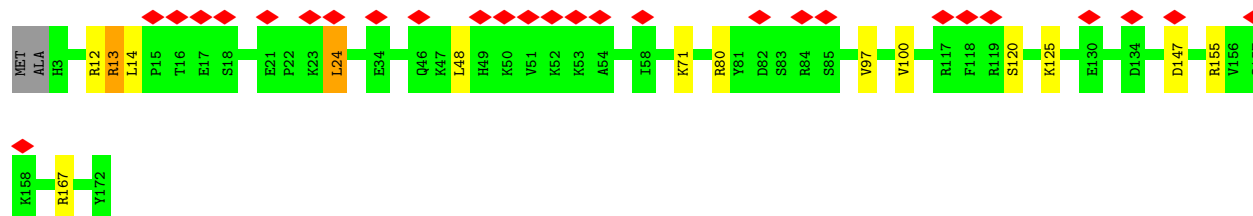
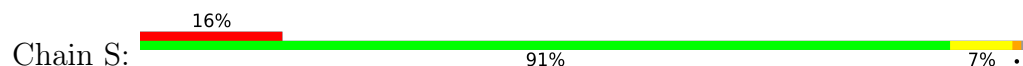


- Molecule 7: 60S ribosomal protein L19-A

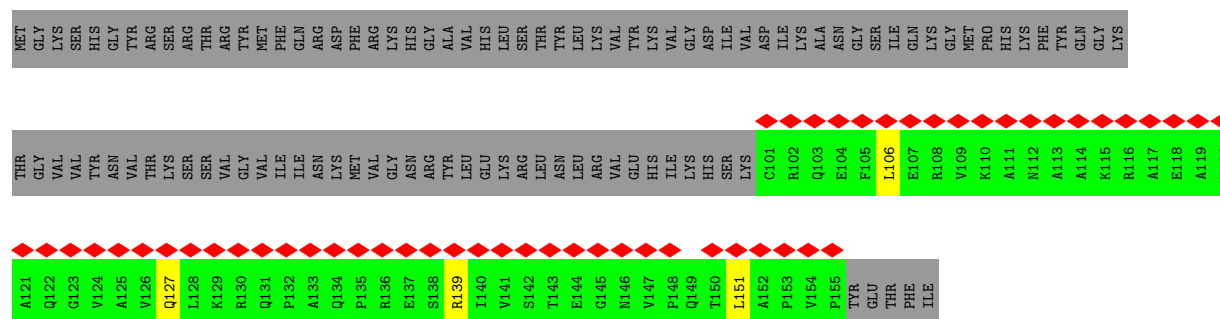




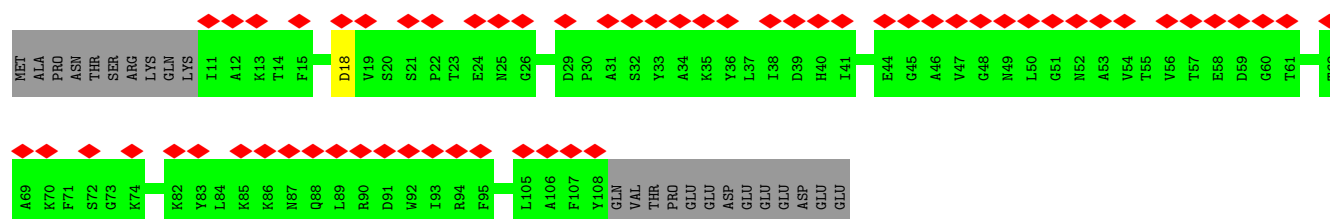
• Molecule 8: 60S ribosomal protein L20-A



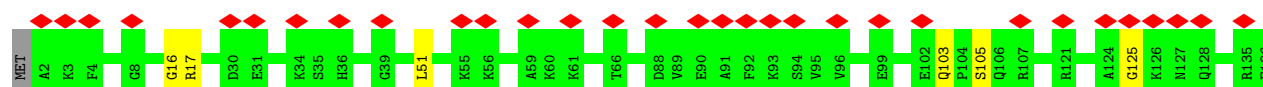
• Molecule 9: 60S ribosomal protein L21-A



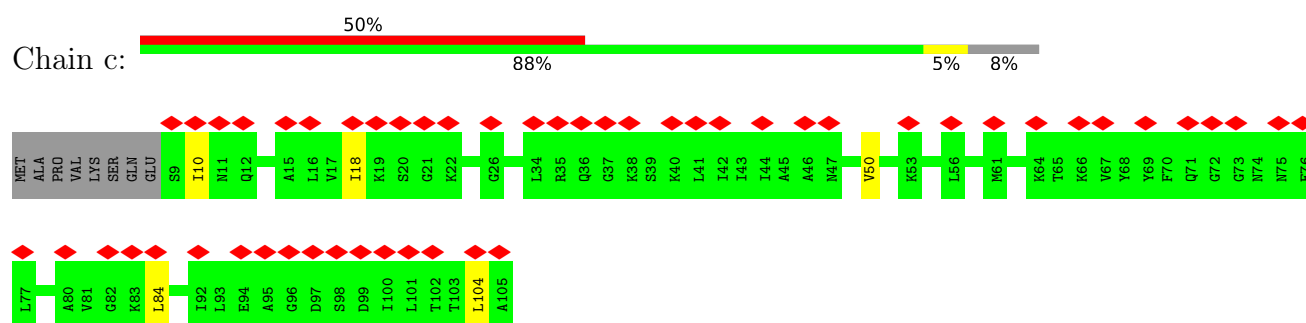
• Molecule 10: 60S ribosomal protein L22-A



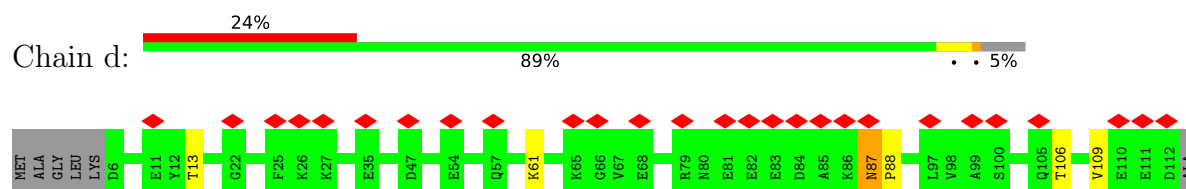
• Molecule 11: 60S ribosomal protein L27-A



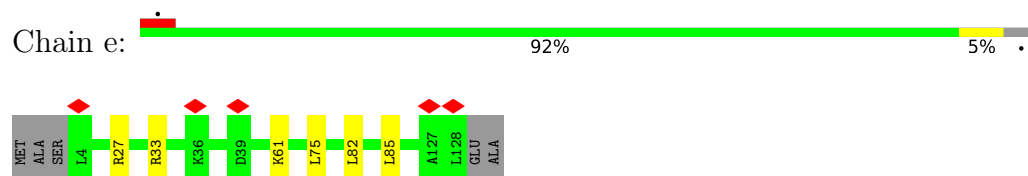
• Molecule 12: 60S ribosomal protein L30



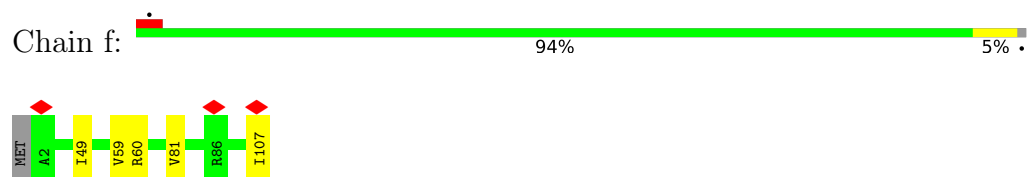
- Molecule 13: 60S ribosomal protein L31-A



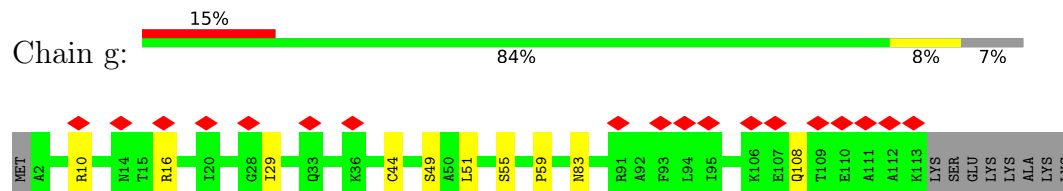
- Molecule 14: 60S ribosomal protein L32



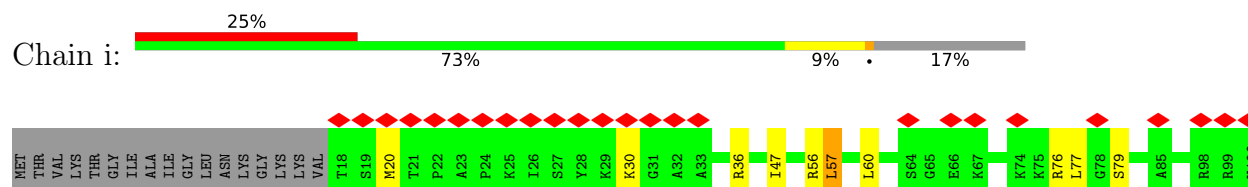
- Molecule 15: 60S ribosomal protein L33-A



- Molecule 16: 60S ribosomal protein L34-A

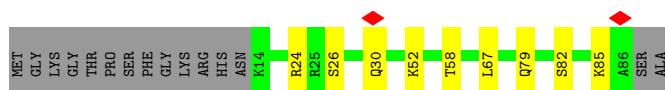


- Molecule 17: 60S ribosomal protein L36-A

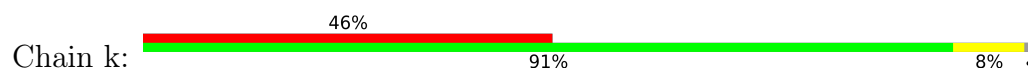


- Molecule 18: 60S ribosomal protein L37-A

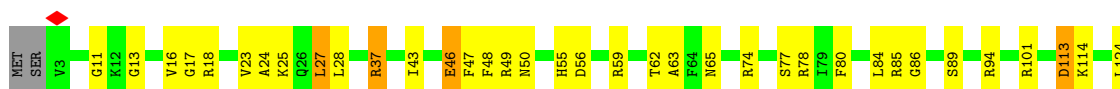




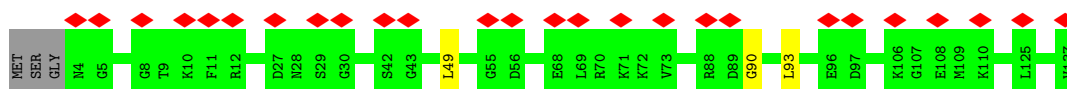
- Molecule 19: 60S ribosomal protein L38



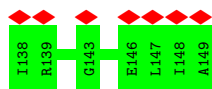
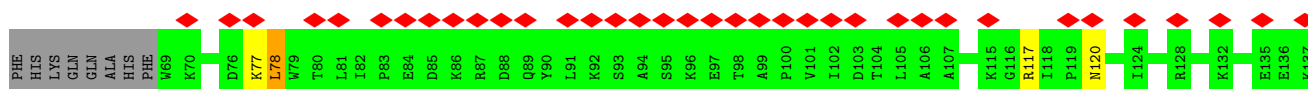
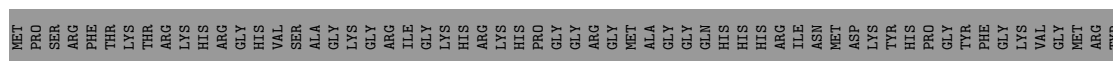
- Molecule 20: 60S ribosomal protein L16-A



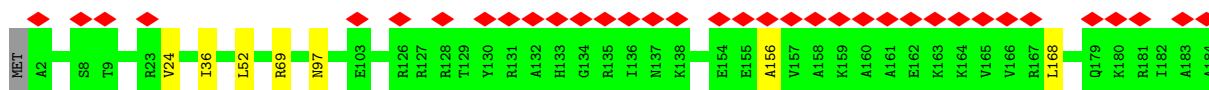
- Molecule 21: 60S ribosomal protein L23-A



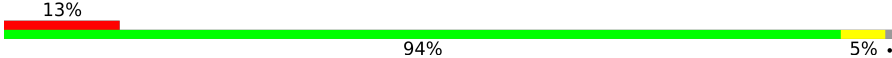
- Molecule 22: 60S ribosomal protein L28

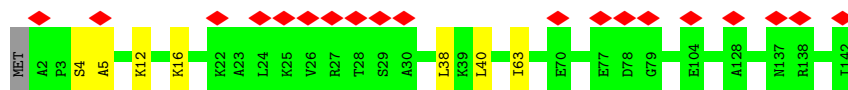


- Molecule 23: 60S ribosomal protein L17-A



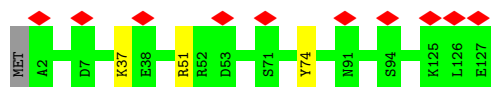
- Molecule 24: 60S ribosomal protein L25

Chain X: 



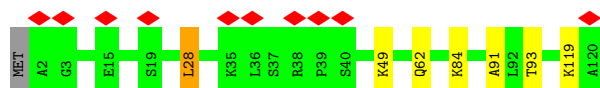
- Molecule 25: 60S ribosomal protein L26-A

Chain Y: 




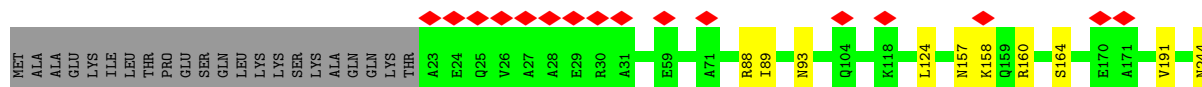
- Molecule 26: 60S ribosomal protein L35-A

Chain h: 




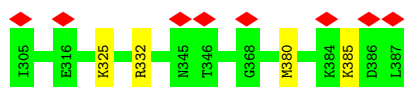
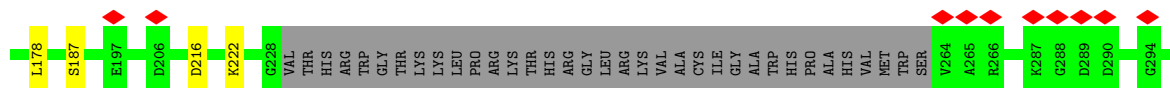
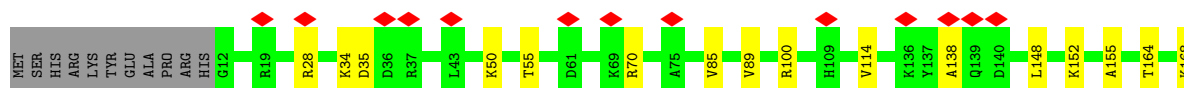
- Molecule 27: 60S ribosomal protein L7-A

Chain F: 

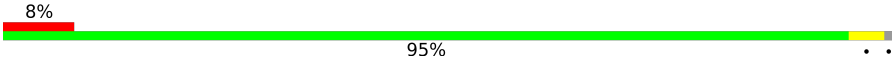


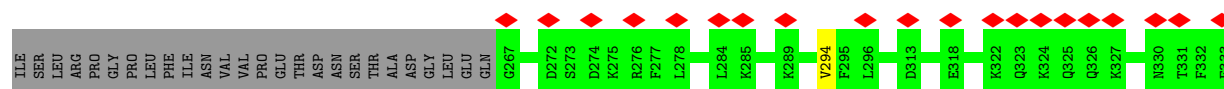
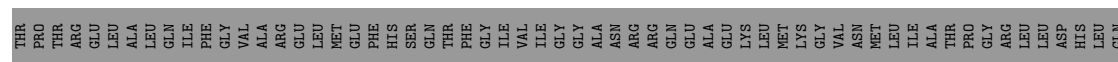
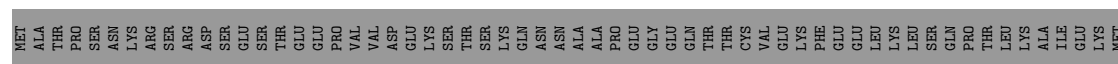
- Molecule 28: 60S ribosomal protein L3

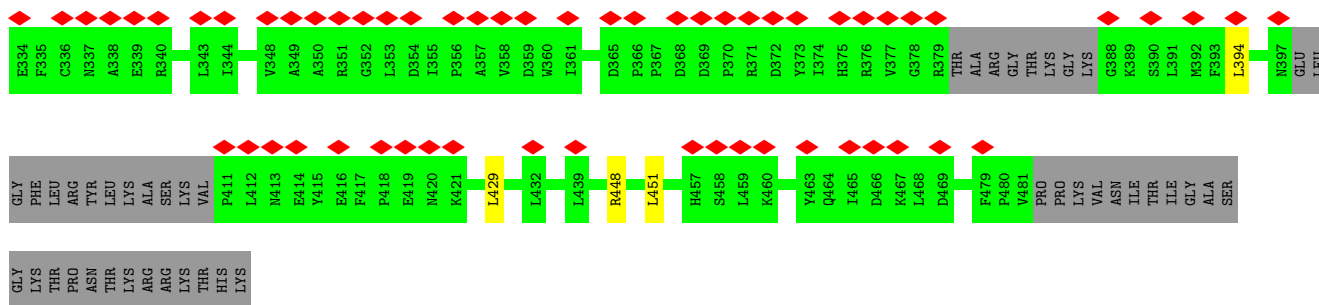
Chain B: 



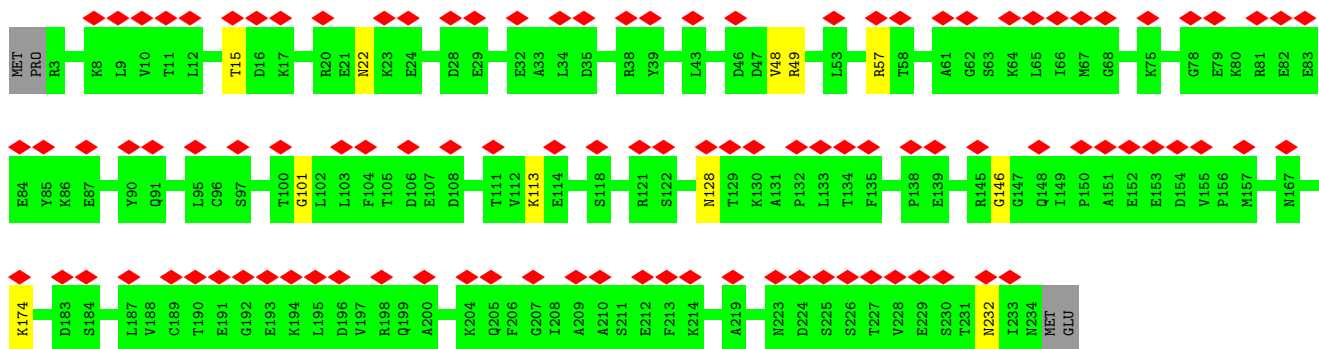
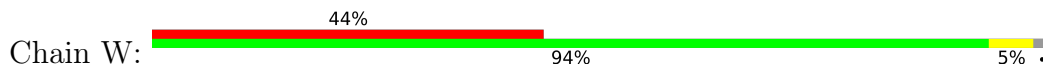
- Molecule 29: 60S ribosomal protein L4-A

Chain C: 

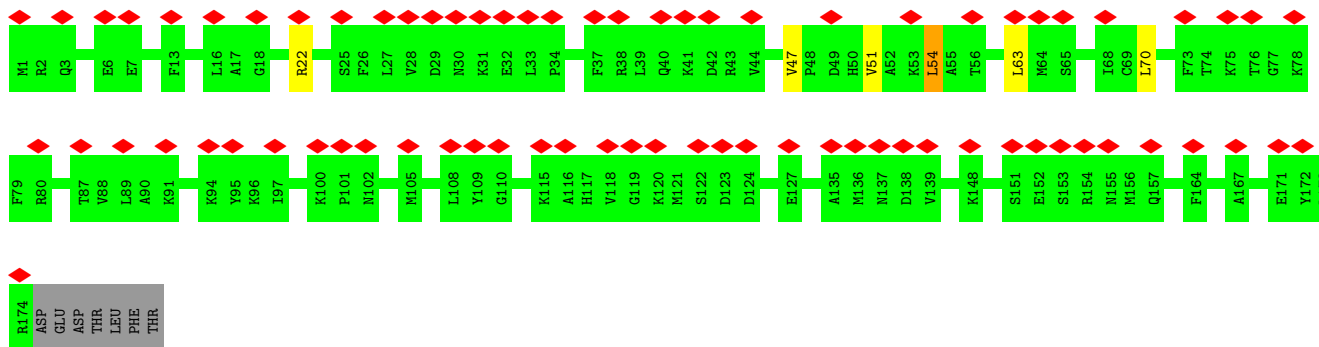
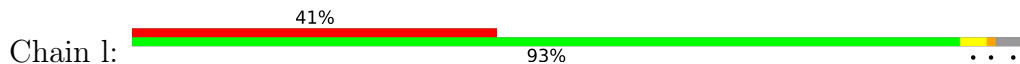




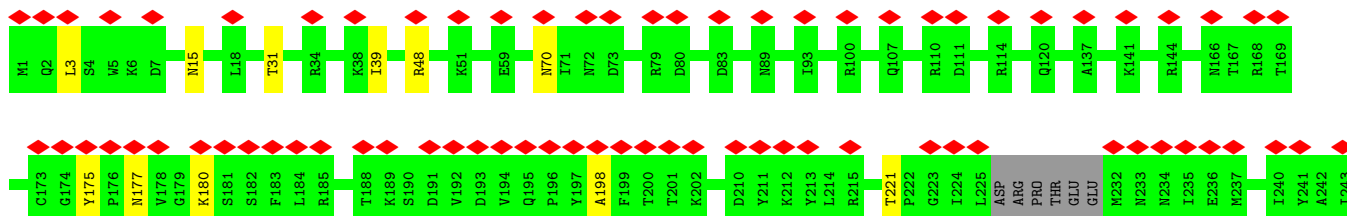
• Molecule 35: Ribosome assembly factor MRT4

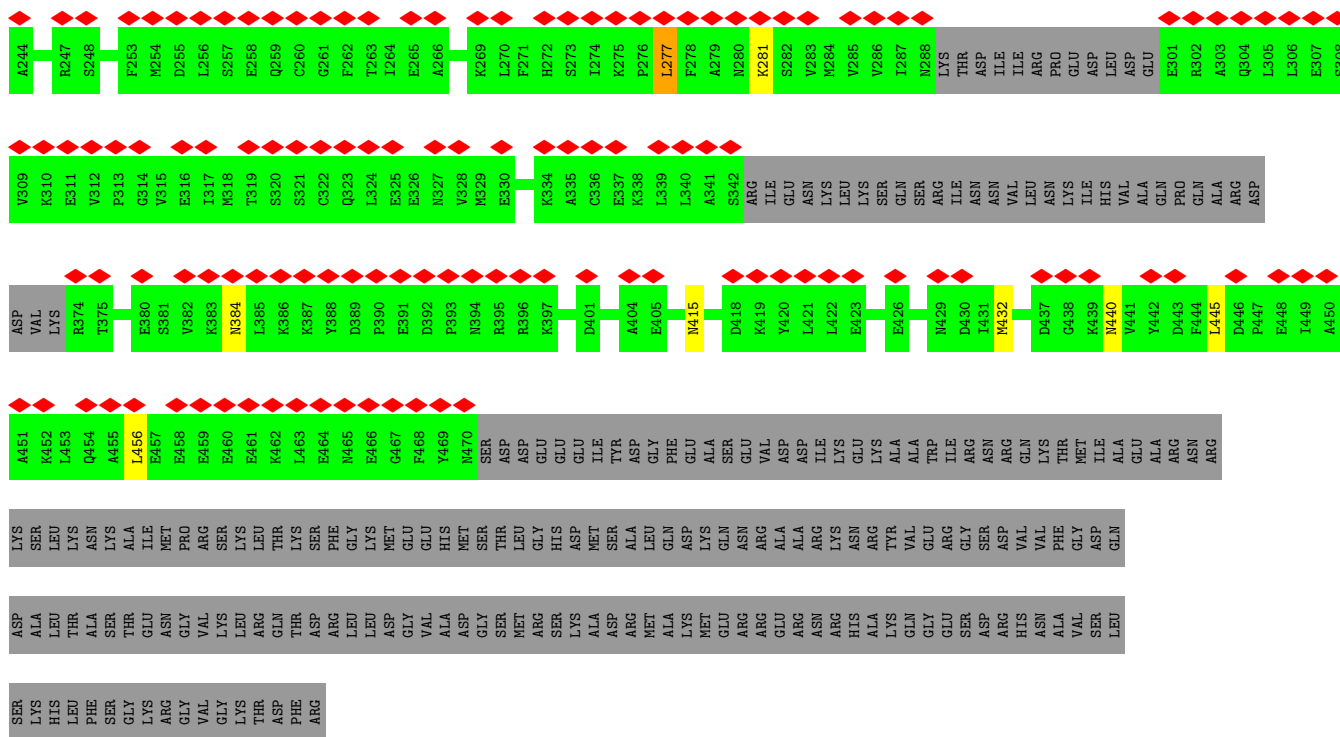


• Molecule 36: 60S ribosome subunit biogenesis protein NIP7

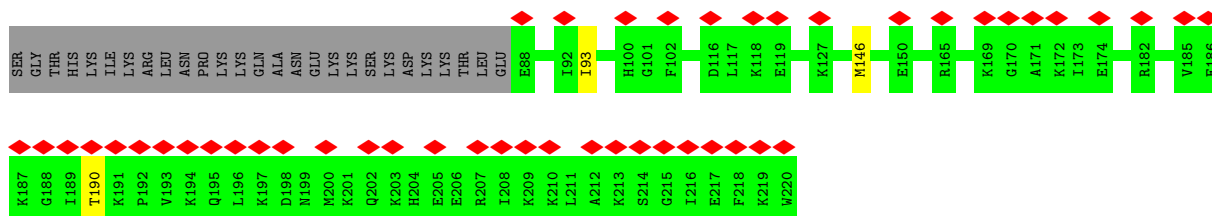
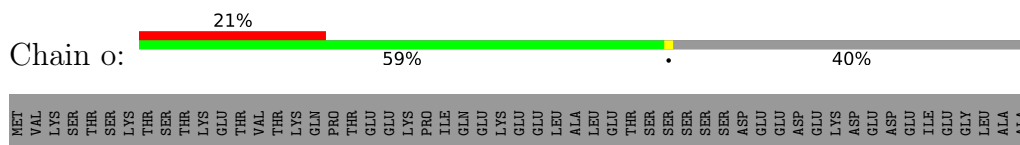


• Molecule 37: Nucleolar GTP-binding protein 1

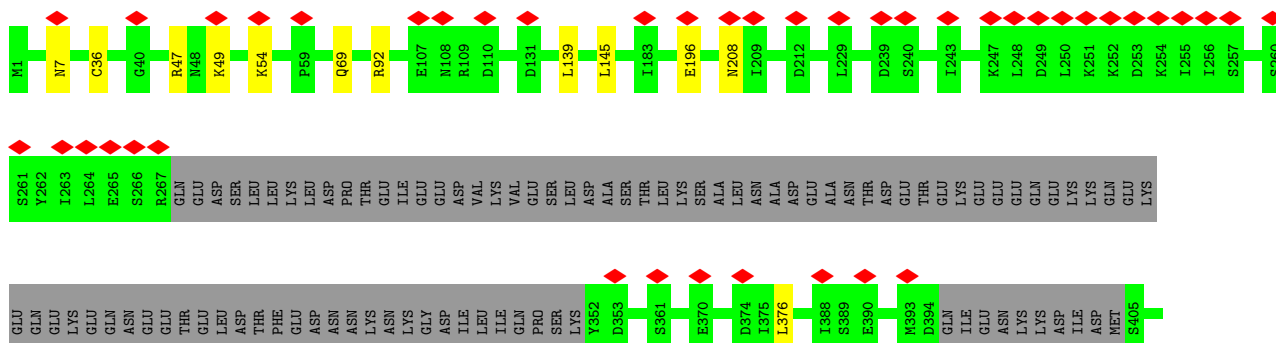


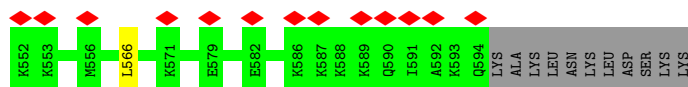
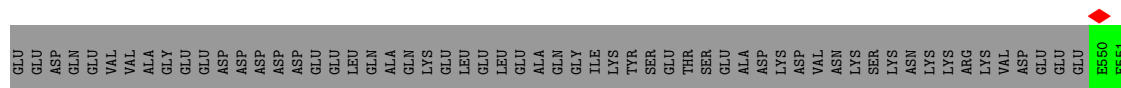
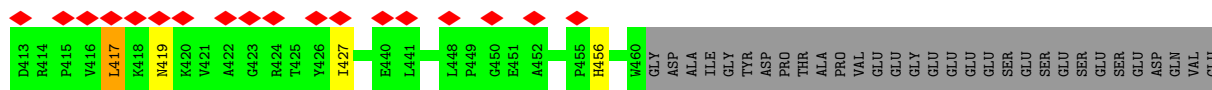


- Molecule 38: Ribosome biogenesis protein 15

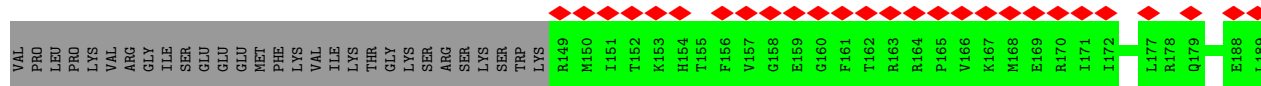
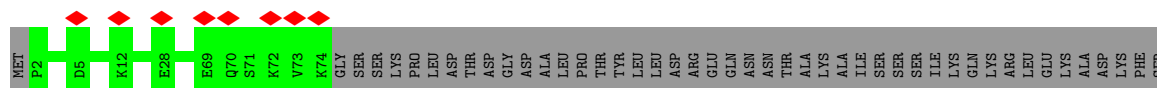


- Molecule 39: Pescadillo homolog

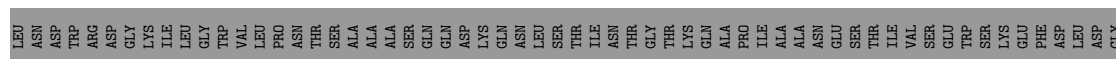
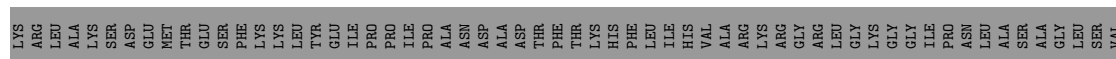
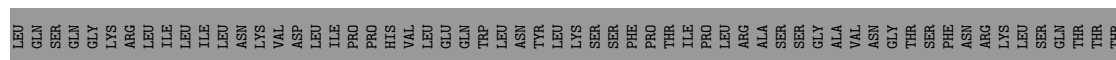
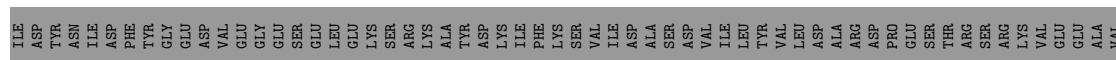
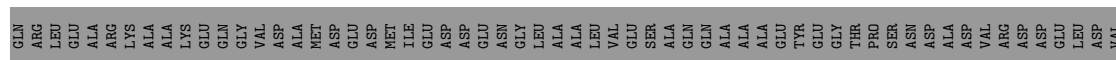
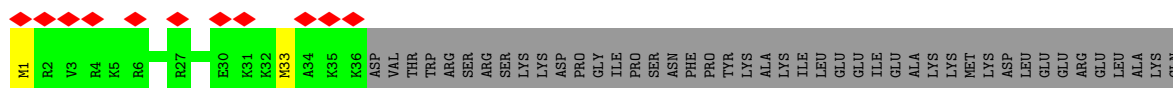


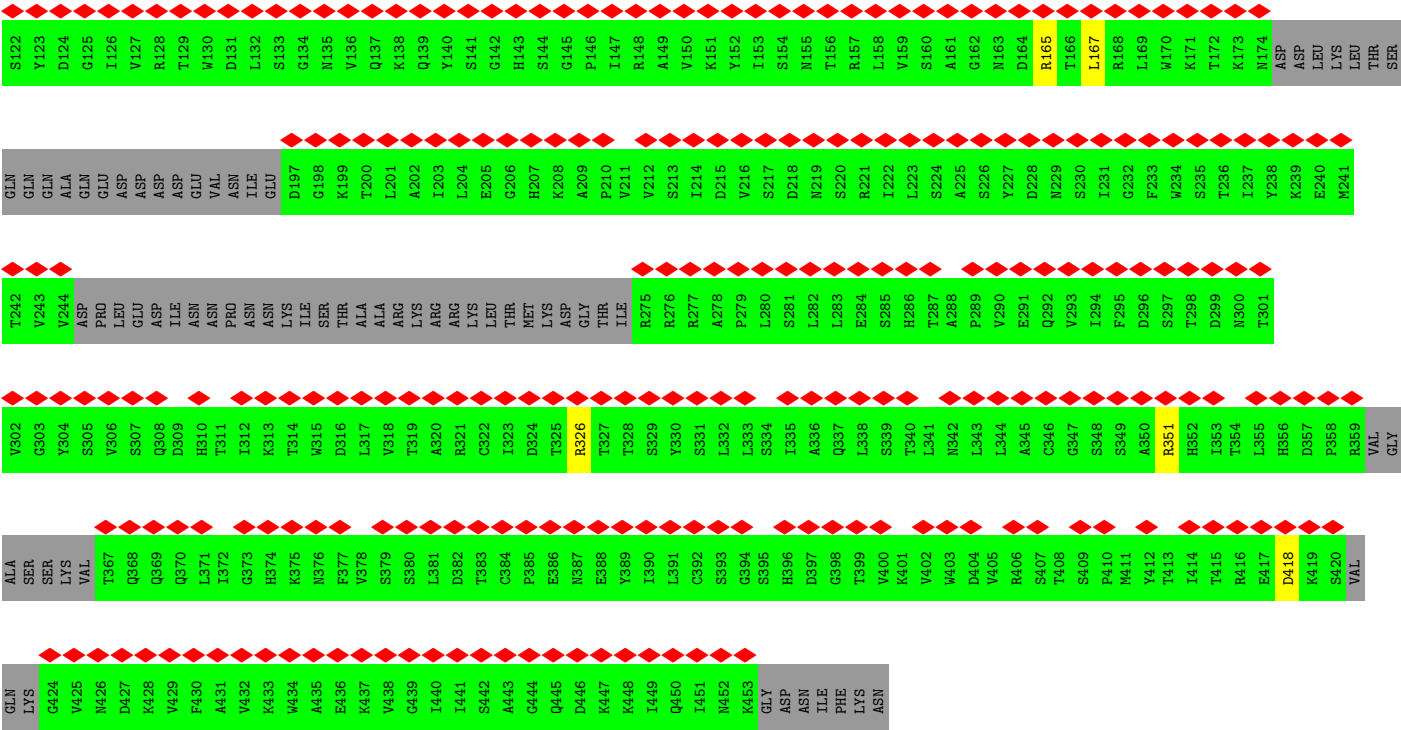


• Molecule 40: Ribosome biogenesis protein NSA2

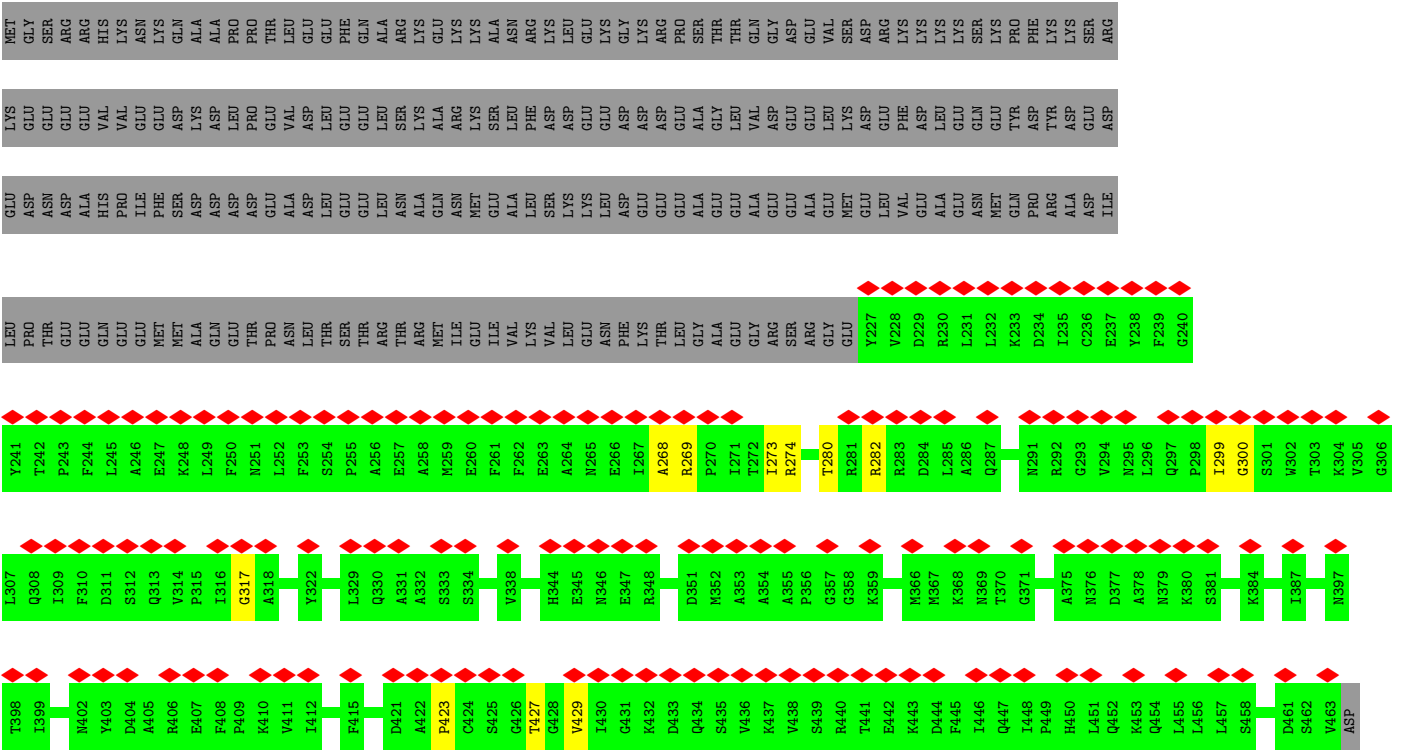


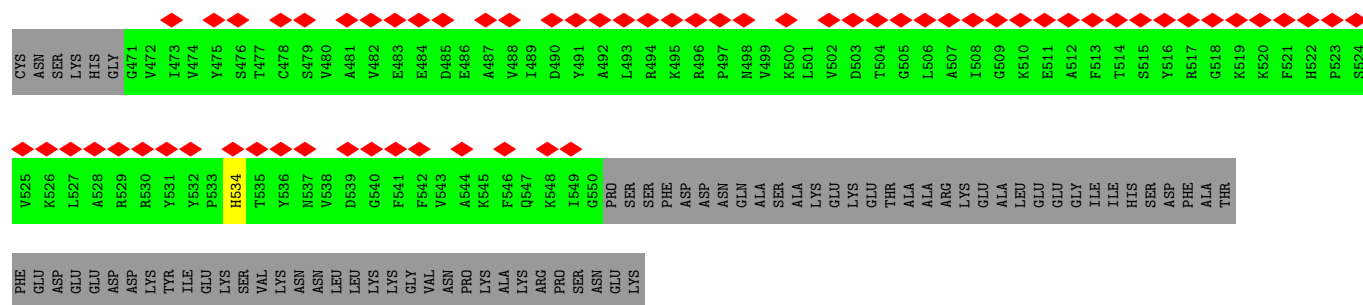
• Molecule 41: Nuclear GTP-binding protein NUG1





● Molecule 46: 25S rRNA (cytosine(2870)-C(5))-methyltransferase





• Molecule 47: Ribosome biogenesis protein RLP24



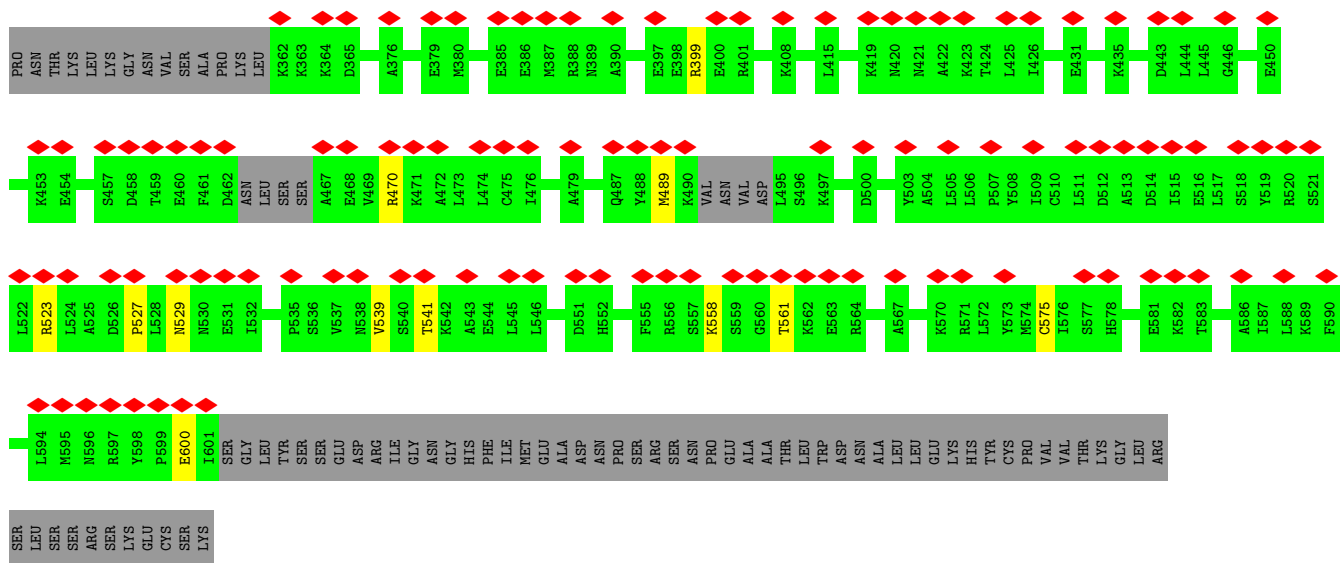
• Molecule 48: Nucleolar protein 16



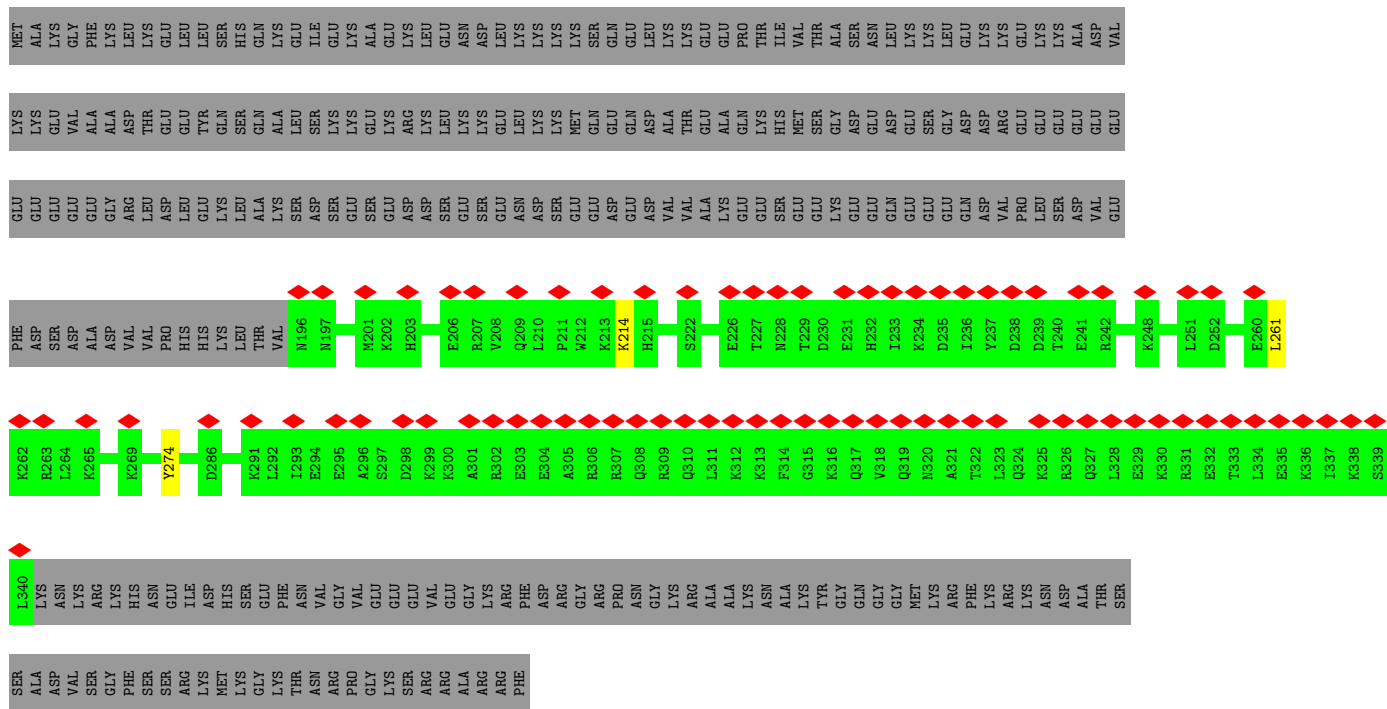
• Molecule 49: 27S pre-rRNA (guanosine(2922)-2'-O)-methyltransferase



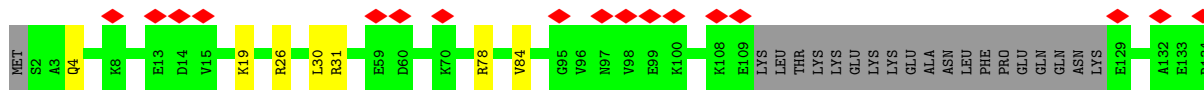
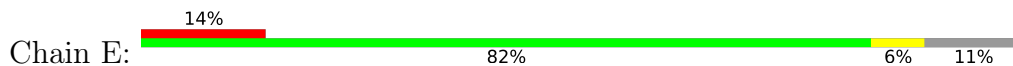


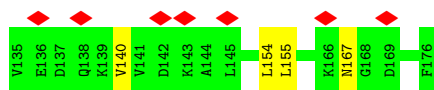


- Molecule 51: rRNA-processing protein EBP2

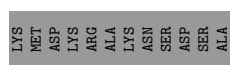
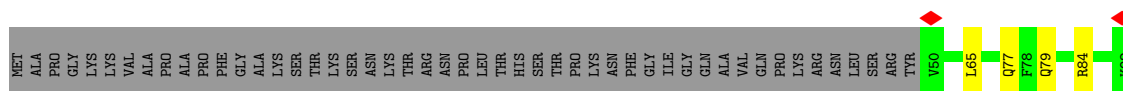


- Molecule 52: 60S ribosomal protein L6-A

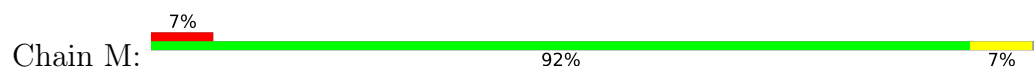




- Molecule 53: 60S ribosomal protein L8-A



- Molecule 54: 60S ribosomal protein L14-A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	112099	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	27	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.521	Depositor
Minimum map value	-0.290	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.07	Depositor
Map size (\AA)	455.28, 455.28, 455.28	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.084, 1.084, 1.084	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

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	1	0.26	2/58862 (0.0%)	0.70	18/91746 (0.0%)
2	2	0.25	0/3746	0.67	1/5832 (0.0%)
3	6	0.27	0/1527	0.75	0/2371
4	L	0.39	0/1016	0.70	0/1363
5	N	0.38	0/1619	0.69	0/2166
6	Q	0.40	0/1050	0.68	0/1419
7	R	0.38	0/977	0.66	0/1310
8	S	0.41	0/1468	0.64	0/1973
9	T	0.41	0/427	0.70	0/576
10	U	0.45	0/794	0.59	0/1076
11	Z	0.41	0/1118	0.65	0/1497
12	c	0.42	0/751	0.63	0/1008
13	d	0.38	0/887	0.64	1/1191 (0.1%)
14	e	0.38	0/1030	0.65	1/1379 (0.1%)
15	f	0.37	0/868	0.63	0/1168
16	g	0.37	0/891	0.65	0/1191
17	i	0.40	0/665	0.76	1/884 (0.1%)
18	j	0.39	0/592	0.68	0/785
19	k	0.39	0/618	0.66	0/826
20	O	0.28	0/1585	0.44	0/2128
21	V	0.39	0/1008	0.63	0/1356
22	a	0.41	0/637	0.63	0/862
23	P	0.38	0/1464	0.62	0/1965
24	X	0.39	0/1116	0.64	1/1503 (0.1%)
25	Y	0.37	0/1004	0.66	0/1341
26	h	0.37	0/978	0.63	1/1301 (0.1%)
27	F	0.40	0/1821	0.63	0/2451
28	B	0.41	0/2756	0.66	0/3702
29	C	0.38	0/2782	0.64	1/3766 (0.0%)
30	H	0.38	0/1531	0.60	0/2062
31	A	0.40	0/1663	0.67	0/2248
32	K	0.42	0/2107	0.65	0/2845

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	m	0.40	0/5356	0.65	1/7264 (0.0%)
34	D	0.44	0/1626	0.65	0/2193
35	W	0.42	0/1902	0.64	0/2564
36	l	0.42	0/1407	0.66	1/1896 (0.1%)
37	b	0.42	0/3474	0.63	1/4683 (0.0%)
38	o	0.42	0/1129	0.65	0/1502
39	n	0.40	0/3441	0.61	1/4625 (0.0%)
40	r	0.37	0/1462	0.60	0/1952
41	s	0.32	0/301	0.60	0/386
42	t	0.39	0/2355	0.65	0/3158
43	y	0.40	0/1722	0.62	0/2343
44	z	0.36	0/445	0.62	0/585
45	p	0.42	0/2362	0.67	1/3200 (0.0%)
46	q	0.44	0/2536	0.64	0/3433
47	u	0.41	0/996	0.61	0/1324
48	v	0.38	0/1100	0.59	0/1456
49	w	0.40	0/3571	0.63	2/4789 (0.0%)
50	I	0.41	0/3515	0.63	0/4725
51	J	0.39	0/1232	0.62	0/1642
52	E	0.39	0/1260	0.66	0/1694
53	G	0.41	0/1463	0.70	0/1978
54	M	0.38	0/1068	0.63	0/1438
All	All	0.34	2/143081 (0.0%)	0.67	32/206121 (0.0%)

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
5	N	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2981	U	C1'-N1	5.54	1.57	1.48
1	1	2942	C	C1'-N1	5.06	1.56	1.48

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	649	A	C2'-C3'-O3'	8.32	127.80	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	932	U	N1-C1'-C2'	7.62	123.90	114.00
33	m	719	LEU	CA-CB-CG	7.58	132.74	115.30
17	i	57	LEU	CA-CB-CG	7.46	132.46	115.30
37	b	277	LEU	CA-CB-CG	6.73	130.77	115.30
45	p	109	LEU	CA-CB-CG	6.72	130.75	115.30
1	1	1227	C	C2'-C3'-O3'	6.68	124.39	113.70
1	1	644	G	C2'-C3'-O3'	6.41	123.95	113.70
36	l	54	LEU	CA-CB-CG	6.25	129.67	115.30
1	1	2922	G	C2'-C3'-O3'	6.25	123.69	113.70
39	n	417	LEU	CA-CB-CG	6.10	129.32	115.30
14	e	82	LEU	CA-CB-CG	6.03	129.18	115.30
2	2	123	G	C2'-C3'-O3'	5.95	123.21	113.70
29	C	313	LEU	CA-CB-CG	5.85	128.75	115.30
1	1	1307	G	C2'-C3'-O3'	5.81	123.00	113.70
1	1	239	G	C2'-C3'-O3'	5.79	122.97	113.70
1	1	292	U	O4'-C1'-N1	5.59	112.67	108.20
49	w	213	LEU	CA-CB-CG	5.59	128.15	115.30
1	1	2954	U	C2'-C3'-O3'	5.54	122.57	113.70
26	h	28	LEU	CA-CB-CG	5.46	127.86	115.30
1	1	221	A	O4'-C1'-N9	5.35	112.48	108.20
49	w	73	LEU	CA-CB-CG	5.26	127.41	115.30
1	1	1203	A	N9-C1'-C2'	5.22	120.78	114.00
1	1	1299	U	N1-C1'-C2'	-5.19	106.29	112.00
1	1	720	A	C2'-C3'-O3'	5.14	121.93	113.70
1	1	2940	A	C4'-C3'-O3'	5.12	123.24	113.00
1	1	1861	G	C2'-C3'-O3'	5.12	121.89	113.70
1	1	1299	U	C5'-C4'-O4'	5.10	115.22	109.10
13	d	87	ASN	C-N-CD	-5.10	109.38	120.60
24	X	40	LEU	CA-CB-CG	5.06	126.93	115.30
1	1	1820	U	C2'-C3'-O3'	5.02	121.72	113.70
1	1	1108	U	O4'-C1'-N1	5.00	112.20	108.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	N	92	LEU	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
4	L	119/199 (60%)	107 (90%)	8 (7%)	4 (3%)	3	22
5	N	182/204 (89%)	166 (91%)	13 (7%)	3 (2%)	9	36
6	Q	132/186 (71%)	123 (93%)	9 (7%)	0	100	100
7	R	116/189 (61%)	109 (94%)	6 (5%)	1 (1%)	17	48
8	S	168/172 (98%)	151 (90%)	13 (8%)	4 (2%)	6	28
9	T	53/160 (33%)	46 (87%)	6 (11%)	1 (2%)	8	34
10	U	96/121 (79%)	90 (94%)	6 (6%)	0	100	100
11	Z	133/136 (98%)	117 (88%)	13 (10%)	3 (2%)	6	29
12	c	95/105 (90%)	92 (97%)	3 (3%)	0	100	100
13	d	105/113 (93%)	96 (91%)	7 (7%)	2 (2%)	8	34
14	e	123/130 (95%)	120 (98%)	3 (2%)	0	100	100
15	f	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
16	g	110/121 (91%)	106 (96%)	4 (4%)	0	100	100
17	i	81/100 (81%)	68 (84%)	12 (15%)	1 (1%)	13	42
18	j	71/88 (81%)	67 (94%)	3 (4%)	1 (1%)	11	38
19	k	75/78 (96%)	69 (92%)	5 (7%)	1 (1%)	12	40
20	O	195/199 (98%)	125 (64%)	38 (20%)	32 (16%)	0	1
21	V	132/137 (96%)	123 (93%)	8 (6%)	1 (1%)	19	51
22	a	79/149 (53%)	72 (91%)	5 (6%)	2 (2%)	5	27
23	P	179/184 (97%)	164 (92%)	14 (8%)	1 (1%)	25	57
24	X	139/142 (98%)	122 (88%)	15 (11%)	2 (1%)	11	38
25	Y	124/127 (98%)	115 (93%)	9 (7%)	0	100	100
26	h	117/120 (98%)	108 (92%)	6 (5%)	3 (3%)	5	27
27	F	220/244 (90%)	204 (93%)	11 (5%)	5 (2%)	6	29
28	B	337/387 (87%)	293 (87%)	38 (11%)	6 (2%)	8	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	C	357/362 (99%)	317 (89%)	33 (9%)	7 (2%)	7	32
30	H	188/191 (98%)	173 (92%)	14 (7%)	1 (0%)	29	61
31	A	192/291 (66%)	174 (91%)	16 (8%)	2 (1%)	15	46
32	K	253/376 (67%)	231 (91%)	20 (8%)	2 (1%)	19	51
33	m	641/807 (79%)	576 (90%)	58 (9%)	7 (1%)	14	45
34	D	188/505 (37%)	167 (89%)	21 (11%)	0	100	100
35	W	230/236 (98%)	214 (93%)	14 (6%)	2 (1%)	17	48
36	l	170/181 (94%)	156 (92%)	14 (8%)	0	100	100
37	b	413/647 (64%)	387 (94%)	24 (6%)	2 (0%)	29	61
38	o	131/220 (60%)	121 (92%)	9 (7%)	1 (1%)	19	51
39	n	403/605 (67%)	372 (92%)	29 (7%)	2 (0%)	29	61
40	r	170/261 (65%)	149 (88%)	20 (12%)	1 (1%)	25	57
41	s	34/520 (6%)	33 (97%)	1 (3%)	0	100	100
42	t	286/322 (89%)	260 (91%)	20 (7%)	6 (2%)	7	31
43	y	223/245 (91%)	211 (95%)	11 (5%)	1 (0%)	34	66
44	z	53/106 (50%)	53 (100%)	0	0	100	100
45	p	288/460 (63%)	262 (91%)	24 (8%)	2 (1%)	22	54
46	q	313/618 (51%)	270 (86%)	36 (12%)	7 (2%)	6	30
47	u	114/199 (57%)	107 (94%)	6 (5%)	1 (1%)	17	48
48	v	124/231 (54%)	118 (95%)	6 (5%)	0	100	100
49	w	426/841 (51%)	389 (91%)	37 (9%)	0	100	100
50	I	421/663 (64%)	380 (90%)	35 (8%)	6 (1%)	11	38
51	J	143/427 (34%)	135 (94%)	8 (6%)	0	100	100
52	E	152/176 (86%)	132 (87%)	20 (13%)	0	100	100
53	G	180/256 (70%)	166 (92%)	12 (7%)	2 (1%)	14	45
54	M	134/138 (97%)	124 (92%)	9 (7%)	1 (1%)	22	54
All	All	9512/13782 (69%)	8630 (91%)	756 (8%)	126 (1%)	16	40

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	L	51	LEU
5	N	145	ASP

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Mol	Chain	Res	Type
8	S	13	ARG
11	Z	103	GLN
19	k	33	LYS
20	O	28	LEU
20	O	47	PHE
20	O	48	PHE
20	O	62	THR
20	O	63	ALA
20	O	86	GLY
20	O	89	SER
20	O	113	ASP
20	O	114	LYS
20	O	137	THR
20	O	145	VAL
20	O	162	VAL
20	O	189	ASP
21	V	90	GLY
26	h	91	ALA
27	F	160	ARG
28	B	34	LYS
28	B	222	LYS
29	C	4	PRO
29	C	140	HIS
29	C	339	LEU
33	m	231	GLU
38	o	190	THR
42	t	227	ILE
42	t	269	GLN
50	I	558	LYS
4	L	50	PRO
5	N	144	ARG
11	Z	125	GLY
13	d	87	ASN
17	i	30	LYS
20	O	13	GLY
20	O	16	VAL
20	O	17	GLY
20	O	27	LEU
20	O	77	SER
20	O	190	VAL
20	O	191	ALA
20	O	198	GLY

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Mol	Chain	Res	Type
27	F	191	VAL
28	B	35	ASP
28	B	138	ALA
29	C	269	SER
30	H	22	SER
33	m	177	GLY
33	m	232	GLN
33	m	328	LYS
42	t	277	VAL
46	q	300	GLY
46	q	427	THR
46	q	429	VAL
54	M	29	ALA
4	L	62	THR
4	L	75	PHE
7	R	53	LYS
20	O	11	GLY
20	O	168	TYR
20	O	169	ALA
20	O	192	LYS
22	a	77	LYS
24	X	4	SER
26	h	119	LYS
27	F	157	ASN
27	F	158	LYS
27	F	164	SER
28	B	187	SER
31	A	171	PRO
33	m	406	ASN
37	b	198	ALA
47	u	81	TYR
50	I	541	THR
53	G	232	HIS
5	N	94	TYR
8	S	24	LEU
9	T	127	GLN
18	j	85	LYS
20	O	24	ALA
20	O	37	ARG
20	O	85	ARG
20	O	152	VAL
22	a	78	LEU

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Mol	Chain	Res	Type
23	P	156	ALA
24	X	5	ALA
26	h	84	LYS
28	B	155	ALA
29	C	268	ALA
31	A	63	PRO
32	K	284	ASN
33	m	154	GLN
33	m	435	GLY
42	t	240	GLY
42	t	270	PRO
46	q	317	GLY
50	I	600	GLU
8	S	14	LEU
13	d	88	PRO
29	C	311	HIS
32	K	256	PRO
37	b	432	MET
39	n	196	GLU
39	n	456	HIS
42	t	151	LEU
45	p	351	ARG
45	p	418	ASP
50	I	527	PRO
50	I	561	THR
53	G	79	GLN
20	O	46	GLU
46	q	268	ALA
20	O	43	ILE
35	W	146	GLY
46	q	269	ARG
11	Z	16	GLY
29	C	146	PRO
35	W	101	GLY
50	I	196	PRO
8	S	167	ARG
40	r	190	GLY
43	y	58	ILE
46	q	423	PRO
20	O	153	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
4	L	101/159 (64%)	93 (92%)	8 (8%)	12	37
5	N	161/176 (92%)	146 (91%)	15 (9%)	9	30
6	Q	110/151 (73%)	102 (93%)	8 (7%)	14	41
7	R	101/154 (66%)	95 (94%)	6 (6%)	19	49
8	S	155/156 (99%)	143 (92%)	12 (8%)	13	38
9	T	44/137 (32%)	41 (93%)	3 (7%)	16	44
10	U	85/107 (79%)	84 (99%)	1 (1%)	71	83
11	Z	115/116 (99%)	112 (97%)	3 (3%)	46	71
12	c	81/88 (92%)	76 (94%)	5 (6%)	18	47
13	d	94/97 (97%)	90 (96%)	4 (4%)	29	59
14	e	108/111 (97%)	103 (95%)	5 (5%)	27	58
15	f	90/91 (99%)	85 (94%)	5 (6%)	21	52
16	g	95/103 (92%)	85 (90%)	10 (10%)	7	25
17	i	69/82 (84%)	60 (87%)	9 (13%)	4	17
18	j	60/71 (84%)	52 (87%)	8 (13%)	4	17
19	k	68/69 (99%)	63 (93%)	5 (7%)	13	40
20	O	160/162 (99%)	132 (82%)	28 (18%)	2	8
21	V	103/105 (98%)	101 (98%)	2 (2%)	57	77
22	a	66/119 (56%)	63 (96%)	3 (4%)	27	58
23	P	145/146 (99%)	139 (96%)	6 (4%)	30	61
24	X	117/118 (99%)	113 (97%)	4 (3%)	37	65
25	Y	109/110 (99%)	106 (97%)	3 (3%)	43	70
26	h	104/105 (99%)	100 (96%)	4 (4%)	33	62
27	F	186/205 (91%)	181 (97%)	5 (3%)	44	71
28	B	284/323 (88%)	266 (94%)	18 (6%)	18	47
29	C	286/289 (99%)	280 (98%)	6 (2%)	53	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	H	170/171 (99%)	162 (95%)	8 (5%)	26	57
31	A	185/263 (70%)	181 (98%)	4 (2%)	52	74
32	K	238/346 (69%)	233 (98%)	5 (2%)	53	75
33	m	582/723 (80%)	564 (97%)	18 (3%)	40	67
34	D	175/440 (40%)	170 (97%)	5 (3%)	42	69
35	W	209/213 (98%)	200 (96%)	9 (4%)	29	59
36	l	149/156 (96%)	143 (96%)	6 (4%)	31	61
37	b	377/573 (66%)	360 (96%)	17 (4%)	27	58
38	o	118/199 (59%)	116 (98%)	2 (2%)	60	78
39	n	371/548 (68%)	356 (96%)	15 (4%)	31	61
40	r	156/229 (68%)	153 (98%)	3 (2%)	57	77
41	s	32/445 (7%)	30 (94%)	2 (6%)	18	47
42	t	259/287 (90%)	252 (97%)	7 (3%)	44	71
43	y	193/211 (92%)	186 (96%)	7 (4%)	35	63
44	z	48/95 (50%)	48 (100%)	0	100	100
45	p	265/413 (64%)	260 (98%)	5 (2%)	57	77
46	q	268/535 (50%)	262 (98%)	6 (2%)	52	74
47	u	101/180 (56%)	96 (95%)	5 (5%)	24	55
48	v	116/205 (57%)	113 (97%)	3 (3%)	46	71
49	w	383/745 (51%)	371 (97%)	12 (3%)	40	67
50	I	393/602 (65%)	381 (97%)	12 (3%)	40	67
51	J	133/383 (35%)	130 (98%)	3 (2%)	50	73
52	E	134/153 (88%)	123 (92%)	11 (8%)	11	36
53	G	150/208 (72%)	136 (91%)	14 (9%)	9	30
54	M	107/109 (98%)	99 (92%)	8 (8%)	13	39
All	All	8409/11982 (70%)	8036 (96%)	373 (4%)	32	59

All (373) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L	21	ARG
4	L	34	SER
4	L	49	ARG

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Mol	Chain	Res	Type
4	L	54	LEU
4	L	76	THR
4	L	85	LEU
4	L	100	ARG
4	L	101	ARG
5	N	10	LEU
5	N	19	LEU
5	N	22	LEU
5	N	34	ASN
5	N	41	ARG
5	N	43	THR
5	N	92	LEU
5	N	95	GLN
5	N	108	ARG
5	N	121	VAL
5	N	132	VAL
5	N	133	ILE
5	N	167	THR
5	N	187	ARG
5	N	188	ARG
6	Q	31	LYS
6	Q	38	ARG
6	Q	59	ARG
6	Q	126	GLN
6	Q	136	ASN
6	Q	141	ARG
6	Q	146	SER
6	Q	147	ARG
7	R	10	LEU
7	R	19	LYS
7	R	30	SER
7	R	98	ARG
7	R	106	LEU
7	R	140	GLU
8	S	12	ARG
8	S	13	ARG
8	S	24	LEU
8	S	48	LEU
8	S	71	LYS
8	S	80	ARG
8	S	97	VAL
8	S	100	VAL

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Mol	Chain	Res	Type
8	S	120	SER
8	S	125	LYS
8	S	147	ASP
8	S	155	ARG
9	T	106	LEU
9	T	139	ARG
9	T	151	LEU
10	U	18	ASP
11	Z	17	ARG
11	Z	51	LEU
11	Z	105	SER
12	c	10	ILE
12	c	18	ILE
12	c	50	VAL
12	c	84	LEU
12	c	104	LEU
13	d	13	THR
13	d	61	LYS
13	d	106	THR
13	d	109	VAL
14	e	27	ARG
14	e	33	ARG
14	e	61	LYS
14	e	75	LEU
14	e	85	LEU
15	f	49	ILE
15	f	59	VAL
15	f	60	ARG
15	f	81	VAL
15	f	107	ILE
16	g	10	ARG
16	g	16	ARG
16	g	29	ILE
16	g	44	CYS
16	g	49	SER
16	g	51	LEU
16	g	55	SER
16	g	59	PRO
16	g	83	ASN
16	g	108	GLN
17	i	20	MET
17	i	36	ARG

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Mol	Chain	Res	Type
17	i	47	ILE
17	i	56	ARG
17	i	57	LEU
17	i	60	LEU
17	i	76	ARG
17	i	77	LEU
17	i	79	SER
18	j	24	ARG
18	j	26	SER
18	j	30	GLN
18	j	52	LYS
18	j	58	THR
18	j	67	LEU
18	j	79	GLN
18	j	82	SER
19	k	6	THR
19	k	12	LEU
19	k	22	THR
19	k	46	ARG
19	k	65	LEU
20	O	18	ARG
20	O	23	VAL
20	O	25	LYS
20	O	27	LEU
20	O	37	ARG
20	O	46	GLU
20	O	49	ARG
20	O	50	ASN
20	O	55	HIS
20	O	56	ASP
20	O	59	ARG
20	O	65	ASN
20	O	74	ARG
20	O	78	ARG
20	O	80	PHE
20	O	84	LEU
20	O	94	ARG
20	O	101	ARG
20	O	113	ASP
20	O	124	LEU
20	O	125	ARG
20	O	129	LEU

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Mol	Chain	Res	Type
20	O	133	ARG
20	O	135	TYR
20	O	137	THR
20	O	152	VAL
20	O	156	LEU
20	O	160	ARG
21	V	49	LEU
21	V	93	LEU
22	a	78	LEU
22	a	117	ARG
22	a	120	ASN
23	P	24	VAL
23	P	36	ILE
23	P	52	LEU
23	P	69	ARG
23	P	97	ASN
23	P	168	LEU
24	X	12	LYS
24	X	16	LYS
24	X	38	LEU
24	X	63	ILE
25	Y	37	LYS
25	Y	51	ARG
25	Y	74	TYR
26	h	28	LEU
26	h	49	LYS
26	h	62	GLN
26	h	93	THR
27	F	88	ARG
27	F	89	ILE
27	F	93	ASN
27	F	124	LEU
27	F	244	ASN
28	B	28	ARG
28	B	50	LYS
28	B	55	THR
28	B	70	ARG
28	B	85	VAL
28	B	89	VAL
28	B	100	ARG
28	B	114	VAL
28	B	148	LEU

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Mol	Chain	Res	Type
28	B	152	LYS
28	B	164	THR
28	B	168	LYS
28	B	178	LEU
28	B	216	ASP
28	B	325	LYS
28	B	332	ARG
28	B	380	MET
28	B	385	LYS
29	C	52	VAL
29	C	154	THR
29	C	179	LEU
29	C	194	TYR
29	C	206	LEU
29	C	259	ASP
30	H	26	LYS
30	H	41	ILE
30	H	63	LYS
30	H	118	LEU
30	H	138	THR
30	H	151	VAL
30	H	157	ASN
30	H	161	LEU
31	A	84	ASN
31	A	106	ASN
31	A	189	ARG
31	A	225	LEU
32	K	75	LYS
32	K	240	ARG
32	K	248	LEU
32	K	256	PRO
32	K	262	ASN
33	m	153	THR
33	m	156	THR
33	m	168	MET
33	m	175	ILE
33	m	178	LYS
33	m	192	LEU
33	m	203	THR
33	m	223	LEU
33	m	238	ASN
33	m	263	LYS

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Mol	Chain	Res	Type
33	m	323	HIS
33	m	324	LEU
33	m	390	ARG
33	m	428	ARG
33	m	440	VAL
33	m	688	ILE
33	m	696	ILE
33	m	719	LEU
34	D	294	VAL
34	D	394	LEU
34	D	429	LEU
34	D	448	ARG
34	D	451	LEU
35	W	15	THR
35	W	22	ASN
35	W	48	VAL
35	W	49	ARG
35	W	57	ARG
35	W	113	LYS
35	W	128	ASN
35	W	174	LYS
35	W	232	ASN
36	l	22	ARG
36	l	47	VAL
36	l	51	VAL
36	l	54	LEU
36	l	63	LEU
36	l	70	LEU
37	b	3	LEU
37	b	15	ASN
37	b	31	THR
37	b	39	ILE
37	b	48	ARG
37	b	70	ASN
37	b	175	TYR
37	b	177	ASN
37	b	180	LYS
37	b	221	THR
37	b	277	LEU
37	b	281	LYS
37	b	384	ASN
37	b	415	ASN

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Mol	Chain	Res	Type
37	b	440	ASN
37	b	445	LEU
37	b	456	LEU
38	o	93	ILE
38	o	146	MET
39	n	7	ASN
39	n	36	CYS
39	n	47	ARG
39	n	49	LYS
39	n	54	LYS
39	n	69	GLN
39	n	92	ARG
39	n	139	LEU
39	n	145	LEU
39	n	208	ASN
39	n	376	LEU
39	n	417	LEU
39	n	419	ASN
39	n	427	ILE
39	n	566	LEU
40	r	203	ASN
40	r	217	LYS
40	r	225	VAL
41	s	1	MET
41	s	33	MET
42	t	15	ASN
42	t	66	LEU
42	t	151	LEU
42	t	157	ASN
42	t	187	LEU
42	t	275	ARG
42	t	291	GLN
43	y	100	ARG
43	y	101	LEU
43	y	114	VAL
43	y	145	ASN
43	y	146	ILE
43	y	154	LEU
43	y	173	LEU
45	p	109	LEU
45	p	111	VAL
45	p	165	ARG

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Mol	Chain	Res	Type
45	p	167	LEU
45	p	326	ARG
46	q	273	ILE
46	q	274	ARG
46	q	280	THR
46	q	282	ARG
46	q	299	ILE
46	q	534	HIS
47	u	27	LYS
47	u	45	ASN
47	u	76	ASN
47	u	100	ARG
47	u	113	ARG
48	v	30	ILE
48	v	33	ASN
48	v	200	PHE
49	w	28	ARG
49	w	73	LEU
49	w	82	MET
49	w	164	LYS
49	w	167	ASN
49	w	186	PRO
49	w	211	ARG
49	w	315	PHE
49	w	665	LEU
49	w	671	LEU
49	w	678	ASP
49	w	742	ARG
50	I	161	ARG
50	I	260	ILE
50	I	304	GLU
50	I	328	ASN
50	I	329	ILE
50	I	399	ARG
50	I	470	ARG
50	I	489	MET
50	I	523	ARG
50	I	529	ASN
50	I	539	VAL
50	I	575	CYS
51	J	214	LYS
51	J	261	LEU

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Mol	Chain	Res	Type
51	J	274	TYR
52	E	4	GLN
52	E	19	LYS
52	E	26	ARG
52	E	30	LEU
52	E	31	ARG
52	E	78	ARG
52	E	84	VAL
52	E	140	VAL
52	E	154	LEU
52	E	155	LEU
52	E	167	ASN
53	G	65	LEU
53	G	77	GLN
53	G	84	ARG
53	G	136	LEU
53	G	150	LEU
53	G	166	LEU
53	G	169	LEU
53	G	190	VAL
53	G	197	VAL
53	G	200	LEU
53	G	204	ARG
53	G	213	LYS
53	G	214	LEU
53	G	229	VAL
54	M	15	VAL
54	M	25	LYS
54	M	38	ILE
54	M	63	VAL
54	M	72	LEU
54	M	77	ARG
54	M	131	VAL
54	M	135	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
4	L	12	ASN
4	L	37	ASN
4	L	120	GLN
5	N	34	ASN

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Mol	Chain	Res	Type
5	N	37	HIS
5	N	95	GLN
6	Q	58	ASN
6	Q	73	GLN
6	Q	136	ASN
7	R	92	GLN
8	S	89	ASN
11	Z	57	HIS
15	f	42	GLN
19	k	40	GLN
20	O	26	GLN
20	O	31	GLN
20	O	42	ASN
20	O	50	ASN
20	O	65	ASN
20	O	72	HIS
20	O	122	GLN
21	V	98	ASN
22	a	120	ASN
23	P	34	GLN
23	P	37	ASN
23	P	96	GLN
24	X	111	ASN
26	h	59	ASN
27	F	209	ASN
28	B	182	GLN
28	B	184	ASN
28	B	279	ASN
28	B	345	ASN
29	C	48	GLN
29	C	87	GLN
29	C	114	ASN
29	C	291	ASN
30	H	58	HIS
31	A	73	GLN
31	A	75	ASN
31	A	150	GLN
31	A	175	HIS
32	K	42	ASN
32	K	262	ASN
33	m	232	GLN
33	m	238	ASN

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Mol	Chain	Res	Type
33	m	629	HIS
33	m	748	HIS
34	D	310	ASN
35	W	128	ASN
35	W	205	GLN
35	W	232	ASN
36	l	50	HIS
36	l	82	HIS
36	l	112	HIS
37	b	70	ASN
37	b	78	HIS
37	b	217	GLN
37	b	415	ASN
38	o	113	GLN
39	n	73	HIS
39	n	164	ASN
39	n	419	ASN
39	n	437	ASN
40	r	4	ASN
42	t	51	ASN
42	t	238	GLN
43	y	9	ASN
43	y	11	ASN
45	p	139	GLN
45	p	337	GLN
45	p	452	ASN
46	q	447	GLN
47	u	45	ASN
47	u	76	ASN
48	v	33	ASN
48	v	39	ASN
49	w	118	HIS
49	w	130	GLN
49	w	137	GLN
49	w	167	ASN
49	w	276	ASN
49	w	694	ASN
50	I	155	ASN
50	I	335	ASN
50	I	344	HIS
50	I	596	ASN
51	J	215	HIS

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Mol	Chain	Res	Type
51	J	220	HIS
51	J	221	GLN
52	E	4	GLN
53	G	95	ASN
53	G	137	ASN
54	M	56	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2439/3396 (71%)	742 (30%)	70 (2%)
2	2	157/158 (99%)	35 (22%)	3 (1%)
3	6	63/232 (27%)	30 (47%)	2 (3%)
All	All	2659/3786 (70%)	807 (30%)	75 (2%)

All (807) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	U
1	1	7	C
1	1	14	U
1	1	22	G
1	1	40	A
1	1	41	G
1	1	42	C
1	1	43	A
1	1	44	U
1	1	48	A
1	1	49	A
1	1	57	A
1	1	59	G
1	1	60	A
1	1	65	A
1	1	66	A
1	1	72	C
1	1	73	C
1	1	74	G
1	1	75	G
1	1	77	A
1	1	85	A
1	1	92	G

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Mol	Chain	Res	Type
1	1	94	G
1	1	96	G
1	1	110	G
1	1	111	C
1	1	113	C
1	1	117	U
1	1	118	U
1	1	120	G
1	1	121	A
1	1	122	A
1	1	135	C
1	1	136	G
1	1	143	G
1	1	148	G
1	1	150	A
1	1	154	U
1	1	155	G
1	1	156	G
1	1	157	A
1	1	164	A
1	1	165	A
1	1	166	C
1	1	170	G
1	1	173	G
1	1	190	U
1	1	191	U
1	1	196	G
1	1	197	G
1	1	200	C
1	1	205	C
1	1	206	G
1	1	210	U
1	1	211	A
1	1	212	G
1	1	213	A
1	1	218	G
1	1	219	A
1	1	220	G
1	1	234	G
1	1	240	U
1	1	241	G
1	1	243	G

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Mol	Chain	Res	Type
1	1	249	U
1	1	250	U
1	1	251	G
1	1	252	U
1	1	264	G
1	1	265	A
1	1	266	A
1	1	268	A
1	1	269	G
1	1	283	G
1	1	284	A
1	1	285	A
1	1	295	A
1	1	298	U
1	1	299	G
1	1	305	U
1	1	311	C
1	1	323	A
1	1	329	U
1	1	338	A
1	1	339	C
1	1	352	A
1	1	368	G
1	1	370	U
1	1	376	G
1	1	390	G
1	1	398	A
1	1	399	A
1	1	401	U
1	1	403	C
1	1	404	G
1	1	421	G
1	1	422	A
1	1	437	G
1	1	438	A
1	1	439	C
1	1	440	A
1	1	495	G
1	1	496	C
1	1	498	A
1	1	503	C
1	1	510	G

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Mol	Chain	Res	Type
1	1	515	C
1	1	517	G
1	1	518	G
1	1	520	U
1	1	521	A
1	1	523	A
1	1	533	A
1	1	534	U
1	1	535	G
1	1	536	U
1	1	542	G
1	1	543	C
1	1	547	G
1	1	550	A
1	1	551	A
1	1	552	G
1	1	555	U
1	1	556	U
1	1	557	A
1	1	558	U
1	1	559	A
1	1	569	A
1	1	578	A
1	1	579	G
1	1	589	A
1	1	592	A
1	1	593	C
1	1	597	G
1	1	603	A
1	1	604	G
1	1	609	G
1	1	611	A
1	1	620	U
1	1	621	A
1	1	622	A
1	1	623	U
1	1	634	C
1	1	636	C
1	1	643	U
1	1	644	G
1	1	645	A
1	1	649	A

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Mol	Chain	Res	Type
1	1	650	C
1	1	660	A
1	1	676	G
1	1	677	A
1	1	681	U
1	1	690	A
1	1	691	A
1	1	705	A
1	1	710	A
1	1	720	A
1	1	721	G
1	1	722	G
1	1	733	G
1	1	734	C
1	1	735	A
1	1	742	G
1	1	743	C
1	1	757	C
1	1	759	U
1	1	760	G
1	1	761	A
1	1	770	G
1	1	772	U
1	1	774	G
1	1	775	A
1	1	776	U
1	1	777	U
1	1	779	G
1	1	780	A
1	1	781	G
1	1	784	A
1	1	785	G
1	1	786	A
1	1	799	G
1	1	801	A
1	1	806	A
1	1	808	A
1	1	813	G
1	1	815	G
1	1	818	C
1	1	819	U
1	1	820	A

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Mol	Chain	Res	Type
1	1	822	G
1	1	826	G
1	1	830	A
1	1	849	C
1	1	854	G
1	1	857	G
1	1	859	G
1	1	860	G
1	1	861	C
1	1	864	G
1	1	871	U
1	1	874	U
1	1	875	G
1	1	877	C
1	1	878	G
1	1	879	U
1	1	880	G
1	1	881	C
1	1	882	A
1	1	883	A
1	1	884	A
1	1	886	C
1	1	887	G
1	1	891	G
1	1	892	U
1	1	893	C
1	1	894	G
1	1	895	A
1	1	896	A
1	1	898	U
1	1	899	U
1	1	900	G
1	1	904	A
1	1	906	A
1	1	909	G
1	1	910	G
1	1	918	C
1	1	919	U
1	1	920	A
1	1	921	A
1	1	932	U
1	1	936	A

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Mol	Chain	Res	Type
1	1	938	C
1	1	944	C
1	1	957	C
1	1	958	C
1	1	959	C
1	1	960	U
1	1	961	C
1	1	962	A
1	1	963	G
1	1	964	G
1	1	970	A
1	1	977	C
1	1	978	G
1	1	979	U
1	1	980	A
1	1	981	U
1	1	982	C
1	1	984	G
1	1	985	U
1	1	991	G
1	1	992	A
1	1	1059	G
1	1	1060	U
1	1	1098	A
1	1	1103	A
1	1	1104	G
1	1	1105	A
1	1	1108	U
1	1	1111	U
1	1	1112	A
1	1	1116	G
1	1	1117	G
1	1	1126	G
1	1	1127	G
1	1	1129	A
1	1	1132	C
1	1	1135	A
1	1	1136	A
1	1	1139	G
1	1	1142	G
1	1	1144	U
1	1	1151	U

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Mol	Chain	Res	Type
1	1	1153	A
1	1	1155	C
1	1	1159	A
1	1	1160	C
1	1	1174	G
1	1	1177	G
1	1	1180	A
1	1	1181	U
1	1	1186	G
1	1	1192	C
1	1	1193	A
1	1	1196	C
1	1	1197	A
1	1	1198	C
1	1	1199	C
1	1	1200	A
1	1	1201	C
1	1	1204	A
1	1	1213	G
1	1	1217	A
1	1	1218	U
1	1	1221	A
1	1	1222	G
1	1	1227	C
1	1	1228	C
1	1	1233	G
1	1	1235	U
1	1	1237	G
1	1	1241	U
1	1	1242	G
1	1	1244	A
1	1	1245	A
1	1	1250	G
1	1	1251	A
1	1	1252	A
1	1	1253	U
1	1	1258	U
1	1	1259	A
1	1	1262	G
1	1	1263	A
1	1	1264	G
1	1	1266	G

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Mol	Chain	Res	Type
1	1	1272	C
1	1	1273	A
1	1	1277	C
1	1	1278	A
1	1	1279	C
1	1	1283	C
1	1	1284	C
1	1	1286	A
1	1	1287	A
1	1	1299	U
1	1	1300	G
1	1	1302	A
1	1	1303	A
1	1	1304	A
1	1	1305	U
1	1	1307	G
1	1	1308	A
1	1	1309	U
1	1	1325	U
1	1	1330	A
1	1	1331	U
1	1	1332	A
1	1	1348	U
1	1	1349	G
1	1	1350	A
1	1	1351	U
1	1	1352	A
1	1	1353	U
1	1	1354	G
1	1	1355	A
1	1	1356	U
1	1	1357	G
1	1	1364	C
1	1	1367	G
1	1	1380	G
1	1	1386	A
1	1	1391	C
1	1	1397	C
1	1	1399	A
1	1	1400	G
1	1	1419	A
1	1	1421	G

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Mol	Chain	Res	Type
1	1	1429	G
1	1	1434	G
1	1	1437	C
1	1	1443	G
1	1	1446	A
1	1	1450	G
1	1	1452	A
1	1	1453	A
1	1	1454	A
1	1	1455	U
1	1	1477	A
1	1	1481	A
1	1	1483	G
1	1	1484	U
1	1	1485	G
1	1	1487	G
1	1	1495	U
1	1	1503	A
1	1	1508	C
1	1	1512	U
1	1	1533	U
1	1	1536	G
1	1	1539	A
1	1	1544	G
1	1	1546	A
1	1	1547	G
1	1	1555	U
1	1	1556	C
1	1	1557	A
1	1	1560	G
1	1	1561	G
1	1	1562	C
1	1	1566	A
1	1	1567	U
1	1	1568	U
1	1	1569	U
1	1	1571	A
1	1	1573	G
1	1	1574	C
1	1	1575	A
1	1	1580	A
1	1	1581	C

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Mol	Chain	Res	Type
1	1	1582	C
1	1	1587	A
1	1	1589	A
1	1	1590	G
1	1	1593	A
1	1	1596	C
1	1	1605	A
1	1	1608	C
1	1	1613	A
1	1	1619	A
1	1	1620	U
1	1	1627	U
1	1	1628	C
1	1	1630	U
1	1	1639	C
1	1	1641	U
1	1	1642	A
1	1	1643	A
1	1	1647	A
1	1	1656	A
1	1	1657	C
1	1	1658	G
1	1	1683	A
1	1	1685	C
1	1	1687	U
1	1	1688	U
1	1	1713	G
1	1	1715	A
1	1	1716	U
1	1	1717	U
1	1	1724	U
1	1	1725	C
1	1	1730	G
1	1	1736	G
1	1	1741	A
1	1	1742	U
1	1	1743	G
1	1	1749	A
1	1	1750	A
1	1	1751	G
1	1	1756	C
1	1	1764	U

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Mol	Chain	Res	Type
1	1	1765	U
1	1	1766	G
1	1	1768	U
1	1	1770	G
1	1	1775	G
1	1	1780	G
1	1	1792	C
1	1	1794	G
1	1	1795	U
1	1	1796	G
1	1	1797	A
1	1	1808	G
1	1	1813	A
1	1	1814	A
1	1	1815	U
1	1	1816	A
1	1	1817	G
1	1	1820	U
1	1	1821	U
1	1	1852	G
1	1	1853	U
1	1	1862	U
1	1	1865	A
1	1	1866	C
1	1	1867	A
1	1	1868	G
1	1	1869	C
1	1	1871	U
1	1	1878	G
1	1	1879	A
1	1	1880	U
1	1	1881	A
1	1	1884	A
1	1	1886	A
1	1	1900	A
1	1	1906	G
1	1	1947	G
1	1	1948	G
1	1	1951	C
1	1	1952	G
1	1	1953	G
1	1	2095	G

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Mol	Chain	Res	Type
1	1	2098	C
1	1	2100	A
1	1	2101	C
1	1	2123	G
1	1	2130	G
1	1	2322	C
1	1	2323	G
1	1	2324	A
1	1	2325	G
1	1	2334	U
1	1	2335	G
1	1	2336	U
1	1	2347	U
1	1	2363	A
1	1	2370	G
1	1	2371	G
1	1	2372	A
1	1	2373	A
1	1	2374	C
1	1	2377	G
1	1	2385	G
1	1	2388	U
1	1	2392	C
1	1	2393	G
1	1	2394	G
1	1	2395	G
1	1	2405	C
1	1	2410	U
1	1	2411	U
1	1	2412	G
1	1	2414	G
1	1	2418	G
1	1	2419	A
1	1	2434	U
1	1	2597	U
1	1	2606	G
1	1	2607	G
1	1	2805	G
1	1	2807	U
1	1	2811	A
1	1	2812	C
1	1	2813	A

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Mol	Chain	Res	Type
1	1	2818	U
1	1	2819	A
1	1	2820	A
1	1	2821	C
1	1	2822	U
1	1	2823	G
1	1	2824	G
1	1	2825	C
1	1	2826	U
1	1	2836	C
1	1	2837	A
1	1	2838	A
1	1	2841	G
1	1	2842	U
1	1	2845	A
1	1	2846	U
1	1	2849	C
1	1	2855	U
1	1	2857	C
1	1	2858	U
1	1	2877	G
1	1	2878	G
1	1	2879	C
1	1	2880	U
1	1	2887	A
1	1	2889	C
1	1	2898	G
1	1	2899	C
1	1	2911	A
1	1	2916	U
1	1	2919	A
1	1	2920	U
1	1	2921	U
1	1	2922	G
1	1	2923	U
1	1	2924	U
1	1	2925	C
1	1	2926	A
1	1	2927	C
1	1	2929	C
1	1	2930	A
1	1	2935	U

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Mol	Chain	Res	Type
1	1	2936	A
1	1	2941	A
1	1	2942	C
1	1	2943	G
1	1	2944	U
1	1	2945	G
1	1	2946	A
1	1	2947	G
1	1	2949	U
1	1	2950	G
1	1	2951	G
1	1	2952	G
1	1	2953	U
1	1	2954	U
1	1	2955	U
1	1	2956	A
1	1	2964	G
1	1	2965	U
1	1	2966	G
1	1	2967	A
1	1	2968	G
1	1	2969	A
1	1	2970	C
1	1	2971	A
1	1	2972	G
1	1	2975	U
1	1	2976	A
1	1	2977	G
1	1	2979	U
1	1	2980	U
1	1	2981	U
1	1	2982	A
1	1	2983	C
1	1	2984	C
1	1	2987	A
1	1	2990	G
1	1	2992	U
1	1	2996	U
1	1	2997	G
1	1	3003	G
1	1	3012	A
1	1	3017	A

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Mol	Chain	Res	Type
1	1	3019	U
1	1	3020	U
1	1	3021	A
1	1	3022	G
1	1	3023	U
1	1	3026	G
1	1	3029	A
1	1	3030	G
1	1	3032	A
1	1	3037	U
1	1	3046	A
1	1	3056	U
1	1	3057	U
1	1	3058	U
1	1	3065	G
1	1	3069	G
1	1	3070	A
1	1	3071	U
1	1	3072	C
1	1	3074	G
1	1	3076	C
1	1	3078	U
1	1	3079	U
1	1	3086	A
1	1	3090	U
1	1	3092	C
1	1	3093	C
1	1	3094	A
1	1	3099	C
1	1	3100	U
1	1	3102	G
1	1	3104	U
1	1	3109	G
1	1	3116	G
1	1	3122	A
1	1	3124	G
1	1	3129	A
1	1	3130	A
1	1	3131	U
1	1	3141	A
1	1	3142	A
1	1	3143	C

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Mol	Chain	Res	Type
1	1	3150	A
1	1	3151	U
1	1	3153	U
1	1	3154	C
1	1	3155	U
1	1	3156	U
1	1	3157	U
1	1	3158	G
1	1	3160	U
1	1	3161	C
1	1	3164	C
1	1	3165	A
1	1	3170	A
1	1	3172	A
1	1	3173	G
1	1	3174	A
1	1	3175	U
1	1	3176	G
1	1	3179	U
1	1	3180	A
1	1	3181	C
1	1	3186	A
1	1	3187	A
1	1	3188	G
1	1	3196	U
1	1	3199	G
1	1	3206	C
1	1	3207	U
1	1	3216	G
1	1	3217	C
1	1	3218	A
1	1	3219	G
1	1	3227	A
1	1	3228	C
1	1	3229	G
1	1	3242	G
1	1	3243	A
1	1	3244	A
1	1	3245	A
1	1	3247	G
1	1	3249	C
1	1	3252	G

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Mol	Chain	Res	Type
1	1	3256	G
1	1	3259	U
1	1	3263	G
1	1	3268	A
1	1	3269	U
1	1	3270	U
1	1	3271	G
1	1	3276	G
1	1	3281	U
1	1	3283	U
1	1	3287	U
1	1	3288	G
1	1	3289	G
1	1	3290	G
1	1	3293	U
1	1	3294	A
1	1	3295	A
1	1	3303	G
1	1	3304	U
1	1	3306	U
1	1	3307	A
1	1	3309	G
1	1	3313	U
1	1	3316	A
1	1	3317	U
1	1	3319	U
1	1	3324	C
1	1	3328	G
1	1	3341	U
1	1	3342	A
1	1	3344	A
1	1	3345	G
1	1	3350	C
1	1	3351	U
1	1	3352	U
1	1	3353	G
1	1	3355	U
1	1	3356	G
1	1	3363	U
1	1	3366	G
1	1	3369	G
1	1	3375	A

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Mol	Chain	Res	Type
1	1	3378	C
1	1	3386	G
1	1	3387	U
1	1	3390	G
1	1	3396	U
2	2	34	U
2	2	35	C
2	2	39	G
2	2	51	G
2	2	59	A
2	2	62	C
2	2	63	G
2	2	71	A
2	2	78	G
2	2	79	A
2	2	81	U
2	2	82	U
2	2	84	C
2	2	85	G
2	2	86	U
2	2	87	G
2	2	90	U
2	2	95	G
2	2	97	A
2	2	104	A
2	2	106	C
2	2	107	G
2	2	111	A
2	2	113	U
2	2	116	G
2	2	124	G
2	2	125	U
2	2	126	A
2	2	128	U
2	2	134	G
2	2	136	G
2	2	151	C
2	2	152	G
2	2	157	U
2	2	158	U
3	6	4	U
3	6	5	C

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Mol	Chain	Res	Type
3	6	6	U
3	6	7	C
3	6	8	A
3	6	9	A
3	6	13	U
3	6	14	U
3	6	15	C
3	6	16	U
3	6	17	G
3	6	23	U
3	6	24	A
3	6	34	A
3	6	36	U
3	6	39	U
3	6	40	U
3	6	42	G
3	6	43	A
3	6	47	A
3	6	52	G
3	6	53	A
3	6	54	A
3	6	56	U
3	6	57	U
3	6	58	G
3	6	59	C
3	6	228	U
3	6	231	A
3	6	232	A

All (75) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	40	A
1	1	153	U
1	1	154	U
1	1	165	A
1	1	239	G
1	1	297	G
1	1	376	G
1	1	494	G
1	1	518	G
1	1	533	A

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Mol	Chain	Res	Type
1	1	556	U
1	1	557	A
1	1	588	G
1	1	644	G
1	1	649	A
1	1	720	A
1	1	734	C
1	1	818	C
1	1	873	C
1	1	878	G
1	1	899	U
1	1	917	A
1	1	978	G
1	1	1102	A
1	1	1103	A
1	1	1104	G
1	1	1128	U
1	1	1159	A
1	1	1227	C
1	1	1241	U
1	1	1299	U
1	1	1302	A
1	1	1307	G
1	1	1329	U
1	1	1331	U
1	1	1355	A
1	1	1428	A
1	1	1451	C
1	1	1481	A
1	1	1502	C
1	1	1574	C
1	1	1581	C
1	1	1641	U
1	1	1716	U
1	1	1813	A
1	1	1820	U
1	1	1861	G
1	1	1947	G
1	1	2323	G
1	1	2837	A
1	1	2857	C
1	1	2878	G

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Mol	Chain	Res	Type
1	1	2922	G
1	1	2940	A
1	1	2946	A
1	1	2954	U
1	1	2986	U
1	1	3016	A
1	1	3055	U
1	1	3093	C
1	1	3116	G
1	1	3121	U
1	1	3171	U
1	1	3218	A
1	1	3228	C
1	1	3267	A
1	1	3269	U
1	1	3340	G
1	1	3350	C
1	1	3389	U
2	2	85	G
2	2	112	U
2	2	123	G
3	6	16	U
3	6	56	U

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	2
36	1	1
4	L	1
23	P	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	135:ALA	C	136:MET	N	6.21
1	1	1792:C	O3'	1793:C	P	5.60
1	L	8:PRO	C	9:ILE	N	4.88
1	1	966:U	O3'	967:A	P	4.55
1	P	131:ARG	C	132:ALA	N	3.63

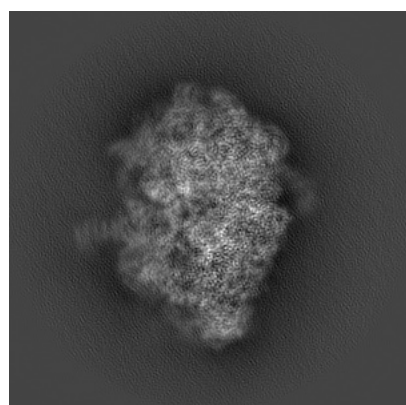
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3891. These allow visual inspection of the internal detail of the map and identification of artifacts.

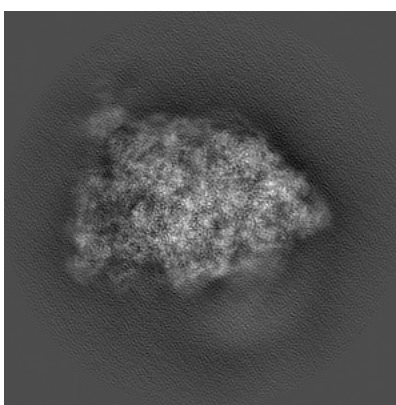
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

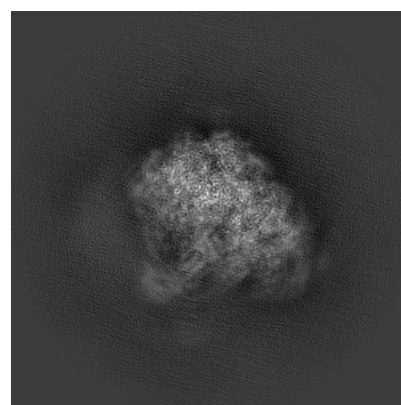
6.1.1 Primary map



X



Y

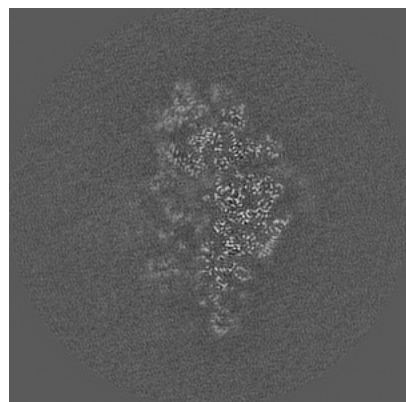


Z

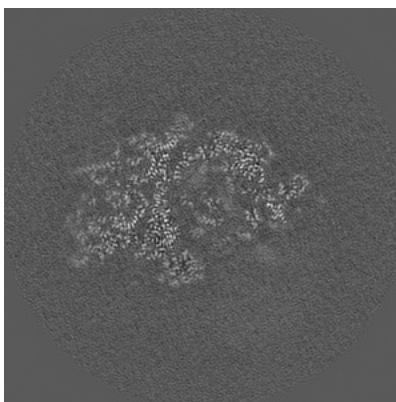
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

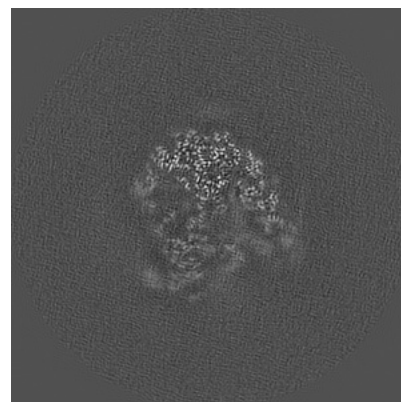
6.2.1 Primary map



X Index: 210



Y Index: 210

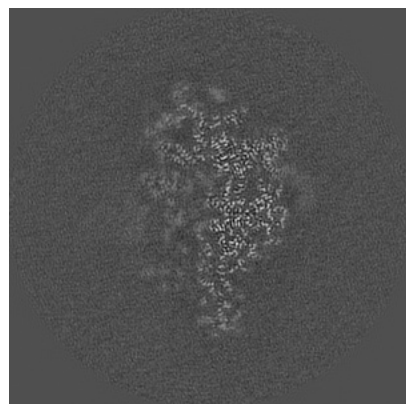


Z Index: 210

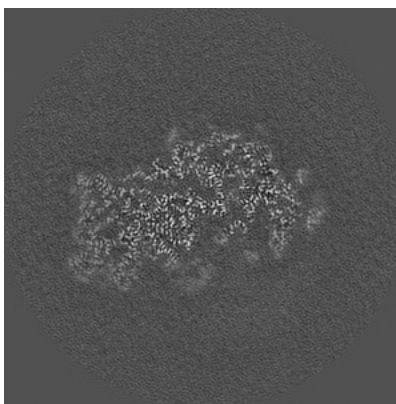
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

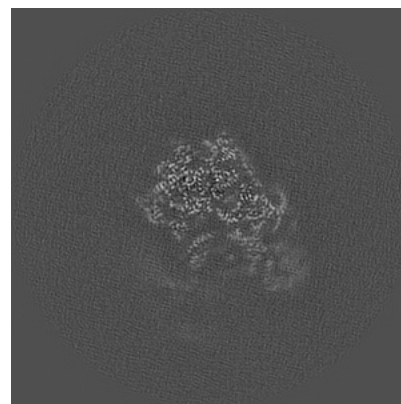
6.3.1 Primary map



X Index: 216



Y Index: 227



Z Index: 172

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

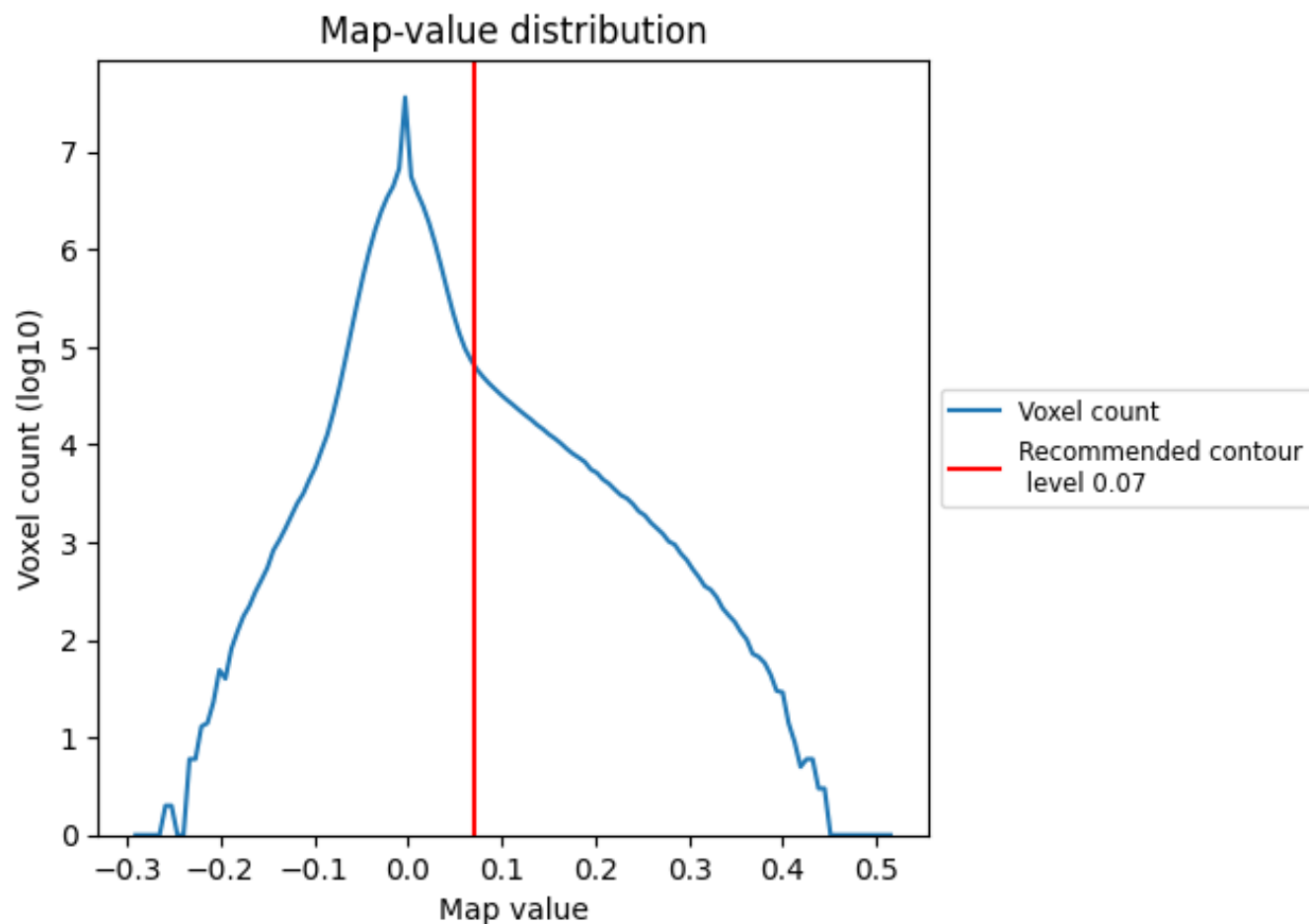
6.5 Mask visualisation

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

7 Map analysis [i](#)

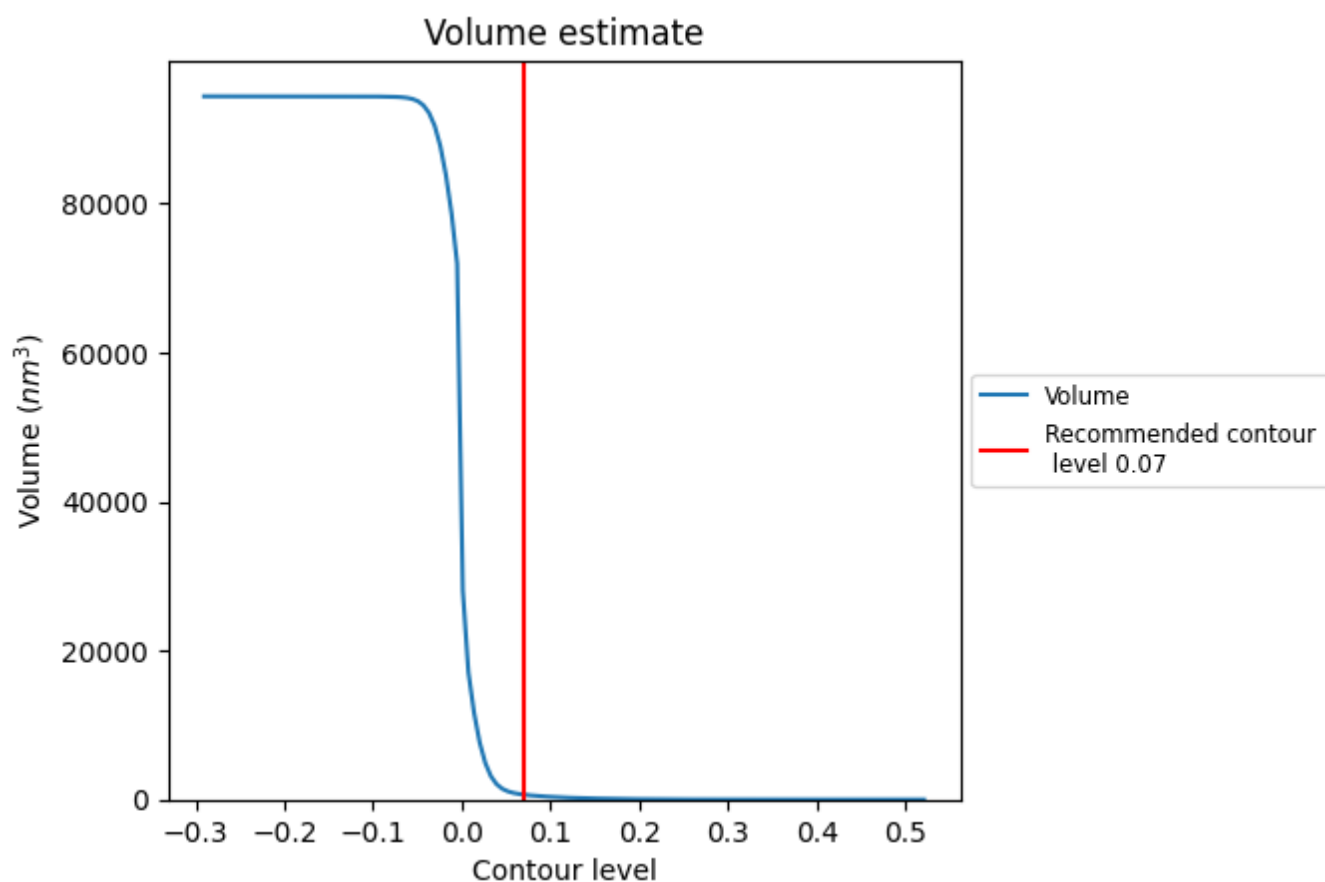
This section contains the results of statistical analysis of the map.

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.

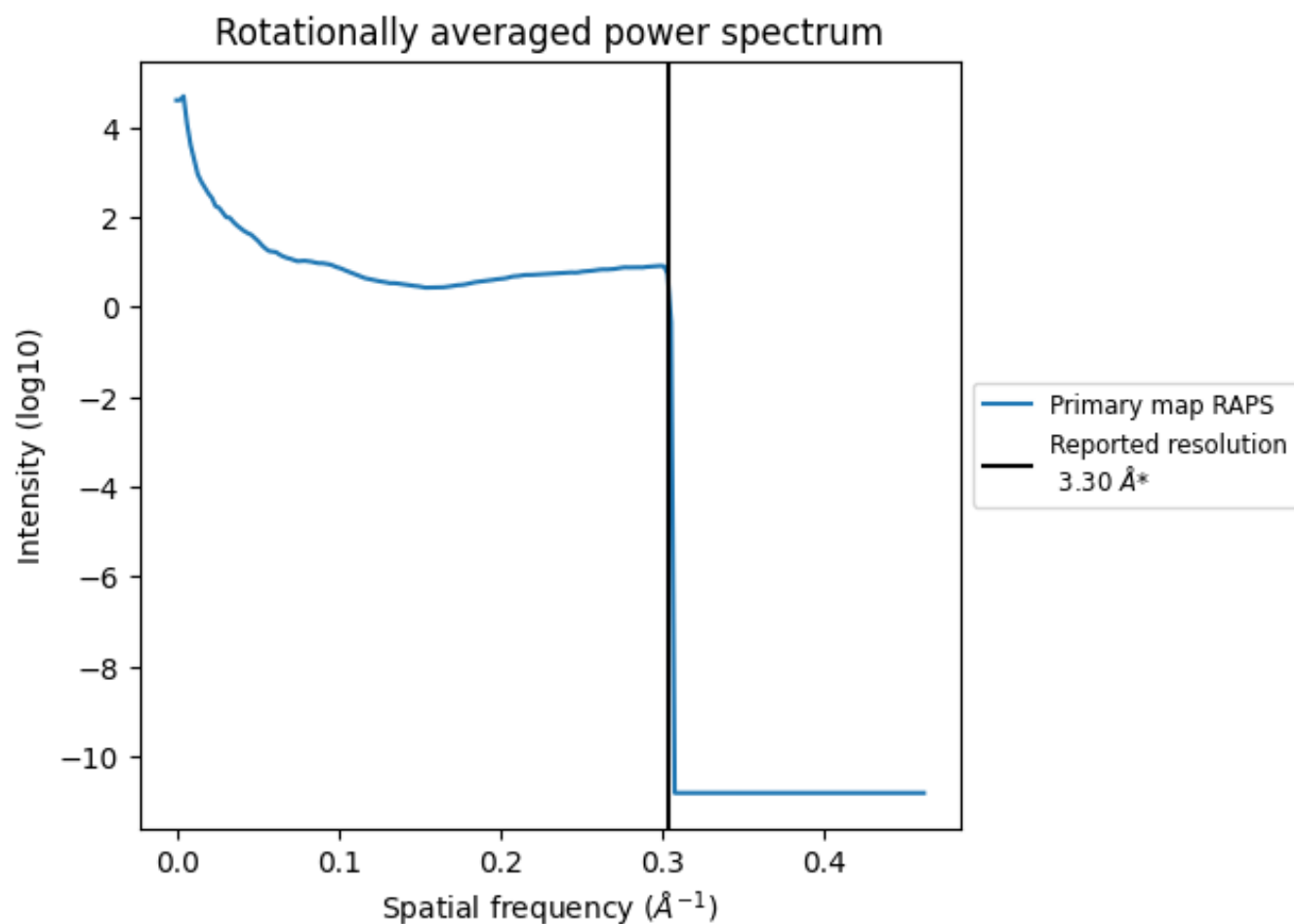
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 662 nm^3 ; this corresponds to an approximate mass of 598 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 ⓘ

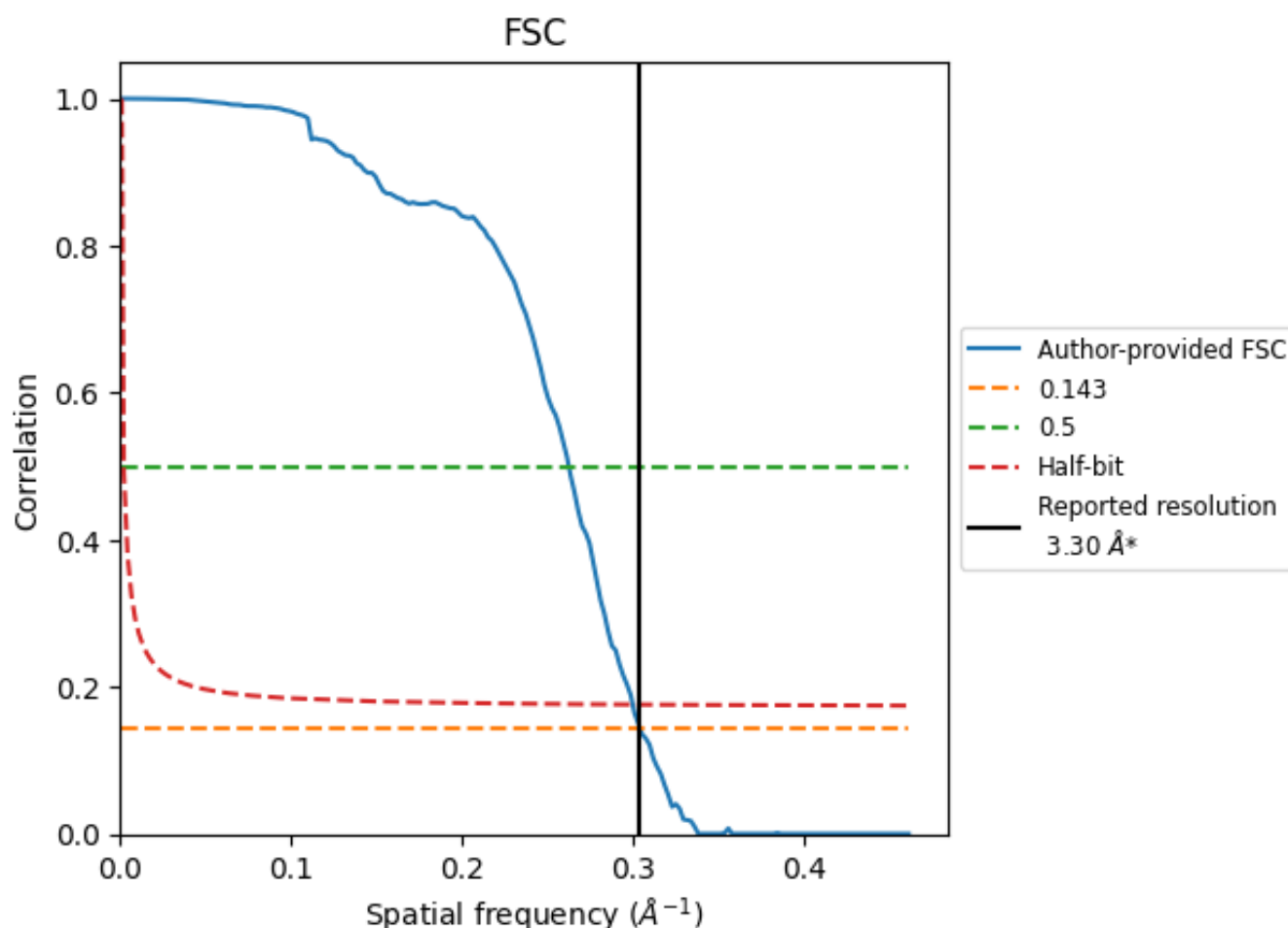


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

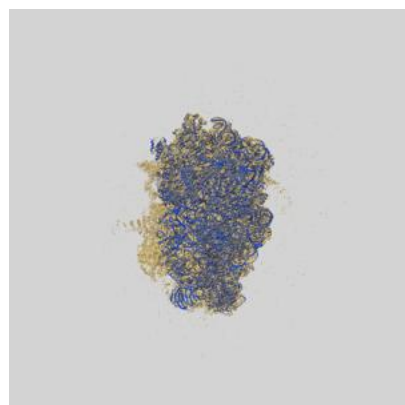
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.81	3.33
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

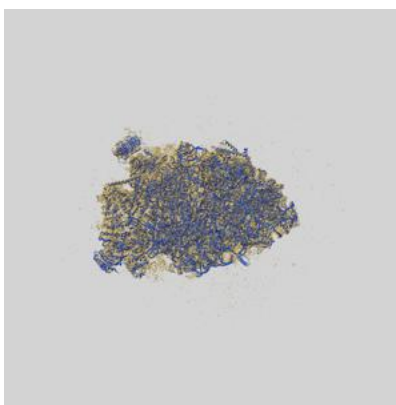
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3891 and PDB model 6ELZ. Per-residue inclusion information can be found in section [3](#) on page [13](#).

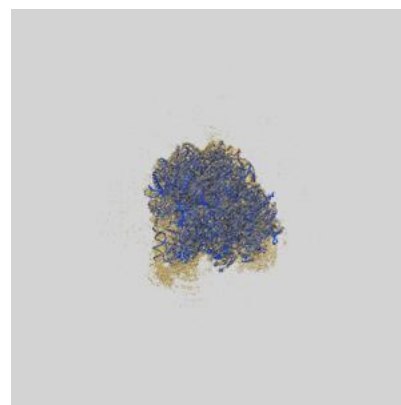
9.1 Map-model overlay [i](#)



X



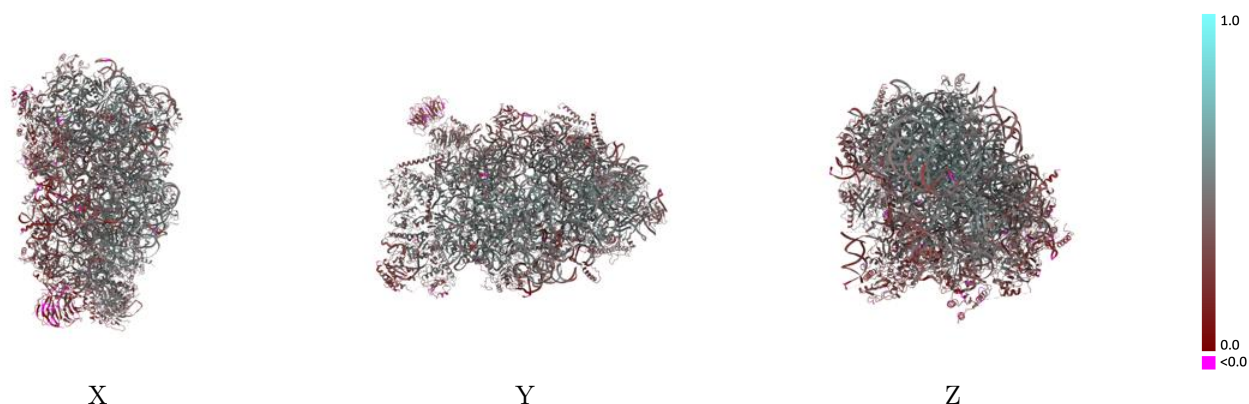
Y



Z

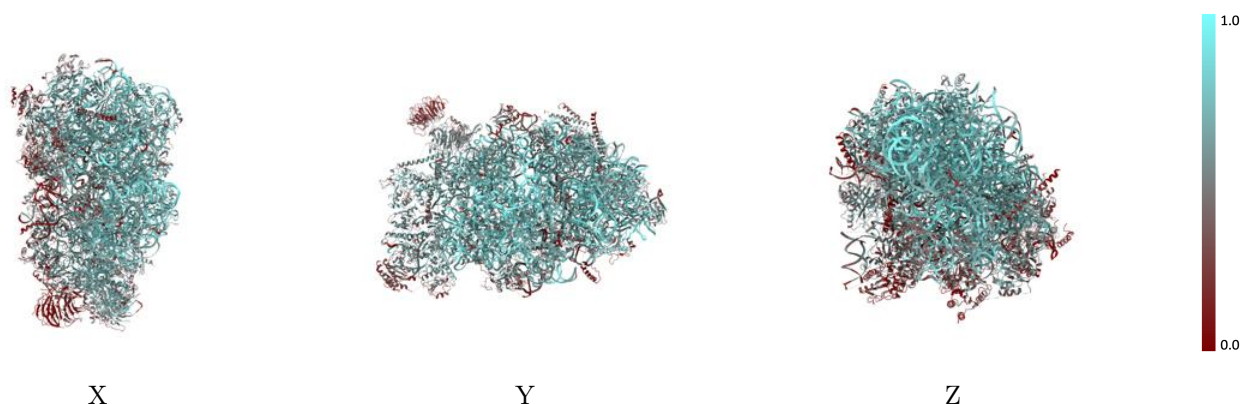
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



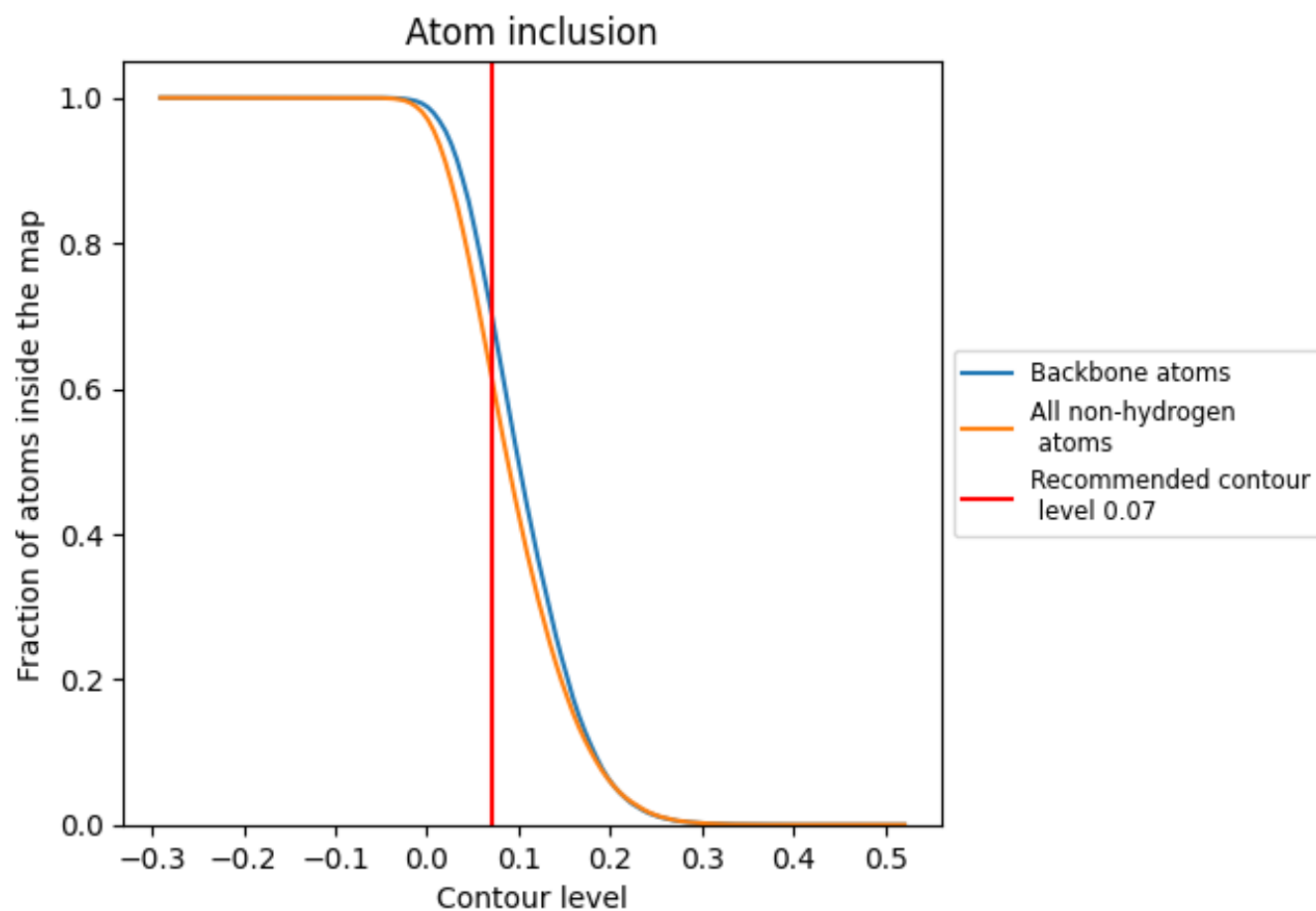
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 62% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6207	 0.4140
1	 0.7352	 0.4370
2	 0.8357	 0.5050
6	 0.6277	 0.3820
A	 0.5842	 0.4050
B	 0.6707	 0.4390
C	 0.7145	 0.4860
D	 0.4698	 0.3600
E	 0.6356	 0.4550
F	 0.6866	 0.4660
G	 0.6780	 0.4760
H	 0.6660	 0.4790
I	 0.3953	 0.3330
J	 0.3860	 0.3260
K	 0.4157	 0.3330
L	 0.7109	 0.4840
M	 0.6949	 0.4880
N	 0.7753	 0.5280
O	 0.7801	 0.5250
P	 0.6383	 0.4320
Q	 0.6465	 0.4450
R	 0.4941	 0.3330
S	 0.6335	 0.4590
T	 0.0585	 0.2390
U	 0.3076	 0.2610
V	 0.5862	 0.4250
W	 0.4401	 0.3520
X	 0.6568	 0.4540
Y	 0.7143	 0.4770
Z	 0.5359	 0.3570
a	 0.4039	 0.3420
b	 0.4125	 0.3440
c	 0.3995	 0.3100
d	 0.5537	 0.4020
e	 0.7070	 0.5100



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Chain	Atom inclusion	Q-score
f	 0.7674	 0.5370
g	 0.6068	 0.4100
h	 0.6607	 0.4800
i	 0.5190	 0.3550
j	 0.7935	 0.5330
k	 0.4591	 0.3270
l	 0.4371	 0.3620
m	 0.5001	 0.3630
n	 0.6012	 0.4280
o	 0.5032	 0.3730
p	 0.1297	 0.1550
q	 0.2686	 0.2930
r	 0.4557	 0.4030
s	 0.4983	 0.4580
t	 0.5312	 0.3940
u	 0.5187	 0.3490
v	 0.6277	 0.4400
w	 0.4276	 0.3650
y	 0.5347	 0.3550
z	 0.2442	 0.3400