



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 06:08 am GMT

PDB ID : 6GZ3
EMDB ID : EMD-0098
Title : tRNA translocation by the eukaryotic 80S ribosome and the impact of GTP hydrolysis, Translocation-intermediate-POST-1 (TI-POST-1)
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:

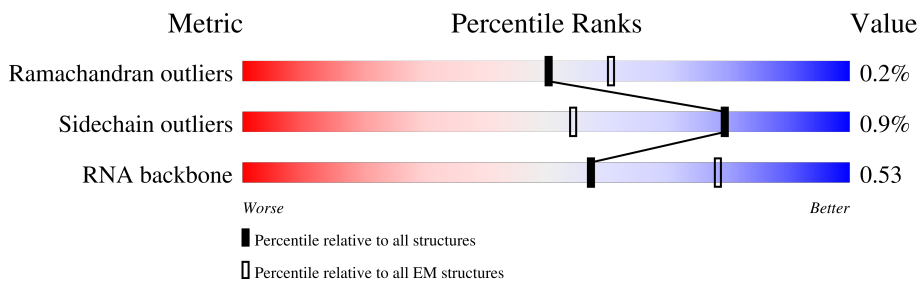
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : 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	A2	3612	
2	Bv	76	
3	Bx	12	
4	Bw	76	
5	B1	1708	
6	BD	220	
7	BF	190	
8	BK	98	

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Mol	Chain	Length	Quality of chain
9	BM	120	98% 100%
10	BP	120	52% 98%
11	BQ	139	47% 99%
12	BR	125	58% 100%
13	BS	139	53% 97%
14	BT	143	50% 99%
15	BU	97	53% 100%
16	BZ	86	79% 99%
17	Bc	62	56% 95%
18	Bd	51	27% 100%
19	Bf	73	99% 100%
20	Bg	314	84% 100%
21	BA	215	44% 99%
22	BB	212	37% 99%
23	BC	222	19% 100%
24	BE	257	26% 97%
25	BG	232	50% 99%
26	BH	183	67% 100%
27	BI	207	32% 99%
28	BJ	179	23% 97%
29	BL	153	35% 98%
30	BN	149	26% 99%
31	BO	136	22% 99%
32	BV	81	30% 98%
33	BW	129	17% 98%

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Mol	Chain	Length	Quality of chain
34	BX	141	22% 99%
35	BY	125	43% 99%
36	Ba	97	19% 99%
37	Bb	80	44% 100%
38	Be	55	38% 95% 5%
39	A3	157	10% 75% 22%
40	A4	119	78% 20%
41	AA	252	6% 100%
42	AB	394	10% 99%
43	AC	363	10% 98%
44	AD	294	13% 98%
45	AE	194	29% 97%
46	AF	234	10% 99%
47	AG	234	21% 100%
48	AH	191	9% 98%
49	AI	211	11% 98%
50	AJ	169	19% 99%
51	AL	205	19% 99%
52	AM	139	13% 99%
53	AN	203	100%
54	AO	195	8% 98%
55	AP	153	6% 99%
56	AQ	187	12% 98%
57	AR	181	16% 99%
58	AS	175	7% 100%

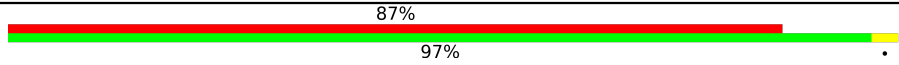
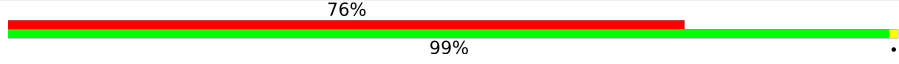
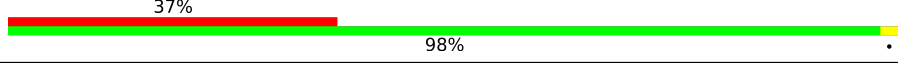
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Mol	Chain	Length	Quality of chain
59	AT	157	12% 99%
60	AU	99	23% 98%
61	AV	129	8% 100%
62	AW	121	55% 99%
63	AX	117	9% 100%
64	AY	127	10% 99%
65	AZ	134	14% 99%
66	Aa	147	10% 99%
67	Ab	68	26% 96%
68	Ac	103	21% 100%
69	Ad	106	14% 100%
70	Ae	129	5% 100%
71	Af	109	6% 98%
72	Ag	114	14% 100%
73	Ah	122	20% 96%
74	Ai	97	19% 100%
75	Aj	84	98%
76	Ak	69	29% 99%
77	Al	50	14% 94% 6%
78	Am	50	10% 98%
79	An	25	84% 100%
80	Ao	105	8% 97%
81	Ap	91	7% 99%
82	At	122	12% 96%
83	Au	217	99% 97%

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Mol	Chain	Length	Quality of chain
84	Aq	151	
85	AK	202	
86	Ct	853	

2 Entry composition [i](#)

There are 89 unique types of molecules in this entry. The entry contains 225624 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 28S ribosomal RNA.

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

- Molecule 2 is a RNA chain called ap/P-site tRNA.

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

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	Bx	12	257	115	46	84	12	0	0

- Molecule 4 is a RNA chain called pe/E-site-tRNA.

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

- Molecule 5 is a RNA chain called 18S ribosomal RNA.

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

- Molecule 6 is a protein called ribosomal protein uS3.

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

- Molecule 7 is a protein called Ribosomal protein S5.

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

- Molecule 8 is a protein called ribosomal protein eS10.

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

- Molecule 9 is a protein called 40S ribosomal protein S12.

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

- Molecule 10 is a protein called ribosomal protein uS19.

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

- Molecule 11 is a protein called ribosomal protein uS9.

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

- Molecule 12 is a protein called ribosomal protein eS17.

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

- Molecule 13 is a protein called ribosomal protein uS13.

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

- Molecule 14 is a protein called ribosomal protein eS19.

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

- Molecule 15 is a protein called ribosomal protein uS10.

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

- Molecule 16 is a protein called ribosomal protein eS25.

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

- Molecule 17 is a protein called Ribosomal protein S28.

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

- Molecule 18 is a protein called ribosomal protein uS14.

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

- Molecule 19 is a protein called Ribosomal protein S27a.

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

- Molecule 20 is a protein called ribosomal protein RACK 1.

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

- Molecule 21 is a protein called ribosomal protein uS2.

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

- Molecule 22 is a protein called 40S ribosomal protein S3a.

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

- Molecule 23 is a protein called ribosomal protein uS5.

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

- Molecule 24 is a protein called ribosomal protein eS4.

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

- Molecule 25 is a protein called 40S ribosomal protein S6.

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

- Molecule 26 is a protein called 40S ribosomal protein S7.

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

- Molecule 27 is a protein called ribosomal protein eS8.

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

- Molecule 28 is a protein called Ribosomal protein S9 (Predicted).

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

- Molecule 29 is a protein called Ribosomal protein S11.

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

- Molecule 30 is a protein called ribosomal protein uS15.

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

- Molecule 31 is a protein called ribosomal protein uS11.

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

- Molecule 32 is a protein called ribosomal protein eS21.

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

- Molecule 33 is a protein called Ribosomal protein S15a.

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

- Molecule 34 is a protein called Ribosomal protein S23.

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

- Molecule 35 is a protein called ribosomal protein eS24.

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

- Molecule 36 is a protein called ribosomal protein eS26.

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

- Molecule 37 is a protein called ribosomal protein eS27.

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

- Molecule 38 is a protein called ribosomal protein eS30.

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

- Molecule 39 is a RNA chain called 5.8S ribosomal RNA.

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

- Molecule 40 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 41 is a protein called Ribosomal protein L8.

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

- Molecule 42 is a protein called ribosomal protein uL3.

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

- Molecule 43 is a protein called ribosomal protein uL4.

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

- Molecule 44 is a protein called ribosomal protein uL18.

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

- Molecule 45 is a protein called ribosomal protein eL6.

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

- Molecule 46 is a protein called ribosomal protein uL30.

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

- Molecule 47 is a protein called ribosomal protein eL8.

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

- Molecule 48 is a protein called ribosomal protein uL6.

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

- Molecule 49 is a protein called Ribosomal protein L10 (Predicted).

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	149	ILE	VAL	conflict	UNP B7NZQ2

- Molecule 50 is a protein called Ribosomal protein L11.

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 L15.

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 L23.

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
62	AW	121	Total	C	N	O	S	0	0
			989	617	202	167	3		

- Molecule 63 is a protein called ribosomal protein uL23.

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

- Molecule 64 is a protein called Ribosomal protein L26.

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

- Molecule 65 is a protein called 60S ribosomal protein L27.

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

- Molecule 66 is a protein called ribosomal protein uL15.

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

- Molecule 67 is a protein called ribosomal protein eL29.

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

- Molecule 68 is a protein called ribosomal protein eL30.

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

- 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 L37.

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
			Total	C	N	O	S		
77	Al	50	444	281	98	64	1	0	0

- Molecule 78 is a protein called ribosomal protein eL40.

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

- Molecule 79 is a protein called ribosomal protein eL41.

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

- Molecule 80 is a protein called ribosomal protein eL42.

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

- Molecule 81 is a protein called ribosomal protein eL43.

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

- Molecule 82 is a protein called ribosomal protein eL28.

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

- Molecule 83 is a protein called Ribosomal protein.

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 L12.

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	A2	230	Total	Mg	0
			230	230	
87	Bx	2	Total	Mg	0
			2	2	
87	B1	69	Total	Mg	0
			69	69	
87	BD	2	Total	Mg	0
			2	2	
87	BS	1	Total	Mg	0
			1	1	
87	Bd	1	Total	Mg	0
			1	1	
87	Ba	1	Total	Mg	0
			1	1	
87	A3	6	Total	Mg	0
			6	6	
87	A4	8	Total	Mg	0
			8	8	

Continued on next page...

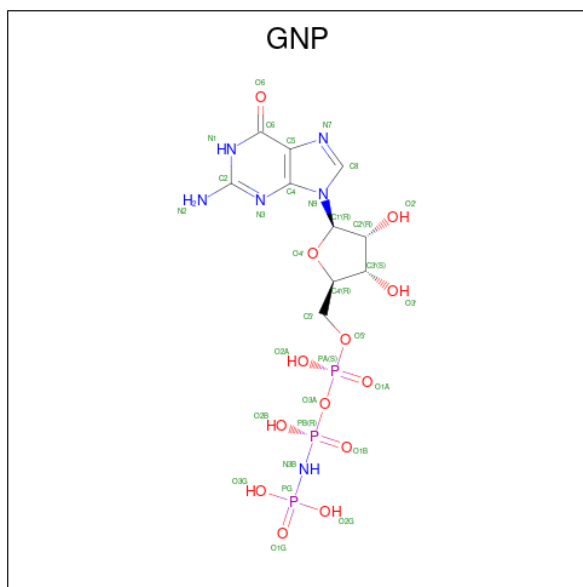
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
87	AA	1	Total 1	Mg 1	0
87	AL	1	Total 1	Mg 1	0
87	AN	1	Total 1	Mg 1	0
87	AP	1	Total 1	Mg 1	0
87	AY	1	Total 1	Mg 1	0
87	Al	1	Total 1	Mg 1	0
87	An	1	Total 1	Mg 1	0

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

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

- Molecule 89 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

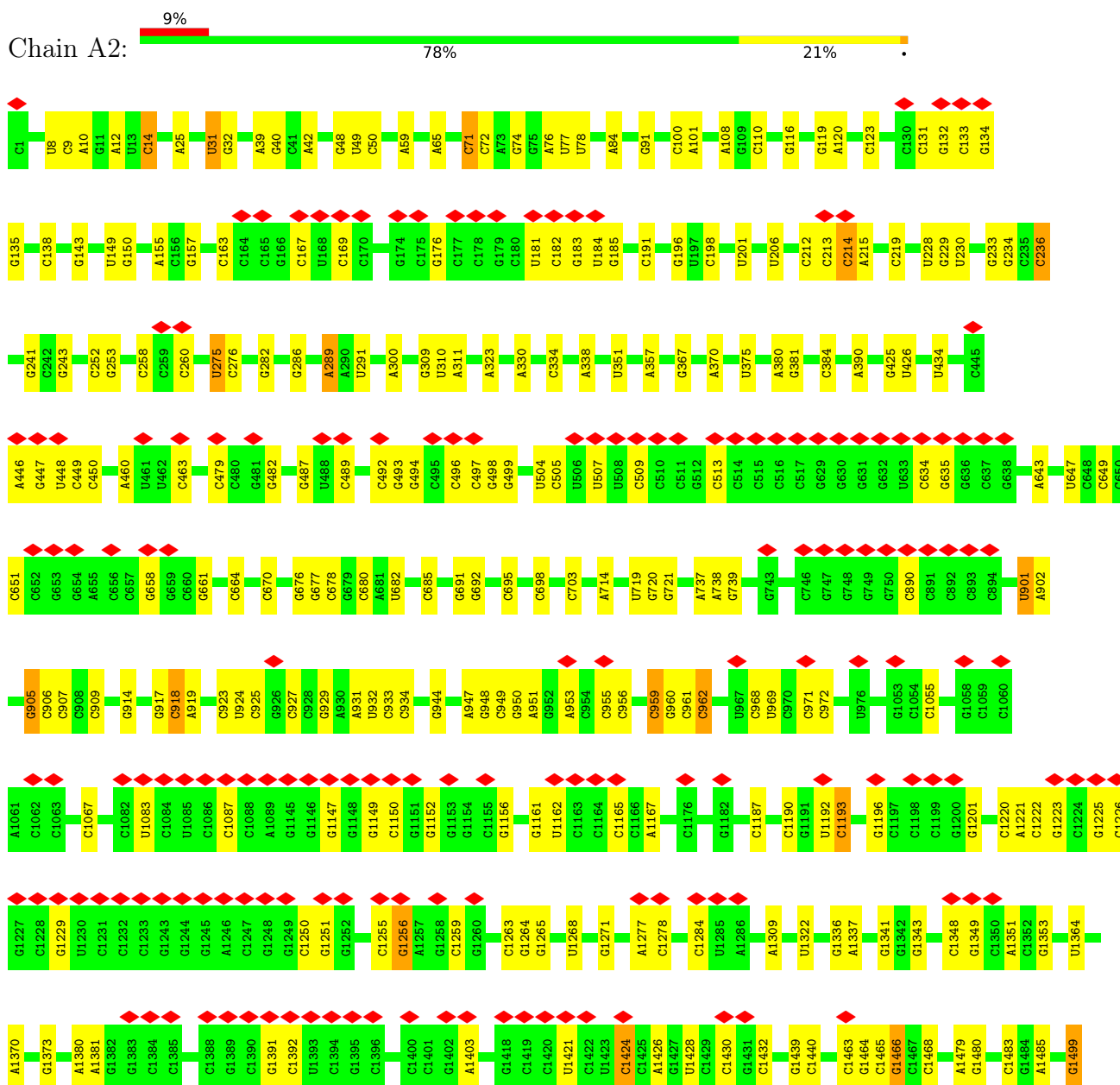


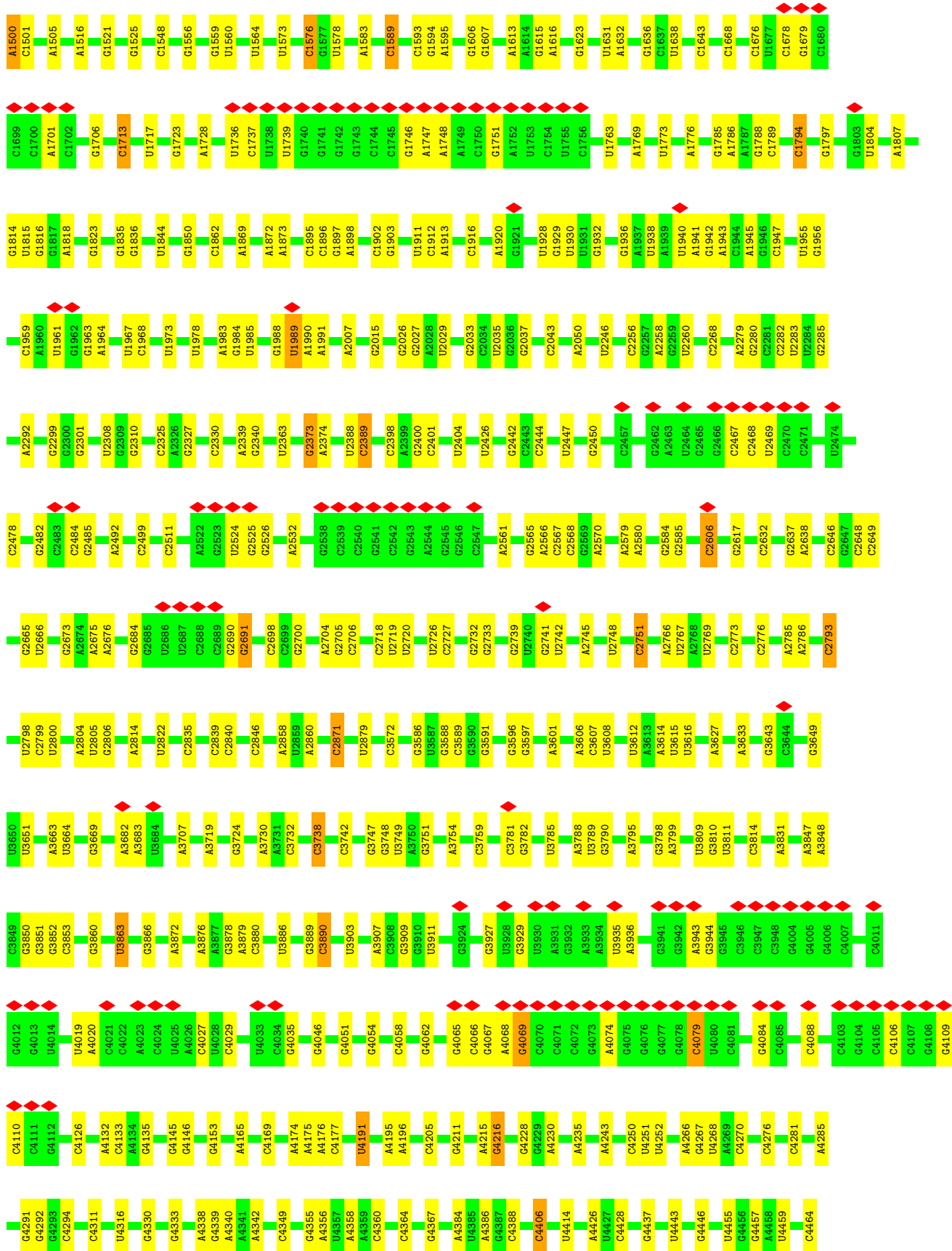
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
89	Ct	1	32	10	6	13	3	0

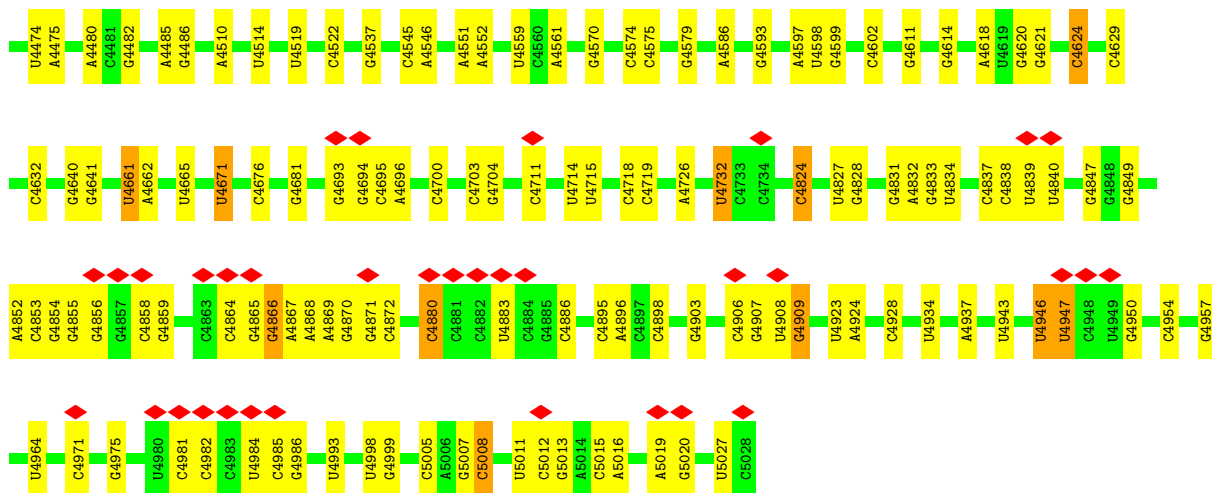
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

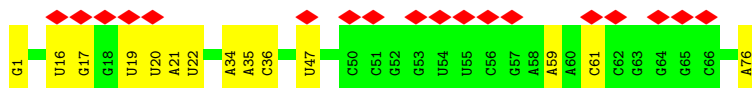
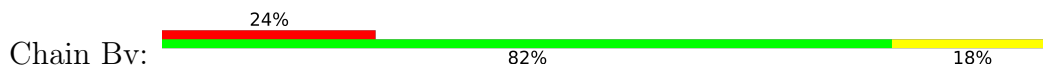
- Molecule 1: 28S ribosomal RNA



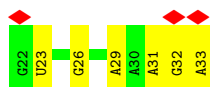




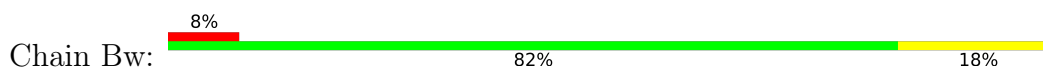
• Molecule 2: ap/P-site tRNA



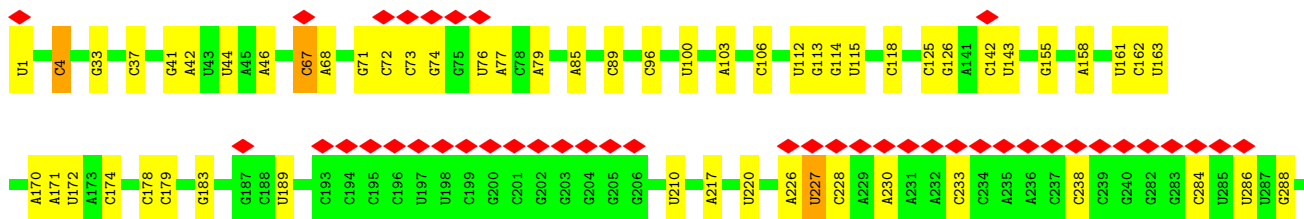
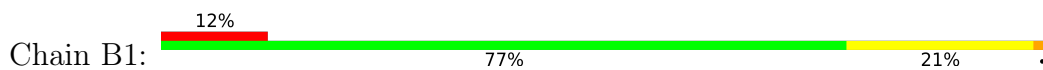
• Molecule 3: mRNA

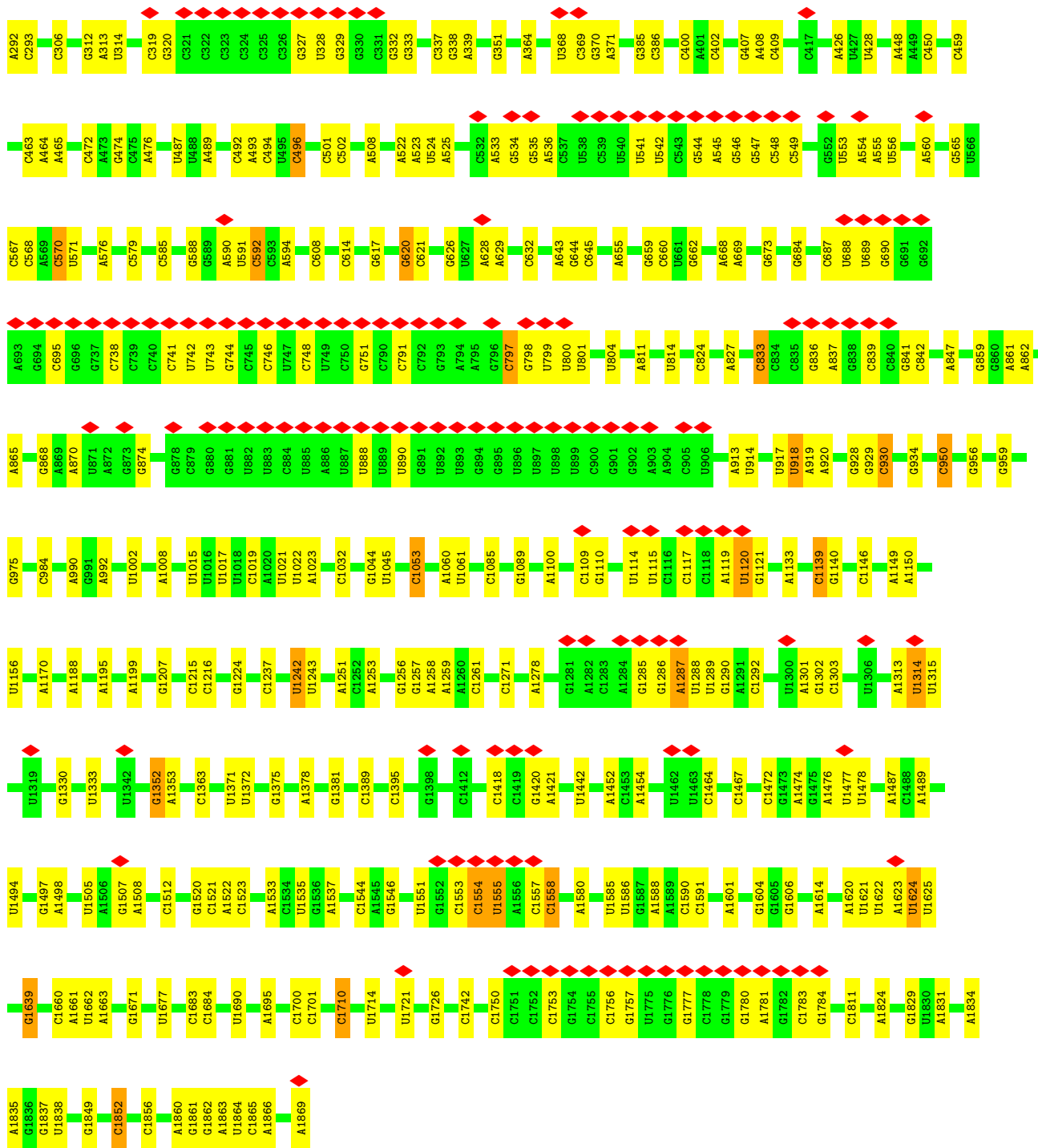


• Molecule 4: pe/E-site-tRNA

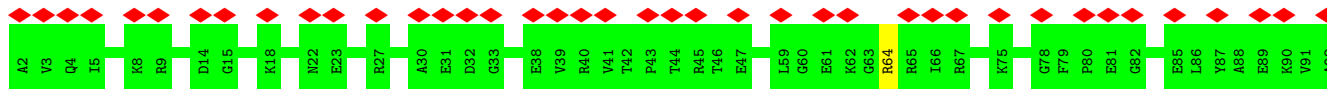


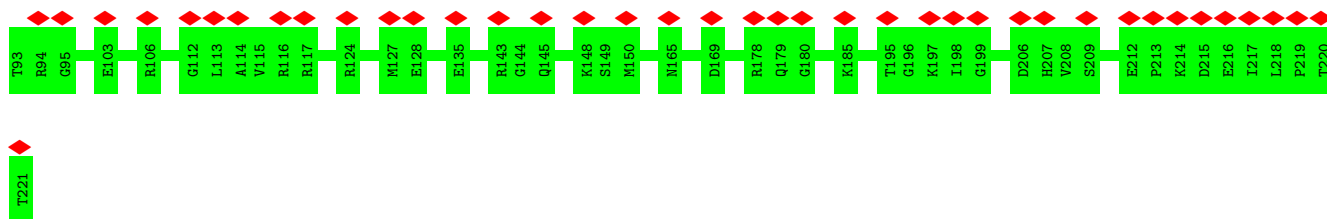
• Molecule 5: 18S ribosomal RNA



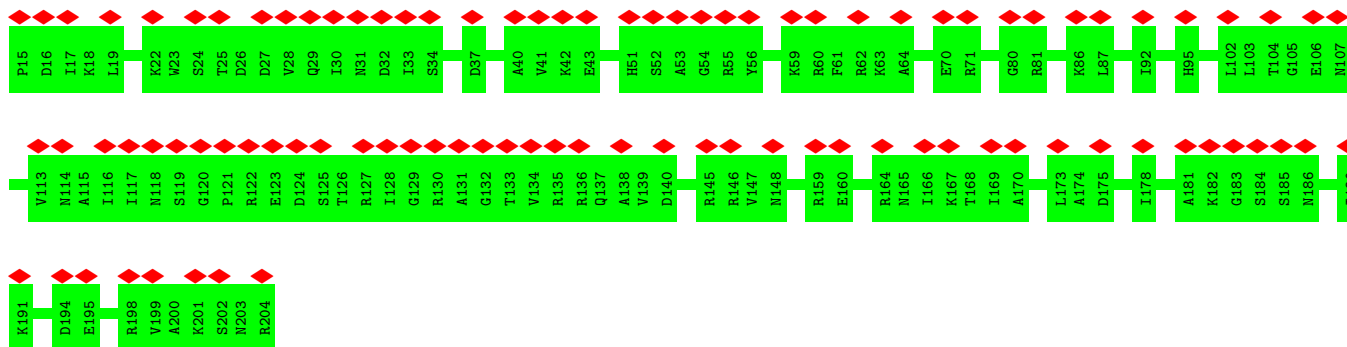


• Molecule 6: ribosomal protein uS3

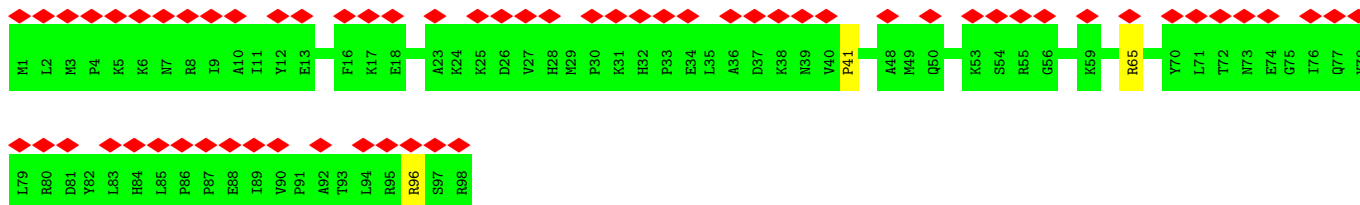




- Molecule 7: Ribosomal protein S5



- Molecule 8: ribosomal protein eS10

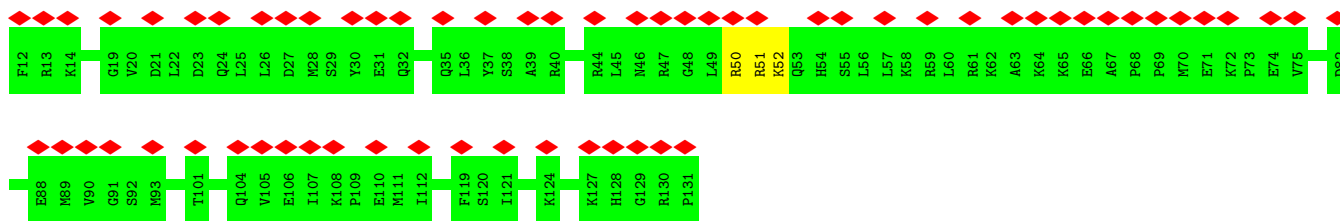


- Molecule 9: 40S ribosomal protein S12



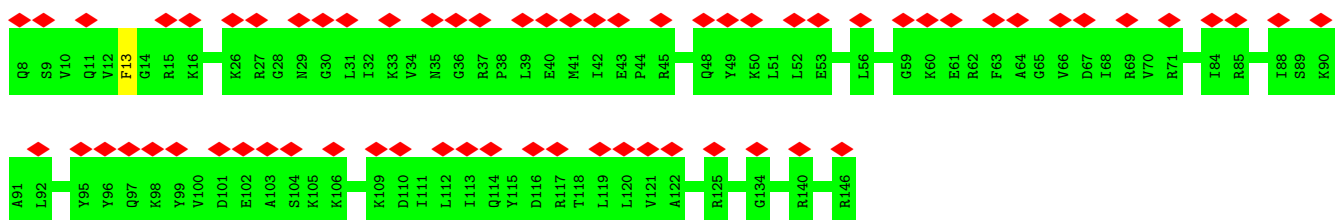
- Molecule 10: ribosomal protein uS19





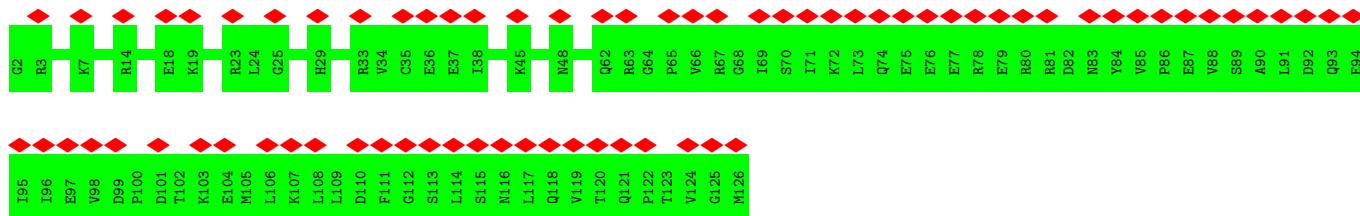
- Molecule 11: ribosomal protein uS9

Chain BQ: 47% 99%



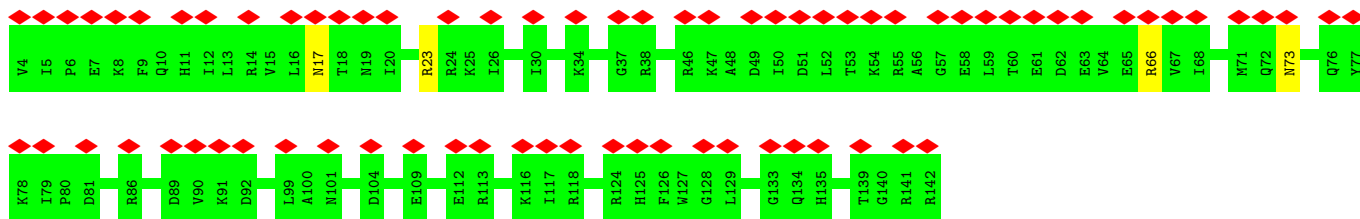
- Molecule 12: ribosomal protein eS17

Chain BR: 58% 100%



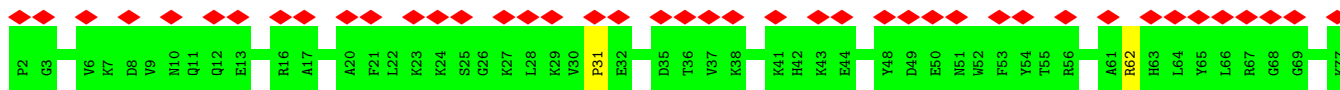
- Molecule 13: ribosomal protein uS13

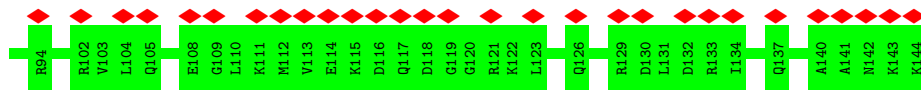
Chain BS: 53% 97%



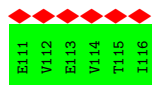
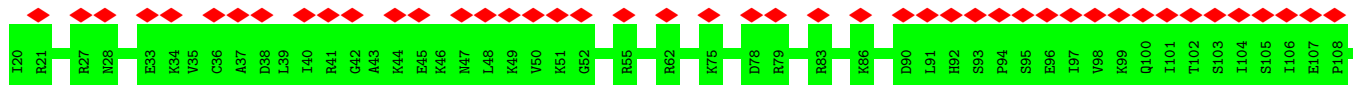
- Molecule 14: ribosomal protein eS19

Chain BT: 50% 99%

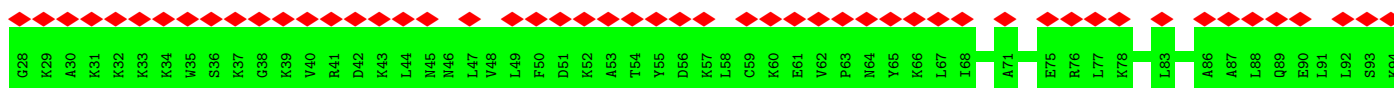
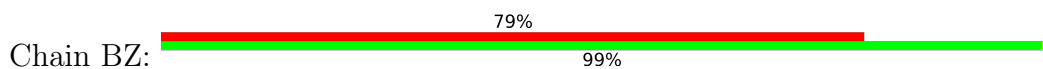




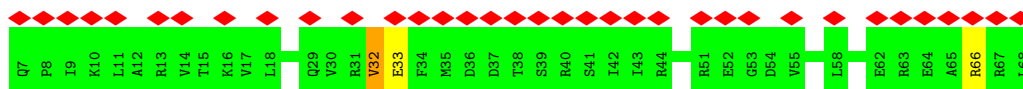
• Molecule 15: ribosomal protein uS10



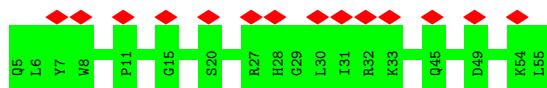
• Molecule 16: ribosomal protein eS25



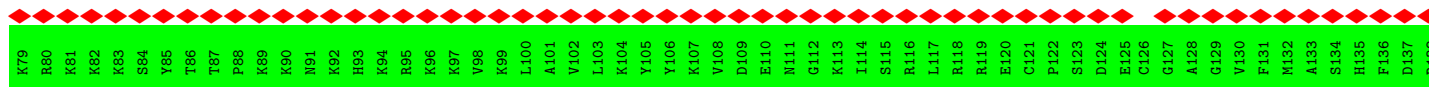
• Molecule 17: Ribosomal protein S28

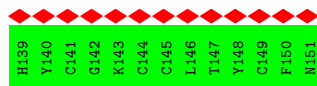


• Molecule 18: ribosomal protein uS14

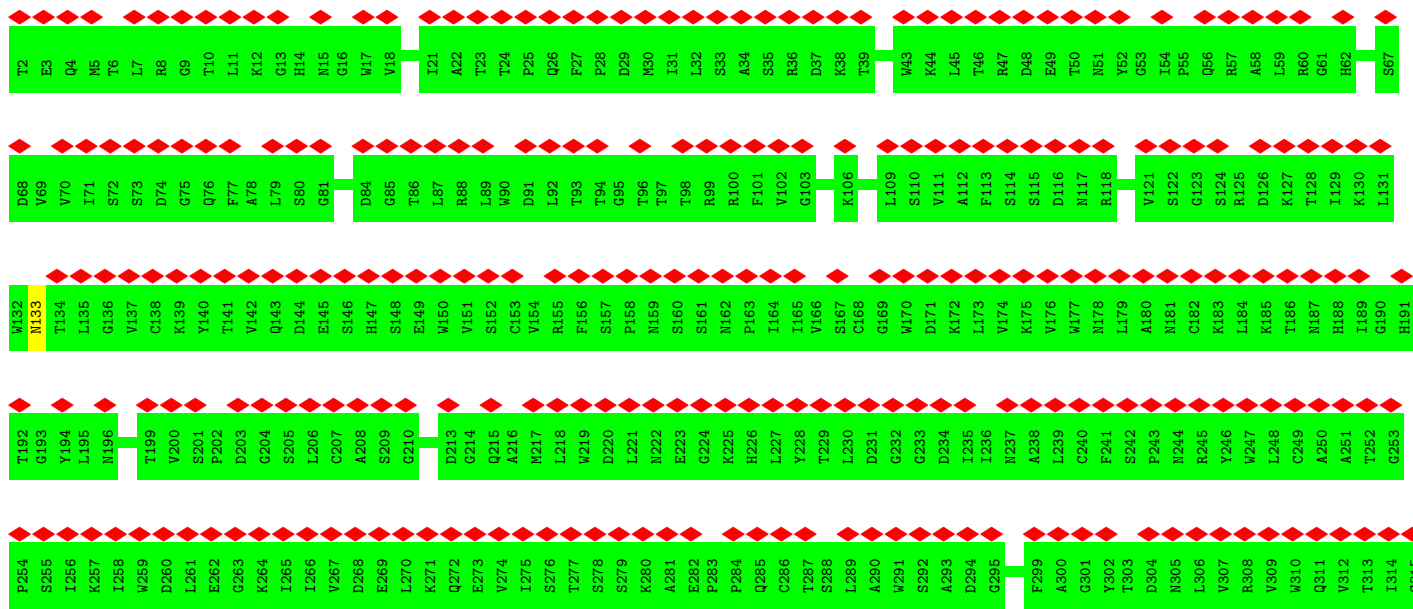
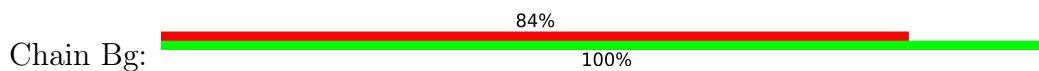


• Molecule 19: Ribosomal protein S27a

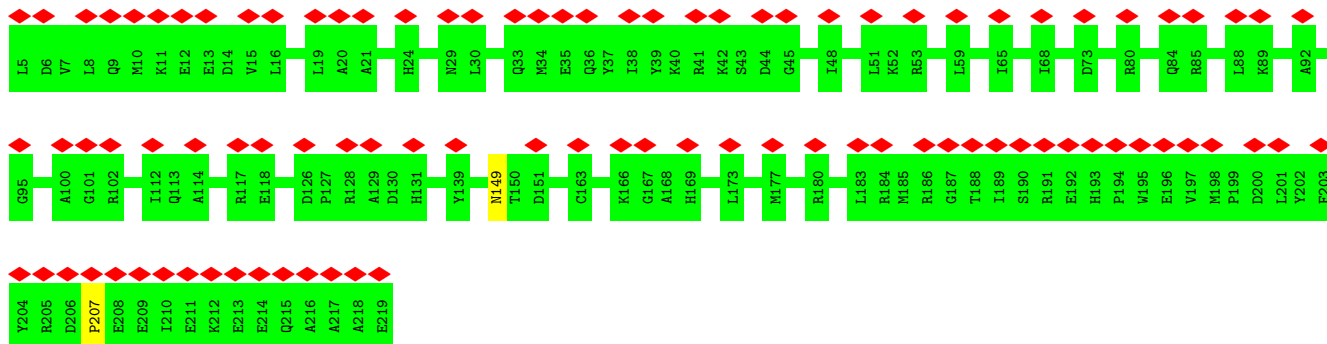




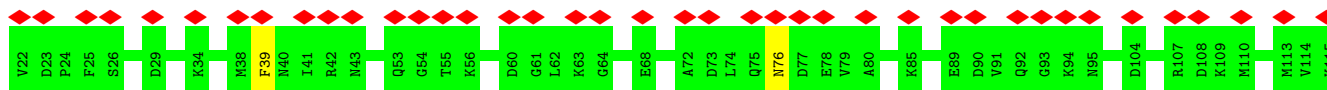
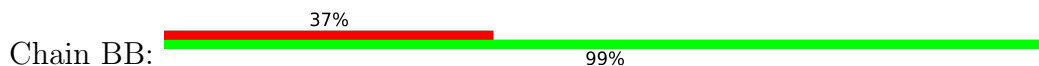
- Molecule 20: ribosomal protein RACK 1

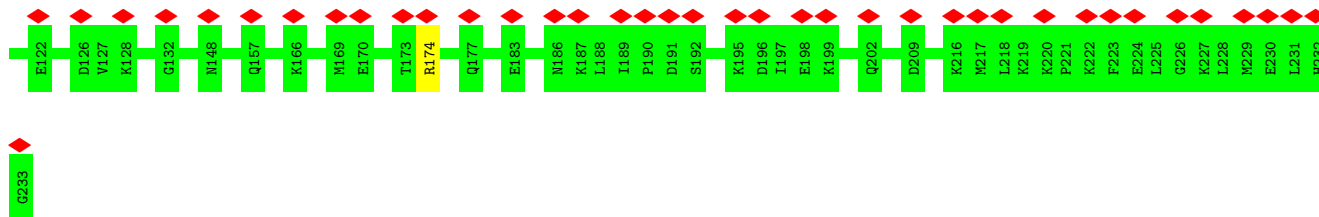


- Molecule 21: ribosomal protein uS2

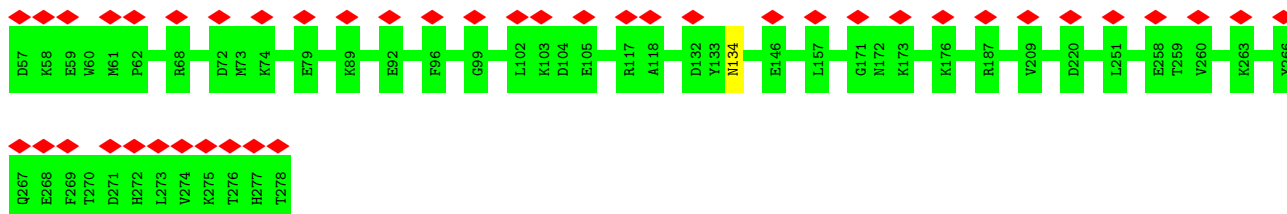


- Molecule 22: 40S ribosomal protein S3a

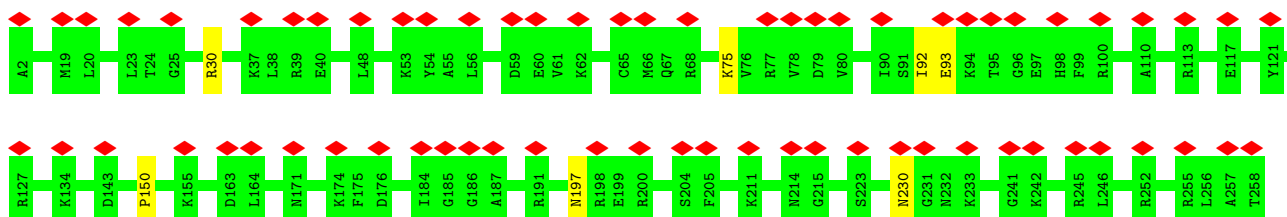




- Molecule 23: ribosomal protein uS5



- Molecule 24: ribosomal protein eS4

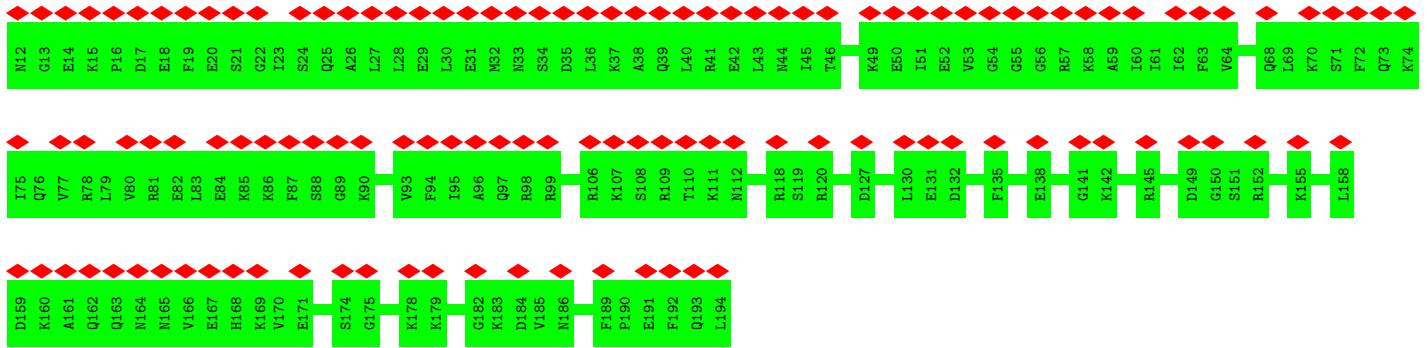


- Molecule 25: 40S ribosomal protein S6

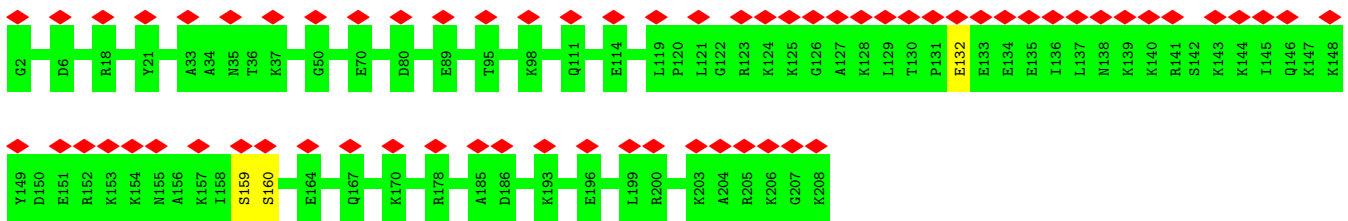


- Molecule 26: 40S ribosomal protein S7

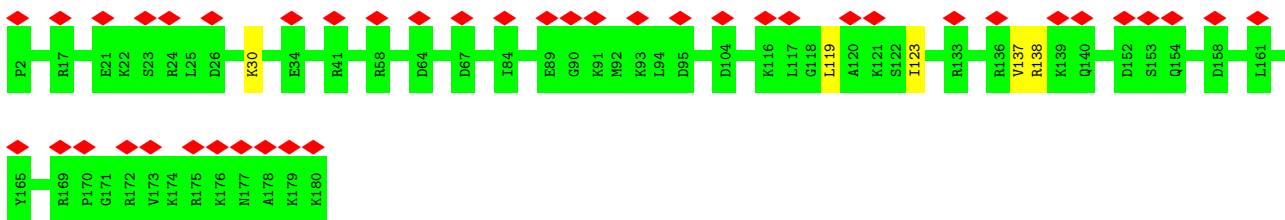




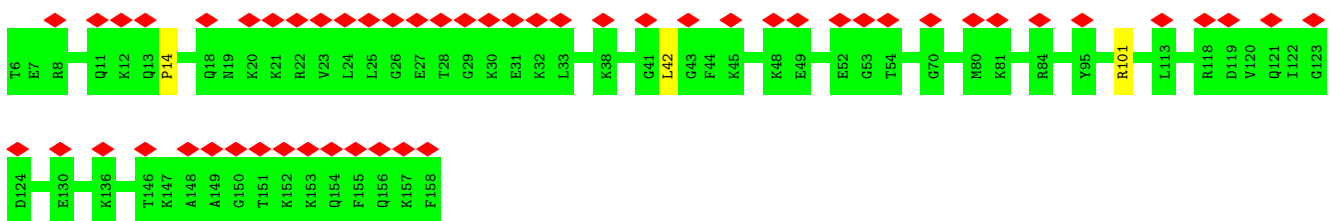
• Molecule 27: ribosomal protein eS8



• Molecule 28: Ribosomal protein S9 (Predicted)

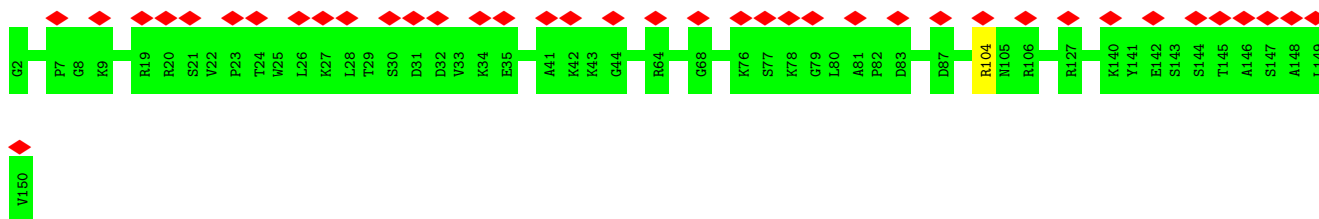


• Molecule 29: Ribosomal protein S11

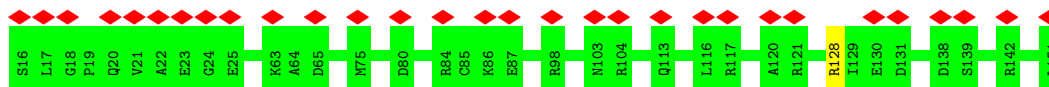


• Molecule 30: ribosomal protein uS15

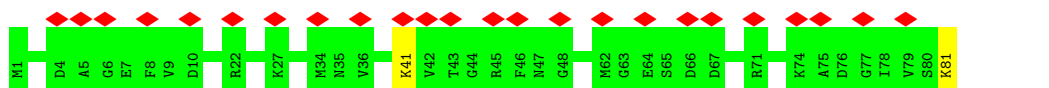




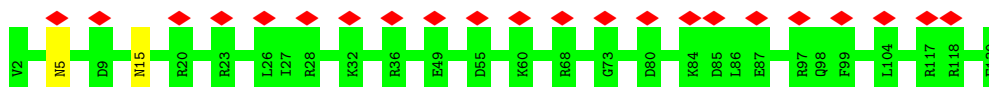
- Molecule 31: ribosomal protein uS11



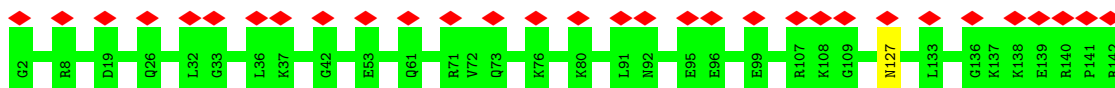
- Molecule 32: ribosomal protein eS21



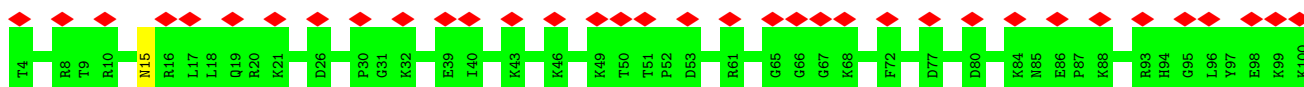
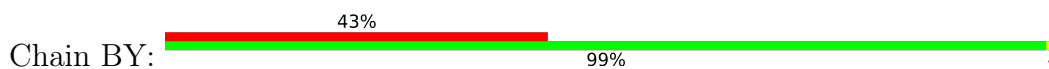
- Molecule 33: Ribosomal protein S15a



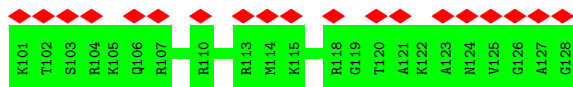
- Molecule 34: Ribosomal protein S23

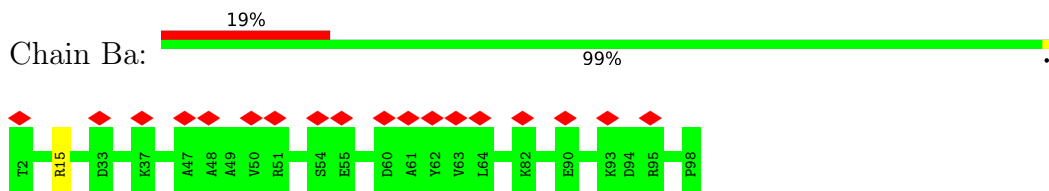


- Molecule 35: ribosomal protein eS24

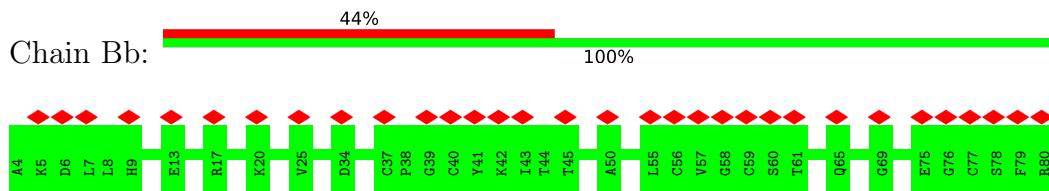


- Molecule 36: ribosomal protein eS26

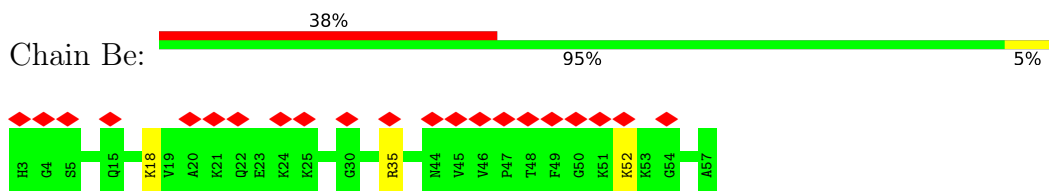




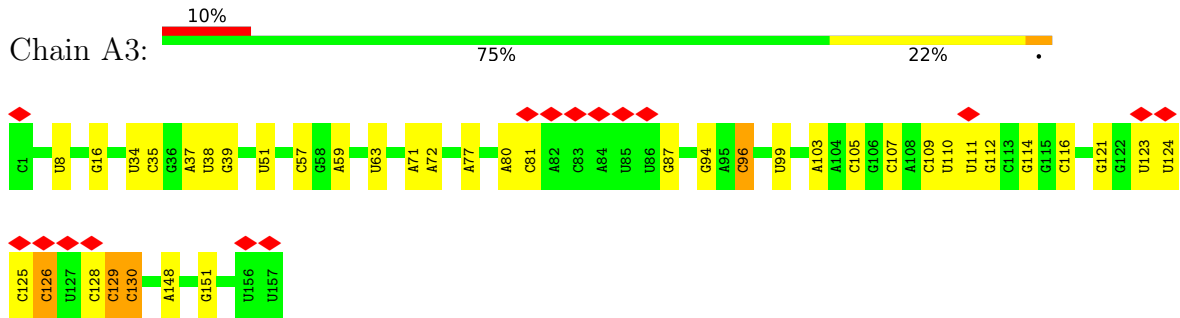
• Molecule 37: ribosomal protein eS27



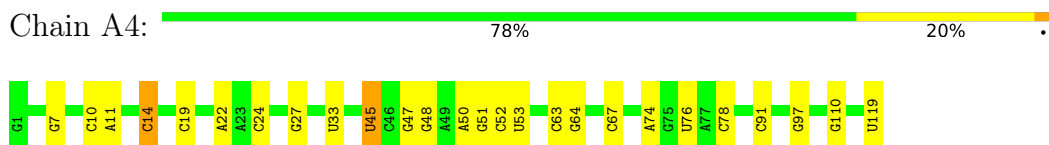
• Molecule 38: ribosomal protein eS30



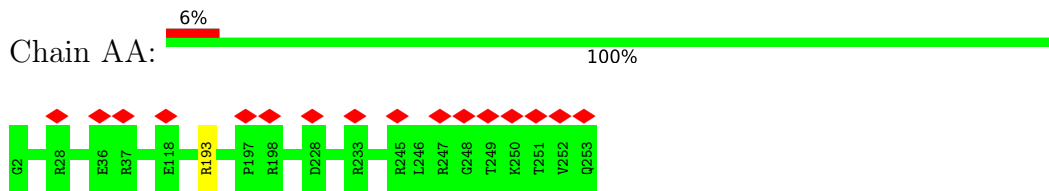
• Molecule 39: 5.8S ribosomal RNA



• Molecule 40: 5S ribosomal RNA

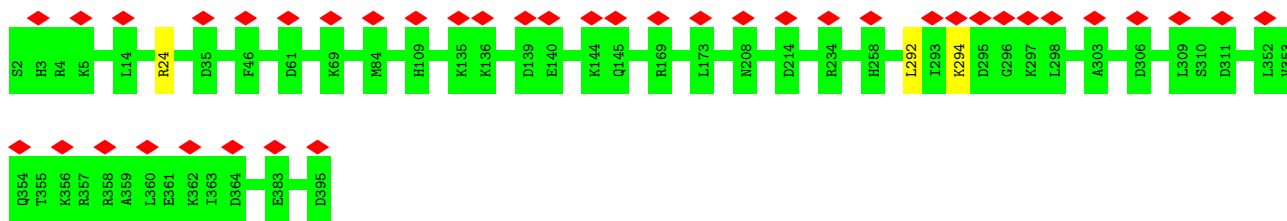


• Molecule 41: Ribosomal protein L8



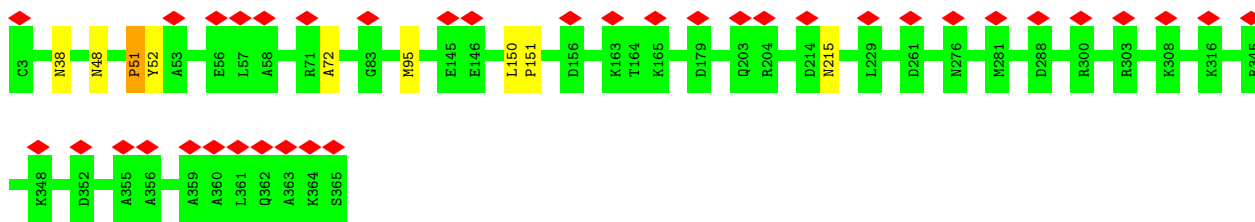
• Molecule 42: ribosomal protein uL3





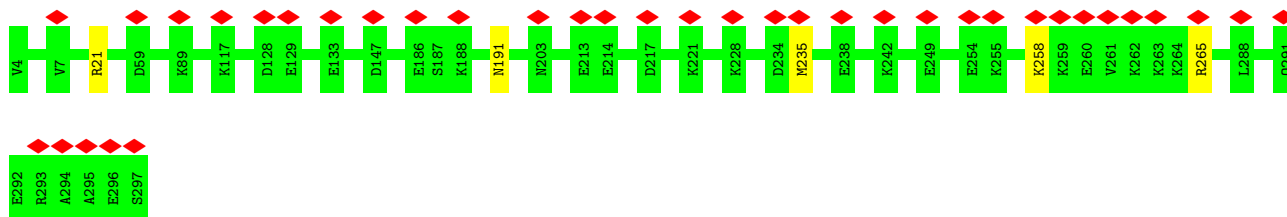
- Molecule 43: ribosomal protein uL4

Chain AC: 10% 98%



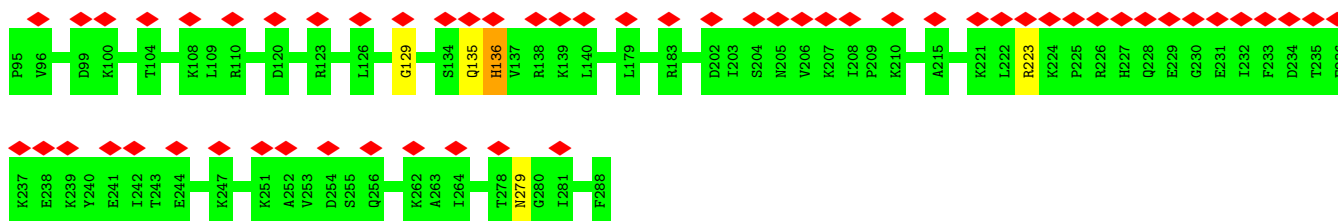
- Molecule 44: ribosomal protein uL18

Chain AD: 13% 98%



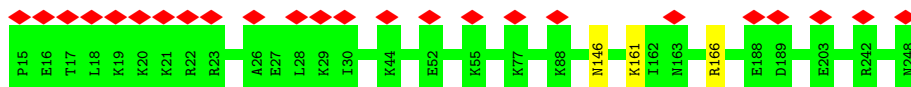
- Molecule 45: ribosomal protein eL6

Chain AE: 29% 97%

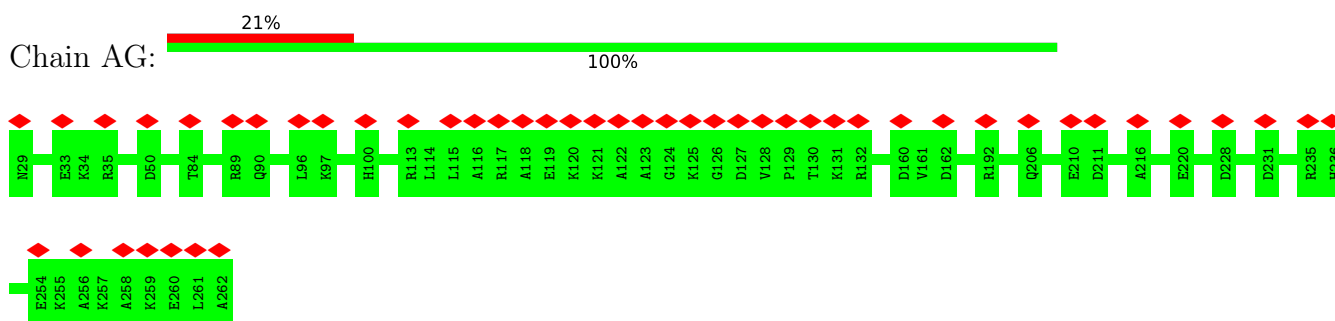


- Molecule 46: ribosomal protein uL30

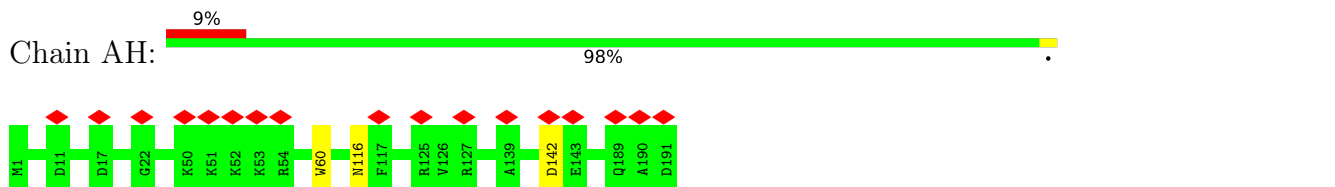
Chain AF: 10% 99%



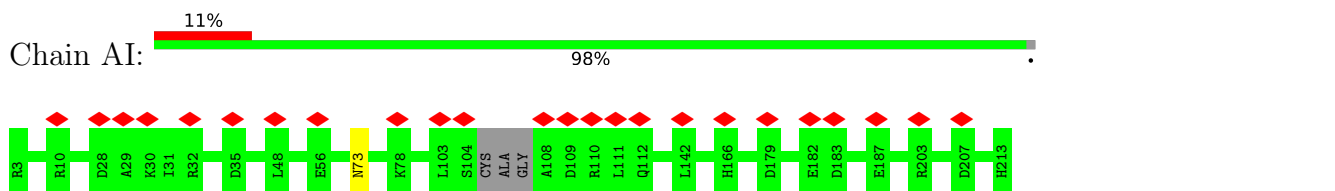
- Molecule 47: ribosomal protein eL8



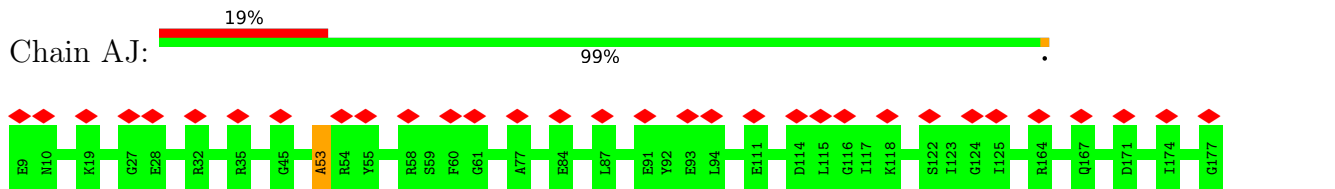
- Molecule 48: ribosomal protein uL6



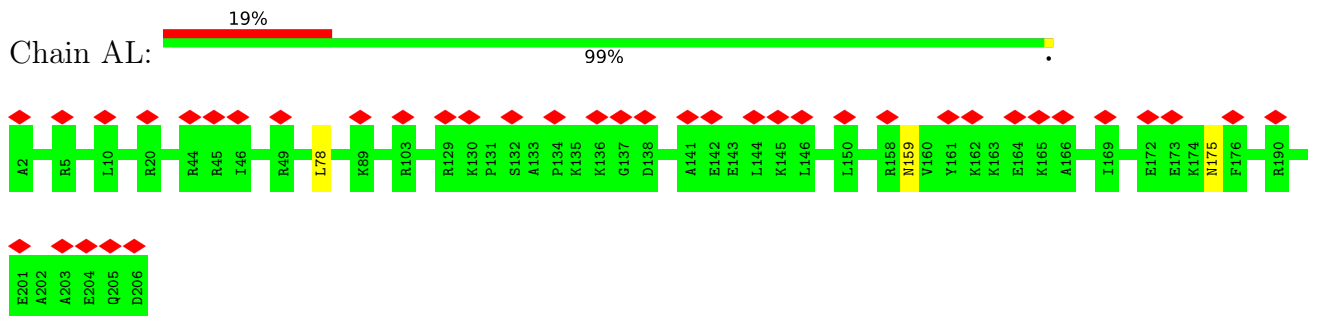
- Molecule 49: Ribosomal protein L10 (Predicted)



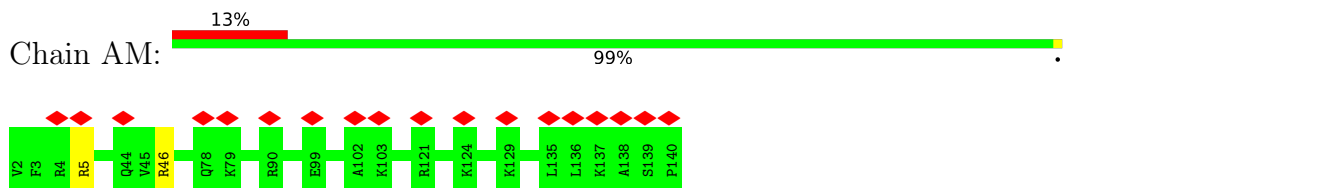
- Molecule 50: Ribosomal protein L11



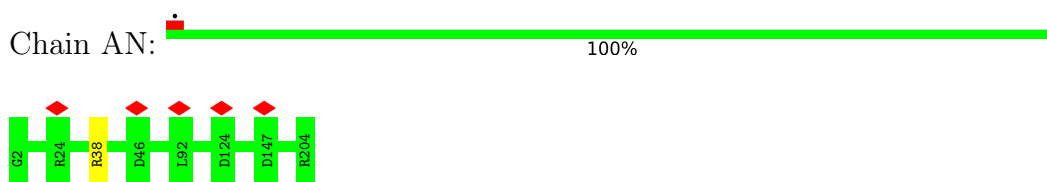
- Molecule 51: ribosomal protein eL13



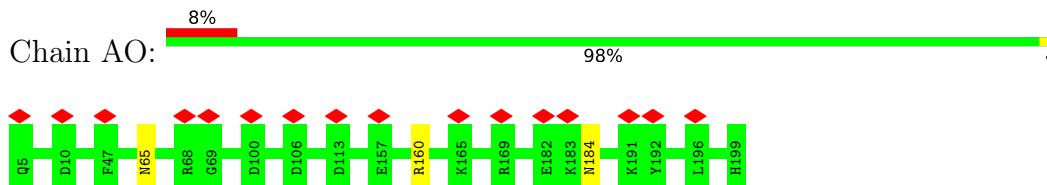
- Molecule 52: ribosomal protein eL14



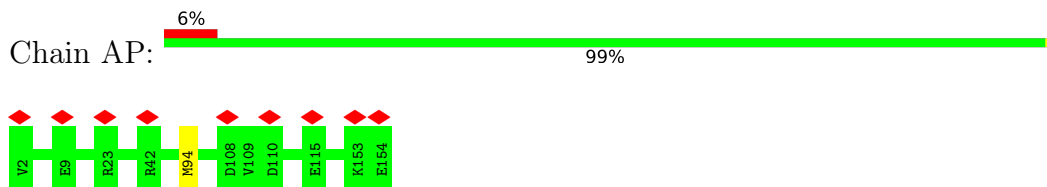
- Molecule 53: Ribosomal protein L15



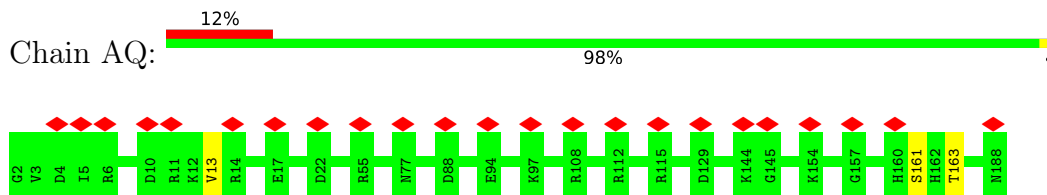
- Molecule 54: ribosomal protein uL13



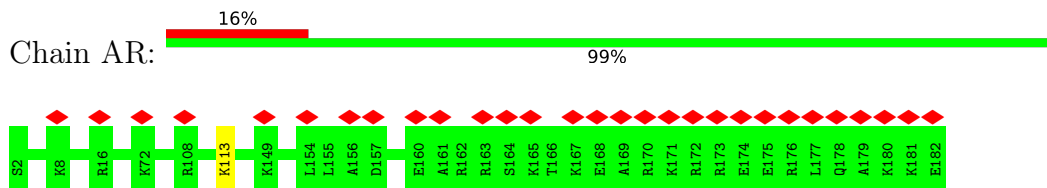
- Molecule 55: ribosomal protein uL22



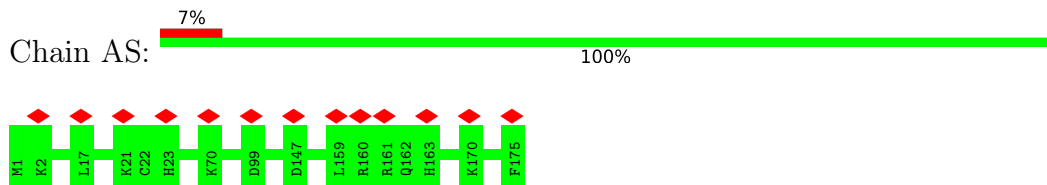
- Molecule 56: ribosomal protein eL18



- Molecule 57: ribosomal protein eL19

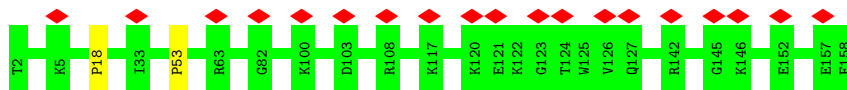


- Molecule 58: ribosomal protein eL20

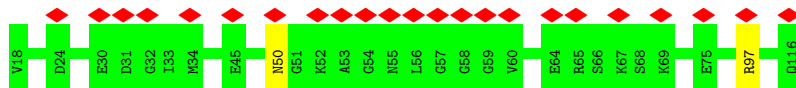


- Molecule 59: ribosomal protein eL21

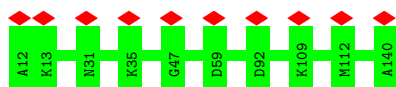




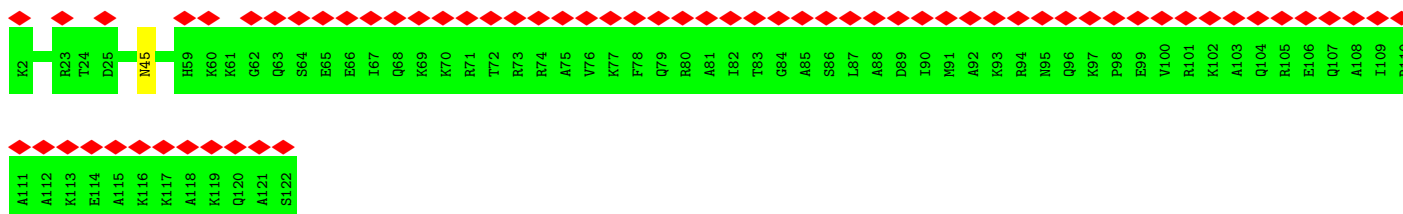
- Molecule 60: ribosomal protein eL22



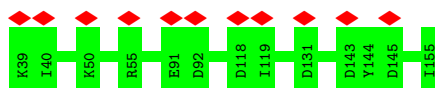
- Molecule 61: Ribosomal protein L23



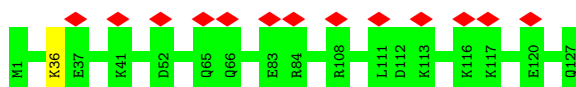
- Molecule 62: ribosomal protein eL24



- Molecule 63: ribosomal protein uL23

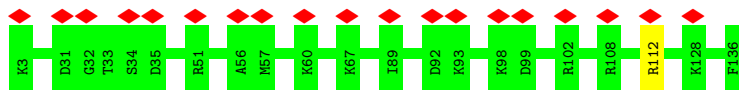


- Molecule 64: Ribosomal protein L26

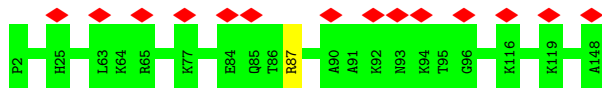


- Molecule 65: 60S ribosomal protein L27

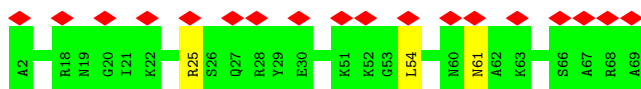




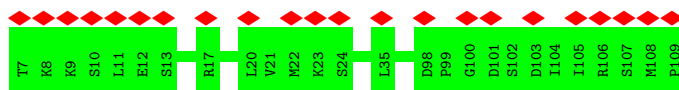
- Molecule 66: ribosomal protein uL15



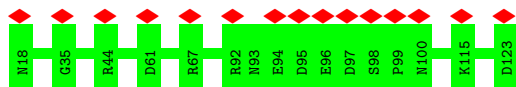
- Molecule 67: ribosomal protein eL29



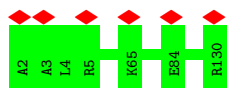
- Molecule 68: ribosomal protein eL30



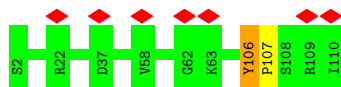
- Molecule 69: ribosomal protein eL31



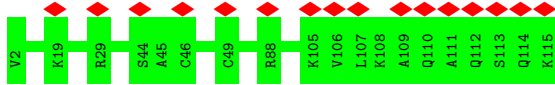
- Molecule 70: ribosomal protein eL32



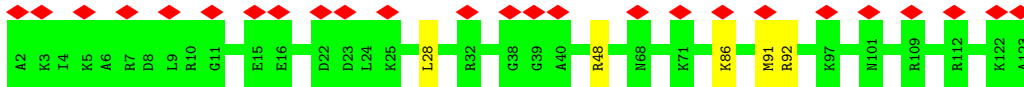
- Molecule 71: ribosomal protein eL33



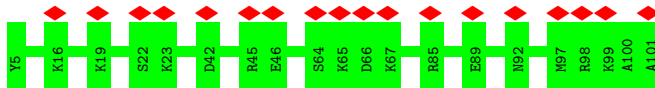
- Molecule 72: ribosomal protein eL34



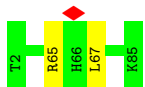
- Molecule 73: ribosomal protein uL29



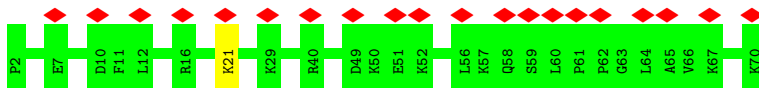
- Molecule 74: ribosomal protein eL36



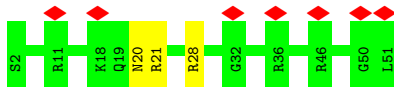
- Molecule 75: Ribosomal protein L37



- Molecule 76: ribosomal protein eL38

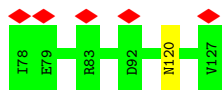


- Molecule 77: ribosomal protein eL39

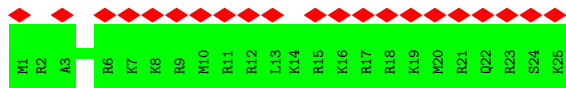
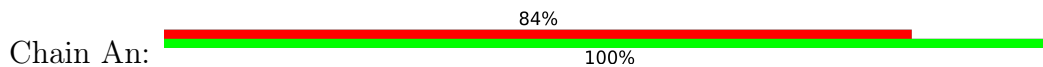


- Molecule 78: ribosomal protein eL40

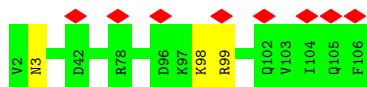




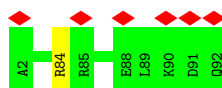
• Molecule 79: ribosomal protein eL41



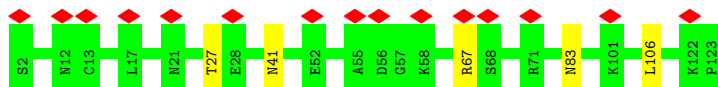
• Molecule 80: ribosomal protein eL42



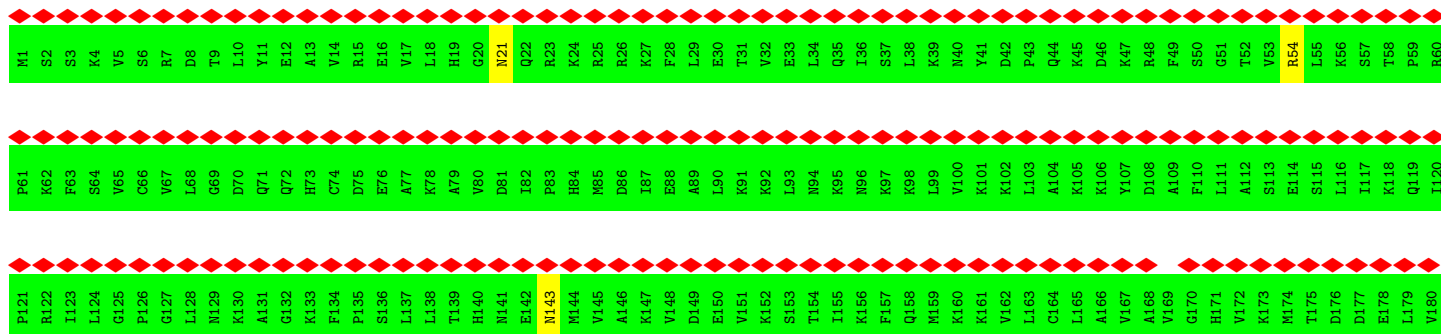
• Molecule 81: ribosomal protein eL43

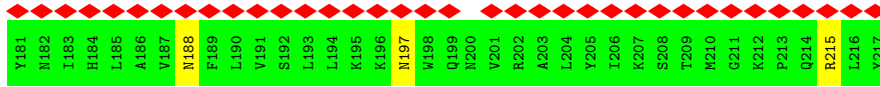


• Molecule 82: ribosomal protein eL28

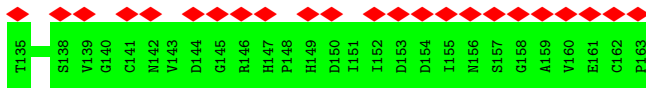
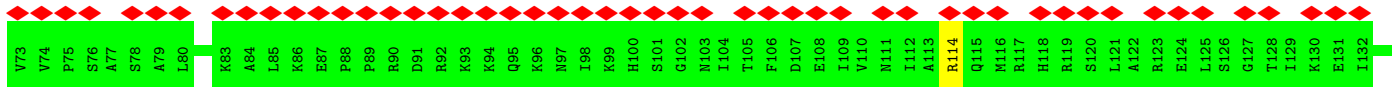
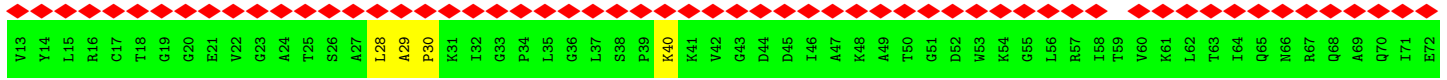


• Molecule 83: Ribosomal protein

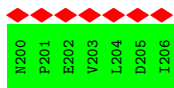
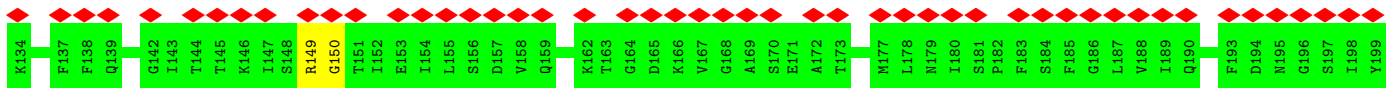
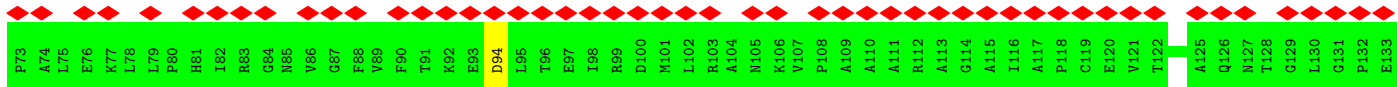
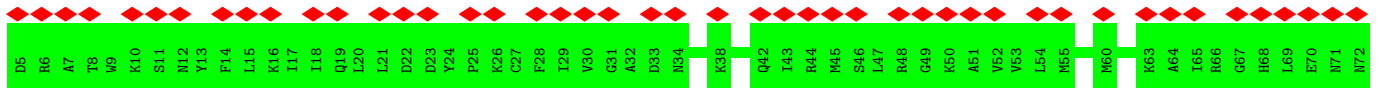
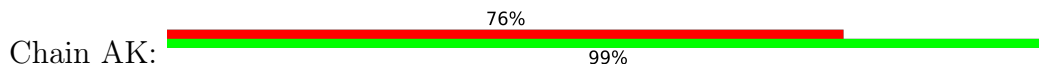




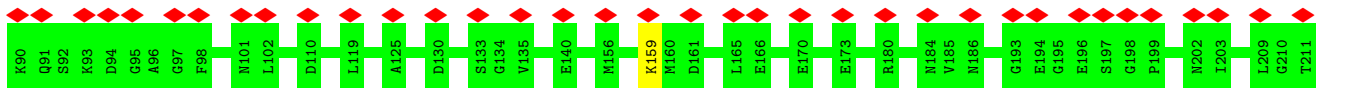
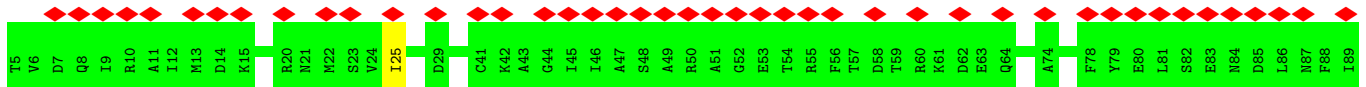
- Molecule 84: Ribosomal protein L12

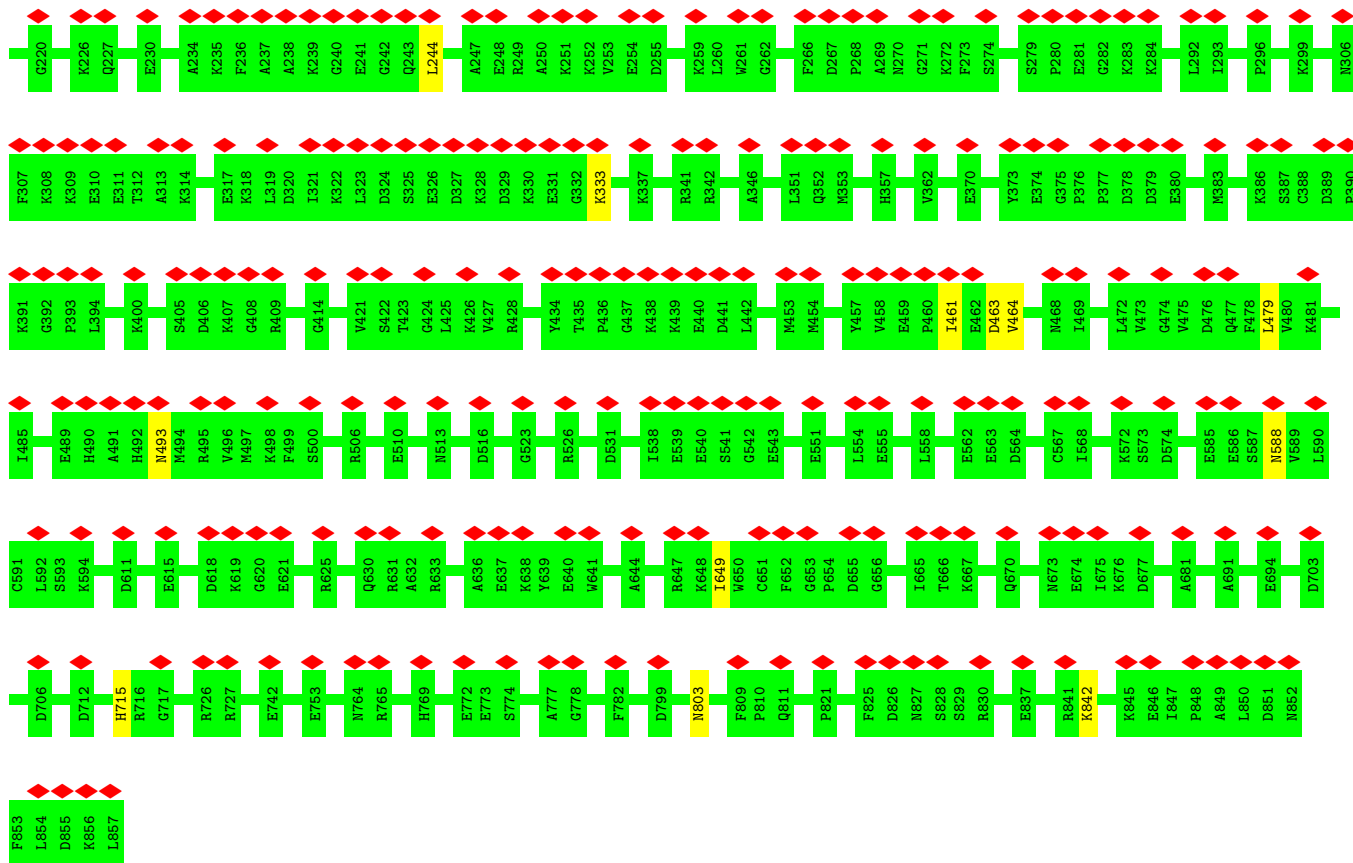


- Molecule 85: ribosomal protein uL10



- Molecule 86: eukaryotic elongation factor 2 (eEF2)





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	32386	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	11.639	Depositor
Minimum map value	-3.647	Depositor
Average map value	0.347	Depositor
Map value standard deviation	0.655	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, ZN, DDE, GNP

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	A2	0.32	0/86613	1.02	277/135108 (0.2%)
2	Bv	0.37	1/1810 (0.1%)	0.98	2/2817 (0.1%)
3	Bx	0.26	0/287	0.95	0/445
4	Bw	0.36	1/1819 (0.1%)	0.91	0/2833
5	B1	0.31	1/40767 (0.0%)	1.03	200/63536 (0.3%)
6	BD	0.27	0/1736	0.51	0/2338
7	BF	0.27	0/1524	0.55	0/2048
8	BK	0.27	0/851	0.58	0/1147
9	BM	0.25	0/941	0.57	0/1264
10	BP	0.31	0/1019	0.67	1/1361 (0.1%)
11	BQ	0.26	0/1126	0.55	0/1506
12	BR	0.26	0/1023	0.52	0/1373
13	BS	0.26	0/1172	0.53	0/1570
14	BT	0.27	0/1131	0.54	0/1515
15	BU	0.25	0/778	0.52	0/1045
16	BZ	0.27	0/696	0.61	0/929
17	Bc	0.26	0/490	0.53	0/656
18	Bd	0.29	0/437	0.56	0/580
19	Bf	0.25	0/613	0.47	0/811
20	Bg	0.27	0/2497	0.53	0/3399
21	BA	0.27	0/1741	0.54	0/2366
22	BB	0.27	0/1749	0.60	0/2340
23	BC	0.28	0/1761	0.53	0/2379
24	BE	0.27	0/2072	0.53	0/2793
25	BG	0.26	0/1907	0.51	0/2538
26	BH	0.26	0/1501	0.52	0/2009
27	BI	0.27	0/1725	0.55	0/2298
28	BJ	0.26	0/1520	0.53	1/2030 (0.0%)
29	BL	0.28	0/1281	0.56	1/1710 (0.1%)
30	BN	0.26	0/1226	0.53	0/1649
31	BO	0.26	0/1029	0.51	0/1380
32	BV	0.27	0/623	0.50	0/833

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BW	0.28	0/1051	0.53	0/1406
34	BX	0.28	0/1116	0.53	0/1490
35	BY	0.26	0/1032	0.50	0/1371
36	Ba	0.26	0/786	0.53	0/1053
37	Bb	0.26	0/637	0.50	0/854
38	Be	0.27	0/443	0.55	0/583
39	A3	0.32	0/3726	1.02	11/5804 (0.2%)
40	A4	0.34	0/2839	1.06	10/4425 (0.2%)
41	AA	0.28	0/1968	0.54	0/2639
42	AB	0.28	0/3246	0.54	1/4345 (0.0%)
43	AC	0.27	0/2942	0.53	0/3951
44	AD	0.28	0/2437	0.53	0/3262
45	AE	0.28	0/1603	0.59	0/2153
46	AF	0.27	0/1986	0.52	0/2644
47	AG	0.28	0/1913	0.55	0/2576
48	AH	0.28	0/1545	0.58	1/2077 (0.0%)
49	AI	0.26	0/1730	0.49	0/2311
50	AJ	0.27	0/1376	0.55	1/1841 (0.1%)
51	AL	0.28	0/1688	0.56	0/2260
52	AM	0.29	0/1161	0.52	0/1554
53	AN	0.28	0/1746	0.51	0/2338
54	AO	0.27	0/1638	0.48	0/2191
55	AP	0.26	0/1268	0.48	0/1701
56	AQ	0.27	0/1537	0.61	0/2052
57	AR	0.25	0/1533	0.48	0/2025
58	AS	0.27	0/1488	0.51	0/1997
59	AT	0.27	0/1312	0.48	0/1753
60	AU	0.27	0/822	0.49	0/1103
61	AV	0.27	0/983	0.49	0/1319
62	AW	0.27	0/1004	0.51	0/1332
63	AX	0.26	0/975	0.51	0/1312
64	AY	0.26	0/1081	0.46	0/1439
65	AZ	0.27	0/1126	0.54	0/1502
66	Aa	0.27	0/1191	0.52	0/1591
67	Ab	0.27	0/569	0.64	1/750 (0.1%)
68	Ac	0.26	0/812	0.53	0/1089
69	Ad	0.26	0/894	0.53	0/1204
70	Ae	0.27	0/1082	0.53	0/1443
71	Af	0.29	0/895	0.57	0/1198
72	Ag	0.28	0/916	0.58	0/1220
73	Ah	0.25	0/1023	0.56	1/1351 (0.1%)
74	Ai	0.26	0/805	0.50	0/1065
75	Aj	0.29	0/703	0.59	1/929 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	Ak	0.26	0/575	0.57	0/761
77	Al	0.25	0/454	0.53	0/599
78	Am	0.25	0/417	0.53	0/553
79	An	0.22	0/241	0.44	0/305
80	Ao	0.28	0/877	0.53	0/1156
81	Ap	0.27	0/718	0.57	0/953
82	At	0.28	0/995	0.65	1/1334 (0.1%)
83	Au	0.27	0/1772	0.54	0/2375
84	Aq	0.29	0/1155	0.72	1/1558 (0.1%)
85	AK	0.28	0/1580	0.59	1/2133 (0.0%)
86	Ct	0.29	0/6767	0.60	3/9139 (0.0%)
All	All	0.30	3/241644 (0.0%)	0.87	515/353975 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	BK	0	1
11	BQ	0	1
17	Bc	0	1
21	BA	0	1
22	BB	0	1
24	BE	0	1
27	BI	0	2
28	BJ	0	1
43	AC	0	2
44	AD	0	1
45	AE	0	3
48	AH	0	2
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	1
86	Ct	0	4
All	All	0	30

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Bv	1	G	OP3-P	-10.62	1.48	1.61
5	B1	1	U	OP3-P	-10.57	1.48	1.61
4	Bw	1	G	OP3-P	-10.55	1.48	1.61

All (515) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1440	C	N1-C2-O2	10.37	125.12	118.90
1	A2	252	C	N1-C2-O2	10.20	125.02	118.90
1	A2	191	C	N3-C2-O2	-9.77	115.06	121.90
5	B1	1315	U	C2-N1-C1'	9.42	129.01	117.70
5	B1	1315	U	N1-C2-O2	9.29	129.30	122.80
1	A2	972	C	N3-C2-O2	-9.15	115.49	121.90
5	B1	96	C	C2-N1-C1'	9.11	128.82	118.80
1	A2	2388	U	C2-N1-C1'	9.05	128.56	117.70
1	A2	2388	U	N1-C2-O2	9.00	129.10	122.80
1	A2	2388	U	N3-C2-O2	-8.91	115.96	122.20
5	B1	1315	U	N3-C2-O2	-8.81	116.03	122.20
5	B1	96	C	N1-C2-O2	8.79	124.17	118.90
5	B1	44	U	C2-N1-C1'	8.76	128.21	117.70
1	A2	1440	C	C2-N1-C1'	8.65	128.32	118.80
5	B1	1558	C	N1-C2-O2	8.63	124.08	118.90
1	A2	1895	C	N3-C2-O2	-8.58	115.89	121.90
1	A2	252	C	C2-N1-C1'	8.40	128.04	118.80
1	A2	2606	C	N1-C2-O2	8.35	123.91	118.90
1	A2	1576	C	N1-C2-O2	8.32	123.89	118.90
1	A2	1440	C	N3-C2-O2	-8.28	116.11	121.90
1	A2	3880	C	N1-C2-O2	8.25	123.85	118.90
5	B1	44	U	N1-C2-O2	8.24	128.57	122.80
5	B1	1512	C	C2-N1-C1'	8.22	127.84	118.80
1	A2	3890	C	C2-N1-C1'	8.18	127.80	118.80
1	A2	1440	C	C6-N1-C2	-8.16	117.03	120.30
1	A2	163	C	N1-C2-O2	8.16	123.80	118.90
5	B1	1591	C	N1-C2-O2	8.15	123.79	118.90
1	A2	2727	C	C2-N1-C1'	8.05	127.66	118.80
1	A2	1187	C	N3-C2-O2	-8.03	116.28	121.90
1	A2	2398	C	C2-N1-C1'	8.03	127.63	118.80
1	A2	703	C	N1-C2-O2	8.00	123.70	118.90
5	B1	1520	G	N3-C4-C5	-7.97	124.62	128.60
1	A2	191	C	N1-C2-O2	7.96	123.68	118.90
5	B1	118	C	N1-C2-O2	7.94	123.66	118.90
1	A2	905	G	C4-N9-C1'	7.89	136.76	126.50
1	A2	252	C	N3-C2-O2	-7.89	116.38	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B1	67	C	C2-N1-C1'	7.85	127.44	118.80
1	A2	1256	G	C4-N9-C1'	7.84	136.69	126.50
1	A2	1576	C	N3-C2-O2	-7.79	116.45	121.90
5	B1	1271	C	N1-C2-O2	7.77	123.56	118.90
5	B1	67	C	N1-C2-O2	7.76	123.56	118.90
5	B1	44	U	N3-C2-O2	-7.74	116.78	122.20
5	B1	1019	C	N3-C2-O2	-7.73	116.49	121.90
5	B1	579	C	N1-C2-O2	7.70	123.52	118.90
1	A2	2398	C	N1-C2-O2	7.70	123.52	118.90
5	B1	1117	C	N1-C2-O2	7.68	123.51	118.90
5	B1	96	C	N3-C2-O2	-7.64	116.55	121.90
5	B1	621	C	C2-N1-C1'	7.63	127.20	118.80
1	A2	1256	G	N3-C4-N9	7.63	130.58	126.00
5	B1	1237	C	N1-C2-O2	7.62	123.47	118.90
1	A2	1256	G	N3-C4-C5	-7.59	124.81	128.60
40	A4	24	C	N1-C2-O2	7.57	123.44	118.90
1	A2	1576	C	C6-N1-C2	-7.54	117.28	120.30
1	A2	77	U	N3-C2-O2	-7.52	116.94	122.20
1	A2	905	G	N3-C4-C5	-7.51	124.84	128.60
5	B1	1389	C	C2-N1-C1'	7.50	127.05	118.80
1	A2	972	C	N1-C2-O2	7.50	123.40	118.90
5	B1	918	U	N1-C2-O2	7.47	128.03	122.80
5	B1	1117	C	C6-N1-C2	-7.47	117.31	120.30
1	A2	138	C	N1-C2-O2	7.43	123.36	118.90
1	A2	4671	U	N1-C2-O2	7.41	127.99	122.80
1	A2	4079	C	N1-C2-O2	7.41	123.34	118.90
5	B1	1389	C	N1-C2-O2	7.41	123.34	118.90
5	B1	1019	C	N1-C2-O2	7.38	123.33	118.90
1	A2	3880	C	N3-C2-O2	-7.35	116.76	121.90
1	A2	4464	C	N1-C2-O2	7.35	123.31	118.90
5	B1	1558	C	C2-N1-C1'	7.30	126.83	118.80
5	B1	496	C	N1-C2-O2	7.29	123.27	118.90
5	B1	1464	C	N1-C2-O2	7.28	123.27	118.90
1	A2	2260	U	N1-C2-O2	7.25	127.87	122.80
5	B1	210	U	N1-C2-O2	7.23	127.86	122.80
5	B1	1710	C	N1-C2-O2	7.22	123.23	118.90
5	B1	1558	C	N3-C2-O2	-7.22	116.85	121.90
5	B1	1520	G	C4-N9-C1'	7.20	135.86	126.50
1	A2	4880	C	C2-N1-C1'	7.20	126.72	118.80
1	A2	2373	G	C4-N9-C1'	7.19	135.85	126.50
5	B1	797	C	P-O3'-C3'	7.18	128.32	119.70
1	A2	1746	G	C4-N9-C1'	7.16	135.81	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	905	G	N3-C4-N9	7.15	130.29	126.00
1	A2	1466	G	C4-N9-C1'	7.15	135.79	126.50
1	A2	4909	G	C4-N9-C1'	7.15	135.79	126.50
1	A2	4946	U	OP1-P-O3'	7.14	120.90	105.20
5	B1	402	C	N1-C2-O2	7.10	123.16	118.90
1	A2	2260	U	N3-C2-O2	-7.09	117.24	122.20
5	B1	227	U	P-O3'-C3'	7.07	128.19	119.70
1	A2	2606	C	C2-N1-C1'	7.05	126.56	118.80
1	A2	14	C	C2-N1-C1'	7.02	126.52	118.80
1	A2	4671	U	N3-C2-O2	-7.01	117.29	122.20
5	B1	1389	C	C6-N1-C2	-6.98	117.51	120.30
1	A2	2727	C	N1-C2-O2	6.97	123.08	118.90
1	A2	2499	C	C2-N1-C1'	6.97	126.46	118.80
1	A2	4909	G	N3-C4-N9	6.94	130.17	126.00
1	A2	1440	C	C5-C6-N1	6.92	124.46	121.00
5	B1	570	C	N1-C2-O2	6.89	123.03	118.90
1	A2	2478	C	N3-C2-O2	-6.89	117.08	121.90
1	A2	918	C	N1-C2-O2	6.85	123.01	118.90
5	B1	1464	C	C6-N1-C2	-6.85	117.56	120.30
1	A2	2798	U	N3-C2-O2	-6.85	117.41	122.20
1	A2	3880	C	C6-N1-C2	-6.85	117.56	120.30
1	A2	2798	U	N1-C2-O2	6.84	127.59	122.80
1	A2	2499	C	N1-C2-O2	6.83	123.00	118.90
5	B1	1117	C	N3-C2-O2	-6.83	117.12	121.90
5	B1	1624	U	N1-C2-O2	6.83	127.58	122.80
1	A2	1193	C	N1-C2-O2	6.82	122.99	118.90
1	A2	1576	C	C2-N1-C1'	6.80	126.28	118.80
5	B1	1237	C	C2-N1-C1'	6.80	126.28	118.80
1	A2	252	C	C6-N1-C2	-6.79	117.59	120.30
5	B1	842	C	C2-N1-C1'	6.78	126.26	118.80
5	B1	1520	G	N3-C4-N9	6.78	130.07	126.00
1	A2	4946	U	P-O3'-C3'	6.76	127.82	119.70
1	A2	1746	G	N3-C4-C5	-6.76	125.22	128.60
1	A2	2606	C	N3-C2-O2	-6.76	117.17	121.90
5	B1	210	U	N3-C2-O2	-6.76	117.47	122.20
42	AB	292	LEU	CA-CB-CG	6.74	130.81	115.30
1	A2	1187	C	N1-C2-O2	6.74	122.94	118.90
1	A2	1466	G	N3-C4-N9	6.73	130.04	126.00
5	B1	620	G	N3-C4-C5	-6.73	125.23	128.60
5	B1	918	U	N3-C2-O2	-6.72	117.50	122.20
1	A2	1256	G	C8-N9-C1'	-6.71	118.28	127.00
5	B1	1512	C	C6-N1-C2	-6.68	117.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	163	C	N3-C2-O2	-6.67	117.23	121.90
5	B1	1389	C	N3-C2-O2	-6.67	117.23	121.90
1	A2	50	C	N1-C2-O2	6.67	122.90	118.90
82	At	106	LEU	CA-CB-CG	6.64	130.58	115.30
5	B1	1558	C	C6-N1-C2	-6.63	117.65	120.30
1	A2	2478	C	N1-C2-O2	6.61	122.86	118.90
1	A2	1466	G	N3-C4-C5	-6.60	125.30	128.60
1	A2	2256	C	C2-N1-C1'	6.60	126.06	118.80
86	Ct	244	LEU	CA-CB-CG	6.60	130.47	115.30
1	A2	31	U	P-O3'-C3'	6.58	127.59	119.70
1	A2	1083	U	N3-C2-O2	-6.57	117.60	122.20
39	A3	126	C	N1-C2-O2	6.57	122.84	118.90
5	B1	1314	U	N1-C2-O2	6.56	127.39	122.80
5	B1	620	G	N3-C4-N9	6.56	129.94	126.00
1	A2	905	G	C8-N9-C1'	-6.54	118.50	127.00
1	A2	2649	C	C2-N1-C1'	6.54	126.00	118.80
5	B1	1591	C	N3-C2-O2	-6.53	117.33	121.90
1	A2	3607	C	C6-N1-C2	-6.52	117.69	120.30
1	A2	77	U	N1-C2-O2	6.51	127.36	122.80
1	A2	1746	G	N3-C4-N9	6.50	129.90	126.00
5	B1	118	C	C2-N1-C1'	6.50	125.95	118.80
1	A2	703	C	N3-C2-O2	-6.47	117.37	121.90
1	A2	4909	G	C8-N9-C1'	-6.47	118.58	127.00
1	A2	3880	C	C2-N1-C1'	6.46	125.91	118.80
1	A2	4079	C	C2-N1-C1'	6.46	125.90	118.80
1	A2	2373	G	N3-C4-C5	-6.44	125.38	128.60
1	A2	2373	G	N3-C4-N9	6.43	129.86	126.00
5	B1	118	C	N3-C2-O2	-6.43	117.40	121.90
5	B1	1684	C	N1-C2-O2	6.41	122.75	118.90
67	Ab	54	LEU	CA-CB-CG	6.41	130.05	115.30
5	B1	233	C	N1-C2-O2	6.40	122.74	118.90
5	B1	96	C	C6-N1-C1'	-6.39	113.13	120.80
39	A3	126	C	C2-N1-C1'	6.38	125.82	118.80
1	A2	2398	C	N3-C2-O2	-6.38	117.43	121.90
5	B1	621	C	N3-C2-O2	-6.38	117.44	121.90
5	B1	1624	U	N3-C2-O2	-6.38	117.74	122.20
40	A4	52	C	N3-C2-O2	-6.37	117.44	121.90
1	A2	1989	U	O4'-C1'-N1	6.37	113.30	108.20
5	B1	1237	C	C6-N1-C2	-6.37	117.75	120.30
5	B1	1464	C	N3-C2-O2	-6.37	117.44	121.90
1	A2	4575	C	N1-C2-O2	6.35	122.71	118.90
5	B1	89	C	C2-N1-C1'	6.35	125.78	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	4928	C	N1-C2-O2	6.33	122.70	118.90
5	B1	1156	U	N1-C2-O2	6.33	127.23	122.80
5	B1	496	C	C2-N1-C1'	6.32	125.75	118.80
1	A2	2798	U	C2-N1-C1'	6.31	125.27	117.70
5	B1	1472	C	C2-N1-C1'	6.30	125.73	118.80
5	B1	1753	C	C2-N1-C1'	6.30	125.73	118.80
1	A2	971	C	N3-C2-O2	-6.29	117.50	121.90
5	B1	1292	C	N1-C2-O2	6.28	122.67	118.90
1	A2	2389	C	C2-N1-C1'	6.28	125.70	118.80
5	B1	1117	C	C2-N1-C1'	6.28	125.70	118.80
1	A2	4464	C	N3-C2-O2	-6.27	117.51	121.90
1	A2	3890	C	C6-N1-C2	-6.25	117.80	120.30
5	B1	496	C	N3-C2-O2	-6.25	117.53	121.90
2	Bv	36	C	C2-N1-C1'	6.24	125.66	118.80
1	A2	219	C	C2-N1-C1'	6.24	125.66	118.80
5	B1	106	C	C2-N1-C1'	6.23	125.65	118.80
73	Ah	28	LEU	CA-CB-CG	6.23	129.63	115.30
1	A2	1083	U	C2-N1-C1'	6.23	125.17	117.70
5	B1	918	U	C2-N1-C1'	6.22	125.17	117.70
1	A2	1668	C	N1-C2-O2	6.22	122.63	118.90
1	A2	2727	C	N3-C2-O2	-6.22	117.54	121.90
1	A2	4514	U	N1-C2-O2	6.21	127.14	122.80
5	B1	579	C	N3-C2-O2	-6.20	117.56	121.90
5	B1	950	C	N1-C2-O2	6.20	122.62	118.90
1	A2	901	U	P-O3'-C3'	6.19	127.13	119.70
1	A2	14	C	C6-N1-C2	-6.19	117.83	120.30
1	A2	1500	A	P-O3'-C3'	6.19	127.12	119.70
1	A2	493	G	N3-C4-N9	6.18	129.71	126.00
5	B1	1512	C	N1-C2-O2	6.18	122.61	118.90
5	B1	1710	C	C2-N1-C1'	6.18	125.60	118.80
1	A2	4671	U	C2-N1-C1'	6.17	125.10	117.70
5	B1	659	G	C4-N9-C1'	6.15	134.49	126.50
1	A2	71	C	P-O3'-C3'	6.14	127.06	119.70
1	A2	4069	G	C4-N9-C1'	6.13	134.47	126.50
5	B1	1156	U	N3-C2-O2	-6.12	117.91	122.20
5	B1	1557	C	C2-N1-C1'	6.12	125.53	118.80
5	B1	67	C	N3-C2-O2	-6.11	117.62	121.90
5	B1	824	C	N1-C2-O2	6.11	122.56	118.90
1	A2	4880	C	N1-C2-O2	6.10	122.56	118.90
1	A2	2606	C	C6-N1-C2	-6.10	117.86	120.30
5	B1	1271	C	C2-N1-C1'	6.10	125.51	118.80
1	A2	1938	U	N3-C2-O2	-6.09	117.93	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1564	U	C2-N1-C1'	6.08	125.00	117.70
5	B1	579	C	C2-N1-C1'	6.08	125.48	118.80
75	Aj	67	LEU	CA-CB-CG	6.07	129.27	115.30
1	A2	493	G	C4-N9-C1'	6.06	134.38	126.50
40	A4	24	C	N3-C2-O2	-6.06	117.66	121.90
1	A2	2835	C	N1-C2-O2	6.06	122.53	118.90
5	B1	210	U	C2-N1-C1'	6.05	124.96	117.70
1	A2	4133	C	N1-C2-O2	6.05	122.53	118.90
1	A2	703	C	C2-N1-C1'	6.04	125.45	118.80
1	A2	703	C	C6-N1-C2	-6.04	117.88	120.30
1	A2	1938	U	N1-C2-O2	6.04	127.03	122.80
5	B1	100	U	N1-C2-O2	6.03	127.02	122.80
5	B1	1271	C	N3-C2-O2	-6.02	117.69	121.90
1	A2	1466	G	C8-N9-C1'	-6.02	119.18	127.00
1	A2	4602	C	N1-C2-O2	6.00	122.50	118.90
5	B1	1557	C	N1-C2-O2	6.00	122.50	118.90
5	B1	1156	U	C2-N1-C1'	5.99	124.89	117.70
1	A2	1638	U	N1-C2-O2	5.99	127.00	122.80
5	B1	621	C	N1-C2-O2	5.98	122.49	118.90
5	B1	1590	C	N1-C2-O2	5.96	122.48	118.90
1	A2	2871	C	C2-N1-C1'	5.96	125.36	118.80
1	A2	918	C	C2-N1-C1'	5.96	125.36	118.80
1	A2	236	C	N1-C2-O2	5.96	122.47	118.90
1	A2	4824	C	N1-C2-O2	5.96	122.47	118.90
1	A2	962	C	N1-C2-O2	5.95	122.47	118.90
1	A2	4676	C	N1-C2-O2	5.95	122.47	118.90
1	A2	2799	C	N1-C2-O2	5.95	122.47	118.90
1	A2	3890	C	C5-C6-N1	5.95	123.97	121.00
5	B1	118	C	C6-N1-C2	-5.95	117.92	120.30
5	B1	1315	U	C6-N1-C1'	-5.93	112.89	121.20
39	A3	116	C	C2-N1-C1'	5.93	125.33	118.80
1	A2	3903	U	N3-C2-O2	-5.93	118.05	122.20
5	B1	179	C	N1-C2-O2	5.93	122.46	118.90
1	A2	1746	G	C8-N9-C1'	-5.92	119.30	127.00
1	A2	252	C	C5-C6-N1	5.92	123.96	121.00
5	B1	1852	C	C2-N1-C1'	5.91	125.31	118.80
1	A2	1668	C	N3-C2-O2	-5.90	117.77	121.90
5	B1	620	G	C4-N9-C1'	5.90	134.16	126.50
1	A2	163	C	C2-N1-C1'	5.89	125.28	118.80
1	A2	4909	G	N3-C4-C5	-5.88	125.66	128.60
1	A2	2388	U	C6-N1-C1'	-5.88	112.97	121.20
5	B1	1464	C	C2-N1-C1'	5.88	125.26	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B1	1591	C	C2-N1-C1'	5.88	125.26	118.80
1	A2	664	C	N1-C2-O2	5.87	122.42	118.90
1	A2	3903	U	N1-C2-O2	5.87	126.91	122.80
5	B1	1554	C	P-O3'-C3'	5.87	126.74	119.70
5	B1	1022	U	C2-N1-C1'	5.85	124.72	117.70
1	A2	2373	G	C8-N9-C1'	-5.85	119.39	127.00
1	A2	138	C	N3-C2-O2	-5.85	117.81	121.90
1	A2	4079	C	N3-C2-O2	-5.84	117.81	121.90
5	B1	1520	G	C2-N3-C4	5.84	114.82	111.90
5	B1	1314	U	N3-C2-O2	-5.83	118.12	122.20
1	A2	670	C	C2-N1-C1'	5.82	125.21	118.80
1	A2	1256	G	C2-N3-C4	5.82	114.81	111.90
5	B1	1237	C	N3-C2-O2	-5.82	117.83	121.90
1	A2	1424	C	N1-C2-O2	5.81	122.39	118.90
1	A2	685	C	N1-C2-O2	5.81	122.38	118.90
5	B1	1742	C	C2-N1-C1'	5.80	125.18	118.80
5	B1	1512	C	C5-C6-N1	5.80	123.90	121.00
5	B1	842	C	N1-C2-O2	5.78	122.37	118.90
1	A2	4514	U	N3-C2-O2	-5.78	118.16	122.20
1	A2	1737	C	N1-C2-O2	5.75	122.35	118.90
1	A2	4866	G	O5'-P-OP1	-5.75	100.53	105.70
1	A2	3738	C	N1-C2-O2	5.74	122.34	118.90
1	A2	275	U	N3-C2-O2	-5.73	118.19	122.20
39	A3	99	U	C2-N1-C1'	5.73	124.57	117.70
1	A2	100	C	N1-C2-O2	5.72	122.33	118.90
1	A2	1193	C	N3-C2-O2	-5.71	117.90	121.90
1	A2	1794	C	C2-N1-C1'	5.71	125.08	118.80
1	A2	3759	C	N1-C2-O2	5.71	122.33	118.90
5	B1	1523	C	C2-N1-C1'	5.71	125.08	118.80
1	A2	651	C	N3-C2-O2	-5.70	117.91	121.90
1	A2	4624	C	C6-N1-C2	-5.70	118.02	120.30
5	B1	1714	U	C2-N1-C1'	5.70	124.54	117.70
5	B1	621	C	C6-N1-C2	-5.70	118.02	120.30
5	B1	96	C	C6-N1-C2	-5.67	118.03	120.30
1	A2	3664	U	N1-C2-O2	5.67	126.77	122.80
1	A2	4574	C	N1-C2-O2	5.67	122.30	118.90
1	A2	890	C	N1-C2-O2	5.67	122.30	118.90
1	A2	4177	C	N1-C2-O2	5.66	122.30	118.90
1	A2	1717	U	N1-C2-O2	5.66	126.76	122.80
1	A2	4216	G	N3-C4-C5	-5.66	125.77	128.60
5	B1	570	C	N3-C2-O2	-5.65	117.94	121.90
5	B1	1591	C	C6-N1-C2	-5.64	118.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1930	U	C2-N1-C1'	5.64	124.47	117.70
5	B1	1315	U	C5-C6-N1	5.64	125.52	122.70
1	A2	1713	C	C2-N1-C1'	5.63	125.00	118.80
1	A2	1589	C	N1-C2-O2	5.63	122.28	118.90
1	A2	2691	G	N3-C4-N9	5.63	129.38	126.00
1	A2	4069	G	N3-C4-C5	-5.62	125.79	128.60
1	A2	3890	C	N1-C2-O2	5.62	122.27	118.90
5	B1	1811	C	C2-N1-C1'	5.62	124.98	118.80
5	B1	1710	C	N3-C2-O2	-5.61	117.97	121.90
48	AH	142	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A2	2727	C	C6-N1-C1'	-5.60	114.08	120.80
40	A4	19	C	C2-N1-C1'	5.60	124.96	118.80
1	A2	3607	C	N3-C2-O2	-5.60	117.98	121.90
84	Aq	28	LEU	CA-CB-CG	5.59	128.16	115.30
1	A2	2499	C	N3-C2-O2	-5.59	117.99	121.90
1	A2	3742	C	N3-C2-O2	-5.58	117.99	121.90
5	B1	44	U	C6-N1-C1'	-5.58	113.39	121.20
5	B1	459	C	C2-N1-C1'	5.57	124.93	118.80
5	B1	1710	C	C6-N1-C2	-5.57	118.07	120.30
5	B1	4	C	N1-C2-O2	5.56	122.24	118.90
1	A2	972	C	C6-N1-C2	-5.56	118.08	120.30
50	AJ	53	ALA	C-N-CA	5.55	135.58	121.70
1	A2	1773	U	N1-C2-O2	5.55	126.68	122.80
5	B1	100	U	N3-C2-O2	-5.54	118.32	122.20
1	A2	3607	C	N1-C2-O2	5.54	122.23	118.90
1	A2	4216	G	N3-C4-N9	5.54	129.32	126.00
40	A4	24	C	C2-N1-C1'	5.54	124.89	118.80
1	A2	2398	C	C6-N1-C2	-5.54	118.08	120.30
1	A2	959	C	P-O3'-C3'	5.54	126.34	119.70
1	A2	4406	C	N1-C2-O2	5.53	122.22	118.90
5	B1	579	C	C6-N1-C2	-5.53	118.09	120.30
5	B1	337	C	N3-C2-O2	-5.52	118.03	121.90
1	A2	2325	C	N1-C2-O2	5.52	122.21	118.90
1	A2	163	C	C6-N1-C2	-5.52	118.09	120.30
5	B1	1287	A	C2-N3-C4	5.51	113.36	110.60
1	A2	191	C	C6-N1-C2	-5.51	118.10	120.30
5	B1	89	C	C6-N1-C2	-5.51	118.10	120.30
1	A2	2649	C	N1-C2-O2	5.51	122.20	118.90
1	A2	4711	C	C6-N1-C2	-5.50	118.10	120.30
1	A2	2840	C	N1-C2-O2	5.50	122.20	118.90
40	A4	45	U	C2-N1-C1'	5.50	124.30	117.70
5	B1	1520	G	C8-N9-C1'	-5.50	119.85	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	3664	U	N3-C2-O2	-5.50	118.35	122.20
39	A3	57	C	N3-C2-O2	-5.49	118.06	121.90
1	A2	4270	C	N1-C2-O2	5.48	122.19	118.90
40	A4	14	C	C2-N1-C1'	5.48	124.83	118.80
1	A2	4514	U	C2-N1-C1'	5.48	124.28	117.70
5	B1	1753	C	C6-N1-C2	-5.48	118.11	120.30
5	B1	659	G	C8-N9-C1'	-5.48	119.88	127.00
5	B1	459	C	N1-C2-O2	5.48	122.19	118.90
1	A2	4364	C	N1-C2-O2	5.47	122.19	118.90
1	A2	4856	G	C4-N9-C1'	5.47	133.62	126.50
5	B1	1271	C	C6-N1-C2	-5.46	118.11	120.30
1	A2	2800	U	N1-C2-O2	5.46	126.62	122.80
5	B1	804	U	N1-C2-O2	5.46	126.62	122.80
1	A2	2260	U	C2-N1-C1'	5.45	124.24	117.70
1	A2	4602	C	C2-N1-C1'	5.45	124.79	118.80
5	B1	1472	C	C6-N1-C2	-5.44	118.12	120.30
1	A2	3890	C	C6-N1-C1'	-5.44	114.27	120.80
1	A2	2444	C	N1-C2-O2	5.43	122.16	118.90
40	A4	24	C	C6-N1-C2	-5.43	118.13	120.30
1	A2	2398	C	C6-N1-C1'	-5.43	114.28	120.80
1	A2	289	A	C2-N3-C4	5.42	113.31	110.60
1	A2	682	U	N3-C2-O2	-5.42	118.41	122.20
5	B1	4	C	C2-N1-C1'	5.42	124.76	118.80
5	B1	1551	U	C2-N1-C1'	5.40	124.18	117.70
5	B1	67	C	C6-N1-C1'	-5.39	114.33	120.80
1	A2	252	C	C6-N1-C1'	-5.39	114.33	120.80
5	B1	402	C	N3-C2-O2	-5.39	118.13	121.90
39	A3	8	U	C2-N1-C1'	5.39	124.17	117.70
5	B1	1472	C	N1-C2-O2	5.38	122.13	118.90
5	B1	1117	C	C5-C6-N1	5.38	123.69	121.00
1	A2	685	C	N3-C2-O2	-5.37	118.14	121.90
1	A2	1717	U	N3-C2-O2	-5.37	118.44	122.20
1	A2	214	C	N1-C2-O2	5.37	122.12	118.90
5	B1	1292	C	N3-C2-O2	-5.37	118.14	121.90
1	A2	1737	C	C2-N1-C1'	5.37	124.70	118.80
5	B1	106	C	C5-C6-N1	5.37	123.68	121.00
5	B1	1120	U	C2-N1-C1'	5.37	124.14	117.70
1	A2	2511	C	N1-C2-O2	5.36	122.12	118.90
39	A3	129	C	C2-N1-C1'	5.36	124.69	118.80
1	A2	4216	G	C4-N9-C1'	5.36	133.46	126.50
5	B1	1242	U	N1-C2-O2	5.36	126.55	122.80
1	A2	3749	U	N1-C2-O2	5.35	126.55	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1638	U	N3-C2-O2	-5.35	118.46	122.20
1	A2	493	G	N3-C4-C5	-5.34	125.93	128.60
1	A2	4191	U	N1-C2-O2	5.34	126.54	122.80
1	A2	4947	U	OP1-P-OP2	-5.34	111.59	119.60
5	B1	556	U	N1-C2-O2	5.34	126.54	122.80
5	B1	1237	C	C5-C6-N1	5.34	123.67	121.00
86	Ct	479	LEU	CA-CB-CG	5.34	127.58	115.30
1	A2	493	G	C8-N9-C1'	-5.33	120.07	127.00
1	A2	4406	C	C2-N1-C1'	5.32	124.65	118.80
1	A2	1083	U	N1-C2-O2	5.32	126.52	122.80
1	A2	918	C	N3-C2-O2	-5.32	118.18	121.90
5	B1	556	U	N3-C2-O2	-5.32	118.48	122.20
5	B1	1472	C	N3-C2-O2	-5.31	118.18	121.90
1	A2	2800	U	N3-C2-O2	-5.31	118.48	122.20
1	A2	4545	C	C2-N1-C1'	5.31	124.64	118.80
1	A2	1187	C	C6-N1-C2	-5.31	118.18	120.30
39	A3	130	C	C2-N1-C1'	5.31	124.64	118.80
5	B1	106	C	C6-N1-C2	-5.30	118.18	120.30
1	A2	1938	U	C2-N1-C1'	5.30	124.06	117.70
1	A2	1773	U	N3-C2-O2	-5.30	118.49	122.20
5	B1	1520	G	C8-N9-C4	-5.30	104.28	106.40
5	B1	741	C	N1-C2-O2	5.30	122.08	118.90
1	A2	3863	U	N3-C2-O2	-5.30	118.49	122.20
1	A2	50	C	N3-C2-O2	-5.29	118.19	121.90
5	B1	189	U	N1-C2-O2	5.29	126.50	122.80
1	A2	276	C	N1-C2-O2	5.29	122.07	118.90
5	B1	1512	C	C6-N1-C1'	-5.28	114.46	120.80
39	A3	126	C	N3-C2-O2	-5.28	118.20	121.90
5	B1	568	C	N1-C2-O2	5.28	122.07	118.90
1	A2	1947	C	N1-C2-O2	5.28	122.06	118.90
5	B1	1590	C	C6-N1-C2	-5.27	118.19	120.30
1	A2	150	G	C4-N9-C1'	5.27	133.34	126.50
1	A2	2691	G	C4-N9-C1'	5.26	133.34	126.50
40	A4	78	C	C2-N1-C1'	5.26	124.59	118.80
39	A3	57	C	N1-C2-O2	5.26	122.05	118.90
1	A2	5008	C	C2-N1-C1'	5.25	124.58	118.80
1	A2	2646	C	N1-C2-O2	5.25	122.05	118.90
5	B1	1352	G	C4-N9-C1'	5.24	133.31	126.50
5	B1	833	C	N1-C2-O2	5.24	122.04	118.90
1	A2	4169	C	C2-N1-C1'	5.24	124.56	118.80
5	B1	233	C	C6-N1-C2	-5.23	118.21	120.30
5	B1	337	C	C6-N1-C2	-5.22	118.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BL	42	LEU	CA-CB-CG	5.22	127.31	115.30
5	B1	833	C	C5-C6-N1	5.22	123.61	121.00
1	A2	4954	C	C2-N1-C1'	5.22	124.54	118.80
28	BJ	119	LEU	CA-CB-CG	5.22	127.30	115.30
5	B1	570	C	C6-N1-C2	-5.21	118.22	120.30
5	B1	1032	C	C2-N1-C1'	5.21	124.53	118.80
1	A2	123	C	N1-C2-O2	5.21	122.02	118.90
1	A2	3853	C	C2-N1-C1'	5.21	124.53	118.80
1	A2	4575	C	N3-C2-O2	-5.20	118.26	121.90
5	B1	1555	U	C2-N1-C1'	5.20	123.94	117.70
5	B1	1017	U	N1-C2-O2	5.20	126.44	122.80
1	A2	2325	C	N3-C2-O2	-5.20	118.26	121.90
5	B1	67	C	C6-N1-C2	-5.20	118.22	120.30
5	B1	824	C	C2-N1-C1'	5.20	124.52	118.80
5	B1	1558	C	C5-C6-N1	5.20	123.60	121.00
5	B1	1639	G	C4-N9-C1'	5.20	133.25	126.50
1	A2	5008	C	N1-C2-O2	5.19	122.02	118.90
1	A2	2793	C	N1-C2-O2	5.19	122.01	118.90
5	B1	1684	C	N3-C2-O2	-5.18	118.27	121.90
5	B1	337	C	N1-C2-O2	5.18	122.01	118.90
5	B1	950	C	C6-N1-C2	-5.18	118.23	120.30
5	B1	459	C	C6-N1-C2	-5.17	118.23	120.30
5	B1	984	C	N3-C2-O2	-5.17	118.28	121.90
1	A2	1576	C	C5-C6-N1	5.17	123.58	121.00
1	A2	1789	C	N1-C2-O2	5.17	122.00	118.90
5	B1	1624	U	C2-N1-C1'	5.16	123.90	117.70
1	A2	1440	C	C6-N1-C1'	-5.15	114.62	120.80
5	B1	100	U	C2-N1-C1'	5.14	123.88	117.70
1	A2	219	C	N1-C2-O2	5.14	121.98	118.90
1	A2	384	C	C6-N1-C2	-5.13	118.25	120.30
1	A2	962	C	N3-C2-O2	-5.13	118.31	121.90
1	A2	4993	U	N3-C2-O2	-5.13	118.61	122.20
1	A2	1193	C	C6-N1-C2	-5.13	118.25	120.30
85	AK	94	ASP	C-N-CA	5.13	134.51	121.70
1	A2	2606	C	C5-C6-N1	5.12	123.56	121.00
1	A2	2499	C	C6-N1-C2	-5.12	118.25	120.30
1	A2	2846	C	C2-N1-C1'	5.12	124.43	118.80
1	A2	4443	U	C2-N1-C1'	5.11	123.84	117.70
5	B1	632	C	C2-N1-C1'	5.11	124.42	118.80
5	B1	1753	C	N1-C2-O2	5.11	121.97	118.90
5	B1	571	U	N3-C2-O2	-5.11	118.62	122.20
1	A2	2727	C	C6-N1-C2	-5.11	118.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	3911	U	N3-C2-O2	-5.11	118.62	122.20
5	B1	804	U	N3-C2-O2	-5.11	118.62	122.20
5	B1	1017	U	N3-C2-O2	-5.11	118.62	122.20
1	A2	4069	G	N3-C4-N9	5.10	129.06	126.00
1	A2	971	C	C6-N1-C2	-5.09	118.26	120.30
40	A4	67	C	C6-N1-C2	-5.09	118.26	120.30
5	B1	1242	U	C2-N1-C1'	5.09	123.81	117.70
1	A2	4079	C	C6-N1-C2	-5.08	118.27	120.30
1	A2	2751	C	N1-C2-O2	5.08	121.95	118.90
1	A2	4880	C	N3-C2-O2	-5.08	118.34	121.90
1	A2	4993	U	N1-C2-O2	5.08	126.35	122.80
5	B1	1120	U	N1-C2-O2	5.08	126.35	122.80
5	B1	1523	C	N1-C2-O2	5.08	121.95	118.90
1	A2	14	C	C5-C6-N1	5.08	123.54	121.00
1	A2	3759	C	C2-N1-C1'	5.08	124.38	118.80
1	A2	4732	U	N1-C2-O2	5.08	126.35	122.80
2	Bv	36	C	C6-N1-C2	-5.08	118.27	120.30
1	A2	664	C	N3-C2-O2	-5.07	118.35	121.90
5	B1	930	C	N1-C2-O2	5.07	121.94	118.90
86	Ct	25	ILE	CG1-CB-CG2	-5.07	100.25	111.40
1	A2	1322	U	N1-C2-O2	5.07	126.35	122.80
39	A3	96	C	N1-C2-O2	5.07	121.94	118.90
5	B1	494	C	N1-C2-O2	5.06	121.94	118.90
5	B1	1120	U	N3-C2-O2	-5.06	118.66	122.20
1	A2	4205	C	C6-N1-C2	-5.06	118.28	120.30
1	A2	1499	G	C4-N9-C1'	5.06	133.07	126.50
1	A2	4676	C	N3-C2-O2	-5.06	118.36	121.90
5	B1	1053	C	C2-N1-C1'	5.05	124.36	118.80
1	A2	236	C	C2-N1-C1'	5.05	124.36	118.80
1	A2	2325	C	C2-N1-C1'	5.05	124.36	118.80
5	B1	571	U	N1-C2-O2	5.05	126.33	122.80
5	B1	1139	C	O4'-C1'-N1	5.05	112.24	108.20
1	A2	3608	U	N3-C2-O2	-5.05	118.67	122.20
5	B1	89	C	N1-C2-O2	5.05	121.93	118.90
1	A2	78	U	N1-C2-O2	5.04	126.33	122.80
5	B1	178	C	N1-C2-O2	5.04	121.93	118.90
1	A2	1193	C	C2-N1-C1'	5.04	124.35	118.80
5	B1	44	U	C5-C6-N1	5.04	125.22	122.70
1	A2	1589	C	N3-C2-O2	-5.04	118.37	121.90
5	B1	592	C	N1-C2-O2	5.04	121.92	118.90
1	A2	4545	C	C6-N1-C2	-5.04	118.28	120.30
1	A2	4545	C	N1-C2-O2	5.04	121.92	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1930	U	N1-C2-O2	5.03	126.32	122.80
5	B1	4	C	C6-N1-C2	-5.03	118.29	120.30
1	A2	4661	U	P-O3'-C3'	5.03	125.73	119.70
1	A2	2444	C	N3-C2-O2	-5.03	118.38	121.90
1	A2	1789	C	C2-N1-C1'	5.03	124.33	118.80
1	A2	4824	C	N3-C2-O2	-5.03	118.38	121.90
5	B1	1701	C	C2-N1-C1'	5.03	124.33	118.80
10	BP	50	ARG	CA-CB-CG	5.03	124.46	113.40
5	B1	621	C	C6-N1-C1'	-5.02	114.77	120.80
5	B1	89	C	N3-C2-O2	-5.02	118.39	121.90
1	A2	243	G	C5-C6-O6	5.02	131.61	128.60
5	B1	402	C	C6-N1-C2	-5.01	118.30	120.30
5	B1	814	U	N1-C2-O2	5.01	126.31	122.80
5	B1	1710	C	C5-C6-N1	5.01	123.50	121.00
5	B1	659	G	N3-C4-N9	5.00	129.00	126.00
5	B1	833	C	C2-N1-C1'	5.00	124.30	118.80
5	B1	1053	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
43	AC	150	LEU	Peptide
43	AC	51	PRO	Peptide
44	AD	258	LYS	Peptide
45	AE	129	GLY	Peptide
45	AE	135	GLN	Peptide
45	AE	136	HIS	Peptide
48	AH	116	ASN	Peptide
48	AH	60	TRP	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
82	At	27	THR	Peptide
21	BA	207	PRO	Peptide
22	BB	39	PHE	Peptide
24	BE	92	ILE	Peptide

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Mol	Chain	Res	Type	Group
27	BI	132	GLU	Peptide
27	BI	159	SER	Peptide
28	BJ	137	VAL	Peptide
8	BK	65	ARG	Peptide
11	BQ	13	PHE	Peptide
17	Bc	32	VAL	Peptide
86	Ct	333	LYS	Peptide
86	Ct	461	ILE	Peptide
86	Ct	463	ASP	Peptide
86	Ct	493	ASN	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	
6	BD	218/220 (99%)	209 (96%)	9 (4%)	0	100	100
7	BF	188/190 (99%)	173 (92%)	15 (8%)	0	100	100
8	BK	96/98 (98%)	82 (85%)	13 (14%)	1 (1%)	15	55
9	BM	118/120 (98%)	110 (93%)	8 (7%)	0	100	100
10	BP	118/120 (98%)	105 (89%)	12 (10%)	1 (1%)	19	59
11	BQ	137/139 (99%)	128 (93%)	9 (7%)	0	100	100
12	BR	123/125 (98%)	109 (89%)	14 (11%)	0	100	100
13	BS	137/139 (99%)	125 (91%)	12 (9%)	0	100	100
14	BT	141/143 (99%)	130 (92%)	10 (7%)	1 (1%)	22	61
15	BU	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
16	BZ	84/86 (98%)	74 (88%)	10 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Bc	60/62 (97%)	55 (92%)	3 (5%)	2 (3%)	4	31
18	Bd	49/51 (96%)	46 (94%)	3 (6%)	0	100	100
19	Bf	71/73 (97%)	63 (89%)	8 (11%)	0	100	100
20	Bg	312/314 (99%)	283 (91%)	29 (9%)	0	100	100
21	BA	213/215 (99%)	199 (93%)	14 (7%)	0	100	100
22	BB	210/212 (99%)	180 (86%)	30 (14%)	0	100	100
23	BC	220/222 (99%)	206 (94%)	14 (6%)	0	100	100
24	BE	255/257 (99%)	236 (92%)	17 (7%)	2 (1%)	19	59
25	BG	230/232 (99%)	216 (94%)	14 (6%)	0	100	100
26	BH	181/183 (99%)	166 (92%)	15 (8%)	0	100	100
27	BI	205/207 (99%)	177 (86%)	27 (13%)	1 (0%)	29	68
28	BJ	177/179 (99%)	157 (89%)	18 (10%)	2 (1%)	14	53
29	BL	151/153 (99%)	138 (91%)	12 (8%)	1 (1%)	22	61
30	BN	147/149 (99%)	131 (89%)	16 (11%)	0	100	100
31	BO	134/136 (98%)	122 (91%)	12 (9%)	0	100	100
32	BV	79/81 (98%)	76 (96%)	3 (4%)	0	100	100
33	BW	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
34	BX	139/141 (99%)	122 (88%)	17 (12%)	0	100	100
35	BY	123/125 (98%)	111 (90%)	12 (10%)	0	100	100
36	Ba	95/97 (98%)	87 (92%)	8 (8%)	0	100	100
37	Bb	78/80 (98%)	71 (91%)	7 (9%)	0	100	100
38	Be	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
41	AA	250/252 (99%)	235 (94%)	15 (6%)	0	100	100
42	AB	392/394 (100%)	361 (92%)	31 (8%)	0	100	100
43	AC	361/363 (99%)	335 (93%)	22 (6%)	4 (1%)	14	53
44	AD	292/294 (99%)	269 (92%)	23 (8%)	0	100	100
45	AE	192/194 (99%)	161 (84%)	30 (16%)	1 (0%)	29	68
46	AF	232/234 (99%)	214 (92%)	18 (8%)	0	100	100
47	AG	232/234 (99%)	218 (94%)	14 (6%)	0	100	100
48	AH	189/191 (99%)	175 (93%)	14 (7%)	0	100	100
49	AI	204/211 (97%)	181 (89%)	23 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	AJ	167/169 (99%)	152 (91%)	14 (8%)	1 (1%)	25	64
51	AL	203/205 (99%)	171 (84%)	31 (15%)	1 (0%)	29	68
52	AM	137/139 (99%)	127 (93%)	10 (7%)	0	100	100
53	AN	201/203 (99%)	185 (92%)	16 (8%)	0	100	100
54	AO	193/195 (99%)	186 (96%)	7 (4%)	0	100	100
55	AP	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
56	AQ	185/187 (99%)	163 (88%)	21 (11%)	1 (0%)	29	68
57	AR	179/181 (99%)	168 (94%)	11 (6%)	0	100	100
58	AS	173/175 (99%)	163 (94%)	10 (6%)	0	100	100
59	AT	155/157 (99%)	138 (89%)	15 (10%)	2 (1%)	12	50
60	AU	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
61	AV	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
62	AW	119/121 (98%)	108 (91%)	11 (9%)	0	100	100
63	AX	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
64	AY	125/127 (98%)	119 (95%)	6 (5%)	0	100	100
65	AZ	132/134 (98%)	115 (87%)	17 (13%)	0	100	100
66	Aa	145/147 (99%)	131 (90%)	14 (10%)	0	100	100
67	Ab	66/68 (97%)	56 (85%)	10 (15%)	0	100	100
68	Ac	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
69	Ad	104/106 (98%)	101 (97%)	3 (3%)	0	100	100
70	Ae	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
71	Af	107/109 (98%)	95 (89%)	10 (9%)	2 (2%)	8	42
72	Ag	112/114 (98%)	100 (89%)	12 (11%)	0	100	100
73	Ah	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
74	Ai	95/97 (98%)	85 (90%)	10 (10%)	0	100	100
75	Aj	82/84 (98%)	73 (89%)	9 (11%)	0	100	100
76	Ak	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
77	Al	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
78	Am	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
79	An	23/25 (92%)	23 (100%)	0	0	100	100
80	Ao	103/105 (98%)	96 (93%)	7 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
81	Ap	89/91 (98%)	83 (93%)	6 (7%)	0	100	100
82	At	120/122 (98%)	105 (88%)	15 (12%)	0	100	100
83	Au	215/217 (99%)	197 (92%)	18 (8%)	0	100	100
84	Aq	149/151 (99%)	112 (75%)	37 (25%)	0	100	100
85	AK	200/202 (99%)	179 (90%)	20 (10%)	1 (0%)	29	68
86	Ct	850/853 (100%)	768 (90%)	79 (9%)	3 (0%)	34	71
All	All	12538/12702 (99%)	11449 (91%)	1062 (8%)	27 (0%)	50	79

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	BP	51	ARG
28	BJ	138	ARG
71	Af	107	PRO
24	BE	93	GLU
51	AL	78	LEU
71	Af	106	TYR
85	AK	150	GLY
86	Ct	159	LYS
8	BK	41	PRO
14	BT	31	PRO
43	AC	51	PRO
50	AJ	53	ALA
17	Bc	33	GLU
45	AE	136	HIS
56	AQ	161	SER
86	Ct	649	ILE
24	BE	150	PRO
27	BI	160	SER
29	BL	14	PRO
43	AC	52	TYR
86	Ct	464	VAL
43	AC	72	ALA
59	AT	53	PRO
28	BJ	123	ILE
43	AC	151	PRO
17	Bc	32	VAL
59	AT	18	PRO

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	
6	BD	183/183 (100%)	182 (100%)	1 (0%)	88	95
7	BF	160/160 (100%)	160 (100%)	0	100	100
8	BK	89/89 (100%)	88 (99%)	1 (1%)	73	88
9	BM	102/102 (100%)	102 (100%)	0	100	100
10	BP	109/109 (100%)	108 (99%)	1 (1%)	78	90
11	BQ	115/115 (100%)	115 (100%)	0	100	100
12	BR	113/113 (100%)	113 (100%)	0	100	100
13	BS	121/121 (100%)	117 (97%)	4 (3%)	38	69
14	BT	113/113 (100%)	112 (99%)	1 (1%)	78	90
15	BU	90/90 (100%)	90 (100%)	0	100	100
16	BZ	75/75 (100%)	74 (99%)	1 (1%)	69	86
17	Bc	55/55 (100%)	54 (98%)	1 (2%)	59	81
18	Bd	45/45 (100%)	45 (100%)	0	100	100
19	Bf	66/66 (100%)	66 (100%)	0	100	100
20	Bg	272/272 (100%)	271 (100%)	1 (0%)	91	97
21	BA	180/180 (100%)	179 (99%)	1 (1%)	86	94
22	BB	193/193 (100%)	191 (99%)	2 (1%)	76	88
23	BC	188/188 (100%)	187 (100%)	1 (0%)	88	95
24	BE	220/220 (100%)	216 (98%)	4 (2%)	59	81
25	BG	202/202 (100%)	200 (99%)	2 (1%)	76	88
26	BH	164/164 (100%)	164 (100%)	0	100	100
27	BI	179/179 (100%)	179 (100%)	0	100	100
28	BJ	160/160 (100%)	159 (99%)	1 (1%)	86	94
29	BL	138/138 (100%)	137 (99%)	1 (1%)	84	93
30	BN	130/130 (100%)	129 (99%)	1 (1%)	81	91
31	BO	106/106 (100%)	105 (99%)	1 (1%)	78	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	BV	65/65 (100%)	63 (97%)	2 (3%)	40	71
33	BW	112/112 (100%)	110 (98%)	2 (2%)	59	81
34	BX	113/113 (100%)	112 (99%)	1 (1%)	78	90
35	BY	107/107 (100%)	106 (99%)	1 (1%)	78	90
36	Ba	84/84 (100%)	83 (99%)	1 (1%)	71	87
37	Bb	72/72 (100%)	72 (100%)	0	100	100
38	Be	44/44 (100%)	41 (93%)	3 (7%)	16	50
41	AA	194/194 (100%)	193 (100%)	1 (0%)	88	95
42	AB	343/343 (100%)	341 (99%)	2 (1%)	86	94
43	AC	302/302 (100%)	298 (99%)	4 (1%)	69	86
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	178/179 (99%)	177 (99%)	1 (1%)	86	94
50	AJ	142/142 (100%)	142 (100%)	0	100	100
51	AL	171/171 (100%)	169 (99%)	2 (1%)	71	87
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
61	AV	100/100 (100%)	100 (100%)	0	100	100
62	AW	100/100 (100%)	99 (99%)	1 (1%)	76	88
63	AX	105/105 (100%)	105 (100%)	0	100	100
64	AY	119/119 (100%)	118 (99%)	1 (1%)	81	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	70 (99%)	1 (1%)	67	85
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%)	90 (97%)	3 (3%)	39	70
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%)	190 (97%)	6 (3%)	40	71
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%)	722 (100%)	3 (0%)	91	97
All	All	10924/10925 (100%)	10828 (99%)	96 (1%)	79	90

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	BD	64	ARG
8	BK	96	ARG
10	BP	52	LYS
13	BS	17	ASN
13	BS	23	ARG
13	BS	66	ARG
13	BS	73	ASN

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Mol	Chain	Res	Type
14	BT	62	ARG
16	BZ	112	ASN
17	Bc	66	ARG
20	Bg	133	ASN
21	BA	149	ASN
22	BB	76	ASN
22	BB	174	ARG
23	BC	134	ASN
24	BE	30	ARG
24	BE	75	LYS
24	BE	197	ASN
24	BE	230	ASN
25	BG	85	ARG
25	BG	202	ASN
28	BJ	30	LYS
29	BL	101	ARG
30	BN	104	ARG
31	BO	128	ARG
32	BV	41	LYS
32	BV	81	LYS
33	BW	5	ASN
33	BW	15	ASN
34	BX	127	ASN
35	BY	15	ASN
36	Ba	15	ARG
38	Be	18	LYS
38	Be	35	ARG
38	Be	52	LYS
41	AA	193	ARG
42	AB	24	ARG
42	AB	294	LYS
43	AC	38	ASN
43	AC	48	ASN
43	AC	95	MET
43	AC	215	ASN
44	AD	21	ARG
44	AD	191	ASN
44	AD	235	MET
44	AD	265	ARG
45	AE	223	ARG
45	AE	279	ASN
46	AF	146	ASN

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Mol	Chain	Res	Type
46	AF	161	LYS
46	AF	166	ARG
49	AI	73	ASN
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
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
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
80	Ao	99	ARG
81	Ap	84	ARG
82	At	41	ASN
82	At	67	ARG
82	At	83	ASN
83	Au	21	ASN
83	Au	54	ARG
83	Au	143	ASN
83	Au	188	ASN
83	Au	197	ASN
83	Au	215	ARG

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Mol	Chain	Res	Type
84	Aq	40	LYS
84	Aq	114	ARG
86	Ct	588	ASN
86	Ct	803	ASN
86	Ct	842	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (138) such sidechains are listed below:

Mol	Chain	Res	Type
6	BD	159	HIS
7	BF	82	ASN
7	BF	95	HIS
7	BF	114	ASN
9	BM	55	ASN
10	BP	41	GLN
11	BQ	11	GLN
11	BQ	80	GLN
11	BQ	86	GLN
12	BR	62	GLN
13	BS	10	GLN
13	BS	17	ASN
13	BS	19	ASN
13	BS	105	ASN
14	BT	11	GLN
16	BZ	89	GLN
16	BZ	106	GLN
16	BZ	112	ASN
17	Bc	24	GLN
17	Bc	29	GLN
20	Bg	133	ASN
20	Bg	226	HIS
21	BA	36	GLN
21	BA	149	ASN
22	BB	76	ASN
23	BC	134	ASN
23	BC	272	HIS
24	BE	8	HIS
24	BE	161	GLN
24	BE	179	ASN
24	BE	197	ASN
24	BE	230	ASN
25	BG	187	HIS

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Mol	Chain	Res	Type
25	BG	202	ASN
25	BG	227	GLN
26	BH	91	HIS
26	BH	193	GLN
27	BI	165	GLN
28	BJ	140	GLN
28	BJ	156	HIS
29	BL	11	GLN
29	BL	83	GLN
30	BN	5	HIS
31	BO	79	GLN
31	BO	103	ASN
33	BW	5	ASN
33	BW	15	ASN
33	BW	16	ASN
33	BW	44	HIS
33	BW	92	ASN
33	BW	98	GLN
34	BX	127	ASN
35	BY	15	ASN
35	BY	29	HIS
35	BY	89	HIS
35	BY	112	ASN
36	Ba	25	ASN
38	Be	3	HIS
41	AA	83	HIS
41	AA	97	ASN
41	AA	132	ASN
41	AA	205	ASN
41	AA	209	HIS
41	AA	215	ASN
42	AB	167	GLN
42	AB	179	HIS
42	AB	275	HIS
42	AB	302	ASN
42	AB	380	GLN
43	AC	41	HIS
43	AC	48	ASN
43	AC	50	GLN
43	AC	198	ASN
43	AC	215	ASN
43	AC	347	HIS

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Mol	Chain	Res	Type
44	AD	111	ASN
44	AD	191	ASN
44	AD	222	GLN
45	AE	191	GLN
45	AE	279	ASN
46	AF	146	ASN
47	AG	43	GLN
49	AI	14	ASN
49	AI	51	HIS
50	AJ	112	HIS
51	AL	149	GLN
51	AL	159	ASN
51	AL	175	ASN
52	AM	44	GLN
52	AM	70	GLN
53	AN	8	GLN
53	AN	37	HIS
53	AN	86	HIS
53	AN	87	HIS
53	AN	196	ASN
54	AO	65	ASN
54	AO	184	ASN
55	AP	40	HIS
55	AP	80	GLN
57	AR	178	GLN
58	AS	66	GLN
60	AU	50	ASN
61	AV	101	ASN
62	AW	45	ASN
62	AW	48	GLN
64	AY	18	HIS
64	AY	61	HIS
64	AY	96	HIS
65	AZ	40	HIS
66	Aa	39	HIS
66	Aa	60	HIS
67	Ab	61	ASN
69	Ad	28	ASN
70	Ae	52	GLN
71	Af	21	GLN
72	Ag	73	HIS
73	Ah	63	GLN

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Mol	Chain	Res	Type
75	Aj	57	ASN
77	Al	20	ASN
77	Al	43	HIS
78	Am	120	ASN
80	Ao	3	ASN
80	Ao	36	GLN
82	At	100	ASN
83	Au	21	ASN
83	Au	40	ASN
83	Au	73	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	433	ASN
86	Ct	492	HIS
86	Ct	588	ASN
86	Ct	696	ASN
86	Ct	811	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A2	3600/3612 (99%)	706 (19%)	9 (0%)
2	Bv	75/76 (98%)	12 (16%)	0
3	Bx	11/12 (91%)	6 (54%)	0
39	A3	156/157 (99%)	35 (22%)	0
4	Bw	75/76 (98%)	13 (17%)	0
40	A4	118/119 (99%)	21 (17%)	0
5	B1	1701/1708 (99%)	336 (19%)	4 (0%)
All	All	5736/5760 (99%)	1129 (19%)	13 (0%)

All (1129) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A2	8	U
1	A2	9	C
1	A2	10	A
1	A2	12	A

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Mol	Chain	Res	Type
1	A2	14	C
1	A2	25	A
1	A2	32	G
1	A2	39	A
1	A2	40	G
1	A2	42	A
1	A2	48	G
1	A2	49	U
1	A2	59	A
1	A2	65	A
1	A2	71	C
1	A2	72	C
1	A2	74	G
1	A2	76	A
1	A2	84	A
1	A2	91	G
1	A2	101	A
1	A2	108	A
1	A2	110	C
1	A2	116	G
1	A2	119	G
1	A2	120	A
1	A2	131	C
1	A2	132	G
1	A2	133	C
1	A2	134	G
1	A2	135	G
1	A2	143	G
1	A2	149	U
1	A2	155	A
1	A2	157	G
1	A2	167	C
1	A2	169	C
1	A2	176	G
1	A2	181	U
1	A2	182	C
1	A2	183	G
1	A2	184	U
1	A2	185	G
1	A2	196	G
1	A2	198	C
1	A2	201	U

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Mol	Chain	Res	Type
1	A2	206	U
1	A2	212	C
1	A2	213	C
1	A2	214	C
1	A2	215	A
1	A2	228	U
1	A2	229	G
1	A2	230	U
1	A2	233	G
1	A2	234	G
1	A2	236	C
1	A2	241	G
1	A2	253	G
1	A2	258	C
1	A2	260	C
1	A2	275	U
1	A2	282	G
1	A2	286	G
1	A2	289	A
1	A2	291	U
1	A2	300	A
1	A2	309	G
1	A2	310	U
1	A2	311	A
1	A2	323	A
1	A2	330	A
1	A2	334	C
1	A2	338	A
1	A2	351	U
1	A2	357	A
1	A2	367	G
1	A2	370	A
1	A2	375	U
1	A2	380	A
1	A2	381	G
1	A2	390	A
1	A2	425	G
1	A2	426	U
1	A2	434	U
1	A2	446	A
1	A2	447	G
1	A2	448	U

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Mol	Chain	Res	Type
1	A2	449	C
1	A2	450	C
1	A2	460	A
1	A2	463	C
1	A2	479	C
1	A2	482	G
1	A2	487	G
1	A2	489	C
1	A2	492	C
1	A2	494	G
1	A2	496	C
1	A2	497	C
1	A2	498	G
1	A2	499	G
1	A2	504	U
1	A2	505	C
1	A2	507	U
1	A2	509	C
1	A2	513	C
1	A2	634	C
1	A2	635	G
1	A2	643	A
1	A2	647	U
1	A2	649	C
1	A2	658	G
1	A2	661	G
1	A2	676	G
1	A2	677	G
1	A2	678	C
1	A2	680	C
1	A2	691	G
1	A2	692	G
1	A2	695	C
1	A2	698	C
1	A2	714	A
1	A2	719	U
1	A2	720	G
1	A2	721	G
1	A2	737	A
1	A2	738	A
1	A2	739	G
1	A2	902	A

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Mol	Chain	Res	Type
1	A2	905	G
1	A2	906	C
1	A2	907	C
1	A2	909	C
1	A2	914	G
1	A2	917	G
1	A2	918	C
1	A2	919	A
1	A2	923	C
1	A2	924	U
1	A2	925	C
1	A2	927	C
1	A2	929	G
1	A2	931	A
1	A2	932	U
1	A2	933	C
1	A2	934	C
1	A2	944	G
1	A2	947	A
1	A2	948	G
1	A2	949	C
1	A2	950	G
1	A2	951	A
1	A2	953	A
1	A2	955	C
1	A2	956	C
1	A2	960	G
1	A2	961	C
1	A2	962	C
1	A2	968	C
1	A2	969	U
1	A2	1055	C
1	A2	1067	C
1	A2	1087	C
1	A2	1147	G
1	A2	1149	G
1	A2	1150	C
1	A2	1152	G
1	A2	1156	G
1	A2	1161	G
1	A2	1162	U
1	A2	1165	C

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Mol	Chain	Res	Type
1	A2	1167	A
1	A2	1190	C
1	A2	1192	U
1	A2	1193	C
1	A2	1196	G
1	A2	1201	G
1	A2	1220	C
1	A2	1221	A
1	A2	1222	C
1	A2	1223	G
1	A2	1225	G
1	A2	1226	C
1	A2	1229	G
1	A2	1250	C
1	A2	1251	G
1	A2	1255	C
1	A2	1256	G
1	A2	1259	C
1	A2	1263	C
1	A2	1264	G
1	A2	1265	G
1	A2	1268	U
1	A2	1271	G
1	A2	1277	A
1	A2	1278	C
1	A2	1284	C
1	A2	1309	A
1	A2	1336	G
1	A2	1337	A
1	A2	1341	G
1	A2	1343	G
1	A2	1348	C
1	A2	1349	G
1	A2	1351	A
1	A2	1353	G
1	A2	1364	U
1	A2	1370	A
1	A2	1373	G
1	A2	1380	A
1	A2	1381	A
1	A2	1391	G
1	A2	1392	C

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Mol	Chain	Res	Type
1	A2	1403	A
1	A2	1421	U
1	A2	1424	C
1	A2	1426	A
1	A2	1428	U
1	A2	1430	C
1	A2	1432	C
1	A2	1439	G
1	A2	1463	C
1	A2	1464	G
1	A2	1465	C
1	A2	1466	G
1	A2	1468	C
1	A2	1479	A
1	A2	1480	G
1	A2	1483	C
1	A2	1485	A
1	A2	1499	G
1	A2	1500	A
1	A2	1501	C
1	A2	1505	A
1	A2	1516	A
1	A2	1521	G
1	A2	1525	G
1	A2	1548	C
1	A2	1556	G
1	A2	1559	G
1	A2	1560	U
1	A2	1573	U
1	A2	1576	C
1	A2	1578	U
1	A2	1583	A
1	A2	1589	C
1	A2	1593	C
1	A2	1594	G
1	A2	1595	A
1	A2	1606	G
1	A2	1607	G
1	A2	1613	A
1	A2	1615	G
1	A2	1616	A
1	A2	1623	G

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Mol	Chain	Res	Type
1	A2	1631	U
1	A2	1632	A
1	A2	1636	G
1	A2	1643	C
1	A2	1676	C
1	A2	1678	C
1	A2	1679	G
1	A2	1701	A
1	A2	1706	G
1	A2	1713	C
1	A2	1723	G
1	A2	1728	A
1	A2	1736	U
1	A2	1739	U
1	A2	1747	A
1	A2	1748	A
1	A2	1751	G
1	A2	1763	U
1	A2	1769	A
1	A2	1776	A
1	A2	1785	G
1	A2	1786	A
1	A2	1788	G
1	A2	1794	C
1	A2	1797	G
1	A2	1804	U
1	A2	1807	A
1	A2	1814	G
1	A2	1815	U
1	A2	1816	G
1	A2	1818	A
1	A2	1823	G
1	A2	1835	G
1	A2	1836	G
1	A2	1844	U
1	A2	1850	G
1	A2	1862	C
1	A2	1869	A
1	A2	1872	A
1	A2	1873	A
1	A2	1896	C
1	A2	1897	G

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Mol	Chain	Res	Type
1	A2	1898	A
1	A2	1902	C
1	A2	1903	G
1	A2	1911	U
1	A2	1912	C
1	A2	1913	A
1	A2	1916	C
1	A2	1920	A
1	A2	1928	U
1	A2	1929	G
1	A2	1932	G
1	A2	1936	G
1	A2	1940	U
1	A2	1941	A
1	A2	1942	G
1	A2	1943	A
1	A2	1945	A
1	A2	1955	U
1	A2	1956	G
1	A2	1959	C
1	A2	1961	U
1	A2	1963	G
1	A2	1964	A
1	A2	1967	U
1	A2	1968	C
1	A2	1973	U
1	A2	1978	U
1	A2	1983	A
1	A2	1984	G
1	A2	1985	U
1	A2	1988	G
1	A2	1989	U
1	A2	1990	A
1	A2	1991	A
1	A2	2007	A
1	A2	2015	G
1	A2	2026	G
1	A2	2027	G
1	A2	2029	U
1	A2	2033	G
1	A2	2035	U
1	A2	2037	G

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Mol	Chain	Res	Type
1	A2	2043	C
1	A2	2050	A
1	A2	2246	U
1	A2	2258	A
1	A2	2268	C
1	A2	2279	A
1	A2	2280	G
1	A2	2282	C
1	A2	2283	U
1	A2	2285	G
1	A2	2292	A
1	A2	2299	G
1	A2	2301	G
1	A2	2308	U
1	A2	2310	G
1	A2	2327	G
1	A2	2330	C
1	A2	2339	A
1	A2	2340	G
1	A2	2363	U
1	A2	2373	G
1	A2	2374	A
1	A2	2389	C
1	A2	2400	G
1	A2	2401	C
1	A2	2404	U
1	A2	2426	U
1	A2	2442	G
1	A2	2447	U
1	A2	2450	G
1	A2	2467	C
1	A2	2468	C
1	A2	2469	U
1	A2	2482	G
1	A2	2484	C
1	A2	2485	G
1	A2	2492	A
1	A2	2524	U
1	A2	2525	G
1	A2	2526	G
1	A2	2532	A
1	A2	2561	A

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Mol	Chain	Res	Type
1	A2	2565	G
1	A2	2566	A
1	A2	2567	C
1	A2	2568	C
1	A2	2570	A
1	A2	2579	A
1	A2	2580	A
1	A2	2584	G
1	A2	2585	G
1	A2	2606	C
1	A2	2617	G
1	A2	2632	C
1	A2	2637	G
1	A2	2638	A
1	A2	2648	C
1	A2	2665	G
1	A2	2666	U
1	A2	2673	G
1	A2	2675	A
1	A2	2676	A
1	A2	2684	G
1	A2	2690	G
1	A2	2691	G
1	A2	2698	C
1	A2	2700	G
1	A2	2704	A
1	A2	2705	G
1	A2	2706	C
1	A2	2718	C
1	A2	2719	U
1	A2	2720	U
1	A2	2726	U
1	A2	2732	G
1	A2	2733	G
1	A2	2739	G
1	A2	2741	G
1	A2	2742	U
1	A2	2745	A
1	A2	2748	U
1	A2	2751	C
1	A2	2766	A
1	A2	2767	U

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Mol	Chain	Res	Type
1	A2	2769	U
1	A2	2773	C
1	A2	2776	C
1	A2	2785	A
1	A2	2786	A
1	A2	2793	C
1	A2	2804	A
1	A2	2805	U
1	A2	2806	G
1	A2	2814	A
1	A2	2822	U
1	A2	2839	C
1	A2	2858	A
1	A2	2860	A
1	A2	2871	C
1	A2	2879	U
1	A2	3572	C
1	A2	3586	G
1	A2	3588	G
1	A2	3589	C
1	A2	3591	G
1	A2	3596	G
1	A2	3597	G
1	A2	3601	A
1	A2	3606	A
1	A2	3612	U
1	A2	3614	A
1	A2	3615	U
1	A2	3616	U
1	A2	3627	A
1	A2	3633	A
1	A2	3643	G
1	A2	3649	G
1	A2	3651	U
1	A2	3663	A
1	A2	3669	G
1	A2	3682	A
1	A2	3683	A
1	A2	3707	A
1	A2	3719	A
1	A2	3724	G
1	A2	3730	A

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Mol	Chain	Res	Type
1	A2	3732	C
1	A2	3738	C
1	A2	3747	G
1	A2	3748	G
1	A2	3751	G
1	A2	3754	A
1	A2	3781	C
1	A2	3782	G
1	A2	3785	U
1	A2	3788	A
1	A2	3789	U
1	A2	3790	G
1	A2	3795	A
1	A2	3798	G
1	A2	3799	A
1	A2	3809	U
1	A2	3810	G
1	A2	3811	U
1	A2	3814	C
1	A2	3831	A
1	A2	3847	A
1	A2	3848	A
1	A2	3850	G
1	A2	3851	G
1	A2	3852	G
1	A2	3860	G
1	A2	3863	U
1	A2	3866	G
1	A2	3872	A
1	A2	3876	A
1	A2	3878	G
1	A2	3879	A
1	A2	3886	U
1	A2	3889	G
1	A2	3890	C
1	A2	3907	A
1	A2	3909	G
1	A2	3927	G
1	A2	3929	G
1	A2	3935	U
1	A2	3936	A
1	A2	3943	A

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Mol	Chain	Res	Type
1	A2	3944	G
1	A2	4019	U
1	A2	4020	A
1	A2	4027	C
1	A2	4029	C
1	A2	4035	G
1	A2	4046	G
1	A2	4051	G
1	A2	4054	G
1	A2	4058	C
1	A2	4062	G
1	A2	4065	G
1	A2	4066	C
1	A2	4067	G
1	A2	4068	A
1	A2	4069	G
1	A2	4074	A
1	A2	4079	C
1	A2	4084	G
1	A2	4088	C
1	A2	4106	C
1	A2	4109	G
1	A2	4110	C
1	A2	4126	C
1	A2	4132	A
1	A2	4135	G
1	A2	4145	G
1	A2	4146	G
1	A2	4153	G
1	A2	4165	A
1	A2	4174	A
1	A2	4175	A
1	A2	4176	A
1	A2	4191	U
1	A2	4195	A
1	A2	4196	A
1	A2	4211	G
1	A2	4215	A
1	A2	4216	G
1	A2	4228	G
1	A2	4230	A
1	A2	4235	A

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Mol	Chain	Res	Type
1	A2	4243	A
1	A2	4250	C
1	A2	4251	U
1	A2	4252	U
1	A2	4266	A
1	A2	4267	G
1	A2	4268	U
1	A2	4276	C
1	A2	4281	C
1	A2	4285	A
1	A2	4291	G
1	A2	4292	G
1	A2	4294	C
1	A2	4311	C
1	A2	4316	U
1	A2	4330	G
1	A2	4333	G
1	A2	4338	A
1	A2	4339	G
1	A2	4340	A
1	A2	4342	A
1	A2	4349	C
1	A2	4355	G
1	A2	4356	A
1	A2	4358	A
1	A2	4360	C
1	A2	4367	G
1	A2	4384	A
1	A2	4386	A
1	A2	4388	C
1	A2	4406	C
1	A2	4414	U
1	A2	4426	A
1	A2	4428	C
1	A2	4437	G
1	A2	4446	G
1	A2	4455	U
1	A2	4457	G
1	A2	4459	U
1	A2	4474	U
1	A2	4475	A
1	A2	4480	A

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Mol	Chain	Res	Type
1	A2	4482	G
1	A2	4485	A
1	A2	4486	G
1	A2	4510	A
1	A2	4519	U
1	A2	4522	C
1	A2	4537	G
1	A2	4546	A
1	A2	4551	A
1	A2	4552	A
1	A2	4559	U
1	A2	4561	A
1	A2	4570	G
1	A2	4579	G
1	A2	4586	A
1	A2	4593	G
1	A2	4597	A
1	A2	4598	U
1	A2	4599	G
1	A2	4611	G
1	A2	4614	G
1	A2	4618	A
1	A2	4620	G
1	A2	4621	G
1	A2	4624	C
1	A2	4629	C
1	A2	4632	C
1	A2	4640	G
1	A2	4641	G
1	A2	4662	A
1	A2	4665	U
1	A2	4671	U
1	A2	4681	G
1	A2	4693	G
1	A2	4694	G
1	A2	4695	C
1	A2	4696	A
1	A2	4700	C
1	A2	4703	C
1	A2	4704	G
1	A2	4714	U
1	A2	4715	U

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Mol	Chain	Res	Type
1	A2	4718	C
1	A2	4719	C
1	A2	4726	A
1	A2	4732	U
1	A2	4824	C
1	A2	4827	U
1	A2	4828	G
1	A2	4831	G
1	A2	4832	A
1	A2	4833	G
1	A2	4834	U
1	A2	4837	C
1	A2	4838	C
1	A2	4839	U
1	A2	4840	U
1	A2	4847	G
1	A2	4849	G
1	A2	4852	A
1	A2	4853	C
1	A2	4854	G
1	A2	4855	G
1	A2	4858	C
1	A2	4859	G
1	A2	4864	C
1	A2	4865	G
1	A2	4866	G
1	A2	4867	A
1	A2	4868	A
1	A2	4869	A
1	A2	4870	G
1	A2	4871	G
1	A2	4872	C
1	A2	4880	C
1	A2	4883	U
1	A2	4886	C
1	A2	4895	C
1	A2	4896	A
1	A2	4898	C
1	A2	4903	G
1	A2	4906	C
1	A2	4907	G
1	A2	4908	U

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Mol	Chain	Res	Type
1	A2	4909	G
1	A2	4923	U
1	A2	4924	A
1	A2	4934	U
1	A2	4937	A
1	A2	4943	U
1	A2	4947	U
1	A2	4950	G
1	A2	4957	G
1	A2	4964	U
1	A2	4971	C
1	A2	4975	G
1	A2	4981	C
1	A2	4982	C
1	A2	4984	U
1	A2	4985	C
1	A2	4986	G
1	A2	4998	U
1	A2	4999	G
1	A2	5005	C
1	A2	5007	G
1	A2	5008	C
1	A2	5011	U
1	A2	5012	C
1	A2	5013	G
1	A2	5015	C
1	A2	5016	A
1	A2	5019	A
1	A2	5020	G
1	A2	5027	U
2	Bv	16	U
2	Bv	17	G
2	Bv	19	U
2	Bv	20	U
2	Bv	21	A
2	Bv	22	U
2	Bv	34	A
2	Bv	35	A
2	Bv	47	U
2	Bv	59	A
2	Bv	61	C
2	Bv	76	A

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Mol	Chain	Res	Type
3	Bx	23	U
3	Bx	26	G
3	Bx	29	A
3	Bx	31	A
3	Bx	32	G
3	Bx	33	A
4	Bw	10	G
4	Bw	16	U
4	Bw	17	U
4	Bw	18	G
4	Bw	19	G
4	Bw	21	A
4	Bw	26	G
4	Bw	35	A
4	Bw	36	A
4	Bw	47	U
4	Bw	48	C
4	Bw	56	C
4	Bw	71	G
5	B1	4	C
5	B1	33	G
5	B1	37	C
5	B1	41	G
5	B1	42	A
5	B1	46	A
5	B1	67	C
5	B1	68	A
5	B1	71	G
5	B1	72	C
5	B1	73	C
5	B1	74	G
5	B1	76	U
5	B1	77	A
5	B1	79	A
5	B1	85	A
5	B1	103	A
5	B1	112	U
5	B1	113	G
5	B1	114	G
5	B1	115	U
5	B1	125	C
5	B1	126	G

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Mol	Chain	Res	Type
5	B1	142	C
5	B1	143	U
5	B1	155	G
5	B1	158	A
5	B1	161	U
5	B1	162	C
5	B1	163	U
5	B1	170	A
5	B1	171	A
5	B1	172	U
5	B1	174	C
5	B1	183	G
5	B1	217	A
5	B1	220	U
5	B1	226	A
5	B1	228	C
5	B1	230	A
5	B1	238	C
5	B1	284	C
5	B1	286	U
5	B1	288	G
5	B1	292	A
5	B1	293	C
5	B1	306	C
5	B1	312	G
5	B1	313	A
5	B1	314	U
5	B1	319	C
5	B1	320	G
5	B1	327	G
5	B1	328	U
5	B1	329	G
5	B1	332	G
5	B1	333	G
5	B1	338	G
5	B1	339	A
5	B1	351	G
5	B1	364	A
5	B1	368	U
5	B1	370	G
5	B1	371	A
5	B1	385	G

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Mol	Chain	Res	Type
5	B1	386	C
5	B1	400	C
5	B1	407	G
5	B1	408	A
5	B1	409	C
5	B1	426	A
5	B1	428	U
5	B1	448	A
5	B1	450	C
5	B1	463	C
5	B1	464	A
5	B1	465	A
5	B1	472	C
5	B1	474	G
5	B1	476	A
5	B1	487	U
5	B1	489	A
5	B1	492	C
5	B1	493	A
5	B1	496	C
5	B1	501	C
5	B1	502	C
5	B1	508	A
5	B1	522	A
5	B1	523	A
5	B1	524	U
5	B1	525	A
5	B1	533	A
5	B1	534	G
5	B1	535	G
5	B1	536	A
5	B1	541	U
5	B1	542	U
5	B1	544	G
5	B1	545	A
5	B1	546	G
5	B1	547	G
5	B1	548	C
5	B1	549	C
5	B1	553	U
5	B1	554	A
5	B1	555	A

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Mol	Chain	Res	Type
5	B1	560	A
5	B1	565	G
5	B1	567	C
5	B1	570	C
5	B1	576	A
5	B1	585	C
5	B1	588	G
5	B1	590	A
5	B1	591	U
5	B1	592	C
5	B1	594	A
5	B1	608	C
5	B1	614	C
5	B1	617	G
5	B1	620	G
5	B1	626	G
5	B1	628	A
5	B1	629	A
5	B1	643	A
5	B1	644	G
5	B1	645	C
5	B1	655	A
5	B1	660	C
5	B1	662	G
5	B1	668	A
5	B1	669	A
5	B1	673	G
5	B1	684	G
5	B1	687	C
5	B1	688	U
5	B1	689	U
5	B1	690	G
5	B1	695	C
5	B1	738	C
5	B1	742	U
5	B1	743	U
5	B1	744	G
5	B1	746	C
5	B1	748	C
5	B1	751	G
5	B1	791	C
5	B1	797	C

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Mol	Chain	Res	Type
5	B1	798	G
5	B1	799	U
5	B1	800	U
5	B1	801	U
5	B1	811	A
5	B1	827	A
5	B1	833	C
5	B1	836	G
5	B1	837	A
5	B1	839	C
5	B1	841	G
5	B1	847	A
5	B1	859	G
5	B1	861	A
5	B1	862	A
5	B1	865	A
5	B1	868	G
5	B1	870	A
5	B1	874	G
5	B1	888	U
5	B1	890	U
5	B1	913	A
5	B1	914	U
5	B1	917	U
5	B1	918	U
5	B1	919	A
5	B1	920	A
5	B1	928	G
5	B1	929	G
5	B1	930	C
5	B1	934	G
5	B1	950	C
5	B1	956	G
5	B1	959	G
5	B1	975	G
5	B1	990	A
5	B1	992	A
5	B1	1002	U
5	B1	1008	A
5	B1	1015	U
5	B1	1021	U
5	B1	1023	A

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Mol	Chain	Res	Type
5	B1	1044	G
5	B1	1045	U
5	B1	1053	C
5	B1	1060	A
5	B1	1061	U
5	B1	1085	C
5	B1	1089	G
5	B1	1100	A
5	B1	1109	C
5	B1	1110	G
5	B1	1114	U
5	B1	1115	U
5	B1	1119	A
5	B1	1120	U
5	B1	1121	G
5	B1	1133	A
5	B1	1139	C
5	B1	1140	G
5	B1	1146	C
5	B1	1149	A
5	B1	1150	A
5	B1	1170	A
5	B1	1188	A
5	B1	1195	A
5	B1	1199	A
5	B1	1207	G
5	B1	1215	C
5	B1	1216	C
5	B1	1224	G
5	B1	1242	U
5	B1	1243	U
5	B1	1251	A
5	B1	1253	A
5	B1	1256	G
5	B1	1257	G
5	B1	1258	A
5	B1	1259	A
5	B1	1261	C
5	B1	1278	A
5	B1	1285	G
5	B1	1286	G
5	B1	1287	A

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Mol	Chain	Res	Type
5	B1	1288	U
5	B1	1289	U
5	B1	1290	G
5	B1	1301	A
5	B1	1302	G
5	B1	1303	C
5	B1	1313	A
5	B1	1314	U
5	B1	1330	G
5	B1	1333	U
5	B1	1352	G
5	B1	1353	A
5	B1	1363	C
5	B1	1371	U
5	B1	1372	U
5	B1	1375	G
5	B1	1378	A
5	B1	1381	G
5	B1	1395	C
5	B1	1418	C
5	B1	1420	G
5	B1	1421	A
5	B1	1442	U
5	B1	1452	A
5	B1	1454	A
5	B1	1467	C
5	B1	1474	A
5	B1	1476	A
5	B1	1477	U
5	B1	1478	U
5	B1	1487	A
5	B1	1489	A
5	B1	1494	U
5	B1	1497	G
5	B1	1498	A
5	B1	1505	U
5	B1	1507	G
5	B1	1508	A
5	B1	1521	C
5	B1	1522	A
5	B1	1533	A
5	B1	1535	U

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Mol	Chain	Res	Type
5	B1	1537	A
5	B1	1544	C
5	B1	1546	G
5	B1	1553	C
5	B1	1554	C
5	B1	1555	U
5	B1	1558	C
5	B1	1580	A
5	B1	1585	U
5	B1	1586	U
5	B1	1588	A
5	B1	1601	A
5	B1	1604	G
5	B1	1606	G
5	B1	1614	A
5	B1	1620	A
5	B1	1621	U
5	B1	1622	U
5	B1	1623	A
5	B1	1624	U
5	B1	1625	U
5	B1	1639	G
5	B1	1660	C
5	B1	1661	A
5	B1	1662	U
5	B1	1663	A
5	B1	1671	G
5	B1	1677	U
5	B1	1683	C
5	B1	1690	U
5	B1	1695	A
5	B1	1700	C
5	B1	1710	C
5	B1	1721	U
5	B1	1726	G
5	B1	1750	C
5	B1	1756	C
5	B1	1757	G
5	B1	1777	G
5	B1	1780	G
5	B1	1781	A
5	B1	1783	C

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Mol	Chain	Res	Type
5	B1	1784	G
5	B1	1824	A
5	B1	1829	G
5	B1	1831	A
5	B1	1834	A
5	B1	1835	A
5	B1	1837	G
5	B1	1838	U
5	B1	1849	G
5	B1	1852	C
5	B1	1856	C
5	B1	1860	A
5	B1	1861	G
5	B1	1862	G
5	B1	1863	A
5	B1	1864	U
5	B1	1865	C
5	B1	1866	A
5	B1	1869	A
39	A3	16	G
39	A3	34	U
39	A3	35	C
39	A3	37	A
39	A3	38	U
39	A3	39	G
39	A3	51	U
39	A3	59	A
39	A3	63	U
39	A3	71	A
39	A3	72	A
39	A3	77	A
39	A3	80	A
39	A3	81	C
39	A3	87	G
39	A3	94	G
39	A3	96	C
39	A3	103	A
39	A3	105	C
39	A3	107	C
39	A3	109	C
39	A3	110	U
39	A3	111	U

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Mol	Chain	Res	Type
39	A3	112	G
39	A3	114	G
39	A3	121	G
39	A3	123	U
39	A3	124	U
39	A3	125	C
39	A3	126	C
39	A3	128	C
39	A3	129	C
39	A3	130	C
39	A3	148	A
39	A3	151	G
40	A4	7	G
40	A4	10	C
40	A4	11	A
40	A4	14	C
40	A4	22	A
40	A4	27	G
40	A4	33	U
40	A4	45	U
40	A4	47	G
40	A4	48	G
40	A4	50	A
40	A4	51	G
40	A4	53	U
40	A4	63	C
40	A4	64	G
40	A4	74	A
40	A4	76	U
40	A4	91	C
40	A4	97	G
40	A4	110	G
40	A4	119	U

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A2	31	U
1	A2	71	C
1	A2	901	U
1	A2	959	C
1	A2	1500	A

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Mol	Chain	Res	Type
1	A2	4661	U
1	A2	4865	G
1	A2	4870	G
1	A2	4946	U
5	B1	227	U
5	B1	369	C
5	B1	797	C
5	B1	1554	C

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	3,86	14,20,21	1.11	2 (14%)	14,28,30	1.52	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	3,86	-	10/20/21/23	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	Ct	715	DDE	CD2-NE2	2.23	1.39	1.36
86	Ct	715	DDE	CBW-CBI	2.08	1.56	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	Ct	715	DDE	CBW-CBI-NAD	3.36	119.57	115.28
86	Ct	715	DDE	CB-CA-C	-2.27	107.21	111.47
86	Ct	715	DDE	CAC-NCB-CBW	2.10	115.73	110.51

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	Ct	715	DDE	CA-CB-CG-ND1
86	Ct	715	DDE	CA-CB-CG-CD2
86	Ct	715	DDE	NAD-CBI-CBW-NCB
86	Ct	715	DDE	OAG-CBI-CBW-NCB
86	Ct	715	DDE	CBI-CBW-NCB-CAB
86	Ct	715	DDE	CE1-CAT-CAU-CBW
86	Ct	715	DDE	CAT-CAU-CBW-CBI
86	Ct	715	DDE	OAG-CBI-CBW-CAU
86	Ct	715	DDE	CBI-CBW-NCB-CAC
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	1.58	7 (24%)	33,54,54	2.10	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	-	-	7/14/38/38	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	4.35	1.64	1.59
89	Ct	901	GNP	C6-N1	3.08	1.38	1.33
89	Ct	901	GNP	PG-N3B	2.81	1.70	1.63
89	Ct	901	GNP	PB-O1B	2.79	1.50	1.46
89	Ct	901	GNP	PG-O1G	2.68	1.50	1.46
89	Ct	901	GNP	PB-O2B	-2.30	1.50	1.56
89	Ct	901	GNP	C5-C6	2.03	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	-8.38	111.98	123.43
89	Ct	901	GNP	C2-N1-C6	5.77	125.10	115.93
89	Ct	901	GNP	N3-C2-N1	-2.75	123.55	127.22
89	Ct	901	GNP	C4-C5-C6	-2.55	118.36	120.80
89	Ct	901	GNP	C2-N3-C4	-2.16	112.89	115.36
89	Ct	901	GNP	PB-O3A-PA	-2.14	125.09	132.62
89	Ct	901	GNP	O1B-PB-N3B	-2.09	108.70	111.77

There are no chirality outliers.

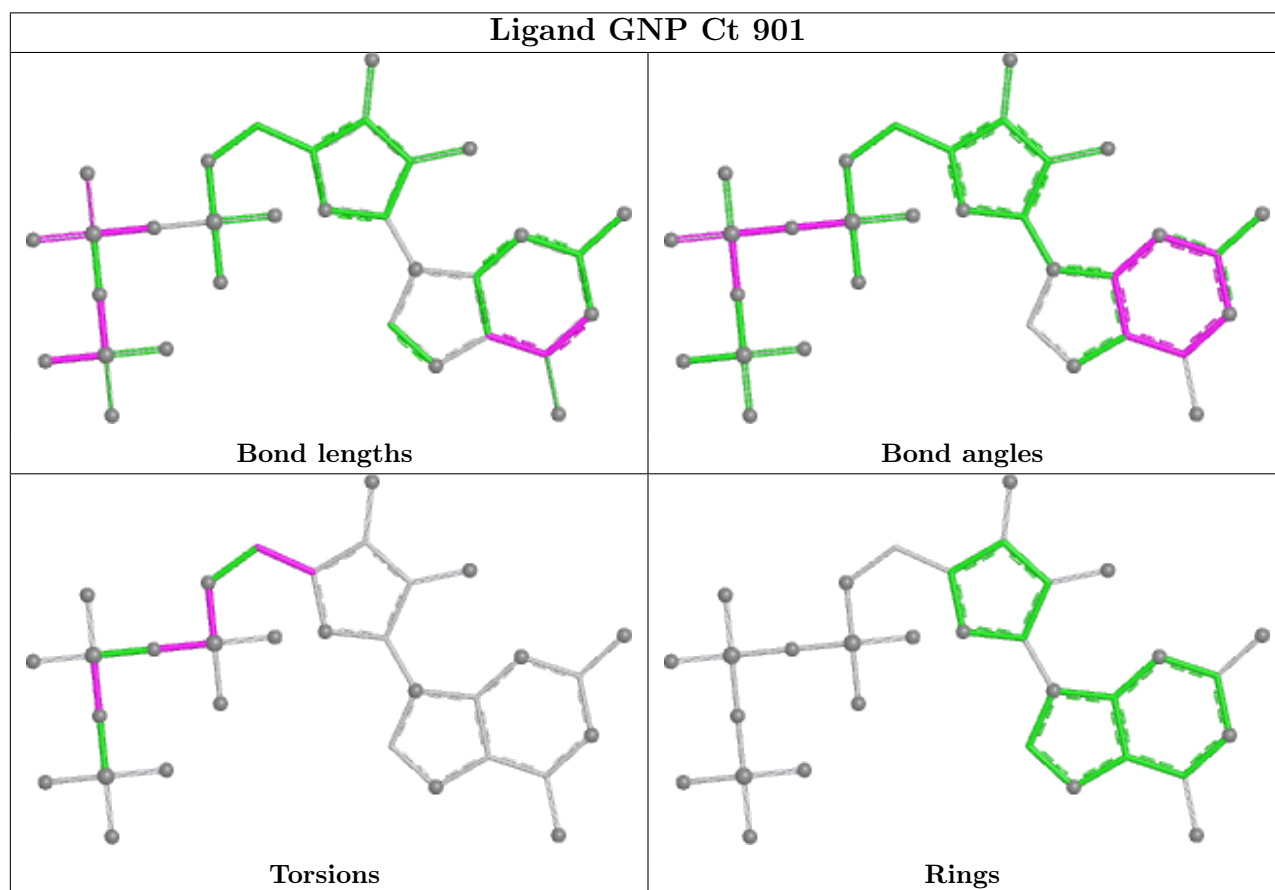
All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
89	Ct	901	GNP	PG-N3B-PB-O1B
89	Ct	901	GNP	C5'-O5'-PA-O3A
89	Ct	901	GNP	C5'-O5'-PA-O1A
89	Ct	901	GNP	C3'-C4'-C5'-O5'
89	Ct	901	GNP	O4'-C4'-C5'-O5'
89	Ct	901	GNP	PB-O3A-PA-O1A
89	Ct	901	GNP	C5'-O5'-PA-O2A

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
1	A2	11
5	B1	6

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	20.66
1	B1	751:G	O3'	790:C	P	20.56
1	A2	517:C	O3'	629:G	P	18.02
1	A2	3948:C	O3'	4004:G	P	17.82
1	B1	1757:G	O3'	1775:U	P	17.75
1	A2	1233:C	O3'	1243:G	P	17.73
1	B1	240:G	O3'	282:G	P	17.66
1	A2	4734:C	O3'	4818:G	P	17.59
1	B1	696:G	O3'	737:G	P	17.05
1	A2	750:G	O3'	890:C	P	16.93
1	A2	976:U	O3'	1047:G	P	16.84
1	A2	2881:G	O3'	3569:C	P	16.75
1	B1	1426:U	O3'	1438:A	P	16.52
1	A2	1089:A	O3'	1145:G	P	16.07
1	A2	1680:C	O3'	1699:C	P	15.11
1	A2	1202:G	O3'	1216:G	P	14.53
1	A2	2068:C	O3'	2245:C	P	14.01

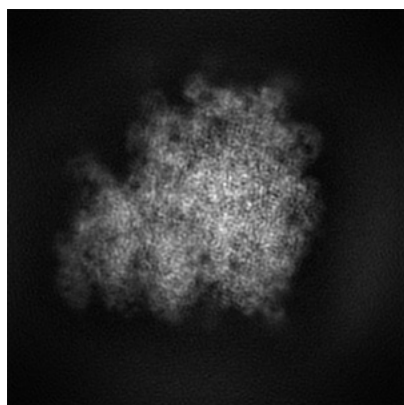
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0098. These allow visual inspection of the internal detail of the map and identification of artifacts.

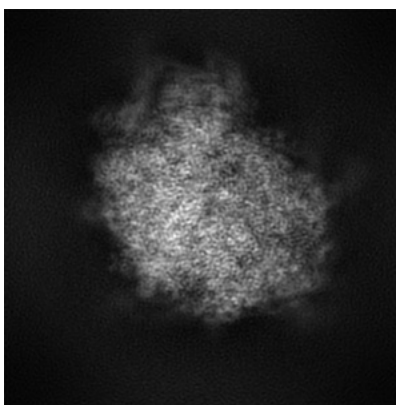
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

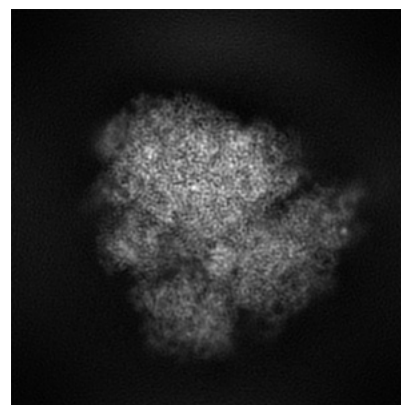
6.1.1 Primary map



X



Y

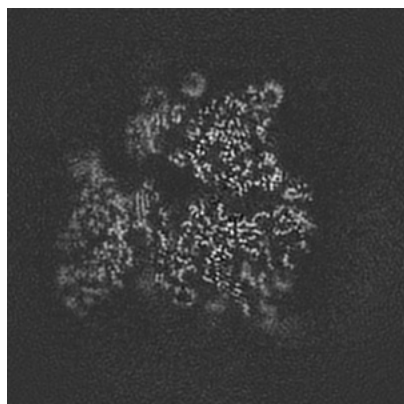


Z

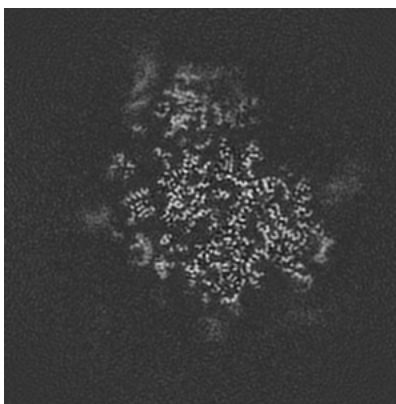
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

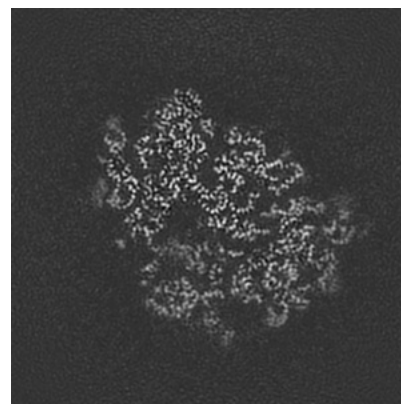
6.2.1 Primary map



X Index: 202



Y Index: 202

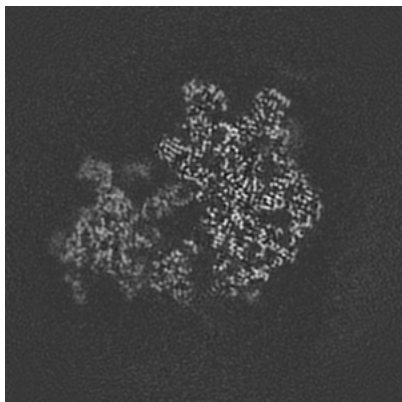


Z Index: 202

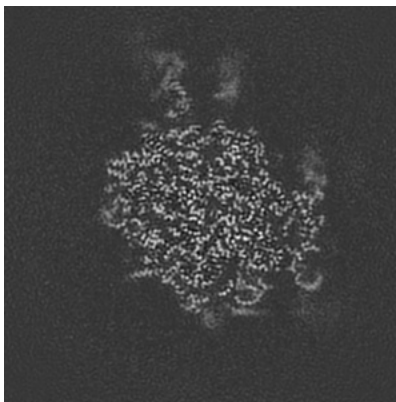
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

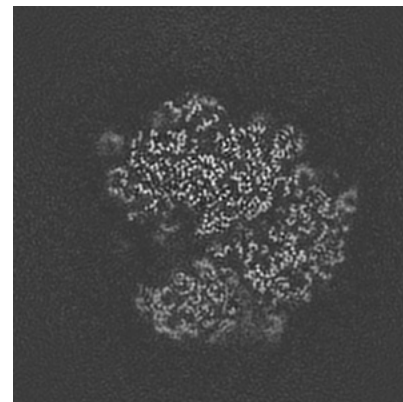
6.3.1 Primary map



X Index: 179



Y Index: 220

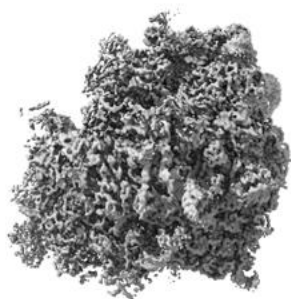


Z Index: 185

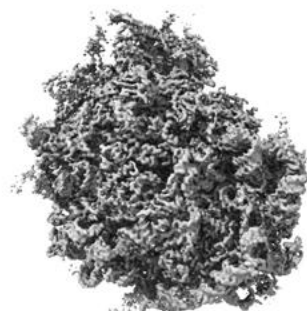
The images above show the largest variance slices of the map in three orthogonal directions.

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.

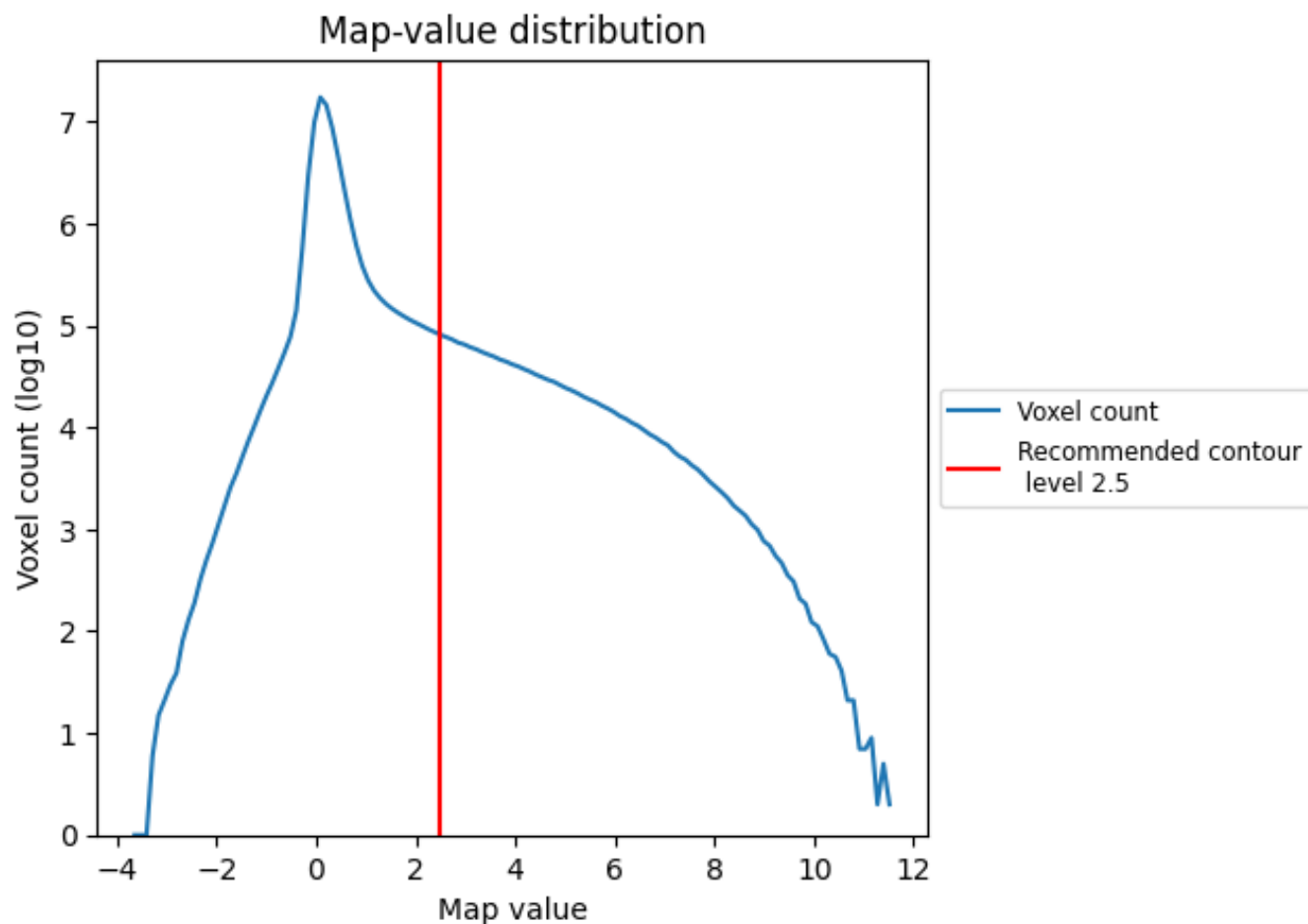
6.5 Mask visualisation

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

7 Map analysis [i](#)

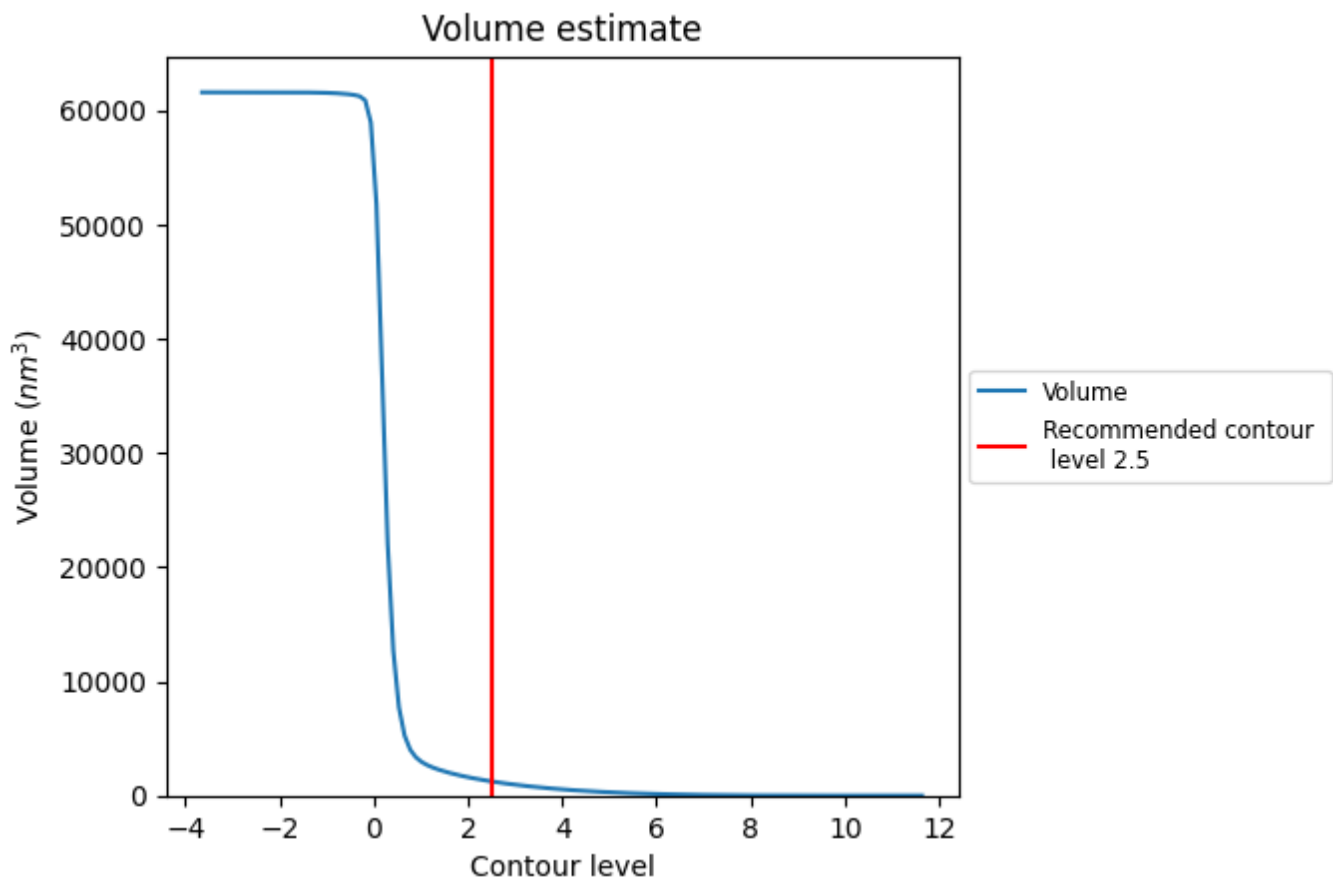
This section contains the results of statistical analysis of the map.

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.

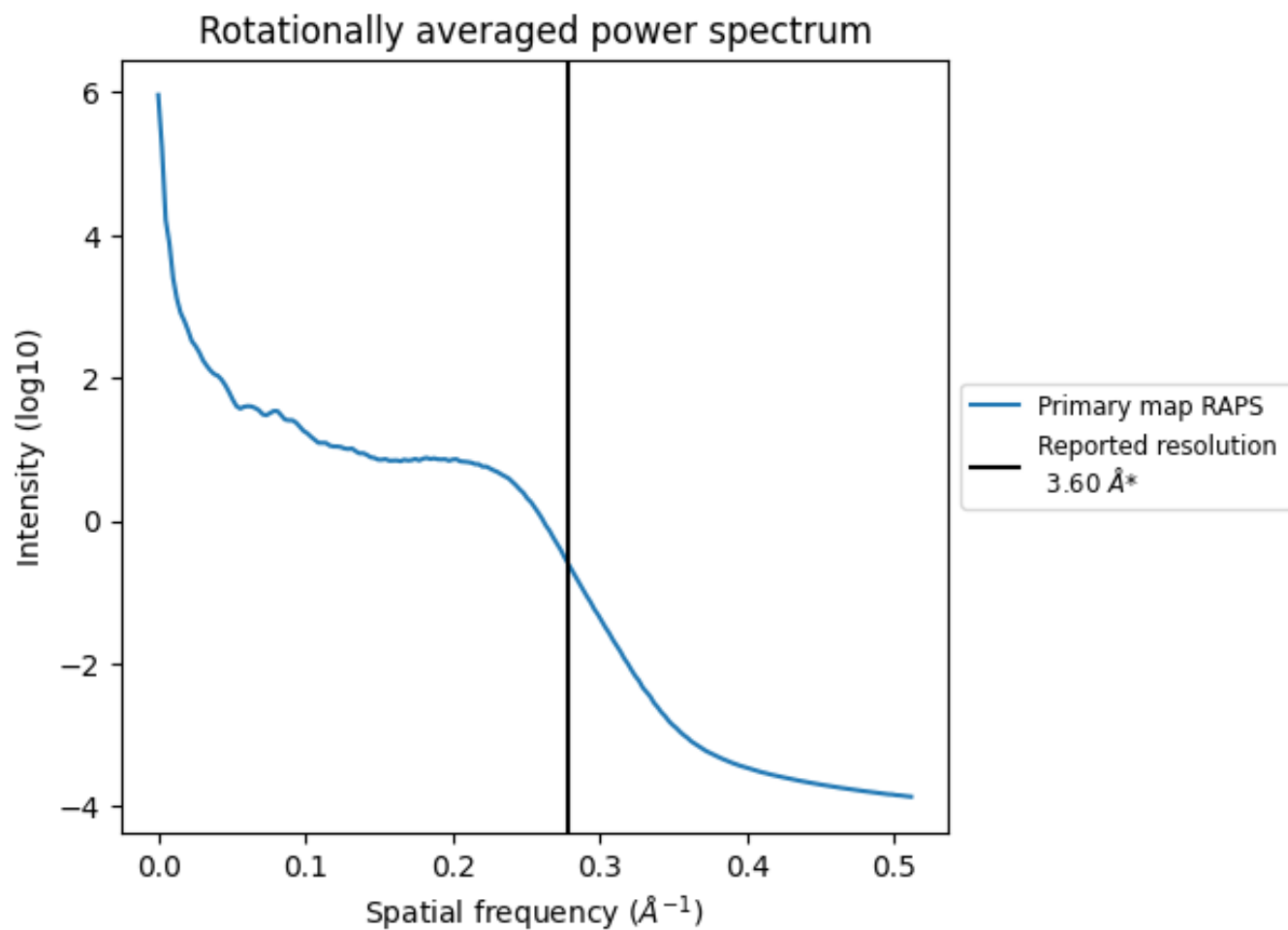
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1237 nm³; this corresponds to an approximate mass of 1118 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 Å⁻¹

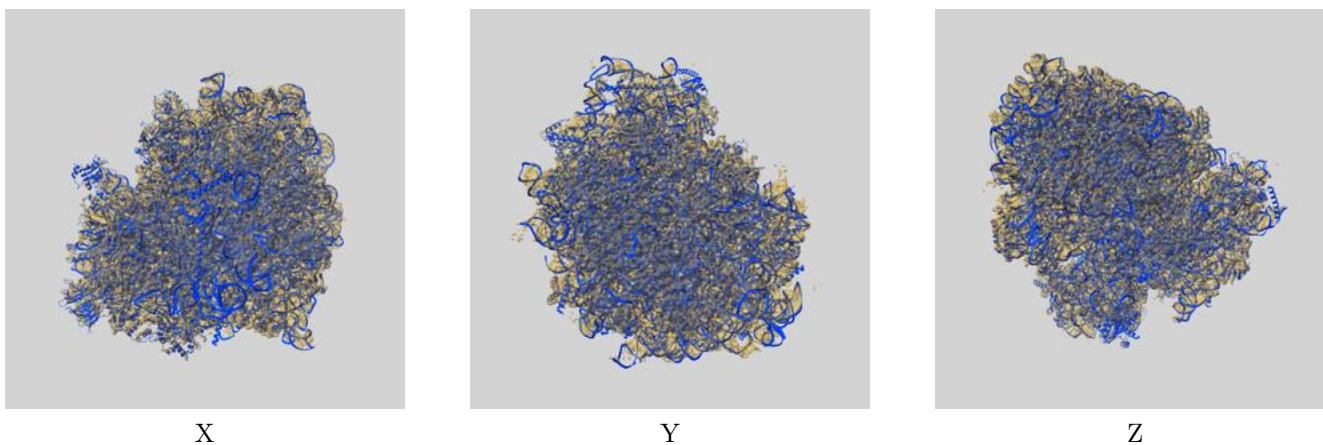
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

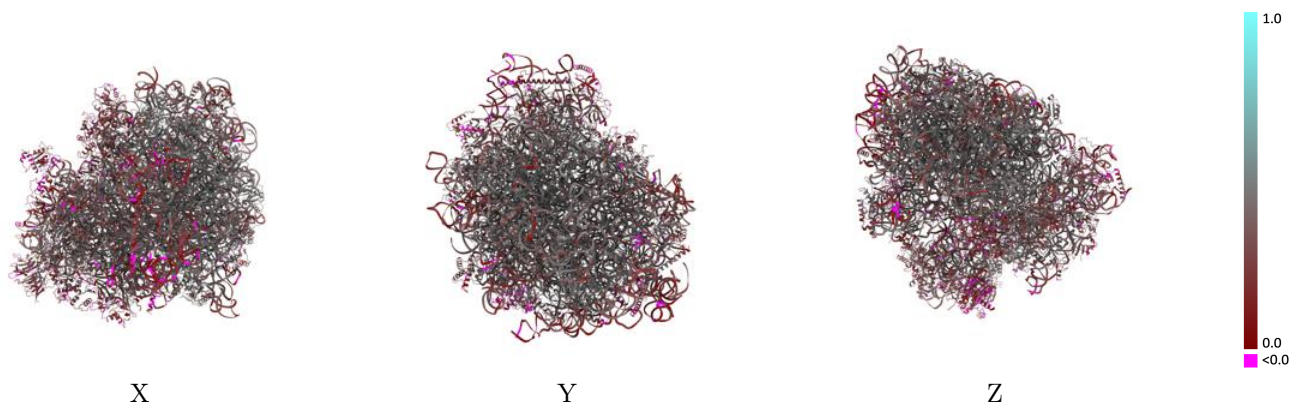
This section contains information regarding the fit between EMDB map EMD-0098 and PDB model 6GZ3. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay [i](#)



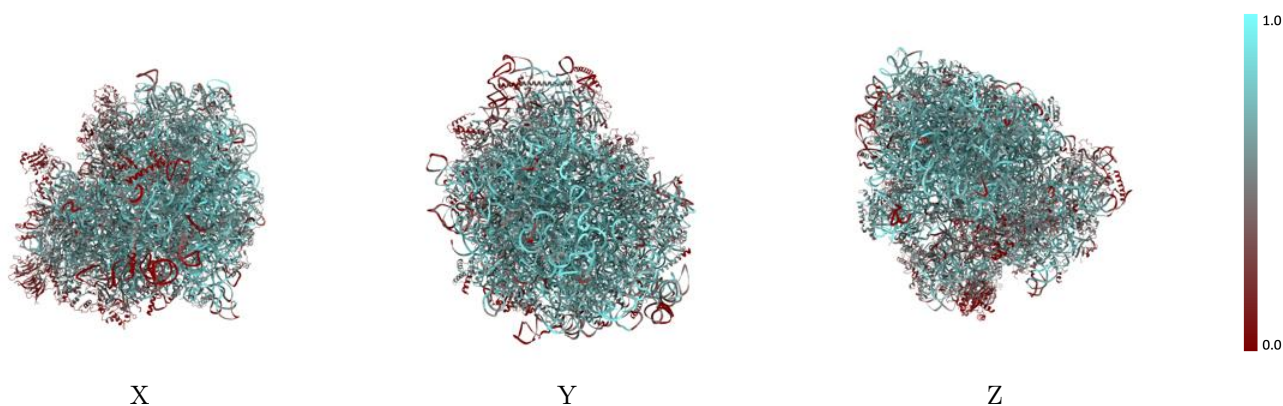
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



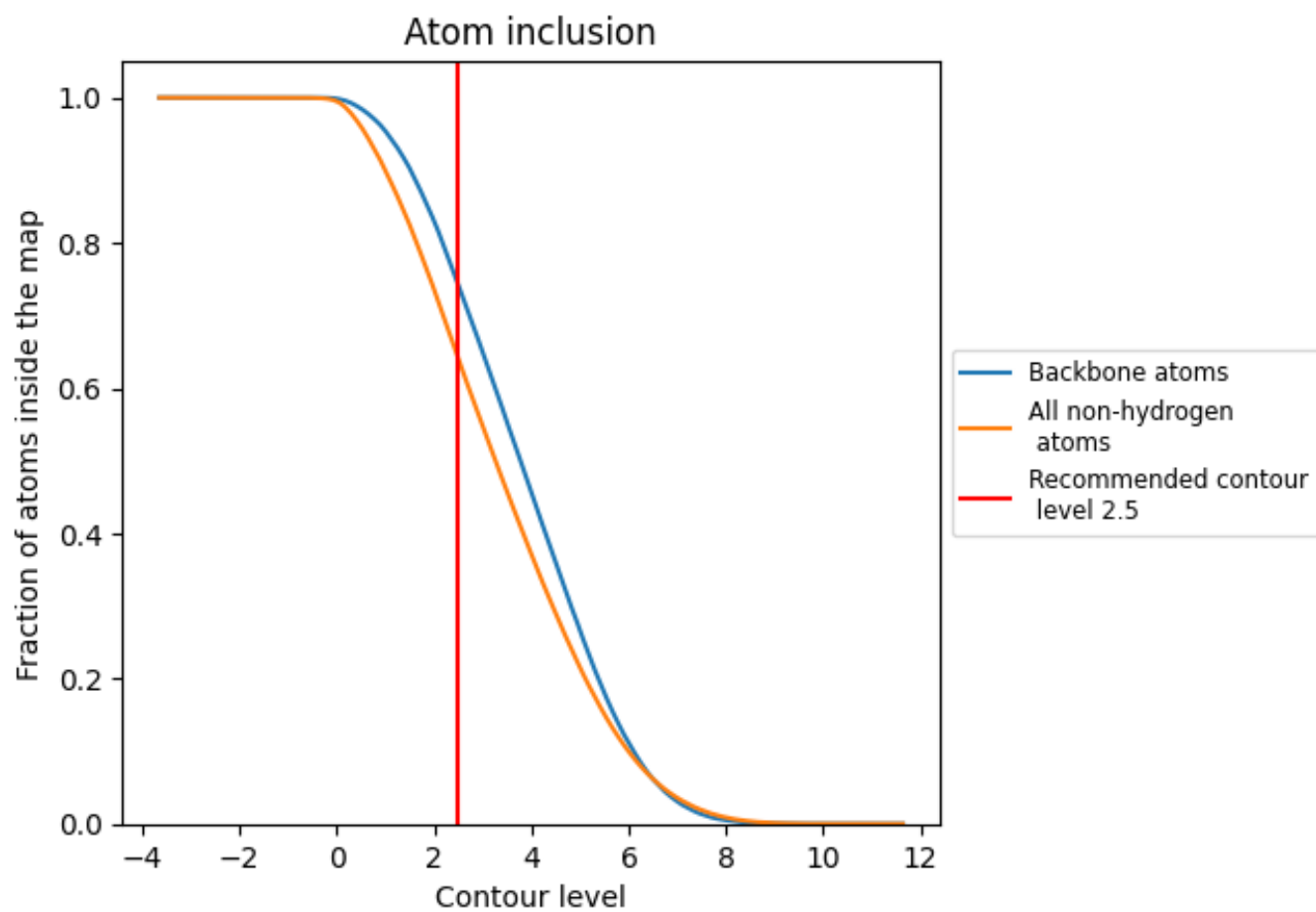
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 74% of all backbone atoms, 64% 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	0.6403	0.3650
A2	0.7652	0.3920
A3	0.7730	0.3970
A4	0.8501	0.4350
AA	0.6617	0.4460
AB	0.6398	0.4200
AC	0.6499	0.4150
AD	0.6158	0.3670
AE	0.5062	0.3230
AF	0.6182	0.3860
AG	0.5591	0.3630
AH	0.5847	0.4080
AI	0.6323	0.4130
AJ	0.5899	0.3710
AK	0.2461	0.2090
AL	0.5902	0.3630
AM	0.6116	0.3790
AN	0.7070	0.4320
AO	0.6430	0.4030
AP	0.6719	0.4380
AQ	0.6450	0.4010
AR	0.5690	0.3590
AS	0.6586	0.4180
AT	0.6253	0.4120
AU	0.5215	0.3620
AV	0.6399	0.4570
AW	0.3249	0.2310
AX	0.6219	0.4310
AY	0.6420	0.4130
AZ	0.6090	0.3860
Aa	0.6717	0.4210
Ab	0.5470	0.3440
Ac	0.5714	0.3640
Ad	0.6321	0.4270
Ae	0.6598	0.4260























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Chain	Atom inclusion	Q-score
Af	 0.6734	 0.4220
Ag	 0.6076	 0.3990
Ah	 0.5739	 0.3710
Ai	 0.6181	 0.3750
Aj	 0.7245	 0.4400
Ak	 0.5009	 0.3570
Al	 0.6392	 0.4160
Am	 0.6423	 0.3990
An	 0.2636	 0.3050
Ao	 0.6337	 0.4200
Ap	 0.6473	 0.4240
Aq	 0.1342	 0.1360
At	 0.6536	 0.3970
Au	 0.0204	 0.0060
B1	 0.7139	 0.3680
BA	 0.4251	 0.3060
BB	 0.4746	 0.3290
BC	 0.5396	 0.3640
BD	 0.4478	 0.3200
BE	 0.5126	 0.3390
BF	 0.3860	 0.2870
BG	 0.3773	 0.2420
BH	 0.2986	 0.2680
BI	 0.4771	 0.3280
BJ	 0.5422	 0.3200
BK	 0.3043	 0.1640
BL	 0.4881	 0.3470
BM	 0.0643	 0.1290
BN	 0.5189	 0.3600
BO	 0.5238	 0.3840
BP	 0.3826	 0.2500
BQ	 0.4157	 0.3100
BR	 0.3357	 0.2710
BS	 0.4092	 0.2540
BT	 0.3845	 0.2450
BU	 0.3413	 0.2890
BV	 0.4909	 0.3430
BW	 0.5653	 0.3820
BX	 0.5640	 0.4040
BY	 0.4284	 0.2680
BZ	 0.2307	 0.2110
Ba	 0.5730	 0.3720

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Chain	Atom inclusion	Q-score
Bb	 0.4405	 0.3290
Bc	 0.3426	 0.3010
Bd	 0.5012	 0.2970
Be	 0.4479	 0.3590
Bf	 0.0634	 0.1410
Bg	 0.2017	 0.2380
Bv	 0.5302	 0.3010
Bw	 0.6595	 0.3310
Bx	 0.5058	 0.2810
Ct	 0.4614	 0.3260