



Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 03:11 AM JST

PDB ID : 6KE6
EMDB ID : EMD-9964
Title : 3.4 angstrom cryo-EM structure of yeast 90S small subunit preribosome
Authors : Du, Y.; Ye, K.; An, W.
Deposited on : 2019-07-03
Resolution : 3.40 Å(reported)
Based on initial models : 5WLC, 5WYJ

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:

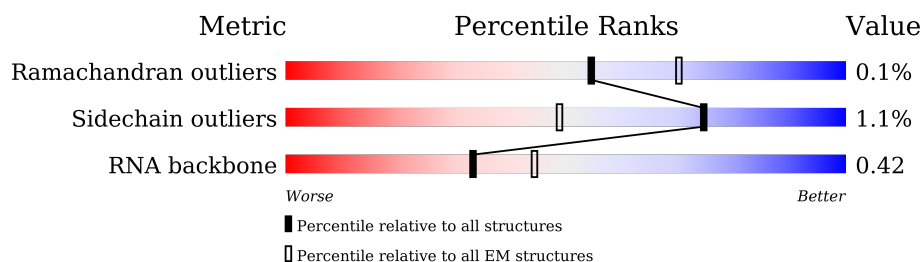
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 3.40 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	3A	333	
2	5A	700	
3	SA	1807	
4	SC	255	
5	SF	261	
6	SG	225	
7	SH	236	
8	SI	190	

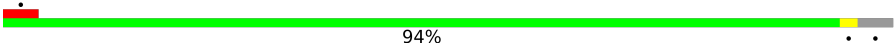
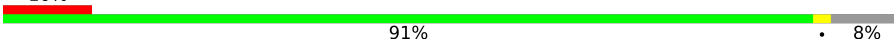


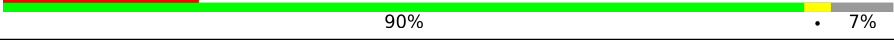

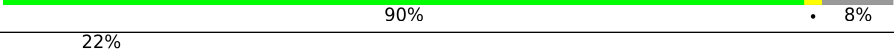
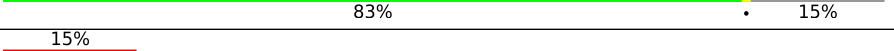
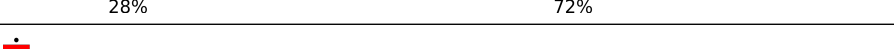
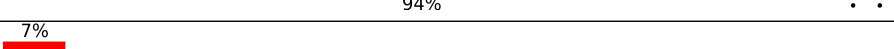
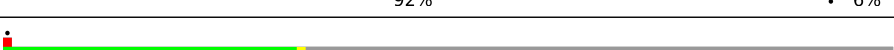

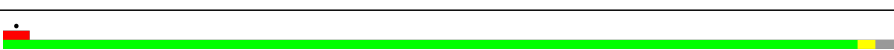

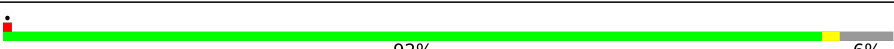





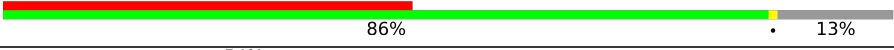




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Mol	Chain	Length	Quality of chain
9	SJ	200	
10	SK	197	
11	SM	156	
12	SN	143	
13	SO	151	
14	SP	137	
15	SR	143	
16	ST	146	
17	SX	130	
18	SY	145	
19	SZ	135	
20	Sc	82	
21	Sd	67	
22	3B	327	
22	3C	327	
23	3D	504	
24	3E	511	
25	3F	573	
26	3G	126	
26	3H	126	
27	A4	776	
28	A5	643	
29	A8	713	
30	A9	575	
31	AE	1769	

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Mol	Chain	Length	Quality of chain
32	AF	513	
33	AG	896	
34	B1	923	
35	B2	943	
36	B3	817	
37	B8	594	
38	BE	939	
39	B6	440	
40	5B	214	
41	5C	554	
42	5D	250	
43	5E	593	
44	5F	183	
45	5G	290	
46	5H	610	
47	5I	489	
48	5J	217	
49	5K	189	
50	RA	707	
51	RB	357	
52	RC	316	
53	RE	1237	
54	RF	297	
55	RG	252	
55	RH	252	

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Mol	Chain	Length	Quality of chain
56	RI	274	
57	RJ	1183	
58	RK	367	
59	RL	1056	
59	RM	1056	
60	RN	810	
61	RO	552	
62	RP	2493	
63	RQ	899	
64	RS	483	
65	RT	326	
66	RV	346	
67	X1	347	

2 Entry composition

There are 70 unique types of molecules in this entry. The entry contains 224791 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 U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3A	175	Total	C	N	O	P	0	0
			3711	1661	648	1227	175		

- Molecule 2 is a RNA chain called 5' ETS.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5A	522	Total	C	N	O	P	0	0
			11143	4979	1982	3660	522		

- Molecule 3 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SA	1310	Total	C	N	O	P	0	0
			27940	12487	4981	9162	1310		

- Molecule 4 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SC	219	Total	C	N	O	S	0	0
			1751	1109	321	317	4		

- Molecule 5 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SF	229	Total	C	N	O	S	0	0
			1815	1161	331	320	3		

- Molecule 6 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SG	213	Total	C	N	O	S	0	0
			1669	1045	307	314	3		

- Molecule 7 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SH	112	Total	C	N	O	S	0	0
			879	562	155	160	2		

- Molecule 8 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SI	165	Total	C	N	O		0	0
			1321	853	226	242			

- Molecule 9 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SJ	166	Total	C	N	O	S	0	0
			1324	824	262	236	2		

- Molecule 10 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SK	171	Total	C	N	O	S	0	0
			1388	879	268	240	1		

- Molecule 11 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SM	123	Total	C	N	O	S	0	0
			997	641	189	164	3		

- Molecule 12 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SN	119	Total	C	N	O	S	0	0
			865	545	151	167	2		

- Molecule 13 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SO	134	Total	C	N	O	S	0	0
			1087	698	202	186	1		

- Molecule 14 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SP	118	Total	C	N	O	S	0	0
			868	536	164	165	3		

- Molecule 15 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SR	125	Total	C	N	O		0	0
			973	625	174	174			

- Molecule 16 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	ST	113	Total	C	N	O	S	0	0
			918	578	174	164	2		

- Molecule 17 is a protein called 40S ribosomal protein S22-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SX	127	Total	C	N	O	S	0	0
			1003	640	183	177	3		

- Molecule 18 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SY	103	Total	C	N	O	S	0	0
			786	503	144	137	2		

- Molecule 19 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SZ	102	Total	C	N	O		0	0
			809	517	148	144			

- Molecule 20 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Sc	80	Total	C	N	O	S	0	0
			603	377	109	112	5		

- Molecule 21 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Sd	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 22 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	3B	240	Total	C	N	O	S	0	0
			1865	1184	333	338	10		
22	3C	225	Total	C	N	O	S	0	0
			1763	1120	316	317	10		

- Molecule 23 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	3D	369	Total	C	N	O	S	0	0
			2848	1811	489	540	8		

- Molecule 24 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	3E	431	Total	C	N	O	S	0	0
			3028	1888	543	588	9		

- Molecule 25 is a protein called Ribosomal RNA-processing protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	3F	434	Total	C	N	O	S	0	0
			3473	2211	603	649	10		

- Molecule 26 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	3G	121	Total	C	N	O	S	0	0
			916	583	158	171	4		
26	3H	121	Total	C	N	O	S	0	0
			916	583	158	171	4		

- Molecule 27 is a protein called U3 small nucleolar RNA-associated protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	A4	662	Total	C	N	O	S	0	0
			5226	3309	910	986	21		

- Molecule 28 is a protein called U3 small nucleolar RNA-associated protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A5	514	Total	C	N	O	S	0	0
			3976	2520	688	755	13		

- Molecule 29 is a protein called U3 small nucleolar RNA-associated protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	A8	548	Total	C	N	O	S	0	0
			3307	2054	608	642	3		

- Molecule 30 is a protein called U3 small nucleolar RNA-associated protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	A9	128	Total	C	N	O	S	0	0
			939	594	173	170	2		

- Molecule 31 is a protein called U3 small nucleolar RNA-associated protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AE	777	Total	C	N	O	S	0	0
			6197	3998	1014	1166	19		

- Molecule 32 is a protein called U3 small nucleolar RNA-associated protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AF	493	Total	C	N	O	S	0	0
			3911	2462	702	735	12		

- Molecule 33 is a protein called NET1-associated nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	AG	826	Total	C	N	O	S	0	0
			6570	4181	1111	1259	19		

- Molecule 34 is a protein called Periodic tryptophan protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B1	834	Total	C	N	O	S	0	0
			6635	4223	1140	1253	19		

- Molecule 35 is a protein called U3 small nucleolar RNA-associated protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	B2	851	Total	C	N	O	S	0	0
			6723	4294	1133	1269	27		

- Molecule 36 is a protein called U3 small nucleolar RNA-associated protein 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	B3	757	Total	C	N	O	S	0	0
			5919	3769	993	1130	27		

- Molecule 37 is a protein called U3 small nucleolar RNA-associated protein 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	B8	477	Total	C	N	O	S	0	0
			3764	2387	662	705	10		

- Molecule 38 is a protein called U3 small nucleolar RNA-associated protein 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BE	865	Total	C	N	O	S	0	0
			6810	4322	1175	1292	21		

- Molecule 39 is a protein called U3 small nucleolar RNA-associated protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	B6	374	Total	C	N	O	S	0	0
			2800	1782	501	505	12		

- Molecule 40 is a protein called Bud site selection protein 21.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	5B	60	Total	C	N	O	0	0
			495	310	101	84		

- Molecule 41 is a protein called U3 small nucleolar RNA-associated protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	5C	535	Total	C	N	O	S	0	0
			4237	2656	762	807	12		

- Molecule 42 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	5D	235	Total	C	N	O	S	0	0
			1972	1226	380	359	7		

- Molecule 43 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	5E	204	Total	C	N	O	S	0	0
			1647	1021	294	328	4		

- Molecule 44 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	5F	182	Total	C	N	O	S	0	0
			1530	967	287	269	7		

- Molecule 45 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	5G	282	Total	C	N	O	S	0	0
			2296	1441	430	418	7		

- Molecule 46 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	5H	136	Total	C	N	O		0	0
			1065	658	211	196			

- Molecule 47 is a protein called Protein SOF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	5I	461	Total	C	N	O	S	0	0
			3765	2354	686	709	16		

- Molecule 48 is a protein called rRNA-processing protein FCF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	5J	144	Total	C	N	O	S	0	0
			1219	769	230	215	5		

- Molecule 49 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	5K	175	Total	C	N	O	S	0	0
			1403	896	256	241	10		

- Molecule 50 is a protein called Ribosome biogenesis protein ENP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	RA	338	Total	C	N	O	S	0	0
			2709	1713	463	524	9		

- Molecule 51 is a protein called U3 small nucleolar ribonucleoprotein protein LCP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	RB	134	Total	C	N	O	S	0	0
			1108	664	227	214	3		

- Molecule 52 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	RC	278	Total	C	N	O	S	0	0
			2207	1408	391	395	13		

- Molecule 53 is a protein called U3 small nucleolar RNA-associated protein 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	RE	1079	Total	C	N	O	S	0	0
			8716	5666	1437	1589	24		

- Molecule 54 is a protein called Ribosomal RNA-processing protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	RF	241	Total	C	N	O	S	0	0
			1963	1253	335	367	8		

- Molecule 55 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	RG	216	Total	C	N	O	S	0	0
			1701	1079	296	315	11		
55	RH	230	Total	C	N	O	S	0	0
			1799	1142	313	333	11		

- Molecule 56 is a protein called Ribosome biogenesis protein UTP30.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	RI	252	Total	C	N	O	S	0	0
			2045	1309	362	366	8		

- Molecule 57 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	RJ	796	Total	C	N	O	S	0	0
			6379	4086	1136	1128	29		

- Molecule 58 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	RK	360	Total	C	N	O	S	0	0
			2781	1781	473	516	11		

- Molecule 59 is a protein called RNA cytidine acetyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	RL	805	Total	C	N	O	S	0	0
			4539	2760	885	887	7		
59	RM	765	Total	C	N	O		0	0
			3774	2244	765	765			

- Molecule 60 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	RN	587	Total	C	N	O	S	0	0
			4363	2758	791	803	11		

- Molecule 61 is a protein called Nucleolar complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	RO	525	Total	C	N	O	S	0	0
			3766	2412	646	696	12		

- Molecule 62 is a protein called U3 small nucleolar RNA-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	RP	2052	Total	C	N	O		0	0
			10202	6098	2052	2052			

- Molecule 63 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	RQ	226	Total	C	N	O	S	0	0
			1651	1023	313	313	2		

- Molecule 64 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	RS	251	Total	C	N	O	S	0	0
			2051	1340	349	359	3		

- Molecule 65 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	RT	171	Total	C	N	O	S	0	0
			1357	864	249	240	4		

- Molecule 66 is a protein called Protein FAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	RV	190	Total	C	N	O	S	0	0
			1448	891	290	264	3		

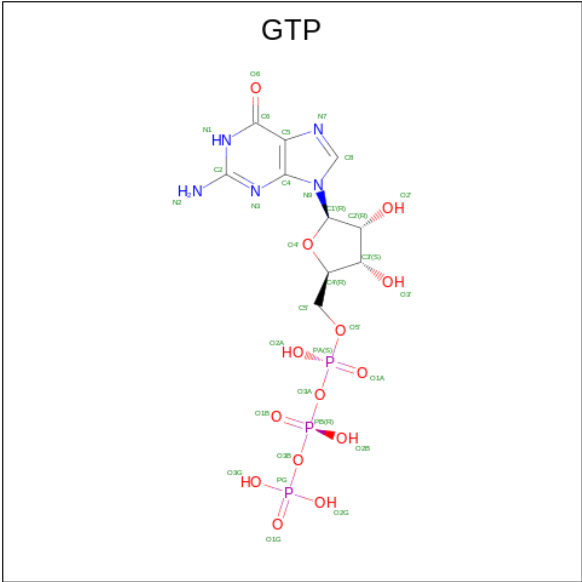
- Molecule 67 is a protein called Unassigned helices.

Mol	Chain	Residues	Atoms				AltConf	Trace
67	X1	127	Total	C	N	O	0	0
			635	381	127	127		

- Molecule 68 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
68	Sc	1	Total	Zn	0
			1	1	
68	5K	1	Total	Zn	0
			1	1	

- Molecule 69 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

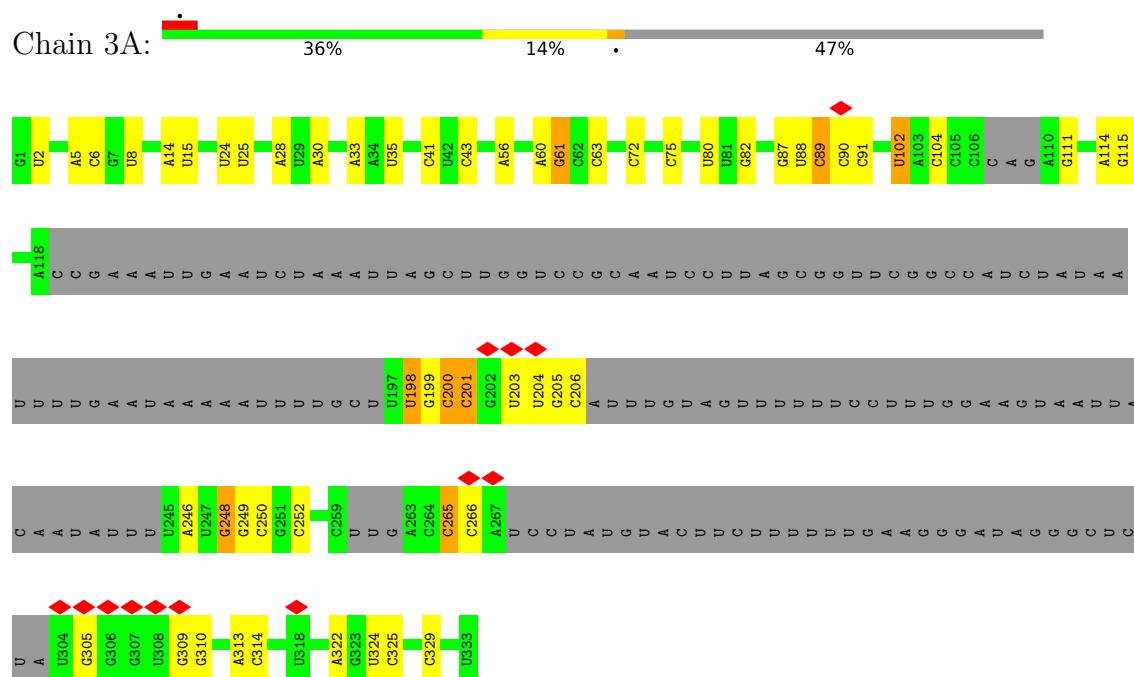
- Molecule 70 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
70	RJ	1	Total	Mg	0
			1	1	

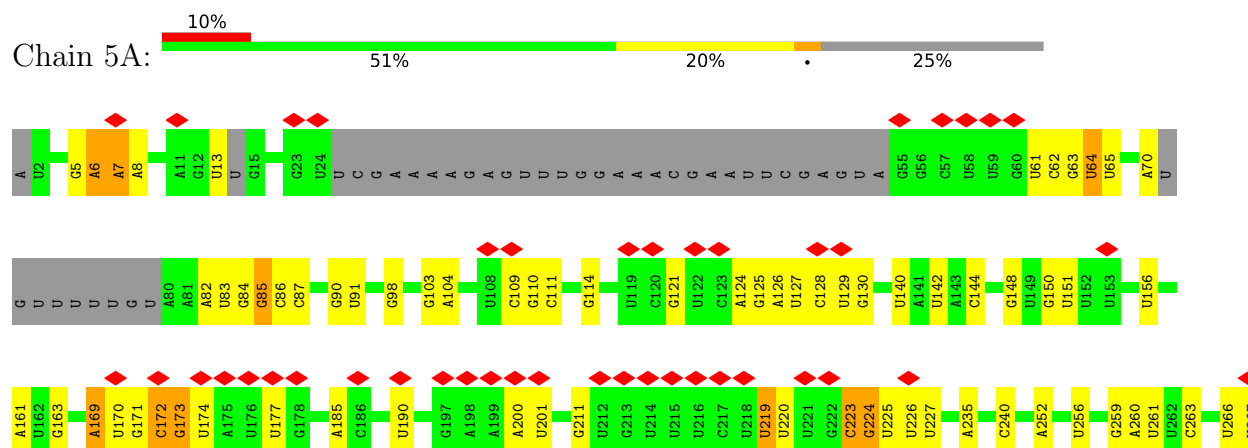
3 Residue-property plots [i](#)

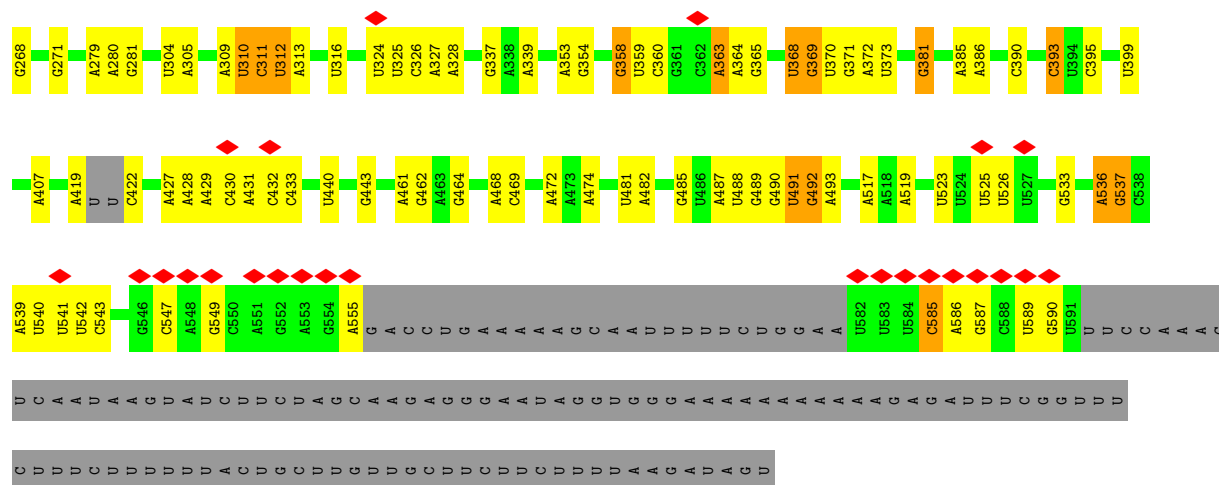
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: U3 snoRNA

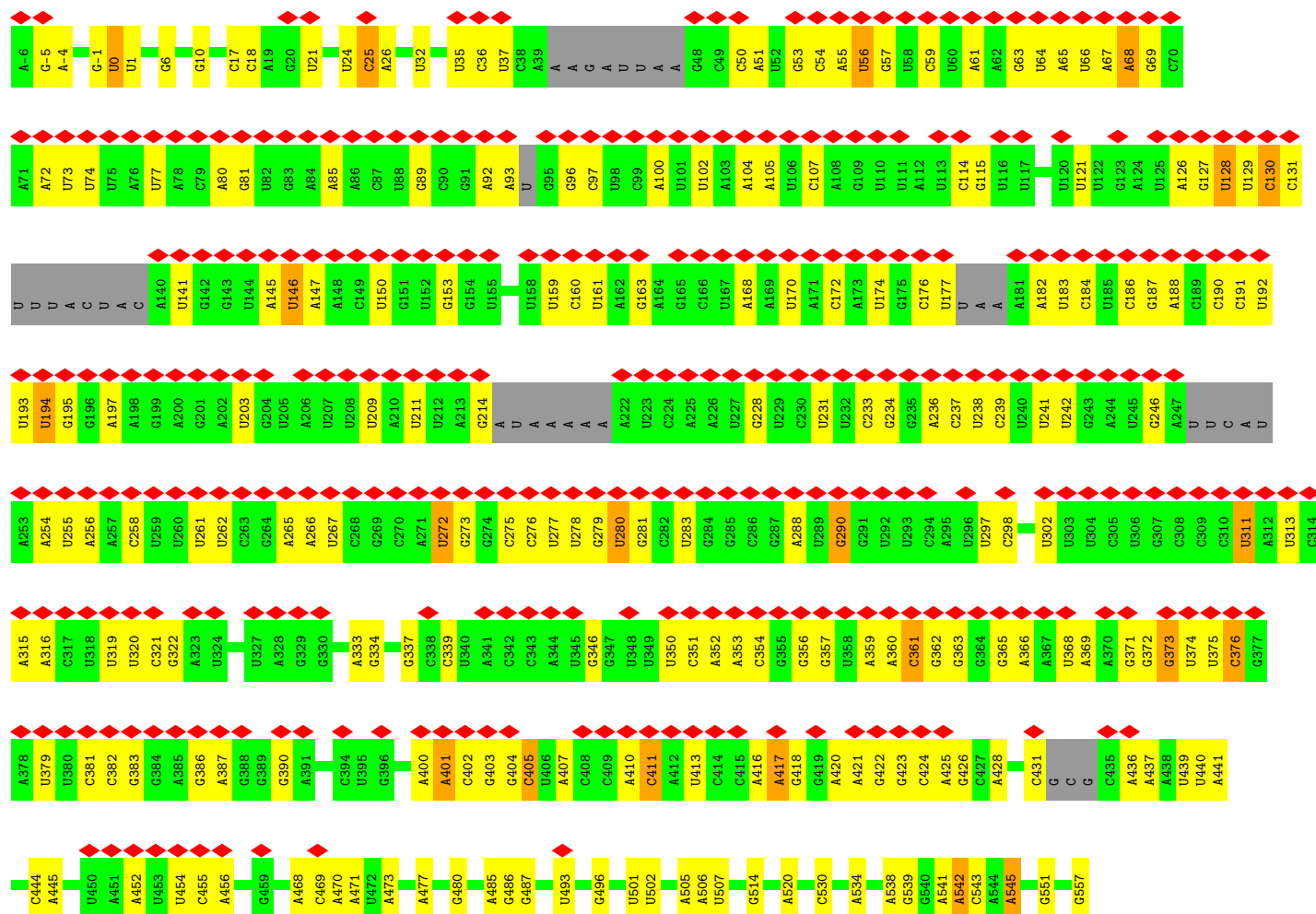
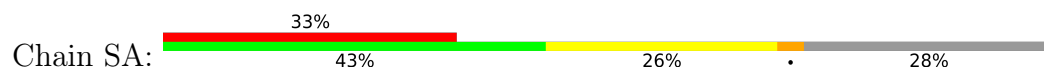


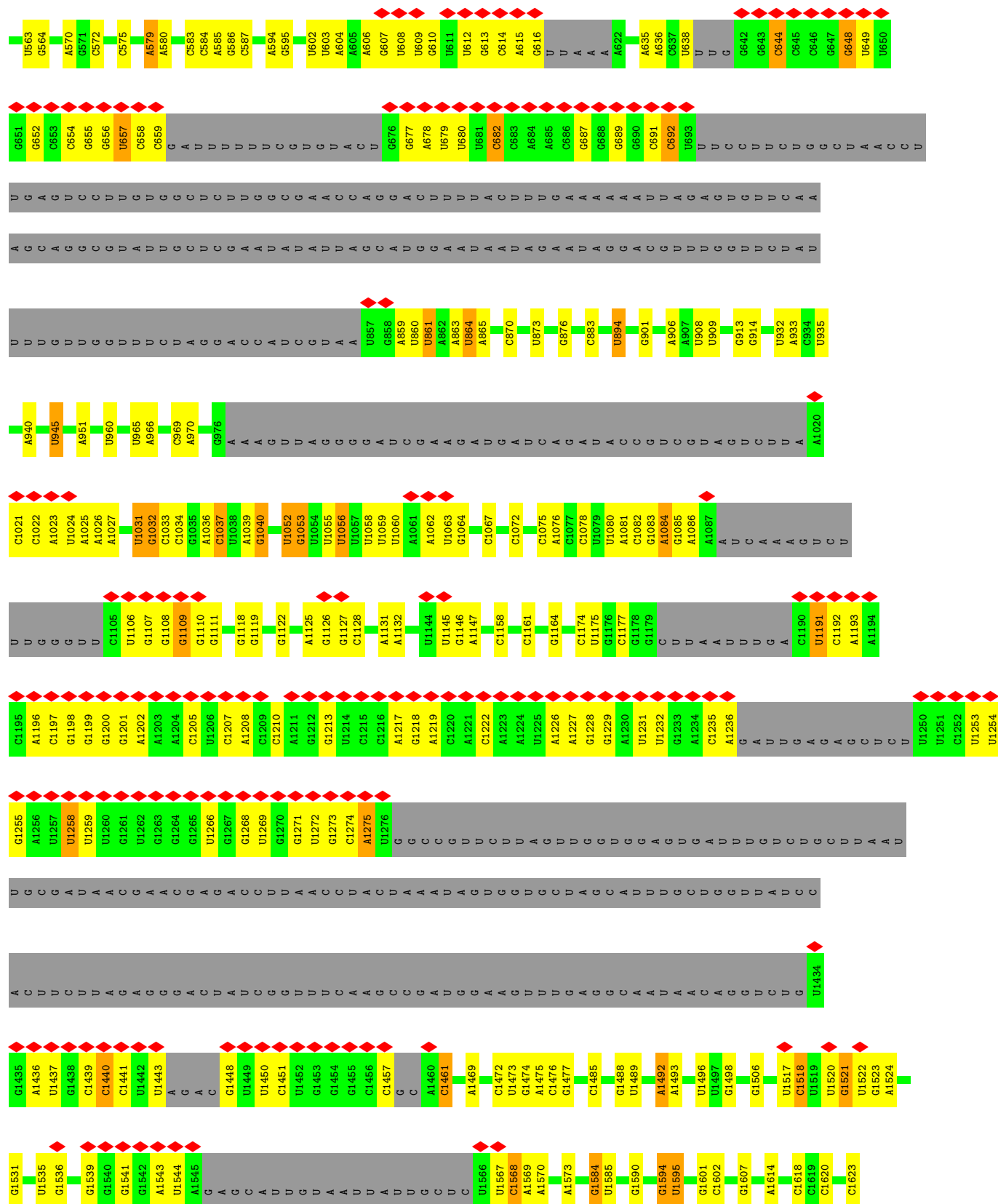
• Molecule 2: 5' ETS





• Molecule 3: 18S rRNA

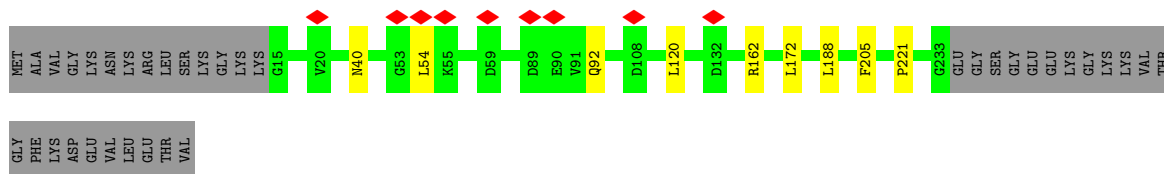






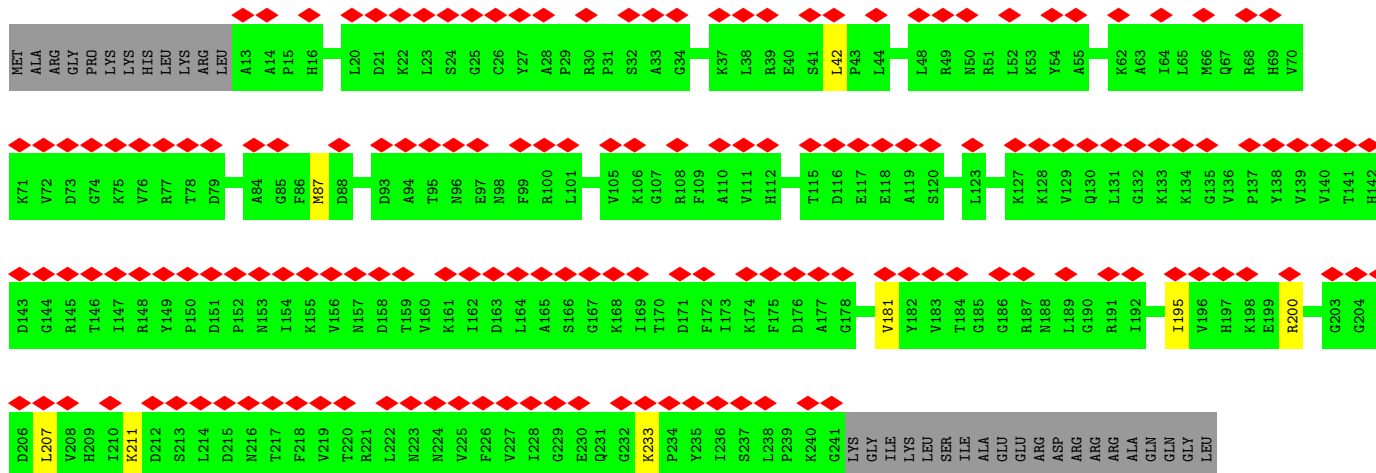
• Molecule 4: 40S ribosomal protein S1-A

Chain SC: 82% 14%



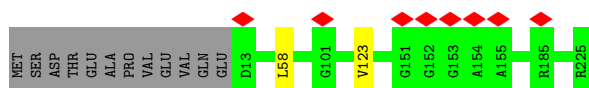
• Molecule 5: 40S ribosomal protein S4-A

Chain SF: 62% 85% 12%

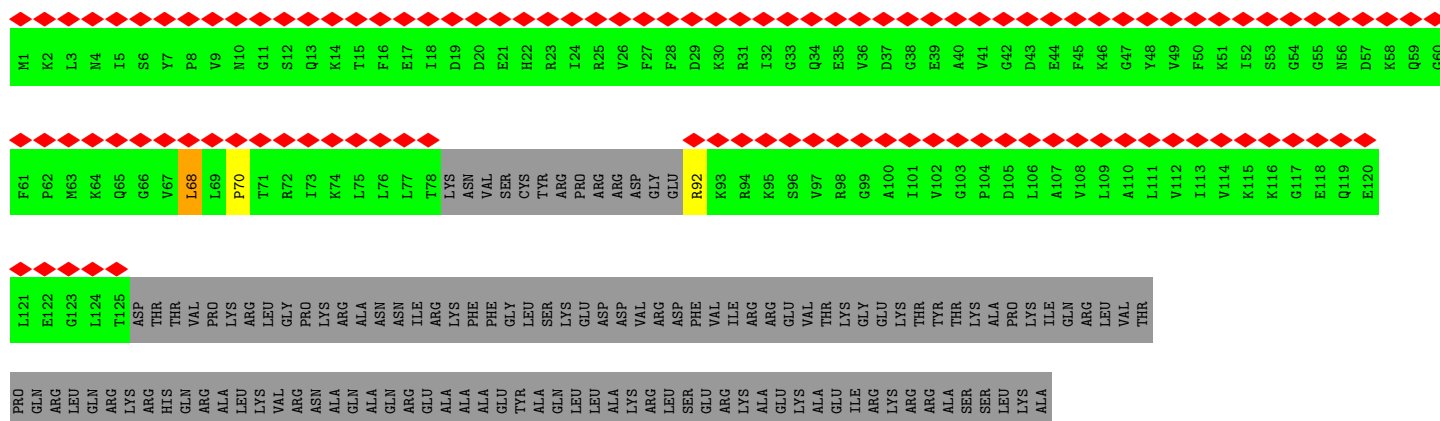


• Molecule 6: 40S ribosomal protein S5

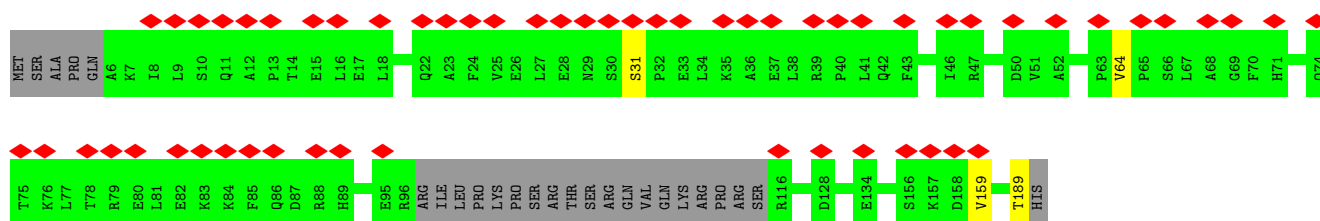
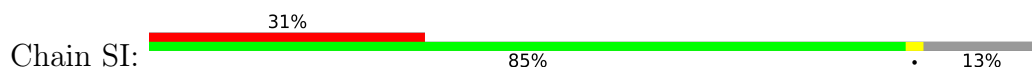
Chain SG: 94% 5%



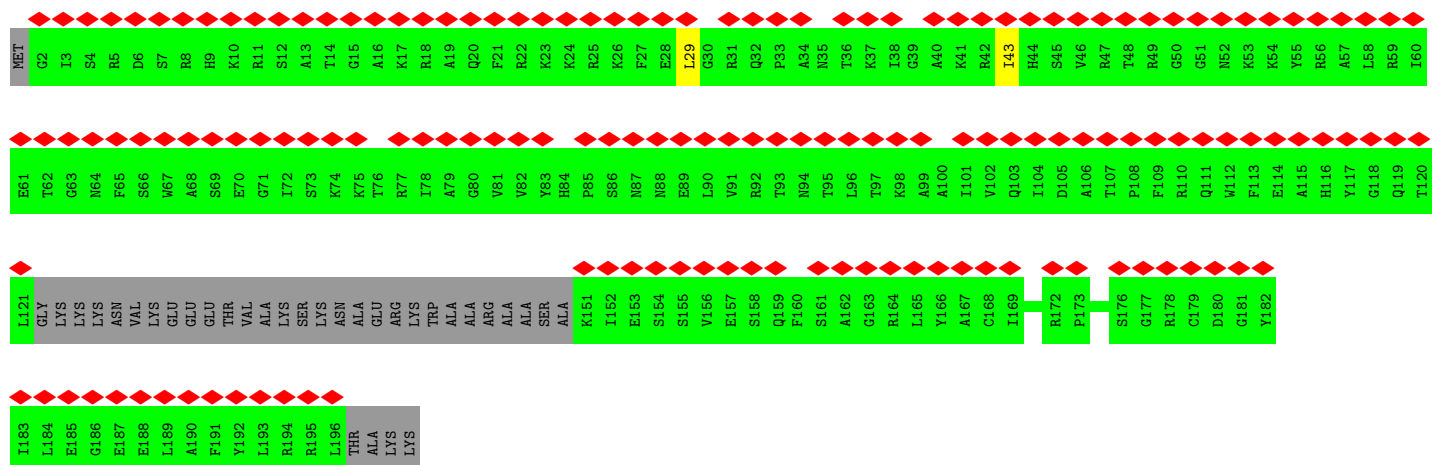
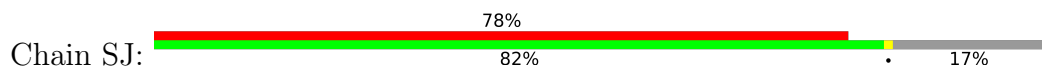
• Molecule 7: 40S ribosomal protein S6-A



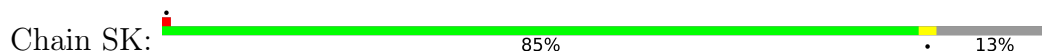
• Molecule 8: 40S ribosomal protein S7-A

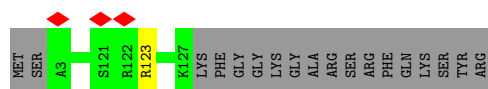


• Molecule 9: 40S ribosomal protein S8-A

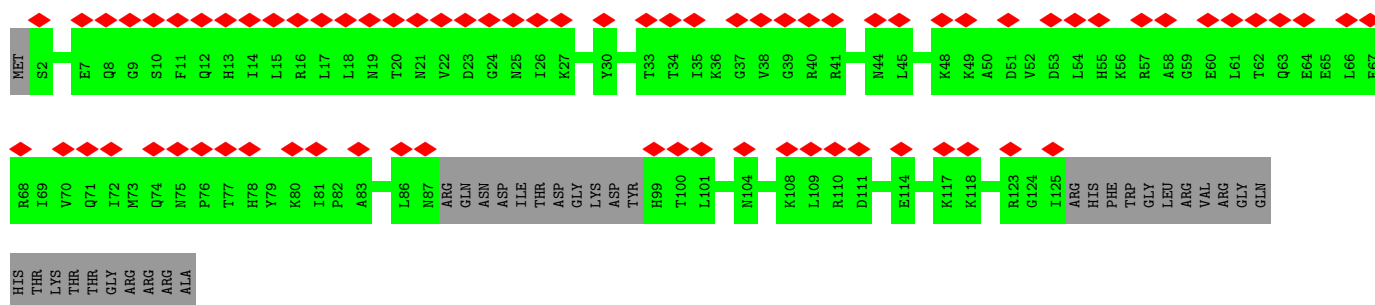
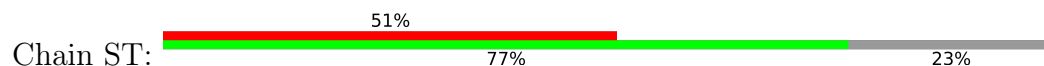


• Molecule 10: 40S ribosomal protein S9-A

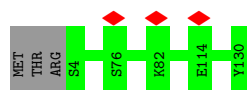




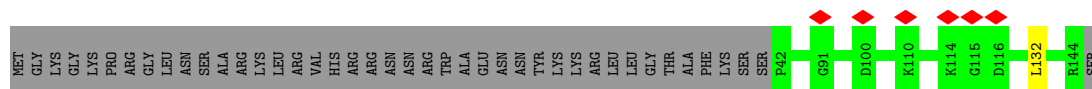
- Molecule 16: 40S ribosomal protein S18-A



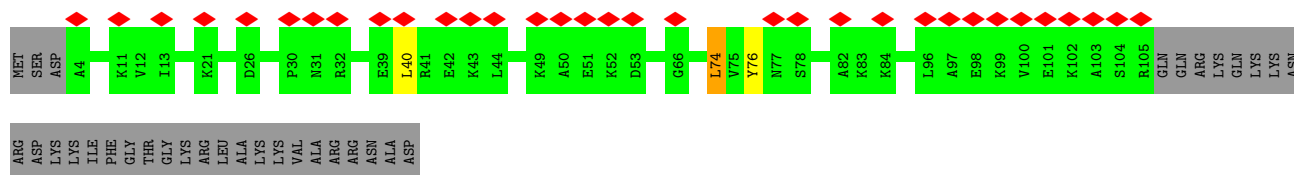
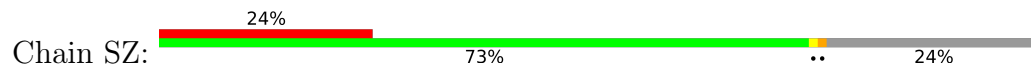
- Molecule 17: 40S ribosomal protein S22-B



- Molecule 18: 40S ribosomal protein S23-A



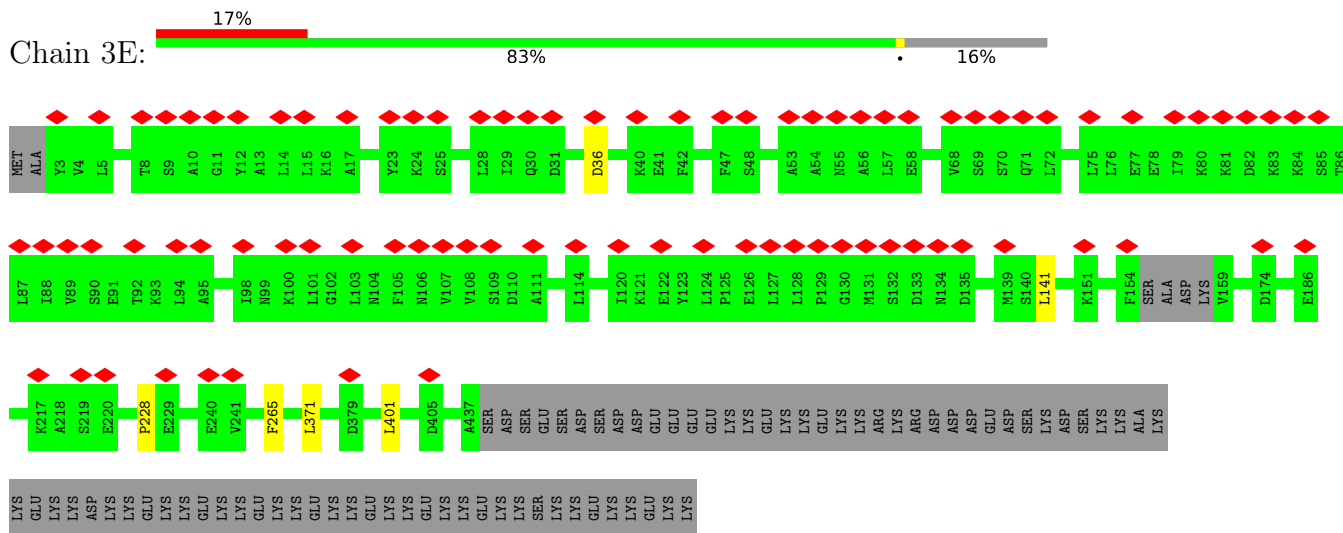
- Molecule 19: 40S ribosomal protein S24-A



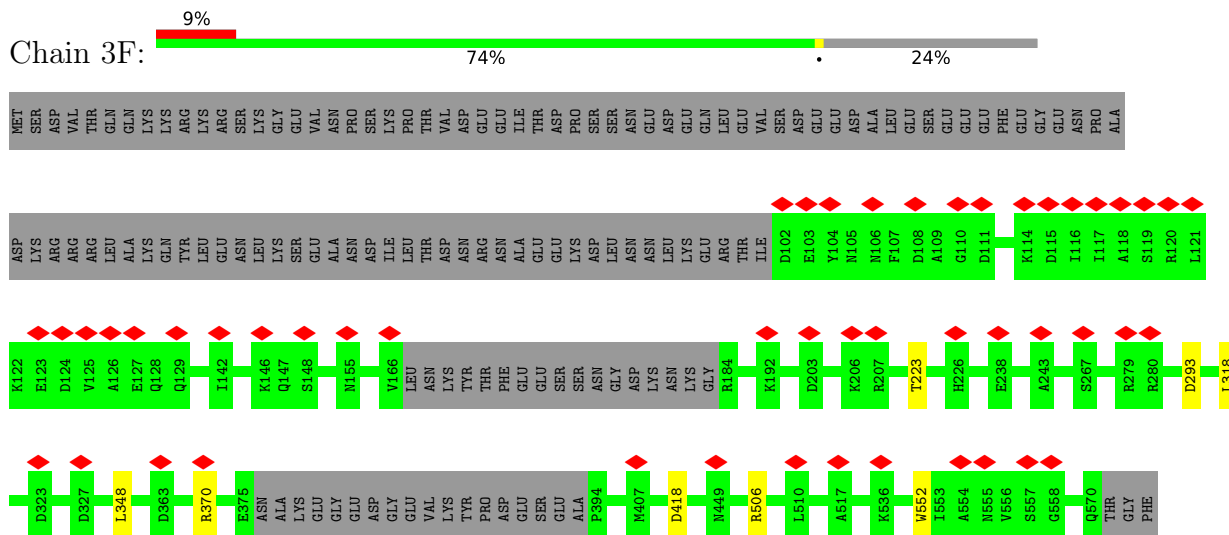
- Molecule 20: 40S ribosomal protein S27-A



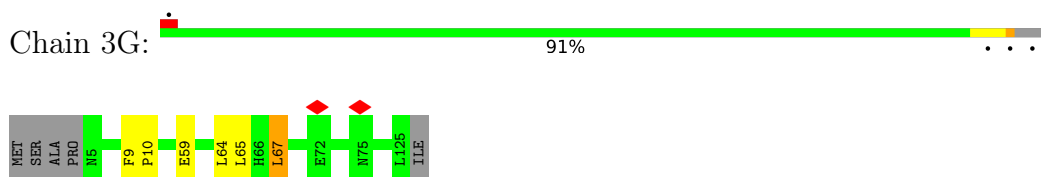
- Molecule 24: Nucleolar protein 58



- Molecule 25: Ribosomal RNA-processing protein 9

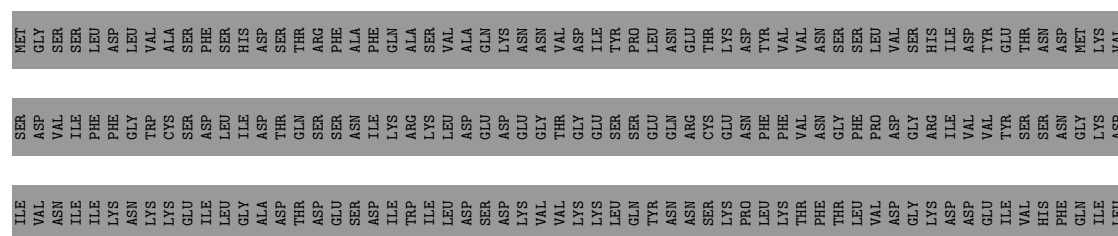


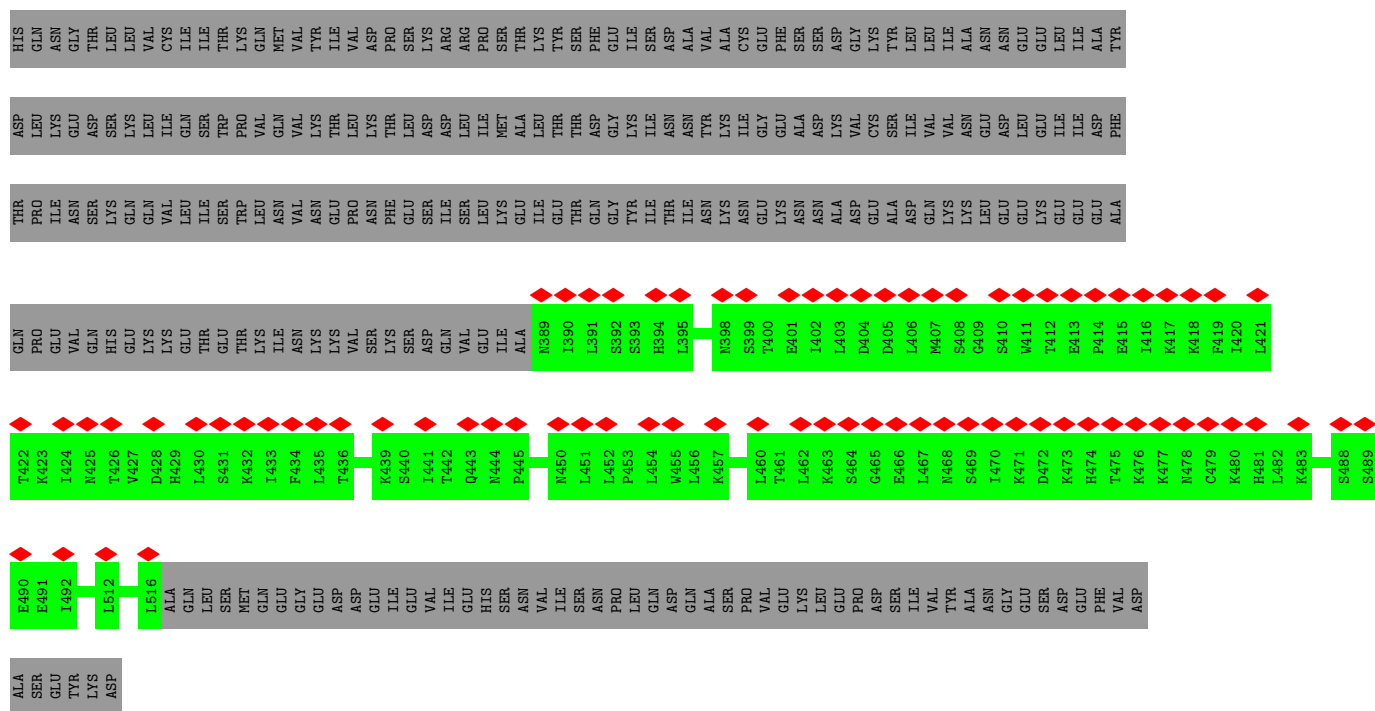
- Molecule 26: 13 kDa ribonucleoprotein-associated protein



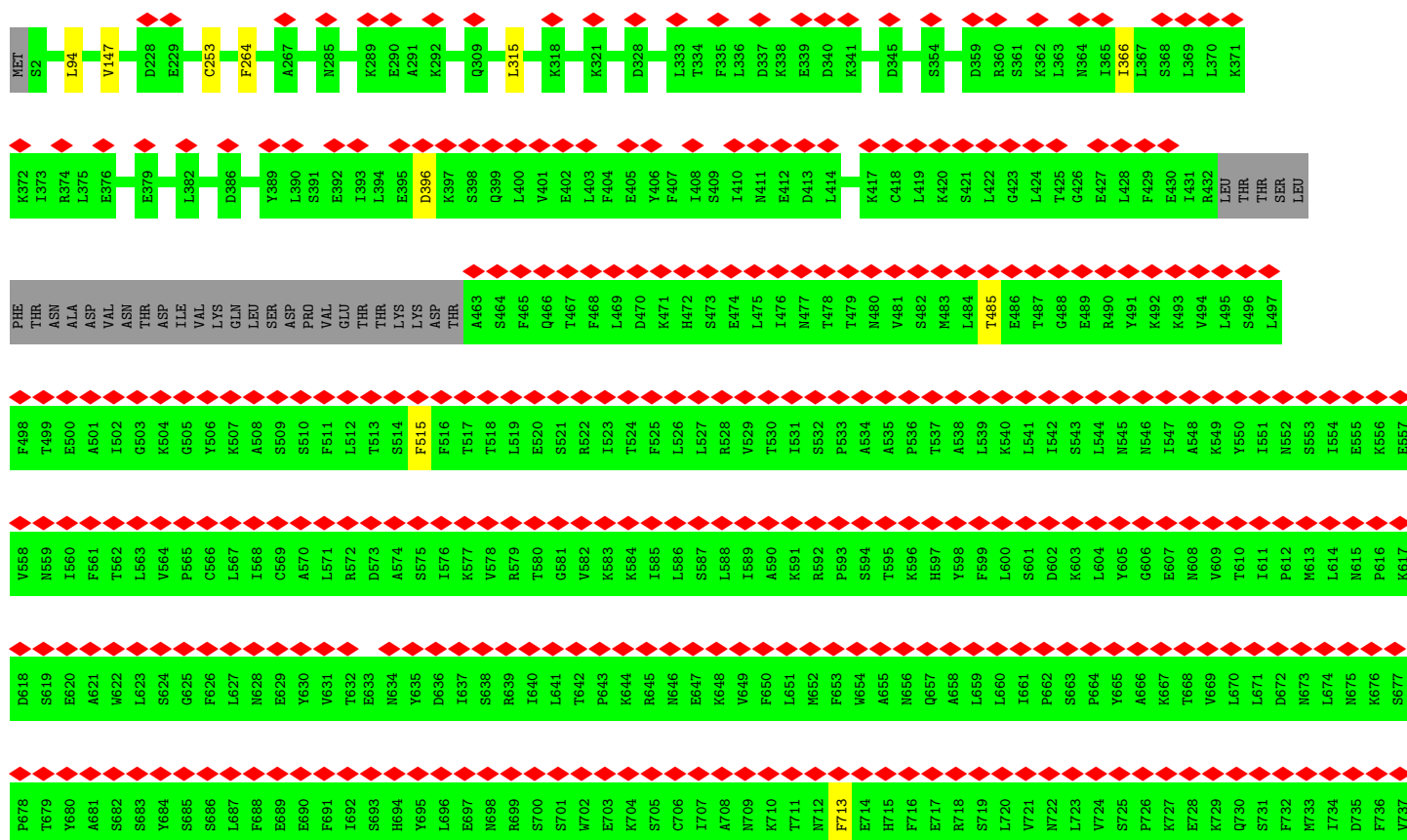
- Molecule 26: 13 kDa ribonucleoprotein-associated protein



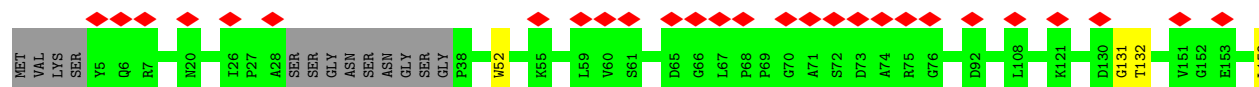


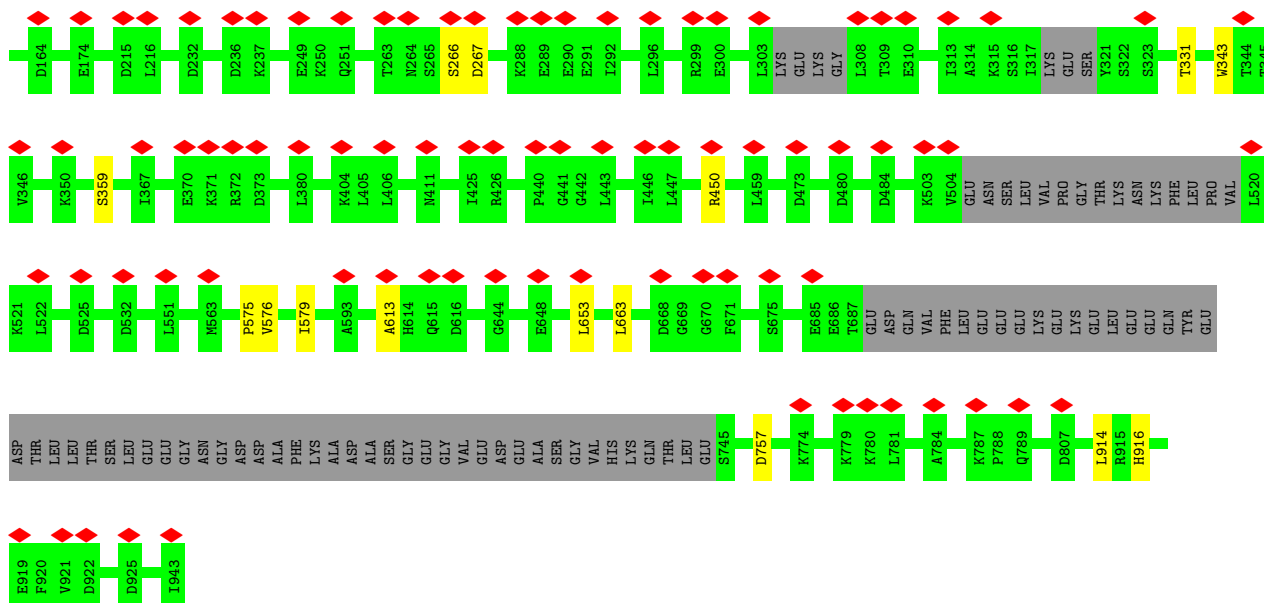


• Molecule 31: U3 small nucleolar RNA-associated protein 10

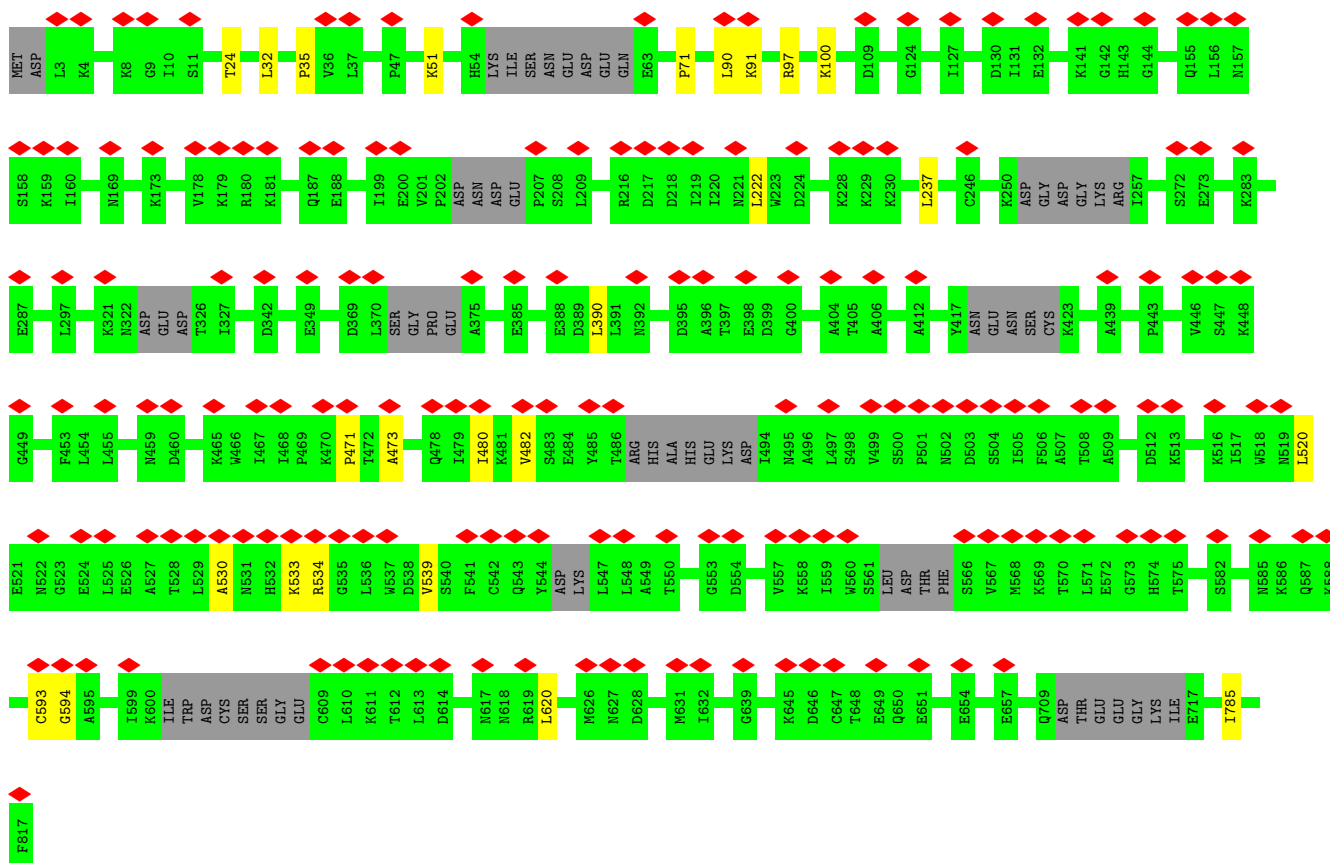
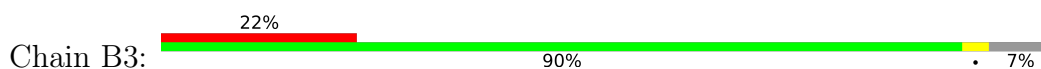




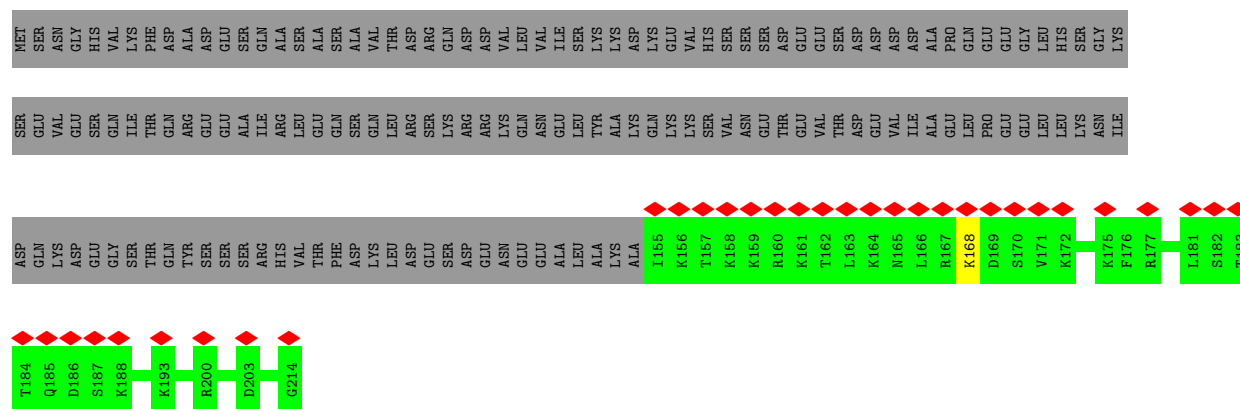




- Molecule 36: U3 small nucleolar RNA-associated protein 13

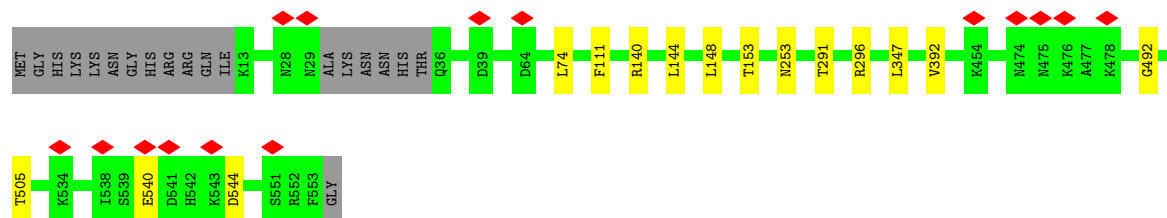


- Molecule 37: U3 small nucleolar RNA-associated protein 18



• Molecule 41: U3 small nucleolar RNA-associated protein 7

Chain 5C: 94%



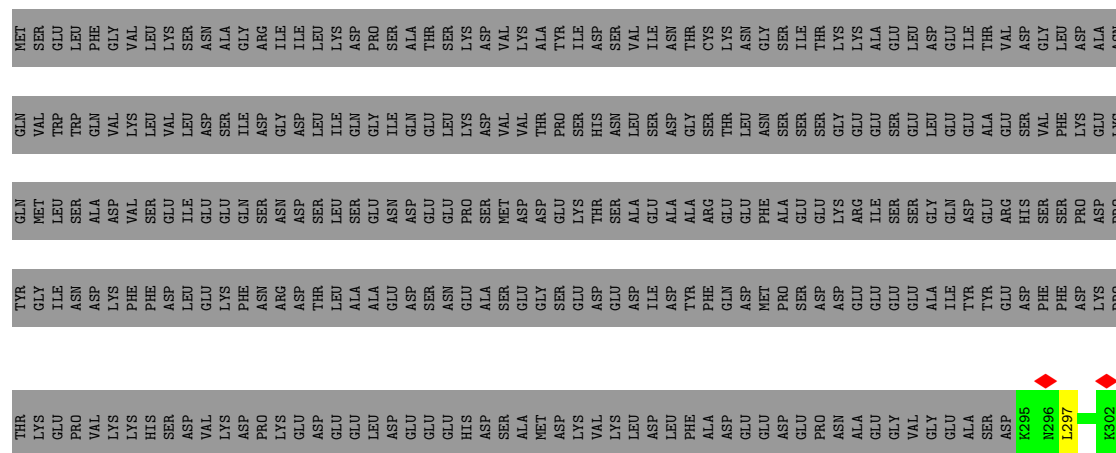
• Molecule 42: U3 small nucleolar RNA-associated protein 11

Chain 5D: 7% 92% 6%



• Molecule 43: U3 small nucleolar RNA-associated protein MPP10

Chain 5E: 33% 66%



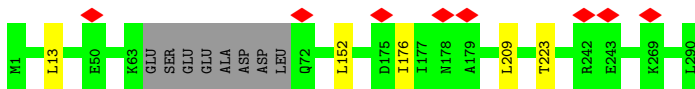
- Molecule 44: U3 small nucleolar ribonucleoprotein protein IMP3

Chain 5F:  97%



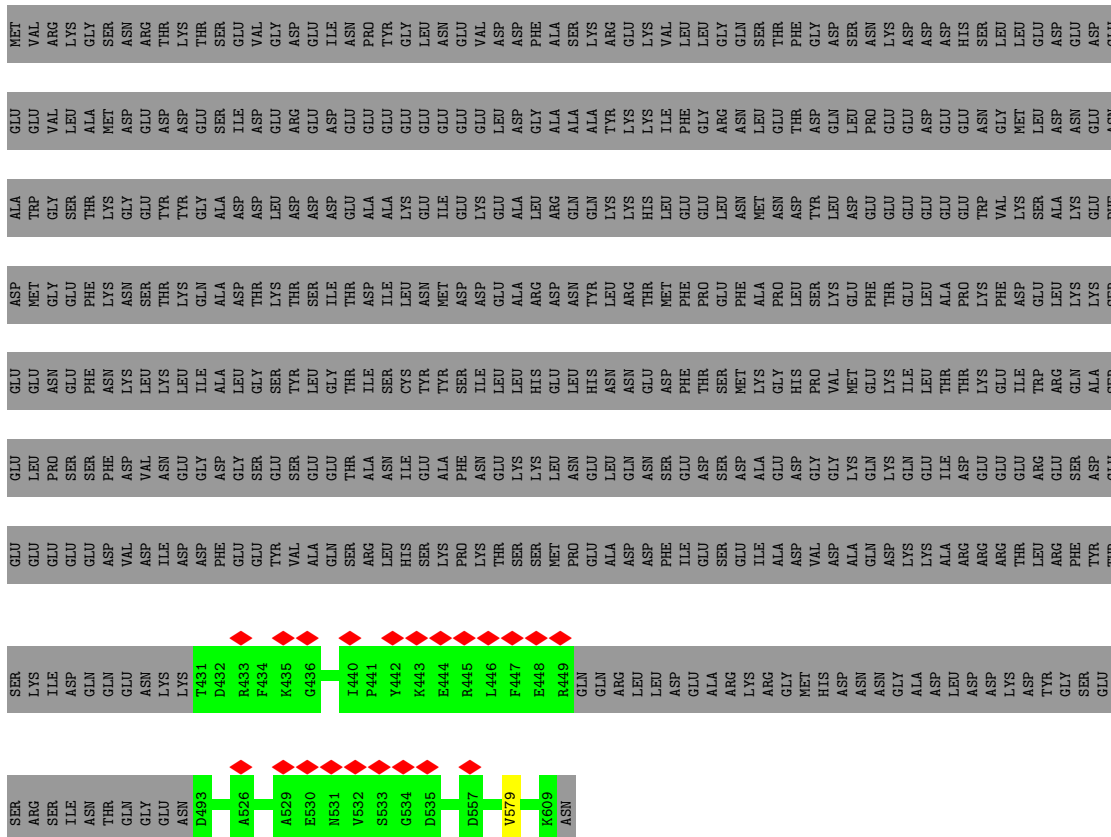
- Molecule 45: U3 small nucleolar ribonucleoprotein protein IMP4

Chain 5G: 96% . .



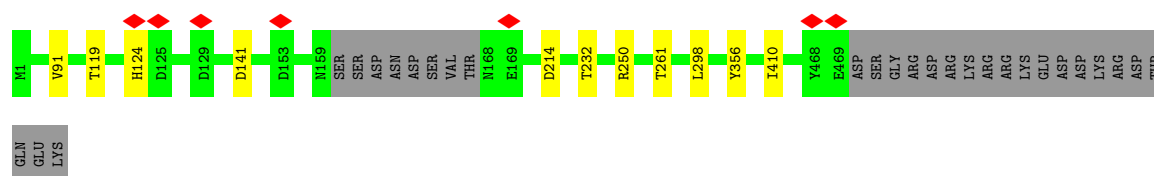
- Molecule 46: Something about silencing protein 10

Chain 5H:  22% 78%



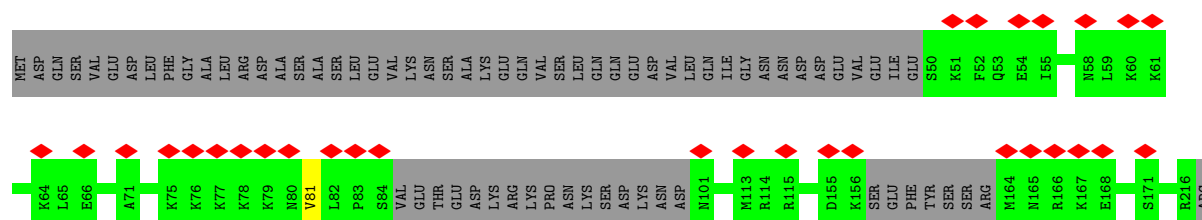
- Molecule 47: Protein SOF1

Chain 5I:  92% 6%



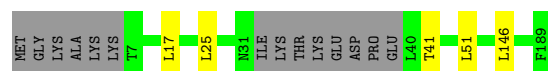
- Molecule 48: rRNA-processing protein FCF2

Chain 5J:  14% 66% 34%



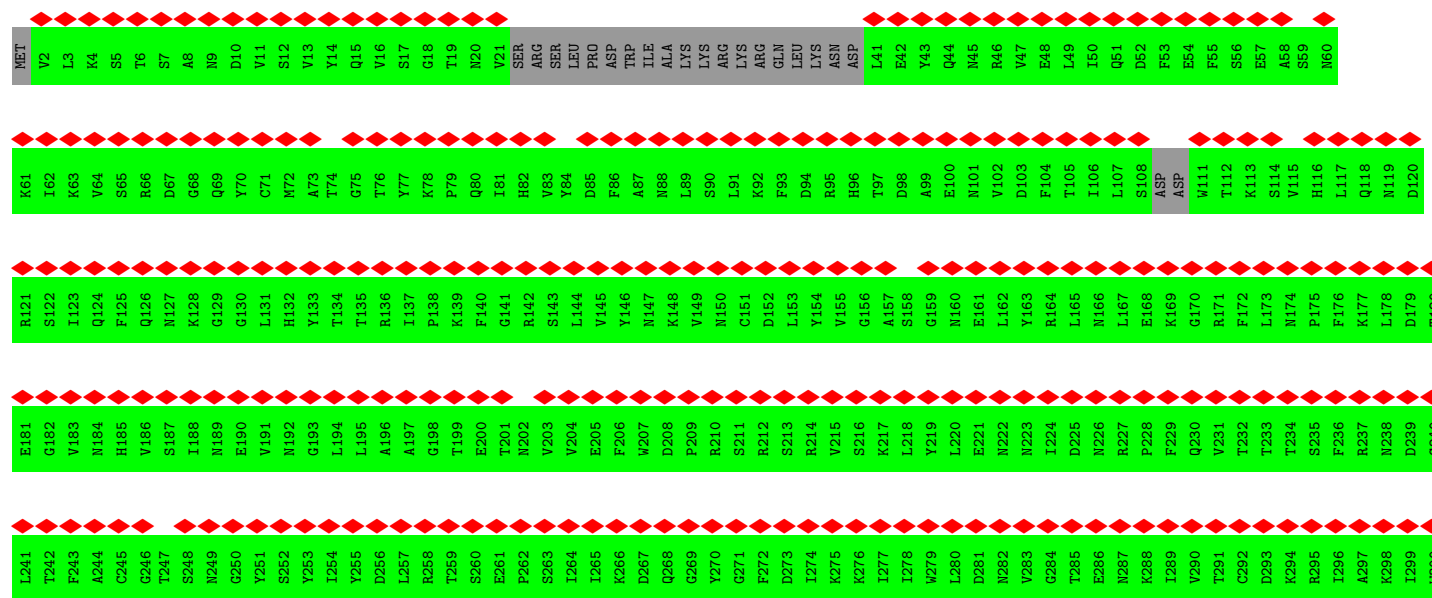
- Molecule 49: rRNA-processing protein FCF1

Chain 5K:  90% 7%

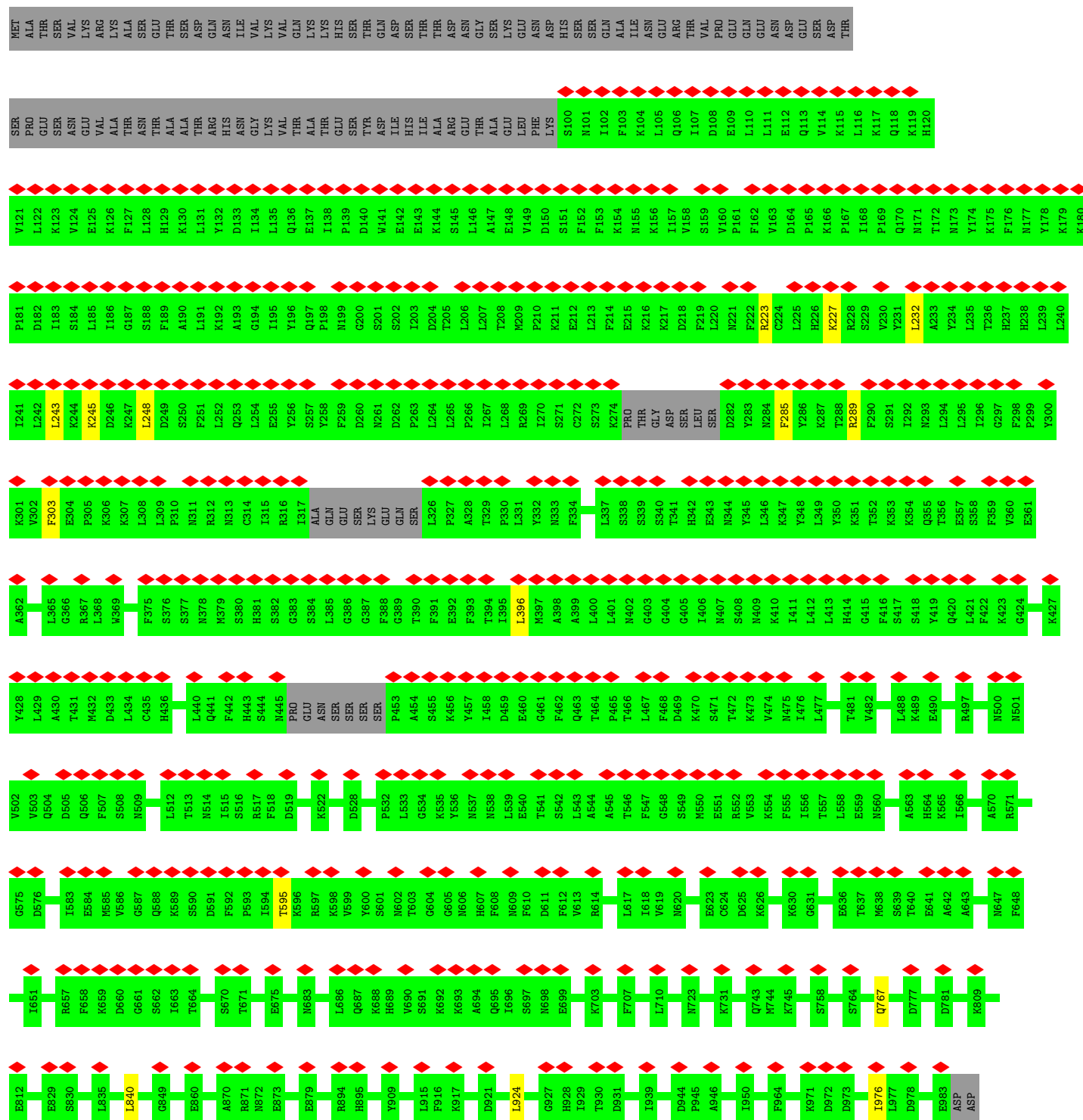


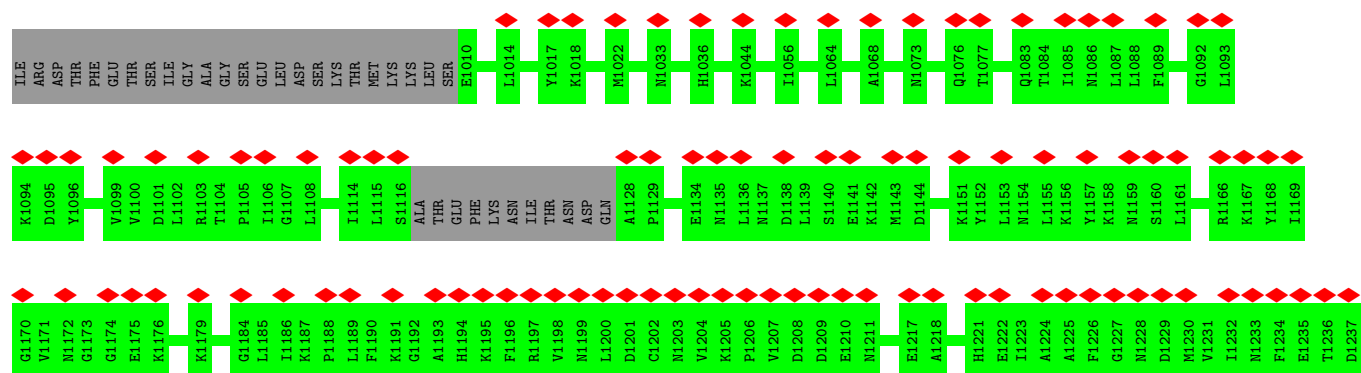
- Molecule 50: Ribosome biogenesis protein ENP2

Chain RA:  47% 48% 52%

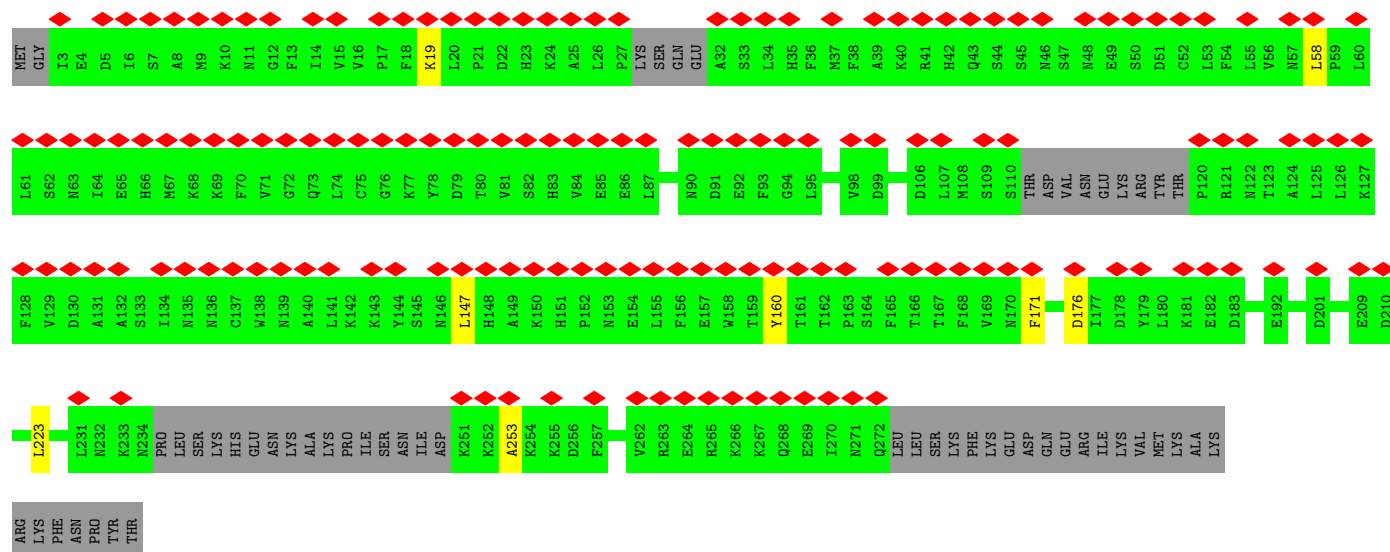




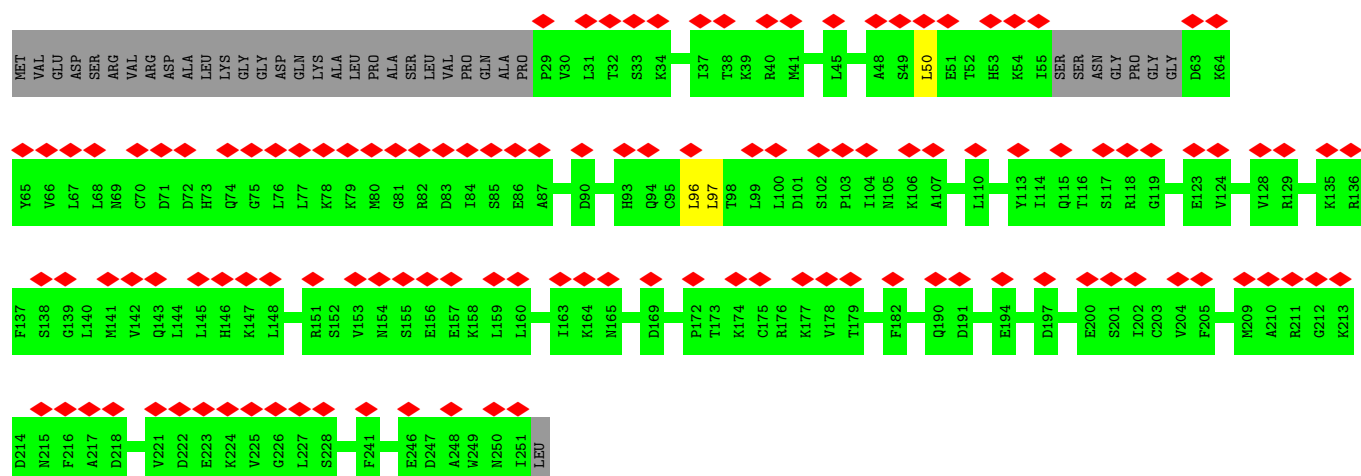
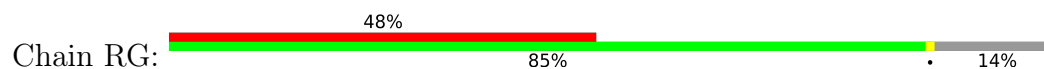




• Molecule 54: Ribosomal RNA-processing protein 7



• Molecule 55: Ribosomal RNA small subunit methyltransferase NEP1

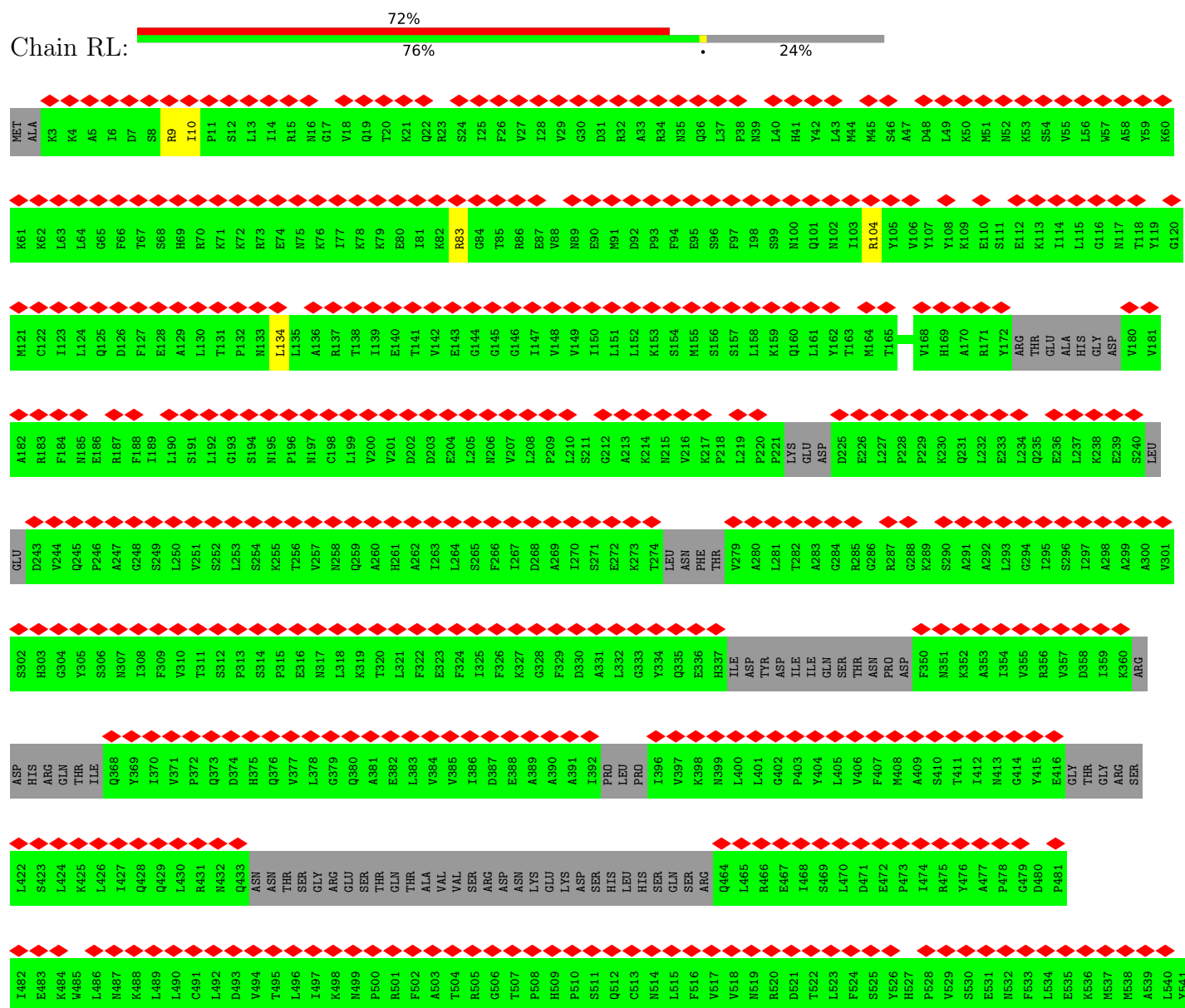




- Molecule 58: RNA 3'-terminal phosphate cyclase-like protein

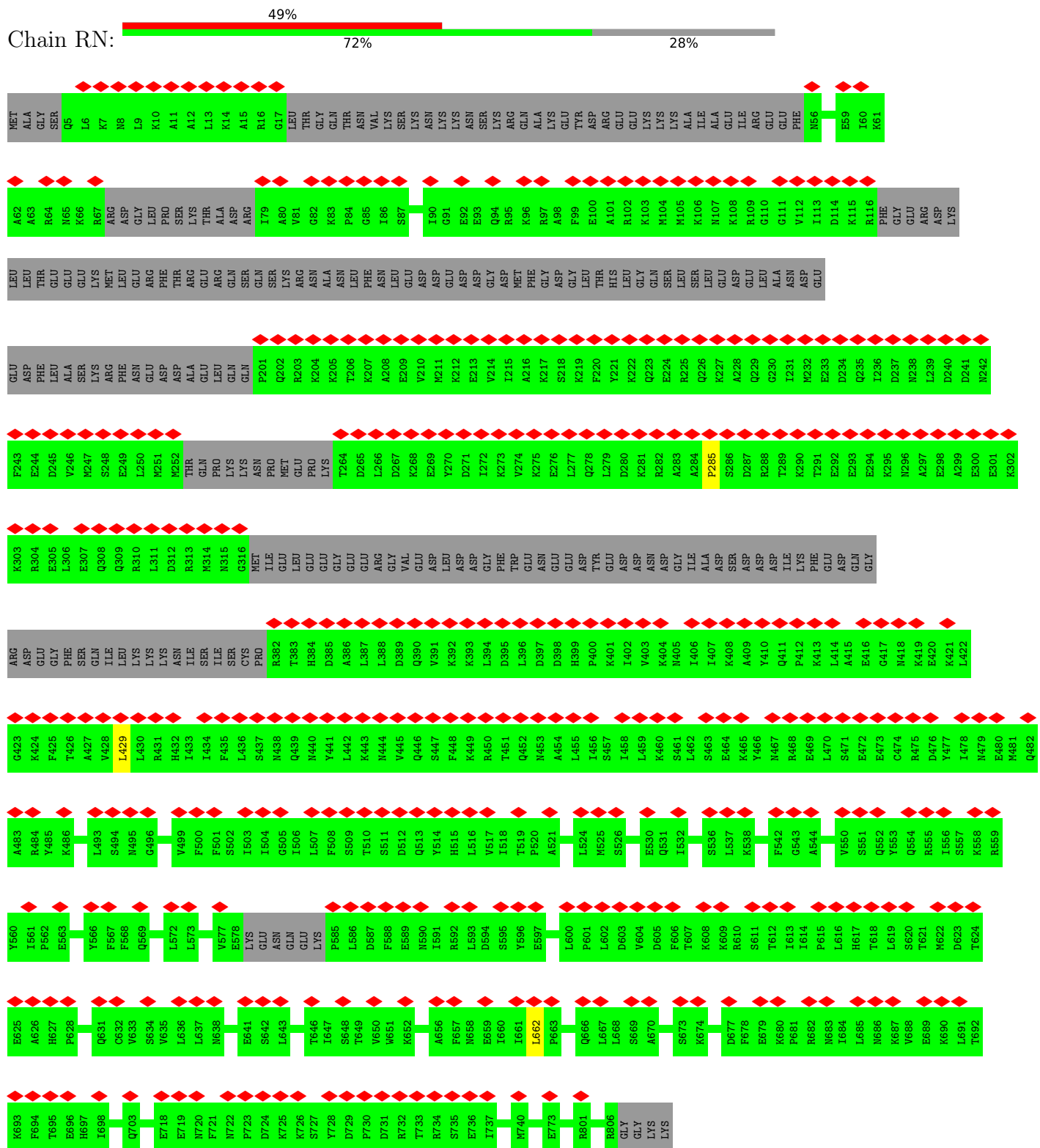


- Molecule 59: RNA cytidine acetyltransferase



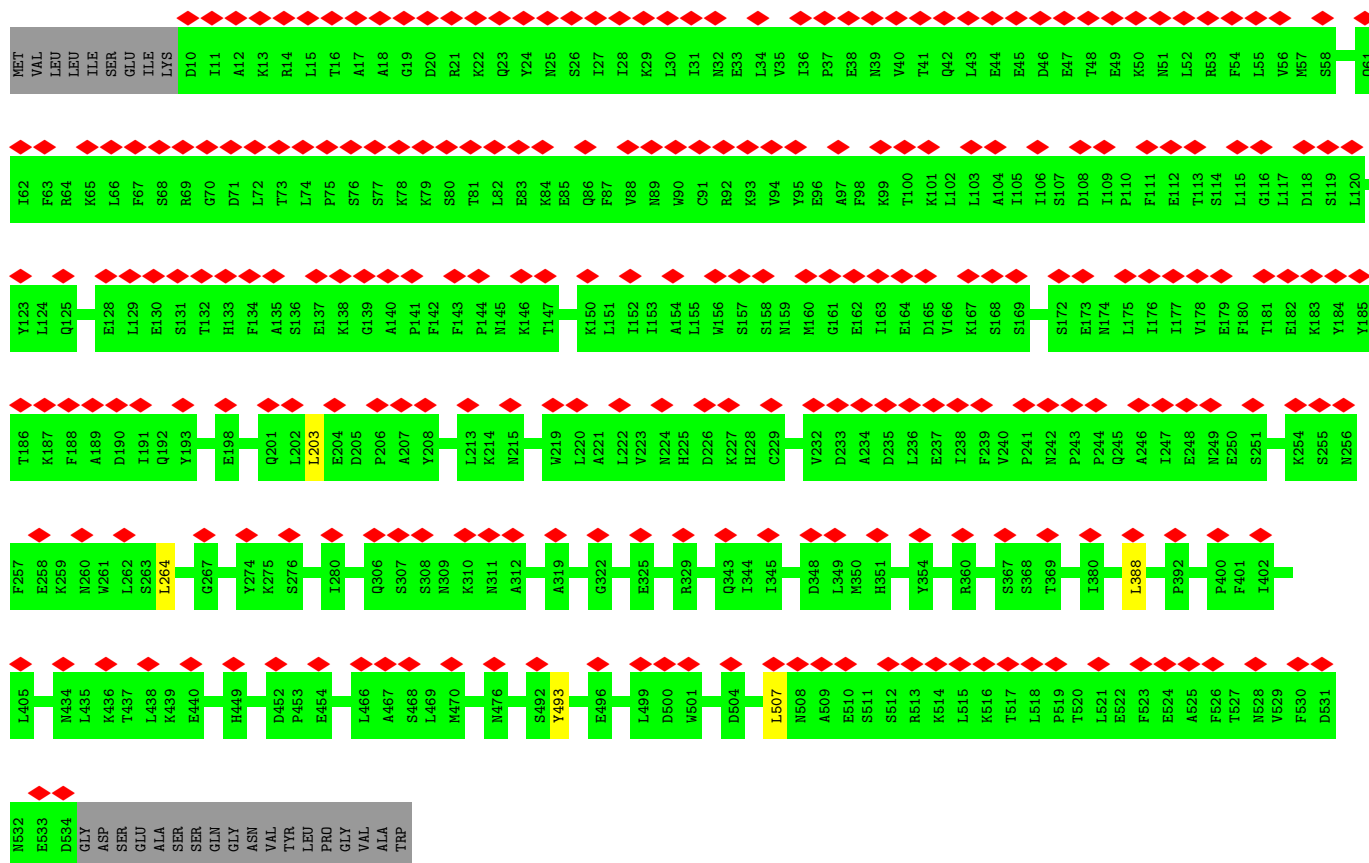
[illegible]

- Molecule 60: Nucleolar complex protein 14



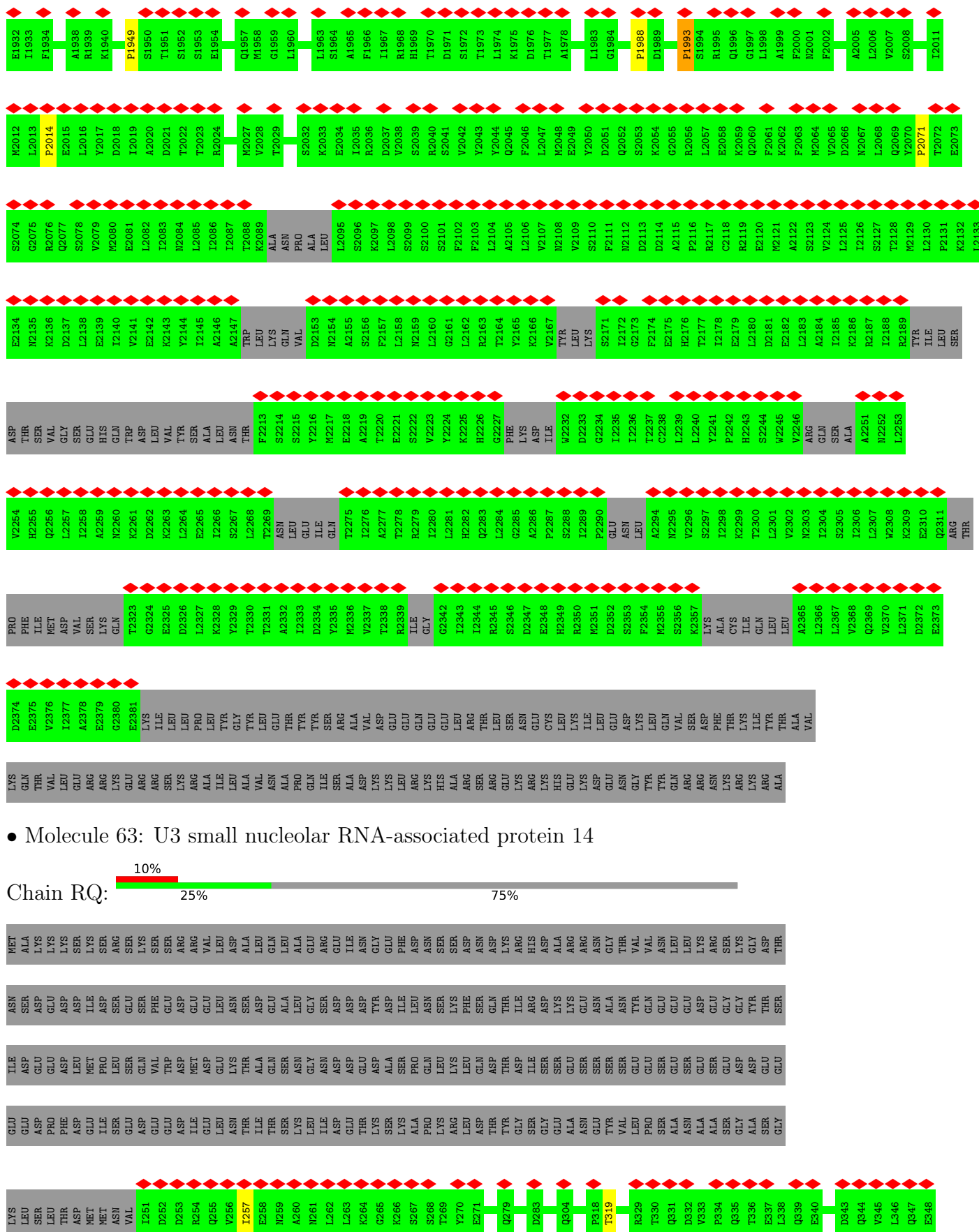
• Molecule 61: Nucleolar complex protein 4

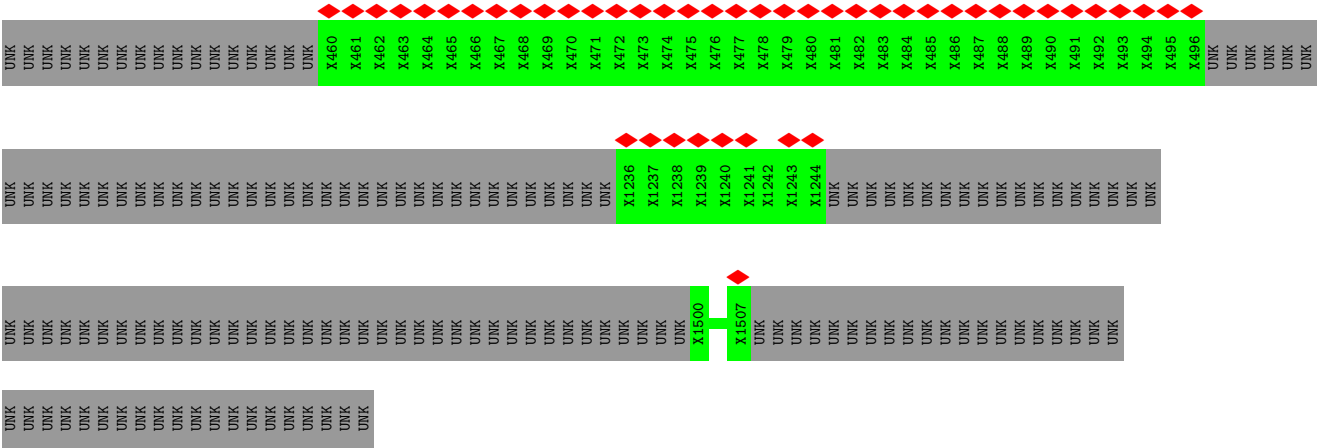




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S1021	V1022	L1023	Q1024	P1025	L1026	I1027	Y1028	S1029	I1030	A1031	M1032	A1033	Y1034	Y1035	V1036	L1037	D1038	T1039	E1040	S1041	T1042	E1043	E1044	V1045	V1046	L1047	R1048	K1049	M1050	A1051	S1052	M1053	L1054	R1055	Q1056	Q1057	G1058	L1059	Q1060	C1061	L1062	S1063	S1064	V1065	F1066	E1067	F1068	V1069	G1070	M1071	T1072	F1073	D1074	W1075	S1076	T1077	S1078	M1079	E1080		
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F661	F662	L663	K664	Y665	L666	F667	G668	L669	L670	T671	V672	R673	F674	S675	P676	V677	W678	T679	G680	V681	F682	D683	L684	I685	P686	N687	V688	Y689	T690	K691	D692	E693	A694	L695	V696	W697	K698	L699	V700	L701	S702	F703	I704	R705	L706	P707	D708	E709	N710	Q711	N712	L713	D714	Y715	Y716	Q717	P718	L719	L720		
E721	D722	G723	A724	M725	K726	V727	L728	M729	D730	S731	S732	V733	V734	R735	L736	D737	D738	T739	I740	D741	T742	F743	S744	H745	L746	W747	S748	K749	V750	S751	T752	E753	Q753	M754	T755	S756	I757	L758	S759	T760	T761	I762	E763	R764	R765	G766	M767	T768	T769	V770	P771	I772	L773	L774	R775	N776	Q777	A778	L779	K780	

S1866	T1867	L1868	E1807	F1871	A1872	L1873	D1874	N1813	F1814	C1815	L1816	Q1817	L1818	F1819	Q1820	E1821	S1822	F1886	L1887	T1888	V1889	S1890	L1891	H1891	L1892	E1893	G1894	P1897	F1898	L1899	R1900	D1901	S1902	L1903	L1904	S1905	E1906	N1907	E1908	V1911	I1912	L1915	R1916	I1917	L1918	I1919	T1920	L1921	I1922	R1923	D1925	F1926	S1927	D1928	S1930	S1931					
K1741	V1742	K1743	E1744	I1745	K1746	K1749	S1750	Y1751	D1752	A1753	G1754	E1755	L1756	L1757	A1758	S1759	N1760	I1761	S1762	L1763	T1764	E1765	F1766	G1767	T1768	L1769	S1770	P1772	V1773	K1774	A1775	M1778	V1779	R1780	I1781	N1782	L1783	R1784	N1787	K1788	L1789	S1790	E1791	L1792	L1793	R1794	R1795	I1796	L1797	L1798	G1799	D1928	S1929	N1801	H1802	N1803					
S1804	E1807	S1808	E1809	S1810	L1813	F1814	C1815	L1816	Q1817	L1818	F1819	Q1820	E1821	S1822	F1886	L1887	T1888	V1889	S1890	L1891	H1891	L1892	E1893	G1894	P1897	F1898	L1899	R1900	D1901	S1902	L1903	L1904	S1905	E1906	N1907	E1908	V1911	I1912	L1915	R1916	I1917	L1918	I1919	T1920	L1921	I1922	R1923	D1925	F1926	S1927	D1928	S1930	S1931								
L1681	K1682	R1683	G1684	Q1685	Q1686	I1687	H1688	V1689	L1690	S1691	Y1692	T1693	V1694	H1695	Y1696	I1697	L1698	K1699	S1700	M1701	H1702	G1703	V1704	F1705	K1706	H1707	S1708	D1709	L1710	D1711	T1712	S1713	S1714	S1715	M1716	I1717	V1718	K1719	I1720	I1721	M1722	E1723	M1724	I1725	F1726	G1727	F1728	A1729	G1730	E1731	E1732	K1733	D1734	S1735	E1736	N1737	Y1738	H1739	T1740		
L1621	G1622	L1623	T1624	N1625	D1626	D1627	I1628	T1629	M1630	F1631	L1632	P1633	S1634	I1635	L1636	T1637	M1638	I1639	C1640	Q1641	V1642	L1643	R1644	S1645	K1646	S1647	E1648	E1649	L1650	R1651	D1652	A1653	S1714	S1715	M1716	I1717	V1718	G1659	K1660	I1661	S1662	I1663	I1664	L1665	G1666	A1667	E1668	Y1669	L1670	V1671	F1672	V1673	I1674	K1675	L1676	L1677	A1678	T1680			
I1561	V1562	R1563	D1564	G1565	A1566	E1567	S1568	L1569	K1570	T1571	L1572	S1573	K1574	F1575	P1576	S1577	ASN	LEU	ASP	GLU	PRO	SER	ASN	PHE	LYS	GLN	GLU	TYR	PRO	LEU	LYS	ILE	GLU	GLY	THR	ARG	ASP	GLU	THR	ILE	E1608	R1609	M1610	P1611	I1612	A1613	E1614	A1615	L1616	V1617	M1618	I1619	V1620								
R1501	N1502	I1503	G1504	N1505	E1506	T1507	Q1508	I1509	A1510	I1511	G1512	G1513	L1514	A1515	Q1516	H1517	M1518	S1519	W1520	N1521	Q1522	Y1523	K1524	A1525	L1526	L1527	R1528	R1529	Y1530	I1531	S1532	M1533	L1534	K1535	T1536	K1537	P1538	M1539	Q1540	M1541	K1542	Q1543	A1544	V1545	Q1546	L1547	I1548	VAL	GLN	LEU	SER	VAL	PRO	ARG	GLU	T1558	L1559	R1560			
L1441	Y1442	M1443	G1444	D1445	E1446	E1447	A1448	D1449	PHE	THR	ASN	VAL	S1573	HIS	ILE	GLN	LEU	HIS	R1461	R1462	Q1463	R1464	A1465	I1466	K1467	R1468	L1469	G1470	E1471	H1472	A1473	H1474	Q1475	L1476	K1477	D1478	M1479	S1480	I1481	S1482	H1483	Y1484	I1486	P1487	M1488	I1489	E1490	H1491	Y1492	V1493	F1494	S1495	D1496	D1497	E1498	R1499	Y1500				
K1381	P1382	N1383	L1384	N1385	E1386	A1387	S1388	K1389	S1390	I1391	S1392	M1393	L1394	K1395	D1396	I1397	L1398	L1399	P1400	PRO	LEU	I1402	R1403	PHE	I1404	G1405	L1406	R1407	D1408	S1409	L1410	E1411	E1412	V1413	GLN	SER	GLU	TYR	VAL	SER	V1420	L1421	S1422	Y1423	M1424	V1425	K1426	N1427	T1428	K1429	Y1430	F1431	T1432	D1433	F1434	E1435	D1436	M1437	A1438	I1439	L1440
F1321	P1322	ARG	ILE	LEU	SER	THR	PHE	LYS	GLY	GLU	ASP	GLY	TYR	LYS	SER	GLN	LEU	GLU	TRP	LEU	PRO	LEU	PHE	THR	PHE	HIS	LEU	PHE	ASN	LYS	GLU	GLU	ALA	LEU	ARG	THR	ASN	ALA	SER	HIS	ILE	MET	LYS	PHE	ILE	D1376	F1377	I1378	M1379	E1380											
H1141	V1142	K1143	E1144	A1145	V1146	I1147	G1148	P1149	T1150	I1151	E1152	A1153	D1154	D1155	S1156	I1157	L1158	R1159	N1160	P1161	M1162	M1163	D1164	D1165	H1166	Y1167	V1168	D1169	L1170	V1171	T1172	L1173	I1174	C1175	T1176	S1177	C1178	L1179	K1180	I1181	L1182	P1183	S1184	L1185	Y1186	V1187	K1188	L1189	S1190	D1191	S1192	M1193	S1194	I1195	S1196	F1197	L1198	L1199	N1200		
L1201	L1202	V1203	S1204	I1205	T1206	E1207	M1208	G1209	T1210	I1211	Q1212	D1213	D1214	H1215	V1216	R1217	S1218	R1219	L1220	I1221	S1222	S1223	I1224	I1225	S1226	I1227	I1228	K1229	G1230	K1231	L1232	K1233	K1234	L1235	Q1236	E1237	N1238	D1239	T1240	Q1241	K1242	I1243	L1244	K1245	I1246	L1247	K1248	L1249	I1250	V1251	F1252	N1253	Y1254	N1255	C1256	S1257	W1258	S1259			
I1261	E1262	E1263	L1264	Y1265	T1266	T1267	I1268	S1269	S1270	L1271	F1272	K1273	T1274	F1275	D1276	E1277	R1278	M1279	L1280	R1281	V1282	S1283	L1284	PHE	T1285	E1286	L1287	F1288	I1289	E1290	L1291	Q1292	R1293	K1294	V1295	P1296	E1297	L1298	E1299	S1300	I1301	S1302	K1303	L1304	V1305	A1306	D1307	L1308	N1309	S1310	Y1311	S1312	S1313	S1314	R1315	M1316	E1317	Y1319	D1320		





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	121139	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	25000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.130	Depositor
Minimum map value	-0.073	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	3A	1.23	0/4141	1.27	34/6433 (0.5%)
2	5A	1.10	0/12462	1.20	78/19411 (0.4%)
3	SA	0.85	0/31237	1.22	263/48637 (0.5%)
4	SC	0.56	0/1777	0.77	4/2388 (0.2%)
5	SF	0.35	0/1854	0.69	2/2504 (0.1%)
6	SG	0.67	0/1690	0.65	0/2285
7	SH	0.36	0/890	0.67	1/1189 (0.1%)
8	SI	0.43	0/1341	0.70	0/1806
9	SJ	0.33	0/1347	0.59	1/1801 (0.1%)
10	SK	0.62	0/1410	0.66	1/1888 (0.1%)
11	SM	0.36	0/1020	0.63	0/1374
12	SN	0.29	0/873	0.66	0/1185
13	SO	0.50	0/1109	0.65	0/1495
14	SP	0.55	0/879	0.66	0/1186
15	SR	0.84	0/990	0.79	2/1335 (0.1%)
16	ST	0.37	0/930	0.64	0/1251
17	SX	0.63	0/1020	0.69	0/1371
18	SY	0.65	0/798	0.74	1/1065 (0.1%)
19	SZ	0.42	0/822	0.69	2/1103 (0.2%)
20	Sc	0.51	0/613	0.68	0/828
21	Sd	0.71	0/499	0.71	0/670
22	3B	0.81	0/1901	0.74	1/2567 (0.0%)
22	3C	0.46	0/1796	0.64	1/2424 (0.0%)
23	3D	0.55	0/2891	0.67	5/3895 (0.1%)
24	3E	0.50	0/3059	0.65	2/4153 (0.0%)
25	3F	0.47	0/3544	0.68	2/4775 (0.0%)
26	3G	0.67	0/928	0.77	2/1262 (0.2%)
26	3H	0.56	0/928	0.71	0/1262
27	A4	0.49	0/5321	0.68	4/7207 (0.1%)
28	A5	0.57	0/4044	0.70	4/5493 (0.1%)
29	A8	0.30	0/3328	0.64	1/4565 (0.0%)
30	A9	0.32	0/951	0.61	0/1287

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	AE	0.48	0/6308	0.67	3/8543 (0.0%)
32	AF	0.54	0/3993	0.68	3/5413 (0.1%)
33	AG	0.46	0/6699	0.66	5/9077 (0.1%)
34	B1	0.87	0/6780	0.75	6/9175 (0.1%)
35	B2	0.45	0/6853	0.69	2/9256 (0.0%)
36	B3	0.45	0/6014	0.72	5/8137 (0.1%)
37	B8	0.72	0/3848	0.71	4/5218 (0.1%)
38	BE	0.75	0/6948	0.70	7/9391 (0.1%)
39	B6	0.53	0/2849	0.60	2/3853 (0.1%)
40	5B	0.36	0/499	0.66	0/659
41	5C	0.79	0/4321	0.72	3/5832 (0.1%)
42	5D	0.67	0/1998	0.71	2/2644 (0.1%)
43	5E	0.58	0/1665	0.66	1/2233 (0.0%)
44	5F	0.96	0/1559	0.85	3/2097 (0.1%)
45	5G	0.72	0/2337	0.71	3/3148 (0.1%)
46	5H	0.57	0/1074	0.58	0/1422
47	5I	0.80	0/3844	0.72	1/5174 (0.0%)
48	5J	0.58	0/1238	0.62	1/1641 (0.1%)
49	5K	0.76	0/1426	0.74	1/1917 (0.1%)
50	RA	0.35	0/2769	0.66	0/3753
51	RB	0.40	0/1121	0.65	0/1487
52	RC	0.55	0/2245	0.63	0/3021
53	RE	0.39	0/8924	0.64	5/12070 (0.0%)
54	RF	0.37	0/2004	0.66	3/2697 (0.1%)
55	RG	0.36	0/1727	0.71	2/2329 (0.1%)
55	RH	0.43	0/1828	0.64	0/2470
56	RI	0.54	0/2080	0.67	0/2797
57	RJ	0.60	0/6514	0.63	2/8768 (0.0%)
58	RK	0.45	0/2832	0.65	0/3825
59	RL	0.29	0/4549	0.52	0/6241
59	RM	0.25	0/3760	0.47	0/5211
60	RN	0.37	0/4423	0.61	2/5965 (0.0%)
61	RO	0.38	0/3849	0.62	2/5261 (0.0%)
62	RP	0.25	0/10172	0.46	11/14158 (0.1%)
63	RQ	0.52	0/1678	0.61	0/2282
64	RS	0.34	0/2104	0.69	1/2854 (0.0%)
65	RT	0.42	0/1379	0.62	1/1853 (0.1%)
66	RV	0.60	0/1456	0.69	2/1937 (0.1%)
All	All	0.65	0/232060	0.82	494/323904 (0.2%)

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
4	SC	0	1
5	SF	0	1
6	SG	0	1
7	SH	0	1
8	SI	0	2
11	SM	0	1
12	SN	0	1
13	SO	0	1
14	SP	0	1
19	SZ	0	1
20	Sc	0	1
22	3B	0	1
23	3D	0	1
24	3E	0	2
26	3G	0	3
26	3H	0	1
28	A5	0	2
29	A8	0	4
33	AG	0	3
34	B1	0	3
35	B2	0	9
36	B3	0	8
37	B8	0	3
38	BE	0	3
39	B6	0	1
41	5C	0	3
42	5D	0	1
43	5E	0	1
44	5F	0	1
47	5I	0	1
49	5K	0	2
51	RB	0	1
53	RE	0	1
54	RF	0	1
56	RI	0	1
57	RJ	0	2
59	RL	0	1
59	RM	0	1
62	RP	0	1
63	RQ	0	1
66	RV	0	1
All	All	0	76

There are no bond length outliers.

All (494) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	5F	13	LEU	CA-CB-CG	10.94	140.47	115.30
3	SA	1034	C	C5-C6-N1	10.38	126.19	121.00
3	SA	1254	U	C2-N1-C1'	10.13	129.85	117.70
2	5A	312	U	O4'-C1'-N1	9.96	116.17	108.20
2	5A	310	U	N3-C2-O2	-9.45	115.59	122.20
3	SA	1451	C	N1-C2-O2	9.36	124.51	118.90
23	3D	283	ASP	CB-CG-OD1	9.26	126.64	118.30
3	SA	1451	C	N3-C2-O2	-9.26	115.42	121.90
2	5A	312	U	P-O3'-C3'	8.84	130.31	119.70
3	SA	1254	U	N1-C2-O2	8.78	128.95	122.80
3	SA	945	U	C5-C6-N1	8.63	127.01	122.70
3	SA	1174	C	N1-C2-O2	8.60	124.06	118.90
4	SC	54	LEU	CA-CB-CG	8.59	135.05	115.30
3	SA	864	U	N1-C2-O2	8.50	128.75	122.80
26	3G	65	LEU	CA-CB-CG	8.47	134.78	115.30
3	SA	864	U	N3-C2-O2	-8.37	116.34	122.20
53	RE	924	LEU	CA-CB-CG	8.35	134.51	115.30
3	SA	864	U	C2-N1-C1'	8.18	127.52	117.70
1	3A	72	C	C6-N1-C2	-8.18	117.03	120.30
1	3A	200	C	N1-C2-O2	8.10	123.76	118.90
2	5A	310	U	N1-C2-O2	8.00	128.40	122.80
3	SA	607	G	C4-N9-C1'	7.97	136.86	126.50
1	3A	89	C	C6-N1-C2	-7.95	117.12	120.30
3	SA	1034	C	C6-N1-C2	-7.91	117.14	120.30
2	5A	399	U	C5-C6-N1	7.91	126.65	122.70
3	SA	1518	C	N1-C2-O2	7.90	123.64	118.90
66	RV	200	ASP	CB-CG-OD1	7.86	125.37	118.30
3	SA	1269	U	N1-C2-O2	7.82	128.27	122.80
3	SA	1258	U	N1-C2-O2	7.77	128.24	122.80
1	3A	89	C	C2-N1-C1'	7.72	127.29	118.80
22	3B	306	LEU	CA-CB-CG	7.71	133.03	115.30
3	SA	172	C	N1-C2-O2	7.70	123.52	118.90
3	SA	354	C	C5-C6-N1	7.70	124.85	121.00
3	SA	1258	U	N3-C2-O2	-7.64	116.85	122.20
1	3A	72	C	C5-C6-N1	7.64	124.82	121.00
35	B2	757	ASP	CB-CG-OD1	7.63	125.17	118.30
3	SA	1177	C	C5-C6-N1	7.62	124.81	121.00
2	5A	523	U	C5-C6-N1	7.59	126.49	122.70
3	SA	1174	C	N3-C2-O2	-7.57	116.60	121.90
1	3A	75	C	C5-C6-N1	7.54	124.77	121.00

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	SA	1665	U	N3-C2-O2	-7.52	116.94	122.20
2	5A	85	G	C5-C6-O6	-7.49	124.10	128.60
2	5A	173	G	P-O3'-C3'	7.49	128.69	119.70
3	SA	1441	C	C2-N1-C1'	7.49	127.04	118.80
2	5A	312	U	C2-N1-C1'	-7.48	108.72	117.70
3	SA	161	U	N3-C2-O2	-7.46	116.98	122.20
19	SZ	74	LEU	CA-CB-CG	7.45	132.43	115.30
3	SA	1760	G	N3-C4-N9	7.43	130.46	126.00
3	SA	405	C	C6-N1-C2	-7.42	117.33	120.30
3	SA	405	C	C2-N1-C1'	7.40	126.94	118.80
3	SA	1674	C	C5-C6-N1	7.35	124.67	121.00
3	SA	1174	C	C2-N1-C1'	7.34	126.87	118.80
15	SR	123	ARG	C-N-CD	-7.33	104.48	120.60
2	5A	219	U	C5-C6-N1	7.33	126.36	122.70
3	SA	172	C	N3-C2-O2	-7.31	116.78	121.90
3	SA	1175	U	N1-C2-O2	7.31	127.92	122.80
3	SA	1760	G	N3-C4-C5	-7.27	124.97	128.60
3	SA	1269	U	C2-N1-C1'	7.26	126.42	117.70
7	SH	68	LEU	CA-CB-CG	7.23	131.94	115.30
3	SA	883	C	C5-C6-N1	7.23	124.62	121.00
38	BE	536	LEU	CA-CB-CG	7.22	131.91	115.30
3	SA	644	C	C5-C6-N1	7.21	124.61	121.00
3	SA	1568	C	N1-C2-O2	7.20	123.22	118.90
60	RN	662	LEU	CA-CB-CG	7.19	131.84	115.30
3	SA	357	G	N3-C4-N9	-7.18	121.69	126.00
3	SA	381	C	N3-C2-O2	-7.17	116.89	121.90
3	SA	1440	C	N1-C2-O2	7.16	123.20	118.90
3	SA	1674	C	C6-N1-C2	-7.15	117.44	120.30
2	5A	111	C	C2-N1-C1'	7.15	126.67	118.80
3	SA	1254	U	C6-N1-C1'	-7.13	111.21	121.20
3	SA	1518	C	C2-N1-C1'	7.10	126.61	118.80
3	SA	258	C	N1-C2-O2	7.10	123.16	118.90
33	AG	601	LEU	CA-CB-CG	7.10	131.62	115.30
2	5A	111	C	C6-N1-C2	-7.08	117.47	120.30
2	5A	61	U	N3-C2-O2	-7.08	117.25	122.20
3	SA	1711	C	N3-C2-O2	-7.06	116.96	121.90
3	SA	405	C	C5-C6-N1	7.03	124.51	121.00
3	SA	1518	C	N3-C2-O2	-7.02	116.98	121.90
2	5A	91	U	C5-C6-N1	7.01	126.20	122.70
3	SA	381	C	N1-C2-O2	7.00	123.10	118.90
3	SA	883	C	C6-N1-C2	-6.98	117.51	120.30
3	SA	1126	G	C4-N9-C1'	6.97	135.56	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	3D	142	LEU	CA-CB-CG	6.96	131.30	115.30
3	SA	361	C	N1-C2-O2	6.94	123.06	118.90
3	SA	1254	U	N3-C2-O2	-6.93	117.35	122.20
3	SA	128	U	C2-N1-C1'	6.90	125.98	117.70
41	5C	74	LEU	CA-CB-CG	6.90	131.17	115.30
3	SA	272	U	P-O3'-C3'	6.88	127.96	119.70
3	SA	161	U	N1-C2-O2	6.88	127.61	122.80
1	3A	200	C	C2-N1-C1'	6.87	126.36	118.80
1	3A	201	C	N1-C2-O2	6.85	123.01	118.90
2	5A	219	U	C2-N1-C1'	6.85	125.92	117.70
28	A5	540	LEU	CA-CB-CG	6.83	131.02	115.30
3	SA	1584	G	C4-N9-C1'	-6.82	117.64	126.50
3	SA	579	A	P-O3'-C3'	6.82	127.88	119.70
3	SA	679	U	C5-C6-N1	6.80	126.10	122.70
41	5C	144	LEU	CA-CB-CG	6.79	130.93	115.30
34	B1	701	LEU	CA-CB-CG	6.79	130.92	115.30
3	SA	1175	U	N3-C2-O2	-6.79	117.45	122.20
3	SA	1053	G	O5'-P-OP1	-6.79	99.59	105.70
1	3A	43	C	C5-C6-N1	6.77	124.39	121.00
3	SA	298	C	C5-C6-N1	6.77	124.39	121.00
3	SA	1664	C	C5-C6-N1	6.76	124.38	121.00
2	5A	90	G	C8-N9-C1'	6.73	135.75	127.00
3	SA	607	G	C8-N9-C1'	-6.73	118.25	127.00
2	5A	358	G	P-O3'-C3'	6.72	127.77	119.70
24	3E	141	LEU	CA-CB-CG	6.72	130.75	115.30
2	5A	252	A	C2-N3-C4	6.72	113.96	110.60
2	5A	172	C	N1-C2-O2	6.69	122.91	118.90
2	5A	399	U	C2-N1-C1'	6.68	125.72	117.70
3	SA	1072	C	C5-C6-N1	6.68	124.34	121.00
3	SA	1258	U	C2-N1-C1'	6.65	125.68	117.70
3	SA	1664	C	C2-N1-C1'	6.64	126.11	118.80
3	SA	1646	C	N1-C2-O2	6.64	122.88	118.90
3	SA	1772	C	C2-N1-C1'	6.64	126.10	118.80
3	SA	258	C	C2-N1-C1'	6.63	126.10	118.80
3	SA	354	C	C6-N1-C2	-6.63	117.65	120.30
3	SA	368	U	C5-C6-N1	6.61	126.01	122.70
3	SA	1441	C	C5-C6-N1	6.61	124.30	121.00
3	SA	1451	C	C6-N1-C2	-6.60	117.66	120.30
2	5A	61	U	N1-C2-O2	6.58	127.41	122.80
44	5F	61	LEU	CA-CB-CG	6.57	130.41	115.30
3	SA	1664	C	C6-N1-C2	-6.57	117.67	120.30
3	SA	607	G	N3-C4-C5	-6.56	125.32	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	SA	861	U	C2-N1-C1'	6.56	125.57	117.70
19	SZ	40	LEU	CB-CG-CD1	-6.54	99.87	111.00
3	SA	894	U	N1-C2-O2	6.54	127.38	122.80
3	SA	107	C	C6-N1-C2	-6.54	117.68	120.30
3	SA	64	U	C5-C6-N1	6.54	125.97	122.70
3	SA	514	G	N7-C8-N9	6.53	116.36	113.10
2	5A	90	G	C4-N9-C1'	-6.52	118.03	126.50
3	SA	1174	C	C6-N1-C2	-6.51	117.69	120.30
3	SA	1772	C	N1-C2-O2	6.51	122.81	118.90
3	SA	1441	C	C6-N1-C2	-6.51	117.70	120.30
2	5A	90	G	O4'-C1'-N9	6.50	113.40	108.20
3	SA	1126	G	N3-C4-N9	6.48	129.89	126.00
1	3A	63	C	C5-C6-N1	6.44	124.22	121.00
2	5A	85	G	C4-C5-N7	6.43	113.37	110.80
28	A5	457	LEU	CA-CB-CG	6.43	130.09	115.30
3	SA	1055	U	N1-C2-O2	6.42	127.30	122.80
3	SA	1254	U	C5-C6-N1	6.42	125.91	122.70
53	RE	303	PHE	C-N-CA	6.42	137.76	121.70
3	SA	401	A	P-O3'-C3'	6.42	127.40	119.70
3	SA	1084	A	P-O3'-C3'	6.42	127.40	119.70
3	SA	1760	G	C4-N9-C1'	6.42	134.84	126.50
62	RP	1949	PRO	N-CA-CB	6.40	110.98	103.30
55	RG	50	LEU	CA-CB-CG	6.39	130.00	115.30
26	3G	67	LEU	CA-CB-CG	6.39	130.00	115.30
24	3E	401	LEU	CA-CB-CG	6.37	129.95	115.30
3	SA	1031	U	P-O3'-C3'	6.36	127.33	119.70
37	B8	521	LEU	CA-CB-CG	6.36	129.92	115.30
3	SA	290	G	C4-N9-C1'	6.35	134.76	126.50
3	SA	1620	C	N3-C2-O2	-6.35	117.46	121.90
3	SA	1677	C	N1-C2-O2	6.34	122.71	118.90
3	SA	607	G	N3-C4-N9	6.34	129.80	126.00
3	SA	1585	U	C5-C6-N1	6.34	125.87	122.70
22	3C	306	LEU	CA-CB-CG	6.34	129.87	115.30
3	SA	56	U	P-O3'-C3'	6.33	127.30	119.70
1	3A	75	C	C6-N1-C2	-6.33	117.77	120.30
3	SA	657	U	N1-C2-O2	6.32	127.22	122.80
28	A5	151	LEU	CA-CB-CG	6.31	129.81	115.30
41	5C	148	LEU	CA-CB-CG	6.31	129.81	115.30
3	SA	514	G	C8-N9-C4	-6.30	103.88	106.40
3	SA	1056	U	N1-C2-O2	6.30	127.21	122.80
4	SC	172	LEU	CA-CB-CG	6.30	129.79	115.30
4	SC	120	LEU	CA-CB-CG	6.27	129.73	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5A	422	C	C2-N1-C1'	6.27	125.70	118.80
1	3A	198	U	P-O3'-C3'	6.25	127.20	119.70
3	SA	1126	G	C8-N9-C1'	-6.25	118.88	127.00
31	AE	315	LEU	CA-CB-CG	6.24	129.65	115.30
34	B1	717	LEU	CA-CB-CG	6.24	129.65	115.30
3	SA	373	G	C4-N9-C1'	6.23	134.60	126.50
1	3A	201	C	C5-C6-N1	6.23	124.11	121.00
3	SA	107	C	C5-C6-N1	6.22	124.11	121.00
2	5A	111	C	C5-C6-N1	6.21	124.10	121.00
3	SA	357	G	C5-C6-O6	6.20	132.32	128.60
48	5J	81	VAL	C-N-CA	6.20	137.20	121.70
3	SA	1033	C	O4'-C1'-N1	6.19	113.15	108.20
3	SA	1665	U	N1-C2-O2	6.19	127.13	122.80
2	5A	390	C	C5-C6-N1	6.18	124.09	121.00
3	SA	1055	U	C2-N1-C1'	6.18	125.11	117.70
27	A4	563	LEU	CA-CB-CG	6.17	129.50	115.30
45	5G	152	LEU	CA-CB-CG	6.16	129.47	115.30
1	3A	102	U	N3-C2-O2	-6.15	117.89	122.20
3	SA	873	U	N3-C2-O2	-6.15	117.89	122.20
3	SA	368	U	C5-C4-O4	-6.15	122.21	125.90
37	B8	22	LEU	CA-CB-CG	6.14	129.43	115.30
3	SA	1584	G	C8-N9-C1'	6.14	134.98	127.00
1	3A	248	G	P-O3'-C3'	6.14	127.07	119.70
3	SA	1052	U	O4'-C1'-N1	6.13	113.11	108.20
3	SA	417	A	P-O3'-C3'	6.12	127.04	119.70
2	5A	263	C	C5-C6-N1	6.11	124.06	121.00
3	SA	1269	U	N3-C2-O2	-6.11	117.93	122.20
2	5A	312	U	OP1-P-O3'	6.08	118.59	105.20
42	5D	224	LEU	CB-CG-CD2	-6.08	100.67	111.00
3	SA	648	G	C4-N9-C1'	6.06	134.38	126.50
3	SA	1760	G	C2-N3-C4	6.05	114.93	111.90
3	SA	530	C	N1-C2-O2	6.04	122.53	118.90
38	BE	522	LEU	CA-CB-CG	6.04	129.20	115.30
33	AG	323	LEU	CA-CB-CG	6.04	129.19	115.30
3	SA	1711	C	N1-C2-O2	6.03	122.52	118.90
38	BE	614	LEU	CA-CB-CG	6.03	129.17	115.30
2	5A	368	U	P-O3'-C3'	6.02	126.93	119.70
2	5A	7	A	O4'-C1'-N9	6.01	113.01	108.20
9	SJ	29	LEU	CA-CB-CG	5.99	129.08	115.30
23	3D	292	LEU	CA-CB-CG	5.99	129.07	115.30
1	3A	248	G	OP1-P-O3'	5.98	118.37	105.20
3	SA	1620	C	N1-C2-O2	5.97	122.48	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	SA	1568	C	N3-C2-O2	-5.97	117.72	121.90
2	5A	312	U	N1-C1'-C2'	5.97	121.75	114.00
34	B1	603	LEU	CA-CB-CG	5.96	129.02	115.30
3	SA	1072	C	C6-N1-C2	-5.95	117.92	120.30
2	5A	172	C	P-O3'-C3'	5.93	126.82	119.70
18	SY	132	LEU	CA-CB-CG	5.93	128.95	115.30
3	SA	290	G	N3-C4-N9	5.93	129.56	126.00
3	SA	1439	C	C5-C6-N1	5.93	123.97	121.00
3	SA	311	U	C2-N1-C1'	5.93	124.81	117.70
27	A4	611	LEU	CA-CB-CG	5.92	128.93	115.30
1	3A	201	C	C2-N1-C1'	5.92	125.31	118.80
2	5A	219	U	N1-C2-O2	5.90	126.93	122.80
61	RO	388	LEU	CA-CB-CG	5.90	128.87	115.30
2	5A	393	C	O5'-P-OP1	-5.89	100.40	105.70
3	SA	1078	C	C5-C6-N1	5.88	123.94	121.00
3	SA	1080	U	N3-C2-O2	-5.87	118.09	122.20
25	3F	348	LEU	CA-CB-CG	5.87	128.80	115.30
2	5A	369	G	O5'-P-OP1	-5.86	100.43	105.70
38	BE	417	LEU	CA-CB-CG	5.86	128.77	115.30
1	3A	89	C	C5-C6-N1	5.85	123.93	121.00
3	SA	1769	U	N3-C2-O2	-5.85	118.10	122.20
3	SA	361	C	C2-N1-C1'	5.85	125.24	118.80
1	3A	102	U	N1-C2-O2	5.85	126.89	122.80
3	SA	280	U	N1-C2-O2	5.85	126.89	122.80
3	SA	280	U	C2-N1-C1'	5.84	124.71	117.70
3	SA	1177	C	C6-N1-C2	-5.84	117.97	120.30
34	B1	69	LEU	CA-CB-CG	5.83	128.72	115.30
2	5A	90	G	N9-C4-C5	5.82	107.73	105.40
3	SA	298	C	C6-N1-C2	-5.82	117.97	120.30
1	3A	61	G	C2-N3-C4	5.82	114.81	111.90
2	5A	311	C	O4'-C1'-N1	5.80	112.84	108.20
3	SA	1760	G	P-O3'-C3'	5.80	126.66	119.70
27	A4	416	LEU	CA-CB-CG	5.80	128.64	115.30
65	RT	250	LEU	CA-CB-CG	5.80	128.64	115.30
3	SA	657	U	C2-N1-C1'	5.80	124.66	117.70
1	3A	201	C	C6-N1-C2	-5.79	117.98	120.30
36	B3	620	LEU	CA-CB-CG	5.79	128.62	115.30
3	SA	1439	C	C6-N1-C2	-5.77	117.99	120.30
5	SF	42	LEU	CA-CB-CG	5.76	128.56	115.30
3	SA	1585	U	C2-N1-C1'	5.76	124.61	117.70
3	SA	1521	G	P-O3'-C3'	5.76	126.61	119.70
3	SA	1594	G	O4'-C1'-N9	5.76	112.81	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	SA	909	U	N3-C2-O2	-5.75	118.17	122.20
1	3A	203	U	N1-C2-O2	5.75	126.82	122.80
3	SA	290	G	N3-C4-C5	-5.74	125.73	128.60
3	SA	545	A	O4'-C1'-N9	5.74	112.79	108.20
3	SA	1646	C	C5-C6-N1	5.74	123.87	121.00
27	A4	225	LEU	CA-CB-CG	5.74	128.50	115.30
3	SA	1191	U	N1-C2-O2	5.74	126.82	122.80
3	SA	1083	G	C4-N9-C1'	5.74	133.96	126.50
2	5A	65	U	N3-C2-O2	-5.72	118.20	122.20
62	RP	2071	PRO	N-CA-CB	5.72	110.16	103.30
45	5G	13	LEU	CA-CB-CG	5.72	128.45	115.30
62	RP	78	PRO	N-CA-CB	5.71	110.16	103.30
3	SA	1037	C	C6-N1-C2	-5.71	118.02	120.30
3	SA	965	U	C2-N1-C1'	5.71	124.55	117.70
44	5F	67	THR	C-N-CA	-5.70	107.45	121.70
3	SA	1769	U	N1-C2-O2	5.70	126.79	122.80
3	SA	1675	C	N1-C2-O2	5.69	122.32	118.90
2	5A	390	C	C6-N1-C2	-5.68	118.03	120.30
3	SA	1759	C	C6-N1-C2	-5.68	118.03	120.30
3	SA	1760	G	C8-N9-C1'	-5.68	119.61	127.00
3	SA	657	U	N3-C2-O2	-5.68	118.22	122.20
3	SA	945	U	C6-N1-C2	-5.67	117.60	121.00
3	SA	1594	G	P-O3'-C3'	5.67	126.51	119.70
2	5A	543	C	C6-N1-C2	-5.67	118.03	120.30
3	SA	542	A	P-O3'-C3'	5.67	126.50	119.70
3	SA	1053	G	C8-N9-C4	-5.67	104.13	106.40
3	SA	1440	C	C2-N1-C1'	5.66	125.03	118.80
57	RJ	845	LEU	CA-CB-CG	5.66	128.31	115.30
2	5A	312	U	C6-N1-C1'	5.66	129.12	121.20
54	RF	58	LEU	CA-CB-CG	5.65	128.30	115.30
3	SA	870	C	C6-N1-C2	-5.65	118.04	120.30
3	SA	1222	C	C5-C6-N1	5.65	123.82	121.00
3	SA	1743	U	C2-N1-C1'	5.64	124.47	117.70
3	SA	1078	C	C6-N1-C2	-5.64	118.05	120.30
62	RP	2014	PRO	N-CA-CB	5.63	110.06	103.30
2	5A	537	G	N3-C4-N9	5.63	129.38	126.00
3	SA	1275	A	C2-N3-C4	5.63	113.42	110.60
62	RP	179	PRO	N-CA-CB	5.63	110.06	103.30
39	B6	18	LEU	CA-CB-CG	5.63	128.25	115.30
3	SA	128	U	N1-C2-O2	5.62	126.74	122.80
3	SA	1665	U	C2-N1-C1'	5.62	124.44	117.70
62	RP	119	PRO	N-CA-CB	5.62	110.04	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	SA	1734	U	N3-C2-O2	-5.62	118.27	122.20
34	B1	29	LEU	CA-CB-CG	5.62	128.22	115.30
37	B8	164	LEU	CA-CB-CG	5.61	128.21	115.30
32	AF	195	LEU	CA-CB-CG	5.61	128.20	115.30
3	SA	1037	C	N1-C2-O2	5.61	122.26	118.90
62	RP	1988	PRO	N-CA-CB	5.61	110.03	103.30
1	3A	89	C	N1-C2-O2	5.60	122.26	118.90
3	SA	405	C	N1-C2-O2	5.60	122.26	118.90
3	SA	894	U	N3-C2-O2	-5.60	118.28	122.20
43	5E	314	LEU	CA-CB-CG	5.60	128.17	115.30
3	SA	311	U	N1-C2-O2	5.59	126.71	122.80
3	SA	607	G	C2-N3-C4	5.59	114.69	111.90
2	5A	492	G	P-O3'-C3'	5.58	126.39	119.70
2	5A	7	A	C8-N9-C4	-5.57	103.57	105.80
3	SA	373	G	N3-C4-C5	-5.57	125.82	128.60
62	RP	105	PRO	N-CA-CB	5.56	109.98	103.30
1	3A	203	U	N3-C2-O2	-5.56	118.31	122.20
3	SA	1440	C	N3-C2-O2	-5.56	118.01	121.90
3	SA	0	U	P-O3'-C3'	5.56	126.37	119.70
3	SA	302	U	N3-C2-O2	-5.56	118.31	122.20
3	SA	1595	U	O5'-P-OP1	-5.55	100.70	105.70
1	3A	200	C	C6-N1-C1'	-5.55	114.14	120.80
3	SA	655	G	N3-C4-N9	-5.55	122.67	126.00
3	SA	1585	U	N1-C2-O2	5.55	126.69	122.80
3	SA	411	C	C6-N1-C2	-5.55	118.08	120.30
3	SA	161	U	C2-N1-C1'	5.54	124.35	117.70
3	SA	1067	C	C6-N1-C2	-5.54	118.08	120.30
34	B1	585	TYR	CB-CG-CD2	-5.54	117.67	121.00
3	SA	1584	G	N3-C4-N9	-5.54	122.68	126.00
3	SA	1772	C	C5-C6-N1	5.54	123.77	121.00
3	SA	50	C	C2-N1-C1'	5.53	124.88	118.80
38	BE	557	LEU	CA-CB-CG	5.53	128.02	115.30
2	5A	263	C	C6-N1-C2	-5.53	118.09	120.30
54	RF	147	LEU	CA-CB-CG	5.53	128.01	115.30
37	B8	328	LEU	CA-CB-CG	5.52	128.00	115.30
2	5A	491	U	N1-C2-O2	5.52	126.67	122.80
3	SA	1034	C	C2-N1-C1'	5.52	124.88	118.80
3	SA	35	U	N1-C2-O2	5.52	126.66	122.80
3	SA	908	U	N3-C2-O2	-5.52	118.34	122.20
3	SA	1717	G	C4-N9-C1'	5.52	133.68	126.50
2	5A	585	C	C6-N1-C2	-5.52	118.09	120.30
3	SA	692	C	N1-C2-O2	5.51	122.21	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5A	252	A	N7-C8-N9	5.51	116.56	113.80
10	SK	105	LEU	CA-CB-CG	5.51	127.97	115.30
23	3D	152	LEU	CA-CB-CG	5.51	127.97	115.30
2	5A	537	G	C4-N9-C1'	5.50	133.66	126.50
3	SA	1191	U	C2-N1-C1'	5.50	124.31	117.70
3	SA	361	C	C6-N1-C2	-5.50	118.10	120.30
3	SA	194	U	C2-N1-C1'	5.50	124.30	117.70
3	SA	1083	G	N7-C8-N9	5.50	115.85	113.10
31	AE	94	LEU	CA-CB-CG	5.49	127.93	115.30
3	SA	894	U	C5-C6-N1	5.49	125.44	122.70
3	SA	1055	U	N3-C2-O2	-5.49	118.36	122.20
2	5A	263	C	C2-N1-C1'	5.47	124.82	118.80
3	SA	1053	G	N9-C4-C5	5.47	107.59	105.40
2	5A	252	A	C4-N9-C1'	5.46	136.13	126.30
3	SA	373	G	N3-C4-N9	5.45	129.27	126.00
3	SA	1779	U	N3-C2-O2	-5.45	118.39	122.20
3	SA	194	U	N1-C2-O2	5.44	126.61	122.80
3	SA	147	A	C2-N3-C4	5.43	113.32	110.60
62	RP	1772	PRO	N-CA-CB	5.43	109.82	103.30
3	SA	413	U	C5-C6-N1	5.43	125.41	122.70
29	A8	563	LEU	CA-CB-CG	5.42	127.77	115.30
35	B2	914	LEU	CA-CB-CG	5.42	127.77	115.30
3	SA	280	U	N3-C2-O2	-5.41	118.41	122.20
3	SA	361	C	C5-C6-N1	5.41	123.71	121.00
3	SA	150	U	N3-C2-O2	-5.41	118.41	122.20
3	SA	1476	C	C2-N1-C1'	5.41	124.75	118.80
3	SA	1109	G	C8-N9-C4	5.40	108.56	106.40
1	3A	6	C	C6-N1-C2	-5.40	118.14	120.30
3	SA	1034	C	N1-C2-O2	5.40	122.14	118.90
36	B3	471	PRO	C-N-CA	5.40	135.20	121.70
3	SA	1032	G	N3-C4-N9	5.40	129.24	126.00
2	5A	252	A	N3-C4-N9	5.40	131.72	127.40
2	5A	381	G	C4-C5-N7	5.39	112.96	110.80
62	RP	1993	PRO	N-CA-CB	5.39	109.77	103.30
3	SA	1056	U	N3-C2-O2	-5.38	118.43	122.20
3	SA	864	U	C6-N1-C1'	-5.38	113.67	121.20
3	SA	530	C	N3-C2-O2	-5.38	118.14	121.90
2	5A	85	G	N1-C6-O6	5.38	123.12	119.90
33	AG	373	LEU	CA-CB-CG	5.37	127.64	115.30
3	SA	682	C	N1-C2-O2	5.36	122.12	118.90
3	SA	873	U	N1-C2-O2	5.36	126.55	122.80
32	AF	118	LEU	CA-CB-CG	5.36	127.63	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	SA	32	U	N3-C2-O2	-5.36	118.45	122.20
3	SA	1646	C	C2-N1-C1'	5.35	124.69	118.80
3	SA	357	G	N9-C4-C5	5.35	107.54	105.40
2	5A	523	U	C6-N1-C2	-5.35	117.79	121.00
2	5A	363	A	P-O3'-C3'	5.34	126.11	119.70
3	SA	1704	U	N1-C2-O2	5.34	126.53	122.80
2	5A	84	G	C4-N9-C1'	5.33	133.43	126.50
2	5A	65	U	N1-C2-O2	5.33	126.53	122.80
1	3A	43	C	C6-N1-C2	-5.32	118.17	120.30
2	5A	6	A	O4'-C1'-N9	5.32	112.46	108.20
2	5A	543	C	C5-C6-N1	5.32	123.66	121.00
3	SA	644	C	C6-N1-C2	-5.32	118.17	120.30
3	SA	1231	U	N3-C2-O2	-5.32	118.48	122.20
2	5A	90	G	N3-C4-N9	-5.32	122.81	126.00
3	SA	346	G	N3-C4-N9	5.31	129.19	126.00
3	SA	1476	C	N1-C2-O2	5.30	122.08	118.90
3	SA	1747	G	C4-N9-C1'	5.30	133.39	126.50
38	BE	834	LEU	CA-CB-CG	-5.30	103.11	115.30
62	RP	1897	PRO	N-CA-CB	5.30	109.66	103.30
57	RJ	829	LEU	CA-CB-CG	5.29	127.46	115.30
3	SA	290	G	C8-N9-C1'	-5.28	120.13	127.00
64	RS	299	LEU	CA-CB-CG	5.28	127.45	115.30
3	SA	1269	U	C6-N1-C1'	-5.28	113.81	121.20
66	RV	204	GLY	N-CA-C	5.28	126.29	113.10
2	5A	85	G	C6-C5-N7	-5.27	127.24	130.40
3	SA	311	U	N3-C2-O2	-5.27	118.51	122.20
2	5A	173	G	OP1-P-O3'	5.26	116.78	105.20
2	5A	169	A	P-O3'-C3'	5.26	126.01	119.70
3	SA	894	U	C2-N1-C1'	5.26	124.01	117.70
49	5K	146	LEU	CA-CB-CG	5.26	127.40	115.30
54	RF	223	LEU	CA-CB-CG	5.26	127.39	115.30
3	SA	1174	C	C5-C6-N1	5.26	123.63	121.00
4	SC	188	LEU	CA-CB-CG	5.26	127.39	115.30
3	SA	648	G	C8-N9-C1'	-5.26	120.17	127.00
53	RE	248	LEU	CA-CB-CG	5.25	127.38	115.30
42	5D	225	LEU	CA-CB-CG	5.25	127.37	115.30
2	5A	98	G	C4-N9-C1'	5.24	133.31	126.50
53	RE	396	LEU	CA-CB-CG	5.24	127.36	115.30
23	3D	184	LEU	CA-CB-CG	5.24	127.35	115.30
3	SA	1759	C	C5-C6-N1	5.23	123.62	121.00
3	SA	1040	G	N9-C4-C5	-5.23	103.31	105.40
3	SA	1451	C	C5-C6-N1	5.23	123.61	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3F	318	LEU	CA-CB-CG	5.23	127.33	115.30
28	A5	63	LEU	CA-CB-CG	5.23	127.33	115.30
31	AE	756	LEU	CA-CB-CG	5.23	127.32	115.30
2	5A	61	U	C2-N1-C1'	5.22	123.97	117.70
33	AG	208	LEU	CA-CB-CG	5.22	127.31	115.30
36	B3	237	LEU	CB-CG-CD2	-5.22	102.12	111.00
3	SA	209	U	N3-C2-O2	-5.22	118.55	122.20
3	SA	121	U	N3-C2-O2	-5.21	118.55	122.20
47	5I	298	LEU	CA-CB-CG	5.21	127.29	115.30
3	SA	1492	A	C4-N9-C1'	5.21	135.68	126.30
2	5A	90	G	C6-C5-N7	5.20	133.52	130.40
2	5A	223	C	N1-C2-O2	5.20	122.02	118.90
3	SA	130	C	N1-C2-O2	5.20	122.02	118.90
3	SA	258	C	N3-C2-O2	-5.20	118.26	121.90
39	B6	23	LEU	CA-CB-CG	5.19	127.24	115.30
3	SA	1779	U	N1-C2-O2	5.19	126.43	122.80
3	SA	908	U	N1-C2-O2	5.18	126.43	122.80
45	5G	209	LEU	CA-CB-CG	5.18	127.22	115.30
3	SA	1518	C	C6-N1-C1'	-5.17	114.59	120.80
1	3A	89	C	N3-C2-O2	-5.17	118.28	121.90
2	5A	536	A	P-O3'-C3'	5.17	125.91	119.70
61	RO	264	LEU	CA-CB-CG	5.17	127.19	115.30
3	SA	146	U	O4'-C1'-N1	5.16	112.33	108.20
32	AF	285	ASP	CB-CG-OD1	5.16	122.94	118.30
3	SA	1461	C	C5-C6-N1	5.16	123.58	121.00
3	SA	357	G	C8-N9-C1'	5.16	133.70	127.00
2	5A	64	U	N3-C2-O2	-5.15	118.59	122.20
2	5A	537	G	C8-N9-C1'	-5.15	120.31	127.00
60	RN	429	LEU	CA-CB-CG	5.14	127.13	115.30
3	SA	692	C	N3-C2-O2	-5.14	118.30	121.90
3	SA	68	A	OP2-P-O3'	5.14	116.50	105.20
3	SA	1161	C	C2-N1-C1'	5.13	124.45	118.80
3	SA	1084	A	OP1-P-O3'	5.13	116.49	105.20
1	3A	61	G	C5-C6-N1	5.12	114.06	111.50
1	3A	250	C	N1-C2-O2	5.12	121.97	118.90
5	SF	87	MET	CA-CB-CG	5.12	122.01	113.30
2	5A	121	G	N7-C8-N9	5.12	115.66	113.10
1	3A	80	U	C2-N1-C1'	5.11	123.84	117.70
3	SA	302	U	C2-N1-C1'	5.11	123.83	117.70
3	SA	1743	U	C6-N1-C1'	-5.10	114.06	121.20
2	5A	252	A	N3-C4-C5	-5.10	123.23	126.80
3	SA	353	A	N1-C6-N6	-5.10	115.54	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3A	8	U	N3-C2-O2	-5.09	118.64	122.20
3	SA	1585	U	N3-C2-O2	-5.09	118.64	122.20
2	5A	310	U	C6-N1-C2	-5.08	117.95	121.00
3	SA	1623	C	C6-N1-C2	-5.07	118.27	120.30
3	SA	275	C	N1-C2-O2	5.07	121.94	118.90
2	5A	224	G	P-O3'-C3'	5.07	125.78	119.70
3	SA	376	C	N1-C2-O2	5.07	121.94	118.90
3	SA	258	C	C5-C6-N1	5.07	123.53	121.00
15	SR	123	ARG	C-N-CA	5.07	143.27	122.00
2	5A	90	G	N1-C6-O6	-5.06	116.86	119.90
3	SA	945	U	C2-N1-C1'	5.06	123.77	117.70
1	3A	41	C	C5-C6-N1	5.06	123.53	121.00
3	SA	909	U	N1-C2-O2	5.06	126.34	122.80
3	SA	1646	C	C6-N1-C2	-5.06	118.28	120.30
3	SA	25	C	N1-C2-O2	5.05	121.93	118.90
3	SA	297	U	N3-C2-O2	-5.05	118.66	122.20
3	SA	150	U	N1-C2-O2	5.05	126.34	122.80
2	5A	585	C	C2-N1-C1'	5.05	124.36	118.80
53	RE	243	LEU	CA-CB-CG	5.05	126.92	115.30
3	SA	363	G	N3-C2-N2	5.04	123.43	119.90
3	SA	1727	G	N3-C4-N9	-5.04	122.97	126.00
38	BE	121	LEU	CA-CB-CG	5.03	126.88	115.30
3	SA	346	G	C4-N9-C1'	5.03	133.04	126.50
36	B3	390	LEU	CA-CB-CG	5.03	126.87	115.30
36	B3	237	LEU	CA-CB-CG	5.03	126.87	115.30
55	RG	96	LEU	CA-CB-CG	5.03	126.86	115.30
3	SA	373	G	C8-N9-C1'	-5.02	120.47	127.00
1	3A	265	C	N1-C2-O2	5.02	121.91	118.90
3	SA	357	G	N1-C6-O6	-5.02	116.89	119.90
3	SA	1568	C	C2-N1-C1'	5.02	124.32	118.80
33	AG	79	LEU	CA-CB-CG	5.01	126.83	115.30
3	SA	186	C	C5-C6-N1	5.01	123.51	121.00
3	SA	130	C	C2-N1-C1'	5.01	124.31	118.80
3	SA	1448	G	N3-C4-N9	-5.01	122.99	126.00

There are no chirality outliers.

All (76) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	3B	176	ALA	Peptide
23	3D	142	LEU	Peptide
24	3E	228	PRO	Peptide

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Mol	Chain	Res	Type	Group
24	3E	36	ASP	Peptide
26	3G	59	GLU	Peptide
26	3G	64	LEU	Peptide
26	3G	9	PHE	Peptide
26	3H	59	GLU	Peptide
41	5C	111	PHE	Peptide
41	5C	140	ARG	Peptide
41	5C	540	GLU	Peptide
42	5D	84	GLY	Peptide
43	5E	453	SER	Peptide
44	5F	101	VAL	Peptide
47	5I	141	ASP	Peptide
49	5K	25	LEU	Peptide
49	5K	51	LEU	Peptide
28	A5	167	SER	Peptide
28	A5	457	LEU	Peptide
29	A8	257	SER	Peptide
29	A8	266	ILE	Peptide
29	A8	529	HIS	Peptide
29	A8	599	MET	Peptide
33	AG	178	PHE	Peptide
33	AG	769	ASN	Peptide
33	AG	780	GLU	Peptide
34	B1	288	ASP	Peptide
34	B1	661	LEU	Peptide
34	B1	733	LYS	Peptide
35	B2	131	GLY	Peptide
35	B2	266	SER	Peptide
35	B2	267	ASP	Peptide
35	B2	359	SER	Peptide
35	B2	52	TRP	Peptide
35	B2	575	PRO	Peptide
35	B2	613	ALA	Peptide
35	B2	653	LEU	Peptide
35	B2	916	HIS	Peptide
36	B3	35	PRO	Peptide
36	B3	473	ALA	Peptide
36	B3	480	ILE	Peptide
36	B3	530	ALA	Peptide
36	B3	593	CYS	Peptide
36	B3	594	GLY	Peptide
36	B3	785	ILE	Peptide

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Mol	Chain	Res	Type	Group
36	B3	90	LEU	Peptide
39	B6	354	ASP	Peptide
37	B8	366	SER	Peptide
37	B8	438	ASN	Peptide
37	B8	501	THR	Peptide
38	BE	173	LEU	Peptide
38	BE	899	ASN	Peptide
38	BE	94	TYR	Peptide
51	RB	273	GLY	Peptide
53	RE	767	GLN	Peptide
54	RF	253	ALA	Peptide
56	RI	50	ARG	Peptide
57	RJ	1026	LYS	Peptide
57	RJ	81	GLY	Peptide
59	RL	743	VAL	Peptide
59	RM	743	VAL	Peptide
62	RP	1907	ASN	Peptide
63	RQ	257	ILE	Peptide
66	RV	203	ILE	Peptide
4	SC	40	ASN	Peptide
5	SF	195	ILE	Peptide
6	SG	58	LEU	Peptide
7	SH	68	LEU	Peptide
8	SI	31	SER	Peptide
8	SI	64	VAL	Peptide
11	SM	128	CYS	Peptide
12	SN	99	GLU	Peptide
13	SO	24	ALA	Peptide
14	SP	90	ARG	Peptide
19	SZ	76	TYR	Peptide
20	Sc	74	SER	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	
4	SC	217/255 (85%)	186 (86%)	30 (14%)	1 (0%)	29	61
5	SF	227/261 (87%)	192 (85%)	35 (15%)	0	100	100
6	SG	211/225 (94%)	197 (93%)	14 (7%)	0	100	100
7	SH	108/236 (46%)	98 (91%)	9 (8%)	1 (1%)	17	49
8	SI	161/190 (85%)	139 (86%)	22 (14%)	0	100	100
9	SJ	162/200 (81%)	141 (87%)	21 (13%)	0	100	100
10	SK	169/197 (86%)	163 (96%)	6 (4%)	0	100	100
11	SM	119/156 (76%)	99 (83%)	20 (17%)	0	100	100
12	SN	117/143 (82%)	96 (82%)	21 (18%)	0	100	100
13	SO	132/151 (87%)	125 (95%)	7 (5%)	0	100	100
14	SP	116/137 (85%)	102 (88%)	14 (12%)	0	100	100
15	SR	123/143 (86%)	113 (92%)	10 (8%)	0	100	100
16	ST	109/146 (75%)	100 (92%)	9 (8%)	0	100	100
17	SX	125/130 (96%)	115 (92%)	10 (8%)	0	100	100
18	SY	101/145 (70%)	91 (90%)	10 (10%)	0	100	100
19	SZ	100/135 (74%)	86 (86%)	14 (14%)	0	100	100
20	Sc	78/82 (95%)	68 (87%)	10 (13%)	0	100	100
21	Sd	61/67 (91%)	55 (90%)	6 (10%)	0	100	100
22	3B	236/327 (72%)	222 (94%)	14 (6%)	0	100	100
22	3C	221/327 (68%)	203 (92%)	18 (8%)	0	100	100
23	3D	359/504 (71%)	344 (96%)	15 (4%)	0	100	100
24	3E	427/511 (84%)	394 (92%)	33 (8%)	0	100	100
25	3F	428/573 (75%)	384 (90%)	43 (10%)	1 (0%)	47	78
26	3G	119/126 (94%)	109 (92%)	9 (8%)	1 (1%)	19	51
26	3H	119/126 (94%)	110 (92%)	9 (8%)	0	100	100
27	A4	648/776 (84%)	576 (89%)	72 (11%)	0	100	100
28	A5	504/643 (78%)	460 (91%)	44 (9%)	0	100	100
29	A8	534/713 (75%)	407 (76%)	124 (23%)	3 (1%)	25	57
30	A9	126/575 (22%)	119 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	AE	773/1769 (44%)	710 (92%)	63 (8%)	0	100	100
32	AF	489/513 (95%)	437 (89%)	51 (10%)	1 (0%)	47	78
33	AG	812/896 (91%)	730 (90%)	82 (10%)	0	100	100
34	B1	830/923 (90%)	752 (91%)	76 (9%)	2 (0%)	47	78
35	B2	839/943 (89%)	750 (89%)	88 (10%)	1 (0%)	51	82
36	B3	733/817 (90%)	599 (82%)	132 (18%)	2 (0%)	41	72
37	B8	469/594 (79%)	423 (90%)	46 (10%)	0	100	100
38	BE	857/939 (91%)	792 (92%)	65 (8%)	0	100	100
39	B6	368/440 (84%)	337 (92%)	31 (8%)	0	100	100
40	5B	58/214 (27%)	55 (95%)	3 (5%)	0	100	100
41	5C	531/554 (96%)	472 (89%)	58 (11%)	1 (0%)	47	78
42	5D	231/250 (92%)	204 (88%)	27 (12%)	0	100	100
43	5E	200/593 (34%)	187 (94%)	11 (6%)	2 (1%)	15	46
44	5F	180/183 (98%)	169 (94%)	11 (6%)	0	100	100
45	5G	278/290 (96%)	249 (90%)	29 (10%)	0	100	100
46	5H	132/610 (22%)	121 (92%)	11 (8%)	0	100	100
47	5I	457/489 (94%)	420 (92%)	37 (8%)	0	100	100
48	5J	138/217 (64%)	129 (94%)	9 (6%)	0	100	100
49	5K	171/189 (90%)	160 (94%)	11 (6%)	0	100	100
50	RA	332/707 (47%)	287 (86%)	45 (14%)	0	100	100
51	RB	132/357 (37%)	116 (88%)	16 (12%)	0	100	100
52	RC	276/316 (87%)	260 (94%)	16 (6%)	0	100	100
53	RE	1067/1237 (86%)	984 (92%)	83 (8%)	0	100	100
54	RF	233/297 (78%)	214 (92%)	19 (8%)	0	100	100
55	RG	212/252 (84%)	186 (88%)	26 (12%)	0	100	100
55	RH	226/252 (90%)	212 (94%)	14 (6%)	0	100	100
56	RI	250/274 (91%)	228 (91%)	22 (9%)	0	100	100
57	RJ	784/1183 (66%)	723 (92%)	61 (8%)	0	100	100
58	RK	358/367 (98%)	335 (94%)	23 (6%)	0	100	100
59	RL	781/1056 (74%)	670 (86%)	109 (14%)	2 (0%)	41	72
59	RM	737/1056 (70%)	640 (87%)	93 (13%)	4 (0%)	29	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	RN	573/810 (71%)	524 (91%)	48 (8%)	1 (0%)	47	78
61	RO	523/552 (95%)	457 (87%)	66 (13%)	0	100	100
62	RP	1992/2493 (80%)	1801 (90%)	189 (10%)	2 (0%)	51	82
63	RQ	220/899 (24%)	197 (90%)	23 (10%)	0	100	100
64	RS	247/483 (51%)	223 (90%)	23 (9%)	1 (0%)	34	67
65	RT	165/326 (51%)	151 (92%)	14 (8%)	0	100	100
66	RV	184/346 (53%)	168 (91%)	16 (9%)	0	100	100
All	All	23995/32886 (73%)	21566 (90%)	2403 (10%)	26 (0%)	54	82

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
43	5E	454	VAL
59	RL	744	PRO
59	RM	744	PRO
62	RP	119	PRO
29	A8	309	PRO
36	B3	91	LYS
59	RM	905	PRO
62	RP	1993	PRO
34	B1	670	LEU
43	5E	460	PRO
59	RM	904	LEU
60	RN	285	PRO
25	3F	552	TRP
29	A8	308	PHE
34	B1	442	GLY
35	B2	132	THR
41	5C	492	GLY
36	B3	71	PRO
59	RL	743	VAL
59	RM	743	VAL
32	AF	49	PRO
64	RS	414	PRO
4	SC	221	PRO
7	SH	70	PRO
26	3G	10	PRO
29	A8	267	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	
4	SC	195/224 (87%)	192 (98%)	3 (2%)	65	82
5	SF	196/222 (88%)	191 (97%)	5 (3%)	46	72
6	SG	180/191 (94%)	179 (99%)	1 (1%)	86	94
7	SH	95/201 (47%)	94 (99%)	1 (1%)	73	86
8	SI	146/170 (86%)	144 (99%)	2 (1%)	67	83
9	SJ	136/161 (84%)	135 (99%)	1 (1%)	84	92
10	SK	147/166 (89%)	144 (98%)	3 (2%)	55	77
11	SM	110/137 (80%)	109 (99%)	1 (1%)	78	90
12	SN	88/119 (74%)	88 (100%)	0	100	100
13	SO	117/128 (91%)	115 (98%)	2 (2%)	60	80
14	SP	90/105 (86%)	88 (98%)	2 (2%)	52	75
15	SR	105/119 (88%)	105 (100%)	0	100	100
16	ST	101/129 (78%)	101 (100%)	0	100	100
17	SX	108/111 (97%)	108 (100%)	0	100	100
18	SY	85/120 (71%)	85 (100%)	0	100	100
19	SZ	85/113 (75%)	84 (99%)	1 (1%)	71	85
20	Sc	69/71 (97%)	69 (100%)	0	100	100
21	Sd	56/60 (93%)	56 (100%)	0	100	100
22	3B	201/240 (84%)	200 (100%)	1 (0%)	88	94
22	3C	190/240 (79%)	190 (100%)	0	100	100
23	3D	296/435 (68%)	292 (99%)	4 (1%)	67	83
24	3E	262/433 (60%)	260 (99%)	2 (1%)	81	91
25	3F	378/503 (75%)	373 (99%)	5 (1%)	69	84
26	3G	100/104 (96%)	99 (99%)	1 (1%)	76	88
26	3H	100/104 (96%)	100 (100%)	0	100	100
27	A4	591/713 (83%)	583 (99%)	8 (1%)	67	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	A5	433/574 (75%)	430 (99%)	3 (1%)	84	92
29	A8	174/657 (26%)	173 (99%)	1 (1%)	86	94
30	A9	89/533 (17%)	89 (100%)	0	100	100
31	AE	708/1633 (43%)	700 (99%)	8 (1%)	73	86
32	AF	437/454 (96%)	432 (99%)	5 (1%)	73	86
33	AG	750/826 (91%)	743 (99%)	7 (1%)	78	90
34	B1	730/812 (90%)	719 (98%)	11 (2%)	65	82
35	B2	736/832 (88%)	729 (99%)	7 (1%)	76	88
36	B3	665/719 (92%)	654 (98%)	11 (2%)	60	80
37	B8	421/529 (80%)	417 (99%)	4 (1%)	76	88
38	BE	757/819 (92%)	748 (99%)	9 (1%)	71	85
39	B6	251/414 (61%)	246 (98%)	5 (2%)	55	77
40	5B	57/196 (29%)	56 (98%)	1 (2%)	59	79
41	5C	465/480 (97%)	457 (98%)	8 (2%)	60	80
42	5D	221/234 (94%)	219 (99%)	2 (1%)	78	90
43	5E	185/535 (35%)	183 (99%)	2 (1%)	73	86
44	5F	171/172 (99%)	171 (100%)	0	100	100
45	5G	251/258 (97%)	249 (99%)	2 (1%)	81	91
46	5H	107/538 (20%)	106 (99%)	1 (1%)	78	90
47	5I	416/443 (94%)	407 (98%)	9 (2%)	52	75
48	5J	133/200 (66%)	133 (100%)	0	100	100
49	5K	157/169 (93%)	155 (99%)	2 (1%)	69	84
50	RA	303/636 (48%)	303 (100%)	0	100	100
51	RB	117/315 (37%)	115 (98%)	2 (2%)	60	80
52	RC	231/289 (80%)	230 (100%)	1 (0%)	91	95
53	RE	984/1125 (88%)	975 (99%)	9 (1%)	78	90
54	RF	221/274 (81%)	217 (98%)	4 (2%)	59	79
55	RG	195/222 (88%)	194 (100%)	1 (0%)	88	94
55	RH	206/222 (93%)	203 (98%)	3 (2%)	65	82
56	RI	235/256 (92%)	231 (98%)	4 (2%)	60	80
57	RJ	683/1039 (66%)	679 (99%)	4 (1%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	RK	307/312 (98%)	305 (99%)	2 (1%)	84	92
59	RL	164/934 (18%)	159 (97%)	5 (3%)	41	68
60	RN	406/732 (56%)	406 (100%)	0	100	100
61	RO	329/506 (65%)	326 (99%)	3 (1%)	78	90
63	RQ	148/808 (18%)	147 (99%)	1 (1%)	84	92
64	RS	225/424 (53%)	221 (98%)	4 (2%)	59	79
65	RT	148/282 (52%)	145 (98%)	3 (2%)	55	77
66	RV	141/304 (46%)	140 (99%)	1 (1%)	84	92
All	All	17584/26026 (68%)	17396 (99%)	188 (1%)	74	86

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	SC	92	GLN
4	SC	162	ARG
4	SC	205	PHE
5	SF	181	VAL
5	SF	200	ARG
5	SF	207	LEU
5	SF	211	LYS
5	SF	233	LYS
6	SG	123	VAL
7	SH	92	ARG
8	SI	159	VAL
8	SI	189	THR
9	SJ	43	ILE
10	SK	57	ARG
10	SK	74	ASN
10	SK	87	SER
11	SM	69	LYS
13	SO	58	HIS
13	SO	135	LEU
14	SP	86	THR
14	SP	117	ASP
19	SZ	74	LEU
22	3B	120	GLU
23	3D	10	GLU
23	3D	48	ILE
23	3D	103	LYS

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Mol	Chain	Res	Type
23	3D	285	ARG
24	3E	265	PHE
24	3E	371	LEU
25	3F	223	THR
25	3F	293	ASP
25	3F	370	ARG
25	3F	418	ASP
25	3F	506	ARG
26	3G	67	LEU
27	A4	33	VAL
27	A4	130	THR
27	A4	282	ASP
27	A4	579	ARG
27	A4	648	PHE
27	A4	745	ASP
27	A4	775	VAL
27	A4	776	PHE
28	A5	139	HIS
28	A5	235	LEU
28	A5	310	THR
29	A8	576	ARG
31	AE	147	VAL
31	AE	253	CYS
31	AE	264	PHE
31	AE	366	ILE
31	AE	396	ASP
31	AE	485	THR
31	AE	515	PHE
31	AE	713	PHE
32	AF	20	THR
32	AF	149	THR
32	AF	199	ARG
32	AF	236	VAL
32	AF	255	VAL
33	AG	109	VAL
33	AG	131	HIS
33	AG	271	LEU
33	AG	336	ARG
33	AG	421	LYS
33	AG	606	HIS
33	AG	716	ARG
34	B1	76	ASP

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Mol	Chain	Res	Type
34	B1	167	ASP
34	B1	173	TRP
34	B1	215	VAL
34	B1	321	SER
34	B1	351	LEU
34	B1	519	LEU
34	B1	526	ASP
34	B1	574	SER
34	B1	603	LEU
34	B1	698	THR
35	B2	159	LEU
35	B2	331	THR
35	B2	343	TRP
35	B2	450	ARG
35	B2	576	VAL
35	B2	579	ILE
35	B2	663	LEU
36	B3	24	THR
36	B3	32	LEU
36	B3	51	LYS
36	B3	97	ARG
36	B3	100	LYS
36	B3	222	LEU
36	B3	482	VAL
36	B3	520	LEU
36	B3	533	LYS
36	B3	534	ARG
36	B3	539	VAL
37	B8	272	LEU
37	B8	344	ARG
37	B8	406	ASP
37	B8	546	LEU
38	BE	207	ASP
38	BE	209	ILE
38	BE	312	THR
38	BE	470	GLN
38	BE	494	LEU
38	BE	570	ILE
38	BE	713	LEU
38	BE	813	PHE
38	BE	899	ASN
39	B6	23	LEU

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Mol	Chain	Res	Type
39	B6	34	LYS
39	B6	67	ARG
39	B6	133	TYR
39	B6	297	ASP
40	5B	168	LYS
41	5C	153	THR
41	5C	253	ASN
41	5C	291	THR
41	5C	296	ARG
41	5C	347	LEU
41	5C	392	VAL
41	5C	505	THR
41	5C	544	ASP
42	5D	91	LEU
42	5D	161	ARG
43	5E	297	LEU
43	5E	330	VAL
45	5G	176	ILE
45	5G	223	THR
46	5H	579	VAL
47	5I	91	VAL
47	5I	119	THR
47	5I	124	HIS
47	5I	214	ASP
47	5I	232	THR
47	5I	250	ARG
47	5I	261	THR
47	5I	356	TYR
47	5I	410	ILE
49	5K	17	LEU
49	5K	41	THR
51	RB	306	ARG
51	RB	341	ARG
52	RC	62	ARG
53	RE	223	ARG
53	RE	227	LYS
53	RE	232	LEU
53	RE	245	LYS
53	RE	285	PHE
53	RE	289	ARG
53	RE	595	THR
53	RE	840	LEU

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Mol	Chain	Res	Type
53	RE	976	ILE
54	RF	19	LYS
54	RF	160	TYR
54	RF	171	PHE
54	RF	176	ASP
55	RG	97	LEU
55	RH	31	LEU
55	RH	82	ARG
55	RH	116	THR
56	RI	17	LEU
56	RI	30	LEU
56	RI	170	LYS
56	RI	171	CYS
57	RJ	214	ARG
57	RJ	868	ARG
57	RJ	973	ARG
57	RJ	1141	LYS
58	RK	213	LYS
58	RK	214	LYS
59	RL	9	ARG
59	RL	10	ILE
59	RL	83	ARG
59	RL	104	ARG
59	RL	134	LEU
61	RO	203	LEU
61	RO	493	TYR
61	RO	507	LEU
63	RQ	319	THR
64	RS	225	THR
64	RS	233	PHE
64	RS	344	LYS
64	RS	390	CYS
65	RT	129	ARG
65	RT	139	LEU
65	RT	182	ILE
66	RV	315	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (285) such sidechains are listed below:

Mol	Chain	Res	Type
4	SC	101	HIS
4	SC	118	GLN

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Mol	Chain	Res	Type
4	SC	183	GLN
5	SF	153	ASN
5	SF	188	ASN
5	SF	224	ASN
6	SG	86	GLN
6	SG	104	ASN
6	SG	127	GLN
6	SG	131	GLN
6	SG	169	ASN
6	SG	186	ASN
7	SH	59	GLN
8	SI	74	GLN
9	SJ	64	ASN
9	SJ	103	GLN
11	SM	92	HIS
11	SM	98	ASN
11	SM	106	ASN
12	SN	38	HIS
12	SN	96	GLN
13	SO	49	GLN
13	SO	58	HIS
15	SR	74	HIS
16	ST	21	ASN
16	ST	44	ASN
17	SX	16	ASN
19	SZ	29	HIS
19	SZ	77	ASN
22	3B	258	HIS
22	3C	145	ASN
23	3D	172	ASN
23	3D	183	GLN
23	3D	302	ASN
23	3D	381	ASN
24	3E	191	HIS
24	3E	254	ASN
24	3E	256	ASN
24	3E	286	ASN
24	3E	289	GLN
24	3E	396	ASN
24	3E	400	GLN
25	3F	226	HIS
25	3F	485	ASN

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Mol	Chain	Res	Type
25	3F	525	GLN
26	3G	29	ASN
26	3G	38	ASN
26	3H	18	GLN
26	3H	45	ASN
26	3H	66	HIS
27	A4	53	HIS
27	A4	140	ASN
27	A4	273	ASN
27	A4	274	GLN
27	A4	279	HIS
27	A4	292	ASN
27	A4	317	ASN
27	A4	452	HIS
27	A4	529	ASN
27	A4	589	ASN
27	A4	621	ASN
27	A4	632	ASN
27	A4	642	ASN
28	A5	103	ASN
28	A5	133	GLN
28	A5	213	ASN
28	A5	302	ASN
28	A5	308	ASN
28	A5	316	ASN
28	A5	324	ASN
28	A5	509	HIS
29	A8	553	GLN
29	A8	609	ASN
30	A9	443	GLN
30	A9	444	ASN
30	A9	474	HIS
30	A9	478	ASN
31	AE	7	GLN
31	AE	51	ASN
31	AE	141	ASN
31	AE	166	ASN
31	AE	202	HIS
31	AE	219	ASN
31	AE	224	ASN
31	AE	309	GLN
31	AE	480	ASN

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Mol	Chain	Res	Type
31	AE	559	ASN
31	AE	709	ASN
31	AE	773	GLN
31	AE	774	ASN
32	AF	24	GLN
32	AF	44	HIS
32	AF	48	ASN
32	AF	64	GLN
32	AF	72	GLN
32	AF	133	HIS
32	AF	217	ASN
32	AF	250	ASN
32	AF	280	HIS
32	AF	289	ASN
32	AF	391	ASN
32	AF	403	ASN
32	AF	481	GLN
32	AF	502	GLN
33	AG	9	GLN
33	AG	169	GLN
33	AG	190	GLN
33	AG	398	HIS
33	AG	424	GLN
33	AG	489	ASN
33	AG	535	ASN
33	AG	624	HIS
33	AG	660	GLN
33	AG	669	ASN
33	AG	759	HIS
33	AG	760	HIS
34	B1	91	HIS
34	B1	142	HIS
34	B1	190	HIS
34	B1	201	HIS
34	B1	302	GLN
34	B1	303	ASN
34	B1	349	ASN
34	B1	386	HIS
34	B1	452	ASN
34	B1	456	HIS
34	B1	650	ASN
34	B1	691	ASN

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Mol	Chain	Res	Type
34	B1	795	ASN
34	B1	813	HIS
34	B1	837	ASN
34	B1	842	ASN
35	B2	128	GLN
35	B2	172	GLN
35	B2	264	ASN
35	B2	276	ASN
35	B2	524	HIS
35	B2	596	ASN
35	B2	657	GLN
35	B2	677	HIS
35	B2	770	ASN
35	B2	798	ASN
35	B2	856	ASN
35	B2	879	GLN
36	B3	143	HIS
36	B3	301	GLN
36	B3	328	GLN
36	B3	392	ASN
36	B3	502	ASN
36	B3	519	ASN
36	B3	616	HIS
36	B3	767	HIS
36	B3	792	HIS
36	B3	802	GLN
37	B8	41	ASN
37	B8	159	HIS
37	B8	162	ASN
37	B8	282	ASN
37	B8	283	HIS
37	B8	308	ASN
37	B8	352	GLN
37	B8	472	GLN
37	B8	492	ASN
38	BE	20	ASN
38	BE	67	HIS
38	BE	203	ASN
38	BE	447	ASN
38	BE	481	ASN
38	BE	501	HIS
38	BE	903	GLN

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Mol	Chain	Res	Type
39	B6	90	GLN
39	B6	115	ASN
40	5B	207	ASN
41	5C	101	ASN
41	5C	124	HIS
41	5C	133	HIS
41	5C	164	GLN
41	5C	170	GLN
41	5C	400	ASN
41	5C	468	GLN
41	5C	480	ASN
41	5C	507	ASN
42	5D	144	ASN
42	5D	221	GLN
43	5E	526	ASN
44	5F	27	HIS
44	5F	39	GLN
44	5F	59	ASN
44	5F	135	HIS
45	5G	18	GLN
45	5G	143	HIS
45	5G	159	HIS
45	5G	208	HIS
46	5H	515	ASN
47	5I	46	ASN
47	5I	76	ASN
47	5I	202	HIS
47	5I	207	ASN
47	5I	260	GLN
47	5I	284	HIS
47	5I	371	ASN
47	5I	392	ASN
47	5I	406	HIS
48	5J	126	HIS
48	5J	184	ASN
48	5J	192	ASN
48	5J	195	GLN
49	5K	43	ASN
50	RA	101	ASN
50	RA	118	GLN
51	RB	301	ASN
51	RB	314	ASN

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Mol	Chain	Res	Type
52	RC	149	ASN
52	RC	151	ASN
52	RC	284	GLN
53	RE	197	GLN
53	RE	221	ASN
53	RE	293	ASN
53	RE	371	GLN
53	RE	414	HIS
53	RE	439	HIS
53	RE	520	ASN
53	RE	607	HIS
53	RE	634	HIS
53	RE	665	HIS
53	RE	834	ASN
53	RE	841	ASN
53	RE	901	ASN
53	RE	1159	ASN
53	RE	1180	ASN
54	RF	23	HIS
55	RG	105	ASN
55	RG	125	ASN
55	RG	170	HIS
55	RG	190	GLN
55	RG	215	ASN
55	RH	69	ASN
56	RI	52	ASN
56	RI	186	ASN
56	RI	192	ASN
56	RI	221	ASN
57	RJ	126	ASN
57	RJ	162	HIS
57	RJ	239	ASN
57	RJ	289	HIS
57	RJ	776	GLN
57	RJ	778	GLN
57	RJ	944	ASN
58	RK	16	ASN
58	RK	88	HIS
58	RK	167	HIS
58	RK	317	GLN
59	RL	16	ASN
59	RL	75	ASN

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Mol	Chain	Res	Type
59	RL	89	ASN
60	RN	452	GLN
60	RN	482	GLN
60	RN	527	GLN
60	RN	569	GLN
60	RN	738	ASN
60	RN	771	ASN
60	RN	797	ASN
61	RO	228	HIS
61	RO	256	ASN
61	RO	268	GLN
61	RO	273	GLN
61	RO	290	HIS
61	RO	304	ASN
61	RO	309	ASN
61	RO	343	GLN
61	RO	346	ASN
61	RO	370	HIS
61	RO	472	HIS
63	RQ	310	HIS
63	RQ	321	HIS
63	RQ	331	GLN
63	RQ	832	ASN
63	RQ	839	ASN
64	RS	302	HIS
64	RS	385	GLN
65	RT	111	ASN
65	RT	218	ASN
65	RT	232	HIS
66	RV	224	HIS
66	RV	225	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3A	169/333 (50%)	46 (27%)	2 (1%)
2	5A	516/700 (73%)	146 (28%)	10 (1%)
3	SA	1290/1807 (71%)	461 (35%)	16 (1%)
All	All	1975/2840 (69%)	653 (33%)	28 (1%)

All (653) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3A	2	U
1	3A	5	A
1	3A	14	A
1	3A	15	U
1	3A	24	U
1	3A	25	U
1	3A	28	A
1	3A	30	A
1	3A	33	A
1	3A	35	U
1	3A	56	A
1	3A	60	A
1	3A	61	G
1	3A	82	G
1	3A	87	G
1	3A	88	U
1	3A	89	C
1	3A	90	C
1	3A	91	C
1	3A	102	U
1	3A	104	C
1	3A	111	G
1	3A	114	A
1	3A	115	G
1	3A	198	U
1	3A	199	G
1	3A	200	C
1	3A	201	C
1	3A	204	U
1	3A	205	G
1	3A	206	C
1	3A	246	A
1	3A	248	G
1	3A	249	G
1	3A	252	C
1	3A	265	C
1	3A	266	C
1	3A	305	G
1	3A	309	G
1	3A	310	G
1	3A	313	A
1	3A	314	C
1	3A	322	A

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Mol	Chain	Res	Type
1	3A	324	U
1	3A	325	C
1	3A	329	C
2	5A	5	G
2	5A	6	A
2	5A	7	A
2	5A	8	A
2	5A	13	U
2	5A	62	C
2	5A	63	G
2	5A	64	U
2	5A	70	A
2	5A	82	A
2	5A	83	U
2	5A	85	G
2	5A	86	C
2	5A	87	C
2	5A	103	G
2	5A	104	A
2	5A	109	C
2	5A	110	G
2	5A	114	G
2	5A	124	A
2	5A	125	G
2	5A	126	A
2	5A	127	U
2	5A	128	C
2	5A	129	U
2	5A	130	G
2	5A	140	U
2	5A	142	U
2	5A	144	C
2	5A	148	G
2	5A	150	G
2	5A	151	U
2	5A	156	U
2	5A	161	A
2	5A	163	G
2	5A	169	A
2	5A	170	U
2	5A	171	G
2	5A	172	C

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Mol	Chain	Res	Type
2	5A	173	G
2	5A	174	U
2	5A	177	U
2	5A	185	A
2	5A	190	U
2	5A	200	A
2	5A	201	U
2	5A	211	G
2	5A	219	U
2	5A	220	U
2	5A	223	C
2	5A	224	G
2	5A	225	U
2	5A	226	U
2	5A	227	U
2	5A	235	A
2	5A	240	C
2	5A	256	U
2	5A	259	G
2	5A	260	A
2	5A	261	U
2	5A	266	U
2	5A	267	U
2	5A	268	G
2	5A	271	G
2	5A	279	A
2	5A	280	A
2	5A	281	G
2	5A	304	U
2	5A	305	A
2	5A	309	A
2	5A	310	U
2	5A	311	C
2	5A	312	U
2	5A	313	A
2	5A	316	U
2	5A	324	U
2	5A	325	U
2	5A	326	C
2	5A	327	A
2	5A	328	A
2	5A	337	G

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Mol	Chain	Res	Type
2	5A	339	A
2	5A	353	A
2	5A	354	G
2	5A	359	U
2	5A	360	C
2	5A	363	A
2	5A	364	A
2	5A	365	G
2	5A	368	U
2	5A	369	G
2	5A	370	U
2	5A	371	G
2	5A	372	A
2	5A	373	U
2	5A	381	G
2	5A	385	A
2	5A	386	A
2	5A	393	C
2	5A	395	C
2	5A	407	A
2	5A	419	A
2	5A	427	A
2	5A	428	A
2	5A	429	A
2	5A	430	C
2	5A	431	A
2	5A	432	C
2	5A	433	C
2	5A	440	U
2	5A	443	G
2	5A	461	A
2	5A	462	G
2	5A	464	G
2	5A	468	A
2	5A	469	C
2	5A	472	A
2	5A	474	A
2	5A	481	U
2	5A	482	A
2	5A	485	G
2	5A	487	A
2	5A	488	U

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Mol	Chain	Res	Type
2	5A	489	G
2	5A	490	G
2	5A	491	U
2	5A	493	A
2	5A	517	A
2	5A	519	A
2	5A	525	U
2	5A	526	U
2	5A	533	G
2	5A	536	A
2	5A	537	G
2	5A	539	A
2	5A	540	U
2	5A	541	U
2	5A	542	U
2	5A	547	C
2	5A	549	G
2	5A	555	A
2	5A	585	C
2	5A	586	A
2	5A	587	G
2	5A	589	U
2	5A	590	G
3	SA	-5	G
3	SA	-4	A
3	SA	-1	G
3	SA	0	U
3	SA	1	U
3	SA	6	G
3	SA	10	G
3	SA	17	C
3	SA	18	C
3	SA	21	U
3	SA	24	U
3	SA	25	C
3	SA	26	A
3	SA	36	C
3	SA	37	U
3	SA	51	A
3	SA	53	G
3	SA	54	C
3	SA	55	A

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Mol	Chain	Res	Type
3	SA	56	U
3	SA	57	G
3	SA	59	C
3	SA	61	A
3	SA	63	G
3	SA	65	A
3	SA	66	U
3	SA	67	A
3	SA	68	A
3	SA	69	G
3	SA	72	A
3	SA	73	U
3	SA	74	U
3	SA	77	U
3	SA	80	A
3	SA	81	G
3	SA	85	A
3	SA	89	G
3	SA	92	A
3	SA	93	A
3	SA	96	G
3	SA	97	C
3	SA	100	A
3	SA	102	U
3	SA	104	A
3	SA	105	A
3	SA	114	C
3	SA	115	G
3	SA	126	A
3	SA	127	G
3	SA	128	U
3	SA	129	U
3	SA	130	C
3	SA	131	C
3	SA	141	U
3	SA	145	A
3	SA	146	U
3	SA	153	G
3	SA	159	U
3	SA	160	C
3	SA	163	G
3	SA	168	A

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Mol	Chain	Res	Type
3	SA	170	U
3	SA	174	U
3	SA	176	C
3	SA	177	U
3	SA	182	A
3	SA	183	U
3	SA	184	C
3	SA	187	G
3	SA	188	A
3	SA	190	C
3	SA	191	C
3	SA	192	U
3	SA	193	U
3	SA	194	U
3	SA	195	G
3	SA	197	A
3	SA	203	U
3	SA	211	U
3	SA	214	G
3	SA	228	G
3	SA	231	U
3	SA	233	C
3	SA	234	G
3	SA	236	A
3	SA	237	C
3	SA	238	U
3	SA	239	C
3	SA	241	U
3	SA	242	U
3	SA	246	G
3	SA	254	A
3	SA	255	U
3	SA	256	A
3	SA	261	U
3	SA	262	U
3	SA	265	A
3	SA	266	A
3	SA	267	U
3	SA	272	U
3	SA	273	G
3	SA	276	C
3	SA	277	U

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Mol	Chain	Res	Type
3	SA	278	U
3	SA	279	G
3	SA	280	U
3	SA	281	G
3	SA	283	U
3	SA	288	A
3	SA	290	G
3	SA	311	U
3	SA	313	U
3	SA	315	A
3	SA	316	A
3	SA	319	U
3	SA	320	U
3	SA	321	C
3	SA	322	G
3	SA	333	A
3	SA	334	G
3	SA	337	G
3	SA	339	C
3	SA	350	U
3	SA	351	C
3	SA	352	A
3	SA	356	G
3	SA	359	A
3	SA	360	A
3	SA	361	C
3	SA	362	G
3	SA	365	G
3	SA	366	A
3	SA	369	A
3	SA	371	G
3	SA	373	G
3	SA	374	U
3	SA	375	U
3	SA	376	C
3	SA	379	U
3	SA	382	C
3	SA	383	G
3	SA	386	G
3	SA	387	A
3	SA	390	G
3	SA	400	A

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Mol	Chain	Res	Type
3	SA	401	A
3	SA	402	C
3	SA	403	G
3	SA	404	G
3	SA	405	C
3	SA	407	A
3	SA	410	A
3	SA	411	C
3	SA	416	A
3	SA	418	G
3	SA	420	A
3	SA	421	A
3	SA	422	G
3	SA	423	G
3	SA	424	C
3	SA	425	A
3	SA	426	G
3	SA	428	A
3	SA	431	C
3	SA	436	A
3	SA	437	A
3	SA	439	U
3	SA	440	U
3	SA	441	A
3	SA	444	C
3	SA	445	A
3	SA	452	A
3	SA	454	U
3	SA	455	C
3	SA	456	A
3	SA	468	A
3	SA	469	C
3	SA	470	A
3	SA	471	A
3	SA	473	A
3	SA	477	A
3	SA	480	G
3	SA	485	A
3	SA	486	G
3	SA	487	G
3	SA	493	U
3	SA	496	G

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Mol	Chain	Res	Type
3	SA	501	U
3	SA	502	U
3	SA	505	A
3	SA	506	A
3	SA	507	U
3	SA	520	A
3	SA	534	A
3	SA	538	A
3	SA	539	G
3	SA	541	A
3	SA	542	A
3	SA	543	C
3	SA	545	A
3	SA	551	G
3	SA	557	G
3	SA	563	U
3	SA	564	G
3	SA	570	A
3	SA	572	C
3	SA	575	C
3	SA	579	A
3	SA	580	A
3	SA	583	C
3	SA	584	C
3	SA	585	A
3	SA	586	G
3	SA	587	C
3	SA	594	A
3	SA	595	G
3	SA	603	U
3	SA	604	A
3	SA	606	A
3	SA	608	U
3	SA	609	U
3	SA	610	G
3	SA	612	U
3	SA	613	G
3	SA	614	C
3	SA	615	A
3	SA	616	G
3	SA	635	A
3	SA	636	A

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Mol	Chain	Res	Type
3	SA	638	U
3	SA	644	C
3	SA	648	G
3	SA	649	U
3	SA	652	G
3	SA	654	C
3	SA	656	G
3	SA	657	U
3	SA	658	C
3	SA	659	C
3	SA	677	G
3	SA	678	A
3	SA	680	U
3	SA	682	C
3	SA	687	G
3	SA	689	G
3	SA	691	C
3	SA	692	C
3	SA	859	A
3	SA	860	U
3	SA	861	U
3	SA	863	A
3	SA	864	U
3	SA	865	A
3	SA	876	G
3	SA	894	U
3	SA	901	G
3	SA	906	A
3	SA	913	G
3	SA	914	G
3	SA	932	U
3	SA	933	A
3	SA	935	U
3	SA	940	A
3	SA	945	U
3	SA	951	A
3	SA	960	U
3	SA	966	A
3	SA	969	C
3	SA	970	A
3	SA	1021	C
3	SA	1022	C

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Mol	Chain	Res	Type
3	SA	1023	A
3	SA	1024	U
3	SA	1025	A
3	SA	1026	A
3	SA	1027	A
3	SA	1031	U
3	SA	1032	G
3	SA	1036	A
3	SA	1037	C
3	SA	1039	A
3	SA	1040	G
3	SA	1052	U
3	SA	1053	G
3	SA	1056	U
3	SA	1058	U
3	SA	1059	U
3	SA	1060	U
3	SA	1062	A
3	SA	1063	U
3	SA	1064	G
3	SA	1075	C
3	SA	1076	A
3	SA	1081	A
3	SA	1082	C
3	SA	1084	A
3	SA	1085	G
3	SA	1086	A
3	SA	1106	U
3	SA	1107	G
3	SA	1108	G
3	SA	1109	G
3	SA	1110	G
3	SA	1111	G
3	SA	1118	G
3	SA	1119	G
3	SA	1122	G
3	SA	1125	A
3	SA	1127	G
3	SA	1128	C
3	SA	1131	A
3	SA	1132	A
3	SA	1145	U

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Mol	Chain	Res	Type
3	SA	1146	G
3	SA	1147	A
3	SA	1158	C
3	SA	1164	G
3	SA	1191	U
3	SA	1192	C
3	SA	1193	A
3	SA	1196	A
3	SA	1197	C
3	SA	1198	G
3	SA	1199	G
3	SA	1200	G
3	SA	1201	G
3	SA	1202	A
3	SA	1205	C
3	SA	1207	C
3	SA	1208	A
3	SA	1210	C
3	SA	1213	G
3	SA	1217	A
3	SA	1218	G
3	SA	1219	A
3	SA	1226	A
3	SA	1227	A
3	SA	1228	G
3	SA	1229	G
3	SA	1232	U
3	SA	1235	C
3	SA	1236	A
3	SA	1253	U
3	SA	1255	G
3	SA	1258	U
3	SA	1259	U
3	SA	1266	U
3	SA	1268	G
3	SA	1271	G
3	SA	1272	U
3	SA	1273	G
3	SA	1274	C
3	SA	1275	A
3	SA	1436	A
3	SA	1437	U

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Mol	Chain	Res	Type
3	SA	1440	C
3	SA	1443	U
3	SA	1450	U
3	SA	1457	C
3	SA	1461	C
3	SA	1469	A
3	SA	1472	C
3	SA	1473	U
3	SA	1474	G
3	SA	1475	A
3	SA	1477	G
3	SA	1485	C
3	SA	1488	G
3	SA	1489	U
3	SA	1492	A
3	SA	1493	A
3	SA	1496	U
3	SA	1498	G
3	SA	1506	G
3	SA	1517	U
3	SA	1518	C
3	SA	1520	U
3	SA	1521	G
3	SA	1522	U
3	SA	1523	G
3	SA	1524	A
3	SA	1531	G
3	SA	1535	U
3	SA	1536	G
3	SA	1539	G
3	SA	1541	G
3	SA	1543	A
3	SA	1544	U
3	SA	1567	U
3	SA	1568	C
3	SA	1569	A
3	SA	1570	A
3	SA	1573	A
3	SA	1584	G
3	SA	1590	G
3	SA	1594	G
3	SA	1595	U

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Mol	Chain	Res	Type
3	SA	1601	G
3	SA	1602	C
3	SA	1607	G
3	SA	1614	A
3	SA	1618	C
3	SA	1628	U
3	SA	1629	G
3	SA	1630	U
3	SA	1631	A
3	SA	1639	C
3	SA	1651	A
3	SA	1658	G
3	SA	1659	A
3	SA	1664	C
3	SA	1670	G
3	SA	1671	A
3	SA	1672	G
3	SA	1677	C
3	SA	1678	A
3	SA	1679	G
3	SA	1680	G
3	SA	1681	A
3	SA	1682	U
3	SA	1683	C
3	SA	1684	U
3	SA	1685	G
3	SA	1690	G
3	SA	1695	G
3	SA	1700	C
3	SA	1702	A
3	SA	1707	A
3	SA	1710	U
3	SA	1711	C
3	SA	1713	G
3	SA	1717	G
3	SA	1718	G
3	SA	1719	A
3	SA	1724	U
3	SA	1725	U
3	SA	1727	G
3	SA	1731	A
3	SA	1732	A

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Mol	Chain	Res	Type
3	SA	1736	G
3	SA	1737	G
3	SA	1742	U
3	SA	1743	U
3	SA	1745	G
3	SA	1747	G
3	SA	1749	A
3	SA	1751	C
3	SA	1756	A
3	SA	1757	G
3	SA	1758	U
3	SA	1759	C
3	SA	1761	U
3	SA	1764	C
3	SA	1765	A
3	SA	1766	A
3	SA	1768	G
3	SA	1772	C
3	SA	1779	U
3	SA	1780	G
3	SA	1781	A
3	SA	1782	A

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	3A	198	U
1	3A	248	G
2	5A	169	A
2	5A	172	C
2	5A	173	G
2	5A	224	G
2	5A	312	U
2	5A	358	G
2	5A	363	A
2	5A	368	U
2	5A	492	G
2	5A	536	A
3	SA	0	U
3	SA	56	U
3	SA	68	A
3	SA	272	U

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Mol	Chain	Res	Type
3	SA	372	G
3	SA	401	A
3	SA	417	A
3	SA	538	A
3	SA	542	A
3	SA	579	A
3	SA	602	U
3	SA	1031	U
3	SA	1052	U
3	SA	1084	A
3	SA	1521	G
3	SA	1594	G

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 4 ligands modelled in this entry, 3 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	$\# Z > 2$
69	GTP	RJ	1201	70	26,34,34	1.23	1 (3%)	32,54,54	1.65	6 (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
69	GTP	RJ	1201	70	-	2/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	RJ	1201	GTP	C5-C6	-4.38	1.38	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	RJ	1201	GTP	PA-O3A-PB	-4.27	118.18	132.83
69	RJ	1201	GTP	PB-O3B-PG	-3.72	120.06	132.83
69	RJ	1201	GTP	C5-C6-N1	3.41	119.98	113.95
69	RJ	1201	GTP	C8-N7-C5	3.09	108.88	102.99
69	RJ	1201	GTP	C2-N1-C6	-3.06	119.46	125.10
69	RJ	1201	GTP	O6-C6-C5	-2.05	120.36	124.37

There are no chirality outliers.

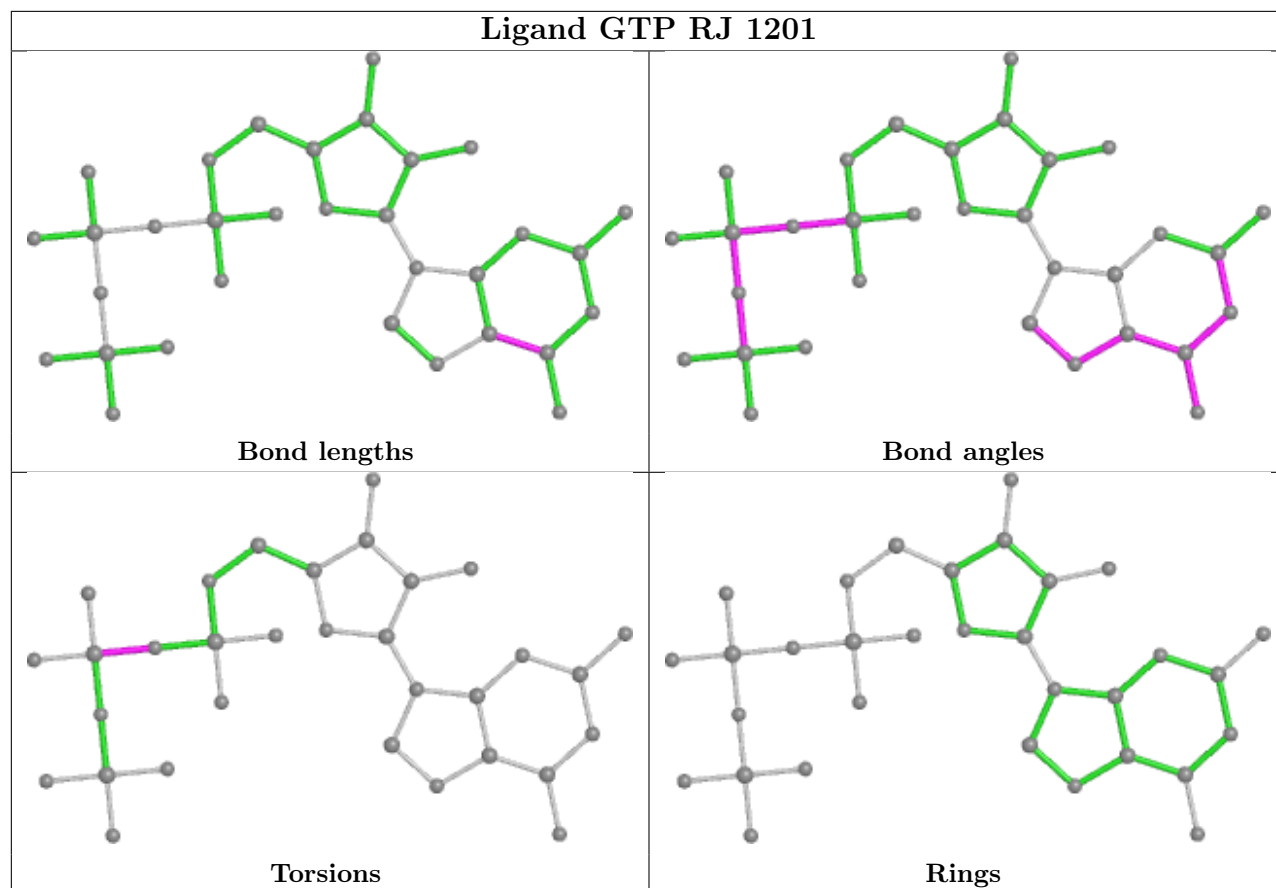
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	RJ	1201	GTP	PA-O3A-PB-O2B
69	RJ	1201	GTP	PA-O3A-PB-O1B

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](#)

There are no chain breaks in this entry.

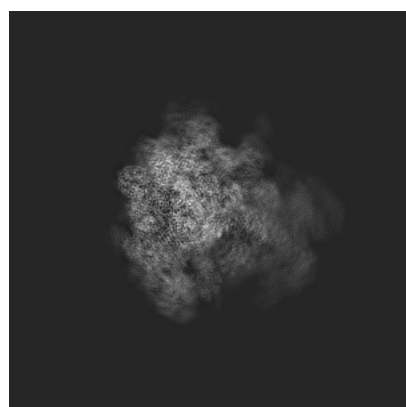
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9964. These allow visual inspection of the internal detail of the map and identification of artifacts.

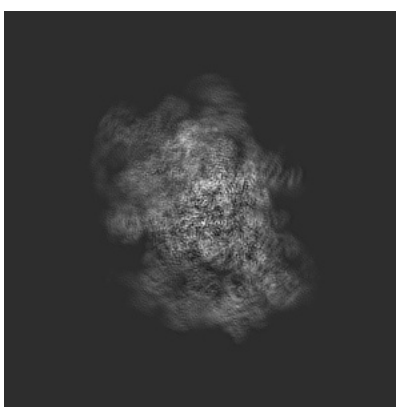
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

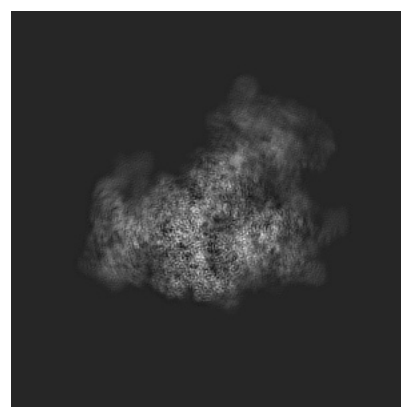
6.1.1 Primary map



X



Y

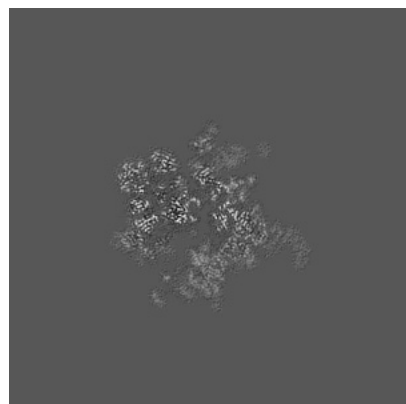


Z

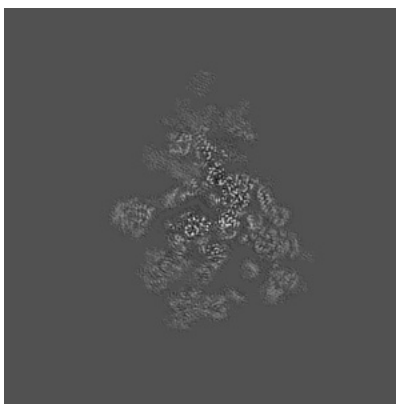
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

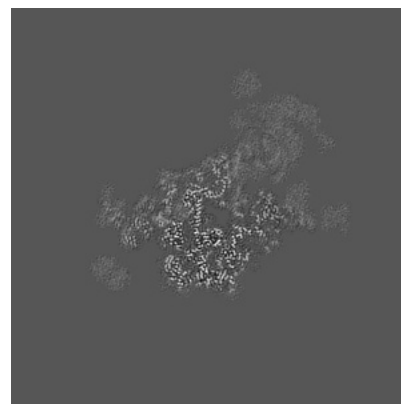
6.2.1 Primary map



X Index: 256



Y Index: 256

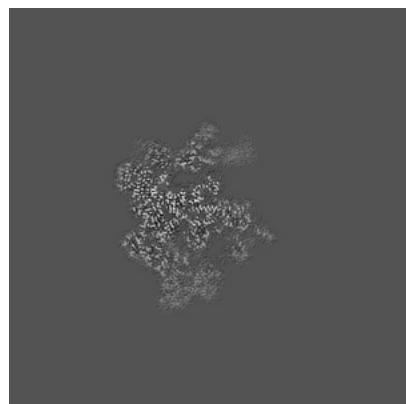


Z Index: 256

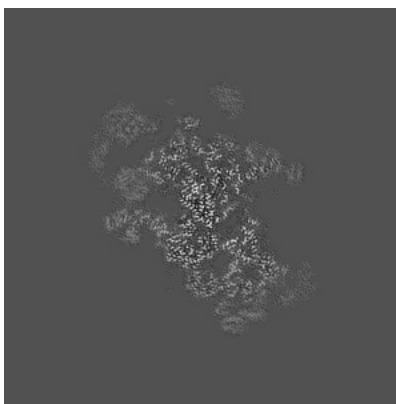
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

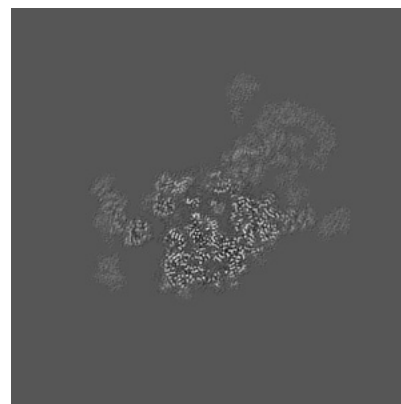
6.3.1 Primary map



X Index: 240



Y Index: 216



Z Index: 267

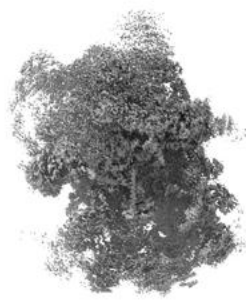
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

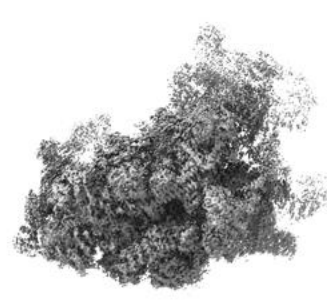
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

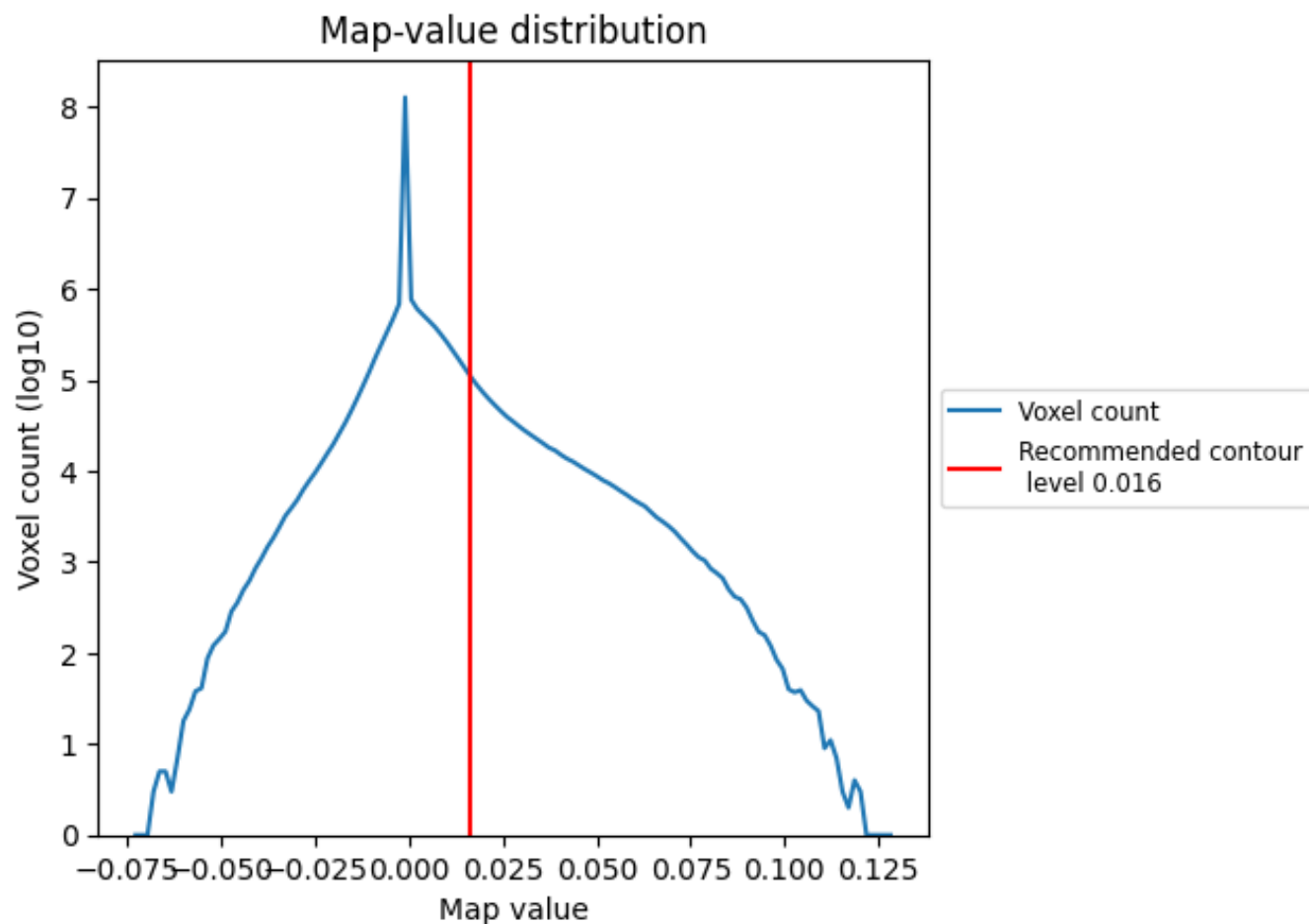
6.5 Mask visualisation

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

7 Map analysis [i](#)

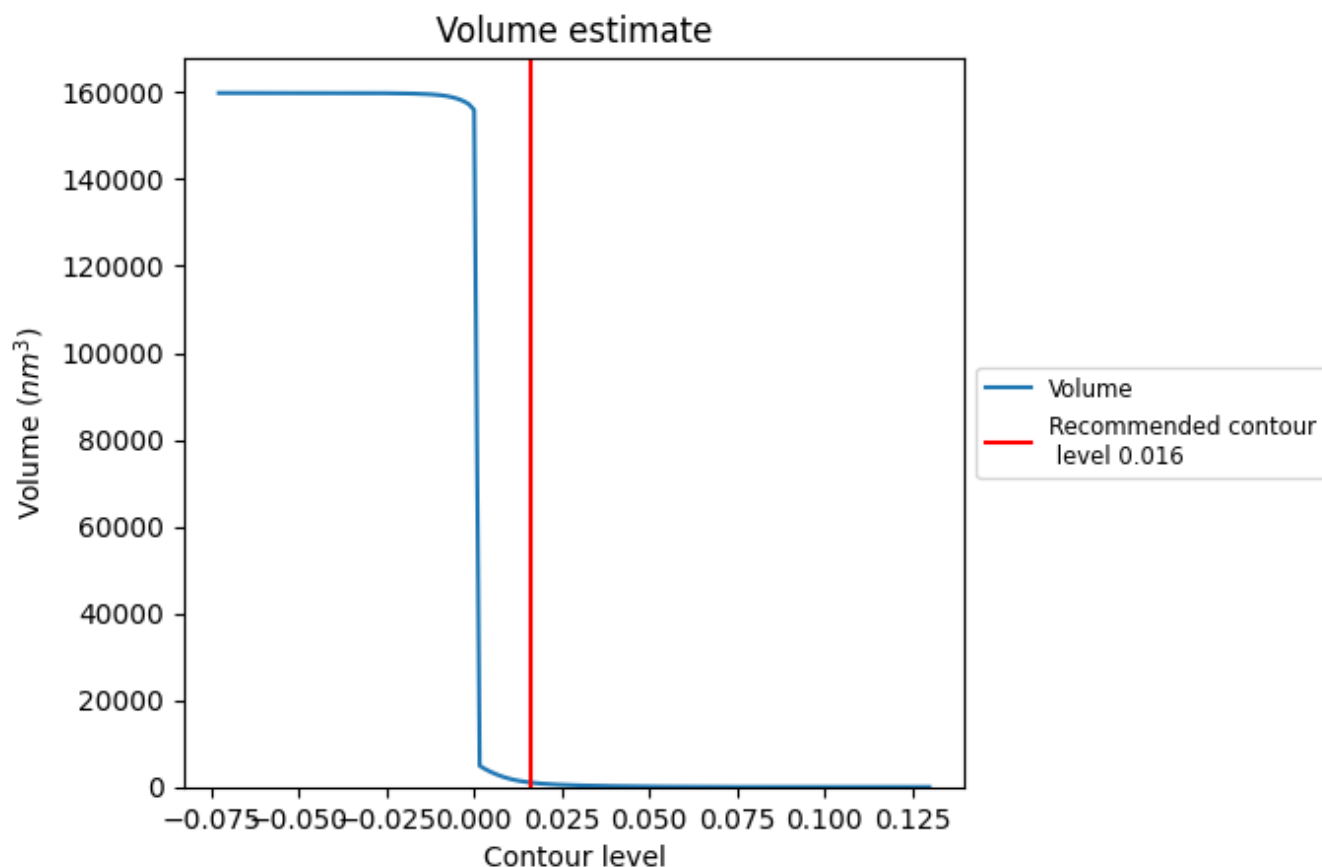
This section contains the results of statistical analysis of the map.

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.

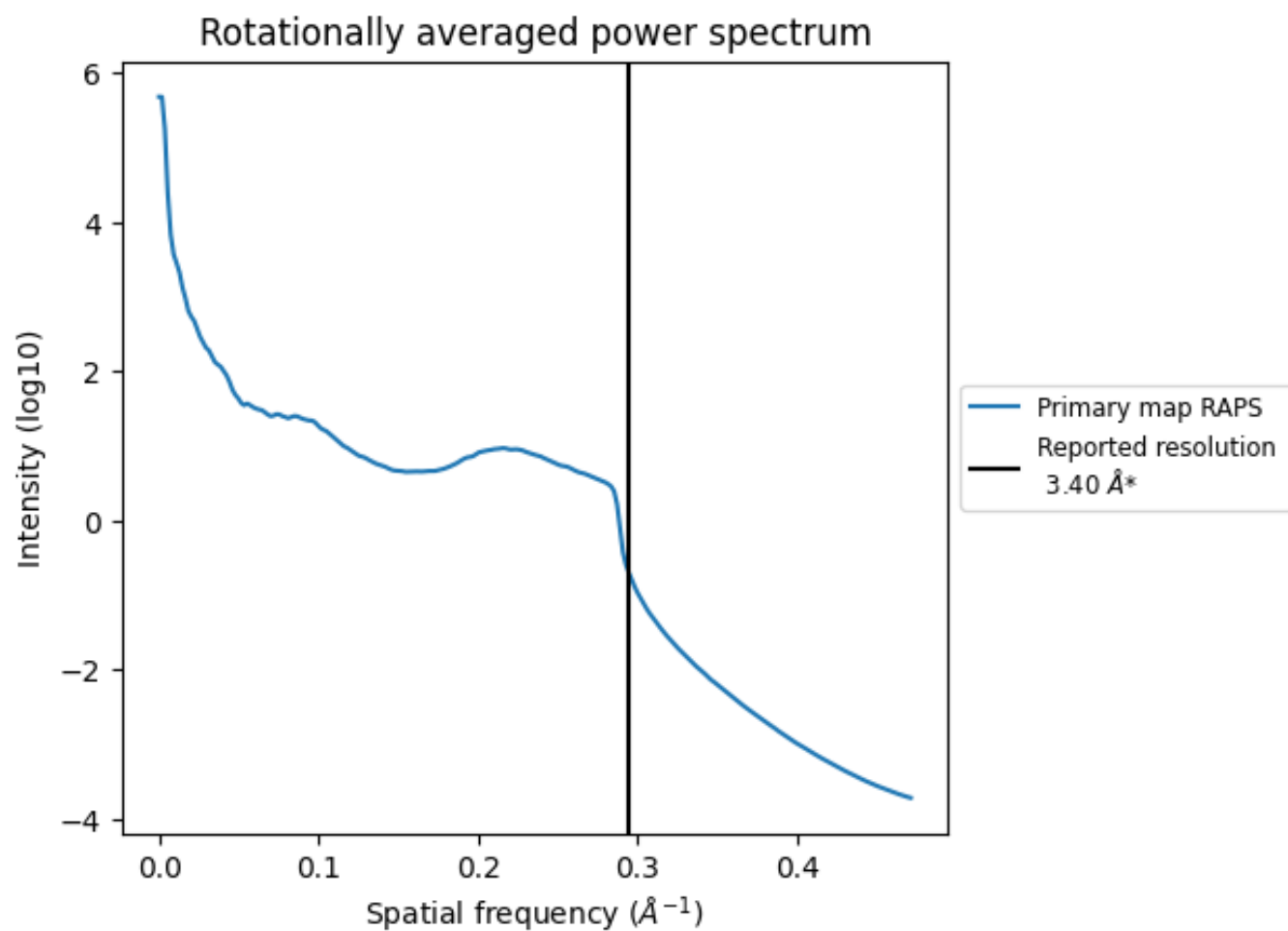
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1022 nm³; this corresponds to an approximate mass of 923 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 ⓘ

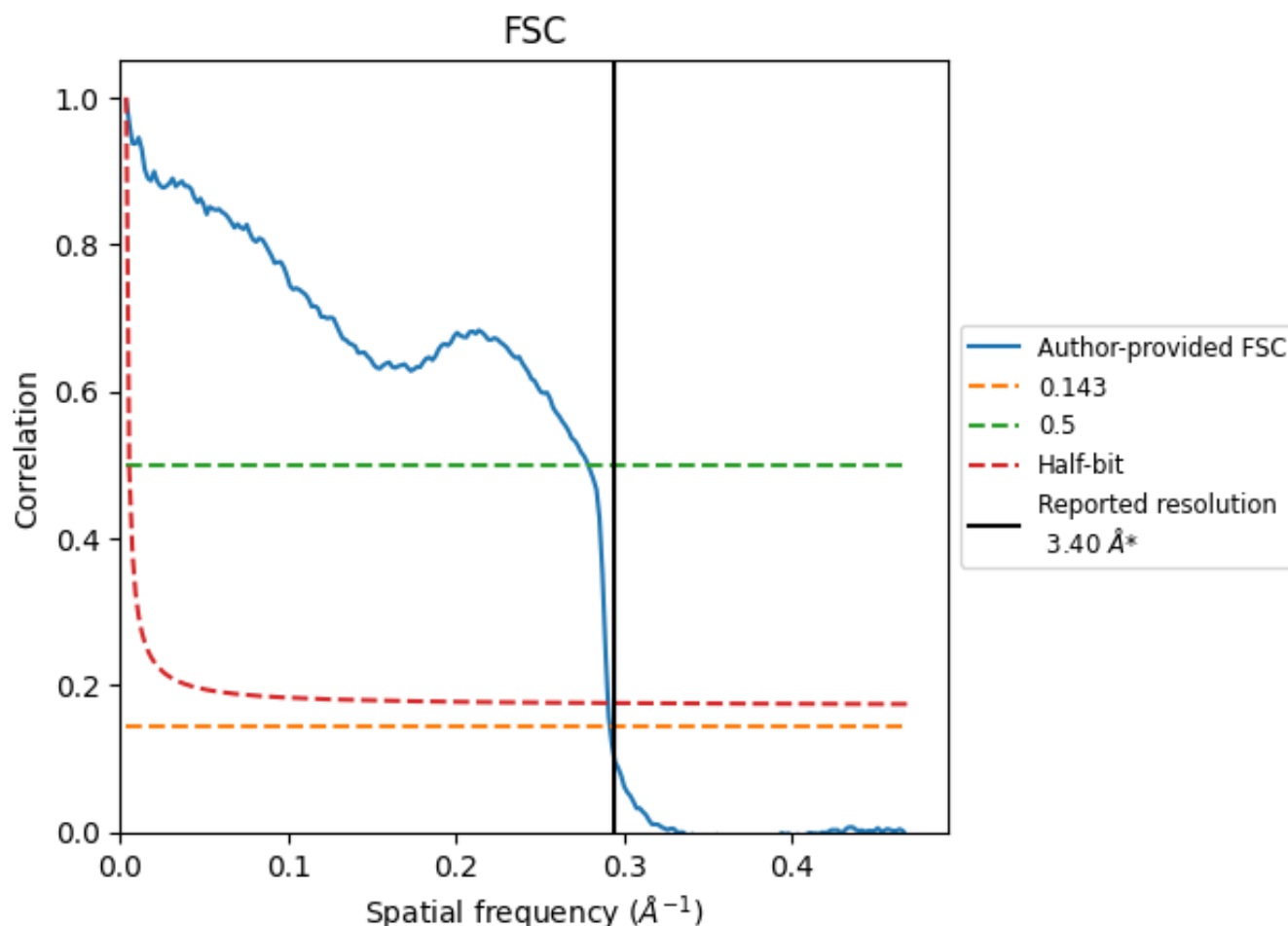


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

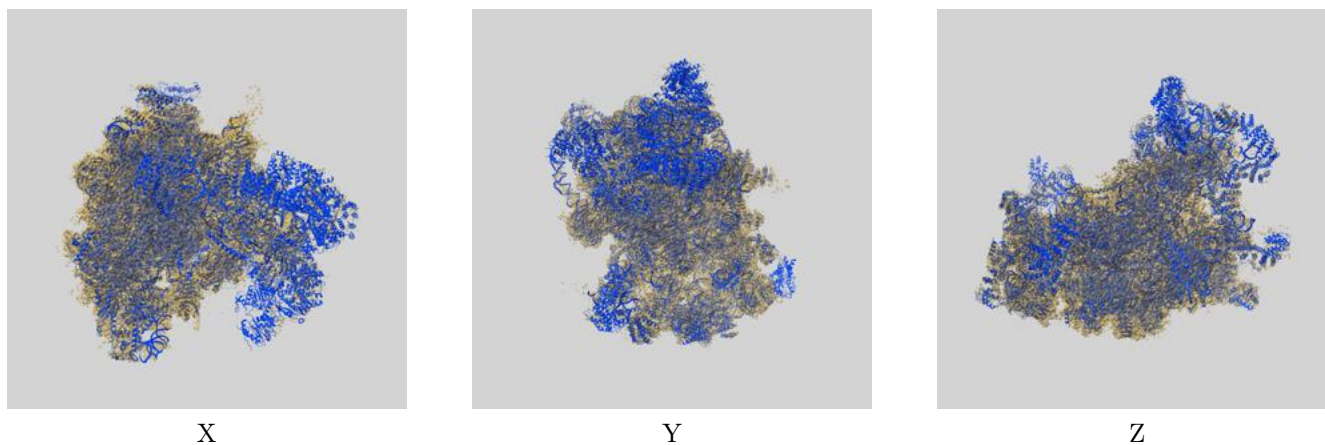
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.43	3.59	3.44
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

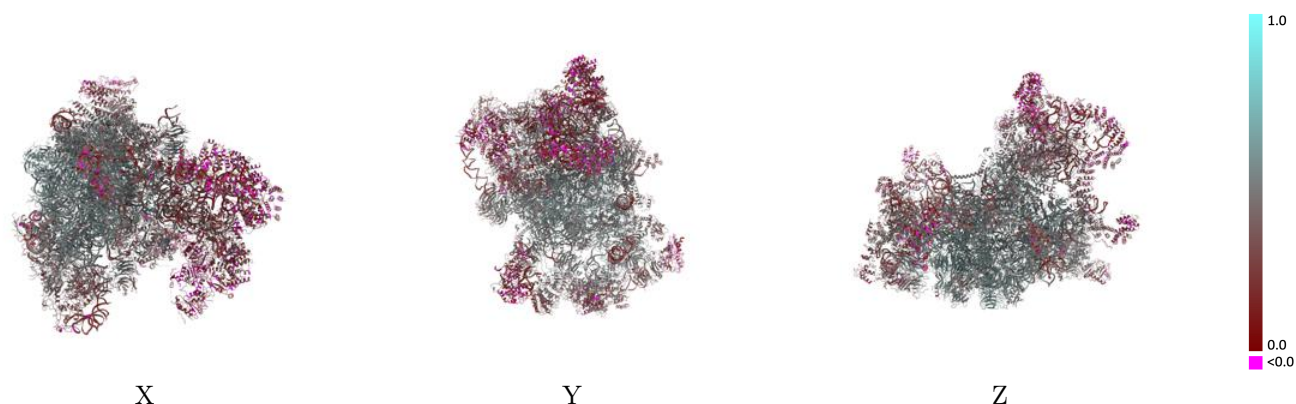
This section contains information regarding the fit between EMDB map EMD-9964 and PDB model 6KE6. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



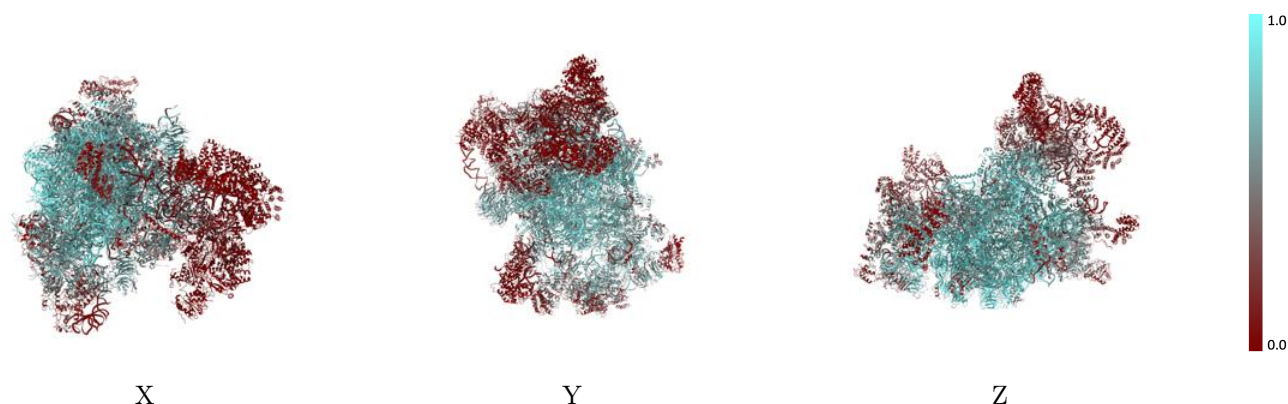
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



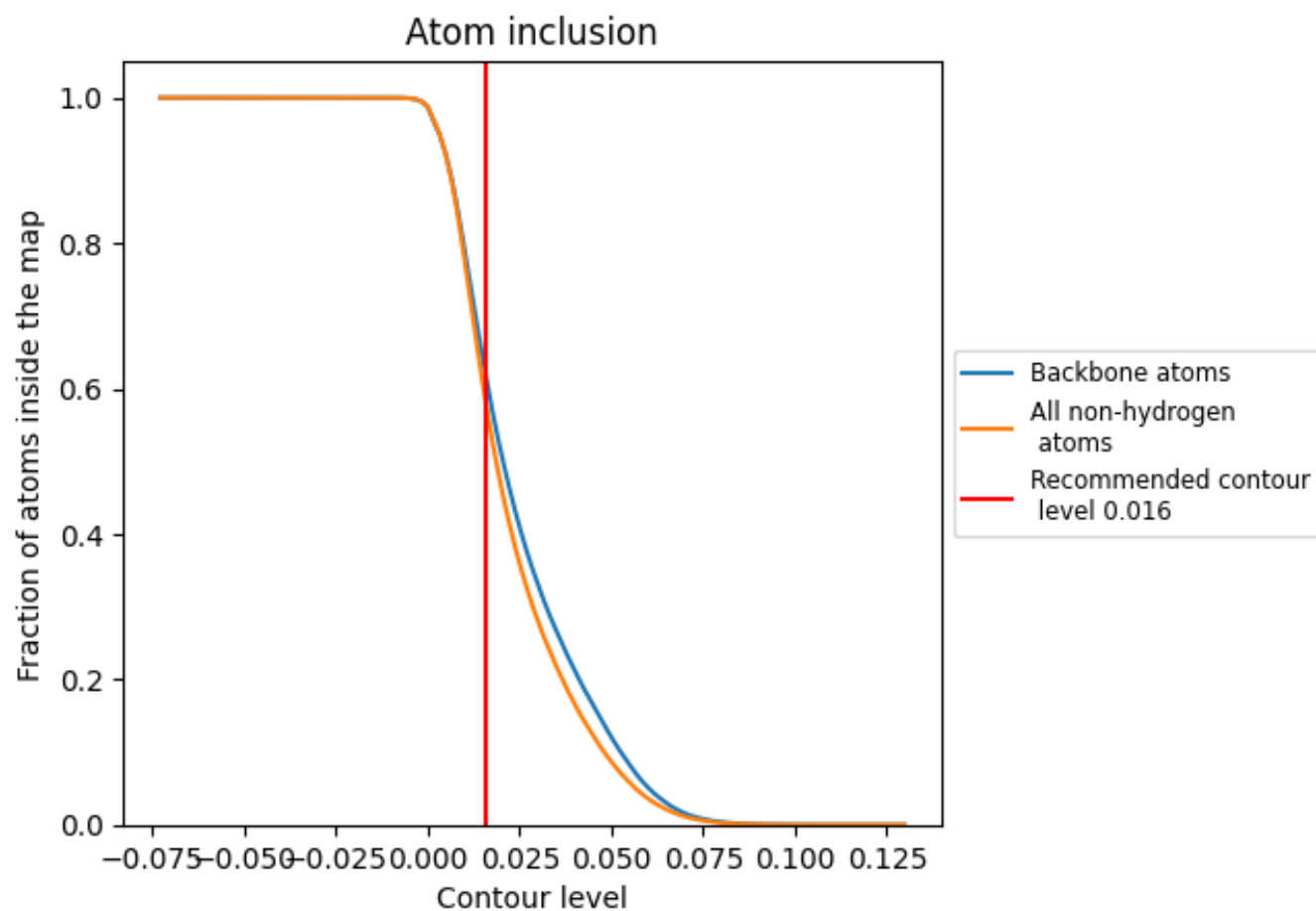
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.016).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 57% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5738	 0.4270
3A	 0.8273	 0.4550
3B	 0.8617	 0.5570
3C	 0.5797	 0.4410
3D	 0.7370	 0.4890
3E	 0.6832	 0.4590
3F	 0.6611	 0.4530
3G	 0.8341	 0.5450
3H	 0.7577	 0.5110
5A	 0.7638	 0.4290
5B	 0.4042	 0.3970
5C	 0.8457	 0.5510
5D	 0.7549	 0.5110
5E	 0.7528	 0.5240
5F	 0.8870	 0.5690
5G	 0.8111	 0.5500
5H	 0.7232	 0.5000
5I	 0.8633	 0.5500
5J	 0.6630	 0.4970
5K	 0.8566	 0.5580
A4	 0.6835	 0.4510
A5	 0.7526	 0.4910
A8	 0.2282	 0.3060
A9	 0.3974	 0.3630
AE	 0.3779	 0.3480
AF	 0.7595	 0.5060
AG	 0.6906	 0.4690
B1	 0.8807	 0.5590
B2	 0.6662	 0.4520
B3	 0.5917	 0.4230
B6	 0.6692	 0.4400
B8	 0.8478	 0.5430
BE	 0.8703	 0.5550
RA	 0.0961	 0.2760
RB	 0.4638	 0.4280



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Chain	Atom inclusion	Q-score
RC	 0.6171	 0.4820
RE	 0.3869	 0.4000
RF	 0.2959	 0.3630
RG	 0.3634	 0.3870
RH	 0.5720	 0.4780
RI	 0.7656	 0.4930
RJ	 0.7419	 0.5030
RK	 0.6827	 0.4860
RL	 0.1198	 0.3130
RM	 0.0188	 0.1970
RN	 0.3311	 0.3780
RO	 0.4476	 0.3860
RP	 0.0911	 0.2260
RQ	 0.5787	 0.4680
RS	 0.0369	 0.2090
RT	 0.6793	 0.4800
RV	 0.7186	 0.5180
SA	 0.5135	 0.3620
SC	 0.7475	 0.5170
SF	 0.2899	 0.3660
SG	 0.8173	 0.5350
SH	 0.0939	 0.3450
SI	 0.5207	 0.4250
SJ	 0.1434	 0.2790
SK	 0.8061	 0.5300
SM	 0.1529	 0.2840
SN	 0.0047	 0.1060
SO	 0.7576	 0.5080
SP	 0.7589	 0.5120
SR	 0.8491	 0.5530
ST	 0.3315	 0.4150
SX	 0.7841	 0.5300
SY	 0.7755	 0.5270
SZ	 0.4905	 0.4280
Sc	 0.7681	 0.5200
Sd	 0.8407	 0.5500
X1	 0.3291	 0.3770