



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 06:27 am GMT

PDB ID : 6GZ4
EMDB ID : EMD-0099
Title : tRNA translocation by the eukaryotic 80S ribosome and the impact of GTP hydrolysis, Translocation-intermediate-POST-2 (TI-POST-2)
Authors : Flis, J.; Holm, M.; Rundlet, E.J.; Loerke, J.; Hilal, T.; Dabrowski, M.; Buerger, J.; Mielke, T.; Blanchard, S.C.; Spahn, C.M.T.; Budkevich, T.V.
Deposited on : 2018-07-03
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

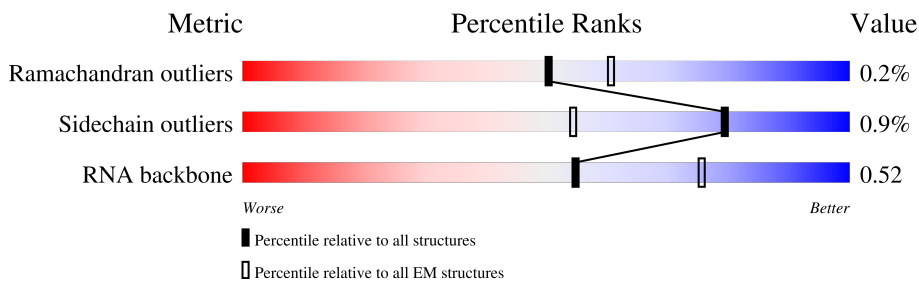
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : 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 3.60 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	AA	252	
2	BA	215	
3	AB	394	
4	BB	212	
5	AC	363	
6	BC	222	
7	A2	3612	
8	Bv	76	

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Mol	Chain	Length	Quality of chain
9	Bx	11	18% 73% 27%
10	Bw	76	7% 83% 17%
11	B1	1708	10% 77% 21%
12	BD	220	35% 100%
13	BF	190	41% 100%
14	BK	98	60% 98%
15	BM	120	97% 100%
16	BP	120	45% 98%
17	BQ	139	32% 99%
18	BR	125	48% 100%
19	BS	139	46% 96%
20	BT	143	42% 99%
21	BU	97	53% 100%
22	BZ	86	64% 98%
23	Bc	62	44% 97%
24	Bd	51	22% 98%
25	Bf	73	92% 100%
26	Bg	314	75% 100%
27	BE	257	19% 97%
28	BG	232	34% 99%
29	BH	183	48% 100%
30	BI	207	20% 99%
31	BJ	179	19% 97%
32	BL	153	25% 98%
33	BN	149	18% 99%

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Mol	Chain	Length	Quality of chain
34	BO	136	13% 99%
35	BV	81	23% 98%
36	BW	129	12% 98%
37	BX	141	15% 99%
38	BY	125	33% 99%
39	Ba	97	15% 99%
40	Bb	80	29% 100%
41	Be	55	33% 95% 5%
42	A3	157	8% 75% 23%
43	A4	119	81% 17%
44	AD	294	13% 99%
45	AE	194	25% 97%
46	AF	234	9% 99%
47	AG	234	17% 100%
48	AH	191	11% 98%
49	AI	208	9% 99%
50	AJ	169	17% 99%
51	AL	205	16% 98%
52	AM	139	12% 99%
53	AN	203	99%
54	AO	195	98%
55	AP	153	5% 99%
56	AQ	187	9% 97%
57	AR	181	10% 99%
58	AS	175	5% 100%

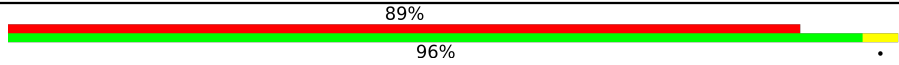
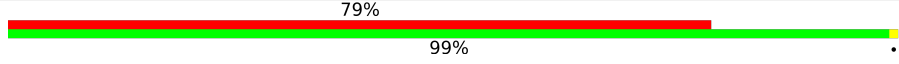
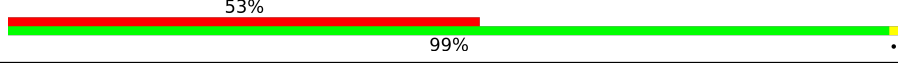
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Mol	Chain	Length	Quality of chain
59	AT	157	10% 99%
60	AU	99	28% 98%
61	AV	129	5% 100%
62	AW	121	52% 98%
63	AX	117	9% 100%
64	AY	127	9% 99%
65	AZ	134	9% 99%
66	Aa	147	7% 99%
67	Ab	68	21% 96%
68	Ac	103	15% 100%
69	Ad	106	9% 100%
70	Ae	129	7% 100%
71	Af	109	7% 98%
72	Ag	114	11% 100%
73	Ah	122	16% 96%
74	Ai	97	16% 100%
75	Aj	84	98%
76	Ak	69	29% 99%
77	Al	50	6% 94% 6%
78	Am	50	10% 98%
79	An	25	92% 100%
80	Ao	105	12% 98%
81	Ap	91	8% 99%
82	At	122	8% 96%
83	Au	217	99% 97%

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Mol	Chain	Length	Quality of chain
84	Aq	151	 89% 96%
85	AK	202	 79% 99%
86	Ct	853	 53% 99%

2 Entry composition [i](#)

There are 89 unique types of molecules in this entry. The entry contains 225601 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AA	252	1930	1209	395	320	6	0	0

- Molecule 2 is a protein called ribosomal protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	BA	215	1704	1083	298	315	8	0	0

- Molecule 3 is a protein called ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AB	394	3178	2024	596	544	14	0	0

- Molecule 4 is a protein called ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	BB	212	1722	1093	308	307	14	0	0

- Molecule 5 is a protein called ribosomal protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AC	363	2888	1817	577	480	14	0	0

- Molecule 6 is a protein called ribosomal protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	BC	222	1724	1114	296	304	10	0	0

- Molecule 7 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	A2	3612	77427	34482	14158	25175	3612	0	0

- Molecule 8 is a RNA chain called ap/P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	Bv	76	1620	723	290	531	76	0	0

- Molecule 9 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	Bx	11	234	105	41	77	11	0	0

- Molecule 10 is a RNA chain called pe/E-site-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	Bw	76	1627	725	294	532	76	0	0

- Molecule 11 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	B1	1708	36456	16274	6546	11928	1708	0	0

- Molecule 12 is a protein called ribosomal protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	BD	220	1709	1090	308	304	7	0	0

- Molecule 13 is a protein called ribosomal protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	BF	190	1502	939	285	271	7	0	0

- Molecule 14 is a protein called ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	BK	98	827	539	148	134	6	0	0

- Molecule 15 is a protein called ribosomal protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	BM	120	931	584	164	174	9	0	0

- Molecule 16 is a protein called ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	BP	120	999	636	188	168	7	0	0

- Molecule 17 is a protein called ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	BQ	139	1109	704	210	192	3	0	0

- Molecule 18 is a protein called ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	BR	125	1011	634	187	186	4	0	0

- Molecule 19 is a protein called ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	BS	139	1154	725	233	195	1	0	0

- Molecule 20 is a protein called ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	BT	143	1112	697	214	198	3	0	0

- Molecule 21 is a protein called ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BU	97	Total	C	N	O	S	0	0
			769	483	144	138	4		

- Molecule 22 is a protein called ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BZ	86	Total	C	N	O	S	0	0
			688	442	129	116	1		

- Molecule 23 is a protein called ribosomal protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Bc	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 24 is a protein called ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Bd	51	Total	C	N	O	S	0	0
			427	269	87	66	5		

- Molecule 25 is a protein called ribosomal protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Bf	73	Total	C	N	O	S	0	0
			601	379	115	100	7		

- Molecule 26 is a protein called ribosomal protein RACK 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Bg	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 27 is a protein called ribosomal protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BE	257	Total	C	N	O	S	0	0
			2031	1298	381	344	8		

- Molecule 28 is a protein called ribosomal protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	BG	232	1884	1176	379	322	7	0	0

- Molecule 29 is a protein called ribosomal protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	BH	183	1479	941	272	265	1	0	0

- Molecule 30 is a protein called ribosomal protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	BI	207	1696	1064	334	293	5	0	0

- Molecule 31 is a protein called ribosomal protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	BJ	179	1495	953	299	241	2	0	0

- Molecule 32 is a protein called ribosomal protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	BL	153	1258	804	235	213	6	0	0

- Molecule 33 is a protein called ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	BN	149	1202	770	228	203	1	0	0

- Molecule 34 is a protein called ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	BO	136	1016	621	199	190	6	0	0

- Molecule 35 is a protein called ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	BV	81	617	380	114	118	5	0	0

- Molecule 36 is a protein called ribosomal protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	BW	129	1034	659	193	176	6	0	0

- Molecule 37 is a protein called ribosomal protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	BX	141	1098	693	219	183	3	0	0

- Molecule 38 is a protein called ribosomal protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	BY	125	1015	642	199	169	5	0	0

- Molecule 39 is a protein called ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	Ba	97	774	481	160	128	5	0	0

- Molecule 40 is a protein called ribosomal protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	Bb	80	625	391	116	111	7	0	0

- Molecule 41 is a protein called ribosomal protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	Be	55	437	272	96	68	1	0	0

- Molecule 42 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
42	A3	157	3337	1489	587	1104	157	0	0

- Molecule 43 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
43	A4	119	2541	1132	454	836	119	0	0

- Molecule 44 is a protein called ribosomal protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	AD	294	2392	1510	436	432	14	0	0

- Molecule 45 is a protein called ribosomal protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	AE	194	1571	1013	294	263	1	0	0

- Molecule 46 is a protein called ribosomal protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	AF	234	1950	1252	376	313	9	0	0

- Molecule 47 is a protein called ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	AG	234	1880	1197	362	317	4	0	0

- Molecule 48 is a protein called ribosomal protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	AH	191	1526	960	285	275	6	0	0

- Molecule 49 is a protein called ribosomal protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	AI	208	1692	1074	327	278	13	0	0

- Molecule 50 is a protein called ribosomal protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	AJ	169	1353	855	252	240	6	0	0

- Molecule 51 is a protein called ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	AL	205	1657	1036	344	273	4	0	0

- Molecule 52 is a protein called ribosomal protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	AM	139	1138	730	218	183	7	0	0

- Molecule 53 is a protein called ribosomal protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	AN	203	1701	1072	359	266	4	0	0

- Molecule 54 is a protein called ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	AO	195	1606	1034	315	252	5	0	0

- Molecule 55 is a protein called ribosomal protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	AP	153	1242	776	241	216	9	0	0

- Molecule 56 is a protein called ribosomal protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	AQ	187	1513	944	314	250	5	0	0

- Molecule 57 is a protein called ribosomal protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	AR	181	1517	938	329	241	9	0	0

- Molecule 58 is a protein called ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	AS	175	1449	921	283	234	11	0	0

- Molecule 59 is a protein called ribosomal protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	AT	157	1284	815	250	214	5	0	0

- Molecule 60 is a protein called ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	AU	99	808	518	141	147	2	0	0

- Molecule 61 is a protein called ribosomal protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	AV	129	969	613	182	169	5	0	0

- Molecule 62 is a protein called ribosomal protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	AW	121	989	617	202	167	3	0	0

- Molecule 63 is a protein called ribosomal protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	AX	117	958	612	180	165	1	0	0

- Molecule 64 is a protein called ribosomal protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	AY	127	1064	668	216	177	3	0	0

- Molecule 65 is a protein called ribosomal protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	AZ	134	1103	712	207	181	3	0	0

- Molecule 66 is a protein called ribosomal protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	Aa	147	1162	736	237	186	3	0	0

- Molecule 67 is a protein called ribosomal protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	Ab	68	559	344	122	90	3	0	0

- Molecule 68 is a protein called ribosomal protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	Ac	103	801	508	141	145	7	0	0

- Molecule 69 is a protein called ribosomal protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	Ad	106	879	555	170	152	2	0	0

- Molecule 70 is a protein called ribosomal protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	Ae	129	1064	673	220	166	5	0	0

- Molecule 71 is a protein called ribosomal protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	Af	109	876	555	174	144	3	0	0

- Molecule 72 is a protein called ribosomal protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	Ag	114	906	566	187	147	6	0	0

- Molecule 73 is a protein called ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	Ah	122	1015	641	205	168	1	0	0

- Molecule 74 is a protein called ribosomal protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	Ai	97	794	497	168	124	5	0	0

- Molecule 75 is a protein called ribosomal protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	Aj	84	689	423	152	109	5	0	0

- Molecule 76 is a protein called ribosomal protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	Ak	69	569	366	103	99	1	0	0

- Molecule 77 is a protein called ribosomal protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Al	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 78 is a protein called ribosomal protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Am	50	Total	C	N	O	S	0	0
			411	254	87	64	6		

- Molecule 79 is a protein called ribosomal protein eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	An	25	Total	C	N	O	S	0	0
			240	145	64	28	3		

- Molecule 80 is a protein called ribosomal protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Ao	105	Total	C	N	O	S	0	0
			863	542	175	140	6		

- Molecule 81 is a protein called ribosomal protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Ap	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 82 is a protein called ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	At	122	Total	C	N	O	S	0	0
			980	607	204	165	4		

- Molecule 83 is a protein called ribosomal protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Au	217	Total	C	N	O	S	0	0
			1744	1114	314	307	9		

- Molecule 84 is a protein called ribosomal protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Aq	151	Total	C	N	O	S	0	0
			1140	708	215	213	4		

- Molecule 85 is a protein called ribosomal protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	AK	202	Total	C	N	O	S	0	0
			1556	989	272	286	9		

- Molecule 86 is a protein called eukaryotic elongation factor 2 (eEF2).

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Ct	853	Total	C	N	O	S	0	0
			6659	4226	1146	1243	44		

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
87	AA	1	Total	Mg	0
			1	1	
87	A2	236	Total	Mg	0
			236	236	
87	Bx	1	Total	Mg	0
			1	1	
87	B1	67	Total	Mg	0
			67	67	
87	BD	2	Total	Mg	0
			2	2	
87	BS	2	Total	Mg	0
			2	2	
87	Bd	2	Total	Mg	0
			2	2	
87	Ba	1	Total	Mg	0
			1	1	
87	A3	4	Total	Mg	0
			4	4	
87	A4	8	Total	Mg	0
			8	8	
87	AL	1	Total	Mg	0
			1	1	
87	AY	1	Total	Mg	0
			1	1	

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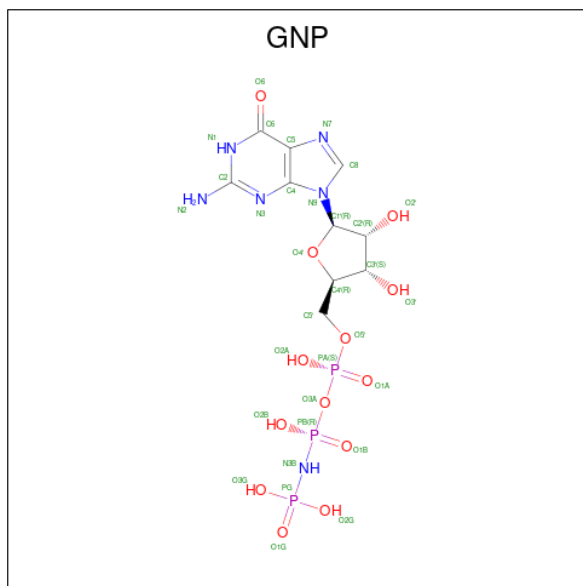
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
87	An	1	Total	Mg	0
			1	1	

- Molecule 88 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
88	Bd	1	Total	Zn	0
			1	1	
88	Ba	1	Total	Zn	0
			1	1	
88	Aj	1	Total	Zn	0
			1	1	
88	Ao	1	Total	Zn	0
			1	1	
88	Ap	1	Total	Zn	0
			1	1	

- Molecule 89 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

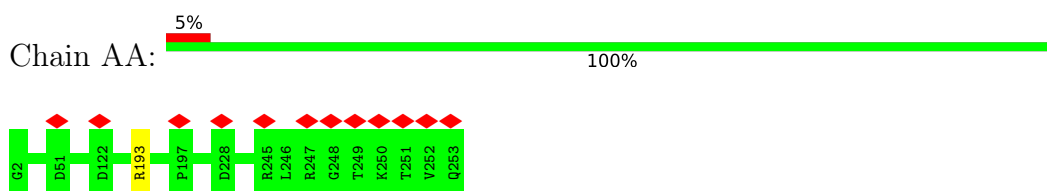


Mol	Chain	Residues	Atoms					AltConf
89	Ct	1	Total	C	N	O	P	0
			32	10	6	13	3	

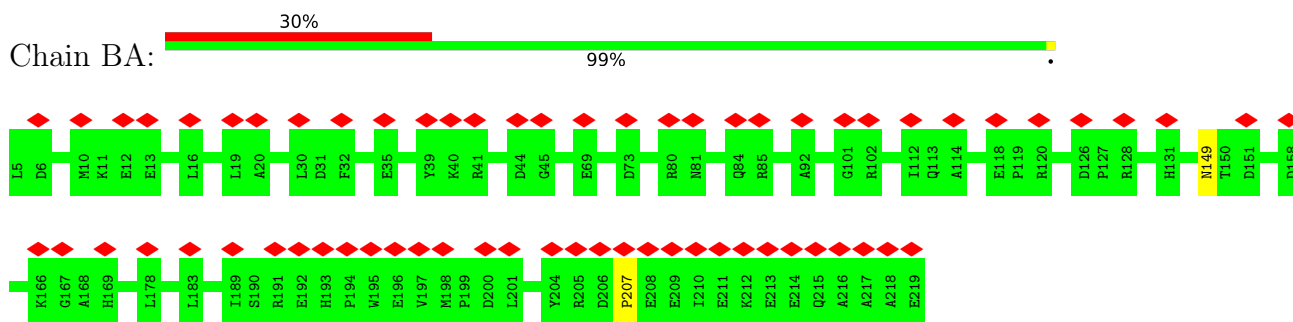
3 Residue-property plots [i](#)

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.

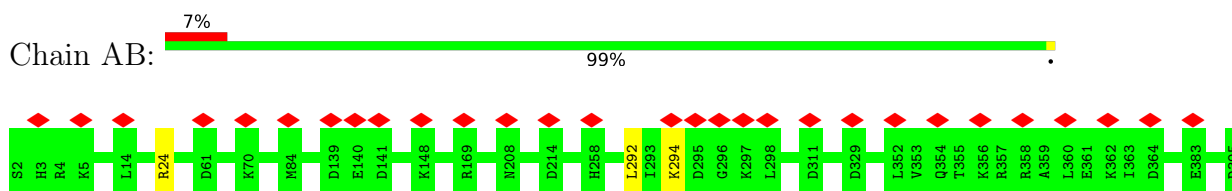
- Molecule 1: ribosomal protein uL2



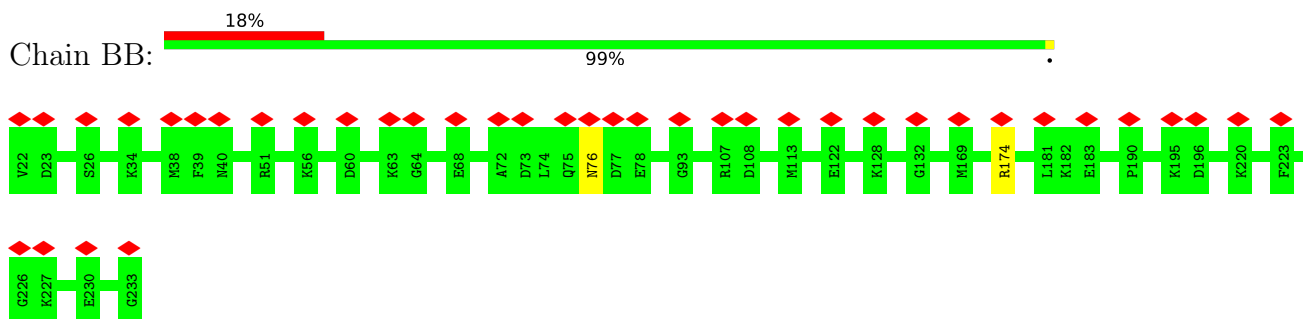
- Molecule 2: ribosomal protein uS2



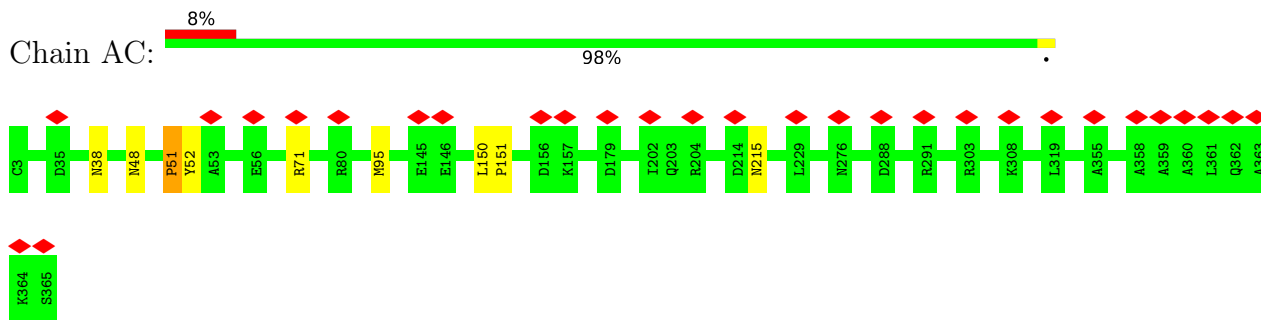
- Molecule 3: ribosomal protein uL3



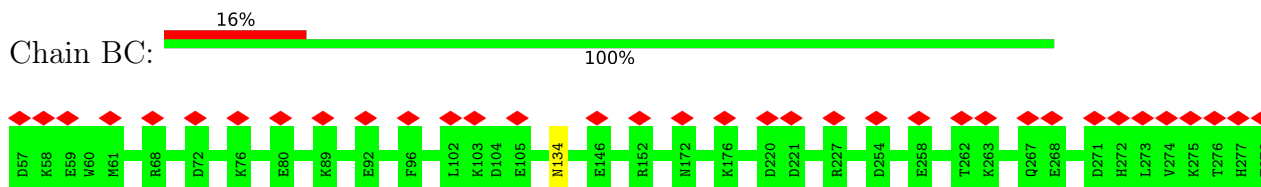
- Molecule 4: ribosomal protein eS1



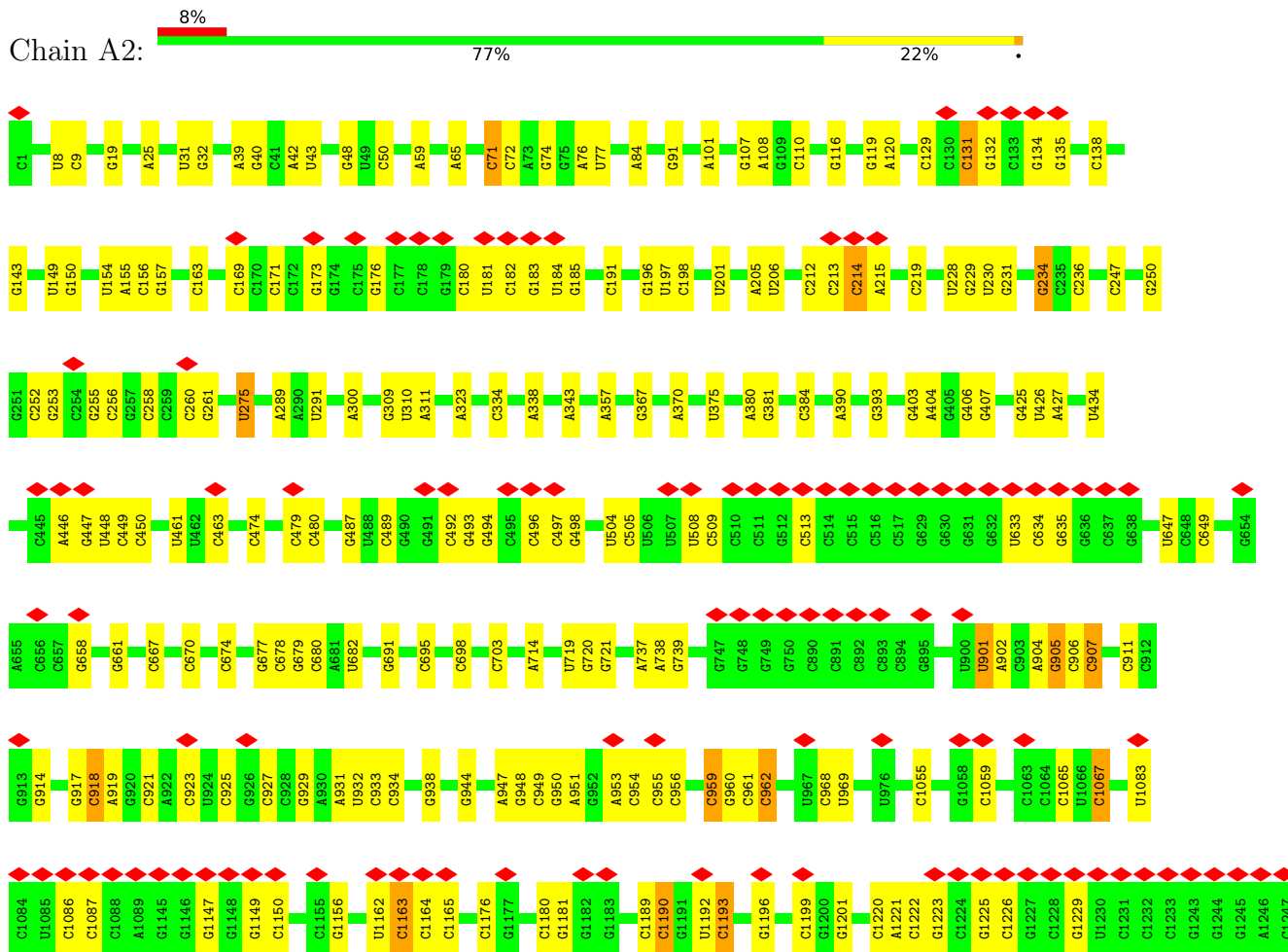
• Molecule 5: ribosomal protein uL4

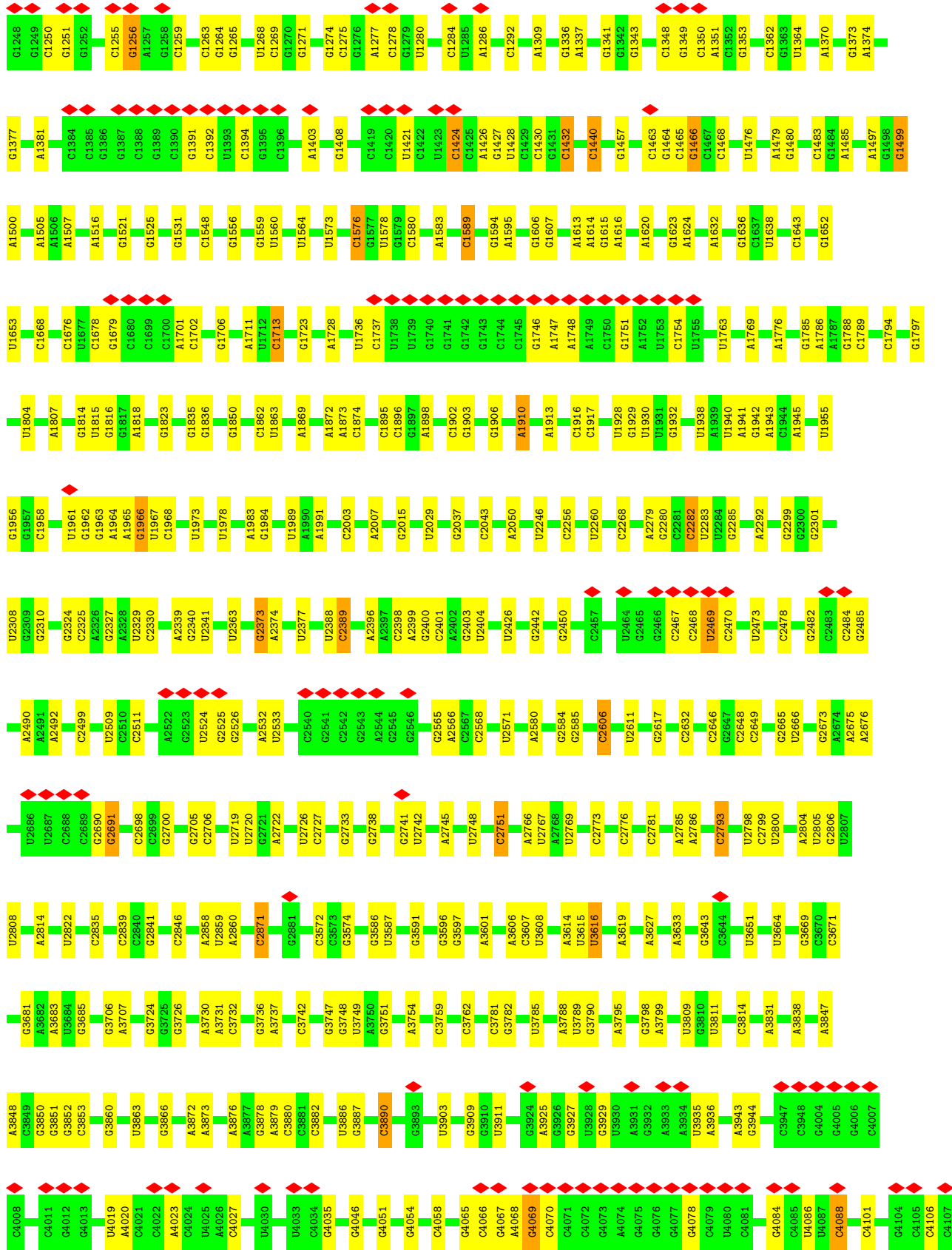


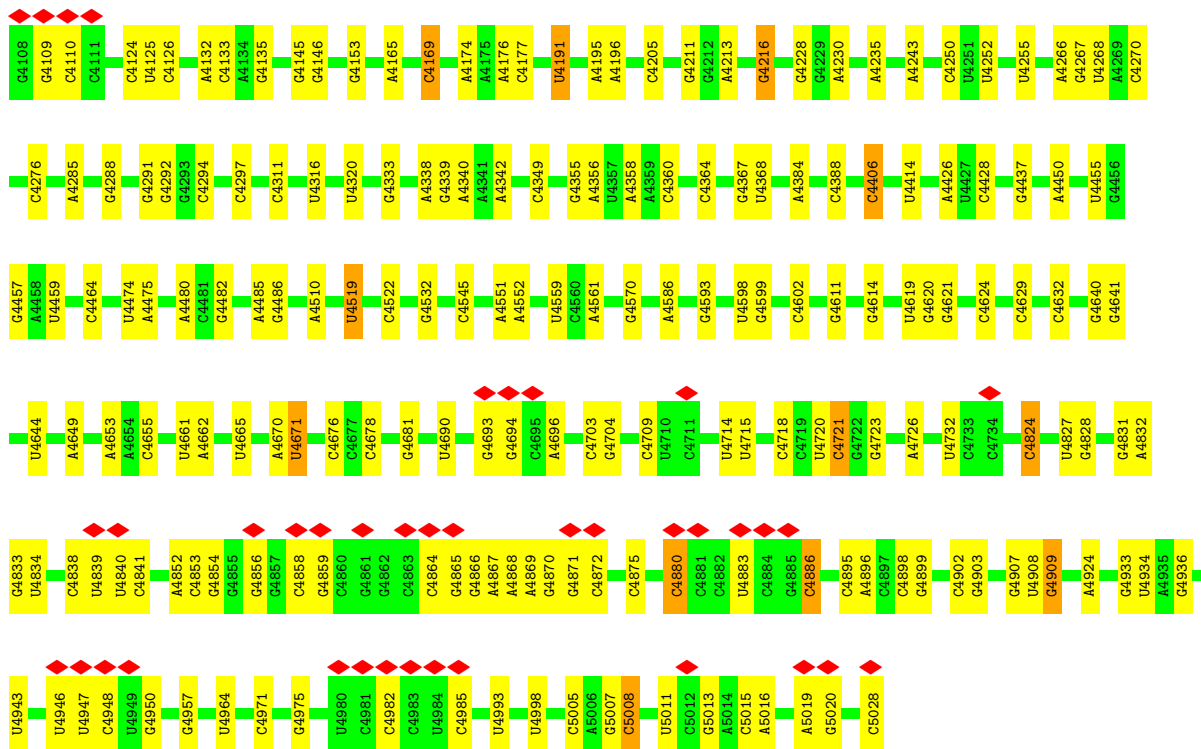
• Molecule 6: ribosomal protein eS28



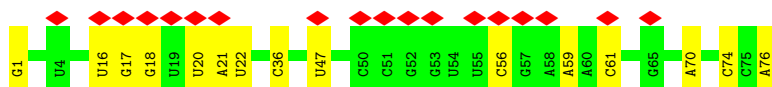
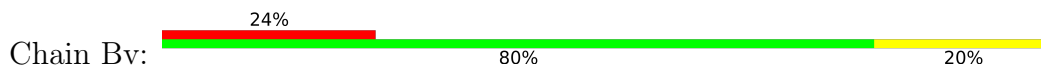
• Molecule 7: 28S ribosomal RNA



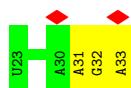
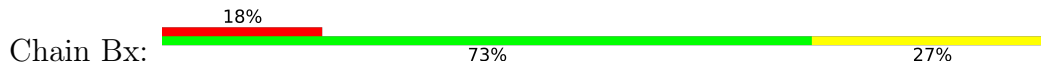




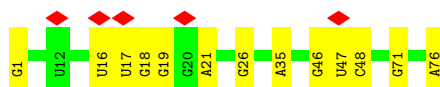
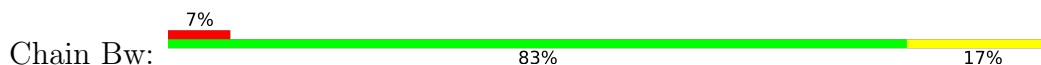
• Molecule 8: ap/P-site tRNA



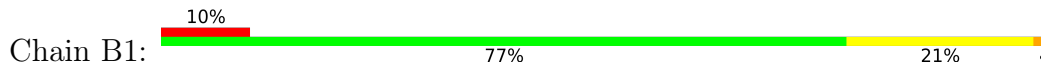
• Molecule 9: mRNA

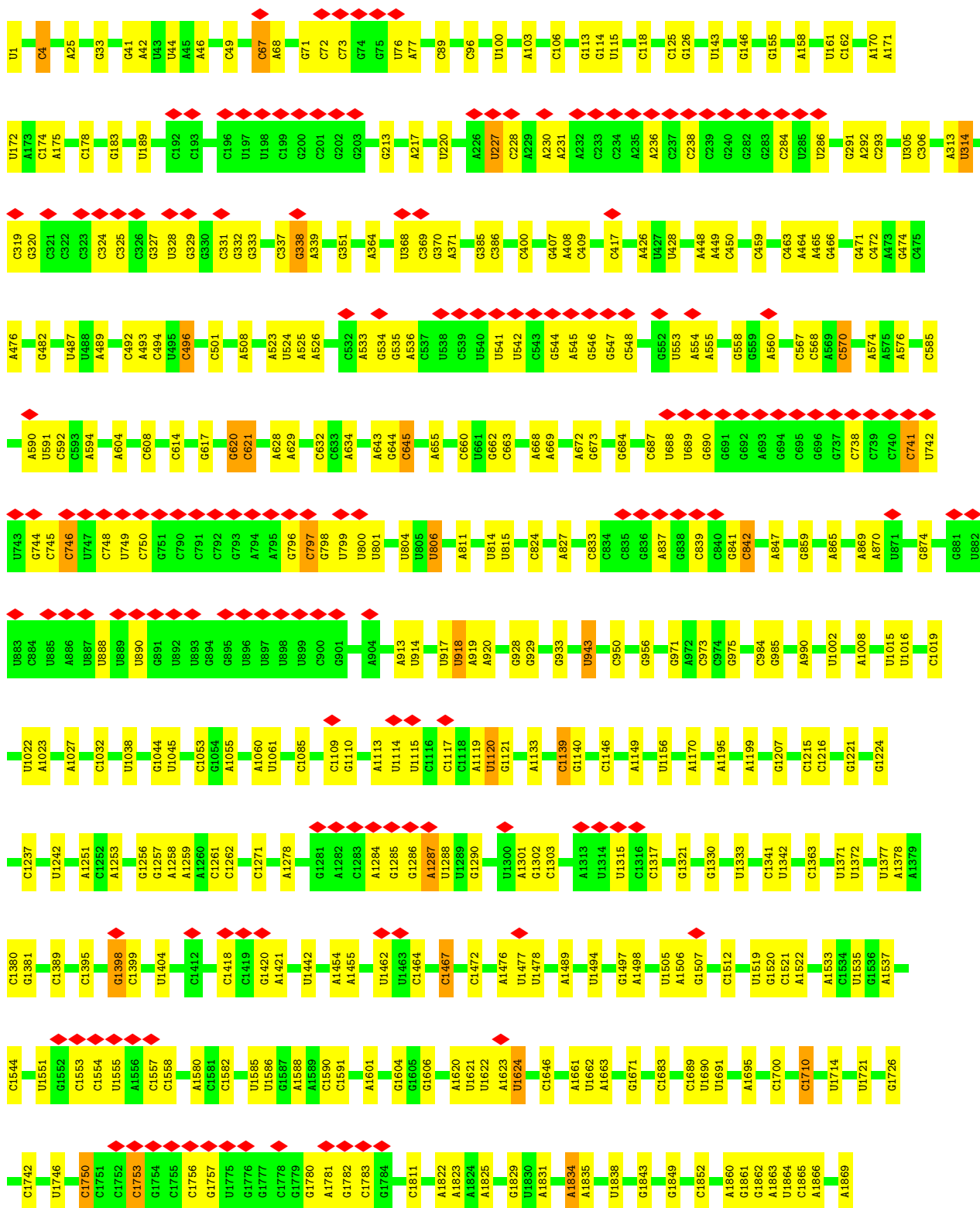


• Molecule 10: pe/E-site-tRNA



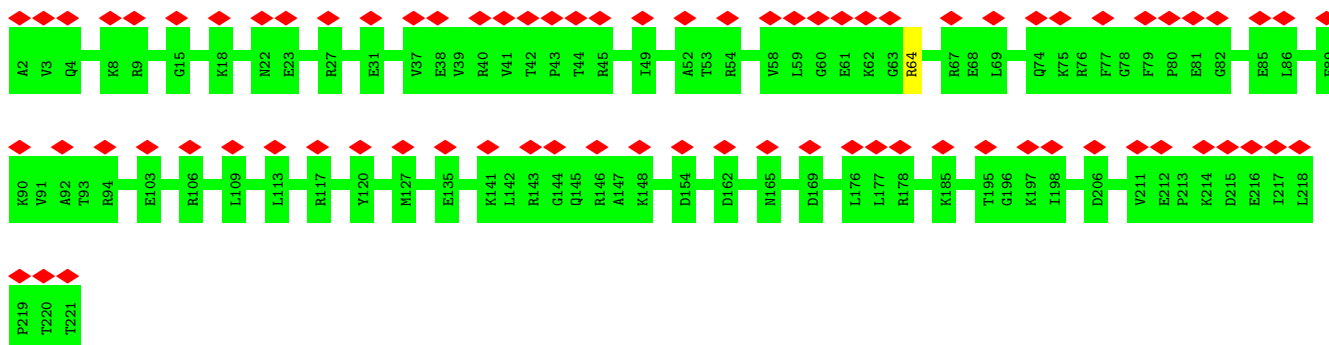
• Molecule 11: 18S ribosomal RNA





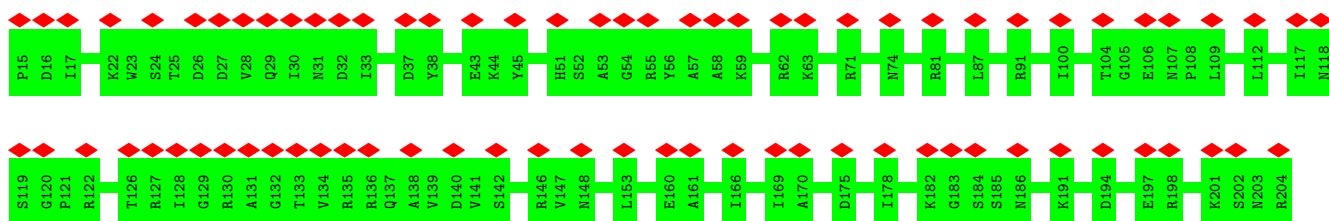
• Molecule 12: ribosomal protein uS3





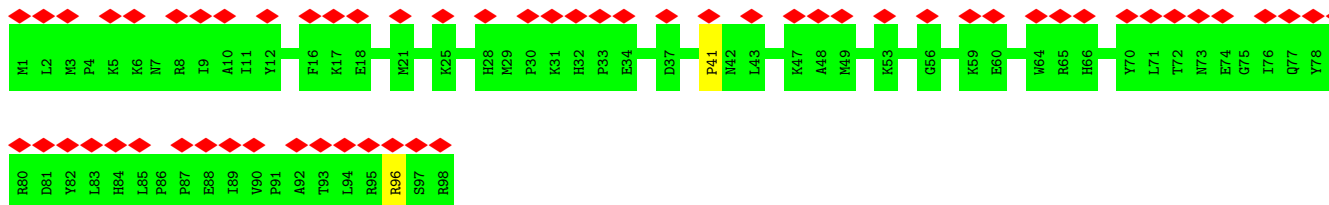
- Molecule 13: ribosomal protein uS7

Chain BF: 41% 100%



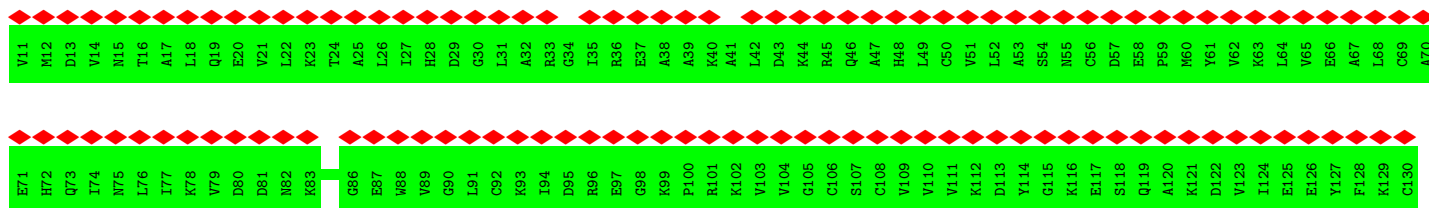
- Molecule 14: ribosomal protein eS10

Chain BK: 60% 98%



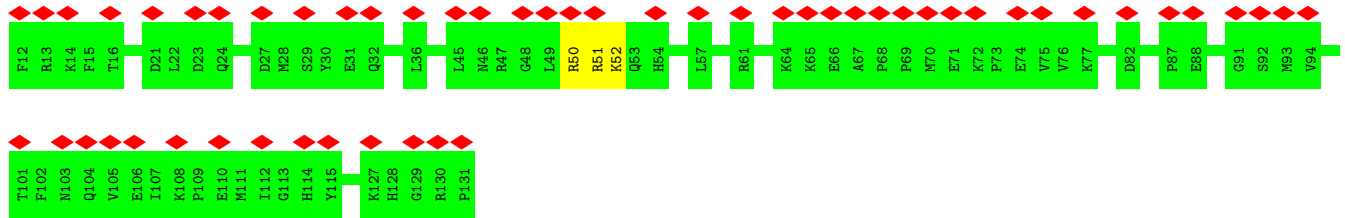
- Molecule 15: ribosomal protein eS12

Chain BM: 97% 100%



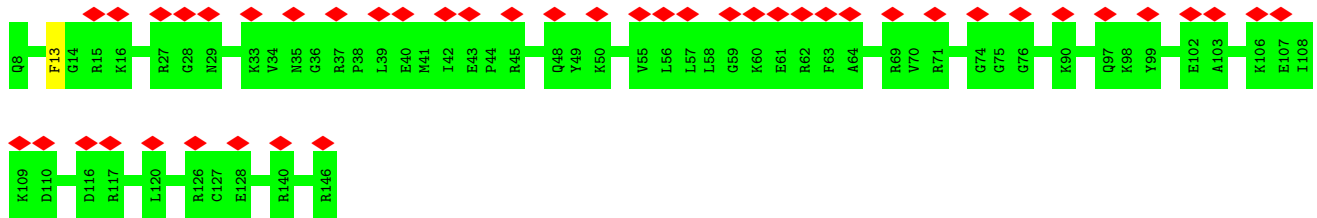
- Molecule 16: ribosomal protein uS19

Chain BP: 45% 98%



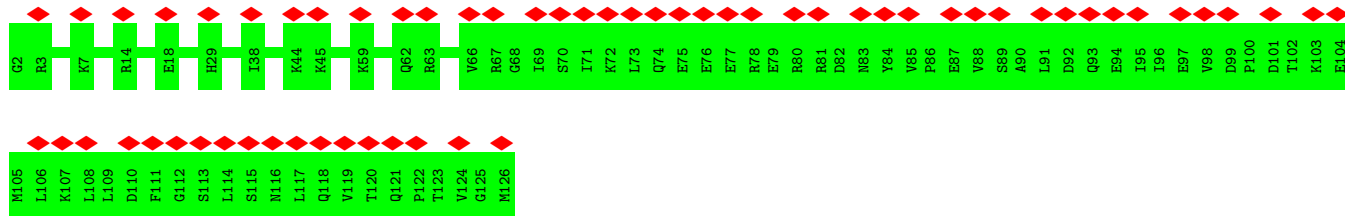
- Molecule 17: ribosomal protein uS9

Chain BQ: 32% 99%



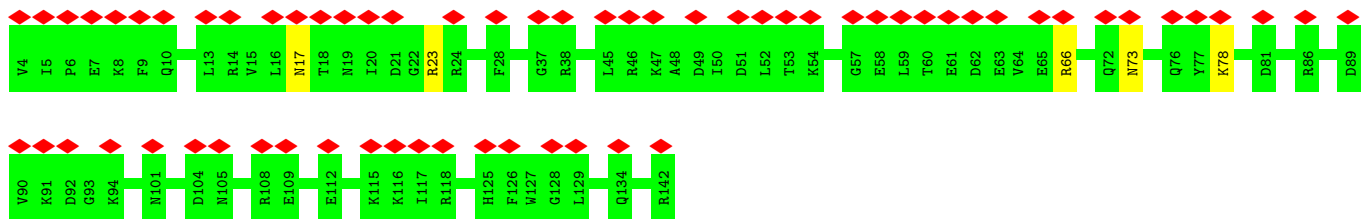
- Molecule 18: ribosomal protein eS17

Chain BR: 48% 100%



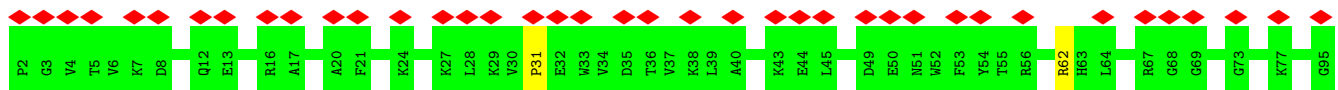
- Molecule 19: ribosomal protein uS13

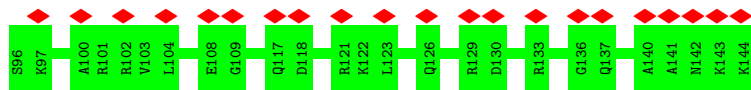
Chain BS: 46% 96%



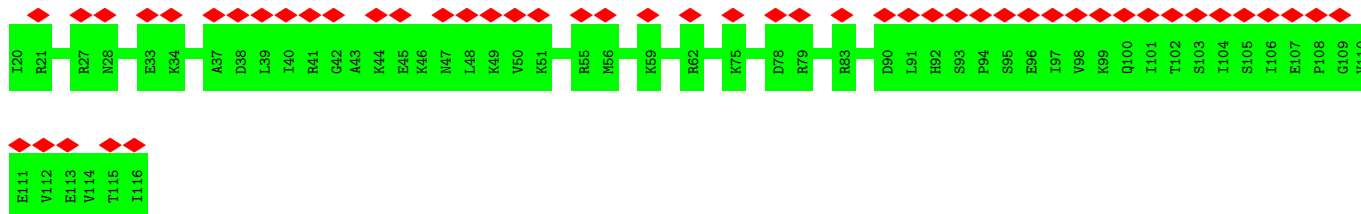
- Molecule 20: ribosomal protein eS19

Chain BT: 42% 99%

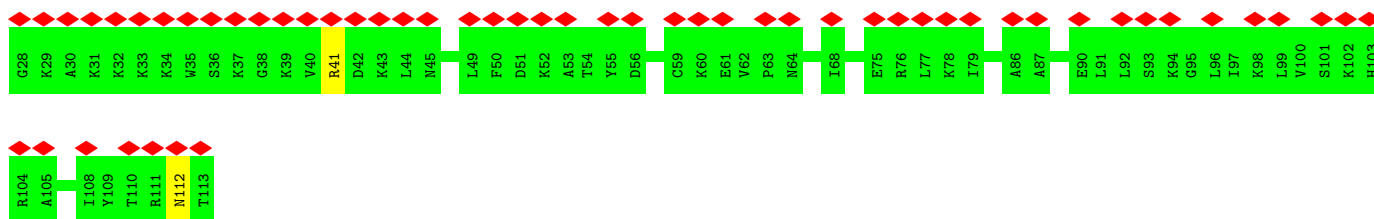




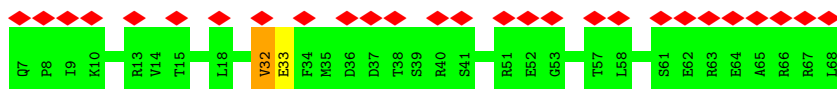
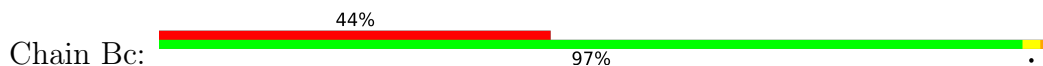
• Molecule 21: ribosomal protein uS10



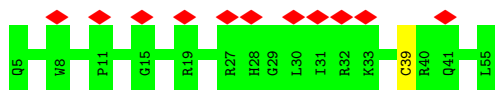
• Molecule 22: ribosomal protein uS10



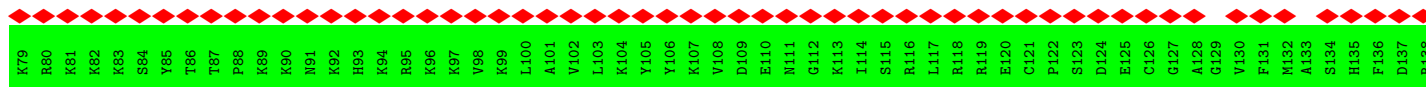
• Molecule 23: ribosomal protein eS28

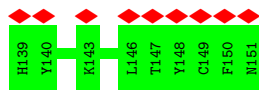


• Molecule 24: ribosomal protein uS14

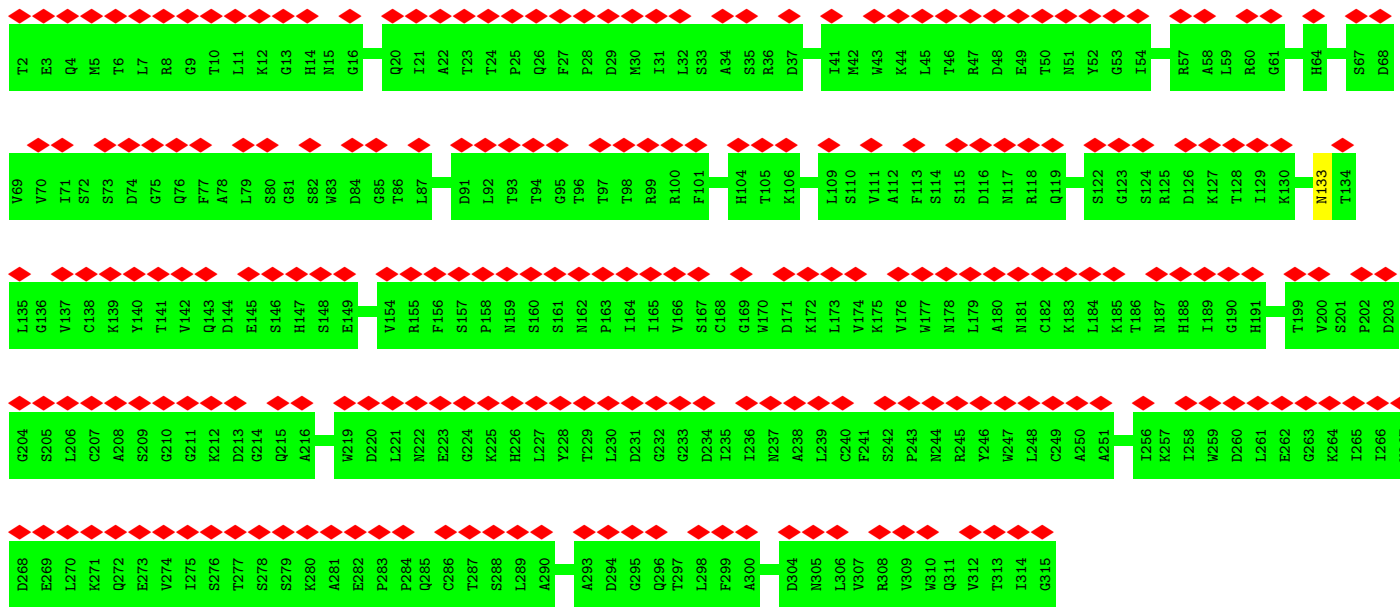
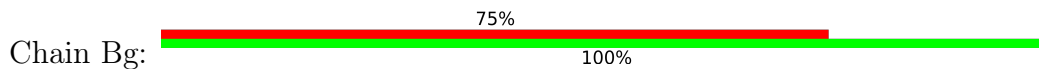


• Molecule 25: ribosomal protein eS31

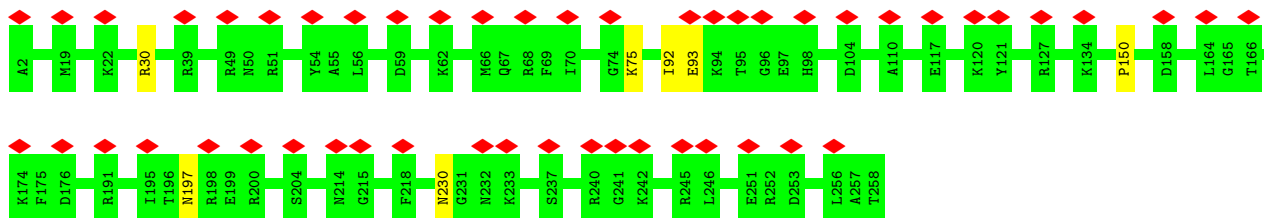




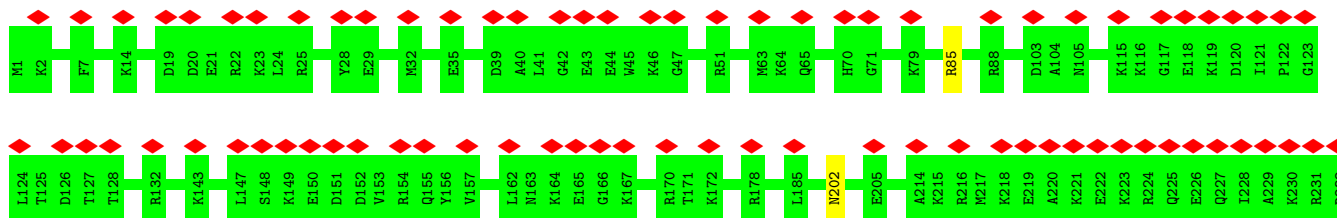
- Molecule 26: ribosomal protein RACK 1



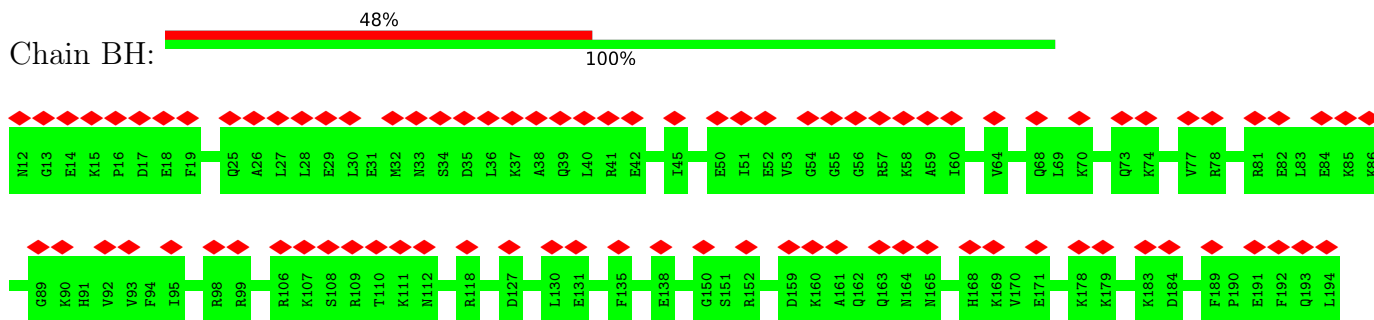
- Molecule 27: ribosomal protein eS4



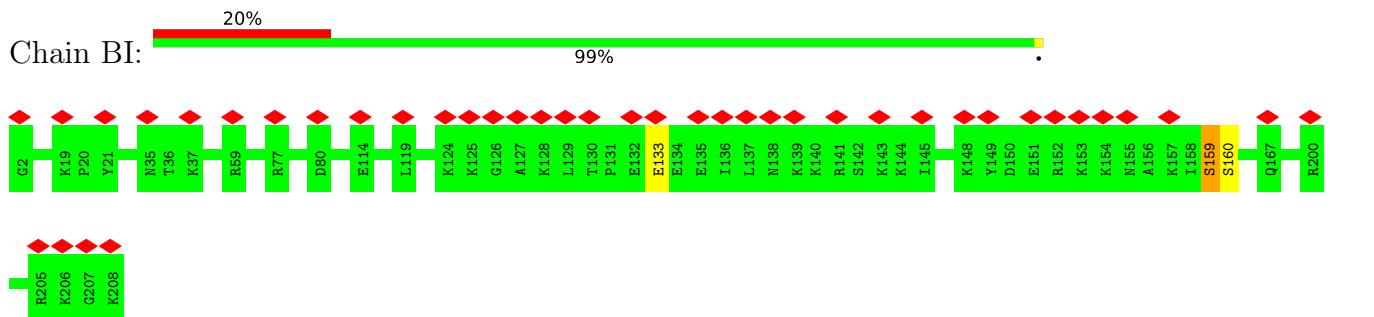
- Molecule 28: ribosomal protein eS6



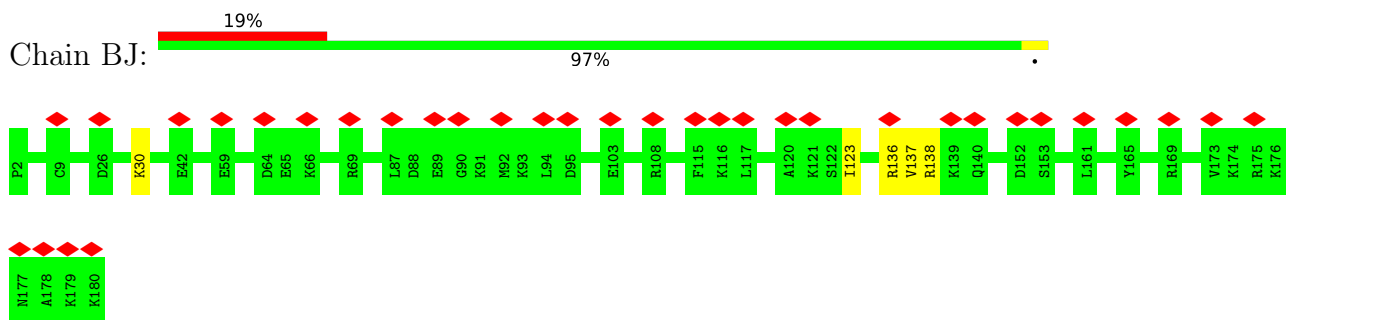
- Molecule 29: ribosomal protein eS7



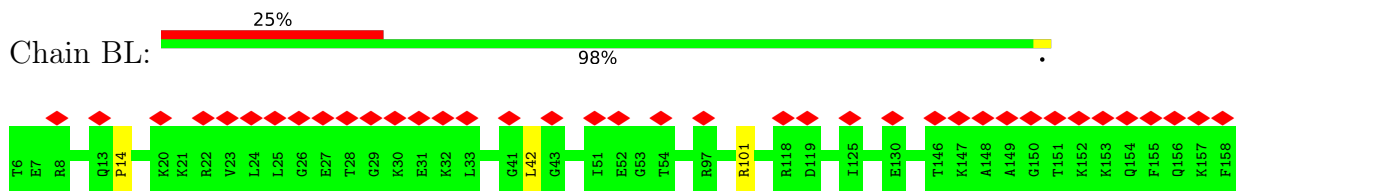
- Molecule 30: ribosomal protein eS8



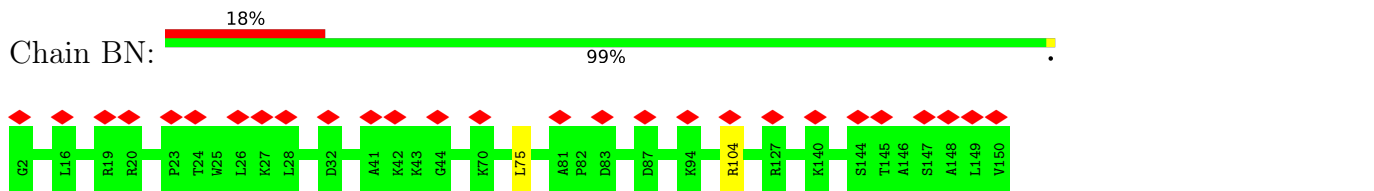
- Molecule 31: ribosomal protein uS4



- Molecule 32: ribosomal protein uS17

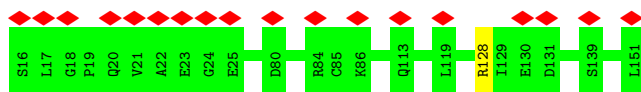


- Molecule 33: ribosomal protein uS15

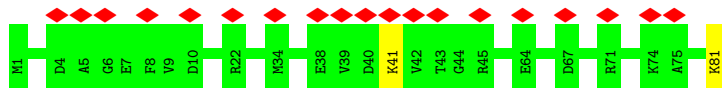


- Molecule 34: ribosomal protein uS11

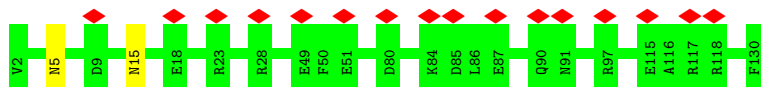




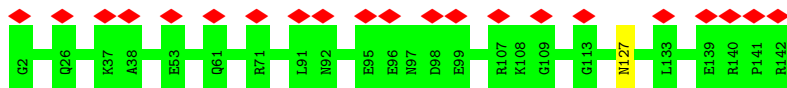
- Molecule 35: ribosomal protein eS21



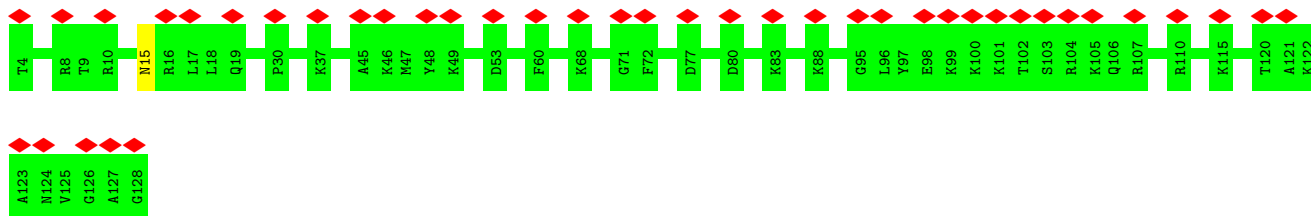
- Molecule 36: ribosomal protein uS8



- Molecule 37: ribosomal protein uS12



- Molecule 38: ribosomal protein eS24

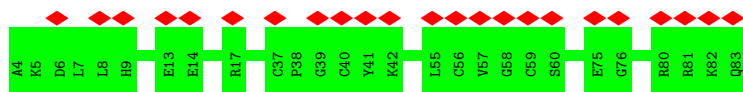


- Molecule 39: ribosomal protein eS26

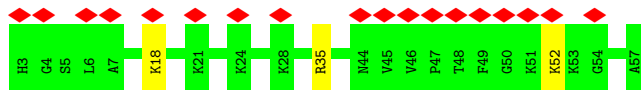


- Molecule 40: ribosomal protein eS27

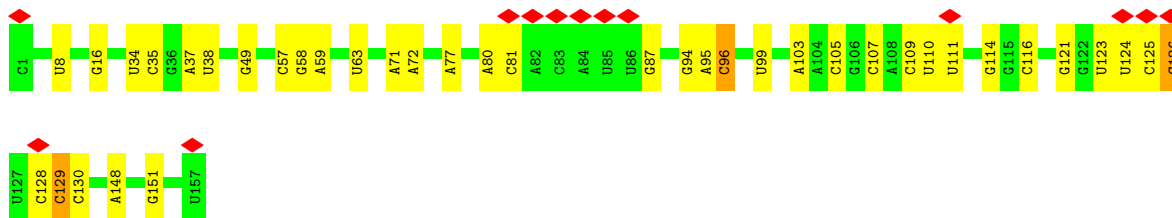
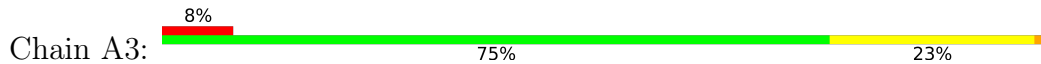




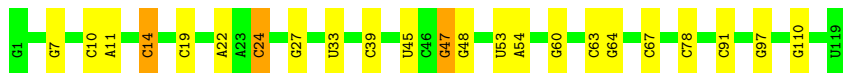
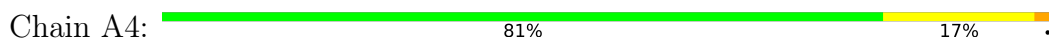
• Molecule 41: ribosomal protein eS30



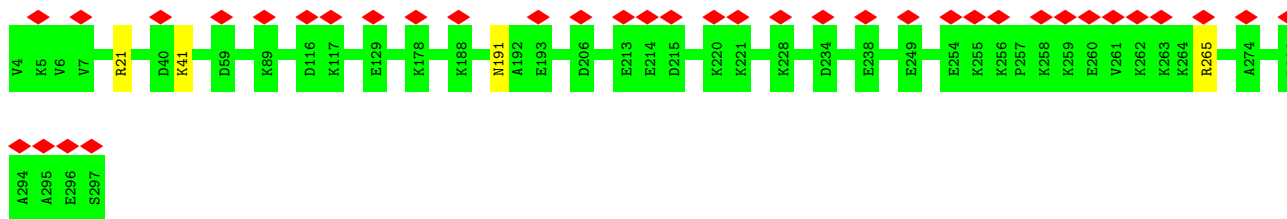
• Molecule 42: 5.8S ribosomal RNA



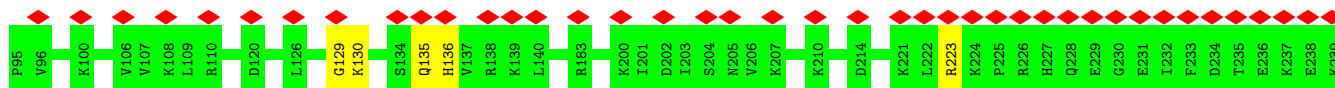
• Molecule 43: 5S ribosomal RNA

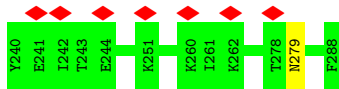


• Molecule 44: ribosomal protein uL18

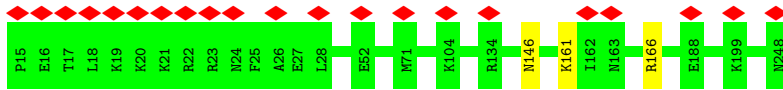


• Molecule 45: ribosomal protein eL6

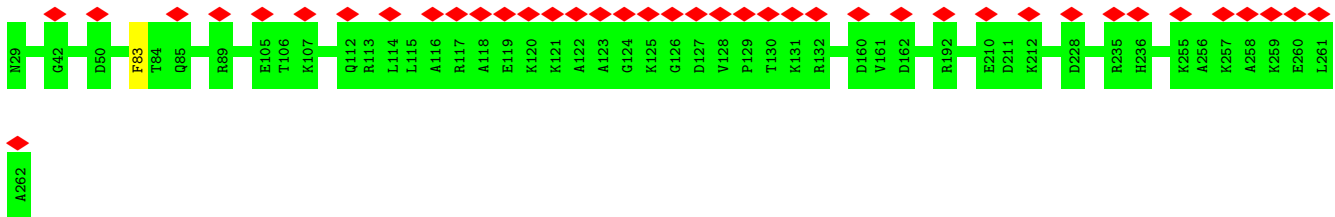




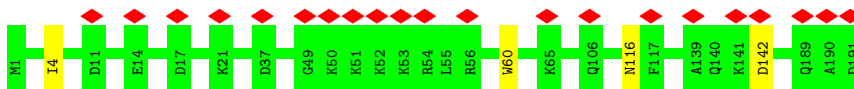
- Molecule 46: ribosomal protein uL30



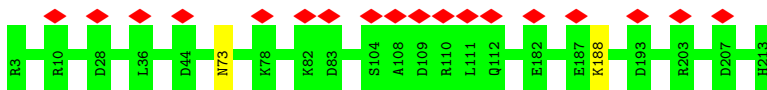
- Molecule 47: ribosomal protein eL8



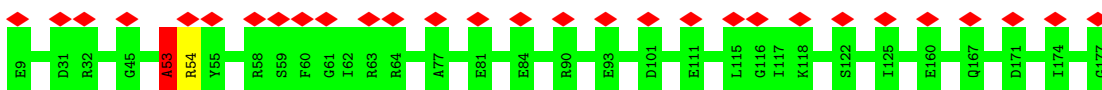
- Molecule 48: ribosomal protein uL6



- Molecule 49: ribosomal protein uL16

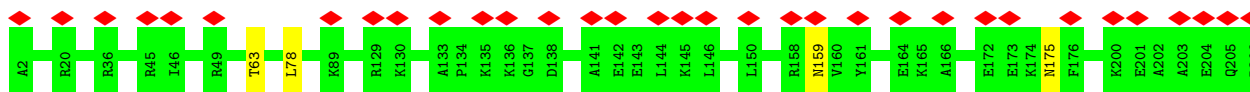


- Molecule 50: ribosomal protein uL5

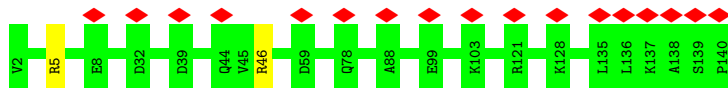


- Molecule 51: ribosomal protein eL13





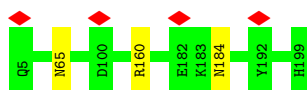
- Molecule 52: ribosomal protein eL14



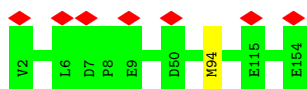
- Molecule 53: ribosomal protein eL15



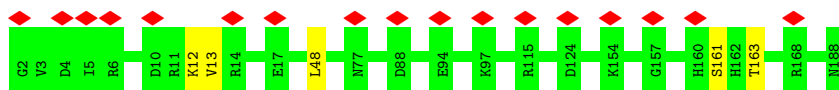
- Molecule 54: ribosomal protein uL13



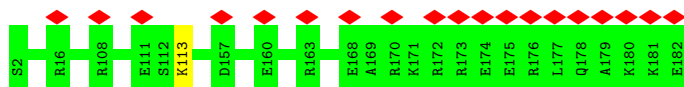
- Molecule 55: ribosomal protein uL22



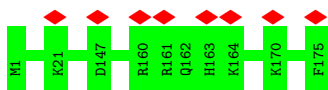
- Molecule 56: ribosomal protein eL18



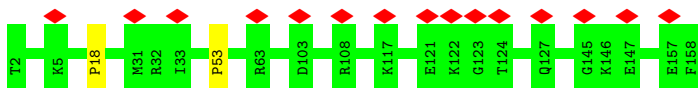
- Molecule 57: ribosomal protein eL19



- Molecule 58: ribosomal protein eL20



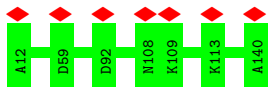
- Molecule 59: ribosomal protein eL21



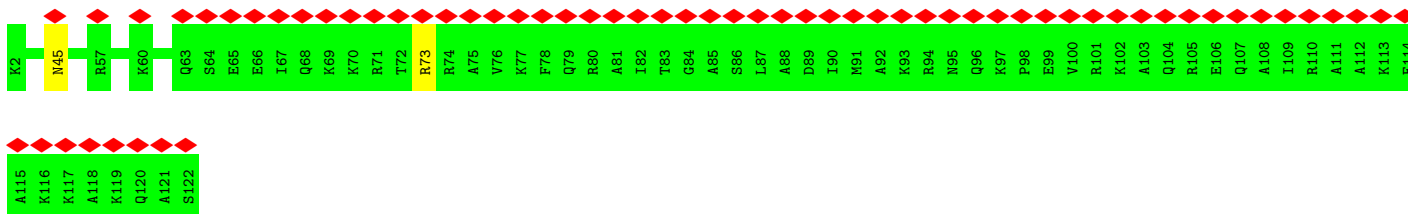
- Molecule 60: ribosomal protein eL22



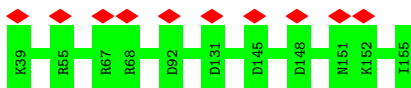
- Molecule 61: ribosomal protein uL14



- Molecule 62: ribosomal protein eL24

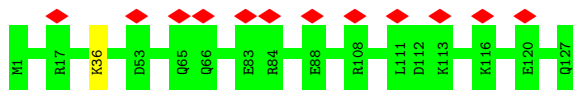


- Molecule 63: ribosomal protein uL23

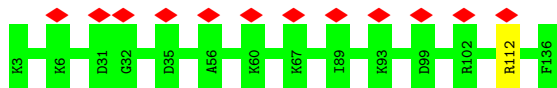


- Molecule 64: ribosomal protein uL24

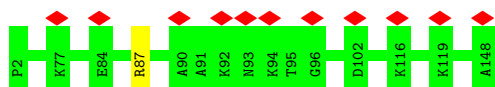




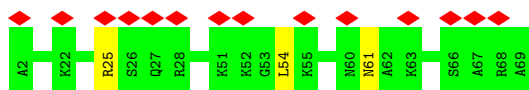
- Molecule 65: ribosomal protein eL27



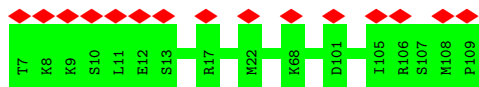
- Molecule 66: ribosomal protein uL15



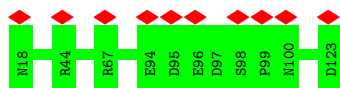
- Molecule 67: ribosomal protein eL29



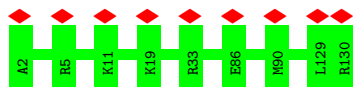
- Molecule 68: ribosomal protein eL30



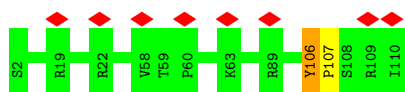
- Molecule 69: ribosomal protein eL31



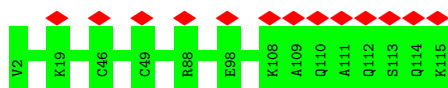
- Molecule 70: ribosomal protein eL32



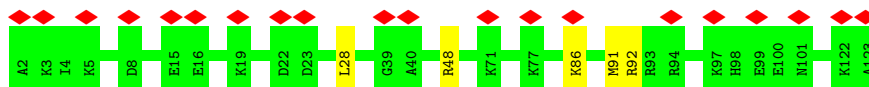
- Molecule 71: ribosomal protein eL33



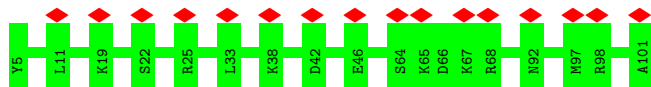
• Molecule 72: ribosomal protein eL34



• Molecule 73: ribosomal protein uL29



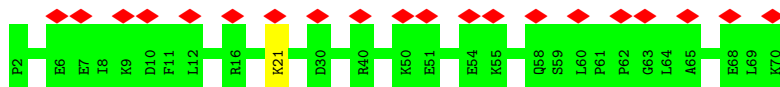
• Molecule 74: ribosomal protein eL36



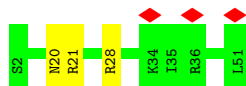
• Molecule 75: ribosomal protein eL37



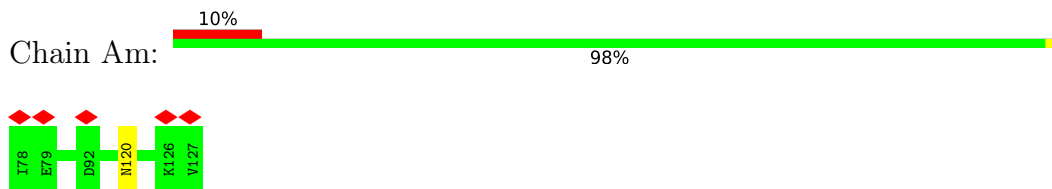
• Molecule 76: ribosomal protein eL38



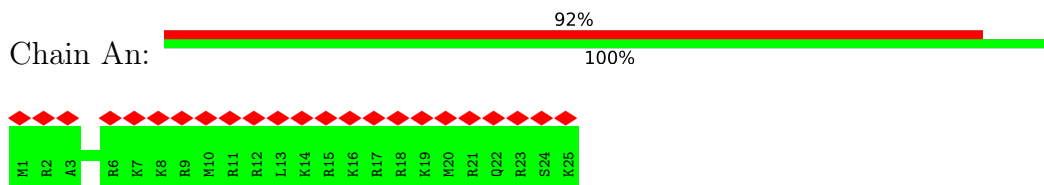
• Molecule 77: ribosomal protein eL39



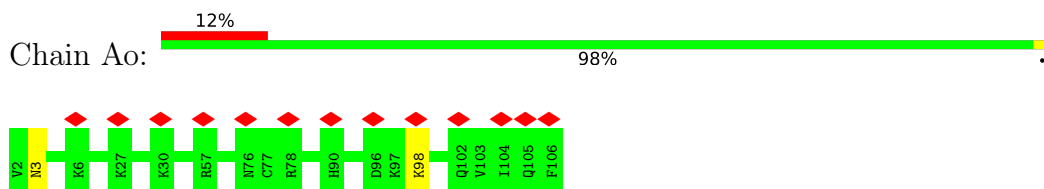
- Molecule 78: ribosomal protein eL40



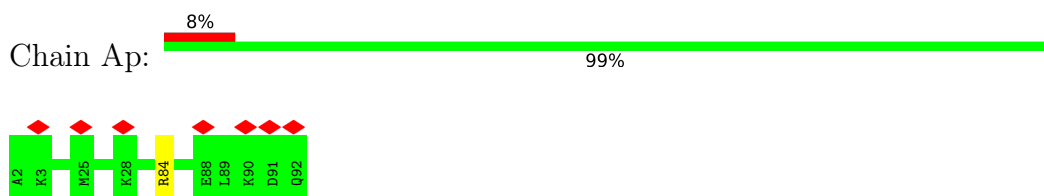
- Molecule 79: ribosomal protein eL41



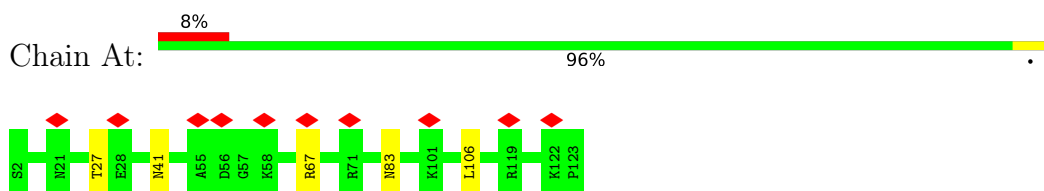
- Molecule 80: ribosomal protein eL42



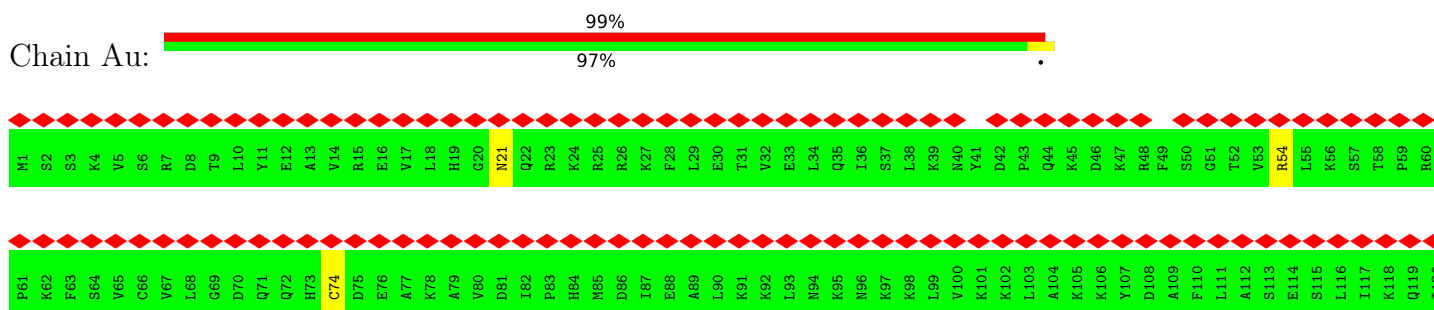
- Molecule 81: ribosomal protein eL43



- Molecule 82: ribosomal protein eL28

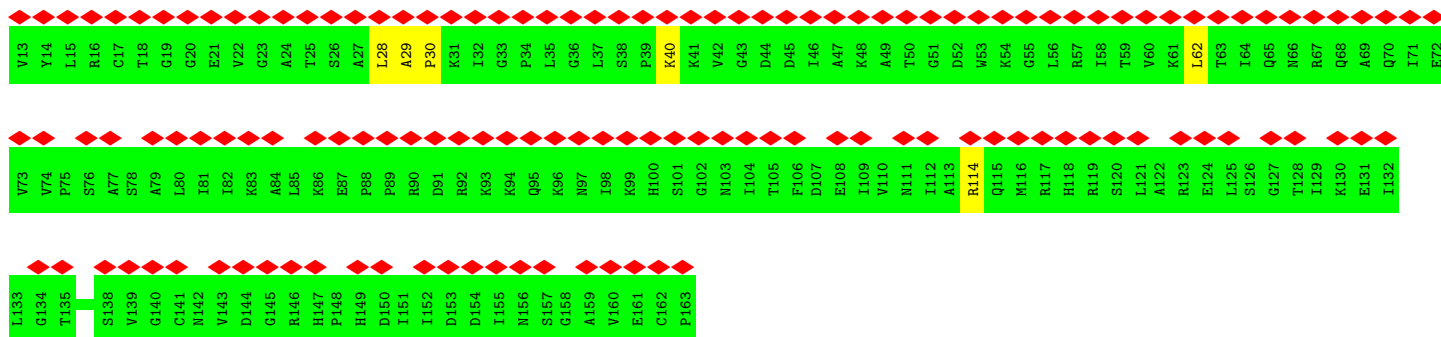
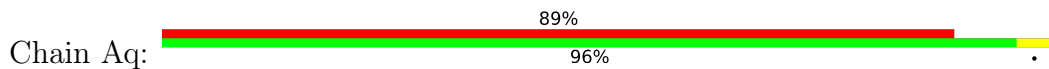


- Molecule 83: ribosomal protein uL1

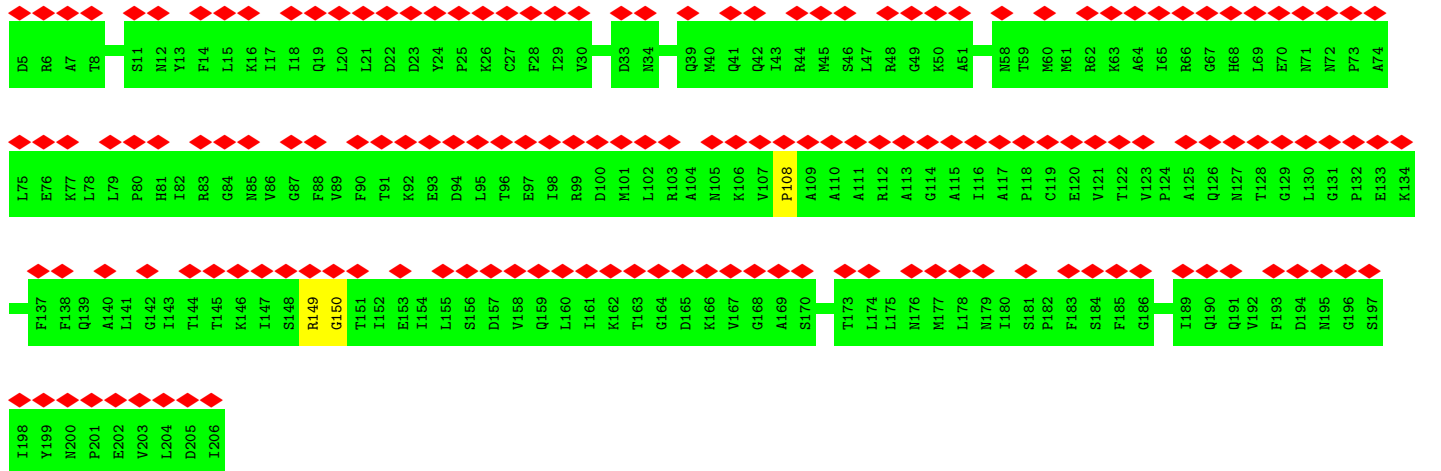
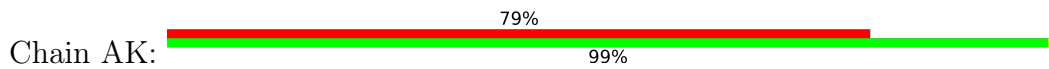




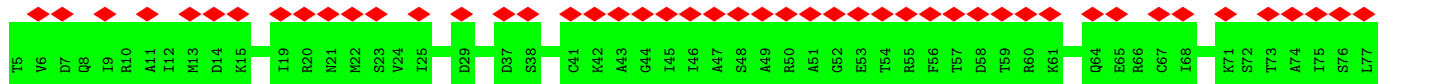
• Molecule 84: ribosomal protein uL11

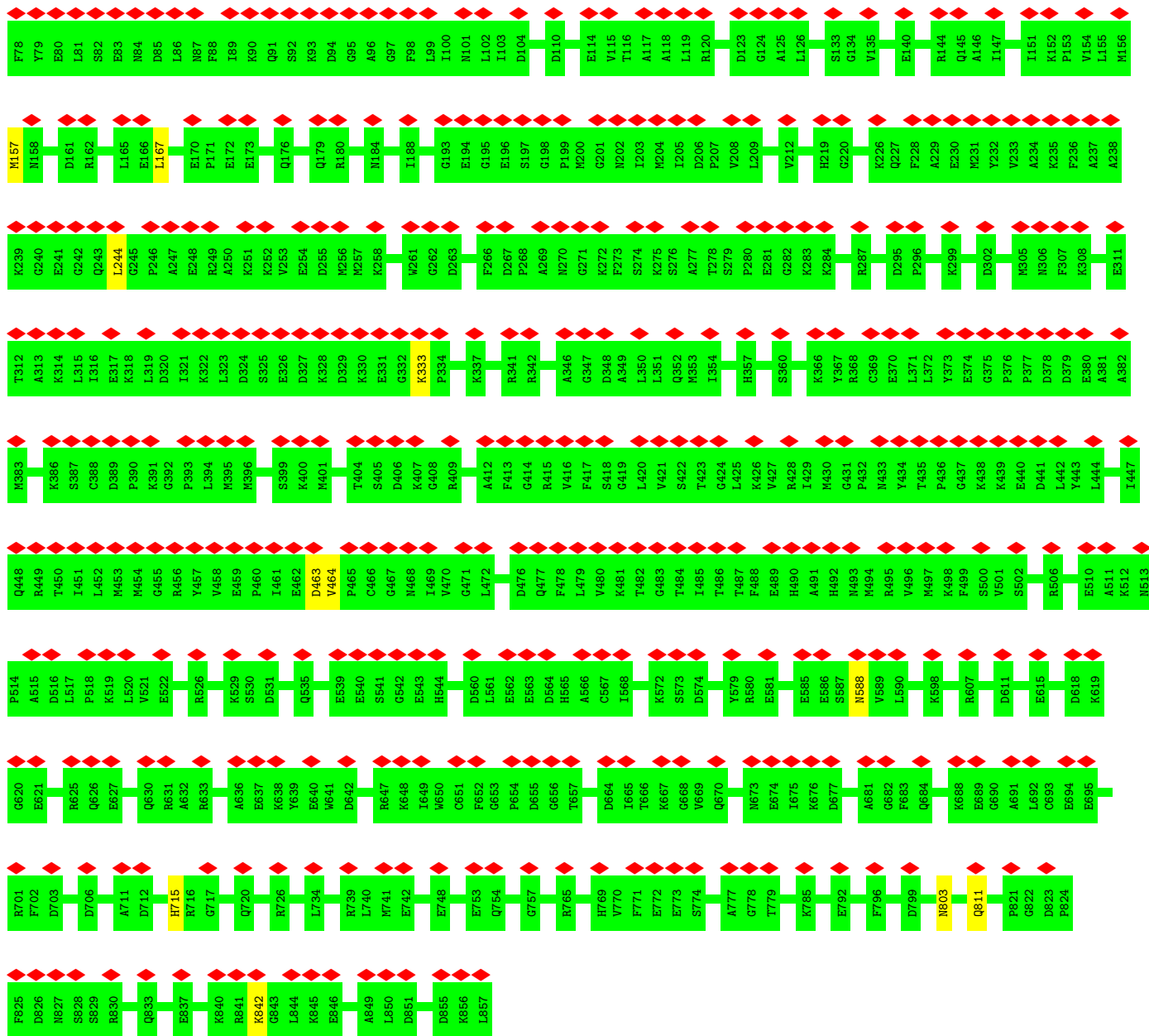


• Molecule 85: ribosomal protein uL10



• Molecule 86: eukaryotic elongation factor 2 (eEF2)





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37941	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	12.587	Depositor
Minimum map value	-3.981	Depositor
Average map value	0.345	Depositor
Map value standard deviation	0.672	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	394.875, 394.875, 394.875	wwPDB
Map dimensions	405, 405, 405	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.975, 0.975, 0.975	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	AA	0.30	0/1968	0.55	0/2639
2	BA	0.28	0/1741	0.54	0/2366
3	AB	0.30	0/3246	0.54	1/4345 (0.0%)
4	BB	0.29	0/1749	0.61	0/2340
5	AC	0.29	0/2942	0.54	0/3951
6	BC	0.30	0/1761	0.54	0/2379
7	A2	0.37	0/86612	1.04	325/135104 (0.2%)
8	Bv	0.38	1/1810 (0.1%)	0.97	2/2817 (0.1%)
9	Bx	0.25	0/261	0.90	0/404
10	Bw	0.39	1/1819 (0.1%)	0.95	0/2833
11	B1	0.35	1/40767 (0.0%)	1.04	189/63536 (0.3%)
12	BD	0.28	0/1736	0.51	0/2338
13	BF	0.27	0/1524	0.57	0/2048
14	BK	0.29	0/851	0.59	0/1147
15	BM	0.26	0/941	0.57	0/1264
16	BP	0.31	0/1019	0.63	1/1361 (0.1%)
17	BQ	0.27	0/1126	0.57	0/1506
18	BR	0.26	0/1023	0.51	0/1373
19	BS	0.27	0/1172	0.53	0/1570
20	BT	0.28	0/1131	0.54	0/1515
21	BU	0.25	0/778	0.53	0/1045
22	BZ	0.27	0/696	0.62	0/929
23	Bc	0.26	0/490	0.56	0/656
24	Bd	0.30	0/437	0.65	1/580 (0.2%)
25	Bf	0.26	0/613	0.46	0/811
26	Bg	0.27	0/2497	0.53	0/3399
27	BE	0.29	0/2072	0.55	0/2793
28	BG	0.26	0/1907	0.51	0/2538
29	BH	0.27	0/1501	0.52	0/2009
30	BI	0.28	0/1725	0.57	1/2298 (0.0%)
31	BJ	0.27	0/1520	0.52	0/2030
32	BL	0.29	0/1281	0.60	1/1710 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BN	0.27	0/1226	0.54	1/1649 (0.1%)
34	BO	0.27	0/1029	0.51	0/1380
35	BV	0.27	0/623	0.52	0/833
36	BW	0.29	0/1051	0.54	0/1406
37	BX	0.29	0/1116	0.56	0/1490
38	BY	0.26	0/1032	0.51	0/1371
39	Ba	0.28	0/786	0.54	0/1053
40	Bb	0.27	0/637	0.50	0/854
41	Be	0.28	0/443	0.56	0/583
42	A3	0.37	0/3726	1.00	13/5804 (0.2%)
43	A4	0.39	0/2839	1.05	12/4425 (0.3%)
44	AD	0.29	0/2437	0.53	0/3262
45	AE	0.29	0/1603	0.59	0/2153
46	AF	0.29	0/1986	0.52	0/2644
47	AG	0.30	0/1913	0.55	1/2576 (0.0%)
48	AH	0.29	0/1545	0.60	1/2077 (0.0%)
49	AI	0.29	0/1730	0.51	0/2311
50	AJ	0.28	0/1376	0.56	1/1841 (0.1%)
51	AL	0.29	0/1688	0.58	0/2260
52	AM	0.31	0/1161	0.52	0/1554
53	AN	0.31	0/1746	0.52	0/2338
54	AO	0.30	0/1638	0.51	0/2191
55	AP	0.29	0/1268	0.49	0/1701
56	AQ	0.28	0/1537	0.62	1/2052 (0.0%)
57	AR	0.26	0/1533	0.49	0/2025
58	AS	0.29	0/1488	0.53	0/1997
59	AT	0.28	0/1312	0.50	0/1753
60	AU	0.28	0/822	0.49	0/1103
61	AV	0.28	0/983	0.51	0/1319
62	AW	0.27	0/1004	0.49	0/1332
63	AX	0.27	0/975	0.51	0/1312
64	AY	0.27	0/1081	0.47	0/1439
65	AZ	0.28	0/1126	0.54	0/1502
66	Aa	0.29	0/1191	0.54	0/1591
67	Ab	0.27	0/569	0.65	1/750 (0.1%)
68	Ac	0.28	0/812	0.53	0/1089
69	Ad	0.27	0/894	0.53	0/1204
70	Ae	0.28	0/1082	0.54	0/1443
71	Af	0.31	0/895	0.57	0/1198
72	Ag	0.30	0/916	0.60	0/1220
73	Ah	0.26	0/1023	0.57	1/1351 (0.1%)
74	Ai	0.26	0/805	0.52	0/1065
75	Aj	0.30	0/703	0.59	0/929

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	Ak	0.27	0/575	0.56	0/761
77	Al	0.26	0/454	0.55	0/599
78	Am	0.26	0/417	0.54	0/553
79	An	0.23	0/241	0.46	0/305
80	Ao	0.29	0/877	0.54	0/1156
81	Ap	0.29	0/718	0.57	0/953
82	At	0.30	0/995	0.66	1/1334 (0.1%)
83	Au	0.27	0/1772	0.53	0/2375
84	Aq	0.30	0/1155	0.70	2/1558 (0.1%)
85	AK	0.28	0/1580	0.60	0/2133
86	Ct	0.28	0/6767	0.58	1/9139 (0.0%)
All	All	0.33	3/241617 (0.0%)	0.88	557/353930 (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
2	BA	0	1
5	AC	0	3
17	BQ	0	1
22	BZ	0	1
23	Bc	0	1
27	BE	0	1
30	BI	0	1
31	BJ	0	2
45	AE	0	3
48	AH	0	3
49	AI	0	1
50	AJ	0	1
56	AQ	0	2
57	AR	0	1
71	Af	0	1
73	Ah	0	1
82	At	0	1
84	Aq	0	2
85	AK	0	2
86	Ct	0	3
All	All	0	32

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Bw	1	G	OP3-P	-10.68	1.48	1.61
8	Bv	1	G	OP3-P	-10.61	1.48	1.61
11	B1	1	U	OP3-P	-10.54	1.48	1.61

All (557) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B1	621	C	N1-C2-O2	9.78	124.77	118.90
11	B1	118	C	N1-C2-O2	9.51	124.61	118.90
11	B1	1315	U	N1-C2-O2	9.42	129.39	122.80
7	A2	2388	U	C2-N1-C1'	9.41	128.99	117.70
11	B1	1019	C	N3-C2-O2	-9.37	115.34	121.90
7	A2	252	C	N1-C2-O2	9.23	124.44	118.90
11	B1	96	C	C2-N1-C1'	9.18	128.90	118.80
11	B1	1019	C	N1-C2-O2	9.03	124.32	118.90
11	B1	118	C	C2-N1-C1'	8.99	128.68	118.80
7	A2	219	C	C2-N1-C1'	8.89	128.57	118.80
11	B1	621	C	N3-C2-O2	-8.85	115.71	121.90
11	B1	1520	G	N3-C4-C5	-8.84	124.18	128.60
7	A2	2388	U	N3-C2-O2	-8.83	116.02	122.20
11	B1	621	C	C2-N1-C1'	8.83	128.51	118.80
7	A2	258	C	N1-C2-O2	8.81	124.19	118.90
7	A2	1895	C	N3-C2-O2	-8.78	115.75	121.90
7	A2	2388	U	N1-C2-O2	8.76	128.94	122.80
7	A2	1576	C	N1-C2-O2	8.60	124.06	118.90
11	B1	1315	U	N3-C2-O2	-8.51	116.24	122.20
7	A2	247	C	N3-C2-O2	-8.50	115.95	121.90
7	A2	3880	C	N1-C2-O2	8.47	123.98	118.90
7	A2	667	C	N3-C2-O2	-8.44	115.99	121.90
11	B1	96	C	N1-C2-O2	8.41	123.95	118.90
7	A2	2606	C	N1-C2-O2	8.29	123.87	118.90
11	B1	1271	C	N1-C2-O2	8.20	123.82	118.90
7	A2	219	C	N1-C2-O2	8.17	123.80	118.90
11	B1	67	C	N1-C2-O2	8.16	123.80	118.90
11	B1	1315	U	C2-N1-C1'	8.15	127.49	117.70
11	B1	67	C	C2-N1-C1'	8.14	127.75	118.80
7	A2	138	C	N1-C2-O2	8.14	123.78	118.90
11	B1	1117	C	N1-C2-O2	8.07	123.74	118.90
7	A2	1432	C	N3-C2-O2	-8.04	116.27	121.90
11	B1	1464	C	N1-C2-O2	8.03	123.72	118.90
7	A2	1576	C	N3-C2-O2	-8.01	116.29	121.90
7	A2	163	C	N1-C2-O2	8.00	123.70	118.90
7	A2	1189	C	N3-C2-O2	-7.99	116.31	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A2	1256	G	C4-N9-C1'	7.96	136.85	126.50
7	A2	2606	C	C2-N1-C1'	7.95	127.54	118.80
11	B1	570	C	N1-C2-O2	7.92	123.65	118.90
11	B1	96	C	N3-C2-O2	-7.89	116.38	121.90
11	B1	918	U	N1-C2-O2	7.87	128.31	122.80
11	B1	1520	G	C4-N9-C1'	7.86	136.71	126.50
11	B1	1710	C	N1-C2-O2	7.84	123.60	118.90
7	A2	3607	C	N3-C2-O2	-7.74	116.48	121.90
7	A2	1256	G	N3-C4-C5	-7.72	124.74	128.60
11	B1	1591	C	N1-C2-O2	7.71	123.53	118.90
11	B1	1237	C	C2-N1-C1'	7.69	127.25	118.80
7	A2	1176	C	N1-C2-O2	7.65	123.49	118.90
11	B1	1520	G	N3-C4-N9	7.58	130.55	126.00
11	B1	496	C	N1-C2-O2	7.58	123.45	118.90
7	A2	918	C	N1-C2-O2	7.55	123.43	118.90
7	A2	252	C	C2-N1-C1'	7.55	127.11	118.80
7	A2	3880	C	N3-C2-O2	-7.54	116.62	121.90
7	A2	1576	C	C6-N1-C2	-7.53	117.29	120.30
7	A2	2727	C	C2-N1-C1'	7.53	127.08	118.80
7	A2	1256	G	N3-C4-N9	7.51	130.51	126.00
11	B1	337	C	N3-C2-O2	-7.50	116.65	121.90
11	B1	1464	C	C6-N1-C2	-7.49	117.30	120.30
7	A2	191	C	N3-C2-O2	-7.49	116.66	121.90
11	B1	745	C	N1-C2-O2	7.48	123.39	118.90
7	A2	905	G	C4-N9-C1'	7.40	136.12	126.50
11	B1	118	C	N3-C2-O2	-7.34	116.76	121.90
7	A2	4671	U	N1-C2-O2	7.29	127.90	122.80
7	A2	4088	C	N1-C2-O2	7.23	123.24	118.90
7	A2	2373	G	C4-N9-C1'	7.22	135.89	126.50
7	A2	4886	C	C2-N1-C1'	7.18	126.69	118.80
7	A2	4909	G	C4-N9-C1'	7.17	135.82	126.50
11	B1	1464	C	C2-N1-C1'	7.16	126.68	118.80
7	A2	77	U	N3-C2-O2	-7.14	117.20	122.20
11	B1	1389	C	C2-N1-C1'	7.12	126.64	118.80
11	B1	1389	C	N1-C2-O2	7.12	123.17	118.90
7	A2	3880	C	C6-N1-C2	-7.11	117.45	120.30
11	B1	1117	C	C6-N1-C2	-7.09	117.47	120.30
7	A2	667	C	N1-C2-O2	7.08	123.15	118.90
7	A2	252	C	N3-C2-O2	-7.06	116.96	121.90
11	B1	797	C	P-O3'-C3'	7.05	128.16	119.70
67	Ab	54	LEU	CA-CB-CG	7.02	131.44	115.30
7	A2	1176	C	C2-N1-C1'	7.00	126.50	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A2	1754	C	N3-C2-O2	-6.99	117.01	121.90
11	B1	1472	C	C2-N1-C1'	6.97	126.47	118.80
7	A2	50	C	N1-C2-O2	6.97	123.08	118.90
7	A2	1424	C	N1-C2-O2	6.96	123.08	118.90
7	A2	2798	U	N3-C2-O2	-6.96	117.33	122.20
7	A2	258	C	N3-C2-O2	-6.95	117.04	121.90
11	B1	1117	C	N3-C2-O2	-6.94	117.04	121.90
11	B1	1117	C	C2-N1-C1'	6.94	126.43	118.80
7	A2	480	C	N1-C2-O2	6.92	123.05	118.90
7	A2	2499	C	C2-N1-C1'	6.92	126.42	118.80
7	A2	2499	C	N1-C2-O2	6.92	123.06	118.90
7	A2	2798	U	N1-C2-O2	6.92	127.65	122.80
11	B1	227	U	P-O3'-C3'	6.92	128.00	119.70
7	A2	3880	C	C2-N1-C1'	6.91	126.40	118.80
11	B1	1464	C	N3-C2-O2	-6.89	117.08	121.90
7	A2	703	C	N1-C2-O2	6.87	123.02	118.90
7	A2	4464	C	N1-C2-O2	6.87	123.02	118.90
11	B1	496	C	C2-N1-C1'	6.87	126.36	118.80
7	A2	2606	C	C6-N1-C2	-6.85	117.56	120.30
7	A2	1576	C	C2-N1-C1'	6.83	126.32	118.80
7	A2	3890	C	C2-N1-C1'	6.82	126.30	118.80
7	A2	219	C	N3-C2-O2	-6.80	117.14	121.90
7	A2	258	C	C2-N1-C1'	6.80	126.28	118.80
7	A2	4671	U	N3-C2-O2	-6.80	117.44	122.20
7	A2	1256	G	C8-N9-C1'	-6.76	118.21	127.00
82	At	106	LEU	CA-CB-CG	6.76	130.84	115.30
7	A2	3607	C	N1-C2-O2	6.73	122.94	118.90
7	A2	5015	C	C2-N1-C1'	6.72	126.19	118.80
11	B1	524	U	N1-C2-O2	6.71	127.50	122.80
11	B1	918	U	C2-N1-C1'	6.71	125.75	117.70
7	A2	4909	G	N3-C4-N9	6.69	130.01	126.00
11	B1	1710	C	C2-N1-C1'	6.69	126.16	118.80
11	B1	1398	G	N3-C4-C5	-6.67	125.27	128.60
7	A2	2835	C	N1-C2-O2	6.66	122.89	118.90
7	A2	4909	G	C8-N9-C1'	-6.65	118.35	127.00
7	A2	2606	C	N3-C2-O2	-6.65	117.25	121.90
7	A2	2260	U	N1-C2-O2	6.63	127.44	122.80
7	A2	905	G	N3-C4-C5	-6.62	125.29	128.60
7	A2	1874	C	C2-N1-C1'	6.59	126.05	118.80
32	BL	42	LEU	CA-CB-CG	6.58	130.44	115.30
11	B1	1022	U	C2-N1-C1'	6.58	125.59	117.70
11	B1	1852	C	C2-N1-C1'	6.58	126.03	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B1	496	C	N3-C2-O2	-6.57	117.30	121.90
7	A2	2649	C	C2-N1-C1'	6.57	126.02	118.80
7	A2	2260	U	N3-C2-O2	-6.54	117.62	122.20
7	A2	959	C	N1-C2-O2	6.53	122.82	118.90
11	B1	89	C	C2-N1-C1'	6.52	125.97	118.80
11	B1	1271	C	N3-C2-O2	-6.51	117.34	121.90
7	A2	4709	C	N3-C2-O2	-6.50	117.35	121.90
7	A2	2389	C	C2-N1-C1'	6.50	125.95	118.80
11	B1	67	C	N3-C2-O2	-6.49	117.36	121.90
7	A2	1176	C	C6-N1-C2	-6.49	117.70	120.30
7	A2	918	C	C2-N1-C1'	6.48	125.93	118.80
11	B1	1520	G	C2-N3-C4	6.47	115.14	111.90
11	B1	174	C	C2-N1-C1'	6.46	125.91	118.80
7	A2	4886	C	C6-N1-C2	-6.46	117.72	120.30
7	A2	1499	G	C4-N9-C1'	6.46	134.89	126.50
7	A2	2727	C	N1-C2-O2	6.45	122.77	118.90
43	A4	24	C	N1-C2-O2	6.45	122.77	118.90
7	A2	1668	C	N1-C2-O2	6.44	122.76	118.90
11	B1	118	C	C6-N1-C1'	-6.43	113.08	120.80
7	A2	163	C	N3-C2-O2	-6.42	117.41	121.90
7	A2	4880	C	C2-N1-C1'	6.40	125.84	118.80
11	B1	96	C	C6-N1-C1'	-6.39	113.13	120.80
11	B1	918	U	N3-C2-O2	-6.39	117.73	122.20
11	B1	1271	C	C2-N1-C1'	6.37	125.80	118.80
7	A2	138	C	N3-C2-O2	-6.36	117.45	121.90
7	A2	911	C	N1-C2-O2	6.35	122.71	118.90
73	Ah	28	LEU	CA-CB-CG	6.35	129.91	115.30
7	A2	4886	C	N1-C2-O2	6.35	122.71	118.90
11	B1	1398	G	C4-N9-C1'	6.35	134.75	126.50
11	B1	1389	C	C6-N1-C2	-6.31	117.78	120.30
7	A2	4665	U	N3-C2-O2	-6.30	117.79	122.20
11	B1	337	C	C6-N1-C2	-6.29	117.78	120.30
11	B1	570	C	N3-C2-O2	-6.29	117.50	121.90
7	A2	4824	C	N1-C2-O2	6.28	122.67	118.90
11	B1	621	C	C6-N1-C2	-6.27	117.79	120.30
7	A2	219	C	C6-N1-C2	-6.27	117.79	120.30
7	A2	493	G	N3-C4-N9	6.27	129.76	126.00
11	B1	746	C	N3-C2-O2	-6.27	117.51	121.90
11	B1	1389	C	N3-C2-O2	-6.25	117.52	121.90
7	A2	901	U	P-O3'-C3'	6.23	127.18	119.70
7	A2	1966	G	C4-N9-C1'	6.22	134.59	126.50
11	B1	1156	U	C2-N1-C1'	6.21	125.16	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A2	3903	U	N1-C2-O2	6.21	127.15	122.80
11	B1	1710	C	C6-N1-C2	-6.20	117.82	120.30
7	A2	2388	U	C6-N1-C1'	-6.20	112.52	121.20
11	B1	1237	C	C6-N1-C2	-6.19	117.82	120.30
11	B1	524	U	N3-C2-O2	-6.18	117.87	122.20
7	A2	493	G	C4-N9-C1'	6.17	134.52	126.50
7	A2	1176	C	N3-C2-O2	-6.16	117.58	121.90
7	A2	1653	U	N3-C2-O2	-6.16	117.89	122.20
7	A2	2373	G	N3-C4-C5	-6.16	125.52	128.60
7	A2	3607	C	C6-N1-C2	-6.16	117.84	120.30
7	A2	4671	U	C2-N1-C1'	6.16	125.09	117.70
11	B1	1557	C	C2-N1-C1'	6.16	125.57	118.80
7	A2	1440	C	N1-C2-O2	6.15	122.59	118.90
11	B1	1750	C	C2-N1-C1'	6.15	125.57	118.80
7	A2	5008	C	C2-N1-C1'	6.14	125.56	118.80
7	A2	4665	U	N1-C2-O2	6.14	127.10	122.80
7	A2	2798	U	C2-N1-C1'	6.14	125.07	117.70
7	A2	3903	U	N3-C2-O2	-6.12	117.91	122.20
3	AB	292	LEU	CA-CB-CG	6.12	129.37	115.30
7	A2	1189	C	N1-C2-O2	6.11	122.57	118.90
11	B1	1591	C	N3-C2-O2	-6.11	117.62	121.90
11	B1	1624	U	N1-C2-O2	6.10	127.07	122.80
7	A2	4069	G	C4-N9-C1'	6.10	134.43	126.50
7	A2	3890	C	C6-N1-C2	-6.09	117.86	120.30
7	A2	2691	G	N3-C4-N9	6.09	129.65	126.00
7	A2	4216	G	N3-C4-C5	-6.08	125.56	128.60
7	A2	2691	G	C4-N9-C1'	6.07	134.39	126.50
7	A2	1067	C	N1-C2-O2	6.07	122.54	118.90
7	A2	2799	C	N1-C2-O2	6.07	122.54	118.90
86	Ct	244	LEU	CA-CB-CG	6.07	129.26	115.30
11	B1	568	C	N1-C2-O2	6.06	122.53	118.90
7	A2	2256	C	C2-N1-C1'	6.05	125.46	118.80
11	B1	337	C	N1-C2-O2	6.05	122.53	118.90
7	A2	1256	G	C2-N3-C4	6.05	114.93	111.90
7	A2	905	G	N3-C4-N9	6.05	129.63	126.00
7	A2	1476	U	N1-C2-O2	6.05	127.03	122.80
7	A2	71	C	P-O3'-C3'	6.04	126.94	119.70
7	A2	2727	C	N3-C2-O2	-6.04	117.67	121.90
11	B1	1237	C	N1-C2-O2	6.04	122.52	118.90
11	B1	1520	G	C8-N9-C1'	-6.03	119.16	127.00
11	B1	570	C	C2-N1-C1'	6.03	125.43	118.80
42	A3	116	C	C2-N1-C1'	6.03	125.43	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B1	1472	C	C6-N1-C2	-6.03	117.89	120.30
11	B1	1710	C	N3-C2-O2	-6.02	117.68	121.90
7	A2	2499	C	N3-C2-O2	-6.01	117.69	121.90
7	A2	905	G	C8-N9-C1'	-6.01	119.19	127.00
11	B1	1557	C	N1-C2-O2	6.01	122.50	118.90
7	A2	3664	U	N1-C2-O2	5.99	127.00	122.80
11	B1	745	C	N3-C2-O2	-5.98	117.71	121.90
7	A2	219	C	C6-N1-C1'	-5.97	113.63	120.80
7	A2	493	G	N3-C4-C5	-5.97	125.61	128.60
11	B1	984	C	N3-C2-O2	-5.96	117.73	121.90
11	B1	1464	C	C5-C6-N1	5.96	123.98	121.00
7	A2	1746	G	C4-N9-C1'	5.95	134.24	126.50
7	A2	2398	C	C2-N1-C1'	5.95	125.35	118.80
11	B1	804	U	N3-C2-O2	-5.95	118.03	122.20
7	A2	1083	U	N3-C2-O2	-5.94	118.04	122.20
43	A4	14	C	C2-N1-C1'	5.94	125.34	118.80
11	B1	1472	C	N3-C2-O2	-5.94	117.74	121.90
7	A2	480	C	C2-N1-C1'	5.93	125.32	118.80
7	A2	1280	U	N1-C2-O2	5.93	126.95	122.80
7	A2	1466	G	C4-N9-C1'	5.93	134.20	126.50
11	B1	621	C	C6-N1-C1'	-5.93	113.69	120.80
7	A2	1638	U	N1-C2-O2	5.92	126.94	122.80
7	A2	163	C	C2-N1-C1'	5.91	125.30	118.80
7	A2	1668	C	N3-C2-O2	-5.91	117.76	121.90
11	B1	804	U	N1-C2-O2	5.91	126.94	122.80
7	A2	50	C	N3-C2-O2	-5.90	117.77	121.90
7	A2	907	C	N1-C2-O2	5.90	122.44	118.90
11	B1	570	C	C6-N1-C2	-5.89	117.94	120.30
11	B1	804	U	C2-N1-C1'	5.89	124.77	117.70
7	A2	2473	U	N3-C2-O2	-5.89	118.08	122.20
7	A2	670	C	C2-N1-C1'	5.89	125.28	118.80
7	A2	1564	U	C2-N1-C1'	5.89	124.77	117.70
11	B1	1472	C	N1-C2-O2	5.89	122.43	118.90
11	B1	1753	C	C2-N1-C1'	5.87	125.25	118.80
11	B1	96	C	C6-N1-C2	-5.86	117.95	120.30
7	A2	4216	G	C4-N9-C1'	5.86	134.12	126.50
7	A2	4464	C	N3-C2-O2	-5.85	117.81	121.90
7	A2	252	C	C6-N1-C2	-5.84	117.96	120.30
7	A2	2871	C	C2-N1-C1'	5.84	125.22	118.80
11	B1	1590	C	N1-C2-O2	5.84	122.40	118.90
7	A2	1466	G	N3-C4-C5	-5.83	125.68	128.60
7	A2	1440	C	C6-N1-C2	-5.83	117.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B1	1287	A	C2-N3-C4	5.83	113.51	110.60
43	A4	78	C	C2-N1-C1'	5.83	125.21	118.80
11	B1	1512	C	C2-N1-C1'	5.82	125.20	118.80
7	A2	4624	C	C6-N1-C2	-5.82	117.97	120.30
11	B1	973	C	C6-N1-C2	-5.81	117.98	120.30
7	A2	1280	U	N3-C2-O2	-5.81	118.13	122.20
7	A2	4177	C	N1-C2-O2	5.81	122.39	118.90
11	B1	645	C	C5-C6-N1	5.81	123.90	121.00
11	B1	950	C	N1-C2-O2	5.80	122.38	118.90
7	A2	911	C	N3-C2-O2	-5.80	117.84	121.90
42	A3	8	U	C2-N1-C1'	5.79	124.64	117.70
7	A2	962	C	N1-C2-O2	5.78	122.37	118.90
7	A2	2003	C	N1-C2-O2	5.78	122.37	118.90
7	A2	4602	C	C2-N1-C1'	5.77	125.15	118.80
7	A2	918	C	N3-C2-O2	-5.77	117.86	121.90
7	A2	191	C	N1-C2-O2	5.77	122.36	118.90
7	A2	2473	U	N1-C2-O2	5.77	126.84	122.80
11	B1	338	G	C4-N9-C1'	-5.77	119.00	126.50
11	B1	1398	G	N3-C4-N9	5.77	129.46	126.00
7	A2	4886	C	C5-C6-N1	5.76	123.88	121.00
7	A2	2691	G	C8-N9-C1'	-5.76	119.51	127.00
11	B1	100	U	N1-C2-O2	5.76	126.83	122.80
11	B1	1591	C	C2-N1-C1'	5.75	125.12	118.80
11	B1	1520	G	C8-N9-C4	-5.74	104.10	106.40
7	A2	1737	C	N1-C2-O2	5.74	122.34	118.90
7	A2	4088	C	C2-N1-C1'	5.74	125.12	118.80
7	A2	1199	C	N1-C2-O2	5.74	122.34	118.90
7	A2	2646	C	N1-C2-O2	5.73	122.34	118.90
7	A2	2003	C	N3-C2-O2	-5.73	117.89	121.90
7	A2	4545	C	N1-C2-O2	5.73	122.34	118.90
7	A2	2282	C	N3-C2-O2	-5.73	117.89	121.90
7	A2	4133	C	N1-C2-O2	5.73	122.34	118.90
11	B1	1271	C	C6-N1-C2	-5.72	118.01	120.30
7	A2	1466	G	N3-C4-N9	5.72	129.43	126.00
7	A2	4676	C	N1-C2-O2	5.72	122.33	118.90
11	B1	1019	C	C6-N1-C2	-5.72	118.01	120.30
7	A2	1275	C	C6-N1-C2	-5.72	118.01	120.30
8	Bv	36	C	C2-N1-C1'	5.72	125.09	118.80
7	A2	1424	C	C2-N1-C1'	5.71	125.09	118.80
7	A2	959	C	C2-N1-C1'	5.71	125.08	118.80
7	A2	5008	C	C6-N1-C2	-5.71	118.02	120.30
7	A2	3664	U	N3-C2-O2	-5.71	118.20	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A2	2373	G	N3-C4-N9	5.71	129.42	126.00
11	B1	1710	C	C5-C6-N1	5.71	123.85	121.00
11	B1	1750	C	C6-N1-C2	-5.71	118.02	120.30
7	A2	4216	G	N3-C4-N9	5.70	129.42	126.00
11	B1	189	U	N1-C2-O2	5.70	126.79	122.80
7	A2	682	U	N3-C2-O2	-5.70	118.21	122.20
7	A2	4602	C	N1-C2-O2	5.69	122.31	118.90
7	A2	4270	C	N1-C2-O2	5.69	122.31	118.90
42	A3	126	C	C2-N1-C1'	5.69	125.06	118.80
7	A2	1193	C	N1-C2-O2	5.68	122.31	118.90
11	B1	106	C	C6-N1-C2	-5.67	118.03	120.30
11	B1	806	U	N1-C2-O2	5.66	126.76	122.80
7	A2	1638	U	N3-C2-O2	-5.66	118.24	122.20
11	B1	459	C	C2-N1-C1'	5.66	125.03	118.80
11	B1	749	U	N1-C2-O2	5.65	126.75	122.80
7	A2	703	C	N3-C2-O2	-5.64	117.95	121.90
7	A2	50	C	C6-N1-C2	-5.64	118.04	120.30
7	A2	2325	C	N1-C2-O2	5.63	122.28	118.90
7	A2	3759	C	N1-C2-O2	5.63	122.28	118.90
11	B1	918	U	C6-N1-C1'	-5.63	113.32	121.20
7	A2	2341	U	N1-C2-O2	5.62	126.74	122.80
7	A2	4205	C	C6-N1-C2	-5.62	118.05	120.30
7	A2	247	C	N1-C2-O2	5.62	122.27	118.90
7	A2	2738	G	C4-N9-C1'	5.61	133.80	126.50
11	B1	1714	U	C2-N1-C1'	5.61	124.44	117.70
7	A2	2606	C	C5-C6-N1	5.61	123.81	121.00
7	A2	1059	C	C6-N1-C2	-5.61	118.06	120.30
43	A4	47	G	C2-N3-C4	5.61	114.70	111.90
11	B1	1156	U	N1-C2-O2	5.61	126.73	122.80
7	A2	4088	C	N3-C2-O2	-5.59	117.99	121.90
7	A2	2470	C	C5-C6-N1	5.58	123.79	121.00
11	B1	1156	U	N3-C2-O2	-5.58	118.30	122.20
7	A2	4169	C	C6-N1-C2	-5.57	118.07	120.30
11	B1	189	U	N3-C2-O2	-5.57	118.30	122.20
43	A4	39	C	N1-C2-O2	5.57	122.24	118.90
11	B1	620	G	N3-C4-N9	5.57	129.34	126.00
7	A2	1476	U	N3-C2-O2	-5.56	118.31	122.20
11	B1	67	C	C6-N1-C1'	-5.56	114.13	120.80
11	B1	1742	C	C2-N1-C1'	5.55	124.91	118.80
7	A2	2341	U	N3-C2-O2	-5.55	118.31	122.20
7	A2	1499	G	C8-N9-C1'	-5.55	119.79	127.00
7	A2	1424	C	N3-C2-O2	-5.54	118.02	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B1	1590	C	C6-N1-C2	-5.54	118.08	120.30
7	A2	907	C	N3-C2-O2	-5.54	118.03	121.90
11	B1	620	G	N3-C4-C5	-5.54	125.83	128.60
11	B1	100	U	N3-C2-O2	-5.53	118.33	122.20
11	B1	67	C	C6-N1-C2	-5.52	118.09	120.30
11	B1	746	C	C6-N1-C2	-5.52	118.09	120.30
7	A2	2846	C	C2-N1-C1'	5.52	124.87	118.80
7	A2	1589	C	N1-C2-O2	5.51	122.21	118.90
7	A2	3911	U	N3-C2-O2	-5.51	118.34	122.20
11	B1	1032	C	C2-N1-C1'	5.50	124.85	118.80
7	A2	1966	G	N3-C4-N9	5.50	129.30	126.00
7	A2	214	C	N1-C2-O2	5.49	122.20	118.90
7	A2	2373	G	C8-N9-C4	-5.49	104.20	106.40
7	A2	4519	U	N3-C2-O2	-5.49	118.36	122.20
11	B1	338	G	N3-C4-N9	-5.49	122.71	126.00
11	B1	950	C	C6-N1-C2	-5.48	118.11	120.30
11	B1	1691	U	C2-N1-C1'	5.48	124.28	117.70
42	A3	99	U	C2-N1-C1'	5.48	124.27	117.70
43	A4	19	C	C2-N1-C1'	5.48	124.83	118.80
7	A2	4624	C	C2-N1-C1'	5.48	124.82	118.80
7	A2	474	C	N1-C2-O2	5.47	122.19	118.90
7	A2	3616	U	N1-C2-O2	5.47	126.63	122.80
11	B1	106	C	C2-N1-C1'	5.47	124.82	118.80
7	A2	252	C	C5-C6-N1	5.47	123.73	121.00
7	A2	1432	C	N1-C2-O2	5.46	122.18	118.90
7	A2	2373	G	C8-N9-C1'	-5.46	119.91	127.00
11	B1	524	U	C2-N1-C1'	5.45	124.24	117.70
11	B1	1691	U	N1-C2-O2	5.45	126.61	122.80
24	Bd	39	CYS	C-N-CA	5.45	135.32	121.70
7	A2	77	U	N1-C2-O2	5.44	126.61	122.80
7	A2	258	C	C6-N1-C2	-5.44	118.12	120.30
7	A2	4205	C	C2-N1-C1'	5.44	124.78	118.80
7	A2	1083	U	C2-N1-C1'	5.43	124.22	117.70
11	B1	314	U	N3-C2-O2	-5.43	118.40	122.20
7	A2	3616	U	N3-C2-O2	-5.43	118.40	122.20
11	B1	1551	U	C2-N1-C1'	5.43	124.21	117.70
11	B1	1624	U	C2-N1-C1'	5.43	124.21	117.70
43	A4	45	U	C2-N1-C1'	5.43	124.21	117.70
7	A2	3616	U	C2-N1-C1'	5.42	124.21	117.70
7	A2	4993	U	N1-C2-O2	5.42	126.60	122.80
11	B1	106	C	C5-C6-N1	5.42	123.71	121.00
7	A2	3759	C	C2-N1-C1'	5.42	124.76	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B1	526	A	N7-C8-N9	5.41	116.51	113.80
7	A2	480	C	C6-N1-C2	-5.41	118.14	120.30
48	AH	142	ASP	CB-CG-OD1	5.40	123.16	118.30
7	A2	4545	C	N3-C2-O2	-5.40	118.12	121.90
7	A2	1059	C	C5-C6-N1	5.39	123.70	121.00
11	B1	494	C	N1-C2-O2	5.39	122.14	118.90
11	B1	585	C	C2-N1-C1'	5.38	124.72	118.80
7	A2	670	C	N1-C2-O2	5.38	122.13	118.90
7	A2	2373	G	N7-C8-N9	5.38	115.79	113.10
11	B1	943	U	N1-C2-O2	5.38	126.56	122.80
7	A2	4909	G	N3-C4-C5	-5.37	125.92	128.60
7	A2	2793	C	N1-C2-O2	5.37	122.12	118.90
7	A2	2835	C	N3-C2-O2	-5.37	118.14	121.90
7	A2	4824	C	N3-C2-O2	-5.37	118.14	121.90
11	B1	645	C	C6-N1-C2	-5.37	118.15	120.30
7	A2	1190	C	N1-C2-O2	5.36	122.12	118.90
7	A2	3742	C	N3-C2-O2	-5.36	118.15	121.90
11	B1	1624	U	N3-C2-O2	-5.36	118.45	122.20
7	A2	480	C	N3-C2-O2	-5.36	118.15	121.90
42	A3	129	C	C2-N1-C1'	5.36	124.69	118.80
11	B1	1834	A	C4-N9-C1'	5.36	135.94	126.30
7	A2	959	C	N3-C2-O2	-5.35	118.15	121.90
11	B1	1315	U	C5-C6-N1	5.35	125.38	122.70
7	A2	1930	U	C2-N1-C1'	5.35	124.12	117.70
11	B1	331	C	C6-N1-C2	-5.34	118.16	120.30
7	A2	234	G	N3-C2-N2	-5.33	116.17	119.90
7	A2	2499	C	C6-N1-C2	-5.33	118.17	120.30
11	B1	1398	G	C2-N3-C4	5.33	114.57	111.90
7	A2	1713	C	C2-N1-C1'	5.33	124.66	118.80
7	A2	703	C	C6-N1-C2	-5.33	118.17	120.30
7	A2	2649	C	N1-C2-O2	5.32	122.09	118.90
11	B1	1467	C	C2-N1-C1'	5.32	124.65	118.80
7	A2	150	G	C4-N9-C1'	5.32	133.41	126.50
7	A2	1176	C	C5-C6-N1	5.32	123.66	121.00
11	B1	943	U	N3-C2-O2	-5.31	118.48	122.20
11	B1	1237	C	C5-C6-N1	5.31	123.66	121.00
7	A2	1163	C	N1-C2-O2	5.31	122.09	118.90
7	A2	2751	C	N1-C2-O2	5.31	122.09	118.90
7	A2	3749	U	N1-C2-O2	5.31	126.52	122.80
7	A2	4993	U	N3-C2-O2	-5.31	118.48	122.20
47	AG	83	PHE	C-N-CA	5.31	134.97	121.70
7	A2	1580	C	N1-C2-O2	5.31	122.08	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A2	3608	U	N1-C2-O2	5.30	126.51	122.80
7	A2	4364	C	N1-C2-O2	5.30	122.08	118.90
7	A2	1966	G	N3-C4-C5	-5.30	125.95	128.60
7	A2	2799	C	N3-C2-O2	-5.30	118.19	121.90
7	A2	2473	U	C2-N1-C1'	5.29	124.05	117.70
7	A2	4088	C	C6-N1-C2	-5.29	118.18	120.30
43	A4	47	G	N3-C4-N9	5.29	129.17	126.00
11	B1	950	C	C2-N1-C1'	5.29	124.62	118.80
7	A2	2325	C	N3-C2-O2	-5.28	118.20	121.90
7	A2	1966	G	C8-N9-C1'	-5.28	120.14	127.00
7	A2	4191	U	N1-C2-O2	5.28	126.49	122.80
11	B1	338	G	N3-C4-C5	5.28	131.24	128.60
7	A2	2511	C	N1-C2-O2	5.27	122.06	118.90
7	A2	5008	C	N1-C2-O2	5.27	122.06	118.90
11	B1	1038	U	N3-C2-O2	-5.27	118.51	122.20
11	B1	1591	C	C6-N1-C2	-5.27	118.19	120.30
50	AJ	53	ALA	C-N-CA	5.27	134.87	121.70
7	A2	2611	U	N1-C2-O2	5.27	126.49	122.80
7	A2	959	C	P-O3'-C3'	5.26	126.02	119.70
7	A2	2727	C	C6-N1-C1'	-5.26	114.48	120.80
11	B1	943	U	C5-C6-N1	5.26	125.33	122.70
7	A2	4909	G	N1-C2-N2	-5.26	111.47	116.20
11	B1	1852	C	C6-N1-C2	-5.26	118.19	120.30
7	A2	493	G	C8-N9-C1'	-5.26	120.16	127.00
42	A3	126	C	N1-C2-O2	5.26	122.05	118.90
11	B1	1139	C	O4'-C1'-N1	5.25	112.40	108.20
7	A2	1895	C	C6-N1-C2	-5.25	118.20	120.30
11	B1	89	C	N1-C2-O2	5.25	122.05	118.90
11	B1	100	U	C2-N1-C1'	5.25	124.00	117.70
11	B1	814	U	N3-C2-O2	-5.25	118.53	122.20
11	B1	1753	C	N1-C2-O2	5.25	122.05	118.90
11	B1	749	U	N3-C2-O2	-5.24	118.53	122.20
56	AQ	48	LEU	CA-CB-CG	5.23	127.34	115.30
8	Bv	56	C	N1-C2-O2	5.23	122.04	118.90
11	B1	1117	C	C5-C6-N1	5.23	123.61	121.00
7	A2	4069	G	C8-N9-C1'	-5.21	120.22	127.00
30	BI	133	GLU	CA-CB-CG	5.21	124.87	113.40
11	B1	1750	C	C5-C6-N1	5.21	123.61	121.00
7	A2	384	C	C6-N1-C2	-5.21	118.22	120.30
7	A2	4644	U	N3-C2-O2	-5.21	118.55	122.20
84	Aq	28	LEU	CA-CB-CG	5.21	127.28	115.30
7	A2	205	A	C2-N3-C4	5.21	113.20	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A2	4255	U	N3-C2-O2	-5.21	118.56	122.20
7	A2	1789	C	C2-N1-C1'	5.20	124.52	118.80
42	A3	129	C	N1-C2-O2	5.20	122.02	118.90
11	B1	824	C	N1-C2-O2	5.20	122.02	118.90
42	A3	57	C	N1-C2-O2	5.20	122.02	118.90
42	A3	116	C	C6-N1-C2	-5.20	118.22	120.30
7	A2	1614	A	C2-N3-C4	5.19	113.19	110.60
42	A3	96	C	N1-C2-O2	5.19	122.01	118.90
7	A2	3608	U	N3-C2-O2	-5.19	118.57	122.20
11	B1	1691	U	N3-C2-O2	-5.19	118.57	122.20
7	A2	2389	C	N1-C2-O2	5.18	122.01	118.90
11	B1	118	C	C6-N1-C2	-5.18	118.23	120.30
42	A3	57	C	N3-C2-O2	-5.18	118.27	121.90
7	A2	129	C	N1-C2-O2	5.18	122.01	118.90
7	A2	4856	G	C4-N9-C1'	5.18	133.24	126.50
7	A2	703	C	C2-N1-C1'	5.18	124.50	118.80
7	A2	3911	U	N1-C2-O2	5.18	126.42	122.80
43	A4	24	C	N3-C2-O2	-5.17	118.28	121.90
7	A2	1910	A	C4-N9-C1'	5.17	135.61	126.30
7	A2	1280	U	C2-N1-C1'	5.17	123.91	117.70
7	A2	1589	C	N3-C2-O2	-5.17	118.28	121.90
11	B1	1811	C	C2-N1-C1'	5.17	124.49	118.80
43	A4	24	C	C6-N1-C2	-5.17	118.23	120.30
7	A2	4368	U	N1-C2-O2	5.17	126.42	122.80
7	A2	131	C	C6-N1-C2	-5.17	118.23	120.30
7	A2	4824	C	C6-N1-C2	-5.17	118.23	120.30
43	A4	78	C	C6-N1-C2	-5.16	118.24	120.30
7	A2	43	U	N1-C2-O2	5.16	126.41	122.80
11	B1	526	A	C8-N9-C4	-5.16	103.74	105.80
7	A2	4545	C	C2-N1-C1'	5.15	124.47	118.80
7	A2	2571	U	N3-C2-O2	-5.15	118.59	122.20
11	B1	741	C	N1-C2-O2	5.15	121.99	118.90
7	A2	4406	C	C2-N1-C1'	5.15	124.46	118.80
7	A2	4101	C	C2-N1-C1'	5.14	124.46	118.80
7	A2	2325	C	C2-N1-C1'	5.14	124.46	118.80
11	B1	314	U	N1-C2-O2	5.14	126.40	122.80
43	A4	67	C	C6-N1-C2	-5.14	118.24	120.30
7	A2	2260	U	C2-N1-C1'	5.14	123.87	117.70
7	A2	4875	C	N1-C2-O2	5.14	121.98	118.90
7	A2	4519	U	N1-C2-O2	5.14	126.39	122.80
7	A2	1653	U	N1-C2-O2	5.13	126.39	122.80
7	A2	1350	C	N1-C2-O2	5.13	121.98	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A2	959	C	C6-N1-C2	-5.12	118.25	120.30
7	A2	1440	C	C5-C6-N1	5.12	123.56	121.00
11	B1	1315	U	C6-N1-C1'	-5.12	114.03	121.20
7	A2	3853	C	C2-N1-C1'	5.12	124.43	118.80
11	B1	89	C	C6-N1-C2	-5.12	118.25	120.30
7	A2	4721	C	C2-N1-C1'	5.11	124.42	118.80
7	A2	4368	U	N3-C2-O2	-5.11	118.62	122.20
7	A2	163	C	C6-N1-C2	-5.11	118.26	120.30
11	B1	89	C	N3-C2-O2	-5.10	118.33	121.90
7	A2	275	U	N3-C2-O2	-5.10	118.63	122.20
11	B1	746	C	N1-C2-O2	5.10	121.96	118.90
11	B1	1753	C	C6-N1-C2	-5.10	118.26	120.30
11	B1	1852	C	C5-C6-N1	5.10	123.55	121.00
7	A2	3880	C	C5-C6-N1	5.10	123.55	121.00
7	A2	219	C	O4'-C1'-N1	5.10	112.28	108.20
11	B1	814	U	N1-C2-O2	5.10	126.37	122.80
11	B1	570	C	C5-C6-N1	5.10	123.55	121.00
11	B1	806	U	N3-C2-O2	-5.10	118.63	122.20
11	B1	796	G	N1-C6-O6	-5.09	116.84	119.90
7	A2	1789	C	N1-C2-O2	5.09	121.96	118.90
84	Aq	62	LEU	CA-CB-CG	5.09	127.01	115.30
7	A2	2469	U	N1-C2-O2	5.09	126.36	122.80
7	A2	4169	C	C2-N1-C1'	5.09	124.40	118.80
11	B1	1120	U	C2-N1-C1'	5.09	123.81	117.70
7	A2	2403	G	C8-N9-C4	-5.08	104.37	106.40
7	A2	1274	G	C4-N9-C1'	5.08	133.11	126.50
11	B1	842	C	C2-N1-C1'	5.08	124.39	118.80
7	A2	2478	C	N1-C2-O2	5.07	121.94	118.90
11	B1	1317	C	N1-C2-O2	5.07	121.94	118.90
7	A2	205	A	N3-C4-N9	5.06	131.45	127.40
7	A2	1576	C	C5-C6-N1	5.06	123.53	121.00
7	A2	1702	C	N1-C2-O2	5.06	121.94	118.90
7	A2	1917	C	N1-C2-O2	5.05	121.93	118.90
11	B1	1467	C	N1-C2-O2	5.05	121.93	118.90
7	A2	43	U	N3-C2-O2	-5.05	118.67	122.20
7	A2	4069	G	N3-C4-N9	5.04	129.03	126.00
7	A2	3890	C	N1-C2-O2	5.04	121.92	118.90
7	A2	3749	U	N3-C2-O2	-5.04	118.67	122.20
7	A2	3890	C	C5-C6-N1	5.04	123.52	121.00
7	A2	1292	C	C5-C6-N1	5.03	123.52	121.00
7	A2	2800	U	N3-C2-O2	-5.03	118.68	122.20
7	A2	2478	C	N3-C2-O2	-5.03	118.38	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B1	632	C	C2-N1-C1'	5.03	124.33	118.80
16	BP	50	ARG	CA-CB-CG	5.02	124.45	113.40
7	A2	219	C	C5-C6-N1	5.02	123.51	121.00
7	A2	3882	C	C5-C6-N1	5.02	123.51	121.00
11	B1	1398	G	C8-N9-C1'	-5.02	120.47	127.00
33	BN	75	LEU	CA-CB-CG	5.02	126.84	115.30
11	B1	4	C	N1-C2-O2	5.02	121.91	118.90
42	A3	116	C	C5-C6-N1	5.01	123.51	121.00
7	A2	4644	U	N1-C2-O2	5.01	126.31	122.80
7	A2	4721	C	N1-C2-O2	5.01	121.91	118.90
11	B1	815	U	N3-C2-O2	-5.01	118.69	122.20
7	A2	4880	C	N1-C2-O2	5.01	121.90	118.90
7	A2	1874	C	N1-C2-O2	5.00	121.90	118.90
7	A2	3762	C	C2-N1-C1'	5.00	124.30	118.80
7	A2	4670	A	C2-N3-C4	5.00	113.10	110.60
42	A3	116	C	N1-C2-O2	5.00	121.90	118.90
7	A2	1910	A	N3-C4-C5	-5.00	123.30	126.80

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	AC	150	LEU	Peptide
5	AC	51	PRO	Peptide
5	AC	71	ARG	Peptide
45	AE	129	GLY	Peptide
45	AE	130	LYS	Peptide
45	AE	135	GLN	Peptide
48	AH	116	ASN	Peptide
48	AH	4	ILE	Peptide
48	AH	60	TRP	Peptide
49	AI	188	LYS	Peptide
50	AJ	53	ALA	Peptide
85	AK	108	PRO	Peptide
85	AK	149	ARG	Peptide
56	AQ	13	VAL	Peptide
56	AQ	163	THR	Peptide
57	AR	113	LYS	Peptide
71	Af	106	TYR	Peptide
73	Ah	86	LYS	Peptide
84	Aq	29	ALA	Peptide
84	Aq	30	PRO	Peptide

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Mol	Chain	Res	Type	Group
82	At	27	THR	Peptide
2	BA	207	PRO	Peptide
27	BE	92	ILE	Peptide
30	BI	159	SER	Peptide
31	BJ	136	ARG	Peptide
31	BJ	137	VAL	Peptide
17	BQ	13	PHE	Peptide
22	BZ	41	ARG	Peptide
23	Bc	32	VAL	Peptide
86	Ct	157	MET	Peptide
86	Ct	333	LYS	Peptide
86	Ct	463	ASP	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	250/252 (99%)	230 (92%)	20 (8%)	0	100	100
2	BA	213/215 (99%)	197 (92%)	16 (8%)	0	100	100
3	AB	392/394 (100%)	354 (90%)	38 (10%)	0	100	100
4	BB	210/212 (99%)	181 (86%)	29 (14%)	0	100	100
5	AC	361/363 (99%)	325 (90%)	33 (9%)	3 (1%)	19	59
6	BC	220/222 (99%)	207 (94%)	13 (6%)	0	100	100
12	BD	218/220 (99%)	205 (94%)	13 (6%)	0	100	100
13	BF	188/190 (99%)	172 (92%)	16 (8%)	0	100	100
14	BK	96/98 (98%)	80 (83%)	15 (16%)	1 (1%)	15	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	BM	118/120 (98%)	110 (93%)	8 (7%)	0	100	100
16	BP	118/120 (98%)	102 (86%)	15 (13%)	1 (1%)	19	59
17	BQ	137/139 (99%)	128 (93%)	9 (7%)	0	100	100
18	BR	123/125 (98%)	111 (90%)	12 (10%)	0	100	100
19	BS	137/139 (99%)	122 (89%)	15 (11%)	0	100	100
20	BT	141/143 (99%)	127 (90%)	13 (9%)	1 (1%)	22	61
21	BU	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
22	BZ	84/86 (98%)	73 (87%)	11 (13%)	0	100	100
23	Bc	60/62 (97%)	53 (88%)	5 (8%)	2 (3%)	4	31
24	Bd	49/51 (96%)	45 (92%)	4 (8%)	0	100	100
25	Bf	71/73 (97%)	63 (89%)	8 (11%)	0	100	100
26	Bg	312/314 (99%)	283 (91%)	29 (9%)	0	100	100
27	BE	255/257 (99%)	237 (93%)	16 (6%)	2 (1%)	19	59
28	BG	230/232 (99%)	215 (94%)	15 (6%)	0	100	100
29	BH	181/183 (99%)	166 (92%)	15 (8%)	0	100	100
30	BI	205/207 (99%)	176 (86%)	27 (13%)	2 (1%)	15	55
31	BJ	177/179 (99%)	154 (87%)	21 (12%)	2 (1%)	14	53
32	BL	151/153 (99%)	136 (90%)	14 (9%)	1 (1%)	22	61
33	BN	147/149 (99%)	133 (90%)	14 (10%)	0	100	100
34	BO	134/136 (98%)	122 (91%)	12 (9%)	0	100	100
35	BV	79/81 (98%)	75 (95%)	4 (5%)	0	100	100
36	BW	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
37	BX	139/141 (99%)	124 (89%)	15 (11%)	0	100	100
38	BY	123/125 (98%)	109 (89%)	14 (11%)	0	100	100
39	Ba	95/97 (98%)	89 (94%)	6 (6%)	0	100	100
40	Bb	78/80 (98%)	71 (91%)	7 (9%)	0	100	100
41	Be	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
44	AD	292/294 (99%)	270 (92%)	22 (8%)	0	100	100
45	AE	192/194 (99%)	159 (83%)	32 (17%)	1 (0%)	29	68
46	AF	232/234 (99%)	215 (93%)	17 (7%)	0	100	100
47	AG	232/234 (99%)	217 (94%)	15 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	AH	189/191 (99%)	175 (93%)	14 (7%)	0	100	100
49	AI	204/208 (98%)	187 (92%)	17 (8%)	0	100	100
50	AJ	167/169 (99%)	149 (89%)	16 (10%)	2 (1%)	13	51
51	AL	203/205 (99%)	170 (84%)	32 (16%)	1 (0%)	29	68
52	AM	137/139 (99%)	127 (93%)	10 (7%)	0	100	100
53	AN	201/203 (99%)	184 (92%)	16 (8%)	1 (0%)	29	68
54	AO	193/195 (99%)	185 (96%)	8 (4%)	0	100	100
55	AP	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
56	AQ	185/187 (99%)	160 (86%)	23 (12%)	2 (1%)	14	53
57	AR	179/181 (99%)	167 (93%)	12 (7%)	0	100	100
58	AS	173/175 (99%)	162 (94%)	11 (6%)	0	100	100
59	AT	155/157 (99%)	139 (90%)	14 (9%)	2 (1%)	12	50
60	AU	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
61	AV	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
62	AW	119/121 (98%)	105 (88%)	14 (12%)	0	100	100
63	AX	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
64	AY	125/127 (98%)	120 (96%)	5 (4%)	0	100	100
65	AZ	132/134 (98%)	117 (89%)	15 (11%)	0	100	100
66	Aa	145/147 (99%)	128 (88%)	17 (12%)	0	100	100
67	Ab	66/68 (97%)	55 (83%)	11 (17%)	0	100	100
68	Ac	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
69	Ad	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
70	Ae	127/129 (98%)	115 (91%)	12 (9%)	0	100	100
71	Af	107/109 (98%)	93 (87%)	12 (11%)	2 (2%)	8	42
72	Ag	112/114 (98%)	101 (90%)	11 (10%)	0	100	100
73	Ah	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
74	Ai	95/97 (98%)	87 (92%)	8 (8%)	0	100	100
75	Aj	82/84 (98%)	75 (92%)	7 (8%)	0	100	100
76	Ak	67/69 (97%)	63 (94%)	4 (6%)	0	100	100
77	Al	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
78	Am	48/50 (96%)	44 (92%)	4 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
79	An	23/25 (92%)	23 (100%)	0	0	100	100
80	Ao	103/105 (98%)	95 (92%)	8 (8%)	0	100	100
81	Ap	89/91 (98%)	81 (91%)	8 (9%)	0	100	100
82	At	120/122 (98%)	106 (88%)	14 (12%)	0	100	100
83	Au	215/217 (99%)	194 (90%)	21 (10%)	0	100	100
84	Aq	149/151 (99%)	119 (80%)	30 (20%)	0	100	100
85	AK	200/202 (99%)	178 (89%)	21 (10%)	1 (0%)	29	68
86	Ct	850/853 (100%)	762 (90%)	87 (10%)	1 (0%)	51	83
All	All	12538/12699 (99%)	11394 (91%)	1116 (9%)	28 (0%)	50	79

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	BE	93	GLU
31	BJ	138	ARG
71	Af	107	PRO
5	AC	51	PRO
16	BP	51	ARG
51	AL	78	LEU
71	Af	106	TYR
85	AK	150	GLY
20	BT	31	PRO
23	Bc	33	GLU
30	BI	159	SER
5	AC	52	TYR
14	BK	41	PRO
27	BE	150	PRO
30	BI	160	SER
32	BL	14	PRO
50	AJ	53	ALA
56	AQ	161	SER
53	AN	95	ALA
56	AQ	12	LYS
45	AE	136	HIS
50	AJ	54	ARG
59	AT	18	PRO
59	AT	53	PRO
31	BJ	123	ILE
86	Ct	464	VAL

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Mol	Chain	Res	Type
5	AC	151	PRO
23	Bc	32	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	194/194 (100%)	193 (100%)	1 (0%)	88	95
2	BA	180/180 (100%)	179 (99%)	1 (1%)	86	94
3	AB	343/343 (100%)	341 (99%)	2 (1%)	86	94
4	BB	193/193 (100%)	191 (99%)	2 (1%)	76	88
5	AC	302/302 (100%)	298 (99%)	4 (1%)	69	86
6	BC	188/188 (100%)	187 (100%)	1 (0%)	88	95
12	BD	183/183 (100%)	182 (100%)	1 (0%)	88	95
13	BF	160/160 (100%)	160 (100%)	0	100	100
14	BK	89/89 (100%)	88 (99%)	1 (1%)	73	88
15	BM	102/102 (100%)	102 (100%)	0	100	100
16	BP	109/109 (100%)	108 (99%)	1 (1%)	78	90
17	BQ	115/115 (100%)	115 (100%)	0	100	100
18	BR	113/113 (100%)	113 (100%)	0	100	100
19	BS	121/121 (100%)	116 (96%)	5 (4%)	30	64
20	BT	113/113 (100%)	112 (99%)	1 (1%)	78	90
21	BU	90/90 (100%)	90 (100%)	0	100	100
22	BZ	75/75 (100%)	74 (99%)	1 (1%)	69	86
23	Bc	55/55 (100%)	55 (100%)	0	100	100
24	Bd	45/45 (100%)	45 (100%)	0	100	100
25	Bf	66/66 (100%)	66 (100%)	0	100	100
26	Bg	272/272 (100%)	271 (100%)	1 (0%)	91	97
27	BE	220/220 (100%)	216 (98%)	4 (2%)	59	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	BG	202/202 (100%)	200 (99%)	2 (1%)	76	88
29	BH	164/164 (100%)	164 (100%)	0	100	100
30	BI	179/179 (100%)	179 (100%)	0	100	100
31	BJ	160/160 (100%)	159 (99%)	1 (1%)	86	94
32	BL	138/138 (100%)	137 (99%)	1 (1%)	84	93
33	BN	130/130 (100%)	129 (99%)	1 (1%)	81	91
34	BO	106/106 (100%)	105 (99%)	1 (1%)	78	90
35	BV	65/65 (100%)	63 (97%)	2 (3%)	40	71
36	BW	112/112 (100%)	110 (98%)	2 (2%)	59	81
37	BX	113/113 (100%)	112 (99%)	1 (1%)	78	90
38	BY	107/107 (100%)	106 (99%)	1 (1%)	78	90
39	Ba	84/84 (100%)	83 (99%)	1 (1%)	71	87
40	Bb	72/72 (100%)	72 (100%)	0	100	100
41	Be	44/44 (100%)	41 (93%)	3 (7%)	16	50
44	AD	248/248 (100%)	244 (98%)	4 (2%)	62	83
45	AE	174/174 (100%)	172 (99%)	2 (1%)	73	88
46	AF	203/203 (100%)	200 (98%)	3 (2%)	65	84
47	AG	199/199 (100%)	199 (100%)	0	100	100
48	AH	170/170 (100%)	170 (100%)	0	100	100
49	AI	178/178 (100%)	177 (99%)	1 (1%)	86	94
50	AJ	142/142 (100%)	142 (100%)	0	100	100
51	AL	171/171 (100%)	168 (98%)	3 (2%)	59	81
52	AM	118/118 (100%)	116 (98%)	2 (2%)	60	82
53	AN	171/171 (100%)	170 (99%)	1 (1%)	86	94
54	AO	168/168 (100%)	165 (98%)	3 (2%)	59	81
55	AP	134/134 (100%)	133 (99%)	1 (1%)	84	93
56	AQ	164/164 (100%)	164 (100%)	0	100	100
57	AR	160/160 (100%)	160 (100%)	0	100	100
58	AS	156/156 (100%)	156 (100%)	0	100	100
59	AT	138/138 (100%)	138 (100%)	0	100	100
60	AU	89/89 (100%)	87 (98%)	2 (2%)	52	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
61	AV	100/100 (100%)	100 (100%)	0	100	100
62	AW	100/100 (100%)	98 (98%)	2 (2%)	55	79
63	AX	105/105 (100%)	105 (100%)	0	100	100
64	AY	119/119 (100%)	118 (99%)	1 (1%)	81	91
65	AZ	117/117 (100%)	116 (99%)	1 (1%)	78	90
66	Aa	120/120 (100%)	119 (99%)	1 (1%)	81	91
67	Ab	58/58 (100%)	56 (97%)	2 (3%)	37	69
68	Ac	88/88 (100%)	88 (100%)	0	100	100
69	Ad	97/97 (100%)	97 (100%)	0	100	100
70	Ae	115/115 (100%)	115 (100%)	0	100	100
71	Af	88/88 (100%)	88 (100%)	0	100	100
72	Ag	98/98 (100%)	98 (100%)	0	100	100
73	Ah	109/109 (100%)	106 (97%)	3 (3%)	43	72
74	Ai	83/83 (100%)	83 (100%)	0	100	100
75	Aj	71/71 (100%)	69 (97%)	2 (3%)	43	72
76	Ak	64/64 (100%)	63 (98%)	1 (2%)	62	83
77	Al	47/47 (100%)	44 (94%)	3 (6%)	17	52
78	Am	46/46 (100%)	45 (98%)	1 (2%)	52	77
79	An	24/24 (100%)	24 (100%)	0	100	100
80	Ao	93/93 (100%)	91 (98%)	2 (2%)	52	77
81	Ap	74/74 (100%)	73 (99%)	1 (1%)	67	85
82	At	106/106 (100%)	103 (97%)	3 (3%)	43	72
83	Au	196/196 (100%)	189 (96%)	7 (4%)	35	67
84	Aq	124/124 (100%)	122 (98%)	2 (2%)	62	83
85	AK	170/170 (100%)	170 (100%)	0	100	100
86	Ct	725/725 (100%)	720 (99%)	5 (1%)	84	93
All	All	10924/10924 (100%)	10823 (99%)	101 (1%)	79	90

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	193	ARG
2	BA	149	ASN

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Mol	Chain	Res	Type
3	AB	24	ARG
3	AB	294	LYS
4	BB	76	ASN
4	BB	174	ARG
5	AC	38	ASN
5	AC	48	ASN
5	AC	95	MET
5	AC	215	ASN
6	BC	134	ASN
12	BD	64	ARG
14	BK	96	ARG
16	BP	52	LYS
19	BS	17	ASN
19	BS	23	ARG
19	BS	66	ARG
19	BS	73	ASN
19	BS	78	LYS
20	BT	62	ARG
22	BZ	112	ASN
26	Bg	133	ASN
27	BE	30	ARG
27	BE	75	LYS
27	BE	197	ASN
27	BE	230	ASN
28	BG	85	ARG
28	BG	202	ASN
31	BJ	30	LYS
32	BL	101	ARG
33	BN	104	ARG
34	BO	128	ARG
35	BV	41	LYS
35	BV	81	LYS
36	BW	5	ASN
36	BW	15	ASN
37	BX	127	ASN
38	BY	15	ASN
39	Ba	15	ARG
41	Be	18	LYS
41	Be	35	ARG
41	Be	52	LYS
44	AD	21	ARG
44	AD	41	LYS

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Mol	Chain	Res	Type
44	AD	191	ASN
44	AD	265	ARG
45	AE	223	ARG
45	AE	279	ASN
46	AF	146	ASN
46	AF	161	LYS
46	AF	166	ARG
49	AI	73	ASN
51	AL	63	THR
51	AL	159	ASN
51	AL	175	ASN
52	AM	5	ARG
52	AM	46	ARG
53	AN	38	ARG
54	AO	65	ASN
54	AO	160	ARG
54	AO	184	ASN
55	AP	94	MET
60	AU	50	ASN
60	AU	97	ARG
62	AW	45	ASN
62	AW	73	ARG
64	AY	36	LYS
65	AZ	112	ARG
66	Aa	87	ARG
67	Ab	25	ARG
67	Ab	61	ASN
73	Ah	48	ARG
73	Ah	91	MET
73	Ah	92	ARG
75	Aj	65	ARG
75	Aj	67	LEU
76	Ak	21	LYS
77	Al	20	ASN
77	Al	21	ARG
77	Al	28	ARG
78	Am	120	ASN
80	Ao	3	ASN
80	Ao	98	LYS
81	Ap	84	ARG
82	At	41	ASN
82	At	67	ARG

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Mol	Chain	Res	Type
82	At	83	ASN
83	Au	21	ASN
83	Au	54	ARG
83	Au	74	CYS
83	Au	143	ASN
83	Au	188	ASN
83	Au	197	ASN
83	Au	215	ARG
84	Aq	40	LYS
84	Aq	114	ARG
86	Ct	167	LEU
86	Ct	588	ASN
86	Ct	803	ASN
86	Ct	811	GLN
86	Ct	842	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (141) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	83	HIS
1	AA	97	ASN
1	AA	132	ASN
1	AA	205	ASN
1	AA	209	HIS
1	AA	218	HIS
2	BA	111	GLN
2	BA	149	ASN
3	AB	167	GLN
3	AB	179	HIS
3	AB	302	ASN
3	AB	322	HIS
3	AB	380	GLN
4	BB	76	ASN
5	AC	41	HIS
5	AC	48	ASN
5	AC	50	GLN
5	AC	198	ASN
5	AC	215	ASN
5	AC	347	HIS
6	BC	113	GLN
6	BC	134	ASN
6	BC	272	HIS

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Mol	Chain	Res	Type
12	BD	179	GLN
13	BF	65	GLN
13	BF	82	ASN
13	BF	95	HIS
13	BF	186	ASN
15	BM	55	ASN
16	BP	41	GLN
16	BP	103	ASN
17	BQ	8	GLN
17	BQ	24	HIS
17	BQ	80	GLN
17	BQ	86	GLN
18	BR	62	GLN
18	BR	74	GLN
19	BS	10	GLN
19	BS	17	ASN
19	BS	19	ASN
19	BS	105	ASN
20	BT	11	GLN
22	BZ	89	GLN
22	BZ	106	GLN
22	BZ	112	ASN
23	Bc	24	GLN
23	Bc	26	GLN
26	Bg	133	ASN
26	Bg	159	ASN
26	Bg	226	HIS
27	BE	179	ASN
27	BE	197	ASN
27	BE	230	ASN
28	BG	56	ASN
28	BG	70	HIS
28	BG	81	HIS
28	BG	202	ASN
28	BG	227	GLN
30	BI	165	GLN
31	BJ	134	HIS
31	BJ	140	GLN
31	BJ	156	HIS
31	BJ	177	ASN
32	BL	11	GLN
32	BL	83	GLN

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Mol	Chain	Res	Type
33	BN	5	HIS
34	BO	103	ASN
36	BW	5	ASN
36	BW	16	ASN
36	BW	98	GLN
37	BX	61	GLN
37	BX	127	ASN
38	BY	15	ASN
38	BY	89	HIS
44	AD	111	ASN
44	AD	191	ASN
44	AD	195	HIS
44	AD	222	GLN
45	AE	191	GLN
45	AE	279	ASN
46	AF	146	ASN
46	AF	163	ASN
49	AI	14	ASN
49	AI	51	HIS
51	AL	149	GLN
51	AL	159	ASN
51	AL	175	ASN
52	AM	33	GLN
52	AM	78	GLN
53	AN	37	HIS
53	AN	86	HIS
53	AN	87	HIS
53	AN	199	GLN
54	AO	65	ASN
54	AO	184	ASN
55	AP	40	HIS
55	AP	80	GLN
55	AP	118	GLN
57	AR	39	GLN
57	AR	178	GLN
58	AS	66	GLN
60	AU	50	ASN
61	AV	101	ASN
62	AW	45	ASN
64	AY	56	GLN
64	AY	96	HIS
65	AZ	40	HIS

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Mol	Chain	Res	Type
66	Aa	40	HIS
66	Aa	60	HIS
66	Aa	74	ASN
67	Ab	12	GLN
67	Ab	42	ASN
69	Ad	28	ASN
70	Ae	52	GLN
70	Ae	124	ASN
71	Af	21	GLN
71	Af	99	HIS
72	Ag	73	HIS
73	Ah	63	GLN
77	Al	20	ASN
77	Al	43	HIS
78	Am	120	ASN
80	Ao	3	ASN
80	Ao	45	GLN
82	At	36	ASN
83	Au	21	ASN
83	Au	140	HIS
83	Au	143	ASN
83	Au	171	HIS
83	Au	188	ASN
83	Au	197	ASN
84	Aq	111	ASN
85	AK	72	ASN
86	Ct	158	ASN
86	Ct	227	GLN
86	Ct	492	HIS
86	Ct	588	ASN
86	Ct	696	ASN
86	Ct	705	HIS
86	Ct	803	ASN
86	Ct	811	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	Bw	75/76 (98%)	12 (16%)	0
11	B1	1701/1708 (99%)	339 (19%)	3 (0%)
42	A3	156/157 (99%)	35 (22%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
43	A4	118/119 (99%)	18 (15%)	0
7	A2	3599/3612 (99%)	720 (20%)	7 (0%)
8	Bv	75/76 (98%)	12 (16%)	0
9	Bx	10/11 (90%)	3 (30%)	0
All	All	5734/5759 (99%)	1139 (19%)	10 (0%)

All (1139) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	A2	8	U
7	A2	9	C
7	A2	19	G
7	A2	25	A
7	A2	32	G
7	A2	39	A
7	A2	40	G
7	A2	42	A
7	A2	48	G
7	A2	59	A
7	A2	65	A
7	A2	71	C
7	A2	72	C
7	A2	74	G
7	A2	76	A
7	A2	84	A
7	A2	91	G
7	A2	101	A
7	A2	107	G
7	A2	108	A
7	A2	110	C
7	A2	116	G
7	A2	119	G
7	A2	120	A
7	A2	131	C
7	A2	132	G
7	A2	134	G
7	A2	135	G
7	A2	143	G
7	A2	149	U
7	A2	154	U
7	A2	155	A
7	A2	156	C

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Mol	Chain	Res	Type
7	A2	157	G
7	A2	169	C
7	A2	171	C
7	A2	173	G
7	A2	176	G
7	A2	180	C
7	A2	181	U
7	A2	182	C
7	A2	183	G
7	A2	184	U
7	A2	185	G
7	A2	196	G
7	A2	197	U
7	A2	198	C
7	A2	201	U
7	A2	206	U
7	A2	212	C
7	A2	213	C
7	A2	214	C
7	A2	215	A
7	A2	228	U
7	A2	229	G
7	A2	230	U
7	A2	231	G
7	A2	234	G
7	A2	236	C
7	A2	250	G
7	A2	253	G
7	A2	255	G
7	A2	256	C
7	A2	260	C
7	A2	261	G
7	A2	275	U
7	A2	289	A
7	A2	291	U
7	A2	300	A
7	A2	309	G
7	A2	310	U
7	A2	311	A
7	A2	323	A
7	A2	334	C
7	A2	338	A

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Mol	Chain	Res	Type
7	A2	343	A
7	A2	357	A
7	A2	367	G
7	A2	370	A
7	A2	375	U
7	A2	380	A
7	A2	381	G
7	A2	390	A
7	A2	393	G
7	A2	403	G
7	A2	404	A
7	A2	406	G
7	A2	407	G
7	A2	425	G
7	A2	426	U
7	A2	427	A
7	A2	434	U
7	A2	446	A
7	A2	447	G
7	A2	448	U
7	A2	449	C
7	A2	450	C
7	A2	461	U
7	A2	463	C
7	A2	479	C
7	A2	487	G
7	A2	489	C
7	A2	492	C
7	A2	494	G
7	A2	496	C
7	A2	497	C
7	A2	498	G
7	A2	504	U
7	A2	505	C
7	A2	508	U
7	A2	509	C
7	A2	513	C
7	A2	633	U
7	A2	634	C
7	A2	635	G
7	A2	647	U
7	A2	649	C

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Mol	Chain	Res	Type
7	A2	658	G
7	A2	661	G
7	A2	674	C
7	A2	677	G
7	A2	678	C
7	A2	679	G
7	A2	680	C
7	A2	691	G
7	A2	695	C
7	A2	698	C
7	A2	714	A
7	A2	719	U
7	A2	720	G
7	A2	721	G
7	A2	737	A
7	A2	738	A
7	A2	739	G
7	A2	901	U
7	A2	902	A
7	A2	904	A
7	A2	905	G
7	A2	906	C
7	A2	907	C
7	A2	914	G
7	A2	917	G
7	A2	918	C
7	A2	919	A
7	A2	921	C
7	A2	923	C
7	A2	925	C
7	A2	927	C
7	A2	929	G
7	A2	931	A
7	A2	932	U
7	A2	933	C
7	A2	934	C
7	A2	938	G
7	A2	944	G
7	A2	947	A
7	A2	948	G
7	A2	949	C
7	A2	950	G

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Mol	Chain	Res	Type
7	A2	951	A
7	A2	953	A
7	A2	954	C
7	A2	955	C
7	A2	956	C
7	A2	960	G
7	A2	961	C
7	A2	962	C
7	A2	968	C
7	A2	969	U
7	A2	1055	C
7	A2	1065	C
7	A2	1067	C
7	A2	1086	C
7	A2	1087	C
7	A2	1147	G
7	A2	1149	G
7	A2	1150	C
7	A2	1156	G
7	A2	1162	U
7	A2	1163	C
7	A2	1164	C
7	A2	1165	C
7	A2	1180	C
7	A2	1181	G
7	A2	1190	C
7	A2	1192	U
7	A2	1193	C
7	A2	1196	G
7	A2	1201	G
7	A2	1220	C
7	A2	1221	A
7	A2	1222	C
7	A2	1223	G
7	A2	1225	G
7	A2	1226	C
7	A2	1229	G
7	A2	1250	C
7	A2	1251	G
7	A2	1255	C
7	A2	1256	G
7	A2	1259	C

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Mol	Chain	Res	Type
7	A2	1263	C
7	A2	1264	G
7	A2	1265	G
7	A2	1268	U
7	A2	1269	C
7	A2	1271	G
7	A2	1277	A
7	A2	1278	C
7	A2	1284	C
7	A2	1286	A
7	A2	1309	A
7	A2	1336	G
7	A2	1337	A
7	A2	1341	G
7	A2	1343	G
7	A2	1348	C
7	A2	1349	G
7	A2	1351	A
7	A2	1353	G
7	A2	1362	C
7	A2	1364	U
7	A2	1370	A
7	A2	1373	G
7	A2	1374	A
7	A2	1377	G
7	A2	1381	A
7	A2	1391	G
7	A2	1392	C
7	A2	1394	C
7	A2	1403	A
7	A2	1408	G
7	A2	1421	U
7	A2	1424	C
7	A2	1426	A
7	A2	1427	G
7	A2	1428	U
7	A2	1430	C
7	A2	1432	C
7	A2	1440	C
7	A2	1457	G
7	A2	1463	C
7	A2	1464	G

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Mol	Chain	Res	Type
7	A2	1465	C
7	A2	1466	G
7	A2	1468	C
7	A2	1479	A
7	A2	1480	G
7	A2	1483	C
7	A2	1485	A
7	A2	1497	A
7	A2	1499	G
7	A2	1500	A
7	A2	1505	A
7	A2	1507	A
7	A2	1516	A
7	A2	1521	G
7	A2	1525	G
7	A2	1531	G
7	A2	1548	C
7	A2	1556	G
7	A2	1559	G
7	A2	1560	U
7	A2	1573	U
7	A2	1576	C
7	A2	1578	U
7	A2	1583	A
7	A2	1589	C
7	A2	1594	G
7	A2	1595	A
7	A2	1606	G
7	A2	1607	G
7	A2	1613	A
7	A2	1615	G
7	A2	1616	A
7	A2	1620	A
7	A2	1623	G
7	A2	1624	A
7	A2	1632	A
7	A2	1636	G
7	A2	1643	C
7	A2	1652	G
7	A2	1676	C
7	A2	1678	C
7	A2	1679	G

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Mol	Chain	Res	Type
7	A2	1701	A
7	A2	1706	G
7	A2	1711	A
7	A2	1713	C
7	A2	1723	G
7	A2	1728	A
7	A2	1736	U
7	A2	1747	A
7	A2	1748	A
7	A2	1751	G
7	A2	1763	U
7	A2	1769	A
7	A2	1776	A
7	A2	1785	G
7	A2	1786	A
7	A2	1788	G
7	A2	1794	C
7	A2	1797	G
7	A2	1804	U
7	A2	1807	A
7	A2	1814	G
7	A2	1815	U
7	A2	1816	G
7	A2	1818	A
7	A2	1823	G
7	A2	1835	G
7	A2	1836	G
7	A2	1850	G
7	A2	1862	C
7	A2	1863	U
7	A2	1869	A
7	A2	1872	A
7	A2	1873	A
7	A2	1896	C
7	A2	1898	A
7	A2	1902	C
7	A2	1903	G
7	A2	1906	G
7	A2	1910	A
7	A2	1913	A
7	A2	1916	C
7	A2	1928	U

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Mol	Chain	Res	Type
7	A2	1929	G
7	A2	1932	G
7	A2	1938	U
7	A2	1940	U
7	A2	1941	A
7	A2	1942	G
7	A2	1943	A
7	A2	1945	A
7	A2	1955	U
7	A2	1956	G
7	A2	1958	C
7	A2	1961	U
7	A2	1962	G
7	A2	1963	G
7	A2	1964	A
7	A2	1965	A
7	A2	1966	G
7	A2	1967	U
7	A2	1968	C
7	A2	1973	U
7	A2	1978	U
7	A2	1983	A
7	A2	1984	G
7	A2	1989	U
7	A2	1991	A
7	A2	2007	A
7	A2	2015	G
7	A2	2029	U
7	A2	2037	G
7	A2	2043	C
7	A2	2050	A
7	A2	2246	U
7	A2	2268	C
7	A2	2279	A
7	A2	2280	G
7	A2	2282	C
7	A2	2283	U
7	A2	2285	G
7	A2	2292	A
7	A2	2299	G
7	A2	2301	G
7	A2	2308	U

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Mol	Chain	Res	Type
7	A2	2310	G
7	A2	2324	G
7	A2	2327	G
7	A2	2329	U
7	A2	2330	C
7	A2	2339	A
7	A2	2340	G
7	A2	2363	U
7	A2	2373	G
7	A2	2374	A
7	A2	2377	U
7	A2	2389	C
7	A2	2396	A
7	A2	2399	A
7	A2	2400	G
7	A2	2401	C
7	A2	2404	U
7	A2	2426	U
7	A2	2442	G
7	A2	2450	G
7	A2	2467	C
7	A2	2468	C
7	A2	2469	U
7	A2	2482	G
7	A2	2484	C
7	A2	2485	G
7	A2	2490	A
7	A2	2492	A
7	A2	2509	U
7	A2	2524	U
7	A2	2525	G
7	A2	2526	G
7	A2	2532	A
7	A2	2533	U
7	A2	2565	G
7	A2	2566	A
7	A2	2568	C
7	A2	2580	A
7	A2	2584	G
7	A2	2585	G
7	A2	2606	C
7	A2	2617	G

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Mol	Chain	Res	Type
7	A2	2632	C
7	A2	2648	C
7	A2	2665	G
7	A2	2666	U
7	A2	2673	G
7	A2	2675	A
7	A2	2676	A
7	A2	2690	G
7	A2	2691	G
7	A2	2698	C
7	A2	2700	G
7	A2	2705	G
7	A2	2706	C
7	A2	2719	U
7	A2	2720	U
7	A2	2722	A
7	A2	2726	U
7	A2	2733	G
7	A2	2741	G
7	A2	2742	U
7	A2	2745	A
7	A2	2748	U
7	A2	2751	C
7	A2	2766	A
7	A2	2767	U
7	A2	2769	U
7	A2	2773	C
7	A2	2776	C
7	A2	2781	C
7	A2	2785	A
7	A2	2786	A
7	A2	2793	C
7	A2	2804	A
7	A2	2805	U
7	A2	2806	G
7	A2	2808	U
7	A2	2814	A
7	A2	2822	U
7	A2	2839	C
7	A2	2841	G
7	A2	2858	A
7	A2	2859	U

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Mol	Chain	Res	Type
7	A2	2860	A
7	A2	2871	C
7	A2	3572	C
7	A2	3574	G
7	A2	3586	G
7	A2	3587	U
7	A2	3591	G
7	A2	3596	G
7	A2	3597	G
7	A2	3601	A
7	A2	3606	A
7	A2	3614	A
7	A2	3615	U
7	A2	3616	U
7	A2	3619	A
7	A2	3627	A
7	A2	3633	A
7	A2	3643	G
7	A2	3651	U
7	A2	3669	G
7	A2	3671	C
7	A2	3681	G
7	A2	3683	A
7	A2	3685	G
7	A2	3706	G
7	A2	3707	A
7	A2	3724	G
7	A2	3726	G
7	A2	3730	A
7	A2	3731	A
7	A2	3732	C
7	A2	3736	G
7	A2	3737	A
7	A2	3747	G
7	A2	3748	G
7	A2	3751	G
7	A2	3754	A
7	A2	3781	C
7	A2	3782	G
7	A2	3785	U
7	A2	3788	A
7	A2	3789	U

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Mol	Chain	Res	Type
7	A2	3790	G
7	A2	3795	A
7	A2	3798	G
7	A2	3799	A
7	A2	3809	U
7	A2	3811	U
7	A2	3814	C
7	A2	3831	A
7	A2	3838	A
7	A2	3847	A
7	A2	3848	A
7	A2	3850	G
7	A2	3851	G
7	A2	3852	G
7	A2	3860	G
7	A2	3863	U
7	A2	3866	G
7	A2	3872	A
7	A2	3873	A
7	A2	3876	A
7	A2	3878	G
7	A2	3879	A
7	A2	3886	U
7	A2	3887	G
7	A2	3890	C
7	A2	3909	G
7	A2	3925	A
7	A2	3927	G
7	A2	3929	G
7	A2	3935	U
7	A2	3936	A
7	A2	3943	A
7	A2	3944	G
7	A2	4019	U
7	A2	4020	A
7	A2	4023	A
7	A2	4027	C
7	A2	4035	G
7	A2	4046	G
7	A2	4051	G
7	A2	4054	G
7	A2	4058	C

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Mol	Chain	Res	Type
7	A2	4065	G
7	A2	4066	C
7	A2	4067	G
7	A2	4068	A
7	A2	4069	G
7	A2	4070	C
7	A2	4078	G
7	A2	4084	G
7	A2	4086	U
7	A2	4088	C
7	A2	4106	C
7	A2	4109	G
7	A2	4110	C
7	A2	4124	C
7	A2	4125	U
7	A2	4126	C
7	A2	4132	A
7	A2	4135	G
7	A2	4145	G
7	A2	4146	G
7	A2	4153	G
7	A2	4165	A
7	A2	4169	C
7	A2	4174	A
7	A2	4176	A
7	A2	4191	U
7	A2	4195	A
7	A2	4196	A
7	A2	4211	G
7	A2	4213	A
7	A2	4216	G
7	A2	4228	G
7	A2	4230	A
7	A2	4235	A
7	A2	4243	A
7	A2	4250	C
7	A2	4252	U
7	A2	4266	A
7	A2	4267	G
7	A2	4268	U
7	A2	4276	C
7	A2	4285	A

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Mol	Chain	Res	Type
7	A2	4288	G
7	A2	4291	G
7	A2	4292	G
7	A2	4294	C
7	A2	4297	C
7	A2	4311	C
7	A2	4316	U
7	A2	4320	U
7	A2	4333	G
7	A2	4338	A
7	A2	4339	G
7	A2	4340	A
7	A2	4342	A
7	A2	4349	C
7	A2	4355	G
7	A2	4356	A
7	A2	4358	A
7	A2	4360	C
7	A2	4367	G
7	A2	4384	A
7	A2	4388	C
7	A2	4406	C
7	A2	4414	U
7	A2	4426	A
7	A2	4428	C
7	A2	4437	G
7	A2	4450	A
7	A2	4455	U
7	A2	4457	G
7	A2	4459	U
7	A2	4474	U
7	A2	4475	A
7	A2	4480	A
7	A2	4482	G
7	A2	4485	A
7	A2	4486	G
7	A2	4510	A
7	A2	4519	U
7	A2	4522	C
7	A2	4532	G
7	A2	4551	A
7	A2	4552	A

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Mol	Chain	Res	Type
7	A2	4559	U
7	A2	4561	A
7	A2	4570	G
7	A2	4586	A
7	A2	4593	G
7	A2	4598	U
7	A2	4599	G
7	A2	4611	G
7	A2	4614	G
7	A2	4619	U
7	A2	4620	G
7	A2	4621	G
7	A2	4629	C
7	A2	4632	C
7	A2	4640	G
7	A2	4641	G
7	A2	4649	A
7	A2	4653	A
7	A2	4655	C
7	A2	4662	A
7	A2	4671	U
7	A2	4678	C
7	A2	4681	G
7	A2	4690	U
7	A2	4693	G
7	A2	4694	G
7	A2	4696	A
7	A2	4703	C
7	A2	4704	G
7	A2	4714	U
7	A2	4715	U
7	A2	4718	C
7	A2	4720	U
7	A2	4721	C
7	A2	4723	G
7	A2	4726	A
7	A2	4732	U
7	A2	4824	C
7	A2	4827	U
7	A2	4828	G
7	A2	4831	G
7	A2	4832	A

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Mol	Chain	Res	Type
7	A2	4833	G
7	A2	4834	U
7	A2	4838	C
7	A2	4839	U
7	A2	4840	U
7	A2	4841	C
7	A2	4852	A
7	A2	4853	C
7	A2	4854	G
7	A2	4858	C
7	A2	4859	G
7	A2	4864	C
7	A2	4865	G
7	A2	4866	G
7	A2	4867	A
7	A2	4868	A
7	A2	4869	A
7	A2	4870	G
7	A2	4871	G
7	A2	4872	C
7	A2	4880	C
7	A2	4883	U
7	A2	4886	C
7	A2	4895	C
7	A2	4896	A
7	A2	4898	C
7	A2	4899	G
7	A2	4902	C
7	A2	4903	G
7	A2	4907	G
7	A2	4908	U
7	A2	4909	G
7	A2	4924	A
7	A2	4933	G
7	A2	4934	U
7	A2	4936	G
7	A2	4943	U
7	A2	4946	U
7	A2	4947	U
7	A2	4948	C
7	A2	4950	G
7	A2	4957	G

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Mol	Chain	Res	Type
7	A2	4964	U
7	A2	4971	C
7	A2	4975	G
7	A2	4982	C
7	A2	4985	C
7	A2	4998	U
7	A2	5005	C
7	A2	5007	G
7	A2	5008	C
7	A2	5011	U
7	A2	5013	G
7	A2	5016	A
7	A2	5019	A
7	A2	5020	G
7	A2	5028	C
8	Bv	16	U
8	Bv	17	G
8	Bv	18	G
8	Bv	20	U
8	Bv	21	A
8	Bv	22	U
8	Bv	47	U
8	Bv	59	A
8	Bv	61	C
8	Bv	70	A
8	Bv	74	C
8	Bv	76	A
9	Bx	31	A
9	Bx	32	G
9	Bx	33	A
10	Bw	16	U
10	Bw	17	U
10	Bw	18	G
10	Bw	19	G
10	Bw	21	A
10	Bw	26	G
10	Bw	35	A
10	Bw	46	G
10	Bw	47	U
10	Bw	48	C
10	Bw	71	G
10	Bw	76	A

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Mol	Chain	Res	Type
11	B1	4	C
11	B1	25	A
11	B1	33	G
11	B1	41	G
11	B1	42	A
11	B1	44	U
11	B1	46	A
11	B1	49	C
11	B1	67	C
11	B1	68	A
11	B1	71	G
11	B1	72	C
11	B1	73	C
11	B1	76	U
11	B1	77	A
11	B1	103	A
11	B1	113	G
11	B1	114	G
11	B1	115	U
11	B1	125	C
11	B1	126	G
11	B1	143	U
11	B1	146	G
11	B1	155	G
11	B1	158	A
11	B1	161	U
11	B1	162	C
11	B1	170	A
11	B1	171	A
11	B1	172	U
11	B1	175	A
11	B1	178	C
11	B1	183	G
11	B1	213	G
11	B1	217	A
11	B1	220	U
11	B1	228	C
11	B1	230	A
11	B1	231	A
11	B1	236	A
11	B1	238	C
11	B1	284	C

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Mol	Chain	Res	Type
11	B1	286	U
11	B1	291	G
11	B1	292	A
11	B1	293	C
11	B1	305	U
11	B1	306	C
11	B1	313	A
11	B1	314	U
11	B1	319	C
11	B1	320	G
11	B1	324	C
11	B1	325	C
11	B1	327	G
11	B1	328	U
11	B1	329	G
11	B1	332	G
11	B1	333	G
11	B1	338	G
11	B1	339	A
11	B1	351	G
11	B1	364	A
11	B1	368	U
11	B1	369	C
11	B1	370	G
11	B1	371	A
11	B1	385	G
11	B1	386	C
11	B1	400	C
11	B1	407	G
11	B1	408	A
11	B1	409	C
11	B1	417	C
11	B1	426	A
11	B1	428	U
11	B1	448	A
11	B1	449	A
11	B1	450	C
11	B1	463	C
11	B1	464	A
11	B1	465	A
11	B1	466	G
11	B1	471	G

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Mol	Chain	Res	Type
11	B1	472	C
11	B1	474	G
11	B1	476	A
11	B1	482	G
11	B1	487	U
11	B1	489	A
11	B1	492	C
11	B1	493	A
11	B1	496	C
11	B1	501	C
11	B1	508	A
11	B1	523	A
11	B1	525	A
11	B1	533	A
11	B1	534	G
11	B1	535	G
11	B1	536	A
11	B1	541	U
11	B1	542	U
11	B1	544	G
11	B1	545	A
11	B1	546	G
11	B1	547	G
11	B1	548	C
11	B1	553	U
11	B1	554	A
11	B1	555	A
11	B1	558	G
11	B1	560	A
11	B1	567	C
11	B1	570	C
11	B1	574	A
11	B1	576	A
11	B1	590	A
11	B1	591	U
11	B1	592	C
11	B1	594	A
11	B1	604	A
11	B1	608	C
11	B1	614	C
11	B1	617	G
11	B1	620	G

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Mol	Chain	Res	Type
11	B1	621	C
11	B1	628	A
11	B1	629	A
11	B1	634	A
11	B1	643	A
11	B1	644	G
11	B1	645	C
11	B1	655	A
11	B1	660	C
11	B1	662	G
11	B1	663	C
11	B1	668	A
11	B1	669	A
11	B1	672	A
11	B1	673	G
11	B1	684	G
11	B1	687	C
11	B1	688	U
11	B1	689	U
11	B1	690	G
11	B1	738	C
11	B1	741	C
11	B1	742	U
11	B1	744	G
11	B1	746	C
11	B1	748	C
11	B1	750	C
11	B1	797	C
11	B1	798	G
11	B1	799	U
11	B1	800	U
11	B1	801	U
11	B1	806	U
11	B1	811	A
11	B1	827	A
11	B1	833	C
11	B1	837	A
11	B1	839	C
11	B1	841	G
11	B1	842	C
11	B1	847	A
11	B1	859	G

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Mol	Chain	Res	Type
11	B1	865	A
11	B1	869	A
11	B1	870	A
11	B1	874	G
11	B1	888	U
11	B1	890	U
11	B1	913	A
11	B1	914	U
11	B1	917	U
11	B1	918	U
11	B1	919	A
11	B1	920	A
11	B1	928	G
11	B1	929	G
11	B1	933	G
11	B1	943	U
11	B1	956	G
11	B1	971	G
11	B1	975	G
11	B1	985	G
11	B1	990	A
11	B1	1002	U
11	B1	1008	A
11	B1	1015	U
11	B1	1016	U
11	B1	1023	A
11	B1	1027	A
11	B1	1044	G
11	B1	1045	U
11	B1	1053	C
11	B1	1055	A
11	B1	1060	A
11	B1	1061	U
11	B1	1085	C
11	B1	1109	C
11	B1	1110	G
11	B1	1113	A
11	B1	1114	U
11	B1	1115	U
11	B1	1119	A
11	B1	1120	U
11	B1	1121	G

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Mol	Chain	Res	Type
11	B1	1133	A
11	B1	1139	C
11	B1	1140	G
11	B1	1146	C
11	B1	1149	A
11	B1	1170	A
11	B1	1195	A
11	B1	1199	A
11	B1	1207	G
11	B1	1215	C
11	B1	1216	C
11	B1	1221	G
11	B1	1224	G
11	B1	1242	U
11	B1	1251	A
11	B1	1253	A
11	B1	1256	G
11	B1	1257	G
11	B1	1258	A
11	B1	1259	A
11	B1	1261	C
11	B1	1262	C
11	B1	1278	A
11	B1	1284	A
11	B1	1285	G
11	B1	1286	G
11	B1	1287	A
11	B1	1288	U
11	B1	1290	G
11	B1	1301	A
11	B1	1302	G
11	B1	1303	C
11	B1	1321	G
11	B1	1330	G
11	B1	1333	U
11	B1	1341	C
11	B1	1342	U
11	B1	1363	C
11	B1	1371	U
11	B1	1372	U
11	B1	1377	U
11	B1	1378	A

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Mol	Chain	Res	Type
11	B1	1380	C
11	B1	1381	G
11	B1	1395	C
11	B1	1398	G
11	B1	1399	C
11	B1	1404	U
11	B1	1418	C
11	B1	1420	G
11	B1	1421	A
11	B1	1442	U
11	B1	1454	A
11	B1	1455	A
11	B1	1462	U
11	B1	1467	C
11	B1	1476	A
11	B1	1477	U
11	B1	1478	U
11	B1	1489	A
11	B1	1494	U
11	B1	1497	G
11	B1	1498	A
11	B1	1505	U
11	B1	1506	A
11	B1	1507	G
11	B1	1519	U
11	B1	1521	C
11	B1	1522	A
11	B1	1533	A
11	B1	1535	U
11	B1	1537	A
11	B1	1544	C
11	B1	1553	C
11	B1	1554	C
11	B1	1555	U
11	B1	1558	C
11	B1	1580	A
11	B1	1582	C
11	B1	1585	U
11	B1	1586	U
11	B1	1588	A
11	B1	1601	A
11	B1	1604	G

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Mol	Chain	Res	Type
11	B1	1606	G
11	B1	1620	A
11	B1	1621	U
11	B1	1622	U
11	B1	1623	A
11	B1	1624	U
11	B1	1646	C
11	B1	1661	A
11	B1	1662	U
11	B1	1663	A
11	B1	1671	G
11	B1	1683	C
11	B1	1690	U
11	B1	1695	A
11	B1	1700	C
11	B1	1710	C
11	B1	1721	U
11	B1	1726	G
11	B1	1746	U
11	B1	1750	C
11	B1	1753	C
11	B1	1756	C
11	B1	1757	G
11	B1	1780	G
11	B1	1781	A
11	B1	1782	G
11	B1	1783	C
11	B1	1822	A
11	B1	1823	A
11	B1	1825	A
11	B1	1829	G
11	B1	1831	A
11	B1	1834	A
11	B1	1835	A
11	B1	1838	U
11	B1	1843	G
11	B1	1849	G
11	B1	1860	A
11	B1	1861	G
11	B1	1862	G
11	B1	1863	A
11	B1	1864	U

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Mol	Chain	Res	Type
11	B1	1865	C
11	B1	1866	A
11	B1	1869	A
42	A3	16	G
42	A3	34	U
42	A3	35	C
42	A3	37	A
42	A3	38	U
42	A3	49	G
42	A3	58	G
42	A3	59	A
42	A3	63	U
42	A3	71	A
42	A3	72	A
42	A3	77	A
42	A3	80	A
42	A3	81	C
42	A3	87	G
42	A3	94	G
42	A3	95	A
42	A3	96	C
42	A3	103	A
42	A3	105	C
42	A3	107	C
42	A3	109	C
42	A3	110	U
42	A3	111	U
42	A3	114	G
42	A3	121	G
42	A3	123	U
42	A3	124	U
42	A3	125	C
42	A3	126	C
42	A3	128	C
42	A3	129	C
42	A3	130	C
42	A3	148	A
42	A3	151	G
43	A4	7	G
43	A4	10	C
43	A4	11	A
43	A4	14	C

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Mol	Chain	Res	Type
43	A4	22	A
43	A4	24	C
43	A4	27	G
43	A4	33	U
43	A4	47	G
43	A4	48	G
43	A4	53	U
43	A4	54	A
43	A4	60	G
43	A4	63	C
43	A4	64	G
43	A4	91	C
43	A4	97	G
43	A4	110	G

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A2	31	U
7	A2	71	C
7	A2	901	U
7	A2	959	C
7	A2	4661	U
7	A2	4870	G
7	A2	4946	U
11	B1	227	U
11	B1	797	C
11	B1	1689	C

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	DDE	Ct	715	86	14,20,21	1.04	1 (7%)	14,28,30	1.42	3 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	DDE	Ct	715	86	-	7/20/21/23	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	Ct	715	DDE	CD2-NE2	2.18	1.39	1.36

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	Ct	715	DDE	CAU-CBW-CBI	-2.89	105.47	111.20
86	Ct	715	DDE	CBW-CBI-NAD	2.67	118.69	115.28
86	Ct	715	DDE	CB-CA-C	-2.16	107.41	111.47

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	Ct	715	DDE	CA-CB-CG-ND1
86	Ct	715	DDE	NAD-CBI-CBW-NCB
86	Ct	715	DDE	OAG-CBI-CBW-NCB
86	Ct	715	DDE	CE1-CAT-CAU-CBW
86	Ct	715	DDE	CA-CB-CG-CD2
86	Ct	715	DDE	OAG-CBI-CBW-CAU
86	Ct	715	DDE	CAU-CBW-NCB-CAB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 333 ligands modelled in this entry, 332 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
89	GNP	Ct	901	-	29,34,34	1.61	7 (24%)	33,54,54	2.12	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	GNP	Ct	901	-	-	3/14/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	Ct	901	GNP	PB-O3A	4.41	1.64	1.59
89	Ct	901	GNP	PB-O1B	2.99	1.50	1.46
89	Ct	901	GNP	C6-N1	2.97	1.38	1.33
89	Ct	901	GNP	PG-N3B	2.87	1.70	1.63
89	Ct	901	GNP	PG-O1G	2.67	1.50	1.46
89	Ct	901	GNP	PB-O2B	-2.25	1.50	1.56
89	Ct	901	GNP	C5-C6	2.08	1.44	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	Ct	901	GNP	C5-C6-N1	-8.39	111.95	123.43
89	Ct	901	GNP	C2-N1-C6	5.81	125.16	115.93
89	Ct	901	GNP	N3-C2-N1	-2.79	123.50	127.22
89	Ct	901	GNP	C4-C5-C6	-2.59	118.33	120.80
89	Ct	901	GNP	O1B-PB-N3B	-2.31	108.36	111.77
89	Ct	901	GNP	PB-O3A-PA	-2.28	124.58	132.62
89	Ct	901	GNP	C2-N3-C4	-2.18	112.87	115.36

There are no chirality outliers.

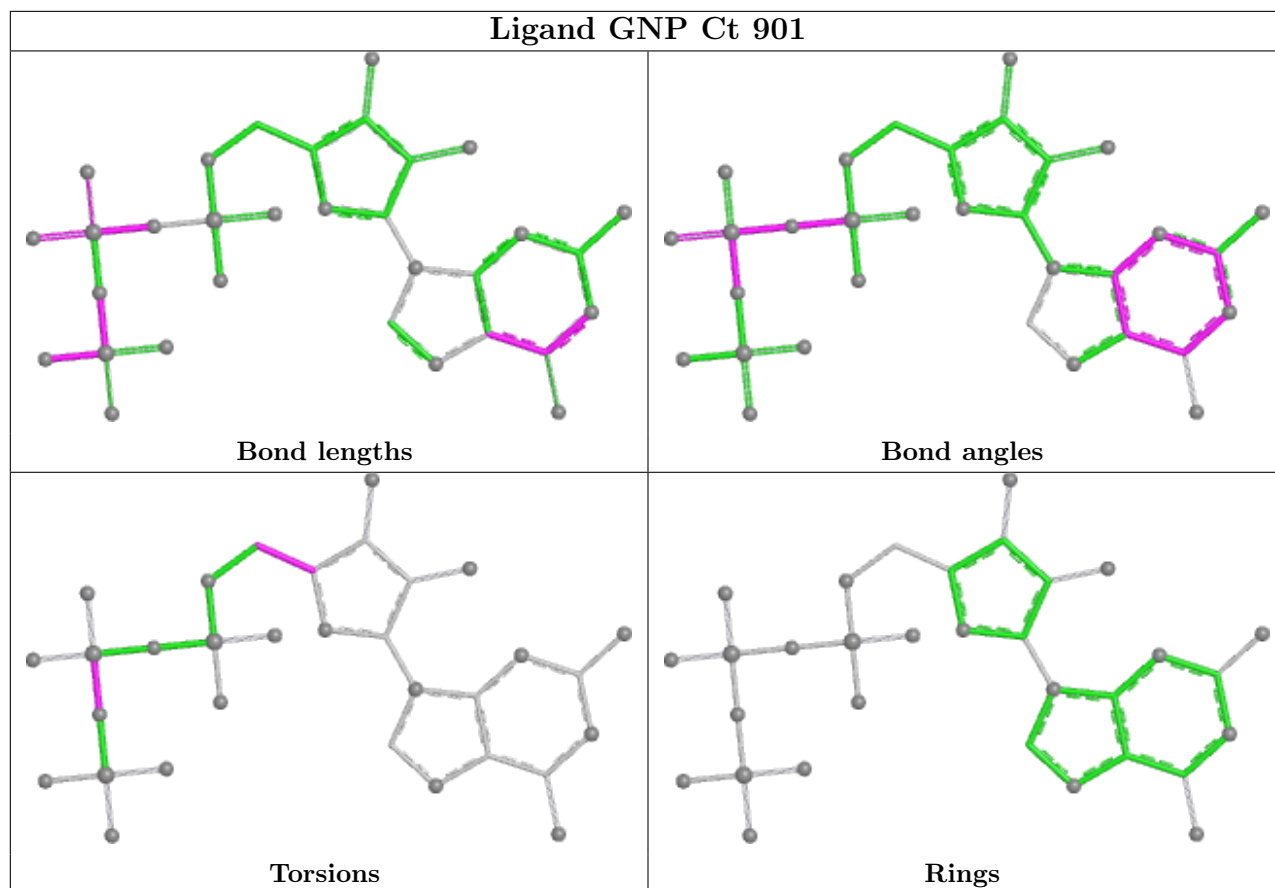
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
89	Ct	901	GNP	PG-N3B-PB-O1B
89	Ct	901	GNP	O4'-C4'-C5'-O5'
89	Ct	901	GNP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	A2	12
11	B1	6
49	AI	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B1	126:G	O3'	141:A	P	22.39
1	B1	751:G	O3'	790:C	P	19.97
1	A2	517:C	O3'	629:G	P	18.43
1	B1	696:G	O3'	737:G	P	17.82

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A2	4734:C	O3'	4818:G	P	17.68
1	A2	2881:G	O3'	3569:C	P	17.61
1	A2	3948:C	O3'	4004:G	P	17.44
1	A2	1233:C	O3'	1243:G	P	17.41
1	A2	750:G	O3'	890:C	P	17.32
1	B1	1426:U	O3'	1438:A	P	16.94
1	B1	1757:G	O3'	1775:U	P	16.84
1	B1	240:G	O3'	282:G	P	16.80
1	A2	976:U	O3'	1047:G	P	16.77
1	A2	1680:C	O3'	1699:C	P	15.45
1	A2	1089:A	O3'	1145:G	P	15.41
1	A2	1202:G	O3'	1216:G	P	15.05
1	A2	2068:C	O3'	2245:C	P	13.71
1	AI	104:SER	C	108:ALA	N	8.09
1	A2	3901:U	O3'	3902:C	P	3.19

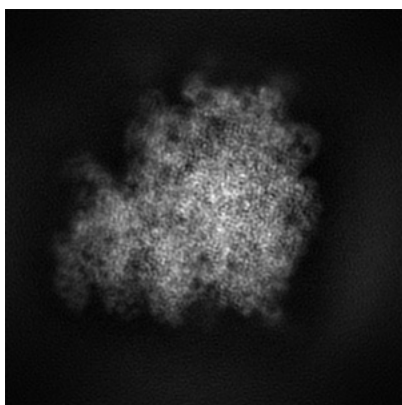
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0099. These allow visual inspection of the internal detail of the map and identification of artifacts.

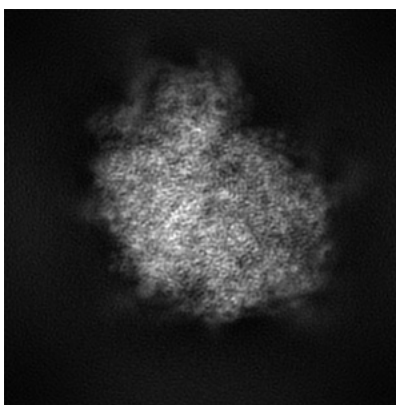
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

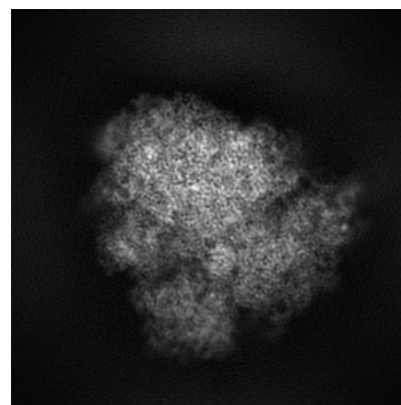
6.1.1 Primary map



X



Y

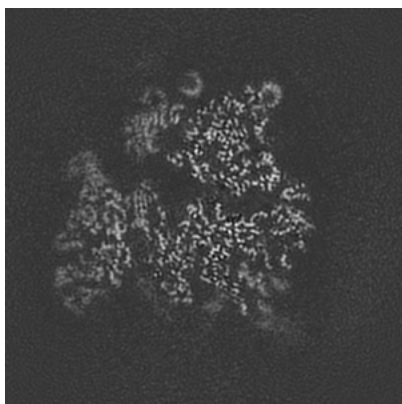


Z

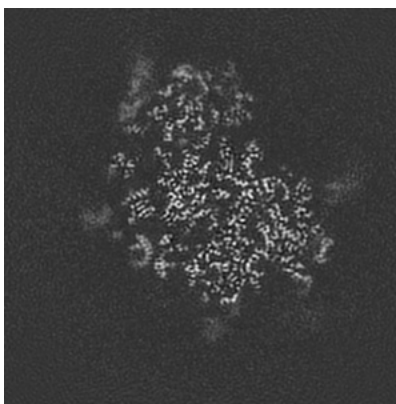
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

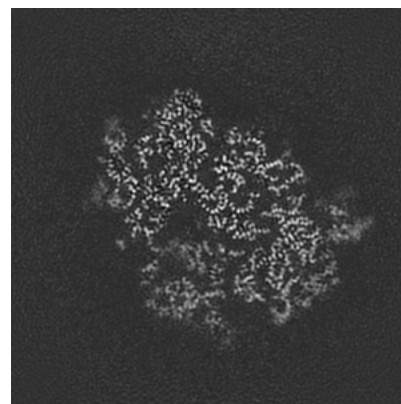
6.2.1 Primary map



X Index: 202



Y Index: 202

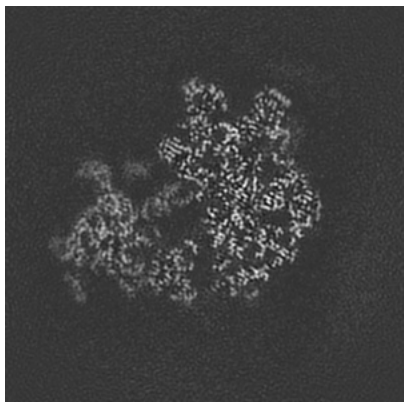


Z Index: 202

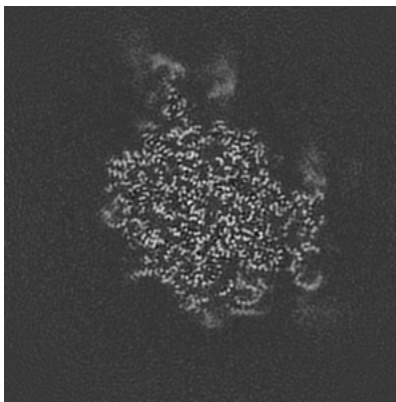
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

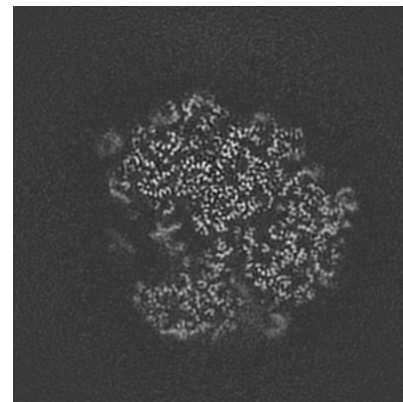
6.3.1 Primary map



X Index: 179



Y Index: 220

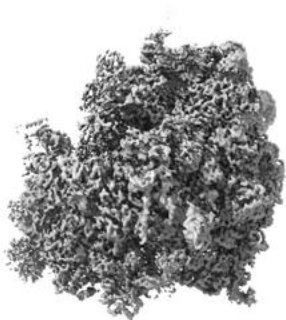


Z Index: 182

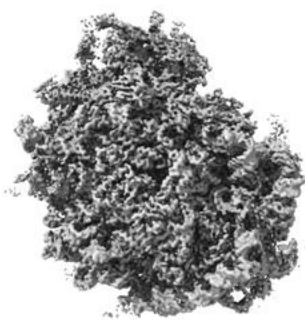
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

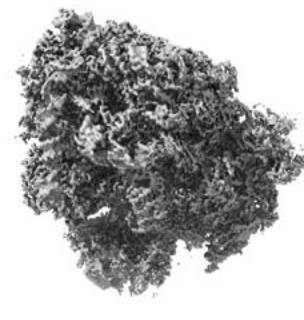
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

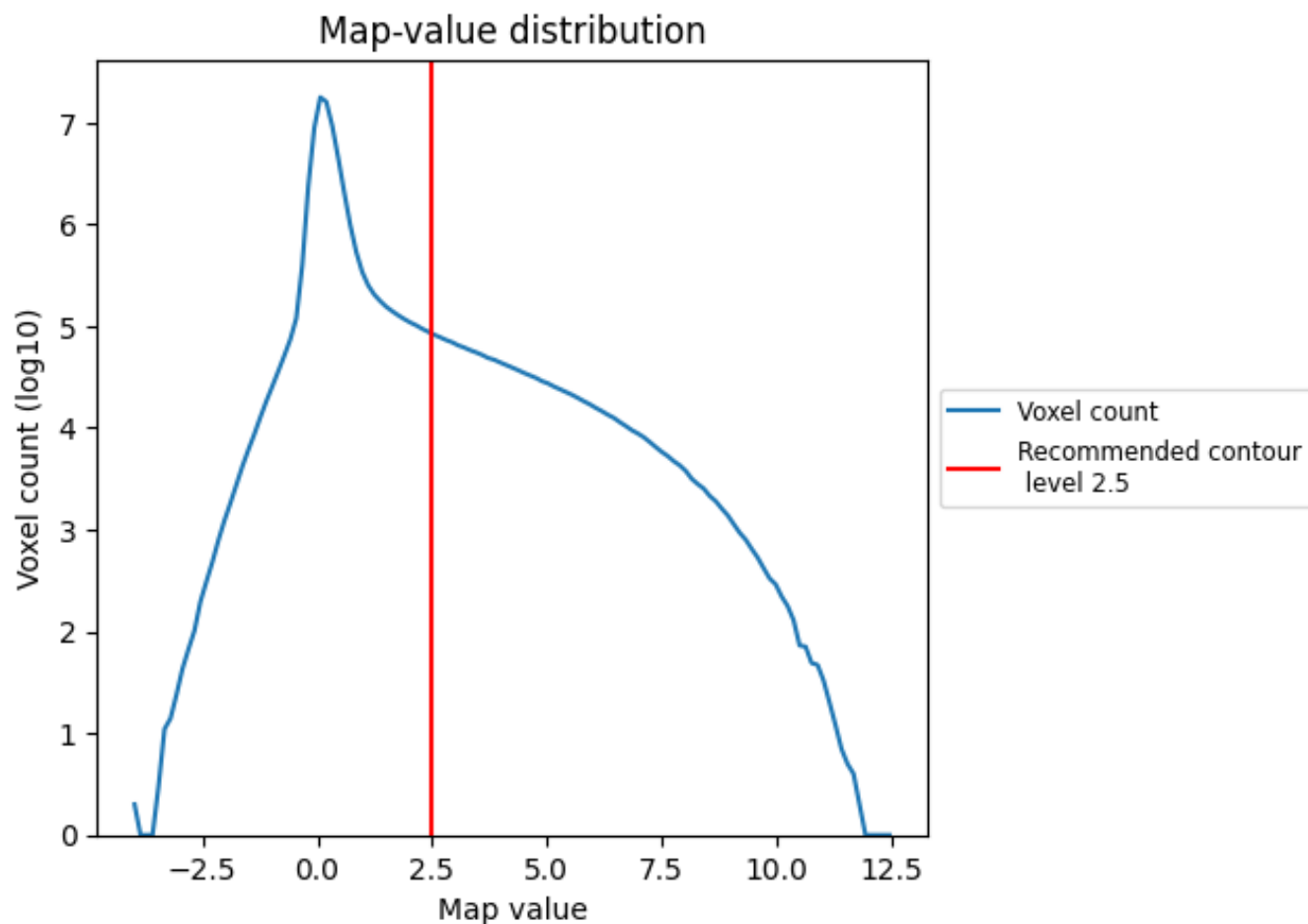
6.5 Mask visualisation

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

7 Map analysis [i](#)

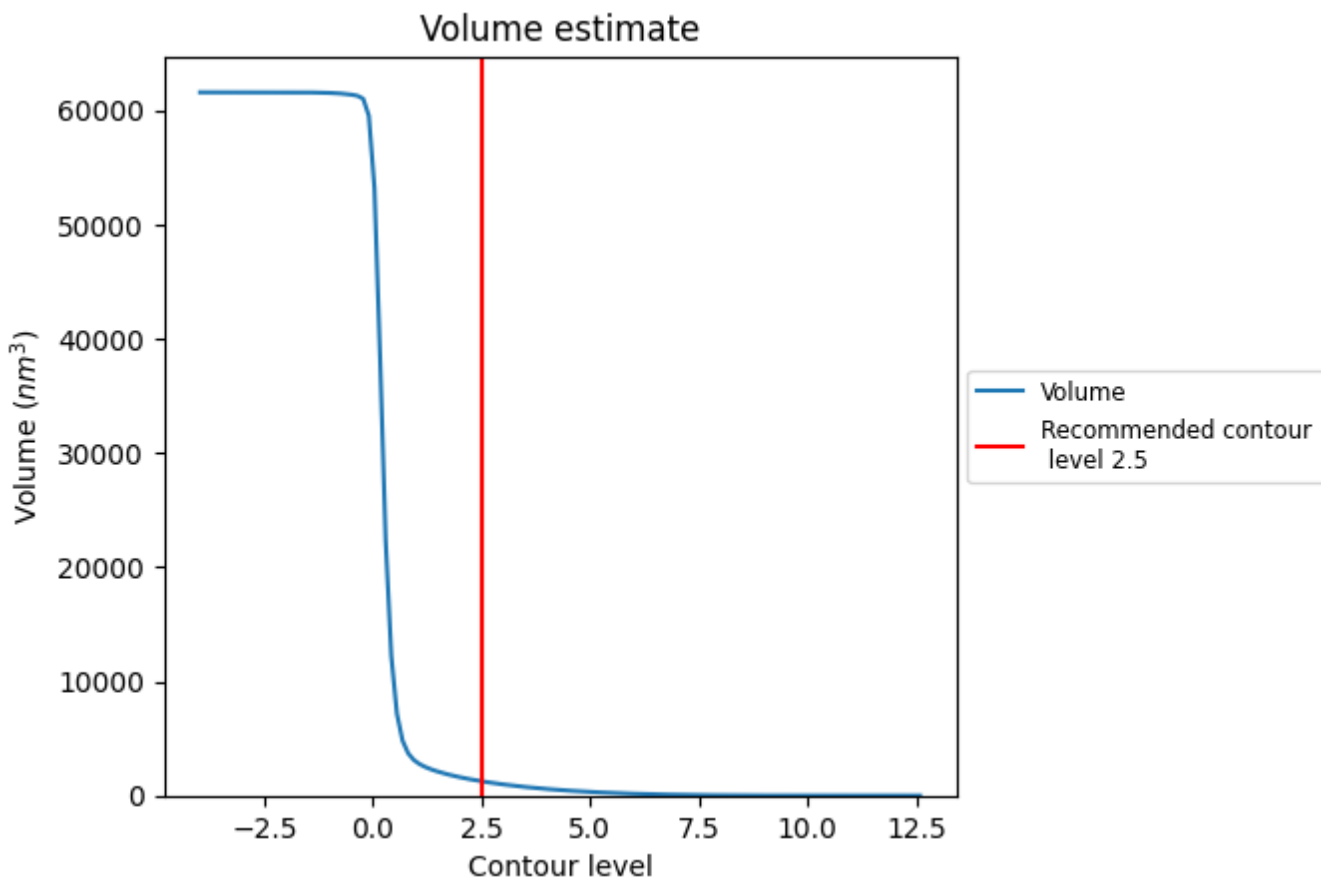
This section contains the results of statistical analysis of the map.

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.

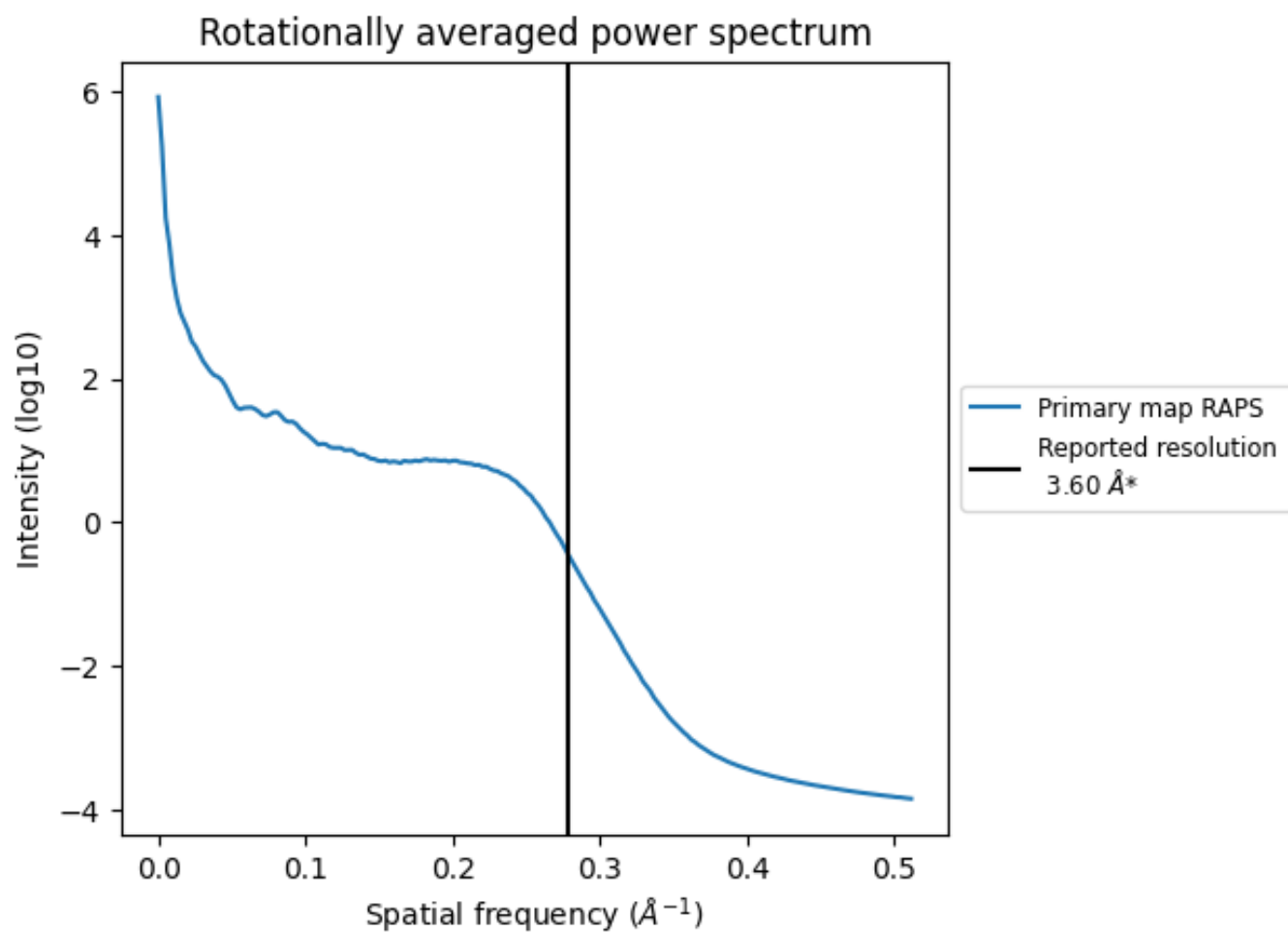
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1249 nm³; this corresponds to an approximate mass of 1128 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.278\AA^{-1}

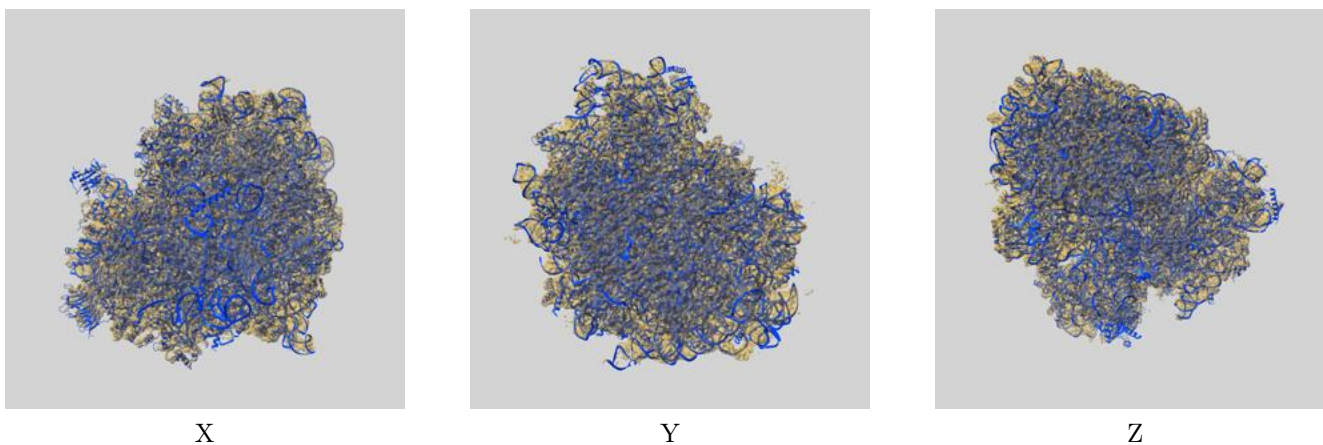
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

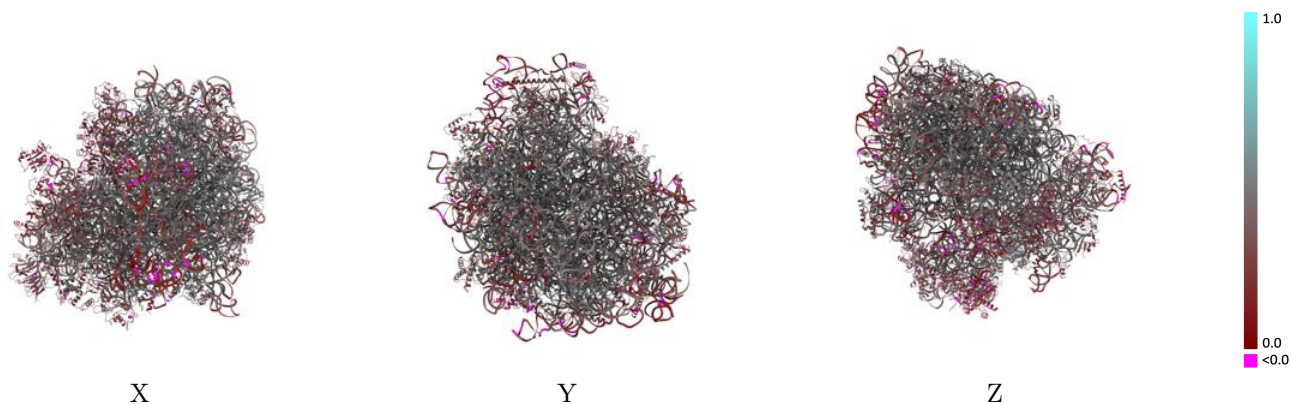
This section contains information regarding the fit between EMDB map EMD-0099 and PDB model 6GZ4. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



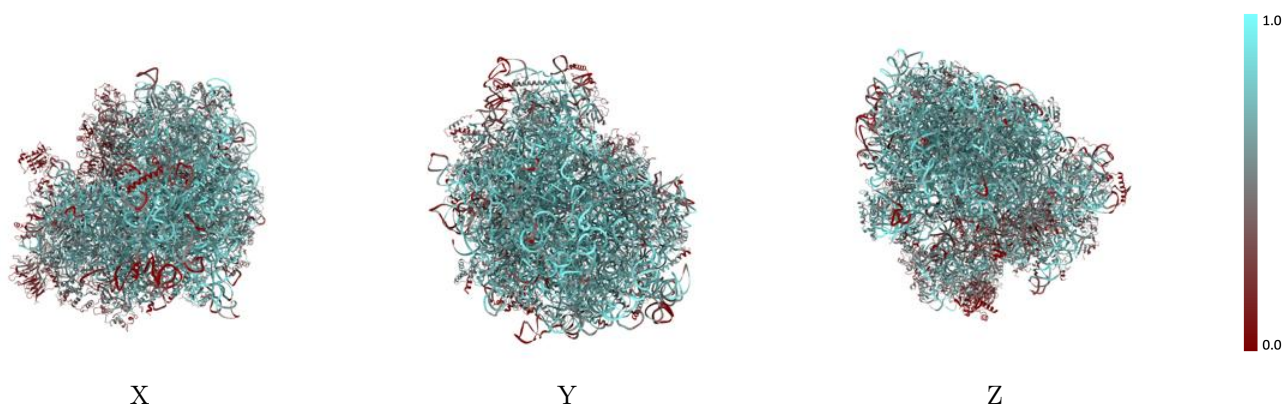
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



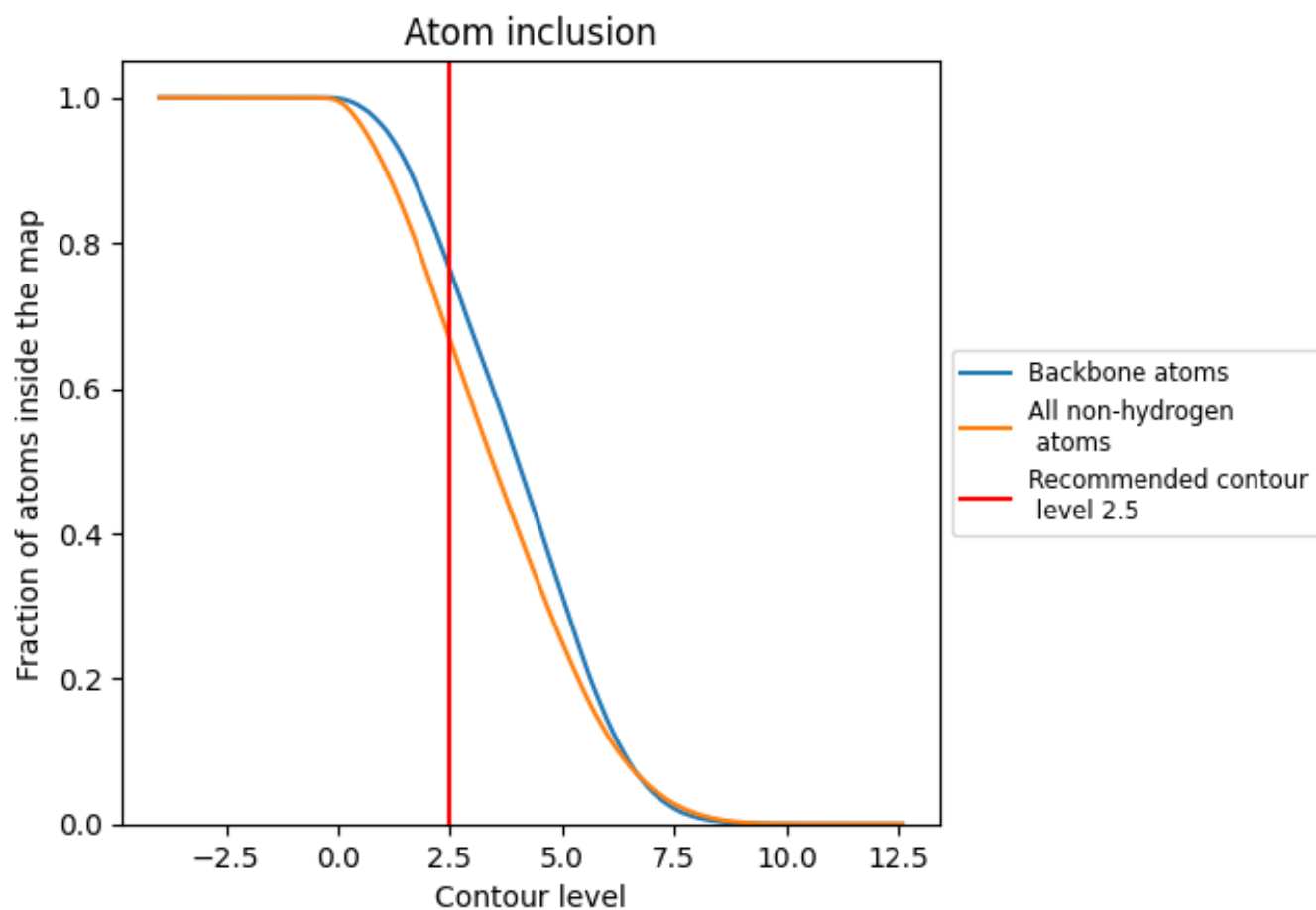
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 66% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6646	 0.3860
A2	 0.7824	 0.4100
A3	 0.7899	 0.4190
A4	 0.8631	 0.4490
AA	 0.6884	 0.4630
AB	 0.6575	 0.4340
AC	 0.6743	 0.4340
AD	 0.6344	 0.3880
AE	 0.5277	 0.3260
AF	 0.6320	 0.4100
AG	 0.5728	 0.3930
AH	 0.6069	 0.4210
AI	 0.6555	 0.4250
AJ	 0.6014	 0.3900
AK	 0.2480	 0.2370
AL	 0.6053	 0.3740
AM	 0.6143	 0.4000
AN	 0.7321	 0.4520
AO	 0.6643	 0.4130
AP	 0.6924	 0.4520
AQ	 0.6637	 0.4310
AR	 0.6221	 0.3990
AS	 0.6764	 0.4420
AT	 0.6605	 0.4300
AU	 0.5367	 0.3720
AV	 0.6621	 0.4620
AW	 0.3553	 0.3030
AX	 0.6445	 0.4420
AY	 0.6537	 0.4280
AZ	 0.6511	 0.4100
Aa	 0.7018	 0.4390
Ab	 0.5838	 0.3540
Ac	 0.6059	 0.3980
Ad	 0.6604	 0.4430
Ae	 0.6667	 0.4480























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Chain	Atom inclusion	Q-score
Af	 0.6770	 0.4320
Ag	 0.6467	 0.4200
Ah	 0.6096	 0.3900
Ai	 0.6142	 0.3880
Aj	 0.7473	 0.4610
Ak	 0.5189	 0.3710
Al	 0.6478	 0.4330
Am	 0.6348	 0.4240
An	 0.2455	 0.3570
Ao	 0.6408	 0.4450
Ap	 0.6531	 0.4300
Aq	 0.1208	 0.1330
At	 0.6897	 0.4130
Au	 0.0297	 0.0570
B1	 0.7522	 0.3930
BA	 0.4961	 0.3600
BB	 0.5650	 0.3730
BC	 0.5751	 0.4010
BD	 0.4532	 0.3430
BE	 0.5616	 0.3850
BF	 0.4470	 0.3250
BG	 0.4670	 0.2890
BH	 0.4041	 0.3090
BI	 0.5657	 0.3760
BJ	 0.5617	 0.3310
BK	 0.3391	 0.2280
BL	 0.5748	 0.3830
BM	 0.0643	 0.1660
BN	 0.5901	 0.3920
BO	 0.5968	 0.4020
BP	 0.4137	 0.2900
BQ	 0.4930	 0.3250
BR	 0.3795	 0.2710
BS	 0.4358	 0.2830
BT	 0.4177	 0.2680
BU	 0.3640	 0.3050
BV	 0.5390	 0.3810
BW	 0.5990	 0.4110
BX	 0.5966	 0.4180
BY	 0.4812	 0.3040
BZ	 0.2961	 0.2300
Ba	 0.6131	 0.4020

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Chain	Atom inclusion	Q-score
Bb	 0.5090	 0.3830
Bc	 0.4106	 0.3370
Bd	 0.5485	 0.3380
Be	 0.5142	 0.3820
Bf	 0.0753	 0.1500
Bg	 0.2472	 0.2730
Bv	 0.5426	 0.3230
Bw	 0.6773	 0.3650
Bx	 0.5872	 0.3640
Ct	 0.3732	 0.2930