Full wwPDB EM Validation Report ⓘ

Apr 2, 2025 – 02:27 am BST

PDB ID	:	5AJ0 / pdb_00005aj0
EMDB ID	:	EMD-2875
Title	:	Cryo electron microscopy of actively translating human polysomes (POST state).
Authors	:	Behrmann, E.; Loerke, J.; Budkevich, T.V.; Yamamoto, K.; Schmidt, A.; Penczek, P.A.; Vos, M.R.; Burger, J.; Mielke, T.; Scheerer, P.; Spahn, C.M.T.
Deposited on	:	2015-02-19
Resolution	:	3.50 Å(reported)
Based on initial model	:	4UJE

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:

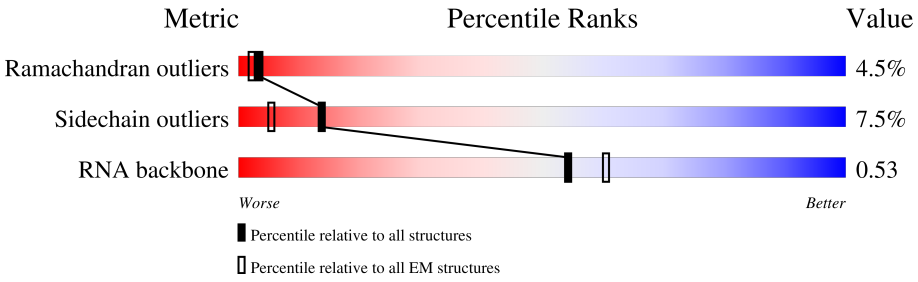
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	A3	194	81% 46% 27% 8% 19%
2	A4	121	98% 44% 49% 6%
3	AA	257	98% 92% 6%
4	AB	403	98% 90% 7%
5	AC	427	85% 76% 8% 15%
6	AD	297	99% 91% 8%
7	AE	288	67% 46% 18% 33%
8	AF	248	94% 88% 6%

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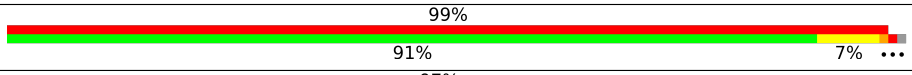
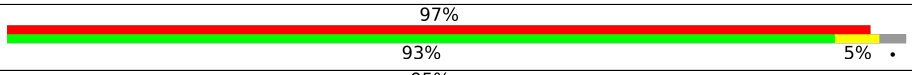
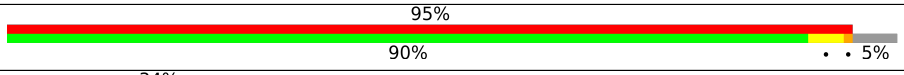
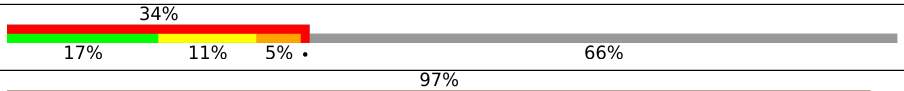
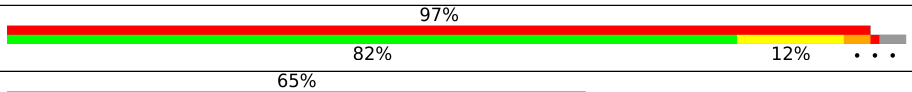
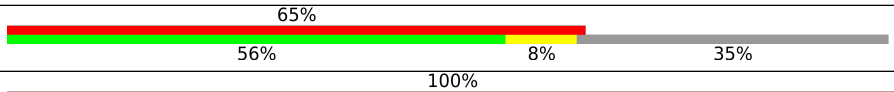
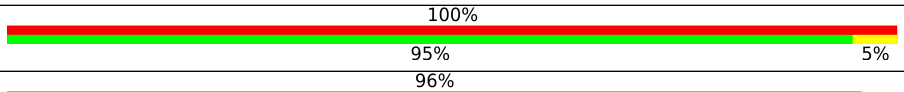
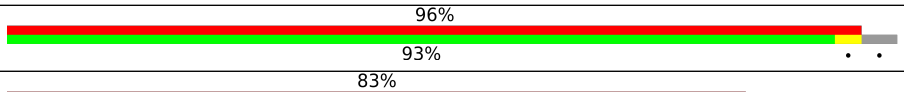
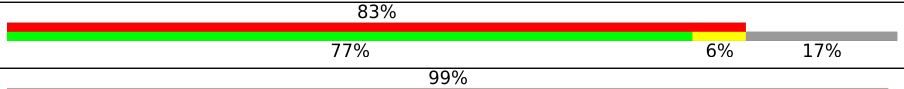
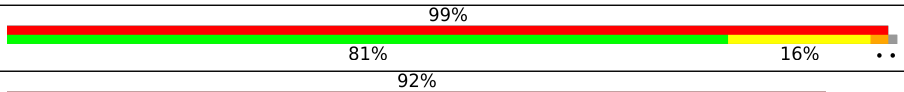
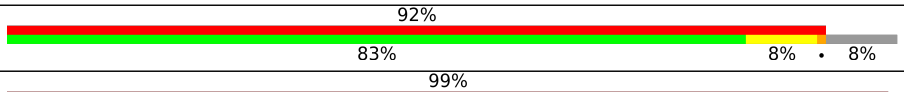
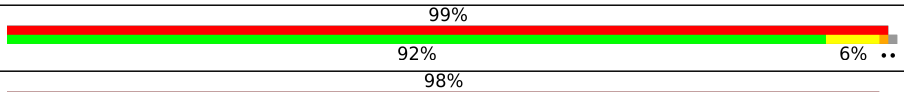
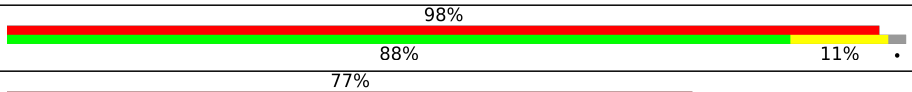
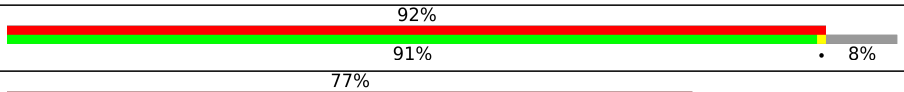
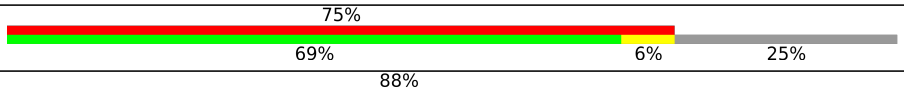
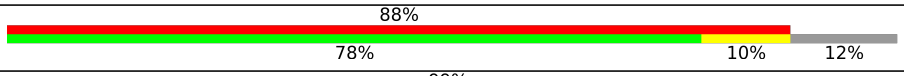
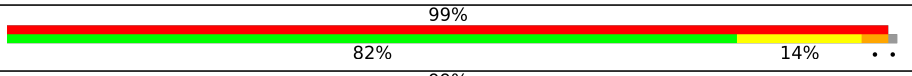
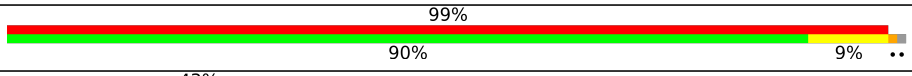
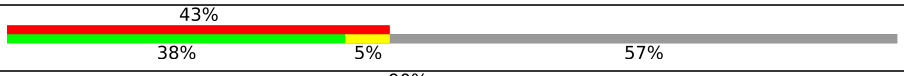
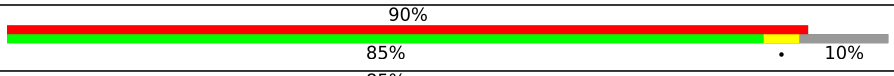
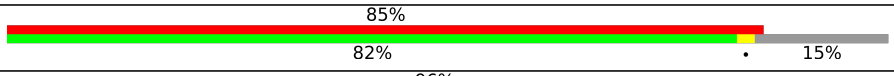
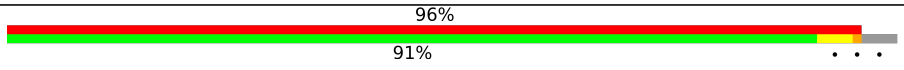
Mol	Chain	Length	Quality of chain
9	AG	266	
10	AH	192	
11	AI	214	
12	AJ	178	
13	AK	317	
14	AL	211	
15	AM	215	
16	AN	204	
17	AO	203	
18	AP	184	
19	AQ	188	
20	AR	196	
21	AS	176	
22	AT	160	
23	AU	128	
24	AV	140	
25	AW	157	
26	AX	156	
27	AY	145	
28	AZ	136	
29	Aa	148	
30	Ab	159	
31	Ac	115	
32	Ad	125	
33	Ae	135	

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Mol	Chain	Length	Quality of chain
34	Af	110	99% 90% 6%
35	Ag	117	97% 91% 6%
36	Ah	123	99% 83% 16%
37	Ai	105	92% 85% 8% 8%
38	Aj	97	87% 72% 12% 13%
39	Ak	70	99% 66% 24% 9%
40	Al	51	98% 92% 6%
41	Am	128	39% 38% 61%
42	An	25	100% 96%
43	Ao	106	99% 88% 11%
44	Ap	92	99% 93% 5%
45	Aq	165	84% 41% 30% 11% 16%
46	At	137	89% 74% 15% 11%
47	Au	217	100% 87% 10%
48	A2	5029	72% 42% 26% 28%
49	B1	1869	91% 54% 34% 9%
50	BA	295	73% 66% 6% 27%
51	BB	264	80% 68% 12% 20%
52	BC	293	76% 69% 7% 24%
53	BD	243	91% 84% 6% 9%
54	BE	263	98% 90% 6%
55	BF	204	93% 85% 7% 7%
56	BG	249	93% 80% 14% 7%
57	BH	194	94% 90% 5% 6%
58	BI	208	100% 93% 7%

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Mol	Chain	Length	Quality of chain
59	BJ	194	92% 81% 10% 8%
60	BK	165	59% 54% 41%
61	BL	158	97% 89% 8%
62	BM	132	91% 87% 9%
63	BN	151	99% 86% 12%
64	BO	151	90% 79% 10% 10%
65	BP	145	83% 65% 12% 17%
66	BQ	146	95% 79% 14% 5%
67	BR	135	93% 74% 15% 7%
68	BS	152	91% 77% 14% 9%
69	BT	145	99% 88% 10%
70	BU	119	82% 75% 7% 18%
71	BV	83	98% 89% 8%
72	BW	130	99% 92% 5%
73	BX	143	97% 86% 10%
74	BY	133	94% 90% 6%
75	BZ	125	69% 52% 17% 31%
76	Ba	115	84% 76% 8% 16%
77	Bb	84	95% 93% 5%
78	Bc	69	90% 84% 10%
79	Bd	56	91% 71% 18% 9%
80	Be	59	93% 80% 14% 7%
81	Bf	156	47% 46% 53%
82	Bg	317	99% 96%
83	Bv	76	100% 46% 51%

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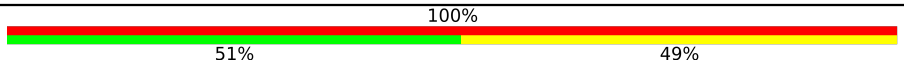
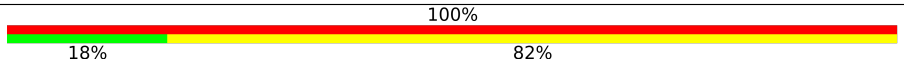
Mol	Chain	Length	Quality of chain
83	Bw	76	
84	Bx	28	
85	By	24	

2 Entry composition (i)

There are 87 unique types of molecules in this entry. The entry contains 218559 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 5.8S ribosomal RNA.

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

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 3 is a protein called 60S ribosomal protein L8.

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

- Molecule 4 is a protein called 60S ribosomal protein L3.

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

- Molecule 5 is a protein called 60S ribosomal protein L4.

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

- Molecule 6 is a protein called 60S ribosomal protein L5.

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

- Molecule 7 is a protein called 60S ribosomal protein L6.

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

- Molecule 8 is a protein called 60S ribosomal protein L7.

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

- Molecule 9 is a protein called 60S ribosomal protein L7a.

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

- Molecule 10 is a protein called 60S ribosomal protein L9.

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

- Molecule 11 is a protein called 60S ribosomal protein L10.

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

- Molecule 12 is a protein called 60S ribosomal protein L11.

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

- Molecule 13 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AK	109	Total	C	N	O	S	0	0
			872	554	159	151	8		

- Molecule 14 is a protein called 60S ribosomal protein L13.

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

- Molecule 15 is a protein called 60S ribosomal protein L14.

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

- Molecule 16 is a protein called 60S ribosomal protein L15.

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

- Molecule 17 is a protein called 60S ribosomal protein L13a.

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

- Molecule 18 is a protein called 60S ribosomal protein L17.

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

- Molecule 19 is a protein called 60S ribosomal protein L18.

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

- Molecule 20 is a protein called 60S ribosomal protein L19.

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

- Molecule 21 is a protein called 60S ribosomal protein L18a.

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

- Molecule 22 is a protein called 60S ribosomal protein L21.

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

- Molecule 23 is a protein called 60S ribosomal protein L22.

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

- Molecule 24 is a protein called 60S ribosomal protein L23.

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

- Molecule 25 is a protein called 60S ribosomal protein L24.

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

- Molecule 26 is a protein called 60S ribosomal protein L23a.

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

- Molecule 27 is a protein called 60S ribosomal protein L26.

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

- Molecule 28 is a protein called 60S ribosomal protein L27.

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

- Molecule 29 is a protein called 60S ribosomal protein L27a.

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

- Molecule 30 is a protein called 60S ribosomal protein L29.

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

- Molecule 31 is a protein called 60S ribosomal protein L30.

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

- Molecule 32 is a protein called 60S ribosomal protein L31.

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

- Molecule 33 is a protein called 60S ribosomal protein L32.

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

- Molecule 34 is a protein called 60S ribosomal protein L35a.

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

- Molecule 35 is a protein called 60S ribosomal protein L34.

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

- Molecule 36 is a protein called 60S ribosomal protein L35.

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

- Molecule 37 is a protein called 60S ribosomal protein L36.

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

- Molecule 38 is a protein called 60S ribosomal protein L37.

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

- Molecule 39 is a protein called 60S ribosomal protein L38.

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

- Molecule 40 is a protein called 60S ribosomal protein L39.

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

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 42 is a protein called 60S ribosomal protein L41.

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

- Molecule 43 is a protein called 60S ribosomal protein L36a.

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

- Molecule 44 is a protein called 60S ribosomal protein L37a.

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

- Molecule 45 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Aq	138	Total	C	N	O	S	0	0
			1046	654	196	193	3		

- Molecule 46 is a protein called 60S ribosomal protein L28.

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

- Molecule 47 is a protein called 60S ribosomal protein L10a.

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

- Molecule 48 is a RNA chain called 28S ribosomal RNA.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	245	C	-	insertion	GB 337381
A2	246	C	-	insertion	GB 337381
A2	247	C	-	insertion	GB 337381
A2	4684	G	-	insertion	GB 337381

- Molecule 49 is a RNA chain called 18S ribosomal RNA.

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

- Molecule 50 is a protein called 40S ribosomal protein SA.

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

- Molecule 51 is a protein called 40S ribosomal protein S3a.

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

- Molecule 52 is a protein called 40S ribosomal protein S2.

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

- Molecule 53 is a protein called 40S ribosomal protein S3.

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

- Molecule 54 is a protein called 40S ribosomal protein S4, Y isoform 1.

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

- Molecule 55 is a protein called 40S ribosomal protein S5.

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

- Molecule 56 is a protein called 40S ribosomal protein S6.

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

- Molecule 57 is a protein called 40S ribosomal protein S7.

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

- Molecule 58 is a protein called 40S ribosomal protein S8.

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

- Molecule 59 is a protein called 40S ribosomal protein S9.

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

- Molecule 60 is a protein called 40S ribosomal protein S10.

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

- Molecule 61 is a protein called 40S ribosomal protein S11.

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

- Molecule 62 is a protein called 40S ribosomal protein S12.

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

- Molecule 63 is a protein called 40S ribosomal protein S13.

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

- Molecule 64 is a protein called 40S ribosomal protein S14.

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

- Molecule 65 is a protein called 40S ribosomal protein S15.

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

- Molecule 66 is a protein called 40S ribosomal protein S16.

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

- Molecule 67 is a protein called 40S ribosomal protein S17-like.

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

- Molecule 68 is a protein called 40S ribosomal protein S18.

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

- Molecule 69 is a protein called 40S ribosomal protein S19.

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

- Molecule 70 is a protein called 40S ribosomal protein S20.

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

- Molecule 71 is a protein called 40S ribosomal protein S21.

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

- Molecule 72 is a protein called 40S ribosomal protein S15a.

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

- Molecule 73 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	BX	139	Total	C	N	O	S	0	0
			1080	682	214	181	3		

- Molecule 74 is a protein called 40S ribosomal protein S24.

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

- Molecule 75 is a protein called 40S ribosomal protein S25.

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

- Molecule 76 is a protein called 40S ribosomal protein S26.

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

- Molecule 77 is a protein called 40S ribosomal protein S27.

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

- Molecule 78 is a protein called 40S ribosomal protein S28.

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

- Molecule 79 is a protein called 40S ribosomal protein S29.

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

- Molecule 80 is a protein called 40S ribosomal protein S30.

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

- Molecule 81 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 82 is a protein called Guanine nucleotide-binding protein subunit beta-2-like 1.

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

- Molecule 83 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Bv	76	Total 1623	C 723	N 290	O 534	P 76	0	0
83	Bw	76	Total 1623	C 723	N 290	O 534	P 76	0	0

- Molecule 84 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Bx	28	Total 561	C 252	N 56	O 225	P 28	0	0

- Molecule 85 is a protein called Nascent protein chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
85	By	24	Total 120	C 72	N 24	O 24	0	0

- Molecule 86 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
86	A3	8	Total 8	Mg 8	0
86	A4	9	Total 9	Mg 9	0
86	AA	1	Total 1	Mg 1	0
86	AB	2	Total 2	Mg 2	0
86	AN	2	Total 2	Mg 2	0
86	AY	1	Total 1	Mg 1	0
86	Aa	3	Total 3	Mg 3	0
86	Ae	2	Total 2	Mg 2	0
86	An	1	Total 1	Mg 1	0
86	A2	220	Total 220	Mg 220	0
86	B1	72	Total 72	Mg 72	0

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Mol	Chain	Residues	Atoms	AltConf
86	BD	1	Total Mg 1 1	0
86	BX	1	Total Mg 1 1	0
86	Bv	2	Total Mg 2 2	0
86	Bx	1	Total Mg 1 1	0

- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

3 Residue-property plots

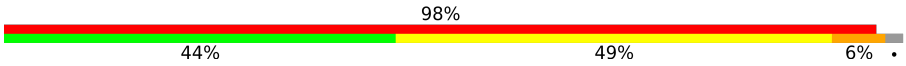
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

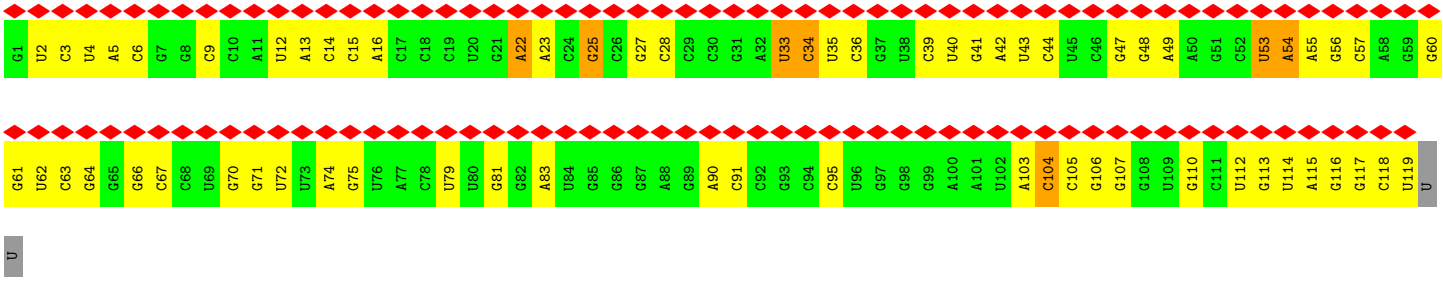
• Molecule 1: 5.8S ribosomal RNA

Chain A3:

• Molecule 2: 5S ribosomal RNA

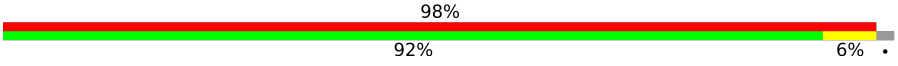
Chain A4:

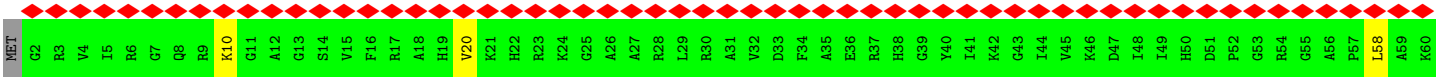




• Molecule 3: 60S ribosomal protein L8

Chain AA:





V61 V62 F63 R64 D65 P66 Y67 R68 F69 K70 K71 R72 T73 E74 L75 F76 I77 A78 A79 E80 G81 I82 H83 T84 G85 Q86 F87 V88 Y89 C90 G91 K92 K93 A94 Q95 L96 N97 I98 G99 N100 V101 L102 P103 V104 G105 T106 M107 P108 E109 G110 T111 I112 V113 C114 C115 L116 E117 E118 K119 P120

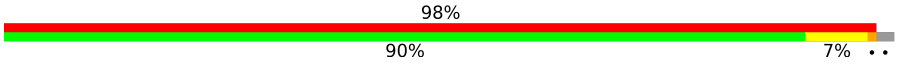
G121 D122 R123 G124 K125 L126 A127 R128 A129 S130 G131 N132 Y133 A134 T135 V136 I137 S138 H139 N140 P141 E142 T143 K144 K145 T146 R147 V148 K149 L150 P151 S152 G153 S154 K155 K156 V157 I158 S159 S160 A161 N162 R163 A164 V165 V166 G167 V168 V169 A170 G171 G172 G173 R174 I175 D176 K177 P178 I179 L180

K181 A182 G183 R184 A185 Y186 H187 K188 Y189 K190 A191 K192 R193 N194 C195 W196 P197 R198 V199 R200 G201 V202 A203 M204 N205 P206 V207 E208 H209 P210 F211 G212 G213 G214 N215 H216 Q217 H218 I219 G220 K221 P222 S223 T224 I225 R226 R227 D228 A229 P230 A231 G232 R233 K234 V235 G236 L237 I238 A239 A240

R241 R242 T243 G244 R245 L246 R247 G248 T249 K250 T251 V252 Q253 GLU LYS GLU ASN

• Molecule 4: 60S ribosomal protein L3

Chain AB:



MET S2 H3 R4 K5 F6 S7 A8 P9 R10 H11 G12 S13 L14 G15 F16 L17 P18 R19 K20 R21 S22 S23 R24 H25 R26 G27 K28 V29 K30 S31 F32 P33 K34 D35 D36 P37 S38 K39 P40 V41 H42 L43 T44 A45 F46 L47 G48 Y49 K50 A51 G52 M53 T54 H55 I56 V57 R58 E59 V60

D61 R62 P63 G64 S65 K66 V67 M68 K69 K70 E71 V72 V73 E74 A75 V76 T77 I78 V79 E80 T81 P82 P83 M84 V85 V86 V87 G88 I89 V90 G91 Y92 V93 E94 T95 P96 R97 G98 L99 R100 T101 F102 K103 T104 V105 F106 A107 E108 H109 I110 S111 D112 E113 C114 K115 R116 R117 F118 Y119 K120

N121 W122 H123 K124 S125 K126 K127 K128 A129 F130 T131 K132 Y133 C134 K135 K136 W137 Q138 D139 E140 D141 G142 K143 K144 Q145 L146 E147 K148 D149 F150 S151 S152 M153 K154 K155 Y156 C157 Q158 V159 I160 R161 V162 I163 A164 H165 T166 Q167 M168 R169 L170 L171 P172 L173 R174 Q175 K176 K177 A178 H179 L180

M181 E182 I183 Q184 V185 N186 G187 G188 T189 V190 A191 E192 K193 L194 D195 W196 A197 R198 E199 R200 L201 E202 Q203 Q204 V205 P206 V207 N208 Q209 V210 F211 G212 Q213 D214 E215 M216 I217 D218 V219 I220 G221 V222 T223 K224 G225 K226 G227 Y228 K229 G230 V231 T232 S233 R234 W235 H236 T237 K238 K239 L240

P241 R242 K243 T244 H245 R246 G247 L248 R249 K250 V251 A252 C253 I254 G255 A256 W257 H258 P259 A260 R261 V262 A263 F264 S265 V266 A267 R268 A269 G270 Q271 K272 G273 Y274 H275 H276 R277 T278 E279 I280 N281 K282 K283 I284 Y285 K286 I287 G288 Q289 G290 Y291 L292 I293 K294 D295 G296 K297 L298 I299 K300

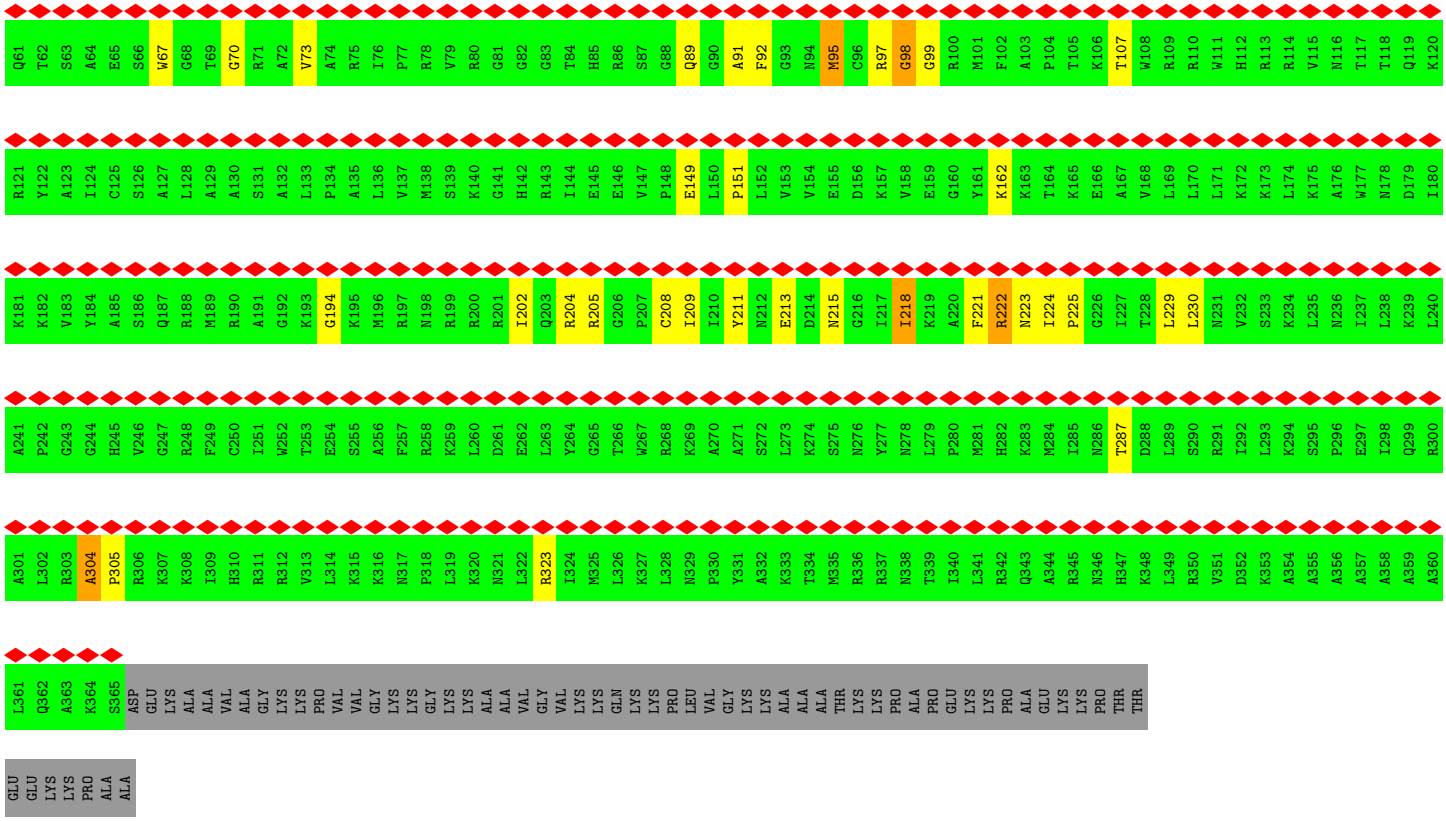
N301 N302 A303 S304 T305 D306 Y307 D308 L309 S310 D311 K312 S313 I314 N315 P316 L317 G318 G319 F320 V321 H322 Y323 G324 E325 V326 T327 N328 D329 F330 V331 M332 L333 K334 G335 C336 V337 V338 G339 T340 K341 K342 R343 V344 L345 T346 L347 R348 K349 S350 L351 L352 Y353 Q354 T355 K356 R357 R358 A359 L360

E361 K362 I363 D364 L365 K366 F367 I368 D369 T370 T371 S372 K373 F374 G375 H376 G377 R378 F379 Q380 T381 M382 E383 E384 K385 K386 A387 F388 M389 G390 P391 L392 K393 K394 D395 ARG ILE ALA LYS GLU GLU GLY ALA

• Molecule 5: 60S ribosomal protein L4

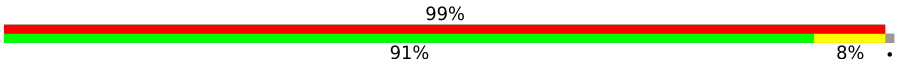
Chain AC:

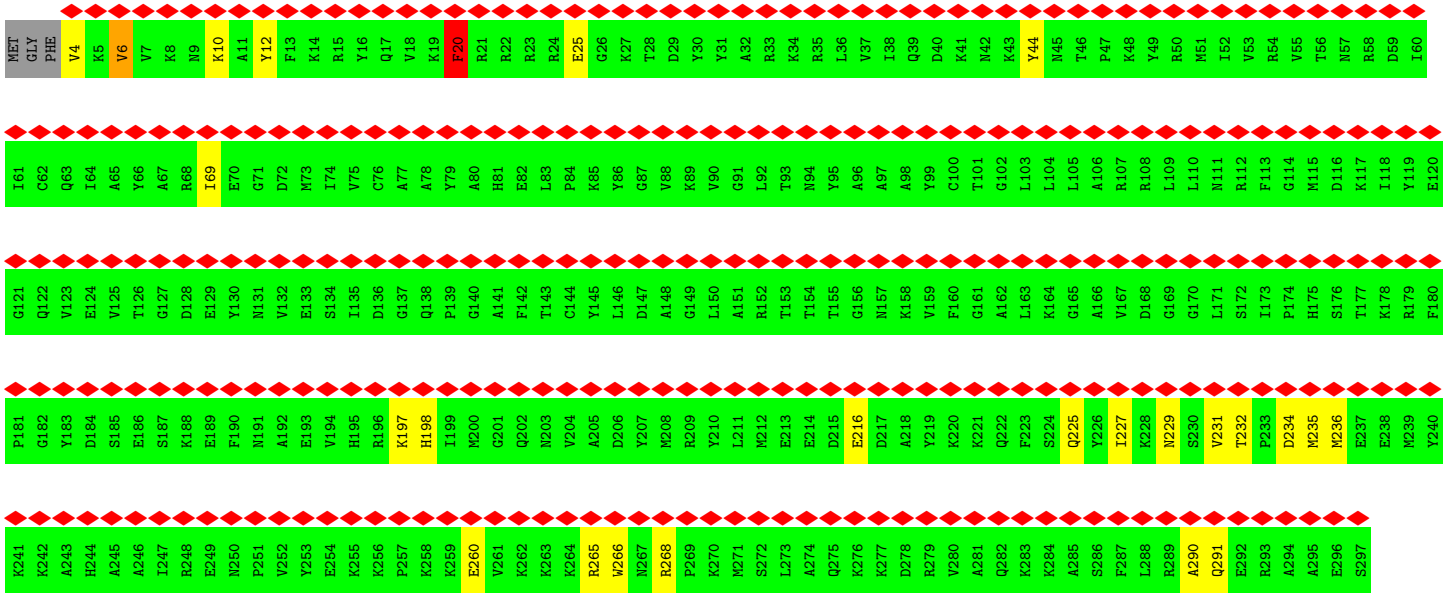
MET ALA C3 A4 R5 P6 L7 I8 S9 V10 Y11 S12 E13 K14 G15 E16 S17 S18 G19 K20 N21 V22 T23 L24 P25 A26 V27 F28 K29 A30 P31 I32 R33 P34 D35 I36 V37 N38 F39 V40 H41 T42 N43 L44 R45 K46 N47 N48 R49 Q50 P51 Y52 A53 V54 S55 E56 L57 A58 G59 H60



• Molecule 6: 60S ribosomal protein L5

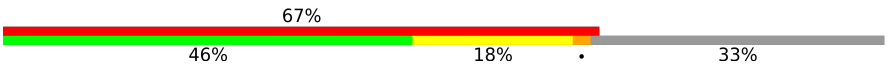
Chain AD:

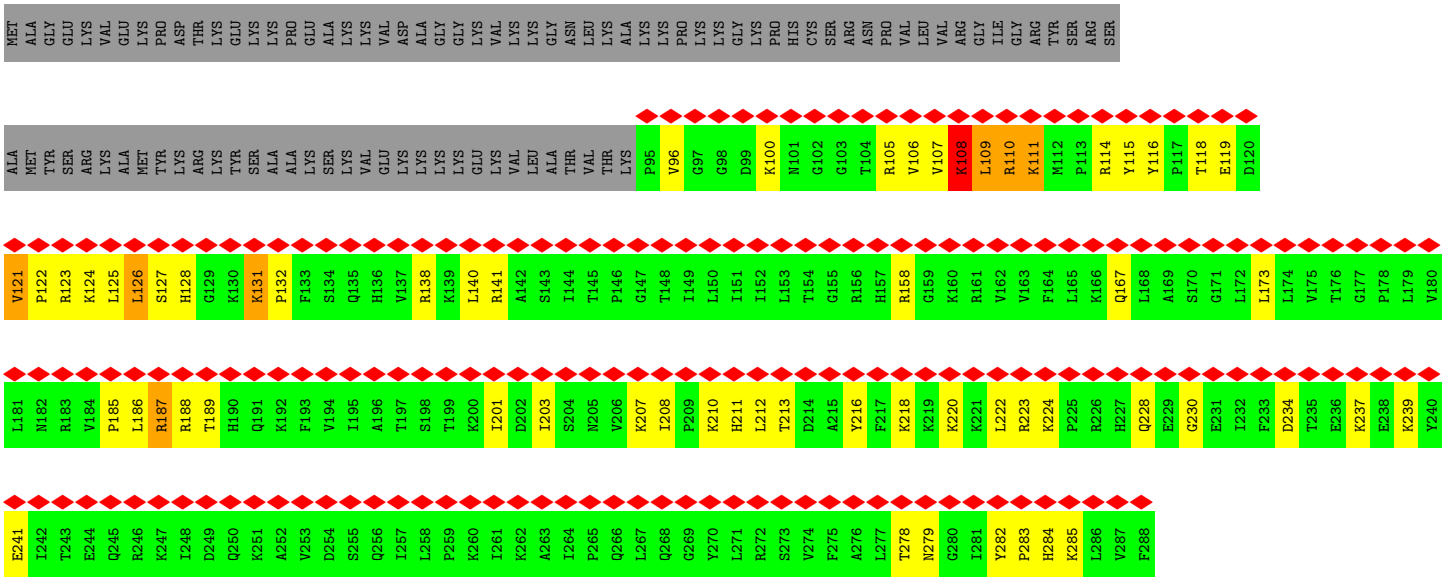




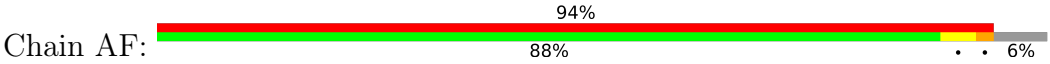
• Molecule 7: 60S ribosomal protein L6

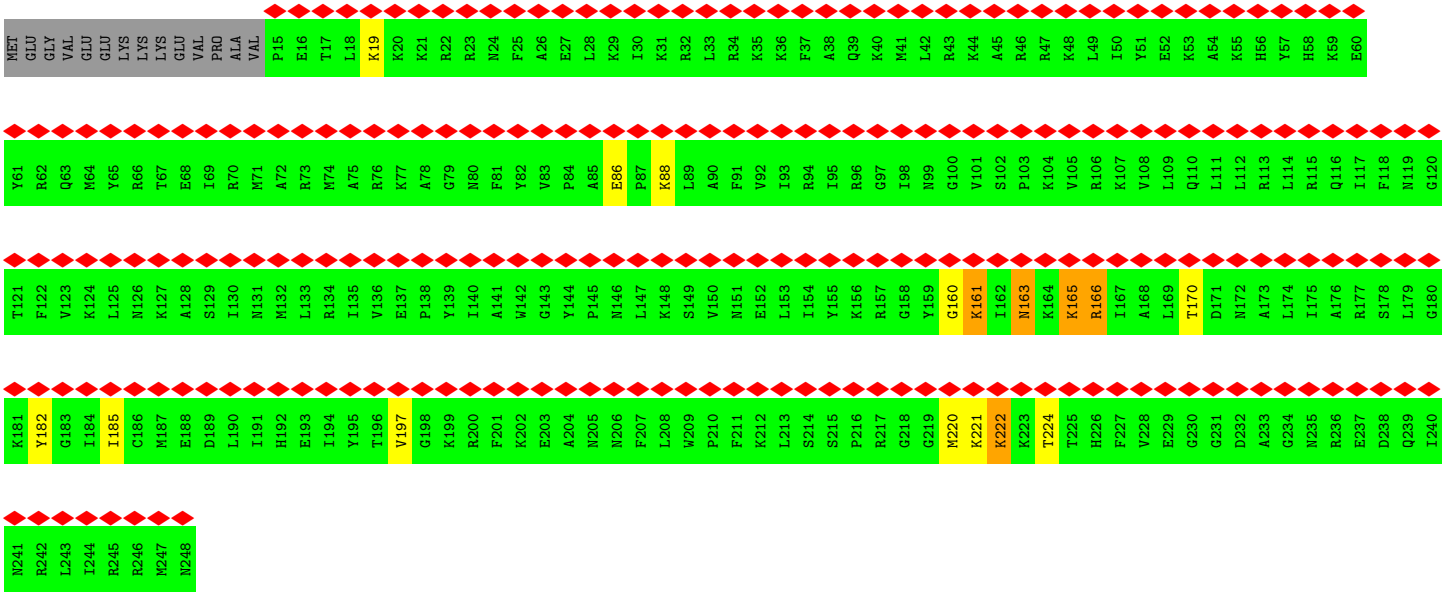
Chain AE:



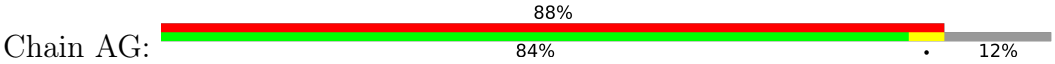


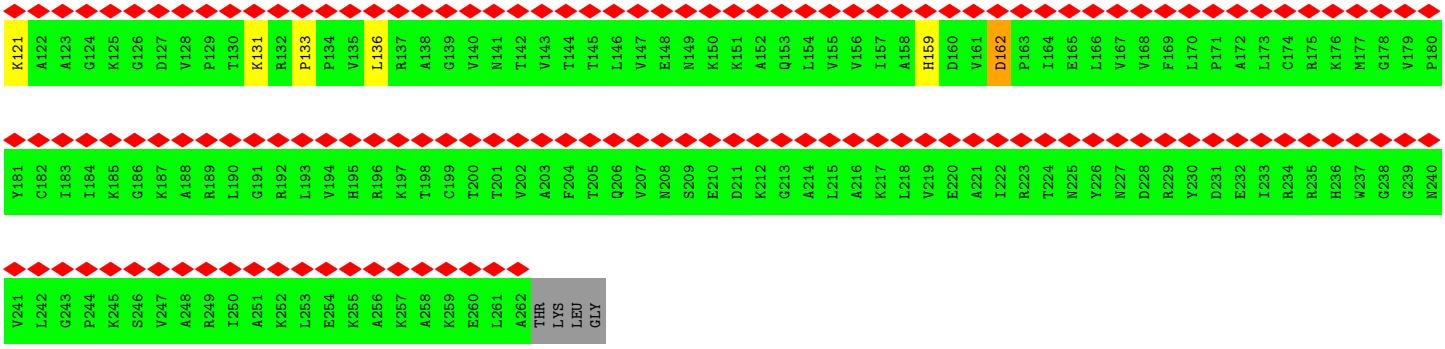
• Molecule 8: 60S ribosomal protein L7





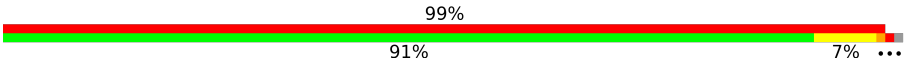
• Molecule 9: 60S ribosomal protein L7a

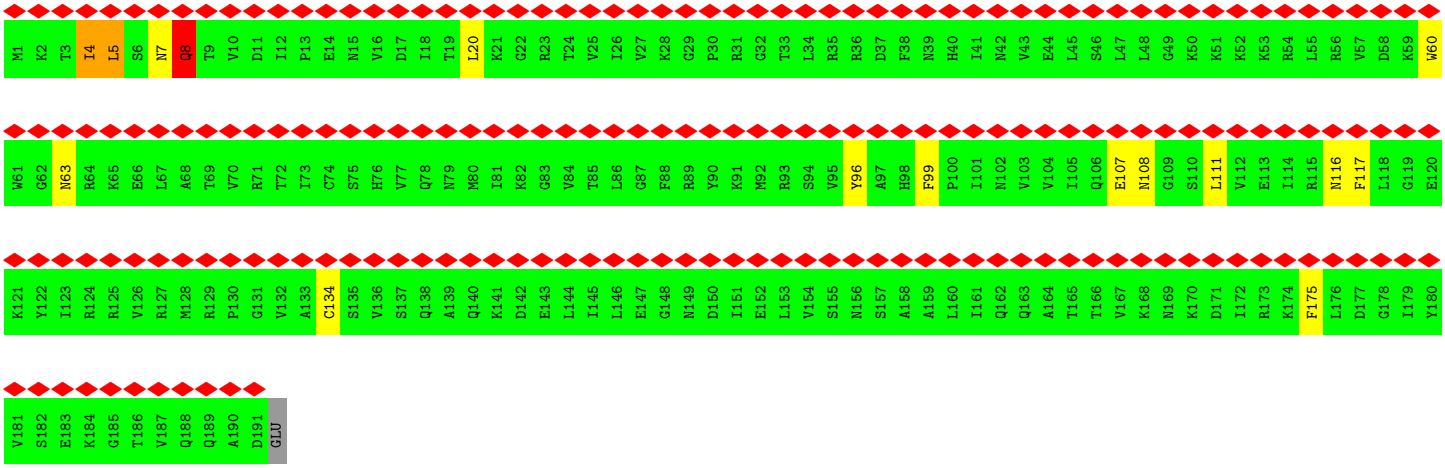




• Molecule 10: 60S ribosomal protein L9

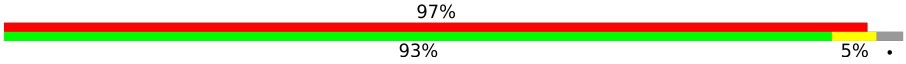
Chain AH:

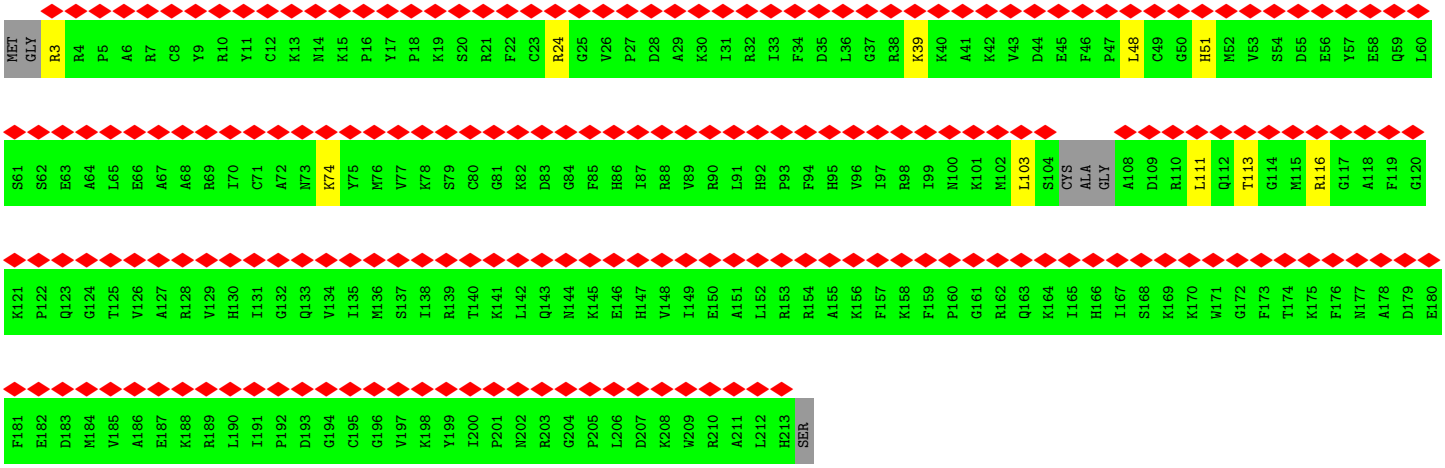




• Molecule 11: 60S ribosomal protein L10

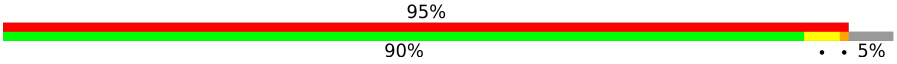
Chain AI:

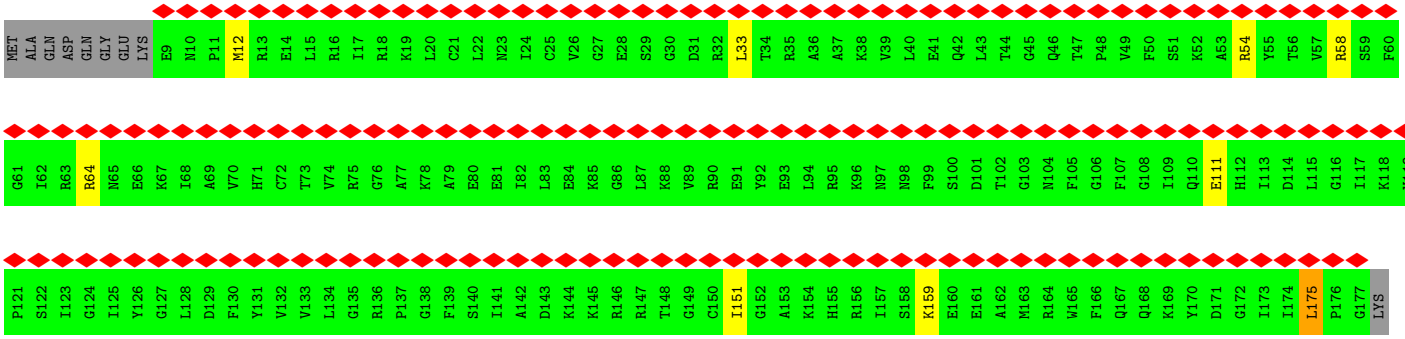




• Molecule 12: 60S ribosomal protein L11

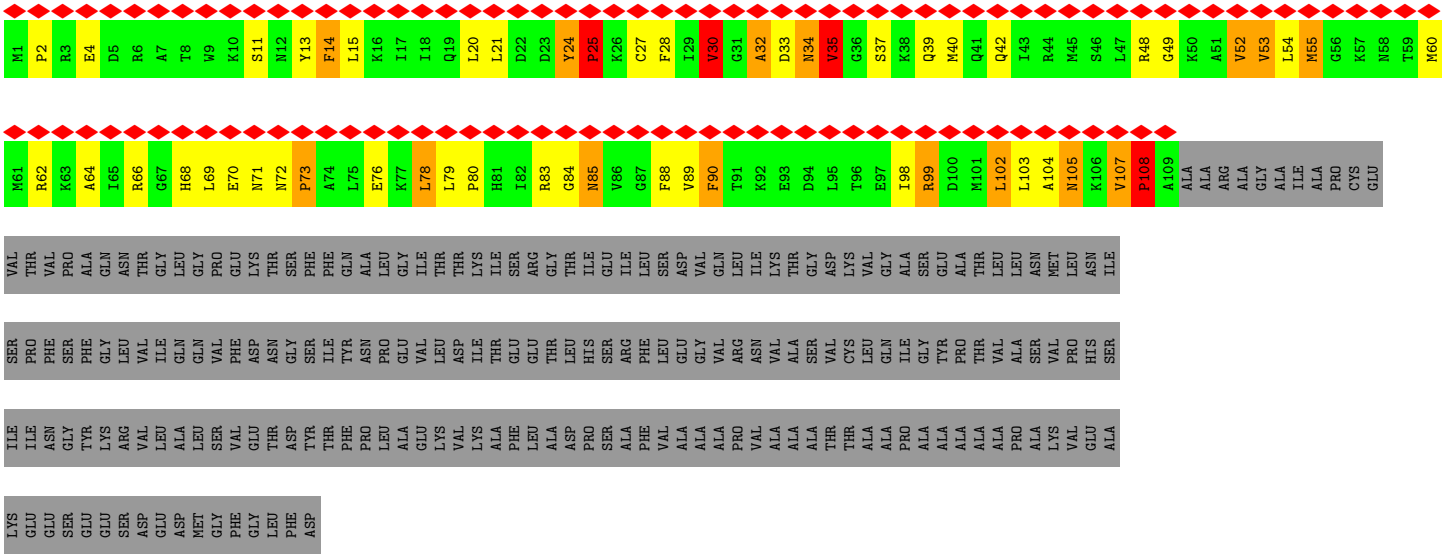
Chain AJ:





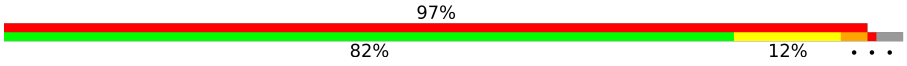
• Molecule 13: 60S acidic ribosomal protein P0

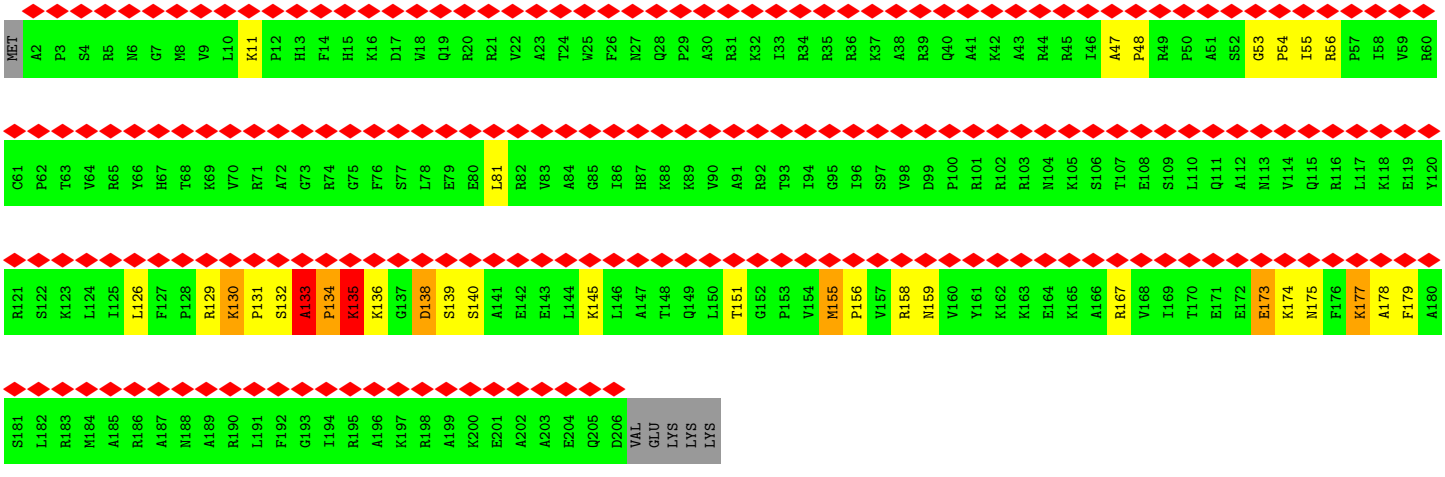
Chain AK:



• Molecule 14: 60S ribosomal protein L13

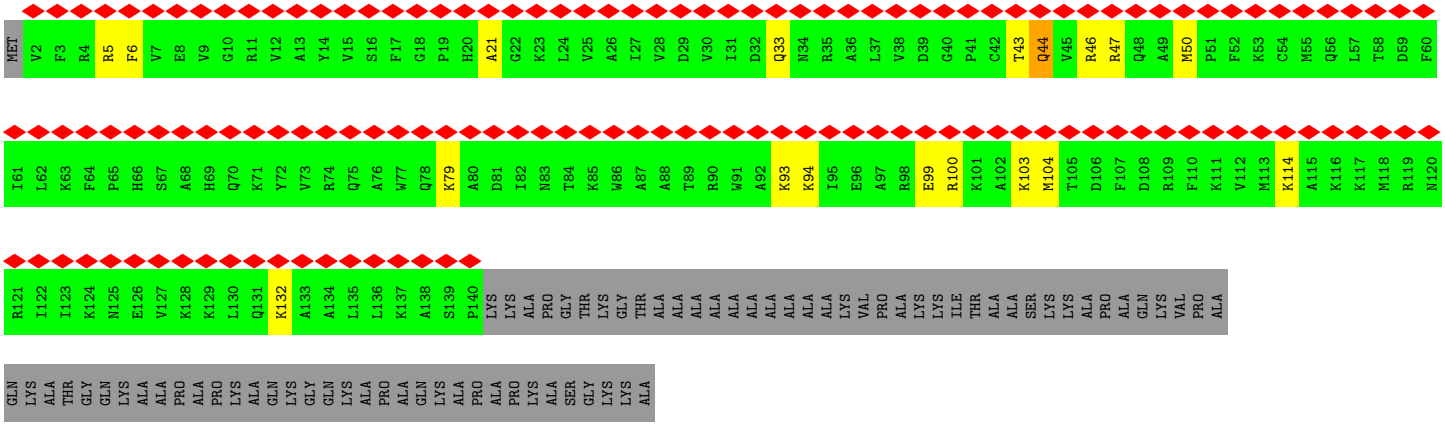
Chain AL:





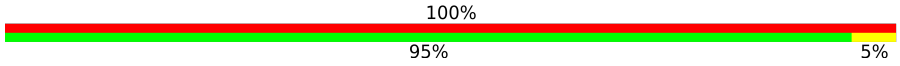
• Molecule 15: 60S ribosomal protein L14

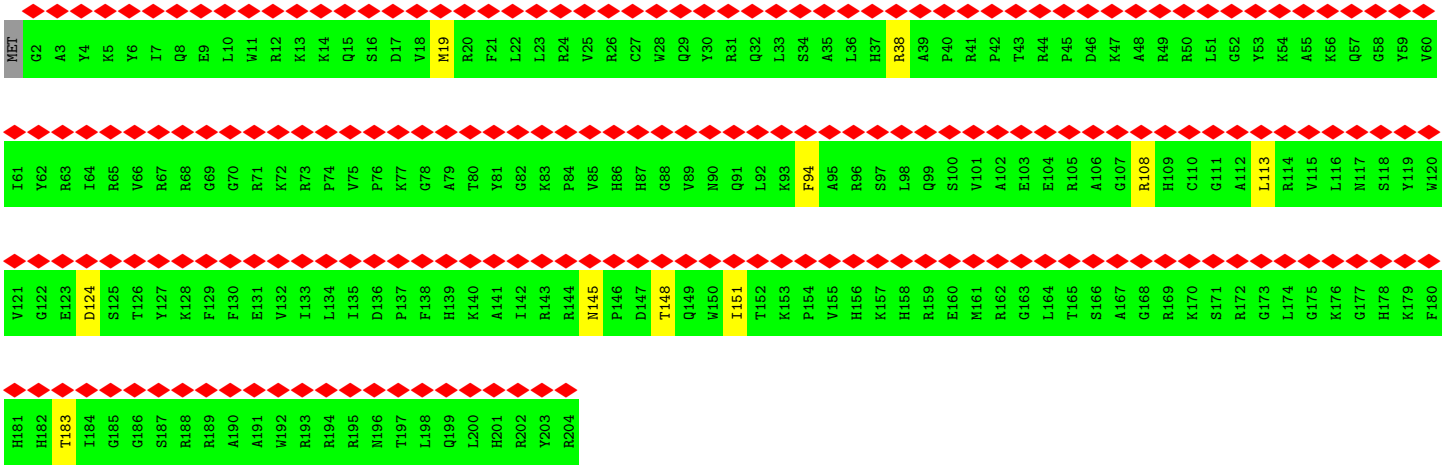
Chain AM:



• Molecule 16: 60S ribosomal protein L15

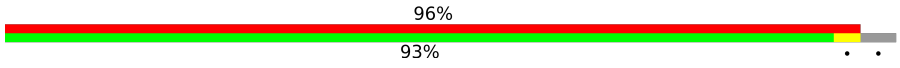
Chain AN:

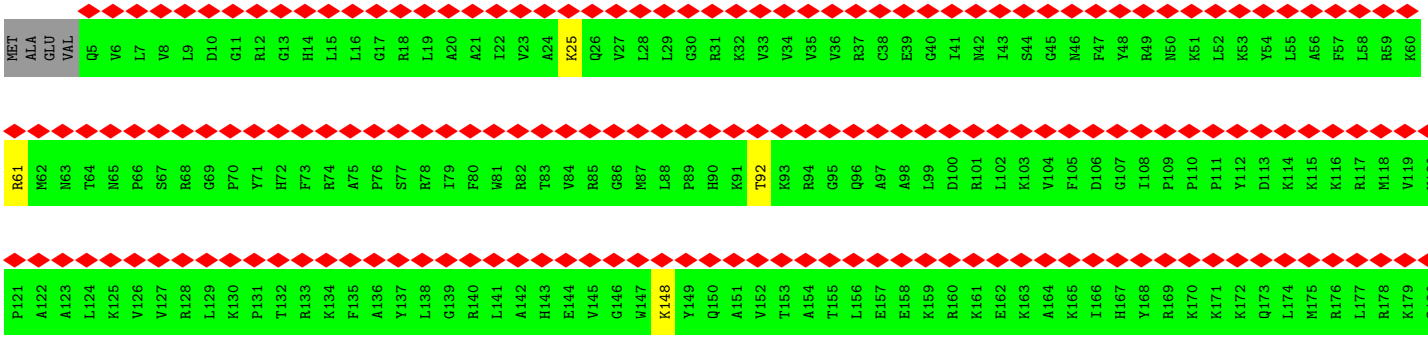


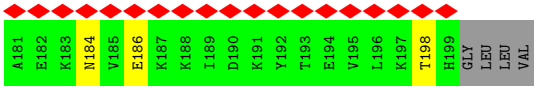


• Molecule 17: 60S ribosomal protein L13a

Chain AO:

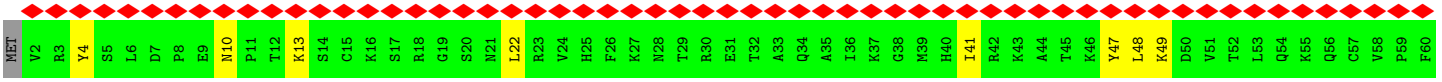


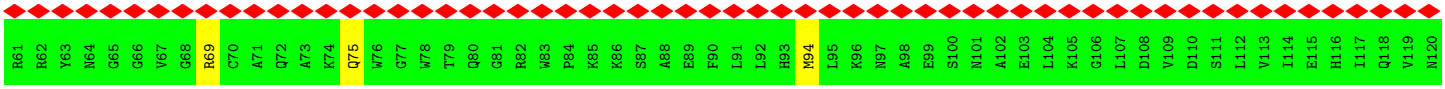


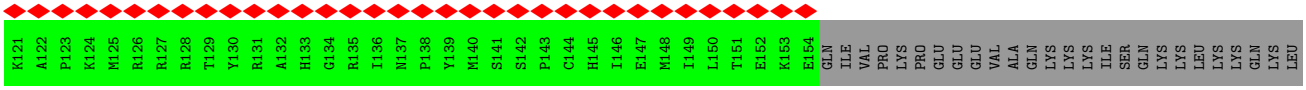


• Molecule 18: 60S ribosomal protein L17

Chain AP:

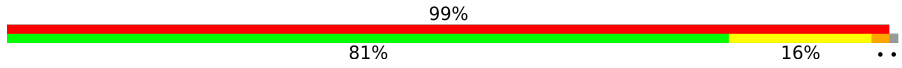


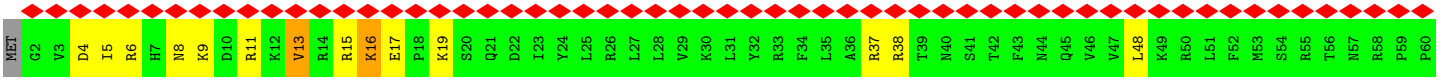


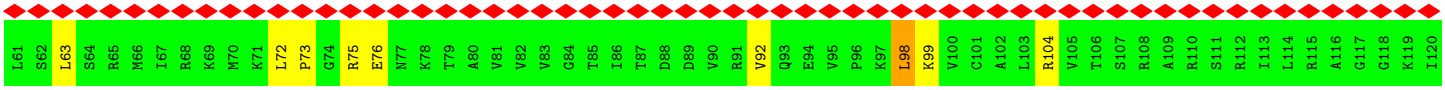


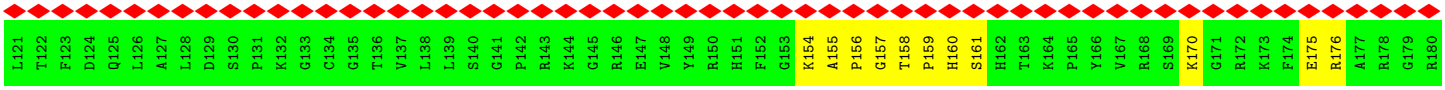
• Molecule 19: 60S ribosomal protein L18

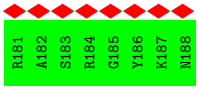
Chain AQ:





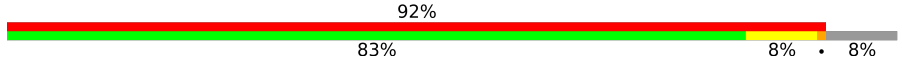


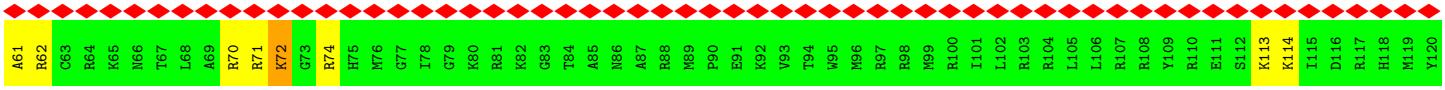


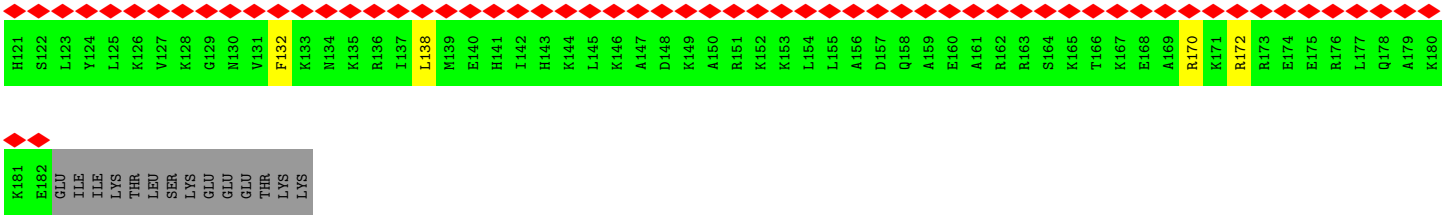


• Molecule 20: 60S ribosomal protein L19

Chain AR:

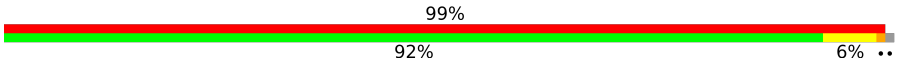


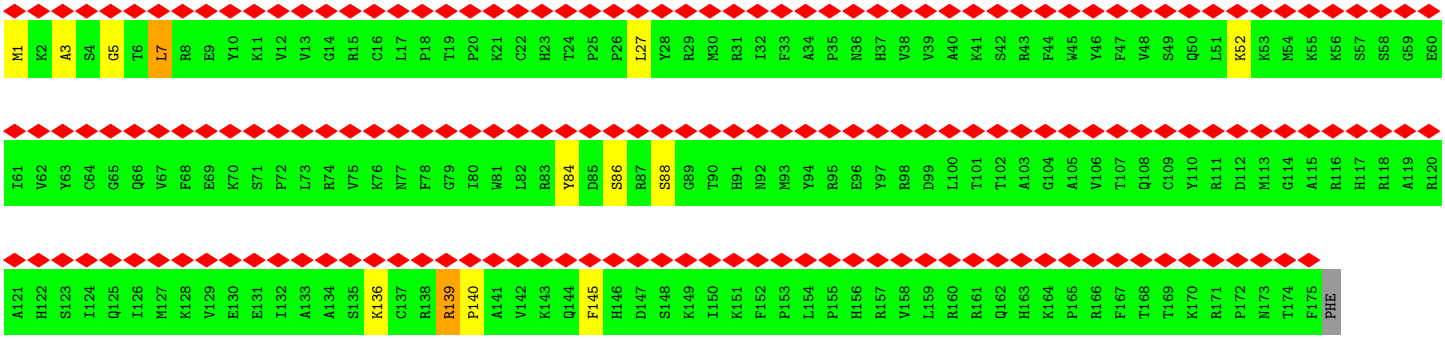




• Molecule 21: 60S ribosomal protein L18a

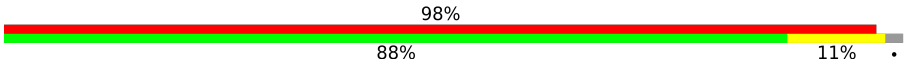
Chain AS:

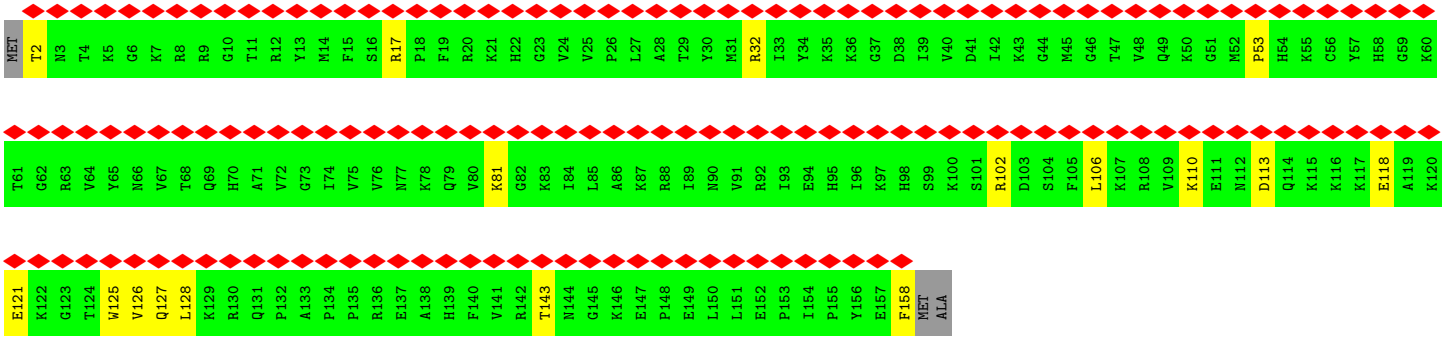




• Molecule 22: 60S ribosomal protein L21

Chain AT:



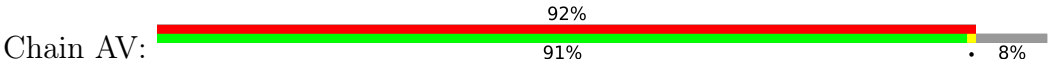


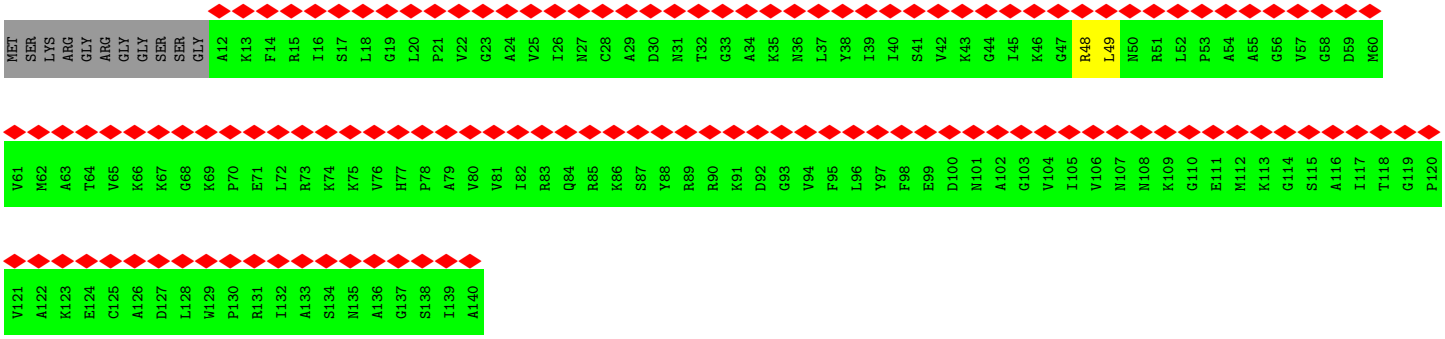
• Molecule 23: 60S ribosomal protein L22

Chain AU:

• Molecule 24: 60S ribosomal protein L23

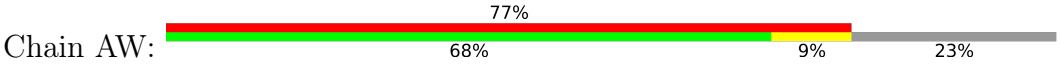
Chain AV:

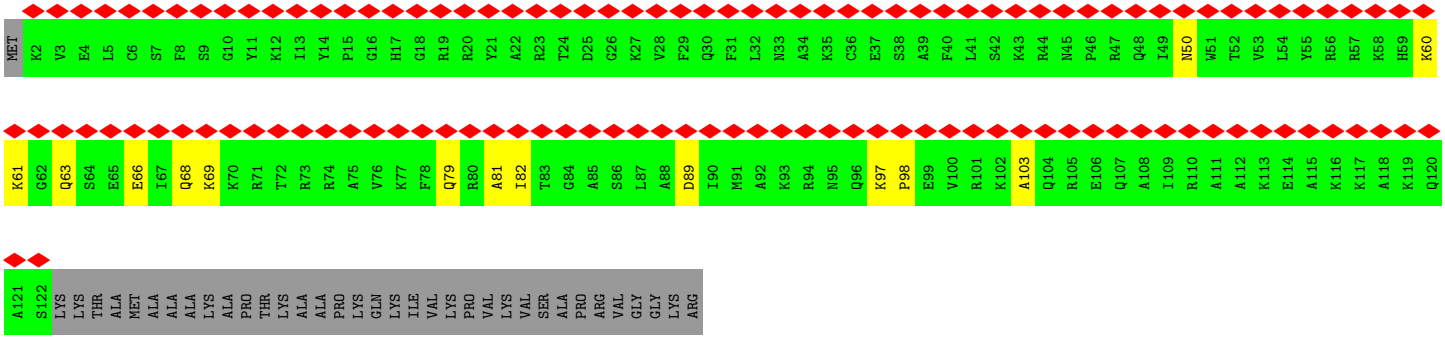




• Molecule 25: 60S ribosomal protein L24

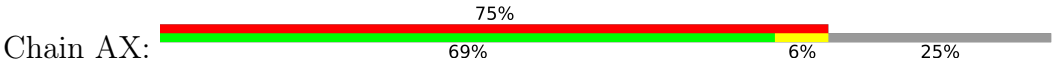
Chain AW:

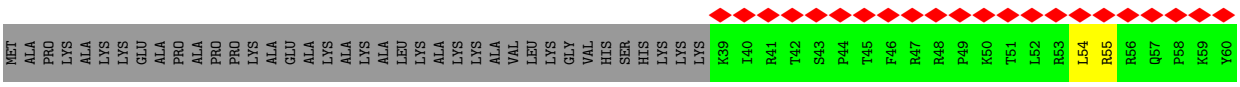


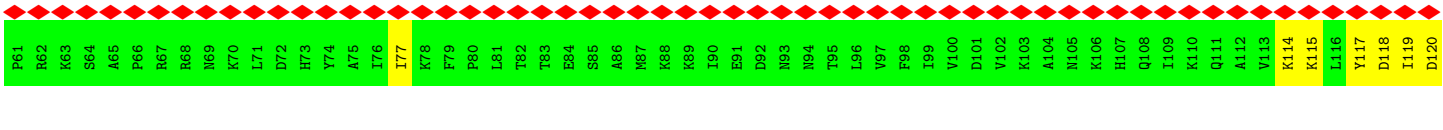


• Molecule 26: 60S ribosomal protein L23a

Chain AX:

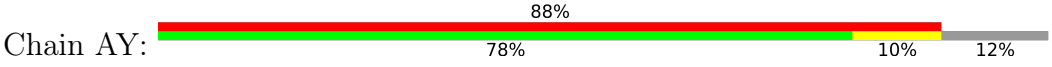


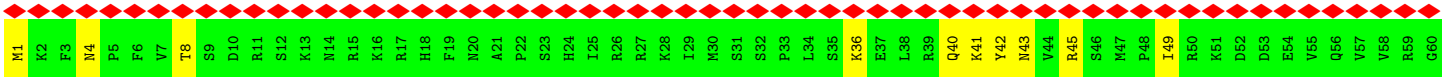


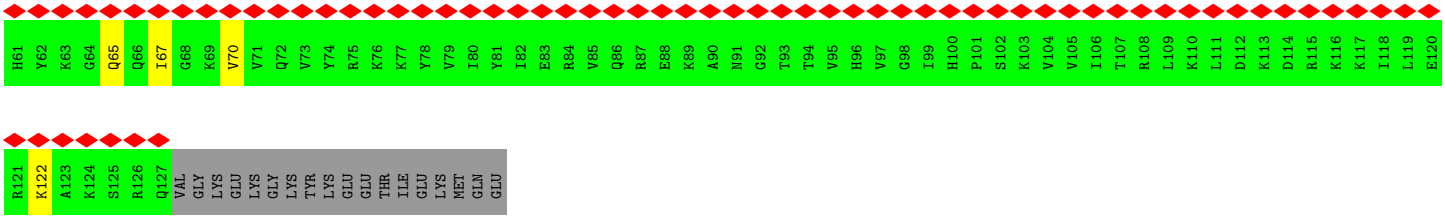


• Molecule 27: 60S ribosomal protein L26

Chain AY:

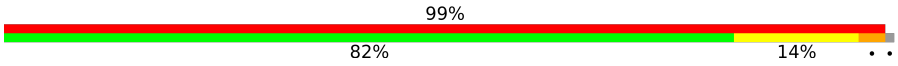


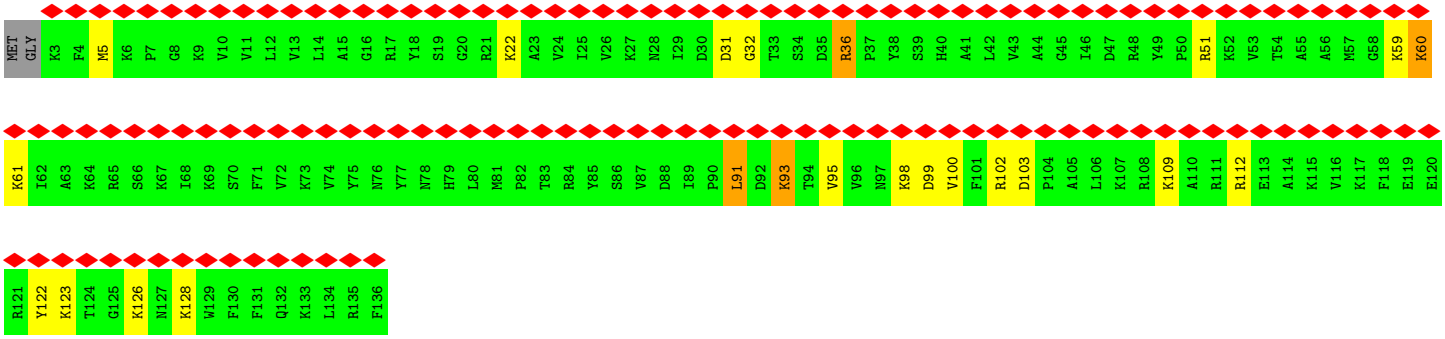




• Molecule 28: 60S ribosomal protein L27

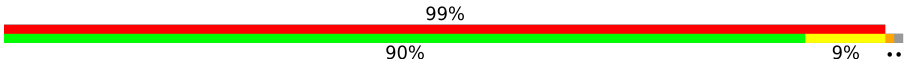
Chain AZ:

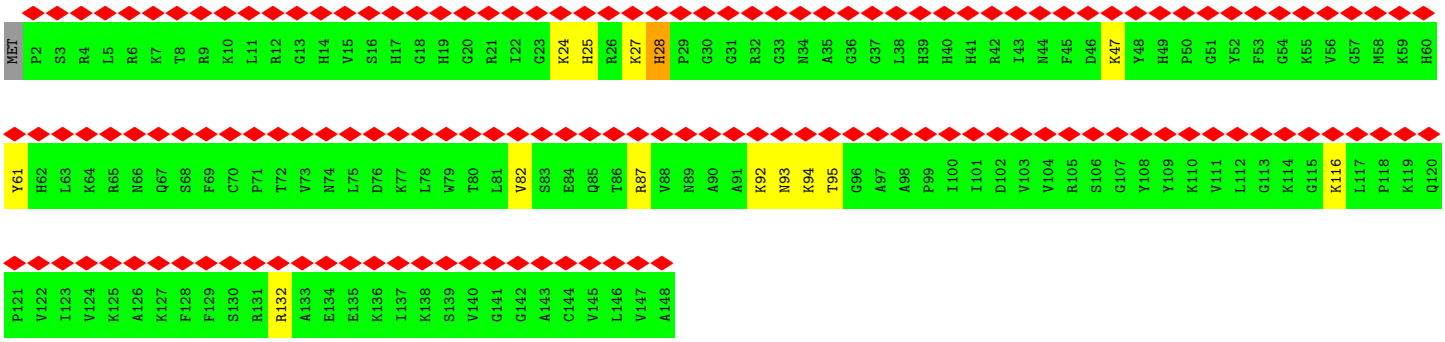




• Molecule 29: 60S ribosomal protein L27a

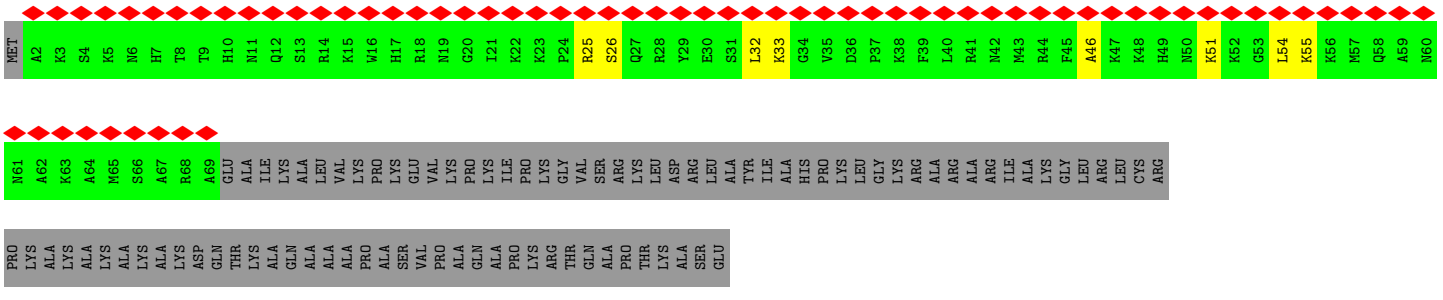
Chain Aa:





• Molecule 30: 60S ribosomal protein L29

Chain Ab:

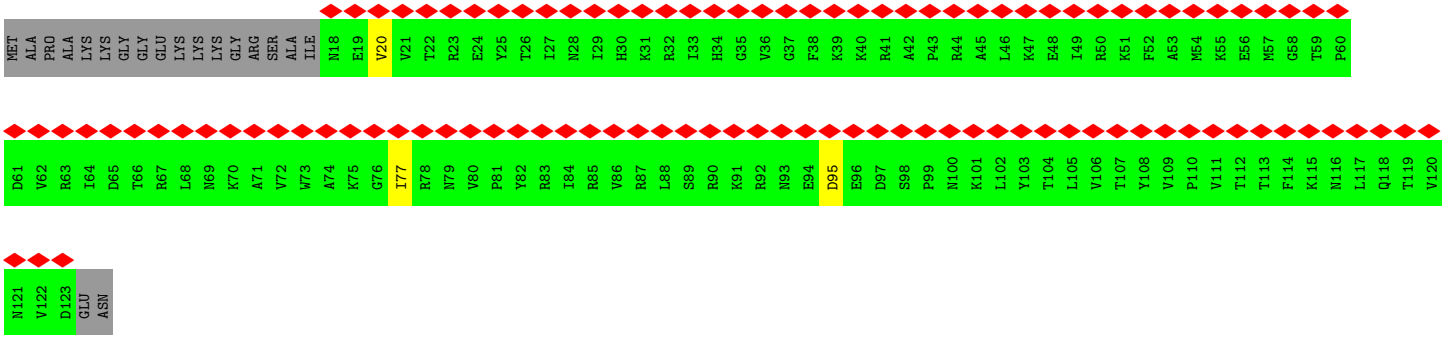


• Molecule 31: 60S ribosomal protein L30

Chain Ac:

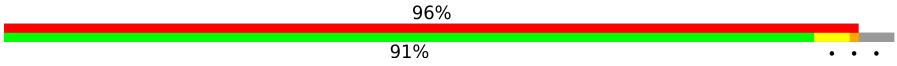
• Molecule 32: 60S ribosomal protein L31

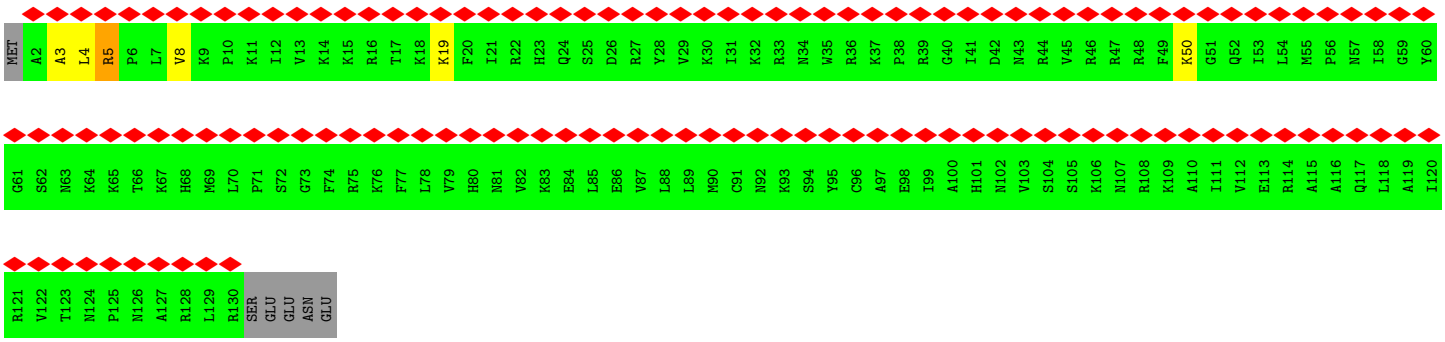
Chain Ad:



• Molecule 33: 60S ribosomal protein L32

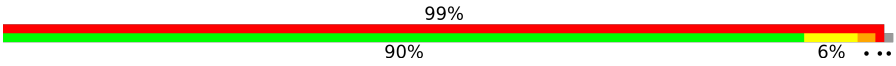
Chain Ae:

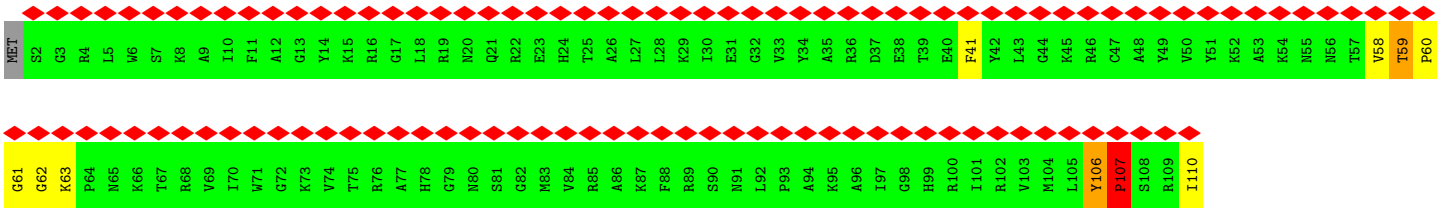




• Molecule 34: 60S ribosomal protein L35a

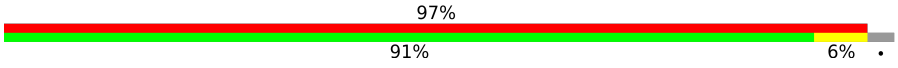
Chain Af:





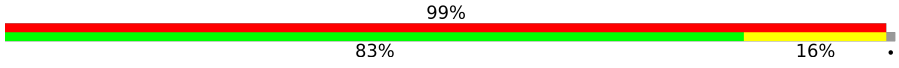
• Molecule 35: 60S ribosomal protein L34

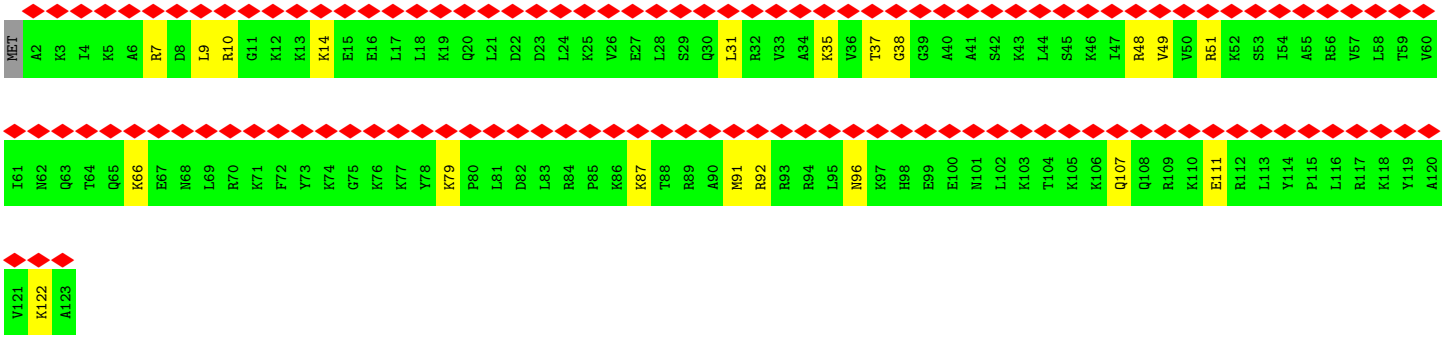
Chain Ag:



- Molecule 36: 60S ribosomal protein L35

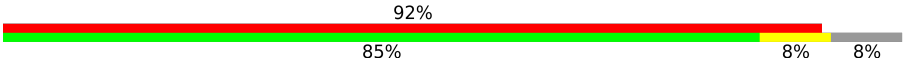
Chain Ah:

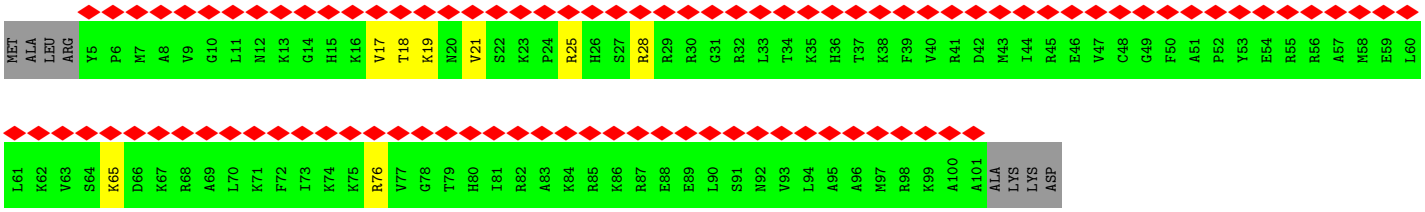




- Molecule 37: 60S ribosomal protein L36

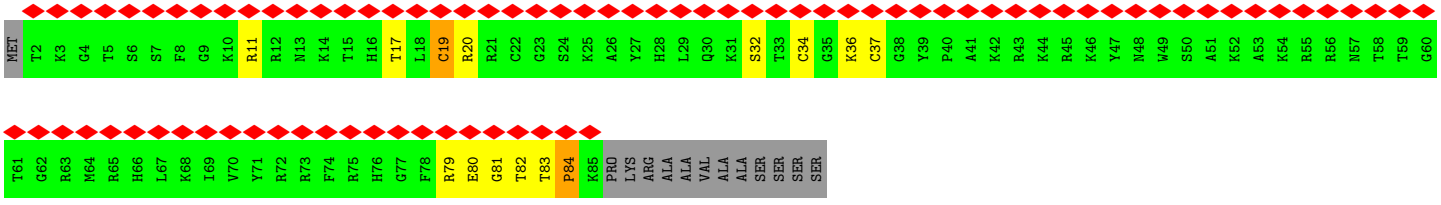
Chain Ai:





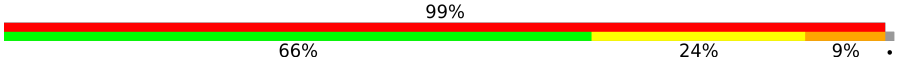
- Molecule 38: 60S ribosomal protein L37

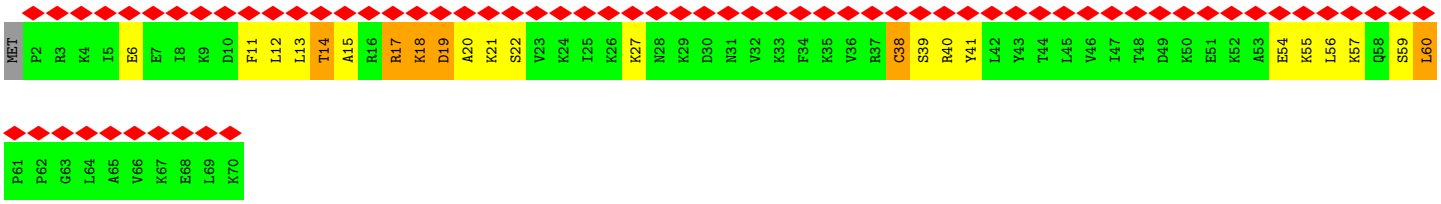
Chain Aj:



- Molecule 39: 60S ribosomal protein L38

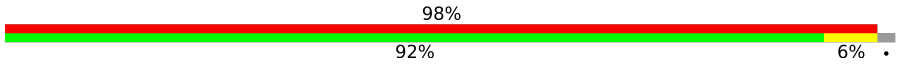
Chain Ak:

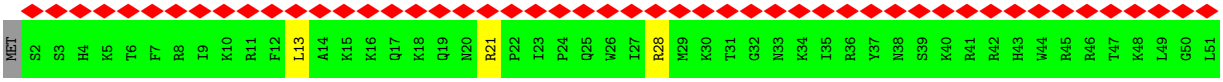




- Molecule 40: 60S ribosomal protein L39

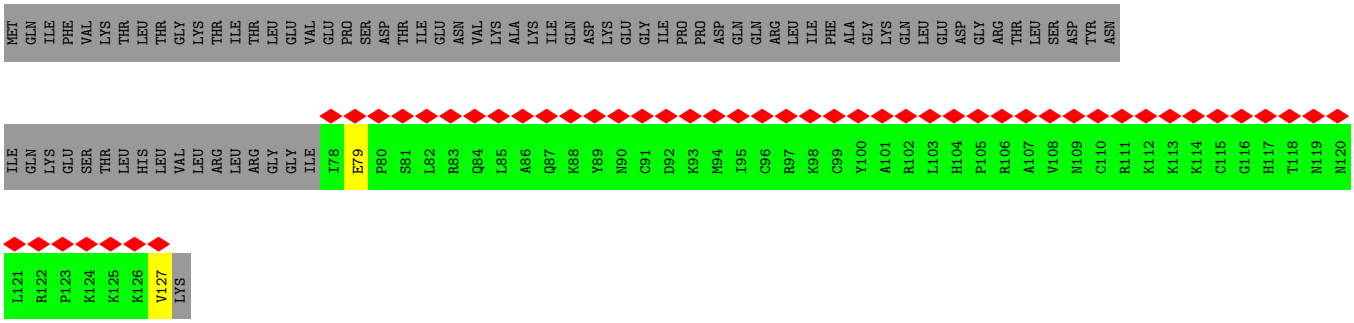
Chain Al:





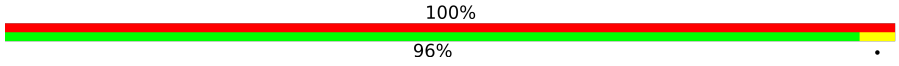
- Molecule 41: Ubiquitin-60S ribosomal protein L40

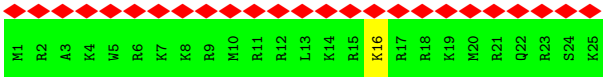
Chain Am:



- Molecule 42: 60S ribosomal protein L41

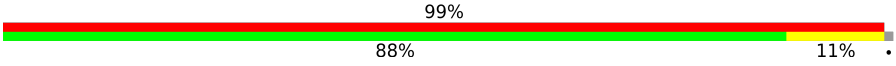
Chain An:

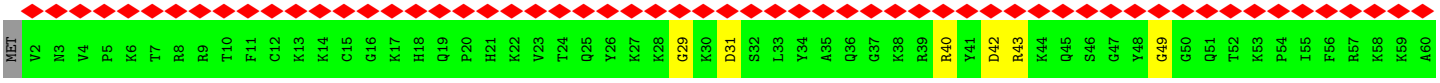


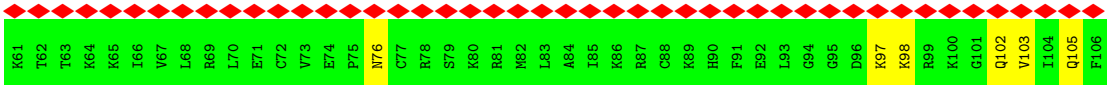


- Molecule 43: 60S ribosomal protein L36a

Chain Ao:







- Molecule 44: 60S ribosomal protein L37a

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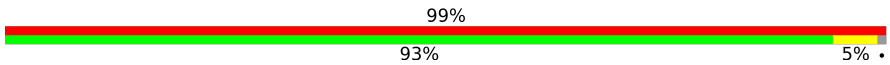
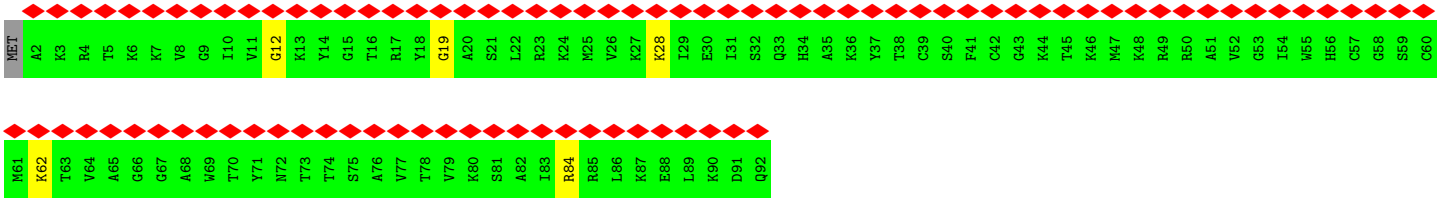
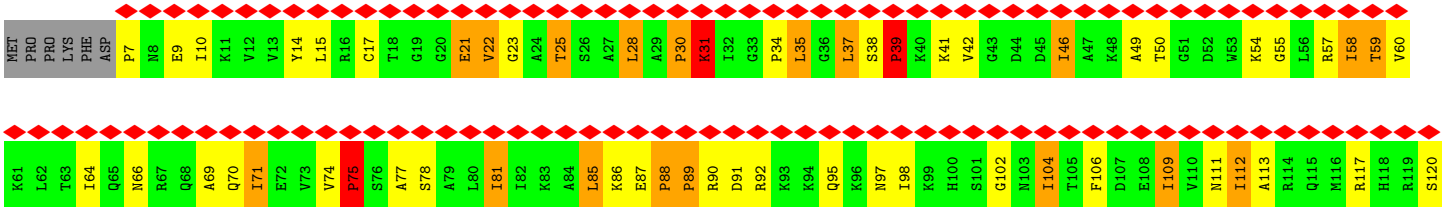




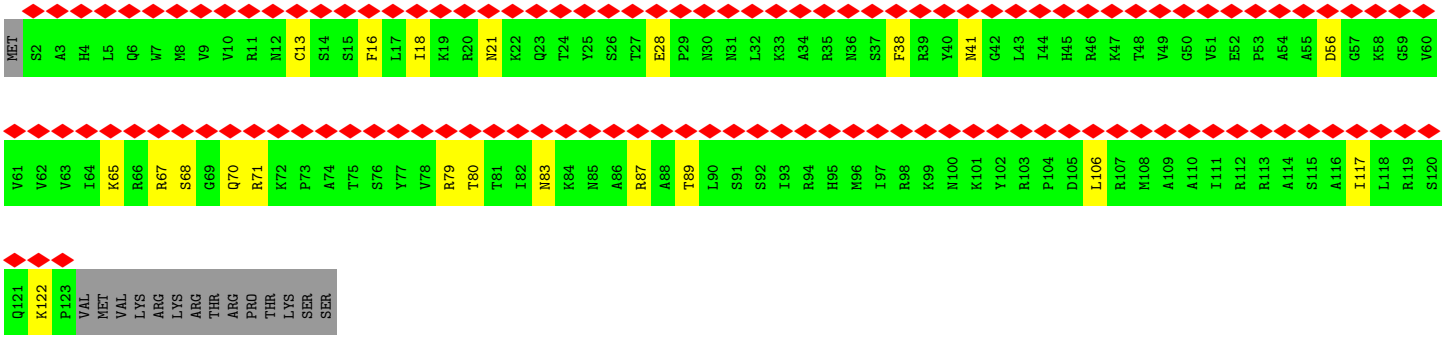
• Molecule 45: 60S ribosomal protein L12

Chain Aq:



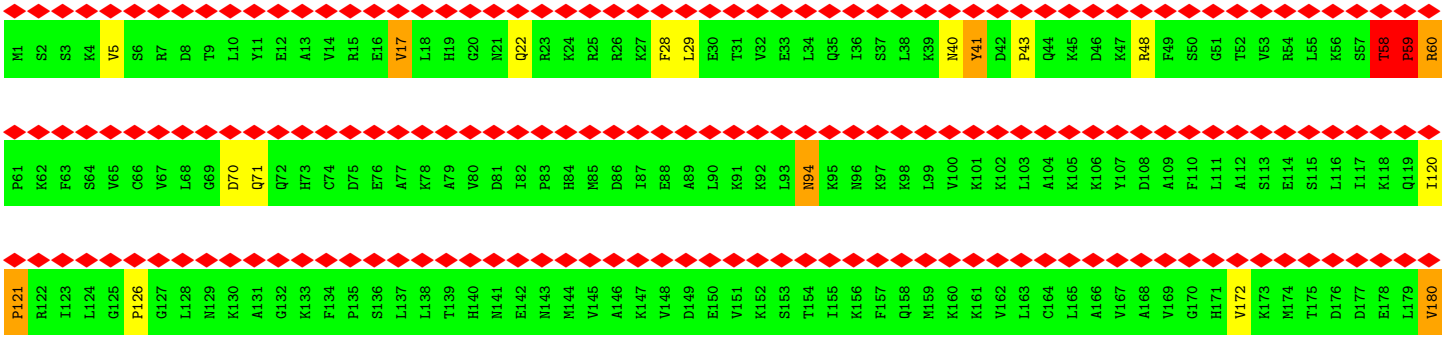
• Molecule 46: 60S ribosomal protein L28

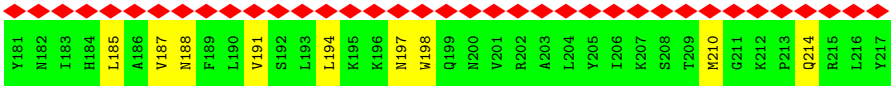
Chain At:



• Molecule 47: 60S ribosomal protein L10a

Chain Au:





• Molecule 48: 28S ribosomal RNA

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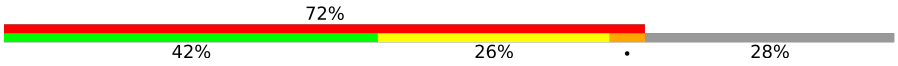

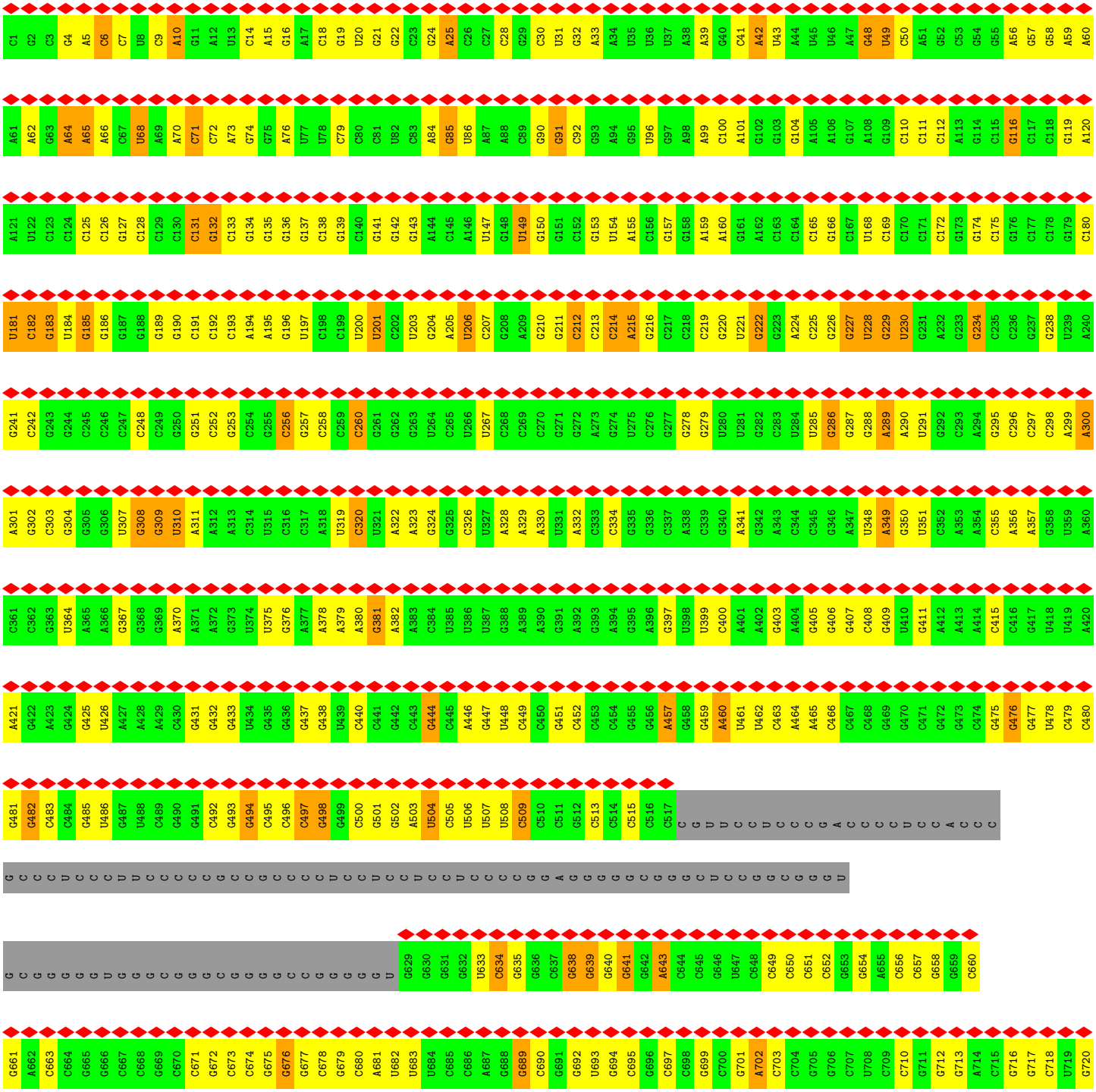

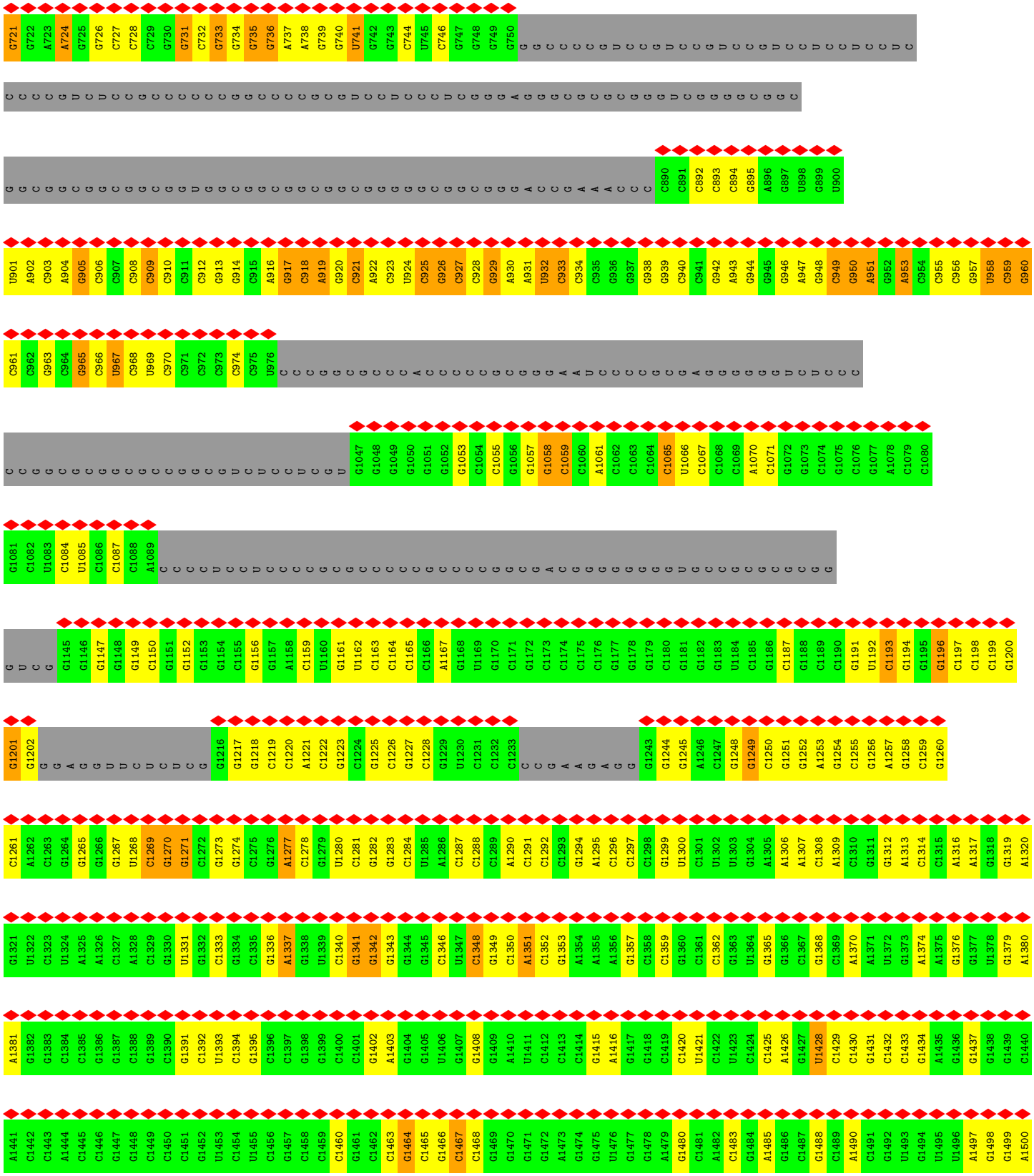
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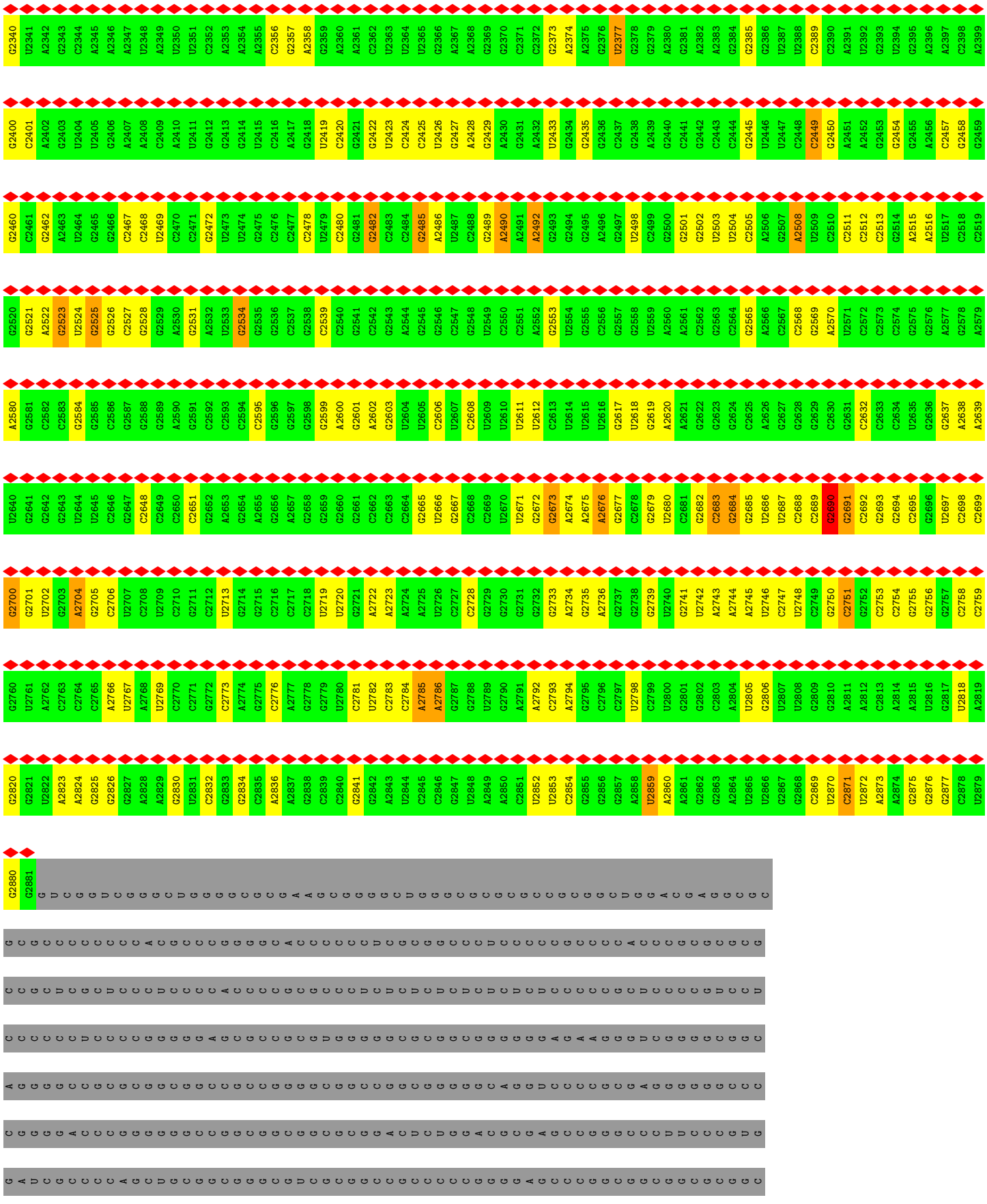
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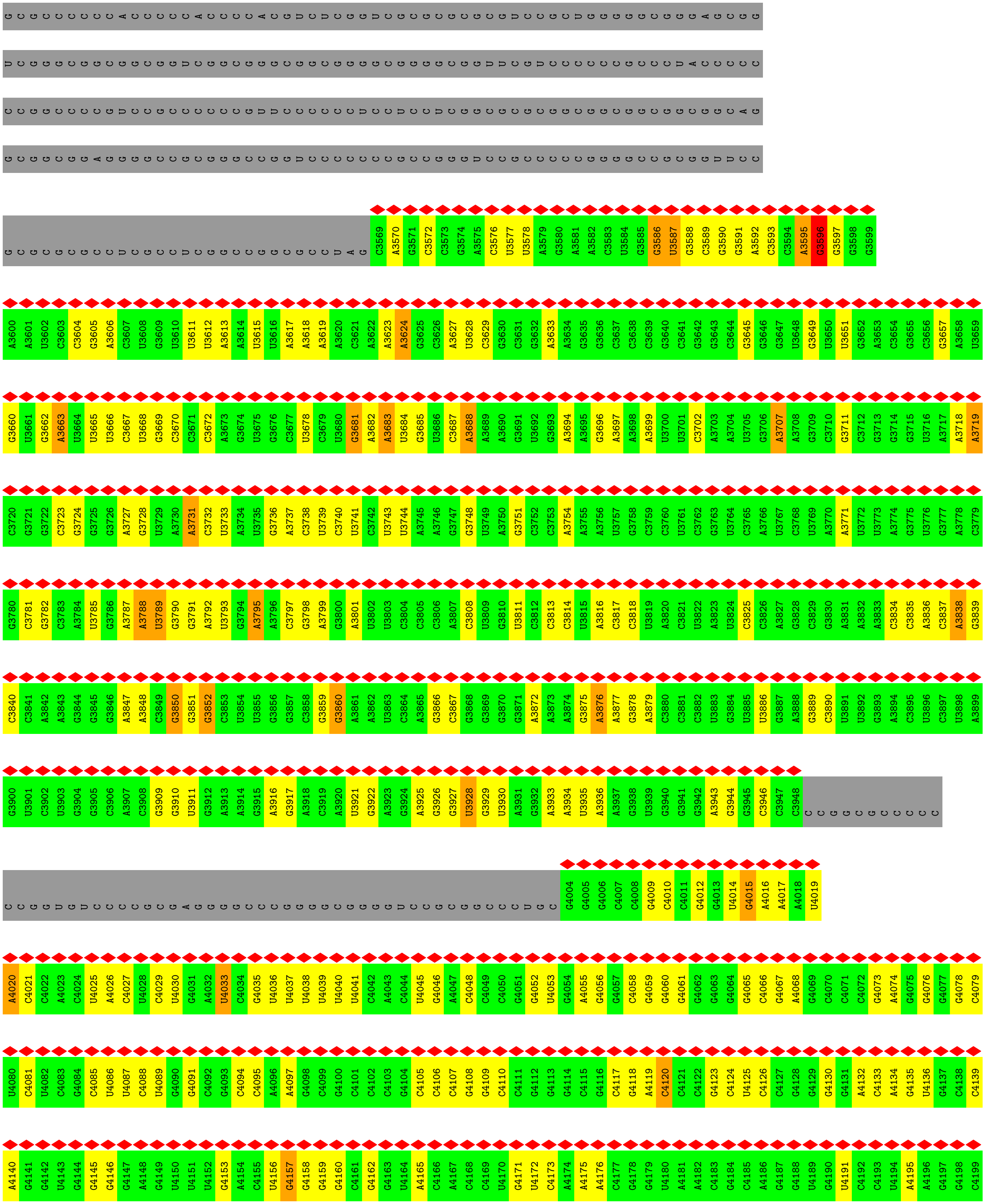
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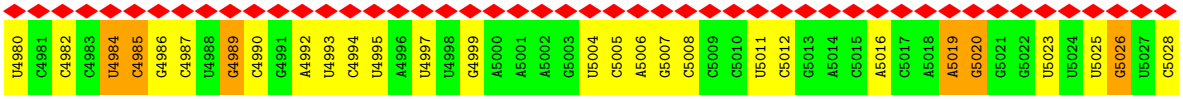
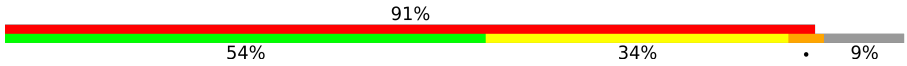
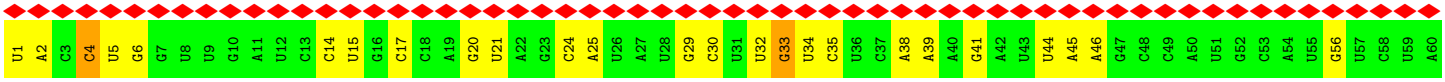
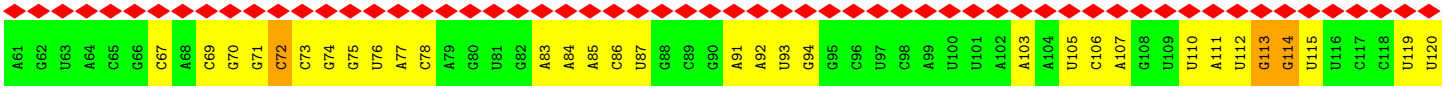


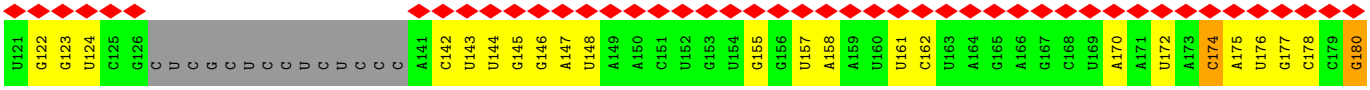
• Molecule 49: 18S ribosomal RNA

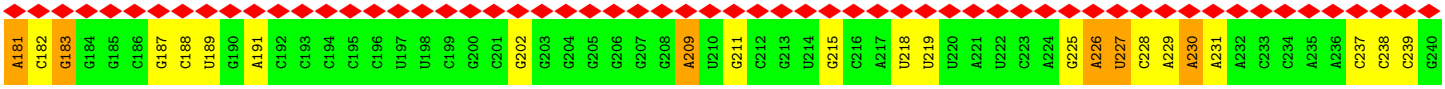
Chain B1:

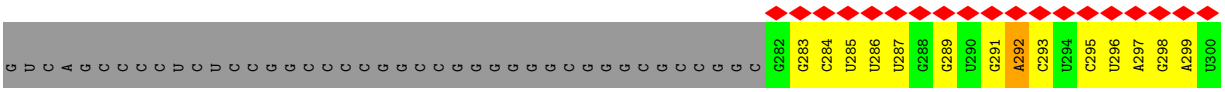


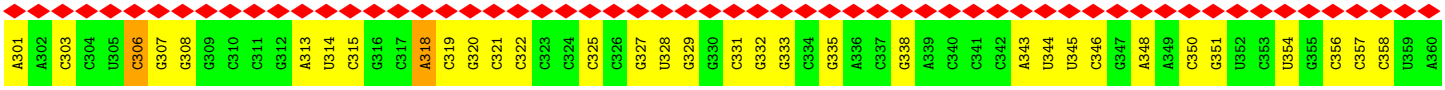


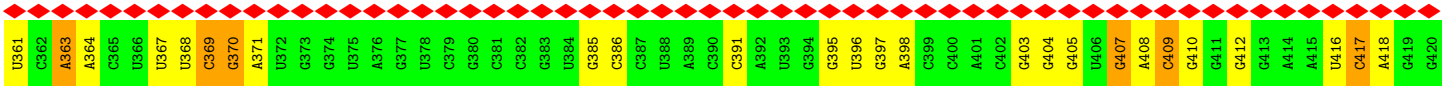


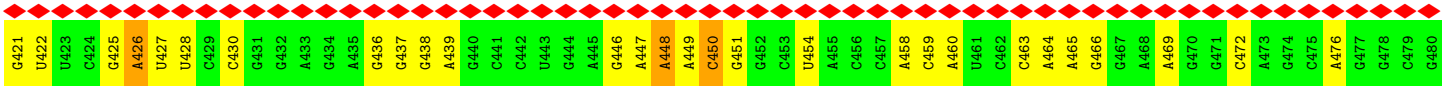


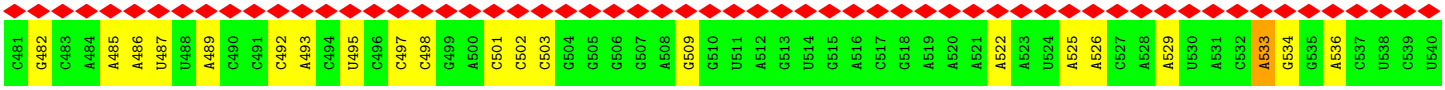


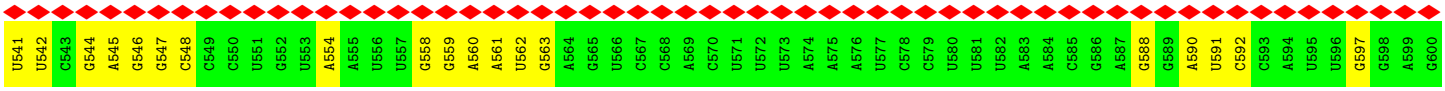


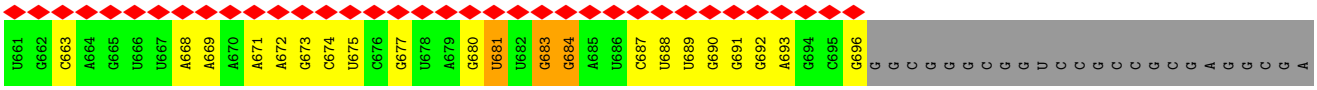


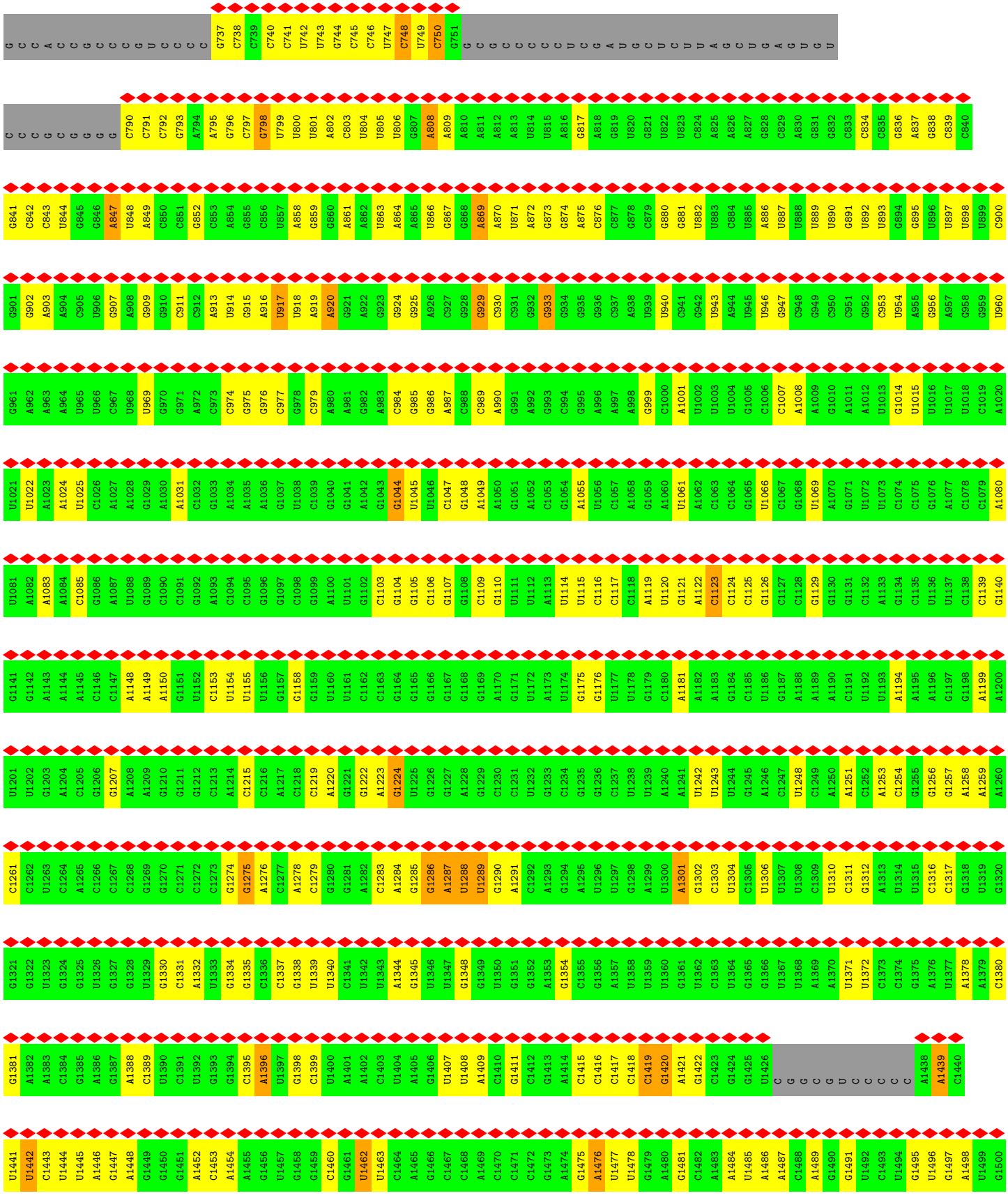








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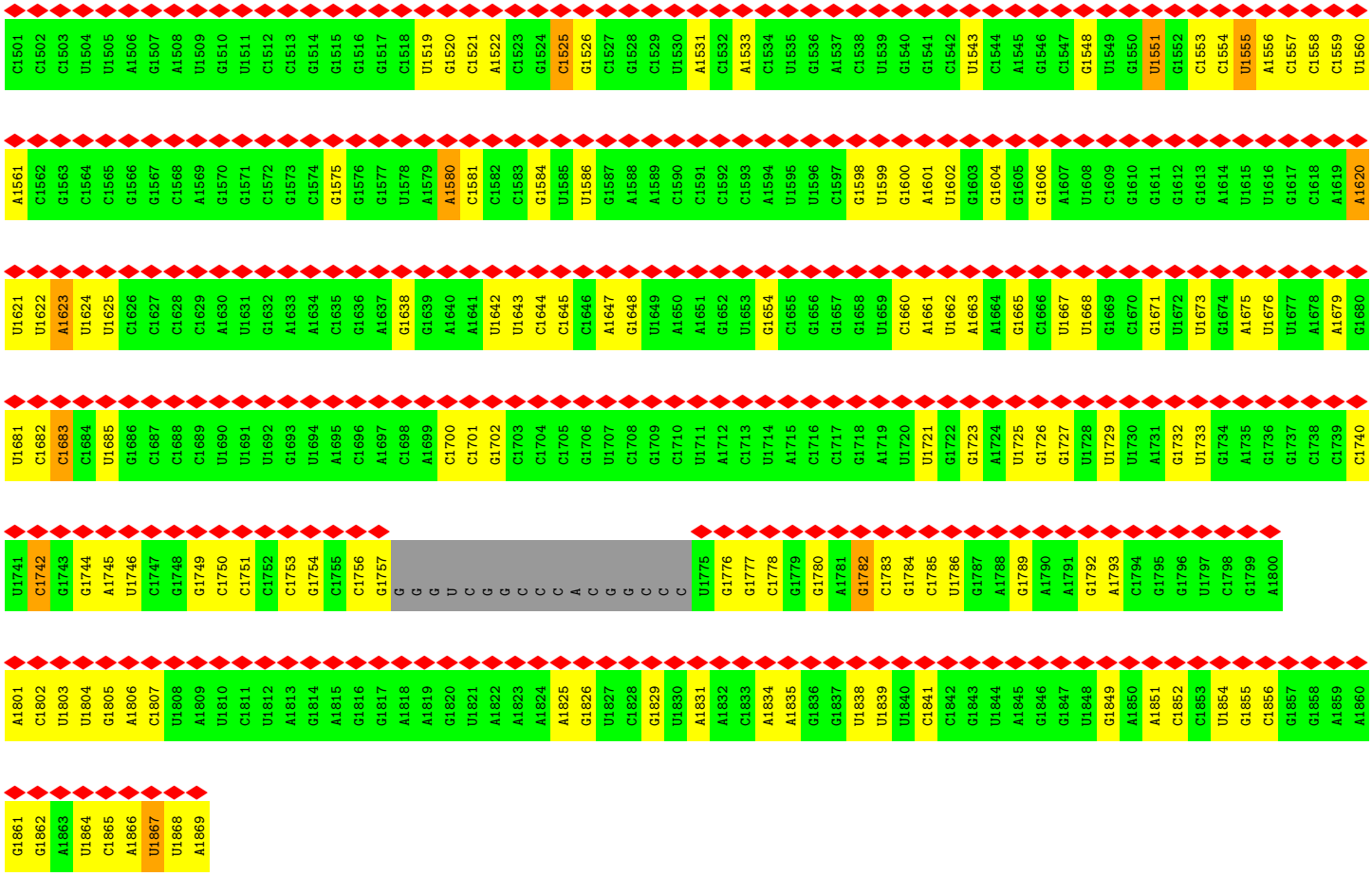
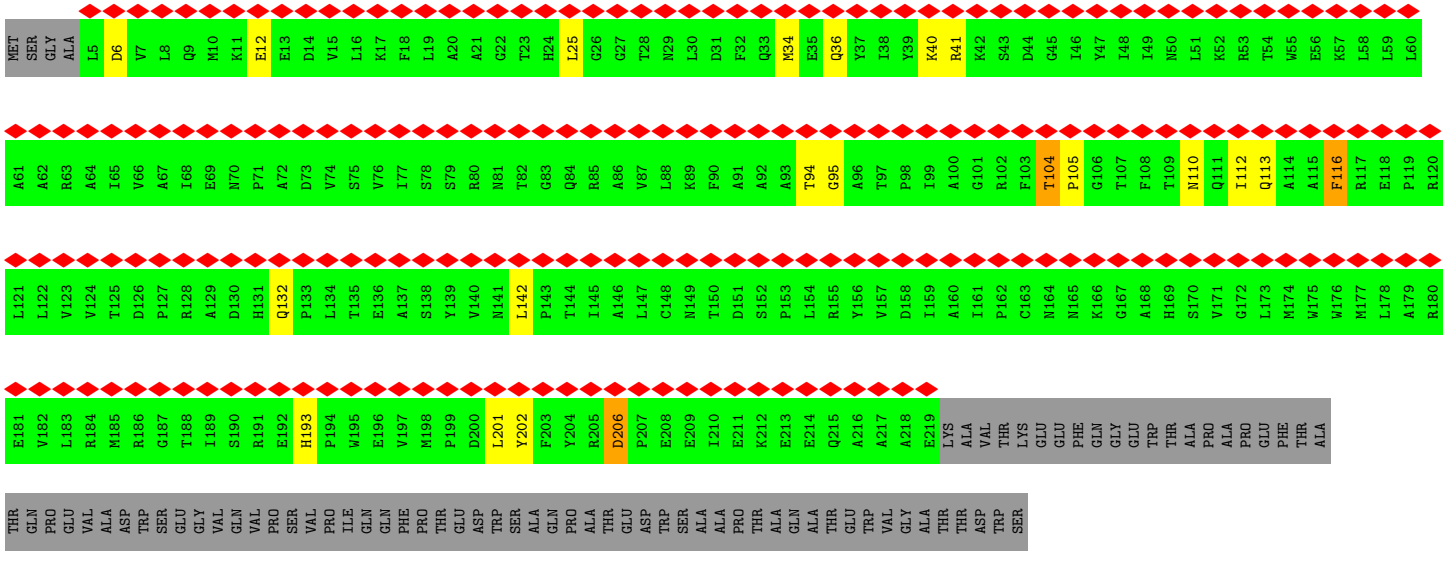


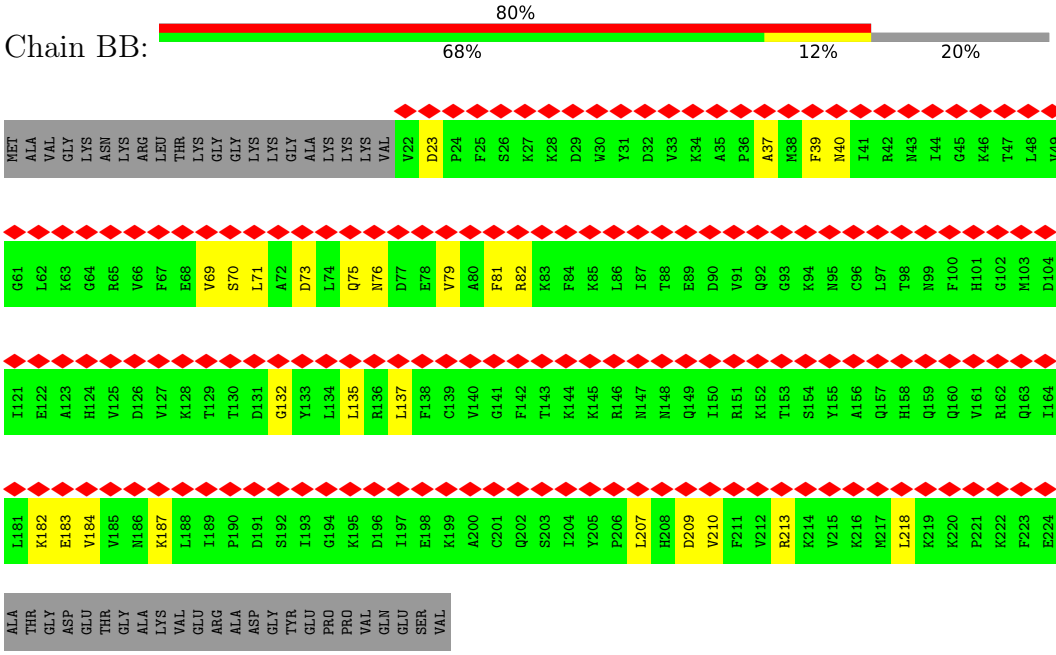
• Molecule 50: 40S ribosomal protein SA

Chain BA:



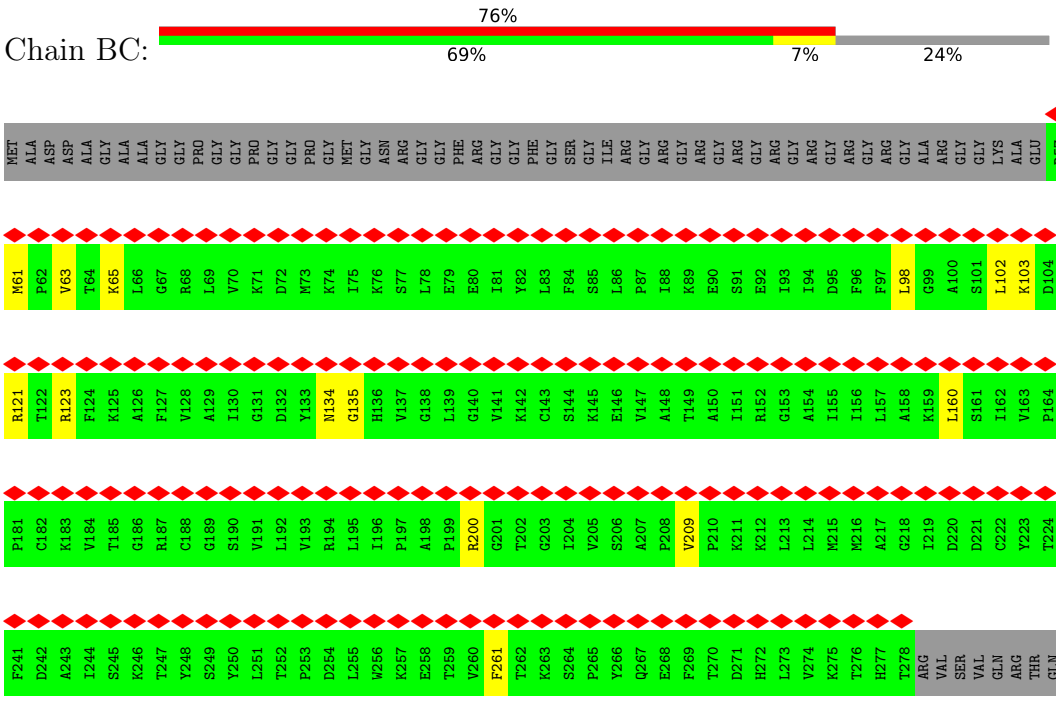
• Molecule 51: 40S ribosomal protein S3a

Chain BB:



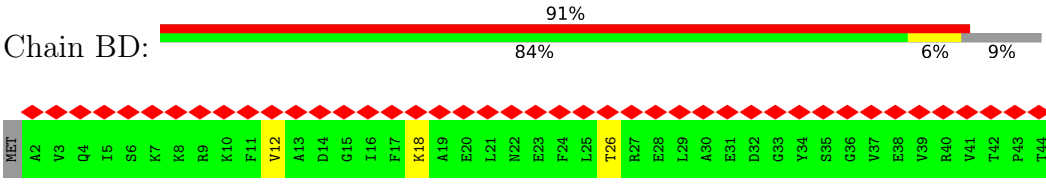
• Molecule 52: 40S ribosomal protein S2

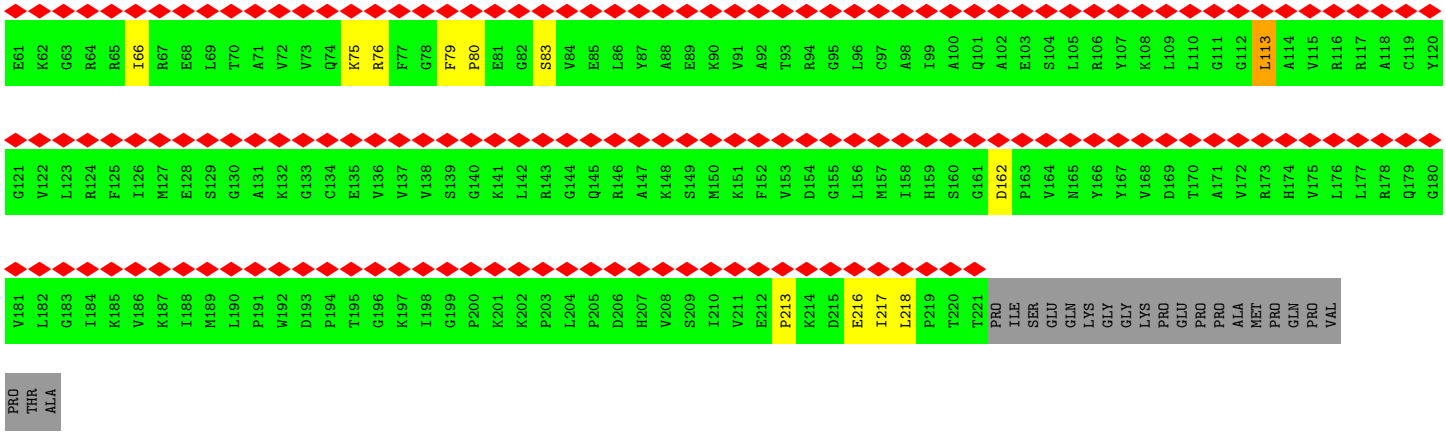
Chain BC:



• Molecule 53: 40S ribosomal protein S3

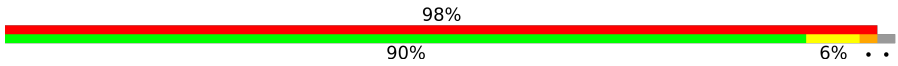
Chain BD:

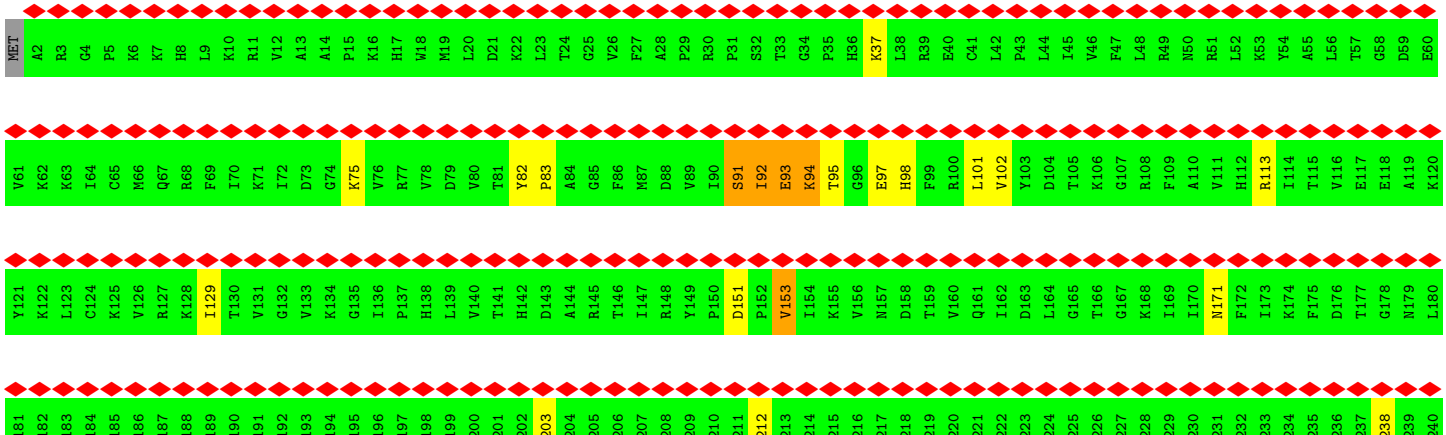




• Molecule 54: 40S ribosomal protein S4, Y isoform 1

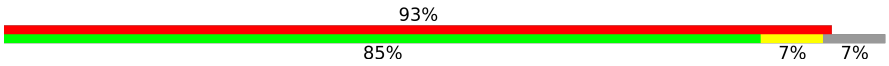
Chain BE:

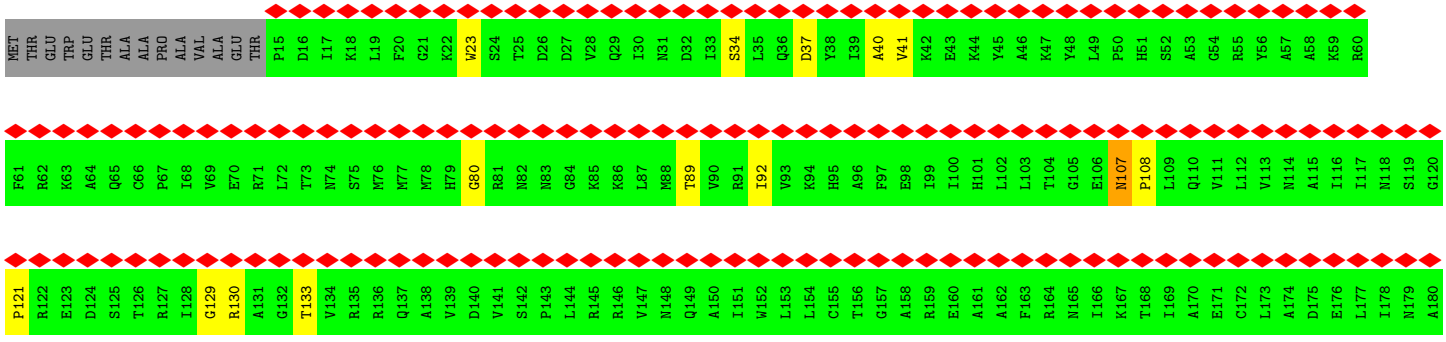


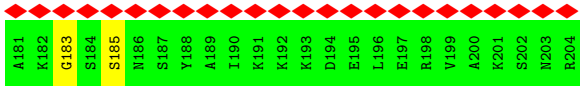


• Molecule 55: 40S ribosomal protein S5

Chain BF:

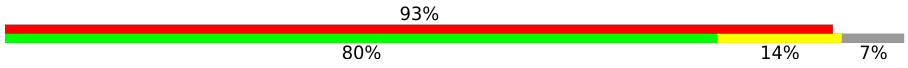


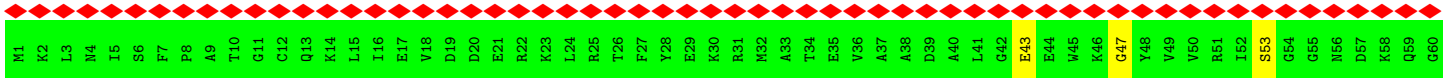


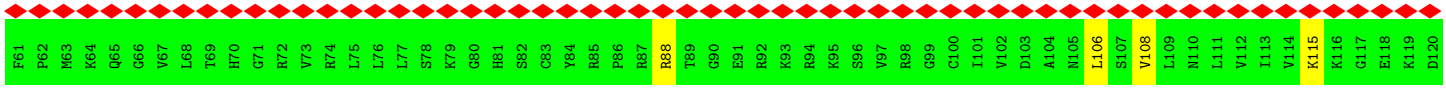


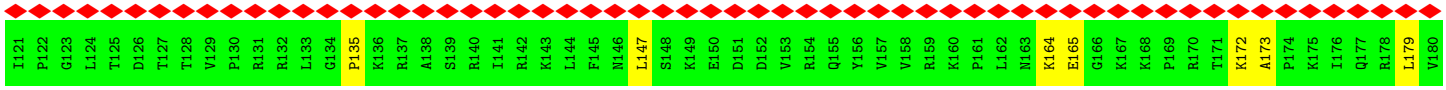
• Molecule 56: 40S ribosomal protein S6

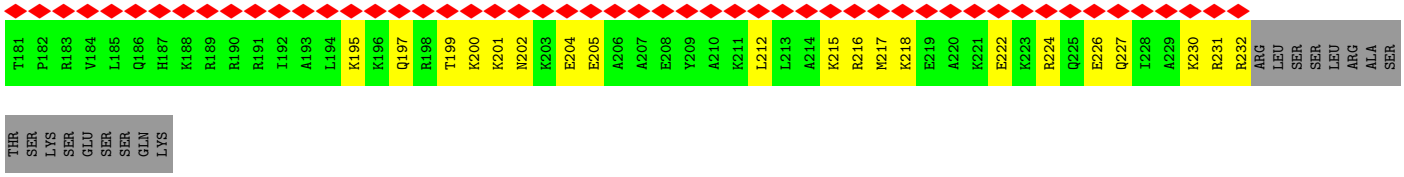
Chain BG:





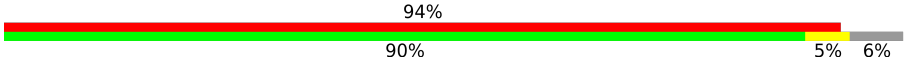


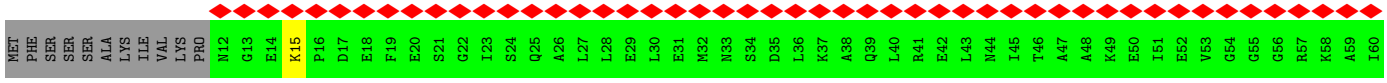


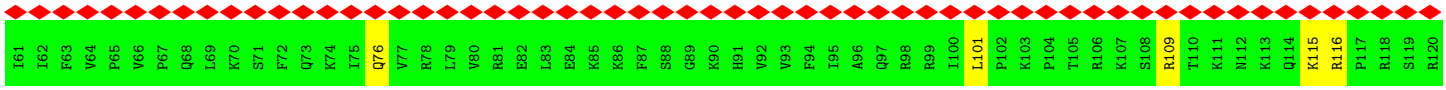


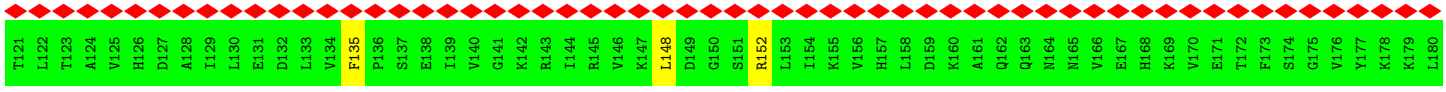
• Molecule 57: 40S ribosomal protein S7

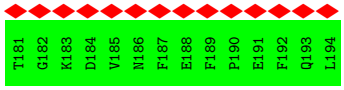
Chain BH:





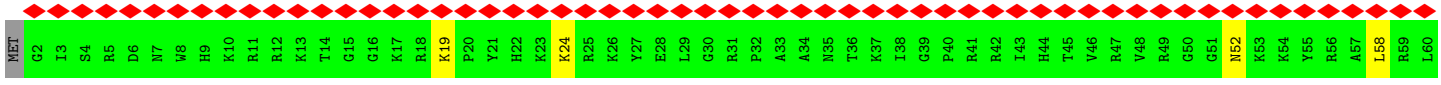






• Molecule 58: 40S ribosomal protein S8

Chain BI:



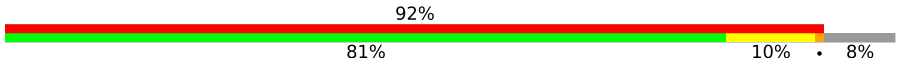
D61 V62 G63 N64 F65 S66 W67 G68 S69 E70 C71 C72 T73 R74 K75 T76 R77 I78 I79 D80 V81 V82 Y83 N84 A85 S86 N87 N88 E89 L90 V91 R92 T93 K94 T95 L96 V97 K98 N99 C100 I101 V102 L103 I104 D105 S106 T107 P108 Y109 R110 Q111 W112 Y113 E114 S115 H116 Y117 A118 L119 P120

L121 G122 R123 K124 K125 G126 A127 K128 L129 T130 P131 E132 E133 E134 E135 I136 L137 N138 K139 K140 R141 S142 K143 K144 I145 Q146 K147 K148 Y149 D150 E151 R152 K153 K154 N155 A156 K157 I158 S159 S160 L161 L162 E163 E164 Q165 F166 Q167 Q168 G169 K170 L171 L172 A173 C174 I175 A176 S177 R178 P179 G180

Q181 C182 G183 R184 A185 D186 G187 Y188 V189 L190 E191 G192 K193 E194 L195 E196 F197 Y198 L199 R200 K201 I202 K203 A204 R205 K206 G207 K208

• Molecule 59: 40S ribosomal protein S9

Chain BJ:



MET P2 V3 A4 R5 S6 W7 V8 C9 R10 K11 T12 Y13 V14 T15 P16 R17 R18 P19 F20 E21 K22 S23 R24 L25 D26 Q27 E28 L29 K30 L31 I32 G33 E34 Y35 G36 L37 R38 N39 K40 R41 E42 V43 W44 R45 V46 K47 F48 T49 L50 A51 K52 I53 R54 K55 A56 A57 R58 E59 L60

L61 T62 L63 D64 E65 K66 D67 P68 R69 R70 L71 F72 E73 G74 N75 A76 L77 L78 R79 R80 L81 V82 R83 I84 G85 V86 L87 D88 E89 G90 K91 M92 K93 L94 D95 Y96 I97 L98 G99 L100 K101 I102 E103 D104 F105 L106 E107 R108 R109 L110 Q111 T112 Q113 V114 F115 K116 L117 G118 L119 A120

K121 S122 I123 H124 H125 A126 R127 V128 L129 I130 R131 Q132 R133 H134 I135 R136 V137 R138 K139 Q140 V141 V142 N143 I144 P145 S146 F147 I148 V149 R150 L151 D152 S153 Q154 K155 H156 I157 D158 F159 S160 L161 R162 S163 P164 Y165 G166 G167 G168 R169 P170 G171 R172 V173 K174 R175 K176 N177 A178 K179 K180

GLY GLN GLY GLY ALA GLY ALA GLY ASP ASP GLU GLU GLU ASP

• Molecule 60: 40S ribosomal protein S10

Chain BK:

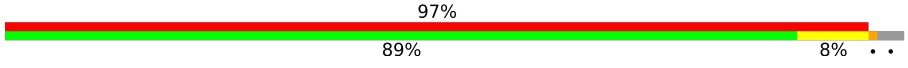
M1 L2 M3 P4 K5 K6 N7 R8 I9 A10 I11 Y12 E13 L14 L15 F16 K17 E18 G19 V20 M21 V22 A23 K24 K25 D26 V27 H28 M29 P30 K31 H32 P33 E34 L35 A36 D37 K38 N39 V40 P41 N42 L43 H44 V45 M46 K47 A48 M49 Q50 S51 L52 K53 S54 R55 G56 Y57 V58 K59 E60

Q61 F62 A63 W64 R65 H66 F67 Y68 W69 Y70 L71 T72 N73 E74 G75 I76 Q77 Y78 L79 R80 D81 Y82 L83 H84 L85 P86 P87 E88 I89 V90 P91 A92 T93 L94 R95 R96 S97 R98 PRO GLU THR GLY ARG PRO ARG PRO LYS GLY GLU GLY GLU ARG PRO ALA ARG LEU THR ARG GLY

GLU ALA ASP ARG ASP THR TYR ARG ARG SER ALA VAL PRO PRO GLY ALA ASP LYS LYS ALA GLU ALA GLY ALA GLY SER ALA THR GLU PHE GLN PHE ARG GLY GLY PHE GLY ARG GLY ARG GLY GLN PRO PRO GLN

• Molecule 61: 40S ribosomal protein S11

Chain BL:



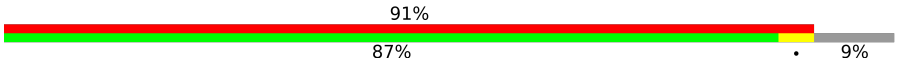
MET ALA ASP ILE GLN T6 E7 R8 A9 Y10 Q11 K12 Q13 P14 T15 I16 F17 Q18 N19 K20 K21 R22 V23 L24 L25 G26 E27 T28 G29 K30 E31 K32 L33 P34 R35 Y36 Y37 K38 N39 I40 G41 L42 G43 F44 K45 T46 P47 K48 E49 A50 I51 E52 G53 T54 Y55 I56 D57 K58 K59 C60

P61 F62 T63 G64 N65 V66 S67 I68 R69 G70 R71 I72 L73 S74 G75 V76 V77 T78 K79 M80 K81 M82 Q83 R84 T85 I86 V87 I88 R89 R90 D91 Y92 L93 H94 Y95 I96 R97 K98 Y99 N100 R101 F102 E103 K104 R105 H106 K107 N108 M109 S110 V111 H112 L113 S114 P115 C116 F117 R118 D119 V120

Q121 I122 G123 D124 I125 V126 T127 V128 G129 E130 C131 R132 P133 L134 S135 K136 T137 V138 R139 F140 N141 V142 L143 K144 V145 T146 K147 A148 A149 G150 T151 K152 K153 Q154 F155 Q156 K157 F158

- Molecule 62: 40S ribosomal protein S12

Chain BM:



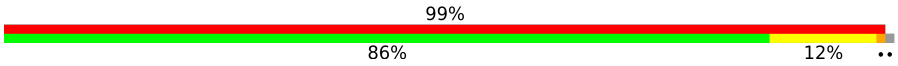
MET ALA GLU GLU GLY ILE ALA ALA GLY GLY V11 M12 D13 V14 N15 T16 A17 L18 Q19 E20 V21 L22 K23 T24 A25 L26 I27 H28 D29 G30 L31 A32 R33 G34 I35 R36 E37 A38 A39 K40 A41 L42 D43 K44 R45 Q46 A47 H48 L49 C50 V51 L52 A53 S54 N55 C56 D57 E58 P59 M60

Y61 V62 K63 L64 V65 E66 A67 L68 C69 A70 E71 H72 Q73 I74 N75 L76 I77 K78 V79 D80 D81 N82 K83 K84 L85 G86 E87 W88 V89 G90 L91 C92 K93 I94 D95 R96 E97 G98 K99 P100 R101 K102 V103 V104 G105 C106 S107 C108 V109 V110 V111 K112 D113 Y114 G115 K116 E117 S118 Q119 A120

K121 D122 V123 I124 E125 E126 Y127 F128 K129 C130 LYS LYS

- Molecule 63: 40S ribosomal protein S13

Chain BN:



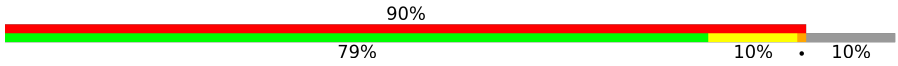
MET G2 R3 M4 H5 A6 P7 G8 K9 G10 L11 S12 Q13 S14 A15 L16 P17 Y18 R19 R20 S21 V22 P23 T24 W25 L26 K27 L28 T29 S30 D31 D32 V33 K34 E35 Q36 I37 Y38 K39 L40 A41 K42 K43 G44 L45 T46 P47 S48 Q49 I50 G51 V52 I53 L54 R55 D56 S57 H58 G59 V60

A61 Q62 V63 R64 F65 V66 T67 G68 N69 K70 I71 L72 R73 I74 L75 K76 S77 K78 G79 L80 A81 P82 D83 L84 P85 E86 D87 L88 Y89 H90 L91 I92 K93 K94 A95 V96 A97 V98 R99 K100 H101 L102 E103 R104 N105 R106 K107 D108 K109 D110 A111 K112 F113 R114 L115 I116 L117 I118 E119 S120

R121 I122 H123 R124 L125 A126 R127 Y128 Y129 K130 T131 K132 R133 V134 L135 P136 P137 N138 W139 K140 Y141 E142 S143 S144 T145 A146 S147 A148 L149 V150 ALA

- Molecule 64: 40S ribosomal protein S14

Chain BO:



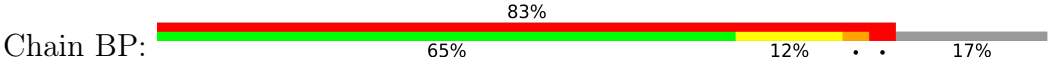
MET ALA PRO ARG LYS GLY LYS GLU LYS LYS GLU GLU GLN VAL ILE S16 L17 G18 P19 Q20 V21 A22 E23 G24 E25 N26 V27 F28 G29 V30 C31 H32 I33 F34 A35 S36 F37 N38 D39 T40 F41 V42 H43 V44 T45 D46 L47 S48 G49 K50 E51 T52 I53 C54 R55 V56 T57 G58 G59 M60

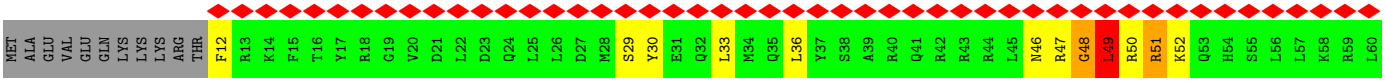
K61 V62 K63 A64 D65 R66 D67 E68 S69 S70 P71 Y72 A73 A74 M75 L76 A77 A78 Q79 D80 V81 A82 Q83 R84 C85 K86 E87 L88 G89 I90 T91 A92 L93 H94 I95 K96 L97 R98 A99 T100 G101 G102 N103 R104 T105 K106 T107 P108 G109 P110 G111 A112 Q113 S114 A115 L116 R117 A118 L119 A120

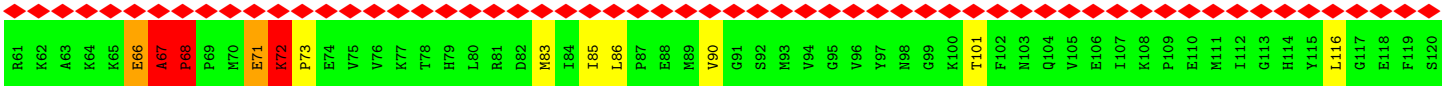
R121 S122 G123 M124 K125 I126 G127 R128 I129 E130 D131 V132 T133 P134 I135 P136 S137 D138 S139 T140 R141 R142 K143 G144 G145 R146 R147 G148 R149 R150 L151

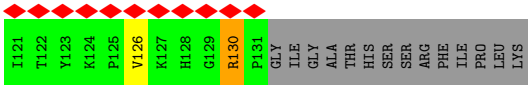
• Molecule 65: 40S ribosomal protein S15

Chain BP:



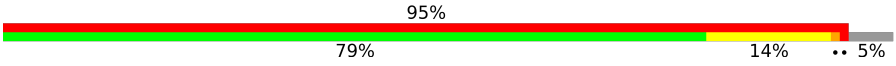


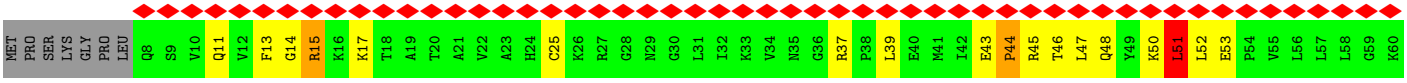


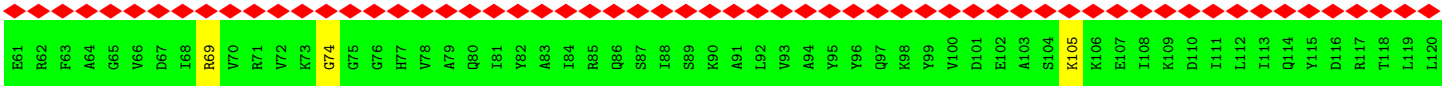


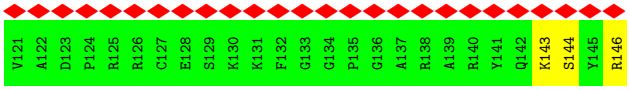
• Molecule 66: 40S ribosomal protein S16

Chain BQ:



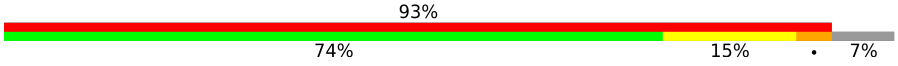


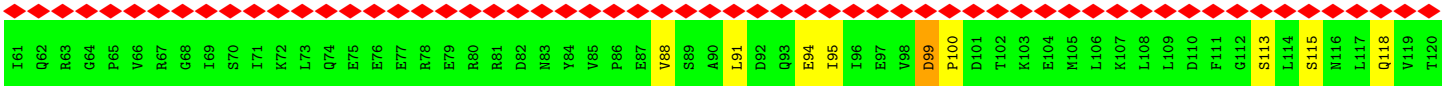


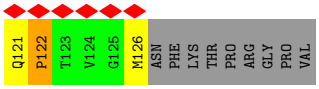


• Molecule 67: 40S ribosomal protein S17-like

Chain BR:

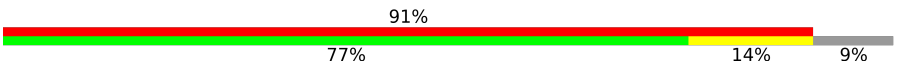


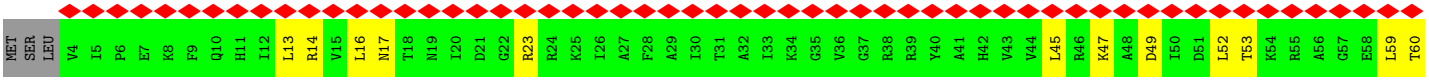


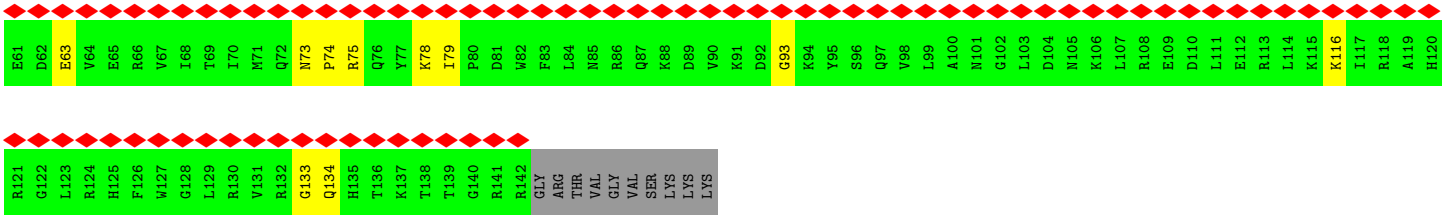


• Molecule 68: 40S ribosomal protein S18

Chain BS:

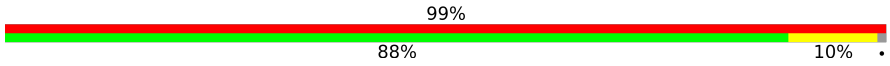


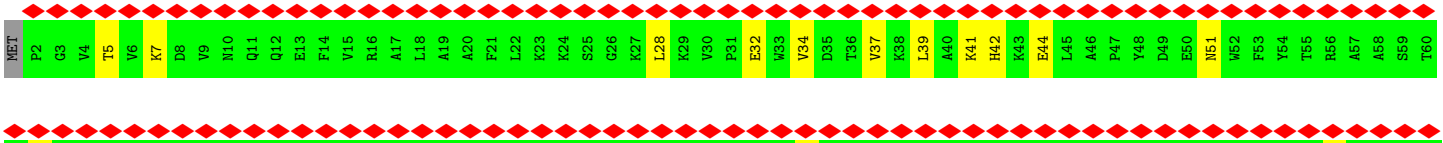




• Molecule 69: 40S ribosomal protein S19

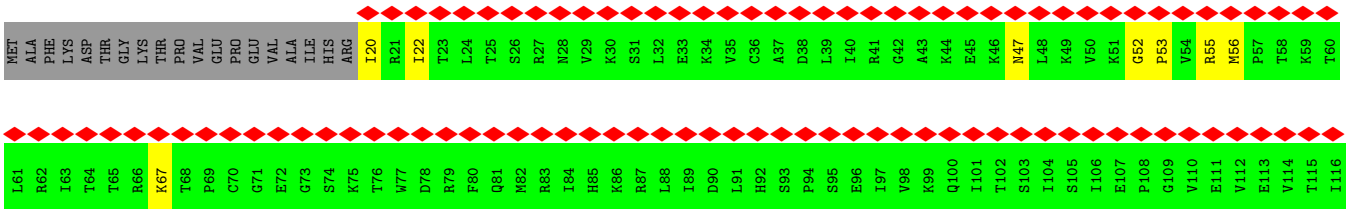
Chain BT:





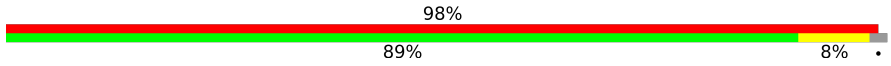
• Molecule 70: 40S ribosomal protein S20

Chain BU:



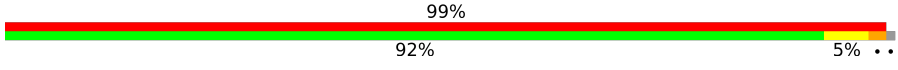
• Molecule 71: 40S ribosomal protein S21

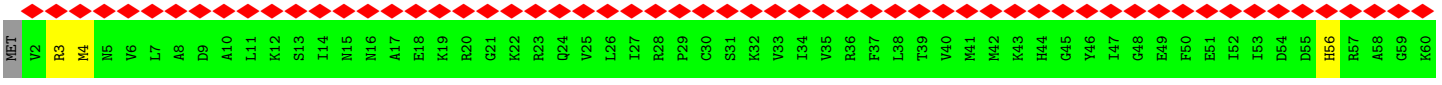
Chain BV:

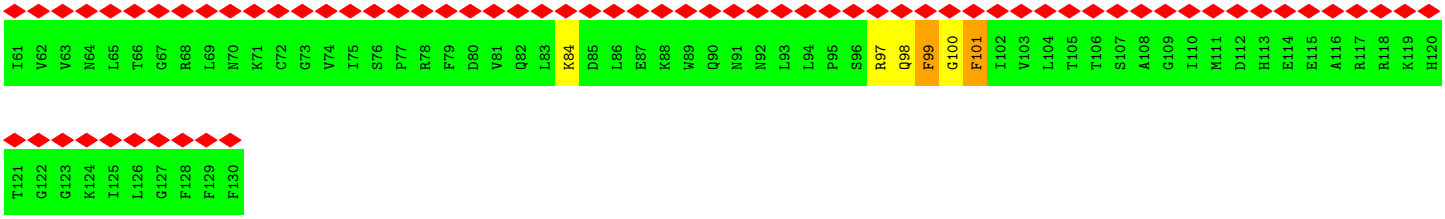


• Molecule 72: 40S ribosomal protein S15a

Chain BW:

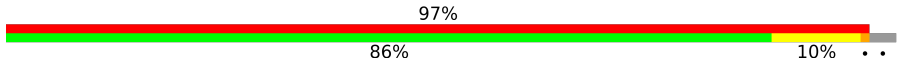






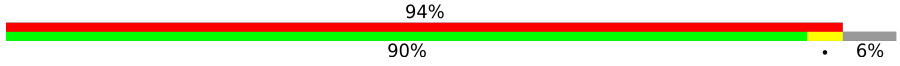
• Molecule 73: 40S ribosomal protein S23

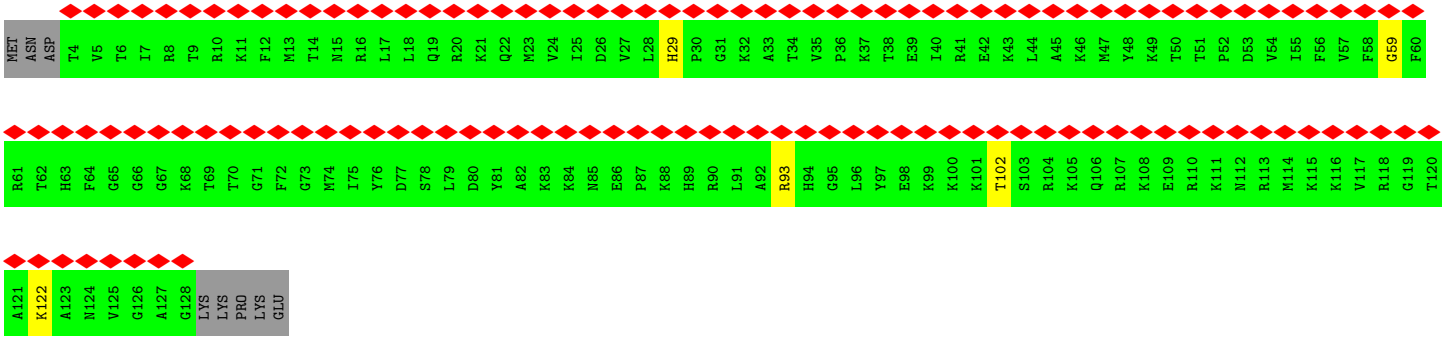
Chain BX:



• Molecule 74: 40S ribosomal protein S24

Chain BY:





• Molecule 75: 40S ribosomal protein S25

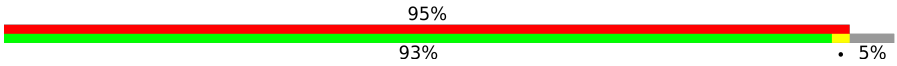
Chain BZ:

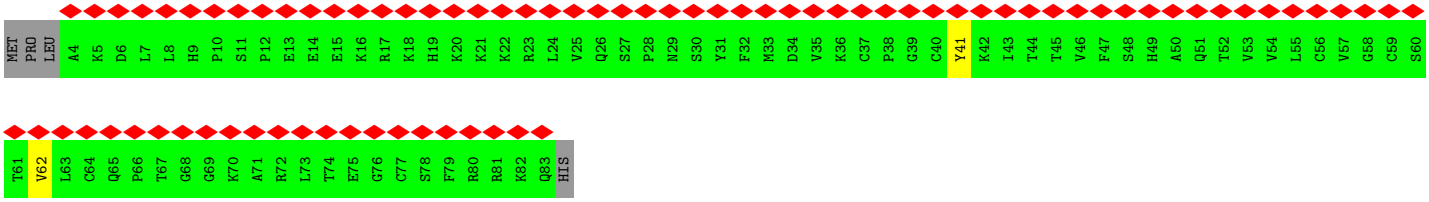
• Molecule 76: 40S ribosomal protein S26

Chain Ba:

• Molecule 77: 40S ribosomal protein S27

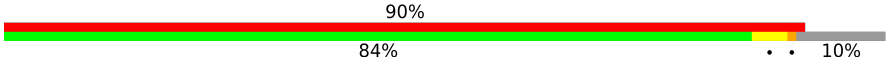
Chain Bb:

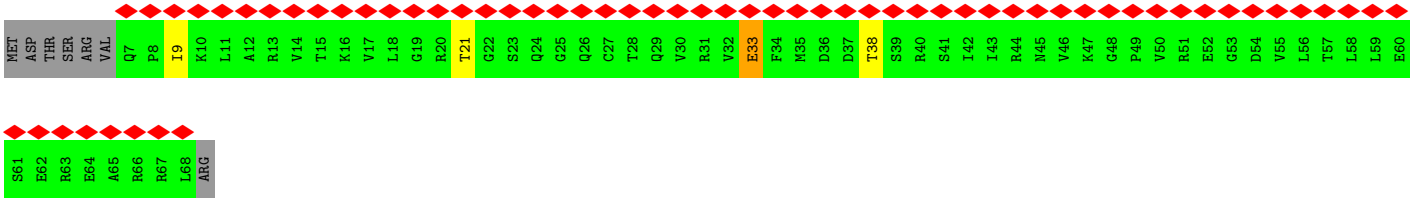




• Molecule 78: 40S ribosomal protein S28

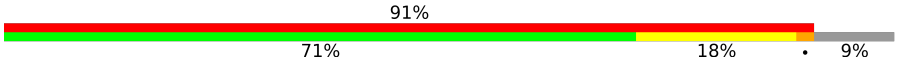
Chain Bc:

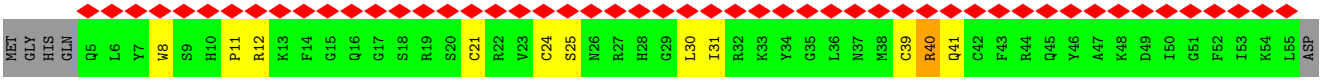




• Molecule 79: 40S ribosomal protein S29

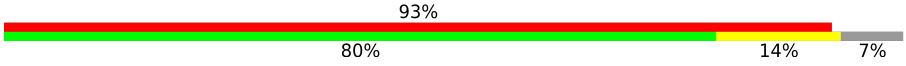
Chain Bd:

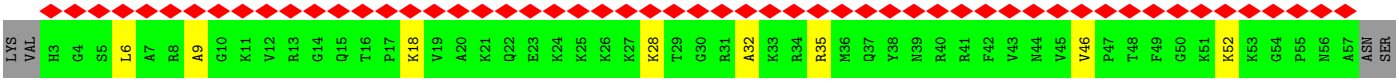




• Molecule 80: 40S ribosomal protein S30

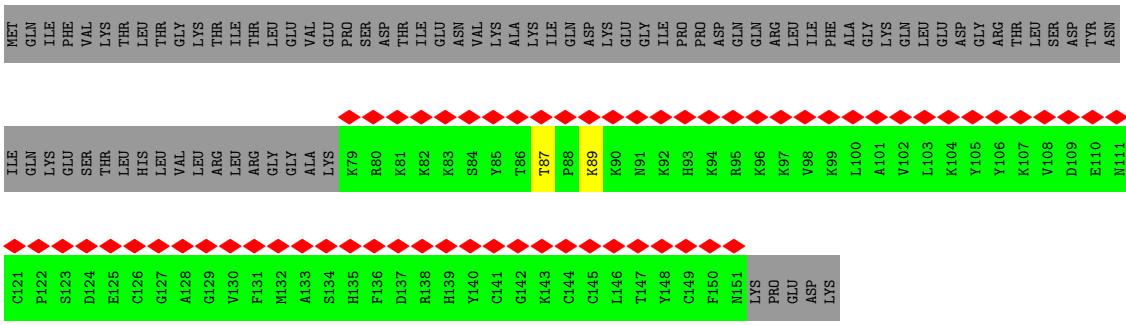
Chain Be:





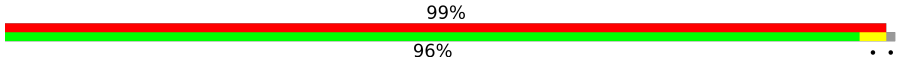
• Molecule 81: Ubiquitin-40S ribosomal protein S27a

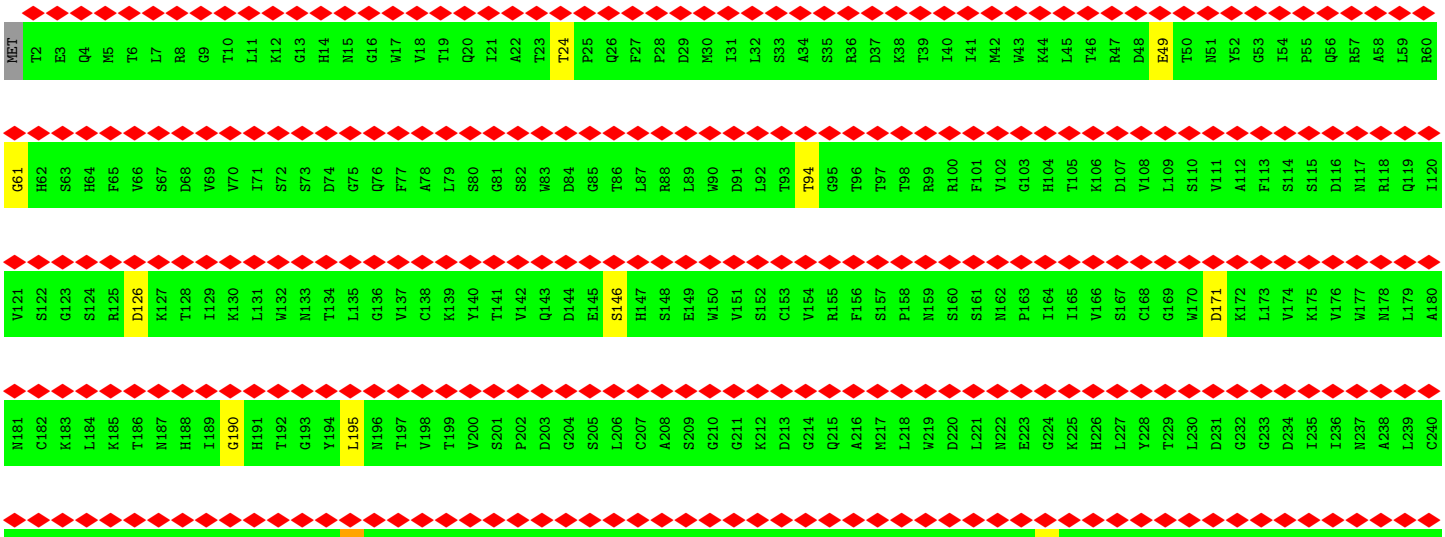
Chain Bf:



• Molecule 82: Guanine nucleotide-binding protein subunit beta-2-like 1

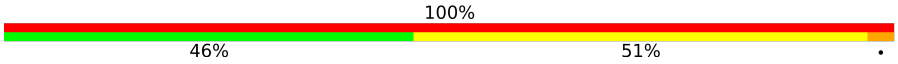
Chain Bg:

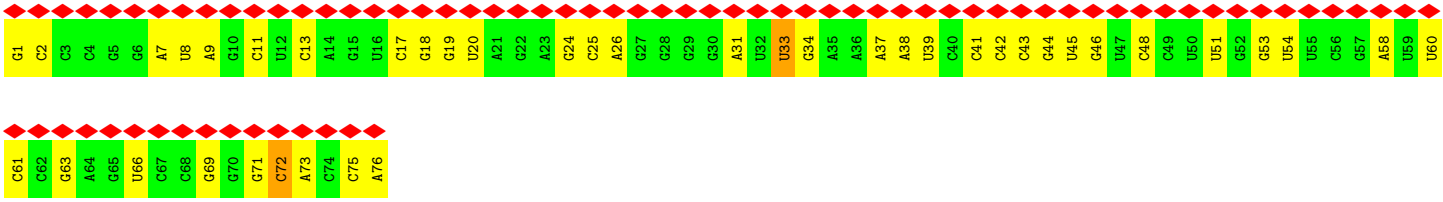




• Molecule 83: tRNA

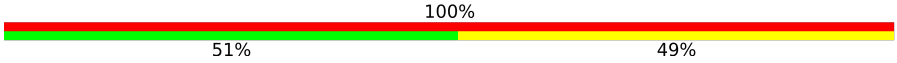
Chain Bv:

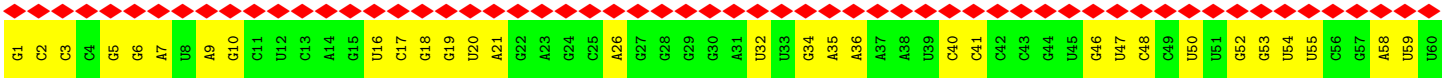


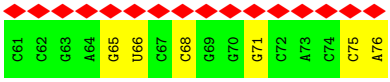


• Molecule 83: tRNA

Chain Bw:

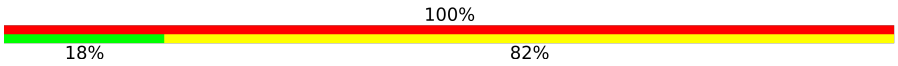


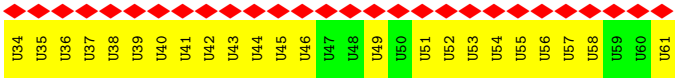




• Molecule 84: mRNA

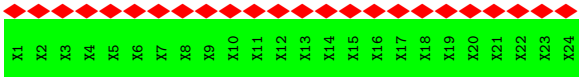
Chain Bx:





• Molecule 85: Nascent protein chain

Chain By:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	313321	Depositor
Resolution determination method	Not provided	
CTF correction method	DEFOCUS GROUPS	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20.00	Depositor
Minimum defocus (nm)	2000.00	Depositor
Maximum defocus (nm)	4500.00	Depositor
Magnification	205000	Depositor
Image detector	TVIPS TEMCAM-F416 (4k x 4k)	Depositor
Maximum map value	15.028	Depositor
Minimum map value	-7.978	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3	Depositor
Map size (Å)	378.0, 378.0, 378.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.945, 0.945, 0.945	Depositor

5 Model quality

5.1 Standard geometry

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

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	A3	1.12	40/3726 (1.1%)	1.17	52/5804 (0.9%)
2	A4	1.10	32/2839 (1.1%)	1.13	40/4425 (0.9%)
3	AA	0.44	0/1968	0.65	1/2639 (0.0%)
4	AB	0.39	0/3246	0.64	0/4345
5	AC	0.41	1/2942 (0.0%)	0.62	3/3951 (0.1%)
6	AD	0.42	0/2437	0.65	2/3262 (0.1%)
7	AE	0.50	0/1603	0.80	4/2153 (0.2%)
8	AF	0.37	0/1986	0.57	0/2644
9	AG	0.38	0/1913	0.57	0/2576
10	AH	0.38	0/1545	0.54	1/2077 (0.0%)
11	AI	0.41	0/1730	0.61	1/2311 (0.0%)
12	AJ	0.39	0/1376	0.59	0/1841
13	AK	0.85	3/886 (0.3%)	1.53	23/1188 (1.9%)
14	AL	0.48	3/1688 (0.2%)	0.73	5/2260 (0.2%)
15	AM	0.39	0/1161	0.64	0/1554
16	AN	0.39	0/1746	0.57	0/2338
17	AO	0.37	0/1638	0.60	0/2191
18	AP	0.42	0/1268	0.70	0/1701
19	AQ	0.47	2/1537 (0.1%)	0.63	3/2052 (0.1%)
20	AR	0.38	0/1533	0.63	1/2025 (0.0%)
21	AS	0.38	1/1488 (0.1%)	0.60	1/1997 (0.1%)
22	AT	0.38	0/1312	0.60	0/1753
23	AU	0.35	0/822	0.58	0/1103
24	AV	0.37	0/983	0.55	0/1319
25	AW	0.42	1/1004 (0.1%)	0.74	3/1332 (0.2%)
26	AX	0.34	0/975	0.51	0/1312
27	AY	0.35	0/1081	0.56	0/1439
28	AZ	0.42	0/1126	0.69	2/1502 (0.1%)
29	Aa	0.50	0/1191	0.70	1/1591 (0.1%)
30	Ab	0.36	0/569	0.58	0/750
31	Ac	0.38	0/812	0.60	0/1089
32	Ad	0.38	0/894	0.58	0/1204

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Ae	0.42	0/1082	0.58	1/1443 (0.1%)
34	Af	0.47	0/895	0.73	2/1198 (0.2%)
35	Ag	0.39	0/916	0.58	0/1220
36	Ah	0.37	0/1023	0.63	1/1351 (0.1%)
37	Ai	0.35	0/805	0.58	0/1065
38	Aj	0.47	1/703 (0.1%)	0.92	3/929 (0.3%)
39	Ak	0.51	0/575	0.74	0/761
40	Al	0.37	0/454	0.54	0/599
41	Am	0.42	0/417	0.59	0/553
42	An	0.36	0/241	0.60	0/305
43	Ao	0.39	0/877	0.66	0/1156
44	Ap	0.39	0/718	0.60	0/953
45	Aq	0.89	3/1058 (0.3%)	1.93	34/1424 (2.4%)
46	At	0.41	0/995	0.69	0/1334
47	Au	0.73	1/1772 (0.1%)	1.28	17/2375 (0.7%)
48	A2	0.98	666/86613 (0.8%)	1.13	1094/135108 (0.8%)
49	B1	0.96	275/40767 (0.7%)	1.13	515/63536 (0.8%)
50	BA	0.52	1/1741 (0.1%)	0.72	5/2366 (0.2%)
51	BB	0.42	0/1749	0.62	0/2340
52	BC	0.37	0/1761	0.58	0/2379
53	BD	0.44	1/1736 (0.1%)	0.63	1/2338 (0.0%)
54	BE	0.41	1/2072 (0.0%)	0.59	1/2793 (0.0%)
55	BF	0.40	1/1524 (0.1%)	0.62	1/2048 (0.0%)
56	BG	0.41	0/1907	0.62	1/2538 (0.0%)
57	BH	0.43	0/1501	0.64	1/2009 (0.0%)
58	BI	0.41	0/1725	0.59	0/2298
59	BJ	0.36	0/1520	0.55	1/2030 (0.0%)
60	BK	0.43	0/851	0.68	0/1147
61	BL	0.44	1/1281 (0.1%)	0.65	2/1710 (0.1%)
62	BM	0.39	0/941	0.63	0/1264
63	BN	0.40	1/1226 (0.1%)	0.57	1/1649 (0.1%)
64	BO	0.43	0/1029	0.64	0/1380
65	BP	0.50	1/1019 (0.1%)	0.74	3/1361 (0.2%)
66	BQ	0.38	0/1126	0.58	2/1506 (0.1%)
67	BR	0.49	3/1023 (0.3%)	0.68	3/1373 (0.2%)
68	BS	0.42	1/1172 (0.1%)	0.63	1/1570 (0.1%)
69	BT	0.36	0/1131	0.60	0/1515
70	BU	0.45	0/778	0.65	1/1045 (0.1%)
71	BV	0.41	0/623	0.60	1/833 (0.1%)
72	BW	0.37	0/1051	0.55	0/1406
73	BX	0.44	1/1097 (0.1%)	0.61	1/1464 (0.1%)
74	BY	0.40	0/1032	0.64	0/1371
75	BZ	0.43	0/696	0.62	0/929

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	Ba	0.49	0/786	0.75	2/1053 (0.2%)
77	Bb	0.42	0/637	0.59	0/854
78	Bc	0.40	0/490	0.66	0/656
79	Bd	0.54	0/437	0.89	3/580 (0.5%)
80	Be	0.37	0/443	0.60	0/583
81	Bf	0.44	0/613	0.62	0/811
82	Bg	0.40	0/2497	0.60	0/3399
83	Bv	0.58	4/1813 (0.2%)	0.84	5/2823 (0.2%)
83	Bw	0.43	2/1813 (0.1%)	0.90	4/2823 (0.1%)
84	Bx	0.60	2/616 (0.3%)	1.20	11/948 (1.2%)
All	All	0.80	1049/234393 (0.4%)	0.98	1861/344230 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	AB	0	3
5	AC	0	2
7	AE	0	1
8	AF	0	2
10	AH	0	3
13	AK	0	3
14	AL	0	6
39	Ak	0	1
48	A2	2	3
49	B1	1	0
54	BE	0	6
63	BN	0	2
64	BO	0	2
65	BP	0	11
66	BQ	0	6
72	BW	0	3
76	Ba	0	1
79	Bd	0	1
All	All	3	56

All (1049) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	A2	3612	U	O3'-P	-21.32	1.35	1.61

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	B1	842	C	O3'-P	20.18	1.85	1.61
48	A2	2689	C	O3'-P	-19.59	1.37	1.61
49	B1	558	G	O3'-P	19.39	1.84	1.61
49	B1	497	C	O3'-P	18.59	1.83	1.61
49	B1	72	C	O3'-P	17.80	1.82	1.61
49	B1	1253	A	O3'-P	17.54	1.82	1.61
49	B1	1439	A	O3'-P	-17.24	1.40	1.61
48	A2	925	C	O3'-P	-17.23	1.40	1.61
49	B1	2	A	O3'-P	-17.22	1.40	1.61
48	A2	1274	G	O3'-P	-17.14	1.40	1.61
48	A2	673	C	O3'-P	-17.07	1.40	1.61
49	B1	38	A	O3'-P	-17.07	1.40	1.61
49	B1	1792	G	O3'-P	-17.07	1.40	1.61
48	A2	1288	C	O3'-P	-17.03	1.40	1.61
48	A2	2335	U	O3'-P	-17.02	1.40	1.61
48	A2	3852	G	O3'-P	-17.01	1.40	1.61
48	A2	4906	C	O3'-P	-17.00	1.40	1.61
48	A2	210	G	O3'-P	-16.98	1.40	1.61
48	A2	4903	G	O3'-P	-16.92	1.40	1.61
49	B1	1389	C	O3'-P	-16.86	1.41	1.61
48	A2	2457	C	O3'-P	-16.84	1.41	1.61
1	A3	124	U	O3'-P	-16.74	1.41	1.61
48	A2	4907	G	O3'-P	-16.74	1.41	1.61
49	B1	619	A	O3'-P	-16.74	1.41	1.61
48	A2	4519	U	O3'-P	-16.69	1.41	1.61
48	A2	238	G	O3'-P	-16.68	1.41	1.61
48	A2	1433	C	O3'-P	-16.65	1.41	1.61
48	A2	3649	G	O3'-P	-16.62	1.41	1.61
48	A2	4117	C	O3'-P	-16.61	1.41	1.61
49	B1	1725	U	O3'-P	-16.59	1.41	1.61
48	A2	4664	G	O3'-P	-16.57	1.41	1.61
48	A2	4538	U	O3'-P	-16.55	1.41	1.61
48	A2	3697	A	O3'-P	-16.55	1.41	1.61
49	B1	348	A	O3'-P	-16.54	1.41	1.61
49	B1	1648	G	O3'-P	-16.37	1.41	1.61
48	A2	1716	G	O3'-P	16.25	1.80	1.61
48	A2	4316	U	O3'-P	-16.23	1.41	1.61
48	A2	3604	C	O3'-P	-16.05	1.41	1.61
2	A4	4	U	O3'-P	-16.04	1.42	1.61
49	B1	426	A	O3'-P	-16.01	1.42	1.61
48	A2	99	A	O3'-P	-15.96	1.42	1.61
49	B1	292	A	O3'-P	-15.91	1.42	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	A2	2602	A	O3'-P	-15.86	1.42	1.61
2	A4	71	G	O3'-P	-15.80	1.42	1.61
49	B1	1420	G	O3'-P	15.78	1.80	1.61
48	A2	4537	G	O3'-P	-15.70	1.42	1.61
49	B1	1475	G	O3'-P	-15.70	1.42	1.61
48	A2	100	C	O3'-P	-15.69	1.42	1.61
49	B1	421	G	O3'-P	-15.68	1.42	1.61
48	A2	3665	U	O3'-P	-15.66	1.42	1.61
48	A2	4457	G	O3'-P	-15.60	1.42	1.61
49	B1	999	G	O3'-P	-15.56	1.42	1.61
48	A2	4488	U	O3'-P	-15.43	1.42	1.61
49	B1	56	G	O3'-P	-15.37	1.42	1.61
2	A4	114	U	O3'-P	-15.37	1.42	1.61
48	A2	2832	C	O3'-P	-15.33	1.42	1.61
49	B1	1122	A	O3'-P	-15.29	1.42	1.61
48	A2	4045	U	O3'-P	-15.29	1.42	1.61
49	B1	368	U	O3'-P	-15.26	1.42	1.61
49	B1	1331	C	O3'-P	-15.24	1.42	1.61
48	A2	4020	A	O3'-P	-15.24	1.42	1.61
49	B1	1291	A	O3'-P	-15.24	1.42	1.61
48	A2	1712	U	O3'-P	-15.21	1.43	1.61
49	B1	1408	U	O3'-P	-15.17	1.43	1.61
48	A2	2330	C	O3'-P	-15.17	1.43	1.61
49	B1	114	G	O3'-P	-15.12	1.43	1.61
48	A2	4135	G	O3'-P	-15.04	1.43	1.61
48	A2	1711	A	O3'-P	-15.01	1.43	1.61
48	A2	111	C	O3'-P	-14.92	1.43	1.61
48	A2	1312	G	O3'-P	-14.91	1.43	1.61
48	A2	4486	G	O3'-P	-14.91	1.43	1.61
48	A2	963	G	O3'-P	-14.89	1.43	1.61
48	A2	4520	U	O3'-P	-14.84	1.43	1.61
49	B1	1683	C	O3'-P	-14.83	1.43	1.61
48	A2	4925	A	O3'-P	-14.79	1.43	1.61
48	A2	2734	A	O3'-P	-14.78	1.43	1.61
48	A2	1760	C	O3'-P	-14.77	1.43	1.61
48	A2	1771	C	O3'-P	-14.71	1.43	1.61
49	B1	1181	A	O3'-P	-14.69	1.43	1.61
49	B1	808	A	O3'-P	-14.68	1.43	1.61
49	B1	677	G	O3'-P	-14.59	1.43	1.61
48	A2	4834	U	O3'-P	-14.58	1.43	1.61
48	A2	295	G	O3'-P	-14.57	1.43	1.61
48	A2	2679	G	O3'-P	-14.56	1.43	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	A2	960	G	O3'-P	-14.54	1.43	1.61
48	A2	503	A	O3'-P	-14.50	1.43	1.61
49	B1	4	C	O3'-P	-14.34	1.44	1.61
49	B1	436	G	O3'-P	-14.32	1.44	1.61
48	A2	3860	G	O3'-P	-14.32	1.44	1.61
48	A2	2502	G	O3'-P	-14.29	1.44	1.61
48	A2	3876	A	O3'-P	-14.28	1.44	1.61
48	A2	4633	C	O3'-P	-14.28	1.44	1.61
48	A2	1376	G	O3'-P	-14.27	1.44	1.61
49	B1	1407	U	O3'-P	-14.27	1.44	1.61
49	B1	684	G	O3'-P	-14.26	1.44	1.61
48	A2	2525	G	O3'-P	-14.13	1.44	1.61
48	A2	4712	G	O3'-P	-14.10	1.44	1.61
48	A2	3593	C	O3'-P	-14.07	1.44	1.61
49	B1	495	U	O3'-P	-14.00	1.44	1.61
48	A2	927	C	O3'-P	-13.95	1.44	1.61
1	A3	139	G	O3'-P	-13.91	1.44	1.61
48	A2	4606	G	O3'-P	-13.91	1.44	1.61
48	A2	9	C	O3'-P	-13.87	1.44	1.61
48	A2	1593	C	O3'-P	-13.82	1.44	1.61
48	A2	2781	C	O3'-P	-13.74	1.44	1.61
48	A2	1854	A	O3'-P	-13.69	1.44	1.61
48	A2	2798	U	O3'-P	-13.67	1.44	1.61
49	B1	291	G	O3'-P	-13.65	1.44	1.61
49	B1	1316	C	O3'-P	-13.65	1.44	1.61
48	A2	2830	G	O3'-P	-13.62	1.44	1.61
48	A2	4461	G	O3'-P	-13.62	1.44	1.61
49	B1	632	C	O3'-P	-13.62	1.44	1.61
48	A2	958	U	C3'-O3'	-13.59	1.23	1.42
48	A2	1346	C	O3'-P	-13.59	1.44	1.61
48	A2	2601	G	O3'-P	-13.55	1.44	1.61
48	A2	1228	C	O3'-P	-13.54	1.45	1.61
49	B1	418	A	O3'-P	-13.54	1.45	1.61
48	A2	3707	A	O3'-P	-13.49	1.45	1.61
48	A2	154	U	O3'-P	-13.47	1.45	1.61
48	A2	5006	A	O3'-P	-13.37	1.45	1.61
48	A2	303	C	O3'-P	-13.33	1.45	1.61
49	B1	297	A	O3'-P	-13.32	1.45	1.61
48	A2	4989	G	O3'-P	-13.29	1.45	1.61
1	A3	15	G	O3'-P	-13.24	1.45	1.61
48	A2	4462	U	O3'-P	-13.23	1.45	1.61
49	B1	1484	A	O3'-P	-13.23	1.45	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	A2	3910	G	O3'-P	-13.22	1.45	1.61
48	A2	2826	G	O3'-P	-13.20	1.45	1.61
48	A2	2751	C	O3'-P	-13.18	1.45	1.61
48	A2	15	A	O3'-P	-13.15	1.45	1.61
48	A2	25	A	O3'-P	-13.14	1.45	1.61
48	A2	2053	C	O3'-P	-13.13	1.45	1.61
49	B1	404	G	O3'-P	-13.13	1.45	1.61
49	B1	1682	C	O3'-P	-13.13	1.45	1.61
48	A2	4990	C	O3'-P	-13.12	1.45	1.61
1	A3	14	U	O3'-P	-13.09	1.45	1.61
48	A2	4521	A	O3'-P	-13.07	1.45	1.61
48	A2	1259	C	O3'-P	-13.05	1.45	1.61
48	A2	2750	G	O3'-P	-13.04	1.45	1.61
49	B1	626	G	O3'-P	-13.02	1.45	1.61
1	A3	126	C	O3'-P	-13.01	1.45	1.61
49	B1	215	G	O3'-P	-13.01	1.45	1.61
48	A2	350	G	O3'-P	-13.01	1.45	1.61
49	B1	188	C	O3'-P	-12.98	1.45	1.61
49	B1	412	G	O3'-P	-12.96	1.45	1.61
48	A2	4823	C	O3'-P	-12.95	1.45	1.61
49	B1	1526	G	O3'-P	-12.91	1.45	1.61
48	A2	1057	G	O3'-P	12.90	1.76	1.61
49	B1	459	C	O3'-P	-12.90	1.45	1.61
48	A2	4976	C	O3'-P	-12.89	1.45	1.61
48	A2	974	C	O3'-P	-12.86	1.45	1.61
48	A2	3792	A	O3'-P	-12.85	1.45	1.61
48	A2	298	C	O3'-P	-12.83	1.45	1.61
49	B1	32	U	O3'-P	-12.81	1.45	1.61
49	B1	1080	A	O3'-P	-12.81	1.45	1.61
49	B1	681	U	O3'-P	-12.79	1.45	1.61
48	A2	958	U	O3'-P	-12.79	1.45	1.61
48	A2	79	C	O3'-P	-12.72	1.45	1.61
49	B1	501	C	O3'-P	-12.72	1.45	1.61
48	A2	4830	G	O3'-P	-12.71	1.45	1.61
49	B1	370	G	O3'-P	-12.71	1.46	1.61
48	A2	1759	C	O3'-P	-12.69	1.46	1.61
48	A2	4682	C	O3'-P	-12.66	1.46	1.61
49	B1	1022	U	O3'-P	-12.65	1.46	1.61
48	A2	1353	G	O3'-P	-12.62	1.46	1.61
48	A2	4677	C	O3'-P	-12.61	1.46	1.61
49	B1	1031	A	O3'-P	-12.60	1.46	1.61
48	A2	1227	G	O3'-P	-12.58	1.46	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	A2	1249	G	O3'-P	12.57	1.76	1.61
48	A2	451	G	O3'-P	-12.54	1.46	1.61
48	A2	4992	A	O3'-P	-12.52	1.46	1.61
1	A3	150	C	O3'-P	-12.52	1.46	1.61
48	A2	1973	U	O3'-P	-12.50	1.46	1.61
1	A3	89	U	O3'-P	-12.48	1.46	1.61
48	A2	452	C	O3'-P	-12.46	1.46	1.61
2	A4	104	C	O3'-P	-12.46	1.46	1.61
49	B1	683	G	O3'-P	12.45	1.76	1.61
48	A2	3624	A	O3'-P	-12.38	1.46	1.61
48	A2	2445	G	O3'-P	-12.36	1.46	1.61
48	A2	2290	C	O3'-P	-12.36	1.46	1.61
48	A2	1295	A	O3'-P	-12.35	1.46	1.61
48	A2	4059	G	O3'-P	-12.33	1.46	1.61
48	A2	3850	G	O3'-P	-12.30	1.46	1.61
48	A2	1061	A	O3'-P	-12.29	1.46	1.61
48	A2	3651	U	O3'-P	-12.29	1.46	1.61
49	B1	351	G	O3'-P	12.28	1.75	1.61
48	A2	2505	C	O3'-P	-12.28	1.46	1.61
48	A2	3839	G	O3'-P	-12.28	1.46	1.61
48	A2	2268	C	O3'-P	-12.22	1.46	1.61
48	A2	1763	U	O3'-P	-12.22	1.46	1.61
49	B1	1220	A	O3'-P	-12.20	1.46	1.61
49	B1	615	C	O3'-P	-12.18	1.46	1.61
48	A2	319	U	O3'-P	-12.15	1.46	1.61
48	A2	3629	C	O3'-P	-12.12	1.46	1.61
1	A3	115	G	O3'-P	-12.07	1.46	1.61
48	A2	1292	C	O3'-P	-12.07	1.46	1.61
1	A3	4	C	O3'-P	-12.06	1.46	1.61
48	A2	1053	G	O3'-P	-12.04	1.46	1.61
2	A4	41	G	O3'-P	-12.04	1.46	1.61
48	A2	4040	U	O3'-P	-12.01	1.46	1.61
48	A2	260	C	O3'-P	-12.00	1.46	1.61
48	A2	959	C	O3'-P	-12.00	1.46	1.61
48	A2	2782	U	O3'-P	-12.00	1.46	1.61
48	A2	4980	U	O3'-P	-11.97	1.46	1.61
48	A2	1981	G	O3'-P	-11.92	1.46	1.61
48	A2	4974	A	O3'-P	-11.91	1.46	1.61
49	B1	105	U	O3'-P	-11.88	1.46	1.61
49	B1	1746	U	O3'-P	-11.88	1.46	1.61
48	A2	200	U	O3'-P	-11.86	1.47	1.61
48	A2	160	A	O3'-P	-11.86	1.47	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	B1	35	C	O3'-P	-11.86	1.47	1.61
48	A2	3859	G	O3'-P	-11.85	1.47	1.61
49	B1	502	C	O3'-P	-11.84	1.47	1.61
48	A2	1357	G	O3'-P	-11.84	1.47	1.61
48	A2	1530	G	O3'-P	-11.83	1.47	1.61
48	A2	2869	C	O3'-P	-11.83	1.47	1.61
49	B1	454	U	O3'-P	-11.82	1.47	1.61
48	A2	1872	A	O3'-P	-11.81	1.47	1.61
48	A2	2292	A	O3'-P	-11.81	1.47	1.61
49	B1	930	C	O3'-P	-11.79	1.47	1.61
48	A2	1271	G	O3'-P	-11.78	1.47	1.61
48	A2	2570	A	O3'-P	-11.72	1.47	1.61
49	B1	405	G	O3'-P	-11.71	1.47	1.61
49	B1	933	G	O3'-P	-11.71	1.47	1.61
49	B1	976	G	O3'-P	-11.64	1.47	1.61
48	A2	2280	G	O3'-P	-11.62	1.47	1.61
49	B1	21	U	O3'-P	-11.61	1.47	1.61
48	A2	19	G	O3'-P	-11.61	1.47	1.61
48	A2	2876	G	O3'-P	-11.58	1.47	1.61
48	A2	703	C	O3'-P	-11.58	1.47	1.61
48	A2	4704	G	O3'-P	-11.55	1.47	1.61
49	B1	1194	A	O3'-P	-11.54	1.47	1.61
49	B1	1806	A	O3'-P	-11.54	1.47	1.61
48	A2	2501	G	O3'-P	-11.51	1.47	1.61
48	A2	716	G	O3'-P	-11.51	1.47	1.61
49	B1	112	U	O3'-P	11.49	1.75	1.61
49	B1	298	G	O3'-P	-11.48	1.47	1.61
48	A2	718	C	O3'-P	-11.47	1.47	1.61
48	A2	2503	U	O3'-P	-11.47	1.47	1.61
1	A3	118	C	O3'-P	-11.46	1.47	1.61
48	A2	421	A	O3'-P	-11.45	1.47	1.61
49	B1	1460	C	O3'-P	-11.44	1.47	1.61
2	A4	106	G	O3'-P	-11.41	1.47	1.61
48	A2	190	G	O3'-P	11.37	1.74	1.61
48	A2	68	U	O3'-P	-11.36	1.47	1.61
49	B1	1395	C	O3'-P	-11.35	1.47	1.61
49	B1	33	G	O3'-P	-11.35	1.47	1.61
48	A2	961	C	O3'-P	-11.32	1.47	1.61
48	A2	2818	U	O3'-P	-11.31	1.47	1.61
48	A2	1488	G	O3'-P	-11.30	1.47	1.61
48	A2	2603	G	O3'-P	-11.28	1.47	1.61
48	A2	226	G	O3'-P	-11.24	1.47	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	B1	1676	U	O3'-P	-11.23	1.47	1.61
49	B1	1855	G	O3'-P	-11.23	1.47	1.61
48	A2	4160	G	O3'-P	-11.22	1.47	1.61
49	B1	361	U	O3'-P	11.22	1.74	1.61
48	A2	2521	G	O3'-P	-11.21	1.47	1.61
1	A3	141	C	O3'-P	-11.18	1.47	1.61
48	A2	2327	G	O3'-P	-11.18	1.47	1.61
48	A2	2458	G	O3'-P	-11.18	1.47	1.61
48	A2	4913	A	O3'-P	-11.16	1.47	1.61
48	A2	3667	C	O3'-P	-11.15	1.47	1.61
48	A2	4602	C	O3'-P	-11.13	1.47	1.61
48	A2	92	C	O3'-P	-11.12	1.47	1.61
48	A2	3617	A	O3'-P	-11.11	1.47	1.61
49	B1	1744	G	O3'-P	-11.10	1.47	1.61
49	B1	660	C	O3'-P	-11.09	1.47	1.61
48	A2	1359	C	O3'-P	-11.06	1.47	1.61
48	A2	204	G	O3'-P	-11.06	1.47	1.61
48	A2	1218	G	O3'-P	-11.05	1.47	1.61
48	A2	1193	C	O3'-P	-11.03	1.48	1.61
49	B1	350	C	O3'-P	-11.03	1.48	1.61
48	A2	49	U	O3'-P	-11.01	1.48	1.61
48	A2	4605	G	O3'-P	-11.01	1.48	1.61
48	A2	296	C	O3'-P	-11.00	1.48	1.61
48	A2	4012	G	O3'-P	-10.99	1.48	1.61
48	A2	1070	A	O3'-P	-10.98	1.48	1.61
49	B1	416	U	O3'-P	-10.98	1.48	1.61
48	A2	2704	A	O3'-P	-10.89	1.48	1.61
48	A2	207	C	O3'-P	-10.88	1.48	1.61
48	A2	4483	U	O3'-P	-10.82	1.48	1.61
48	A2	431	G	O3'-P	-10.78	1.48	1.61
1	A3	67	U	O3'-P	-10.77	1.48	1.61
48	A2	308	G	O3'-P	-10.76	1.48	1.61
48	A2	2786	A	O3'-P	-10.76	1.48	1.61
48	A2	4617	A	O3'-P	-10.76	1.48	1.61
49	B1	1453	C	O3'-P	-10.75	1.48	1.61
48	A2	2753	C	O3'-P	-10.72	1.48	1.61
48	A2	1851	C	O3'-P	-10.71	1.48	1.61
48	A2	90	G	O3'-P	-10.71	1.48	1.61
2	A4	40	U	O3'-P	-10.70	1.48	1.61
48	A2	2569	G	O3'-P	-10.66	1.48	1.61
45	Aq	46	ILE	CB-CG2	-10.65	1.19	1.52
48	A2	3740	C	O3'-P	-10.65	1.48	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	A2	286	G	O3'-P	-10.63	1.48	1.61
48	A2	916	A	O3'-P	10.63	1.74	1.61
49	B1	1123	C	O3'-P	-10.63	1.48	1.61
49	B1	450	C	O3'-P	-10.63	1.48	1.61
48	A2	1616	A	O3'-P	-10.61	1.48	1.61
48	A2	3836	A	O3'-P	-10.58	1.48	1.61
48	A2	4306	U	O3'-P	-10.55	1.48	1.61
48	A2	2269	C	O3'-P	-10.54	1.48	1.61
2	A4	33	U	O3'-P	-10.51	1.48	1.61
48	A2	2694	G	O3'-P	-10.51	1.48	1.61
48	A2	2422	G	O3'-P	-10.50	1.48	1.61
48	A2	1245	G	O3'-P	-10.49	1.48	1.61
48	A2	3818	C	O3'-P	-10.49	1.48	1.61
49	B1	20	G	O3'-P	-10.48	1.48	1.61
49	B1	1276	A	O3'-P	-10.48	1.48	1.61
1	A3	136	U	O3'-P	-10.46	1.48	1.61
48	A2	22	G	O3'-P	-10.45	1.48	1.61
1	A3	25	G	O3'-P	-10.45	1.48	1.61
49	B1	84	A	O3'-P	-10.44	1.48	1.61
48	A2	2841	G	O3'-P	-10.42	1.48	1.61
48	A2	405	G	O3'-P	-10.40	1.48	1.61
48	A2	3623	A	O3'-P	-10.36	1.48	1.61
48	A2	3662	G	O3'-P	-10.35	1.48	1.61
48	A2	2599	G	O3'-P	-10.34	1.48	1.61
49	B1	604	A	O3'-P	-10.34	1.48	1.61
48	A2	1846	G	O3'-P	-10.32	1.48	1.61
2	A4	5	A	O3'-P	-10.28	1.48	1.61
49	B1	106	C	O3'-P	-10.28	1.48	1.61
49	B1	597	G	O3'-P	-10.25	1.48	1.61
49	B1	147	A	O3'-P	-10.24	1.48	1.61
48	A2	2435	G	O3'-P	-10.22	1.48	1.61
48	A2	3687	C	O3'-P	-10.22	1.48	1.61
83	Bw	1	G	OP3-P	-10.21	1.49	1.61
48	A2	1631	U	O3'-P	-10.20	1.49	1.61
49	B1	1742	C	O3'-P	-10.20	1.49	1.61
48	A2	2328	A	O3'-P	-10.18	1.49	1.61
83	Bv	1	G	OP3-P	-10.18	1.49	1.61
1	A3	113	C	O3'-P	-10.17	1.49	1.61
84	Bx	34	U	OP3-P	-10.17	1.49	1.61
49	B1	1561	A	O3'-P	-10.16	1.49	1.61
48	A2	2472	G	O3'-P	-10.15	1.49	1.61
48	A2	356	A	O3'-P	-10.13	1.49	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	B1	219	U	O3'-P	-10.11	1.49	1.61
48	A2	4587	C	O3'-P	-10.10	1.49	1.61
48	A2	3834	C	O3'-P	-10.10	1.49	1.61
48	A2	2783	C	O3'-P	-10.07	1.49	1.61
48	A2	4618	A	O3'-P	-10.01	1.49	1.61
1	A3	3	A	O3'-P	-9.98	1.49	1.61
49	B1	1789	G	O3'-P	-9.98	1.49	1.61
48	A2	4125	U	O3'-P	-9.98	1.49	1.61
48	A2	1572	C	O3'-P	-9.97	1.49	1.61
48	A2	3808	C	O3'-P	-9.96	1.49	1.61
48	A2	1198	C	O3'-P	-9.96	1.49	1.61
48	A2	2758	C	O3'-P	-9.96	1.49	1.61
48	A2	153	G	O3'-P	-9.96	1.49	1.61
2	A4	34	C	O3'-P	9.92	1.73	1.61
48	A2	4924	A	O3'-P	-9.91	1.49	1.61
49	B1	425	G	O3'-P	-9.90	1.49	1.61
49	B1	864	A	O3'-P	-9.86	1.49	1.61
48	A2	432	G	O3'-P	-9.84	1.49	1.61
48	A2	1313	A	O3'-P	-9.84	1.49	1.61
48	A2	656	C	O3'-P	-9.84	1.49	1.61
2	A4	90	A	O3'-P	-9.81	1.49	1.61
49	B1	1643	U	O3'-P	-9.80	1.49	1.61
48	A2	2527	C	O3'-P	-9.80	1.49	1.61
48	A2	4835	G	O3'-P	-9.80	1.49	1.61
48	A2	4041	U	O3'-P	-9.79	1.49	1.61
49	B1	1491	G	O3'-P	-9.79	1.49	1.61
49	B1	1219	C	O3'-P	-9.73	1.49	1.61
48	A2	3738	C	O3'-P	-9.71	1.49	1.61
49	B1	448	A	O3'-P	9.71	1.72	1.61
49	B1	1024	A	O3'-P	-9.70	1.49	1.61
48	A2	3663	A	O3'-P	-9.68	1.49	1.61
48	A2	1612	A	O3'-P	-9.66	1.49	1.61
48	A2	378	A	O3'-P	-9.62	1.49	1.61
48	A2	4590	U	O3'-P	-9.61	1.49	1.61
49	B1	1727	G	O3'-P	-9.60	1.49	1.61
49	B1	1107	G	O3'-P	-9.59	1.49	1.61
48	A2	4060	G	O3'-P	-9.59	1.49	1.61
48	A2	2611	U	O3'-P	-9.58	1.49	1.61
49	B1	689	U	O3'-P	-9.57	1.49	1.61
48	A2	4720	U	O3'-P	-9.56	1.49	1.61
48	A2	4723	G	O3'-P	-9.54	1.49	1.61
49	B1	1306	U	O3'-P	-9.52	1.49	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	A2	4308	U	O3'-P	-9.49	1.49	1.61
48	A2	2302	C	O3'-P	-9.48	1.49	1.61
48	A2	440	C	O3'-P	-9.47	1.49	1.61
2	A4	63	C	O3'-P	-9.46	1.49	1.61
48	A2	1071	C	O3'-P	-9.43	1.49	1.61
48	A2	2746	U	O3'-P	-9.40	1.49	1.61
48	A2	4413	G	O3'-P	-9.38	1.49	1.61
48	A2	1803	G	O3'-P	-9.38	1.49	1.61
1	A3	129	C	O3'-P	-9.37	1.50	1.61
1	A3	23	C	O3'-P	-9.37	1.50	1.61
48	A2	2747	C	O3'-P	-9.37	1.50	1.61
48	A2	2454	G	O3'-P	-9.36	1.50	1.61
49	B1	680	G	O3'-P	-9.35	1.50	1.61
48	A2	1588	U	O3'-P	-9.33	1.50	1.61
49	B1	1856	C	O3'-P	-9.32	1.50	1.61
48	A2	2245	C	O3'-P	-9.31	1.50	1.61
48	A2	4985	C	O3'-P	-9.29	1.50	1.61
48	A2	504	U	O3'-P	-9.27	1.50	1.61
48	A2	466	C	O3'-P	-9.25	1.50	1.61
49	B1	94	G	O3'-P	-9.23	1.50	1.61
48	A2	4828	G	O3'-P	-9.22	1.50	1.61
48	A2	4318	G	O3'-P	-9.21	1.50	1.61
49	B1	817	G	O3'-P	-9.20	1.50	1.61
48	A2	4124	C	O3'-P	-9.20	1.50	1.61
48	A2	2877	G	O3'-P	-9.19	1.50	1.61
48	A2	433	G	O3'-P	-9.18	1.50	1.61
48	A2	929	G	O3'-P	-9.18	1.50	1.61
48	A2	3660	G	O3'-P	-9.18	1.50	1.61
49	B1	1015	U	O3'-P	-9.16	1.50	1.61
48	A2	2872	U	O3'-P	-9.16	1.50	1.61
49	B1	1476	A	O3'-P	-9.14	1.50	1.61
48	A2	4601	G	O3'-P	-9.14	1.50	1.61
48	A2	3718	A	O3'-P	-9.13	1.50	1.61
49	B1	369	C	O3'-P	-9.09	1.50	1.61
48	A2	2523	G	O3'-P	-9.07	1.50	1.61
48	A2	278	G	O3'-P	-9.07	1.50	1.61
1	A3	119	C	O3'-P	-9.07	1.50	1.61
48	A2	2701	G	O3'-P	-9.06	1.50	1.61
48	A2	959	C	P-O5'	-9.05	1.50	1.59
48	A2	3816	A	O3'-P	-9.04	1.50	1.61
48	A2	1736	U	O3'-P	-9.03	1.50	1.61
48	A2	4523	C	O3'-P	-9.02	1.50	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	B1	1047	C	O3'-P	-9.02	1.50	1.61
48	A2	4056	G	O3'-P	-9.02	1.50	1.61
48	A2	892	C	O3'-P	-9.00	1.50	1.61
48	A2	650	C	O3'-P	-8.99	1.50	1.61
48	A2	20	U	O3'-P	-8.99	1.50	1.61
48	A2	4360	C	O3'-P	-8.99	1.50	1.61
48	A2	4162	G	O3'-P	8.98	1.72	1.61
48	A2	4728	C	O3'-P	-8.96	1.50	1.61
48	A2	1368	G	O3'-P	-8.96	1.50	1.61
2	A4	67	C	O3'-P	-8.95	1.50	1.61
48	A2	4406	C	O3'-P	8.94	1.71	1.61
48	A2	4459	U	O3'-P	-8.93	1.50	1.61
49	B1	953	C	O3'-P	-8.91	1.50	1.61
48	A2	4993	U	O3'-P	-8.90	1.50	1.61
48	A2	1314	C	O3'-P	-8.90	1.50	1.61
48	A2	2059	C	O3'-P	-8.90	1.50	1.61
48	A2	3570	A	O3'-P	-8.89	1.50	1.61
48	A2	1987	U	O3'-P	-8.89	1.50	1.61
48	A2	4840	U	O3'-P	-8.88	1.50	1.61
48	A2	1586	G	O3'-P	-8.87	1.50	1.61
49	B1	946	U	O3'-P	-8.87	1.50	1.61
49	B1	1334	G	O3'-P	-8.87	1.50	1.61
48	A2	483	C	O3'-P	-8.84	1.50	1.61
48	A2	216	G	O3'-P	-8.84	1.50	1.61
48	A2	3728	G	O3'-P	-8.84	1.50	1.61
48	A2	4959	U	O3'-P	-8.82	1.50	1.61
49	B1	307	G	O3'-P	-8.82	1.50	1.61
49	B1	1388	A	O3'-P	-8.80	1.50	1.61
49	B1	1645	C	O3'-P	-8.80	1.50	1.61
48	A2	4010	C	O3'-P	-8.79	1.50	1.61
49	B1	1667	U	O3'-P	-8.78	1.50	1.61
48	A2	1788	G	O3'-P	-8.78	1.50	1.61
48	A2	1983	A	O3'-P	-8.74	1.50	1.61
48	A2	2671	U	O3'-P	-8.74	1.50	1.61
49	B1	847	A	O3'-P	-8.73	1.50	1.61
48	A2	3670	C	O3'-P	-8.73	1.50	1.61
48	A2	4456	G	O3'-P	-8.71	1.50	1.61
49	B1	979	C	O3'-P	-8.70	1.50	1.61
48	A2	60	A	O3'-P	-8.70	1.50	1.61
49	B1	295	C	O3'-P	-8.69	1.50	1.61
49	B1	663	C	O3'-P	-8.68	1.50	1.61
49	B1	1644	C	O3'-P	-8.68	1.50	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	A2	1569	G	O3'-P	-8.66	1.50	1.61
49	B1	410	G	O3'-P	-8.63	1.50	1.61
49	B1	844	U	O3'-P	-8.63	1.50	1.61
49	B1	639	C	O3'-P	-8.63	1.50	1.61
49	B1	174	C	O3'-P	-8.62	1.50	1.61
49	B1	1340	U	O3'-P	-8.62	1.50	1.61
49	B1	1729	U	O3'-P	-8.61	1.50	1.61
48	A2	910	C	O3'-P	-8.60	1.50	1.61
49	B1	1224	G	O3'-P	-8.60	1.50	1.61
48	A2	220	G	O3'-P	-8.58	1.50	1.61
49	B1	1868	U	O3'-P	8.57	1.71	1.61
48	A2	1199	C	O3'-P	8.56	1.71	1.61
48	A2	4052	G	O3'-P	-8.55	1.50	1.61
2	A4	55	A	O3'-P	-8.55	1.50	1.61
48	A2	4039	U	O3'-P	-8.54	1.50	1.61
48	A2	4994	C	O3'-P	-8.54	1.50	1.61
49	B1	803	C	O3'-P	-8.52	1.50	1.61
49	B1	940	U	O3'-P	-8.51	1.50	1.61
48	A2	4663	A	O3'-P	8.50	1.71	1.61
49	B1	1445	U	O3'-P	-8.50	1.50	1.61
48	A2	1296	C	O3'-P	-8.50	1.50	1.61
48	A2	3685	G	O3'-P	8.49	1.71	1.61
48	A2	4594	U	O3'-P	-8.48	1.50	1.61
48	A2	1731	A	O3'-P	-8.47	1.50	1.61
48	A2	2433	U	O3'-P	-8.47	1.50	1.61
48	A2	1879	C	O3'-P	-8.46	1.51	1.61
49	B1	918	U	O3'-P	8.45	1.71	1.61
48	A2	1191	G	O3'-P	-8.45	1.51	1.61
48	A2	1340	C	O3'-P	-8.44	1.51	1.61
48	A2	1725	A	O3'-P	-8.44	1.51	1.61
48	A2	4327	C	O3'-P	-8.42	1.51	1.61
48	A2	125	C	O3'-P	8.42	1.71	1.61
48	A2	1319	G	O3'-P	8.39	1.71	1.61
49	B1	804	U	O3'-P	-8.38	1.51	1.61
48	A2	2733	G	O3'-P	-8.37	1.51	1.61
48	A2	1464	G	O3'-P	-8.37	1.51	1.61
48	A2	1727	G	O3'-P	-8.37	1.51	1.61
48	A2	1714	C	O3'-P	-8.36	1.51	1.61
48	A2	2728	C	O3'-P	-8.35	1.51	1.61
49	B1	148	U	O3'-P	-8.34	1.51	1.61
48	A2	3587	U	O3'-P	-8.34	1.51	1.61
48	A2	4890	U	O3'-P	-8.30	1.51	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	B1	1310	U	O3'-P	-8.30	1.51	1.61
48	A2	1613	A	O3'-P	-8.29	1.51	1.61
49	B1	974	C	O3'-P	-8.29	1.51	1.61
48	A2	1957	G	O3'-P	-8.28	1.51	1.61
48	A2	4660	C	O3'-P	-8.27	1.51	1.61
48	A2	1348	C	O3'-P	-8.27	1.51	1.61
1	A3	24	G	O3'-P	-8.26	1.51	1.61
48	A2	917	G	O3'-P	8.24	1.71	1.61
48	A2	1490	A	O3'-P	-8.24	1.51	1.61
1	A3	127	U	O3'-P	8.21	1.71	1.61
48	A2	1972	A	O3'-P	-8.19	1.51	1.61
48	A2	4603	U	O3'-P	-8.18	1.51	1.61
48	A2	3917	G	O3'-P	-8.18	1.51	1.61
49	B1	1248	U	O3'-P	-8.17	1.51	1.61
48	A2	14	C	O3'-P	-8.16	1.51	1.61
48	A2	2061	U	O3'-P	-8.14	1.51	1.61
49	B1	984	C	O3'-P	-8.14	1.51	1.61
49	B1	1304	U	O3'-P	-8.14	1.51	1.61
48	A2	4524	C	O3'-P	-8.13	1.51	1.61
48	A2	4319	G	O3'-P	-8.12	1.51	1.61
48	A2	2270	G	O3'-P	-8.11	1.51	1.61
49	B1	69	C	O3'-P	-8.10	1.51	1.61
48	A2	634	C	O3'-P	8.04	1.70	1.61
48	A2	643	A	O3'-P	-8.03	1.51	1.61
48	A2	2697	U	O3'-P	-8.03	1.51	1.61
48	A2	288	G	O3'-P	-8.03	1.51	1.61
48	A2	1974	C	O3'-P	8.02	1.70	1.61
49	B1	1254	C	O3'-P	-8.02	1.51	1.61
49	B1	1421	A	O3'-P	-8.01	1.51	1.61
2	A4	70	G	O3'-P	-8.00	1.51	1.61
49	B1	1462	U	O3'-P	-7.99	1.51	1.61
45	Aq	75	PRO	N-CD	7.99	1.59	1.47
1	A3	135	C	O3'-P	-7.99	1.51	1.61
48	A2	147	U	O3'-P	7.98	1.70	1.61
45	Aq	75	PRO	CG-CD	7.96	1.76	1.50
2	A4	105	C	O3'-P	-7.96	1.51	1.61
48	A2	348	U	O3'-P	-7.94	1.51	1.61
48	A2	726	G	O3'-P	-7.93	1.51	1.61
1	A3	2	G	O3'-P	-7.90	1.51	1.61
1	A3	93	C	O3'-P	-7.88	1.51	1.61
48	A2	930	A	O3'-P	-7.86	1.51	1.61
48	A2	1954	G	O3'-P	7.85	1.70	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	A2	1845	G	O3'-P	-7.85	1.51	1.61
48	A2	4827	U	C5'-C4'	-7.84	1.42	1.51
48	A2	205	A	O3'-P	-7.83	1.51	1.61
48	A2	110	C	O3'-P	-7.83	1.51	1.61
48	A2	3702	C	O3'-P	7.80	1.70	1.61
48	A2	2672	G	O3'-P	-7.79	1.51	1.61
48	A2	3611	U	O3'-P	-7.76	1.51	1.61
48	A2	3736	G	O3'-P	-7.76	1.51	1.61
48	A2	7	C	O3'-P	-7.75	1.51	1.61
48	A2	2702	U	O3'-P	-7.75	1.51	1.61
48	A2	3719	A	O3'-P	-7.75	1.51	1.61
49	B1	289	G	O3'-P	-7.75	1.51	1.61
48	A2	4094	C	O3'-P	-7.74	1.51	1.61
1	A3	72	A	O3'-P	-7.74	1.51	1.61
48	A2	1560	U	O3'-P	7.73	1.70	1.61
48	A2	2698	C	O3'-P	-7.73	1.51	1.61
48	A2	2759	C	O3'-P	-7.70	1.51	1.61
49	B1	119	U	O3'-P	-7.69	1.51	1.61
48	A2	2736	A	O3'-P	-7.68	1.51	1.61
48	A2	724	A	O3'-P	-7.68	1.51	1.61
49	B1	1642	U	O3'-P	-7.66	1.51	1.61
48	A2	1059	C	O3'-P	7.65	1.70	1.61
49	B1	86	C	O3'-P	-7.65	1.51	1.61
48	A2	5007	G	O3'-P	-7.64	1.51	1.61
48	A2	299	A	O3'-P	-7.63	1.51	1.61
48	A2	4825	G	O3'-P	-7.63	1.51	1.61
48	A2	1804	U	O3'-P	-7.63	1.51	1.61
49	B1	123	G	O3'-P	-7.63	1.51	1.61
48	A2	4173	C	O3'-P	-7.63	1.51	1.61
48	A2	4123	G	O3'-P	-7.62	1.52	1.61
48	A2	919	A	O3'-P	7.61	1.70	1.61
48	A2	2699	C	O3'-P	-7.61	1.52	1.61
49	B1	1726	G	O3'-P	-7.60	1.52	1.61
48	A2	4685	A	O3'-P	-7.59	1.52	1.61
48	A2	1574	G	O3'-P	-7.58	1.52	1.61
48	A2	4707	G	O3'-P	-7.58	1.52	1.61
48	A2	702	A	O3'-P	-7.58	1.52	1.61
48	A2	4837	C	O3'-P	-7.58	1.52	1.61
2	A4	112	U	O3'-P	7.58	1.70	1.61
48	A2	3669	G	O3'-P	-7.54	1.52	1.61
49	B1	849	A	O3'-P	-7.54	1.52	1.61
2	A4	48	G	O3'-P	-7.53	1.52	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	B1	367	U	O3'-P	-7.53	1.52	1.61
48	A2	1282	G	O3'-P	-7.53	1.52	1.61
49	B1	1044	G	O3'-P	-7.52	1.52	1.61
48	A2	1679	G	O3'-P	7.51	1.70	1.61
48	A2	2246	U	O3'-P	-7.50	1.52	1.61
48	A2	4311	C	O3'-P	-7.50	1.52	1.61
48	A2	4009	G	O3'-P	-7.50	1.52	1.61
48	A2	1333	C	O3'-P	-7.49	1.52	1.61
49	B1	447	A	O3'-P	-7.49	1.52	1.61
2	A4	44	C	O3'-P	-7.49	1.52	1.61
49	B1	1554	C	O3'-P	-7.48	1.52	1.61
2	A4	62	U	O3'-P	-7.47	1.52	1.61
48	A2	2489	G	O3'-P	-7.47	1.52	1.61
48	A2	406	G	O3'-P	-7.46	1.52	1.61
48	A2	2677	G	O3'-P	-7.44	1.52	1.61
48	A2	2329	U	O3'-P	-7.44	1.52	1.61
49	B1	346	C	O3'-P	-7.44	1.52	1.61
48	A2	50	C	O3'-P	-7.43	1.52	1.61
49	B1	1278	A	O3'-P	7.43	1.70	1.61
48	A2	182	C	O3'-P	-7.41	1.52	1.61
48	A2	2285	G	O3'-P	-7.41	1.52	1.61
49	B1	338	G	O3'-P	7.41	1.70	1.61
48	A2	2722	A	O3'-P	-7.40	1.52	1.61
48	A2	2824	A	O3'-P	-7.40	1.52	1.61
48	A2	921	C	O3'-P	7.38	1.70	1.61
48	A2	3615	U	O3'-P	-7.37	1.52	1.61
49	B1	977	C	O3'-P	-7.36	1.52	1.61
49	B1	176	U	O3'-P	-7.36	1.52	1.61
48	A2	2673	G	O3'-P	-7.36	1.52	1.61
49	B1	917	U	O3'-P	-7.36	1.52	1.61
48	A2	1467	C	O3'-P	-7.35	1.52	1.61
49	B1	1702	G	O3'-P	-7.35	1.52	1.61
48	A2	3613	A	C5'-C4'	-7.33	1.42	1.51
48	A2	4599	G	O3'-P	7.33	1.70	1.61
49	B1	446	G	O3'-P	-7.33	1.52	1.61
48	A2	2490	A	O3'-P	-7.33	1.52	1.61
48	A2	908	C	O3'-P	-7.31	1.52	1.61
48	A2	3934	A	O3'-P	-7.31	1.52	1.61
48	A2	4686	A	O3'-P	-7.31	1.52	1.61
13	AK	27	CYS	CB-SG	-7.30	1.69	1.82
49	B1	85	A	O3'-P	-7.29	1.52	1.61
48	A2	3688	A	O3'-P	-7.29	1.52	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	A2	1287	C	O3'-P	-7.29	1.52	1.61
1	A3	142	U	O3'-P	-7.28	1.52	1.61
48	A2	326	C	O3'-P	-7.26	1.52	1.61
48	A2	2526	G	O3'-P	-7.26	1.52	1.61
48	A2	3612	U	C3'-O3'	-7.26	1.31	1.42
49	B1	124	U	O3'-P	-7.25	1.52	1.61
48	A2	950	G	O3'-P	7.24	1.69	1.61
1	A3	12	G	O3'-P	-7.22	1.52	1.61
48	A2	3791	G	O3'-P	-7.22	1.52	1.61
48	A2	1299	G	O3'-P	-7.21	1.52	1.61
48	A2	4915	C	O3'-P	7.19	1.69	1.61
49	B1	1335	G	O3'-P	-7.19	1.52	1.61
49	B1	1681	U	O3'-P	-7.19	1.52	1.61
48	A2	3672	C	O3'-P	7.18	1.69	1.61
48	A2	21	G	O3'-P	7.17	1.69	1.61
48	A2	1331	U	O3'-P	-7.17	1.52	1.61
49	B1	407	G	O3'-P	-7.14	1.52	1.61
49	B1	1452	A	O3'-P	-7.14	1.52	1.61
49	B1	1584	G	O3'-P	-7.14	1.52	1.61
49	B1	1575	G	O3'-P	7.12	1.69	1.61
1	A3	116	C	O3'-P	-7.12	1.52	1.61
48	A2	1434	G	O3'-P	-7.11	1.52	1.61
48	A2	180	C	O3'-P	7.09	1.69	1.61
48	A2	1571	C	O3'-P	-7.09	1.52	1.61
48	A2	4713	G	O3'-P	-7.07	1.52	1.61
48	A2	497	C	O3'-P	-7.07	1.52	1.61
49	B1	749	U	C3'-O3'	-7.05	1.32	1.42
49	B1	369	C	P-O5'	-7.04	1.52	1.59
49	B1	1700	C	O3'-P	-7.02	1.52	1.61
83	Bv	33	U	O3'-P	-7.01	1.52	1.61
49	B1	1732	G	O3'-P	-7.00	1.52	1.61
48	A2	478	U	O3'-P	-7.00	1.52	1.61
49	B1	120	U	O3'-P	-6.99	1.52	1.61
48	A2	1416	A	O3'-P	6.98	1.69	1.61
48	A2	3801	A	O3'-P	6.97	1.69	1.61
49	B1	343	A	O3'-P	-6.97	1.52	1.61
48	A2	172	C	O3'-P	-6.96	1.52	1.61
48	A2	1764	U	O3'-P	-6.95	1.52	1.61
49	B1	1647	A	O3'-P	-6.95	1.52	1.61
49	B1	1417	C	O3'-P	6.94	1.69	1.61
48	A2	2313	C	O3'-P	-6.94	1.52	1.61
48	A2	4136	U	O3'-P	-6.94	1.52	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	B1	122	G	O3'-P	-6.93	1.52	1.61
48	A2	4984	U	O3'-P	-6.92	1.52	1.61
49	B1	1442	U	O3'-P	-6.91	1.52	1.61
1	A3	79	G	O3'-P	-6.91	1.52	1.61
1	A3	11	C	O3'-P	-6.90	1.52	1.61
48	A2	713	G	O3'-P	-6.90	1.52	1.61
48	A2	2690	G	P-O5'	-6.89	1.52	1.59
48	A2	1850	G	O3'-P	-6.89	1.52	1.61
49	B1	924	G	O3'-P	-6.88	1.52	1.61
48	A2	66	A	O3'-P	-6.88	1.52	1.61
2	A4	6	C	O3'-P	-6.88	1.52	1.61
48	A2	10	A	O3'-P	-6.88	1.52	1.61
48	A2	4407	U	O3'-P	-6.87	1.52	1.61
48	A2	680	C	O3'-P	-6.86	1.52	1.61
48	A2	2057	G	O3'-P	-6.84	1.52	1.61
48	A2	4648	G	O3'-P	-6.84	1.52	1.61
48	A2	307	U	O3'-P	-6.84	1.52	1.61
1	A3	110	U	O3'-P	-6.83	1.52	1.61
48	A2	150	G	O4'-C1'	6.83	1.50	1.41
49	B1	1581	C	O3'-P	-6.80	1.52	1.61
48	A2	2676	A	O3'-P	-6.80	1.52	1.61
48	A2	4097	A	O3'-P	-6.78	1.53	1.61
49	B1	1158	G	O3'-P	-6.78	1.53	1.61
48	A2	946	G	O3'-P	-6.75	1.53	1.61
48	A2	1944	C	O3'-P	-6.74	1.53	1.61
48	A2	1273	G	O3'-P	-6.74	1.53	1.61
48	A2	355	C	O3'-P	-6.73	1.53	1.61
48	A2	1765	C	O3'-P	-6.73	1.53	1.61
48	A2	2478	C	O3'-P	-6.70	1.53	1.61
48	A2	926	G	O3'-P	6.70	1.69	1.61
2	A4	61	G	O3'-P	-6.69	1.53	1.61
48	A2	1290	A	O3'-P	-6.69	1.53	1.61
49	B1	498	C	O3'-P	-6.69	1.53	1.61
48	A2	1270	G	O3'-P	-6.69	1.53	1.61
48	A2	1225	G	O3'-P	6.67	1.69	1.61
49	B1	1801	A	O3'-P	-6.65	1.53	1.61
48	A2	127	G	C1'-N9	-6.63	1.37	1.46
48	A2	1260	G	P-O5'	-6.62	1.53	1.59
48	A2	328	A	O3'-P	-6.61	1.53	1.61
49	B1	929	G	O3'-P	-6.59	1.53	1.61
48	A2	1365	G	O3'-P	-6.59	1.53	1.61
49	B1	1685	U	O3'-P	-6.59	1.53	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	A2	267	U	O3'-P	-6.57	1.53	1.61
48	A2	2427	G	O3'-P	-6.56	1.53	1.61
49	B1	674	C	O3'-P	-6.56	1.53	1.61
48	A2	2312	G	O3'-P	6.55	1.69	1.61
48	A2	3589	C	O3'-P	-6.55	1.53	1.61
48	A2	457	A	O3'-P	-6.55	1.53	1.61
48	A2	4033	U	O4'-C1'	6.54	1.50	1.41
48	A2	690	C	O3'-P	6.53	1.69	1.61
48	A2	1281	C	O3'-P	-6.52	1.53	1.61
48	A2	1800	G	O3'-P	6.52	1.69	1.61
48	A2	4463	U	O3'-P	-6.51	1.53	1.61
49	B1	985	G	O3'-P	-6.51	1.53	1.61
49	B1	863	U	O3'-P	-6.50	1.53	1.61
48	A2	1797	G	O3'-P	-6.50	1.53	1.61
48	A2	3838	A	O3'-P	6.50	1.69	1.61
48	A2	501	G	O4'-C1'	6.50	1.50	1.41
48	A2	4086	U	O3'-P	-6.50	1.53	1.61
48	A2	3731	A	O3'-P	-6.48	1.53	1.61
49	B1	363	A	O3'-P	6.48	1.69	1.61
1	A3	38	U	O3'-P	-6.46	1.53	1.61
48	A2	2700	G	O3'-P	-6.46	1.53	1.61
48	A2	3678	U	O3'-P	-6.46	1.53	1.61
49	B1	1222	G	O3'-P	-6.46	1.53	1.61
48	A2	4036	U	O3'-P	-6.45	1.53	1.61
48	A2	927	C	O4'-C1'	-6.45	1.33	1.41
48	A2	4156	U	O3'-P	-6.44	1.53	1.61
48	A2	509	C	O3'-P	6.43	1.68	1.61
48	A2	5005	C	O3'-P	-6.42	1.53	1.61
49	B1	218	U	O3'-P	-6.42	1.53	1.61
48	A2	309	G	O3'-P	-6.41	1.53	1.61
48	A2	4091	G	O3'-P	-6.41	1.53	1.61
48	A2	329	A	O3'-P	-6.41	1.53	1.61
48	A2	4175	A	O3'-P	-6.41	1.53	1.61
49	B1	837	A	O3'-P	6.40	1.68	1.61
48	A2	1732	G	O3'-P	-6.40	1.53	1.61
49	B1	345	U	O3'-P	-6.40	1.53	1.61
48	A2	2735	G	O3'-P	-6.40	1.53	1.61
48	A2	1796	C	O3'-P	-6.39	1.53	1.61
83	Bv	1	G	P-OP2	6.39	1.59	1.49
48	A2	1758	A	O3'-P	-6.38	1.53	1.61
84	Bx	34	U	P-OP2	6.38	1.59	1.49
49	B1	1807	C	O3'-P	-6.37	1.53	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	B1	403	G	O3'-P	-6.36	1.53	1.61
83	Bw	1	G	P-OP2	6.36	1.59	1.49
48	A2	1058	G	O3'-P	6.35	1.68	1.61
48	A2	4055	A	O3'-P	6.34	1.68	1.61
48	A2	922	A	O3'-P	-6.33	1.53	1.61
48	A2	4694	G	O3'-P	-6.33	1.53	1.61
49	B1	422	U	O3'-P	-6.33	1.53	1.61
48	A2	86	U	O3'-P	-6.33	1.53	1.61
49	B1	1396	A	O3'-P	-6.32	1.53	1.61
48	A2	4836	C	O3'-P	-6.31	1.53	1.61
48	A2	211	G	O3'-P	6.30	1.68	1.61
48	A2	5025	U	O3'-P	-6.30	1.53	1.61
2	A4	116	G	O3'-P	-6.29	1.53	1.61
48	A2	112	C	O3'-P	-6.29	1.53	1.61
48	A2	3840	C	O3'-P	-6.27	1.53	1.61
48	A2	1955	U	O3'-P	6.27	1.68	1.61
49	B1	451	G	O3'-P	-6.26	1.53	1.61
48	A2	721	G	O3'-P	-6.25	1.53	1.61
48	A2	2480	C	O3'-P	-6.22	1.53	1.61
48	A2	166	G	O3'-P	-6.21	1.53	1.61
48	A2	1065	C	O3'-P	-6.21	1.53	1.61
48	A2	3683	A	O3'-P	-6.21	1.53	1.61
48	A2	4722	G	O3'-P	-6.20	1.53	1.61
49	B1	5	U	O3'-P	6.20	1.68	1.61
49	B1	107	A	O3'-P	-6.19	1.53	1.61
48	A2	657	C	O3'-P	-6.19	1.53	1.61
49	B1	843	C	O3'-P	6.19	1.68	1.61
48	A2	438	G	O3'-P	-6.18	1.53	1.61
49	B1	30	C	O3'-P	-6.18	1.53	1.61
48	A2	4922	C	O3'-P	-6.17	1.53	1.61
48	A2	1260	G	O3'-P	6.17	1.68	1.61
48	A2	893	C	O3'-P	-6.17	1.53	1.61
49	B1	653	A	O3'-P	-6.16	1.53	1.61
48	A2	1248	G	O3'-P	6.16	1.68	1.61
2	A4	42	A	O3'-P	-6.15	1.53	1.61
48	A2	399	U	O3'-P	-6.14	1.53	1.61
48	A2	2322	G	O3'-P	-6.14	1.53	1.61
48	A2	1855	A	O3'-P	-6.14	1.53	1.61
48	A2	48	G	O3'-P	-6.13	1.53	1.61
48	A2	324	G	O3'-P	-6.13	1.53	1.61
48	A2	1433	C	O4'-C1'	6.13	1.49	1.41
49	B1	417	C	O3'-P	-6.13	1.53	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	B1	1103	C	O3'-P	-6.12	1.53	1.61
48	A2	2251	C	O3'-P	-6.11	1.53	1.61
48	A2	671	C	O3'-P	-6.11	1.53	1.61
49	B1	657	U	O3'-P	-6.11	1.53	1.61
48	A2	465	A	O3'-P	-6.10	1.53	1.61
48	A2	3627	A	O3'-P	-6.09	1.53	1.61
48	A2	1614	A	O3'-P	6.08	1.68	1.61
48	A2	300	A	O4'-C1'	-6.08	1.33	1.41
48	A2	320	C	O3'-P	-6.08	1.53	1.61
48	A2	4326	G	O3'-P	-6.08	1.53	1.61
48	A2	4140	A	O3'-P	-6.07	1.53	1.61
48	A2	4623	G	O3'-P	-6.07	1.53	1.61
49	B1	601	G	O3'-P	-6.06	1.53	1.61
48	A2	2836	A	O3'-P	-6.06	1.53	1.61
49	B1	947	G	O3'-P	-6.06	1.53	1.61
48	A2	219	C	O4'-C1'	6.06	1.49	1.41
48	A2	4095	C	O3'-P	-6.04	1.53	1.61
48	A2	104	G	O3'-P	-6.04	1.53	1.61
48	A2	4715	U	O3'-P	-6.04	1.53	1.61
48	A2	2682	G	O4'-C1'	6.04	1.49	1.41
48	A2	43	U	O3'-P	-6.03	1.53	1.61
48	A2	1219	C	O3'-P	-6.03	1.53	1.61
49	B1	1275	G	O3'-P	6.02	1.68	1.61
49	B1	1443	C	O3'-P	-6.01	1.53	1.61
48	A2	1194	G	O3'-P	6.01	1.68	1.61
48	A2	56	A	O3'-P	-6.00	1.53	1.61
48	A2	1916	C	O3'-P	-6.00	1.53	1.61
49	B1	24	C	O3'-P	6.00	1.68	1.61
48	A2	1498	G	O3'-P	-5.99	1.53	1.61
1	A3	33	G	O3'-P	-5.98	1.53	1.61
48	A2	894	C	O3'-P	-5.98	1.53	1.61
49	B1	1223	A	O4'-C1'	5.98	1.49	1.41
48	A2	1294	G	O3'-P	-5.97	1.53	1.61
48	A2	4841	C	O3'-P	-5.97	1.53	1.61
48	A2	1306	A	O3'-P	-5.97	1.53	1.61
49	B1	1049	A	O3'-P	-5.96	1.53	1.61
48	A2	2873	A	O3'-P	-5.95	1.54	1.61
48	A2	57	G	O3'-P	-5.94	1.54	1.61
48	A2	689	G	O3'-P	5.94	1.68	1.61
48	A2	4414	U	O3'-P	-5.93	1.54	1.61
48	A2	3787	A	O3'-P	-5.93	1.54	1.61
49	B1	430	C	O3'-P	-5.92	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	B1	1007	C	O3'-P	-5.92	1.54	1.61
1	A3	152	U	O3'-P	-5.92	1.54	1.61
48	A2	1950	G	O3'-P	5.92	1.68	1.61
48	A2	310	U	O3'-P	-5.90	1.54	1.61
49	B1	29	G	O3'-P	-5.89	1.54	1.61
49	B1	848	U	O3'-P	-5.86	1.54	1.61
48	A2	909	C	O3'-P	-5.84	1.54	1.61
48	A2	475	G	O3'-P	-5.83	1.54	1.61
48	A2	5004	U	O3'-P	-5.83	1.54	1.61
48	A2	287	G	C3'-O3'	-5.83	1.33	1.42
48	A2	4157	G	O3'-P	-5.83	1.54	1.61
48	A2	3837	C	O3'-P	-5.83	1.54	1.61
49	B1	209	A	O3'-P	5.83	1.68	1.61
1	A3	117	C	O3'-P	-5.82	1.54	1.61
49	B1	178	C	O3'-P	-5.82	1.54	1.61
48	A2	62	A	O3'-P	-5.81	1.54	1.61
48	A2	2600	A	O3'-P	-5.80	1.54	1.61
13	AK	25	PRO	N-CD	5.80	1.55	1.47
48	A2	3628	U	O3'-P	-5.80	1.54	1.61
48	A2	256	C	O3'-P	5.79	1.68	1.61
48	A2	1187	C	O3'-P	-5.79	1.54	1.61
48	A2	131	C	O3'-P	5.79	1.68	1.61
48	A2	4827	U	O3'-P	5.79	1.68	1.61
48	A2	1798	C	O3'-P	-5.77	1.54	1.61
48	A2	895	G	O3'-P	-5.77	1.54	1.61
49	B1	395	G	O3'-P	5.76	1.68	1.61
48	A2	1968	C	O3'-P	5.76	1.68	1.61
49	B1	1176	G	O3'-P	-5.76	1.54	1.61
48	A2	155	A	O3'-P	-5.75	1.54	1.61
1	A3	34	U	O3'-P	5.74	1.68	1.61
48	A2	1202	G	O4'-C1'	5.74	1.49	1.41
48	A2	4134	A	O3'-P	-5.74	1.54	1.61
48	A2	1497	A	O3'-P	-5.74	1.54	1.61
48	A2	658	G	O3'-P	-5.72	1.54	1.61
48	A2	437	G	O3'-P	-5.71	1.54	1.61
48	A2	3723	C	O3'-P	5.70	1.68	1.61
48	A2	2871	C	O3'-P	-5.70	1.54	1.61
49	B1	620	G	O3'-P	-5.70	1.54	1.61
48	A2	2332	U	O3'-P	-5.70	1.54	1.61
49	B1	1419	C	O3'-P	-5.69	1.54	1.61
48	A2	215	A	O3'-P	-5.69	1.54	1.61
48	A2	2424	C	O3'-P	-5.69	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	B1	303	C	O3'-P	-5.68	1.54	1.61
83	Bv	34	G	O3'-P	-5.68	1.54	1.61
49	B1	460	A	O3'-P	-5.68	1.54	1.61
48	A2	1428	U	O3'-P	-5.66	1.54	1.61
48	A2	2311	A	O3'-P	-5.65	1.54	1.61
1	A3	106	G	O3'-P	-5.65	1.54	1.61
48	A2	918	C	O3'-P	5.64	1.68	1.61
48	A2	4995	U	O3'-P	-5.63	1.54	1.61
48	A2	4409	C	O3'-P	-5.63	1.54	1.61
48	A2	1778	U	O3'-P	-5.63	1.54	1.61
48	A2	4172	U	O3'-P	-5.63	1.54	1.61
49	B1	1422	G	O3'-P	-5.62	1.54	1.61
25	AW	98	PRO	N-CD	5.61	1.55	1.47
49	B1	1740	C	O3'-P	-5.61	1.54	1.61
49	B1	1804	U	O3'-P	5.60	1.67	1.61
48	A2	4708	C	O3'-P	5.60	1.67	1.61
49	B1	872	A	O3'-P	-5.59	1.54	1.61
48	A2	357	A	O3'-P	-5.57	1.54	1.61
48	A2	332	A	O3'-P	-5.56	1.54	1.61
48	A2	949	C	O3'-P	5.56	1.67	1.61
48	A2	131	C	C3'-O3'	-5.55	1.34	1.42
48	A2	4727	G	O3'-P	-5.54	1.54	1.61
48	A2	142	G	O3'-P	5.54	1.67	1.61
48	A2	2325	C	O3'-P	-5.54	1.54	1.61
49	B1	954	U	O3'-P	-5.54	1.54	1.61
48	A2	41	C	O3'-P	-5.53	1.54	1.61
48	A2	257	G	O3'-P	-5.53	1.54	1.61
49	B1	449	A	O3'-P	-5.52	1.54	1.61
2	A4	95	C	O3'-P	-5.51	1.54	1.61
48	A2	6	C	O3'-P	-5.51	1.54	1.61
48	A2	4021	C	O3'-P	-5.51	1.54	1.61
48	A2	2058	C	O3'-P	5.49	1.67	1.61
48	A2	2785	A	O3'-P	-5.48	1.54	1.61
48	A2	1863	U	O3'-P	-5.47	1.54	1.61
48	A2	1437	G	O3'-P	-5.47	1.54	1.61
49	B1	1803	U	O3'-P	-5.47	1.54	1.61
48	A2	2695	C	O3'-P	-5.46	1.54	1.61
49	B1	690	G	O5'-C5'	5.46	1.53	1.44
49	B1	1446	A	O3'-P	-5.43	1.54	1.61
49	B1	1285	G	C5'-C4'	-5.43	1.44	1.51
48	A2	2875	G	O3'-P	-5.42	1.54	1.61
49	B1	344	U	O3'-P	-5.41	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	BS	74	PRO	N-CD	5.41	1.55	1.47
48	A2	4158	G	O3'-P	-5.41	1.54	1.61
49	B1	745	C	O3'-P	-5.41	1.54	1.61
49	B1	628	A	O3'-P	5.40	1.67	1.61
49	B1	1485	U	O3'-P	-5.39	1.54	1.61
48	A2	302	G	O3'-P	-5.39	1.54	1.61
48	A2	734	G	O3'-P	-5.38	1.54	1.61
48	A2	640	G	O4'-C1'	5.38	1.48	1.41
49	B1	1560	U	O3'-P	-5.38	1.54	1.61
38	Aj	84	PRO	N-CD	5.38	1.55	1.47
48	A2	4410	G	O3'-P	-5.37	1.54	1.61
49	B1	620	G	O4'-C1'	5.37	1.48	1.41
54	BE	83	PRO	N-CD	5.37	1.55	1.47
2	A4	54	A	O3'-P	-5.37	1.54	1.61
48	A2	4684	G	O4'-C1'	5.36	1.48	1.41
2	A4	25	G	O3'-P	-5.35	1.54	1.61
48	A2	4663	A	O4'-C1'	5.35	1.48	1.41
48	A2	951	A	O3'-P	-5.35	1.54	1.61
48	A2	1291	C	O3'-P	-5.34	1.54	1.61
49	B1	1415	C	O3'-P	-5.34	1.54	1.61
48	A2	1201	G	O4'-C1'	5.34	1.48	1.41
53	BD	80	PRO	N-CD	5.33	1.55	1.47
48	A2	681	A	O3'-P	-5.33	1.54	1.61
48	A2	4586	A	O4'-C1'	5.33	1.48	1.41
48	A2	297	C	O3'-P	-5.33	1.54	1.61
2	A4	117	G	O4'-C1'	5.33	1.48	1.41
48	A2	1774	U	O3'-P	-5.33	1.54	1.61
49	B1	1441	U	O3'-P	-5.32	1.54	1.61
49	B1	145	G	O3'-P	-5.32	1.54	1.61
49	B1	1223	A	O3'-P	5.32	1.67	1.61
50	BA	105	PRO	N-CD	5.31	1.55	1.47
48	A2	1226	C	C5'-C4'	5.31	1.57	1.51
48	A2	1644	C	O4'-C1'	5.31	1.48	1.41
48	A2	3835	C	O3'-P	-5.31	1.54	1.61
14	AL	131	PRO	N-CD	5.30	1.55	1.47
48	A2	4910	G	O3'-P	-5.29	1.54	1.61
48	A2	212	C	O4'-C1'	5.29	1.48	1.41
48	A2	3597	G	O3'-P	-5.29	1.54	1.61
49	B1	87	U	O4'-C1'	5.28	1.48	1.41
48	A2	64	A	O3'-P	-5.28	1.54	1.61
48	A2	379	A	O3'-P	5.27	1.67	1.61
48	A2	2756	G	O3'-P	-5.27	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	A2	4310	A	O3'-P	5.26	1.67	1.61
48	A2	1336	G	O3'-P	5.26	1.67	1.61
48	A2	376	G	O4'-C1'	5.25	1.48	1.41
48	A2	476	G	O3'-P	-5.25	1.54	1.61
48	A2	1590	G	O3'-P	-5.25	1.54	1.61
49	B1	1155	U	O3'-P	-5.24	1.54	1.61
49	B1	1317	C	O3'-P	-5.24	1.54	1.61
61	BL	14	PRO	N-CD	5.24	1.55	1.47
14	AL	134	PRO	N-CD	5.23	1.55	1.47
49	B1	144	U	O3'-P	-5.23	1.54	1.61
48	A2	219	C	O3'-P	-5.23	1.54	1.61
48	A2	2754	C	O3'-P	5.22	1.67	1.61
49	B1	299	A	O3'-P	-5.22	1.54	1.61
19	AQ	73	PRO	N-CD	5.22	1.55	1.47
48	A2	21	G	O4'-C1'	5.22	1.48	1.41
48	A2	4977	A	O4'-C1'	5.22	1.48	1.41
49	B1	631	U	O3'-P	-5.21	1.54	1.61
48	A2	252	C	O3'-P	5.21	1.67	1.61
2	A4	36	C	O3'-P	-5.21	1.54	1.61
48	A2	2513	C	O3'-P	-5.20	1.54	1.61
63	BN	82	PRO	N-CD	5.20	1.55	1.47
48	A2	1848	A	O3'-P	-5.20	1.54	1.61
49	B1	1753	C	O3'-P	-5.20	1.54	1.61
21	AS	140	PRO	N-CD	5.19	1.55	1.47
48	A2	2689	C	C3'-O3'	-5.19	1.34	1.42
48	A2	4526	A	O3'-P	-5.19	1.54	1.61
48	A2	4600	U	O3'-P	-5.19	1.54	1.61
49	B1	915	G	C5'-C4'	5.18	1.57	1.51
2	A4	115	A	O3'-P	5.18	1.67	1.61
48	A2	2504	U	O3'-P	5.18	1.67	1.61
49	B1	627	U	O3'-P	-5.18	1.54	1.61
49	B1	690	G	C5'-C4'	5.18	1.57	1.51
48	A2	4467	C	O3'-P	-5.18	1.54	1.61
48	A2	1919	C	O3'-P	-5.18	1.54	1.61
49	B1	356	C	O3'-P	-5.17	1.54	1.61
49	B1	688	U	O3'-P	-5.17	1.54	1.61
49	B1	975	G	O3'-P	-5.17	1.54	1.61
48	A2	660	C	O3'-P	-5.17	1.54	1.61
73	BX	62	PRO	N-CD	5.17	1.55	1.47
2	A4	91	C	O3'-P	-5.17	1.54	1.61
48	A2	2553	G	O3'-P	-5.17	1.54	1.61
49	B1	1733	U	O3'-P	-5.17	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	A2	227	G	O3'-P	-5.16	1.54	1.61
48	A2	4516	G	O3'-P	5.16	1.67	1.61
48	A2	1960	A	O3'-P	5.16	1.67	1.61
48	A2	961	C	O5'-C5'	-5.15	1.34	1.42
48	A2	3684	U	O3'-P	-5.15	1.54	1.61
48	A2	2283	U	O3'-P	5.14	1.67	1.61
48	A2	3817	C	O4'-C1'	5.12	1.48	1.41
1	A3	144	U	O4'-C1'	5.11	1.48	1.41
48	A2	1761	U	O3'-P	-5.11	1.55	1.61
48	A2	3696	G	O3'-P	-5.11	1.55	1.61
2	A4	53	U	O3'-P	-5.11	1.55	1.61
48	A2	1958	C	O3'-P	-5.10	1.55	1.61
1	A3	153	C	O4'-C1'	5.10	1.48	1.41
48	A2	3613	A	O3'-P	-5.10	1.55	1.61
47	Au	121	PRO	N-CD	5.10	1.54	1.47
48	A2	2568	C	O4'-C1'	5.10	1.48	1.41
19	AQ	156	PRO	N-CD	5.09	1.54	1.47
67	BR	42	PRO	N-CD	5.09	1.54	1.47
67	BR	100	PRO	N-CD	5.09	1.54	1.47
48	A2	3697	A	O4'-C1'	-5.08	1.35	1.41
65	BP	68	PRO	N-CD	5.08	1.54	1.47
48	A2	3595	A	O3'-P	-5.08	1.55	1.61
49	B1	370	G	C3'-C2'	-5.08	1.47	1.52
5	AC	225	PRO	N-CD	5.07	1.54	1.47
48	A2	126	C	C1'-N1	5.07	1.56	1.48
48	A2	4726	A	O3'-P	-5.06	1.55	1.61
13	AK	80	PRO	N-CD	5.06	1.54	1.47
49	B1	458	A	O3'-P	-5.05	1.55	1.61
48	A2	712	G	O4'-C1'	5.05	1.48	1.41
48	A2	1954	G	O4'-C1'	5.05	1.48	1.41
48	A2	1468	C	O3'-P	-5.04	1.55	1.61
49	B1	92	A	O3'-P	5.04	1.67	1.61
48	A2	4842	G	O4'-C1'	5.04	1.48	1.41
49	B1	1675	A	O3'-P	-5.03	1.55	1.61
67	BR	122	PRO	N-CD	5.03	1.54	1.47
14	AL	54	PRO	N-CD	5.03	1.54	1.47
48	A2	1969	G	O3'-P	-5.02	1.55	1.61
1	A3	134	G	O3'-P	-5.01	1.55	1.61
55	BF	108	PRO	N-CD	5.01	1.54	1.47
48	A2	159	A	O4'-C1'	5.01	1.48	1.41

All (1861) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	Aq	75	PRO	CA-N-CD	-36.28	60.70	111.50
48	A2	1225	G	O5'-P-OP1	-28.99	75.91	110.70
48	A2	131	C	C4'-C3'-O3'	28.78	170.56	113.00
49	B1	558	G	P-O3'-C3'	-28.42	85.60	119.70
48	A2	137	G	C4'-C3'-O3'	26.49	165.98	113.00
48	A2	132	G	O5'-P-OP1	-26.34	79.09	110.70
49	B1	842	C	O3'-P-O5'	-25.65	55.26	104.00
48	A2	1225	G	O5'-P-OP2	25.02	140.72	110.70
48	A2	1341	G	C4'-C3'-O3'	25.00	162.99	113.00
47	Au	121	PRO	CA-N-CD	-24.11	77.74	111.50
49	B1	837	A	C4'-C3'-O3'	23.94	160.87	113.00
49	B1	111	A	P-O3'-C3'	-23.44	91.57	119.70
49	B1	688	U	C4'-C3'-O3'	-22.29	62.59	109.40
13	AK	52	VAL	CG1-CB-CG2	20.77	144.12	110.90
48	A2	1283	G	P-O3'-C3'	-20.73	94.82	119.70
48	A2	494	G	C4'-C3'-O3'	20.66	154.32	113.00
49	B1	743	U	C4'-C3'-O3'	-20.49	66.37	109.40
48	A2	1300	U	P-O3'-C3'	-20.34	95.29	119.70
45	Aq	75	PRO	CA-CB-CG	-19.95	66.09	104.00
48	A2	958	U	C4'-C3'-O3'	19.67	152.34	113.00
2	A4	34	C	P-O3'-C3'	19.18	142.71	119.70
48	A2	50	C	P-O5'-C5'	18.69	150.81	120.90
48	A2	494	G	P-O3'-C3'	-18.51	97.49	119.70
49	B1	1285	G	O5'-C5'-C4'	18.18	146.23	111.70
48	A2	132	G	O5'-P-OP2	17.88	132.16	110.70
48	A2	203	U	P-O3'-C3'	17.68	140.92	119.70
48	A2	462	U	C4'-C3'-O3'	17.49	147.98	113.00
48	A2	3736	G	P-O3'-C3'	17.00	140.10	119.70
49	B1	1554	C	C4'-C3'-O3'	-16.87	73.97	109.40
48	A2	4619	U	P-O3'-C3'	16.74	139.79	119.70
49	B1	112	U	P-O3'-C3'	16.29	139.25	119.70
49	B1	748	C	C4'-C3'-O3'	-16.13	75.52	109.40
45	Aq	74	VAL	C-N-CD	-15.76	85.94	120.60
49	B1	1778	C	C2'-C3'-O3'	15.71	144.07	109.50
48	A2	191	C	P-O5'-C5'	15.58	145.83	120.90
48	A2	4907	G	P-O3'-C3'	15.55	138.36	119.70
48	A2	5007	G	P-O5'-C5'	-15.20	96.57	120.90
48	A2	309	G	O5'-P-OP2	-15.16	92.06	105.70
48	A2	49	U	O3'-P-O5'	14.96	132.41	104.00
48	A2	309	G	O5'-P-OP1	14.93	128.61	110.70
48	A2	916	A	P-O3'-C3'	14.86	137.53	119.70
48	A2	1716	G	P-O3'-C3'	-14.85	101.88	119.70
48	A2	3682	A	C4'-C3'-O3'	-14.79	78.35	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	1259	C	C4'-C3'-O3'	-14.56	78.81	109.40
48	A2	958	U	C2'-C3'-O3'	-14.55	77.48	109.50
48	A2	2482	G	P-O3'-C3'	-14.51	102.29	119.70
48	A2	1715	G	P-O3'-C3'	-14.47	102.34	119.70
49	B1	368	U	P-O3'-C3'	14.31	136.87	119.70
1	A3	112	G	O5'-P-OP2	-14.20	92.92	105.70
48	A2	2246	U	C2'-C3'-O3'	-14.19	78.29	109.50
48	A2	2689	C	P-O5'-C5'	-14.16	98.25	120.90
48	A2	3727	A	P-O5'-C5'	14.12	143.50	120.90
49	B1	688	U	P-O3'-C3'	14.09	136.61	119.70
48	A2	1226	C	P-O5'-C5'	14.04	143.36	120.90
84	Bx	45	U	C4'-C3'-O3'	14.04	141.08	113.00
48	A2	495	C	P-O3'-C3'	-14.03	102.86	119.70
48	A2	4686	A	P-O5'-C5'	14.00	143.30	120.90
25	AW	97	LYS	C-N-CD	-13.80	90.23	120.60
48	A2	1433	C	P-O3'-C3'	-13.78	103.16	119.70
48	A2	131	C	P-O3'-C3'	-13.72	103.24	119.70
49	B1	803	C	C4'-C3'-O3'	-13.71	80.60	109.40
48	A2	1217	G	P-O3'-C3'	-13.66	103.30	119.70
48	A2	939	G	P-O5'-C5'	13.66	142.75	120.90
48	A2	463	C	P-O5'-C5'	13.62	142.69	120.90
48	A2	5	A	P-O3'-C3'	13.58	136.00	119.70
48	A2	1631	U	C1'-C2'-O2'	-13.54	69.99	110.60
49	B1	836	G	C4'-C3'-O3'	-13.45	81.15	109.40
48	A2	2686	U	P-O5'-C5'	-13.43	99.41	120.90
49	B1	306	C	O5'-P-OP2	-13.33	93.70	105.70
49	B1	1284	A	C2'-C3'-O3'	13.20	138.54	109.50
48	A2	464	A	P-O5'-C5'	13.12	141.90	120.90
48	A2	1350	C	C4'-C3'-O3'	-13.12	81.84	109.40
48	A2	85	G	C4'-C3'-O3'	-13.10	81.88	109.40
48	A2	1342	G	P-O5'-C5'	-13.09	99.96	120.90
48	A2	4306	U	P-O3'-C3'	-12.99	104.11	119.70
49	B1	182	C	P-O5'-C5'	-12.91	100.25	120.90
48	A2	3684	U	C2'-C3'-O3'	12.89	137.87	109.50
48	A2	2748	U	C4'-C3'-O3'	-12.89	82.33	109.40
48	A2	58	G	C3'-C2'-O2'	-12.87	75.98	113.30
49	B1	747	U	C4'-C3'-O3'	12.87	138.73	113.00
49	B1	178	C	P-O3'-C3'	12.86	135.13	119.70
13	AK	24	TYR	C-N-CD	-12.82	92.39	120.60
49	B1	1620	A	C4'-C3'-O3'	12.82	138.64	113.00
49	B1	748	C	O4'-C1'-N1	12.80	118.44	108.20
49	B1	225	G	C4'-C3'-O3'	-12.77	82.59	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	3933	A	P-O3'-C3'	12.74	134.99	119.70
45	Aq	39	PRO	CA-N-CD	-12.74	93.67	111.50
48	A2	2325	C	C3'-C2'-O2'	-12.69	76.49	113.30
48	A2	4617	A	P-O3'-C3'	12.67	134.91	119.70
49	B1	867	G	C4'-C3'-O3'	-12.60	82.95	109.40
49	B1	38	A	P-O3'-C3'	-12.57	104.61	119.70
1	A3	34	U	C3'-C2'-O2'	-12.54	76.92	113.30
48	A2	1341	G	C2'-C3'-O3'	-12.54	81.91	109.50
49	B1	848	U	P-O5'-C5'	-12.50	100.89	120.90
48	A2	3697	A	P-O3'-C3'	12.49	134.69	119.70
48	A2	2859	U	C4'-C3'-O3'	12.47	137.94	113.00
1	A3	110	U	C2'-C3'-O3'	-12.47	82.08	109.50
48	A2	2686	U	O5'-P-OP1	-12.45	94.50	105.70
49	B1	114	G	P-O3'-C3'	-12.43	104.78	119.70
48	A2	3946	C	P-O3'-C3'	-12.40	104.83	119.70
48	A2	1057	G	P-O3'-C3'	-12.37	104.85	119.70
48	A2	2511	C	P-O3'-C3'	12.35	134.52	119.70
48	A2	961	C	C2'-C3'-O3'	12.33	136.63	109.50
48	A2	3851	G	P-O3'-C3'	-12.33	104.90	119.70
48	A2	1429	C	P-O5'-C5'	12.21	140.44	120.90
48	A2	65	A	C3'-C2'-O2'	-12.20	77.94	113.30
48	A2	3682	A	N9-C1'-C2'	-12.17	98.18	114.00
48	A2	2690	G	C5'-C4'-C3'	-12.16	96.54	116.00
1	A3	126	C	P-O3'-C3'	12.08	134.20	119.70
48	A2	3917	G	P-O3'-C3'	-12.08	105.20	119.70
48	A2	4162	G	P-O3'-C3'	12.07	134.19	119.70
48	A2	4666	C	P-O3'-C3'	-12.05	105.24	119.70
48	A2	3611	U	C4'-C3'-O3'	-12.03	84.14	109.40
48	A2	961	C	C5'-C4'-C3'	-12.00	96.79	116.00
48	A2	1244	G	P-O3'-C3'	-11.99	105.32	119.70
48	A2	221	U	C3'-C2'-O2'	-11.94	78.67	113.30
49	B1	740	C	C4'-C3'-O3'	-11.92	84.36	109.40
48	A2	4537	G	P-O3'-C3'	11.91	133.99	119.70
48	A2	2689	C	O5'-P-OP1	-11.90	94.99	105.70
49	B1	306	C	P-O5'-C5'	-11.87	101.91	120.90
48	A2	966	C	P-O3'-C3'	11.86	133.94	119.70
48	A2	3649	G	P-O3'-C3'	11.86	133.93	119.70
48	A2	1341	G	C3'-C2'-O2'	-11.86	78.92	113.30
49	B1	1022	U	P-O3'-C3'	11.82	133.88	119.70
45	Aq	42	VAL	CG1-CB-CG2	11.81	129.79	110.90
48	A2	2523	G	P-O3'-C3'	11.80	133.86	119.70
48	A2	4037	U	P-O3'-C3'	-11.80	105.54	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	212	C	P-O3'-C3'	-11.74	105.61	119.70
1	A3	94	G	C4'-C3'-O3'	-11.72	84.80	109.40
49	B1	804	U	C2'-C3'-O3'	11.71	135.27	109.50
83	Bw	34	G	C4'-C3'-O3'	-11.70	84.82	109.40
48	A2	931	A	C3'-C2'-O2'	-11.66	79.50	113.30
49	B1	533	A	C4'-C3'-O3'	11.63	136.26	113.00
48	A2	2793	C	C4'-C3'-O3'	-11.62	84.99	109.40
49	B1	873	G	P-O3'-C3'	-11.62	105.75	119.70
48	A2	500	C	P-O3'-C3'	11.60	133.62	119.70
49	B1	744	G	O4'-C4'-C3'	-11.59	92.41	104.00
48	A2	1799	U	P-O3'-C3'	11.57	133.59	119.70
48	A2	3613	A	C3'-C2'-O2'	-11.57	79.75	113.30
48	A2	925	C	OP1-P-O3'	11.55	130.61	105.20
49	B1	1786	U	P-O5'-C5'	-11.55	102.42	120.90
1	A3	109	C	O5'-P-OP1	11.54	124.55	110.70
49	B1	437	G	P-O3'-C3'	11.54	133.55	119.70
48	A2	1316	A	P-O3'-C3'	11.53	133.54	119.70
48	A2	507	U	P-O3'-C3'	-11.53	105.87	119.70
48	A2	131	C	C2'-C3'-O3'	-11.52	84.16	109.50
49	B1	744	G	C4'-C3'-O3'	-11.52	85.21	109.40
48	A2	357	A	C3'-C2'-O2'	-11.50	79.95	113.30
48	A2	2751	C	P-O3'-C3'	-11.47	105.94	119.70
49	B1	238	C	C4'-C3'-O3'	11.47	135.93	113.00
48	A2	1260	G	C5'-C4'-C3'	-11.43	97.71	116.00
48	A2	1307	A	C3'-C2'-O2'	-11.42	80.17	113.30
48	A2	3685	G	P-O3'-C3'	11.40	133.38	119.70
49	B1	306	C	O4'-C1'-N1	-11.39	99.09	108.20
48	A2	211	G	P-O3'-C3'	11.38	133.36	119.70
48	A2	4827	U	C4'-C3'-O3'	-11.35	85.56	109.40
49	B1	890	U	C4'-C3'-O3'	-11.35	85.57	109.40
48	A2	1256	G	C4'-C3'-O3'	11.34	135.69	113.00
48	A2	2460	G	P-O3'-C3'	-11.34	106.10	119.70
48	A2	229	G	C4'-C3'-O3'	-11.32	85.62	109.40
38	Aj	34	CYS	CA-CB-SG	11.32	134.38	114.00
48	A2	3590	G	C1'-C2'-O2'	-11.31	76.66	110.60
49	B1	397	G	P-O3'-C3'	-11.31	106.13	119.70
48	A2	3731	A	C4'-C3'-O3'	-11.30	85.68	109.40
48	A2	2690	G	O4'-C1'-N9	11.29	117.23	108.20
1	A3	109	C	O5'-P-OP2	-11.25	95.57	105.70
45	Aq	30	PRO	CA-N-CD	-11.20	95.83	111.50
49	B1	805	U	C2'-C3'-O3'	11.19	134.12	109.50
49	B1	1805	G	P-O3'-C3'	11.16	133.09	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	718	C	C3'-C2'-O2'	-11.15	80.97	113.30
48	A2	185	G	P-O3'-C3'	11.13	133.06	119.70
48	A2	1975	C	P-O3'-C3'	-11.13	106.34	119.70
48	A2	137	G	C2'-C3'-O3'	-11.13	85.01	109.50
49	B1	836	G	C2'-C3'-O3'	11.10	133.91	109.50
1	A3	129	C	P-O3'-C3'	-11.09	106.39	119.70
48	A2	506	U	C4'-C3'-O3'	11.09	135.19	113.00
48	A2	1253	A	P-O3'-C3'	11.08	133.00	119.70
48	A2	2689	C	C4'-C3'-O3'	-11.08	86.14	109.40
48	A2	4980	U	P-O3'-C3'	-11.06	106.43	119.70
2	A4	72	U	P-O3'-C3'	11.04	132.94	119.70
48	A2	1260	G	C4'-C3'-O3'	11.03	135.07	113.00
48	A2	4707	G	P-O3'-C3'	-11.02	106.48	119.70
48	A2	2462	G	P-O3'-C3'	-10.97	106.54	119.70
48	A2	1261	C	P-O5'-C5'	-10.96	103.36	120.90
13	AK	25	PRO	CA-N-CD	-10.94	96.18	111.50
49	B1	1556	A	C4'-C3'-O3'	-10.93	86.44	109.40
48	A2	2688	C	O5'-P-OP1	-10.90	95.89	105.70
13	AK	52	VAL	CA-CB-CG1	-10.89	94.56	110.90
48	A2	2618	U	P-O5'-C5'	-10.89	103.48	120.90
83	Bw	35	A	C4'-C3'-O3'	10.88	134.77	113.00
48	A2	1632	A	C3'-C2'-O2'	-10.84	81.86	113.30
48	A2	2691	G	O5'-P-OP1	-10.83	95.95	105.70
48	A2	2684	G	C4'-C3'-O3'	10.82	134.65	113.00
1	A3	153	C	P-O3'-C3'	-10.82	106.72	119.70
48	A2	1764	U	P-O3'-C3'	-10.80	106.74	119.70
49	B1	1453	C	P-O3'-C3'	-10.80	106.74	119.70
48	A2	25	A	P-O3'-C3'	10.76	132.61	119.70
48	A2	966	C	C4'-C3'-O3'	10.76	134.52	113.00
48	A2	4015	G	C4'-C3'-O3'	10.76	134.52	113.00
49	B1	1289	U	C4'-C3'-O3'	10.74	134.48	113.00
48	A2	5007	G	C3'-C2'-O2'	-10.72	82.20	113.30
48	A2	309	G	C1'-C2'-O2'	-10.71	78.46	110.60
48	A2	2512	C	P-O3'-C3'	-10.71	106.85	119.70
49	B1	738	C	C2'-C3'-O3'	10.71	133.06	109.50
48	A2	4718	C	P-O5'-C5'	10.70	138.02	120.90
48	A2	960	G	N9-C1'-C2'	-10.69	100.11	114.00
49	B1	293	C	P-O3'-C3'	-10.69	106.88	119.70
48	A2	3737	A	C4'-C3'-O3'	10.67	134.34	113.00
49	B1	24	C	P-O3'-C3'	10.65	132.48	119.70
49	B1	744	G	N9-C1'-C2'	-10.62	100.19	114.00
2	A4	75	G	C4'-C3'-O3'	10.62	134.24	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	Au	191	VAL	CA-CB-CG2	10.61	126.81	110.90
48	A2	2691	G	O5'-C5'-C4'	10.60	131.84	111.70
49	B1	1105	G	O5'-P-OP1	-10.58	96.18	105.70
45	Aq	88	PRO	CA-N-CD	-10.57	96.70	111.50
48	A2	2689	C	O5'-P-OP2	10.57	123.38	110.70
48	A2	4715	U	N1-C1'-C2'	-10.54	100.29	114.00
1	A3	34	U	C4'-C3'-O3'	-10.53	87.28	109.40
49	B1	1285	G	C5'-C4'-C3'	10.51	132.82	116.00
48	A2	1353	G	P-O3'-C3'	10.49	132.29	119.70
48	A2	3611	U	C3'-C2'-O2'	-10.48	82.90	113.30
49	B1	106	C	P-O3'-C3'	-10.47	107.14	119.70
48	A2	381	G	C4'-C3'-O3'	10.45	133.90	113.00
48	A2	2328	A	P-O3'-C3'	10.45	132.24	119.70
48	A2	671	C	P-O3'-C3'	-10.44	107.17	119.70
48	A2	4828	G	O5'-P-OP2	-10.41	96.33	105.70
48	A2	958	U	P-O3'-C3'	-10.40	107.22	119.70
48	A2	191	C	C4'-C3'-O3'	-10.38	87.61	109.40
49	B1	795	A	C4'-C3'-O3'	-10.38	87.61	109.40
48	A2	85	G	P-O5'-C5'	-10.37	104.31	120.90
48	A2	186	G	P-O3'-C3'	-10.36	107.27	119.70
49	B1	1286	G	C4'-C3'-O3'	10.35	133.70	113.00
45	Aq	22	VAL	CG1-CB-CG2	-10.35	94.35	110.90
48	A2	2825	G	C2'-C3'-O3'	10.34	132.26	109.50
47	Au	121	PRO	CA-CB-CG	-10.34	84.36	104.00
49	B1	1625	U	P-O5'-C5'	-10.31	104.40	120.90
49	B1	460	A	P-O3'-C3'	-10.31	107.33	119.70
49	B1	793	G	P-O5'-C5'	10.29	137.37	120.90
48	A2	2689	C	C2'-C3'-O3'	10.29	132.14	109.50
48	A2	4596	U	N1-C1'-C2'	10.27	127.35	114.00
13	AK	108	PRO	CA-N-CD	-10.26	97.14	111.50
48	A2	1260	G	P-O3'-C3'	-10.26	107.39	119.70
48	A2	3789	U	P-O3'-C3'	-10.24	107.41	119.70
48	A2	2010	A	P-O3'-C3'	10.24	131.99	119.70
48	A2	2617	G	O5'-P-OP2	-10.23	96.49	105.70
48	A2	221	U	N1-C1'-C2'	10.20	127.26	114.00
49	B1	690	G	O5'-C5'-C4'	10.20	131.07	111.70
48	A2	3928	U	P-O3'-C3'	10.19	131.93	119.70
49	B1	915	G	C5'-C4'-C3'	10.17	132.28	116.00
1	A3	124	U	P-O3'-C3'	-10.17	107.50	119.70
48	A2	4136	U	P-O3'-C3'	-10.17	107.50	119.70
48	A2	727	C	C5'-C4'-C3'	-10.17	99.73	116.00
48	A2	1741	G	O4'-C1'-N9	10.16	116.33	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A3	94	G	C3'-C2'-O2'	-10.15	83.87	113.30
49	B1	791	C	C2'-C3'-O3'	10.15	131.82	109.50
48	A2	2690	G	C5'-C4'-O4'	-10.13	96.94	109.10
49	B1	1854	U	P-O3'-C3'	-10.12	107.55	119.70
49	B1	356	C	O5'-P-OP2	-10.12	96.59	105.70
48	A2	4896	A	P-O5'-C5'	10.11	137.07	120.90
49	B1	639	C	P-O5'-C5'	10.10	137.06	120.90
48	A2	961	C	P-O5'-C5'	-10.07	104.78	120.90
49	B1	369	C	C4'-C3'-O3'	-10.07	88.25	109.40
48	A2	2683	C	C2'-C3'-O3'	10.07	131.65	109.50
48	A2	154	U	C2'-C3'-O3'	10.06	131.63	109.50
48	A2	650	C	P-O3'-C3'	-10.06	107.63	119.70
49	B1	615	C	P-O3'-C3'	10.06	131.77	119.70
45	Aq	59	THR	OG1-CB-CG2	-10.06	86.87	110.00
49	B1	227	U	C4'-C3'-O3'	-10.03	88.34	109.40
49	B1	1289	U	C5'-C4'-C3'	10.03	132.04	116.00
48	A2	651	C	P-O3'-C3'	9.99	131.68	119.70
48	A2	931	A	P-O3'-C3'	9.96	131.66	119.70
48	A2	1225	G	C4'-C3'-O3'	9.95	132.90	113.00
49	B1	690	G	C2'-C3'-O3'	-9.95	87.62	109.50
48	A2	3929	G	P-O5'-C5'	-9.94	104.99	120.90
49	B1	237	C	C4'-C3'-O3'	9.94	132.87	113.00
48	A2	2691	G	P-O5'-C5'	9.91	136.75	120.90
48	A2	2690	G	C4-N9-C1'	-9.90	113.62	126.50
48	A2	111	C	C3'-C2'-O2'	-9.90	84.59	113.30
48	A2	154	U	C5'-C4'-C3'	-9.90	100.16	116.00
48	A2	2792	A	P-O3'-C3'	9.90	131.57	119.70
25	AW	98	PRO	CA-N-CD	-9.88	97.67	111.50
49	B1	746	C	P-O5'-C5'	-9.88	105.09	120.90
49	B1	842	C	OP2-P-O3'	9.88	126.94	105.20
49	B1	1826	G	P-O5'-C5'	-9.87	105.11	120.90
48	A2	206	U	P-O3'-C3'	-9.85	107.88	119.70
48	A2	2601	G	P-O3'-C3'	-9.85	107.88	119.70
48	A2	1258	G	O4'-C1'-N9	9.84	116.07	108.20
48	A2	497	C	P-O3'-C3'	-9.83	107.91	119.70
48	A2	4827	U	C2'-C3'-O3'	9.82	131.11	109.50
48	A2	3613	A	C5'-C4'-C3'	-9.82	100.29	116.00
45	Aq	46	ILE	CG1-CB-CG2	9.80	132.96	111.40
48	A2	287	G	C3'-C2'-O2'	-9.79	84.91	113.30
48	A2	220	G	P-O3'-C3'	-9.78	107.96	119.70
49	B1	1557	C	C4'-C3'-O3'	9.78	132.56	113.00
49	B1	744	G	O4'-C1'-N9	9.77	116.02	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	B1	1454	A	P-O5'-C5'	-9.77	105.27	120.90
48	A2	192	C	O5'-P-OP1	-9.76	96.92	105.70
49	B1	690	G	C5'-C4'-O4'	9.76	120.81	109.10
49	B1	215	G	P-O3'-C3'	9.75	131.40	119.70
48	A2	2793	C	C2'-C3'-O3'	-9.75	88.05	109.50
48	A2	7	C	C4'-C3'-O3'	-9.73	88.97	109.40
48	A2	2825	G	C5'-C4'-C3'	-9.71	100.46	116.00
48	A2	2692	C	P-O5'-C5'	9.71	136.44	120.90
48	A2	4717	G	C4'-C3'-O3'	-9.71	89.00	109.40
48	A2	641	G	P-O3'-C3'	9.70	131.34	119.70
48	A2	1259	C	P-O3'-C3'	-9.69	108.07	119.70
48	A2	4828	G	C2'-C3'-O3'	-9.68	88.21	109.50
49	B1	25	A	O4'-C1'-N9	9.68	115.94	108.20
48	A2	4458	A	P-O3'-C3'	9.64	131.27	119.70
48	A2	3578	U	P-O5'-C5'	9.64	136.32	120.90
48	A2	2682	G	O4'-C1'-N9	9.62	115.90	108.20
48	A2	5006	A	C3'-C2'-O2'	-9.62	85.40	113.30
49	B1	502	C	P-O3'-C3'	-9.62	108.15	119.70
49	B1	1647	A	P-O3'-C3'	9.60	131.22	119.70
48	A2	728	C	P-O3'-C3'	-9.60	108.18	119.70
48	A2	1296	C	P-O5'-C5'	-9.58	105.58	120.90
48	A2	290	A	C2'-C3'-O3'	9.57	130.55	109.50
48	A2	968	C	C5'-C4'-O4'	9.57	120.58	109.10
49	B1	33	G	OP2-P-O3'	9.57	126.25	105.20
48	A2	2299	G	P-O5'-C5'	-9.56	105.60	120.90
49	B1	1802	C	P-O3'-C3'	-9.55	108.24	119.70
48	A2	330	A	P-O3'-C3'	9.53	131.13	119.70
48	A2	4906	C	P-O3'-C3'	-9.52	108.28	119.70
48	A2	4030	U	P-O3'-C3'	-9.51	108.29	119.70
45	Aq	46	ILE	CA-CB-CG1	-9.47	93.00	111.00
49	B1	438	G	P-O3'-C3'	-9.47	108.33	119.70
48	A2	1258	G	P-O5'-C5'	-9.46	105.76	120.90
48	A2	959	C	C5'-C4'-C3'	-9.45	100.88	116.00
49	B1	306	C	O5'-P-OP1	9.44	122.03	110.70
48	A2	4685	A	O5'-P-OP2	-9.43	97.21	105.70
48	A2	4620	G	P-O3'-C3'	9.42	131.01	119.70
48	A2	3737	A	C2'-C3'-O3'	-9.40	88.82	109.50
48	A2	1559	G	P-O3'-C3'	9.39	130.97	119.70
49	B1	1723	G	P-O3'-C3'	-9.35	108.48	119.70
48	A2	49	U	O5'-P-OP1	9.33	121.90	110.70
48	A2	4409	C	P-O3'-C3'	-9.32	108.52	119.70
48	A2	1741	G	P-O5'-C5'	9.31	135.80	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	B1	837	A	C2'-C3'-O3'	-9.31	89.03	109.50
49	B1	804	U	P-O5'-C5'	-9.30	106.02	120.90
1	A3	103	A	P-O5'-C5'	-9.29	106.04	120.90
48	A2	1296	C	C4'-C3'-O3'	-9.29	89.90	109.40
48	A2	3590	G	C2'-C3'-O3'	-9.26	89.12	109.50
48	A2	19	G	P-O3'-C3'	9.25	130.80	119.70
49	B1	1448	A	P-O5'-C5'	9.23	135.67	120.90
48	A2	4827	U	N1-C1'-C2'	9.22	125.98	114.00
48	A2	953	A	P-O3'-C3'	9.21	130.75	119.70
48	A2	967	U	C4'-C3'-O3'	9.20	131.40	113.00
48	A2	295	G	P-O3'-C3'	-9.20	108.67	119.70
49	B1	1481	G	P-O3'-C3'	9.19	130.73	119.70
48	A2	968	C	C4'-C3'-O3'	9.13	131.27	113.00
48	A2	229	G	N9-C1'-C2'	9.12	125.86	114.00
38	Aj	19	CYS	CA-CB-SG	9.12	130.41	114.00
49	B1	1554	C	P-O5'-C5'	-9.11	106.33	120.90
49	B1	792	C	C2'-C3'-O3'	9.10	129.53	109.50
48	A2	4526	A	P-O3'-C3'	9.09	130.61	119.70
48	A2	228	U	C1'-C2'-O2'	-9.09	83.34	110.60
48	A2	917	G	P-O3'-C3'	9.08	130.60	119.70
49	B1	450	C	O5'-P-OP1	-9.08	97.53	105.70
48	A2	968	C	C5'-C4'-C3'	-9.07	101.48	116.00
49	B1	1491	G	P-O3'-C3'	-9.07	108.82	119.70
48	A2	7	C	C3'-C2'-O2'	-9.05	87.07	113.30
48	A2	463	C	C4'-C3'-O3'	9.02	131.04	113.00
2	A4	105	C	O3'-P-O5'	9.02	121.14	104.00
48	A2	229	G	P-O5'-C5'	-9.02	106.47	120.90
48	A2	930	A	C3'-C2'-O2'	-9.02	87.15	113.30
48	A2	4827	U	P-O3'-C3'	-9.02	108.88	119.70
48	A2	3930	U	P-O5'-C5'	9.01	135.32	120.90
48	A2	2054	C	P-O3'-C3'	-9.00	108.90	119.70
48	A2	4586	A	O4'-C1'-N9	9.00	115.40	108.20
48	A2	1357	G	P-O3'-C3'	8.99	130.49	119.70
48	A2	1981	G	P-O3'-C3'	8.98	130.47	119.70
49	B1	308	G	O4'-C1'-N9	8.97	115.38	108.20
49	B1	239	C	O5'-C5'-C4'	8.96	128.73	111.70
48	A2	192	C	O5'-P-OP2	8.96	121.45	110.70
48	A2	3612	U	C3'-C2'-O2'	-8.95	87.35	113.30
49	B1	882	U	P-O5'-C5'	8.95	135.21	120.90
48	A2	1297	C	N1-C1'-C2'	8.94	125.62	114.00
48	A2	2526	G	P-O3'-C3'	8.93	130.42	119.70
48	A2	2284	U	P-O3'-C3'	8.93	130.41	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	B1	903	A	O4'-C1'-N9	8.93	115.34	108.20
48	A2	2485	G	O4'-C1'-N9	8.92	115.34	108.20
13	AK	107	VAL	CA-CB-CG1	8.92	124.27	110.90
49	B1	369	C	C2'-C3'-O3'	8.92	129.12	109.50
49	B1	1285	G	P-O5'-C5'	-8.90	106.67	120.90
49	B1	230	A	C4'-C3'-O3'	8.87	130.75	113.00
48	A2	229	G	P-O3'-C3'	8.87	130.34	119.70
48	A2	2056	G	O4'-C1'-N9	8.87	115.29	108.20
48	A2	1226	C	O5'-C5'-C4'	-8.86	94.87	111.70
48	A2	960	G	C4'-C3'-O3'	-8.86	90.81	109.40
83	Bv	72	C	N1-C1'-C2'	-8.85	102.27	112.00
48	A2	112	C	C5'-C4'-O4'	8.85	119.72	109.10
49	B1	744	G	O5'-C5'-C4'	8.83	128.48	111.70
48	A2	159	A	P-O3'-C3'	-8.83	109.10	119.70
48	A2	279	G	P-O3'-C3'	8.82	130.28	119.70
48	A2	737	A	C4'-C3'-O3'	-8.81	90.90	109.40
49	B1	1301	A	O4'-C1'-N9	8.81	115.25	108.20
13	AK	90	PHE	CA-CB-CG	8.80	135.03	113.90
48	A2	2793	C	P-O3'-C3'	8.80	130.26	119.70
48	A2	319	U	P-O3'-C3'	8.80	130.26	119.70
48	A2	4532	G	P-O3'-C3'	8.80	130.26	119.70
48	A2	2685	G	P-O3'-C3'	-8.79	109.15	119.70
48	A2	326	C	P-O3'-C3'	-8.78	109.17	119.70
48	A2	918	C	P-O3'-C3'	8.76	130.21	119.70
48	A2	3597	G	P-O5'-C5'	-8.75	106.89	120.90
48	A2	3683	A	C4'-C3'-O3'	-8.75	91.02	109.40
48	A2	139	G	C4'-C3'-O3'	8.74	130.48	113.00
48	A2	4119	A	P-O3'-C3'	-8.74	109.21	119.70
48	A2	2329	U	P-O3'-C3'	8.73	130.18	119.70
49	B1	1782	G	C4'-C3'-O3'	8.73	130.46	113.00
48	A2	652	C	P-O3'-C3'	-8.72	109.23	119.70
48	A2	713	G	C1'-C2'-O2'	-8.72	84.43	110.60
48	A2	1227	G	P-O3'-C3'	-8.72	109.23	119.70
48	A2	286	G	C3'-C2'-O2'	-8.72	88.02	113.30
48	A2	328	A	P-O3'-C3'	8.71	130.15	119.70
49	B1	689	U	C5'-C4'-O4'	8.71	119.55	109.10
48	A2	3627	A	P-O3'-C3'	8.71	130.15	119.70
48	A2	228	U	C4'-C3'-O3'	-8.70	91.12	109.40
49	B1	874	G	C4'-C3'-O3'	8.70	130.40	113.00
48	A2	91	G	OP1-P-O3'	-8.70	86.07	105.20
48	A2	1219	C	P-O3'-C3'	-8.69	109.27	119.70
49	B1	21	U	P-O3'-C3'	-8.69	109.27	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	2748	U	C1'-C2'-O2'	-8.69	84.54	110.60
48	A2	4086	U	C4'-C3'-O3'	-8.69	91.16	109.40
49	B1	873	G	C4'-C3'-O3'	-8.68	91.17	109.40
13	AK	73	PRO	CA-N-CD	-8.67	99.36	111.50
48	A2	1467	C	P-O3'-C3'	8.67	130.11	119.70
48	A2	967	U	P-O3'-C3'	-8.67	109.30	119.70
48	A2	741	U	P-O3'-C3'	8.66	130.09	119.70
49	B1	1702	G	C4'-C3'-O3'	-8.65	91.23	109.40
48	A2	1282	G	P-O3'-C3'	-8.65	109.33	119.70
48	A2	713	G	C4'-C3'-O3'	-8.64	91.24	109.40
49	B1	1554	C	O3'-P-O5'	-8.64	87.58	104.00
48	A2	4135	G	P-O3'-C3'	-8.63	109.34	119.70
49	B1	748	C	O5'-C5'-C4'	-8.63	95.30	111.70
48	A2	1742	G	O5'-P-OP1	-8.61	97.95	105.70
48	A2	1201	G	O4'-C1'-N9	8.60	115.08	108.20
50	BA	116	PHE	N-CA-C	-8.59	87.80	111.00
45	Aq	22	VAL	CA-CB-CG2	8.59	123.78	110.90
48	A2	210	G	O3'-P-O5'	-8.59	87.68	104.00
48	A2	1319	G	P-O3'-C3'	8.59	130.01	119.70
48	A2	1269	C	P-O3'-C3'	-8.59	109.40	119.70
49	B1	1339	U	P-O3'-C3'	8.59	130.00	119.70
48	A2	62	A	OP2-P-O3'	8.57	124.05	105.20
48	A2	480	C	P-O3'-C3'	8.57	129.98	119.70
48	A2	3793	U	OP2-P-O3'	8.57	124.05	105.20
48	A2	925	C	O3'-P-O5'	-8.55	87.75	104.00
49	B1	183	G	O5'-C5'-C4'	-8.53	95.49	111.70
48	A2	4119	A	OP2-P-O3'	8.53	123.96	105.20
48	A2	460	A	C4'-C3'-O3'	-8.51	91.53	109.40
48	A2	3911	U	P-O3'-C3'	-8.51	109.49	119.70
49	B1	371	A	O5'-C5'-C4'	8.50	127.86	111.70
48	A2	958	U	O3'-P-O5'	-8.50	87.85	104.00
48	A2	2690	G	C3'-C2'-O2'	-8.50	88.65	113.30
48	A2	1225	G	C5'-C4'-O4'	-8.49	98.91	109.10
49	B1	1683	C	P-O3'-C3'	8.49	129.89	119.70
48	A2	4130	G	P-O3'-C3'	-8.49	109.52	119.70
2	A4	3	C	P-O5'-C5'	8.48	134.47	120.90
48	A2	91	G	OP2-P-O3'	8.47	123.83	105.20
48	A2	1849	A	C4'-C3'-O3'	-8.47	91.62	109.40
49	B1	417	C	P-O3'-C3'	-8.47	109.54	119.70
48	A2	4600	U	P-O3'-C3'	8.46	129.85	119.70
48	A2	5006	A	P-O5'-C5'	-8.46	107.36	120.90
49	B1	909	G	C4'-C3'-O3'	8.45	129.91	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	B1	806	U	P-O5'-C5'	-8.45	107.38	120.90
49	B1	447	A	P-O3'-C3'	-8.45	109.57	119.70
49	B1	1283	C	C4'-C3'-O3'	8.44	129.88	113.00
48	A2	1741	G	C4-N9-C1'	-8.44	115.53	126.50
49	B1	345	U	P-O3'-C3'	-8.43	109.58	119.70
48	A2	150	G	O4'-C1'-N9	8.42	114.93	108.20
48	A2	2617	G	C3'-C2'-O2'	-8.41	88.91	113.30
49	B1	298	G	P-O3'-C3'	-8.40	109.62	119.70
49	B1	533	A	P-O3'-C3'	8.40	129.78	119.70
49	B1	798	G	C4'-C3'-O3'	-8.40	91.76	109.40
49	B1	1556	A	N9-C1'-C2'	8.39	124.91	114.00
48	A2	1066	U	OP2-P-O3'	8.38	123.64	105.20
48	A2	1572	C	P-O3'-C3'	8.38	129.75	119.70
48	A2	959	C	O4'-C1'-N1	8.37	114.89	108.20
48	A2	356	A	C3'-C2'-O2'	-8.36	89.05	113.30
49	B1	320	G	C5'-C4'-C3'	8.35	129.36	116.00
2	A4	56	G	P-O3'-C3'	8.34	129.71	119.70
49	B1	689	U	O4'-C1'-N1	8.34	114.87	108.20
48	A2	2876	G	P-O3'-C3'	-8.34	109.70	119.70
47	Au	180	VAL	CA-CB-CG1	8.33	123.40	110.90
48	A2	85	G	C1'-C2'-O2'	-8.33	85.60	110.60
48	A2	444	G	O4'-C1'-N9	8.32	114.85	108.20
48	A2	4033	U	O4'-C1'-N1	8.31	114.85	108.20
49	B1	180	G	C4'-C3'-O3'	8.31	129.63	113.00
48	A2	938	G	O3'-P-O5'	8.31	119.79	104.00
48	A2	1877	A	P-O5'-C5'	8.31	134.20	120.90
48	A2	732	C	P-O3'-C3'	-8.29	109.75	119.70
48	A2	4319	G	P-O3'-C3'	-8.29	109.75	119.70
48	A2	111	C	P-O3'-C3'	8.28	129.64	119.70
49	B1	748	C	C2'-C3'-O3'	8.28	127.72	109.50
48	A2	85	G	O5'-C5'-C4'	8.28	127.43	111.70
48	A2	4597	A	P-O3'-C3'	8.26	129.61	119.70
49	B1	1753	C	C4'-C3'-O3'	8.25	129.50	113.00
48	A2	228	U	N1-C1'-C2'	8.25	124.72	114.00
49	B1	1525	C	P-O3'-C3'	-8.25	109.80	119.70
48	A2	2508	A	O4'-C1'-N9	8.24	114.79	108.20
49	B1	1015	U	P-O3'-C3'	8.24	129.59	119.70
49	B1	451	G	P-O5'-C5'	-8.24	107.72	120.90
13	AK	89	VAL	CA-CB-CG1	8.23	123.25	110.90
48	A2	3921	U	P-O3'-C3'	-8.23	109.82	119.70
49	B1	110	U	P-O3'-C3'	-8.23	109.82	119.70
49	B1	1223	A	O4'-C1'-N9	8.23	114.78	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	B1	1445	U	C4'-C3'-O3'	-8.22	92.14	109.40
49	B1	604	A	P-O3'-C3'	-8.21	109.84	119.70
49	B1	1554	C	P-O3'-C3'	8.21	129.56	119.70
48	A2	1196	G	P-O3'-C3'	-8.21	109.85	119.70
45	Aq	25	THR	CA-CB-CG2	8.20	123.89	112.40
48	A2	4597	A	N9-C1'-C2'	8.20	124.67	114.00
48	A2	4631	A	P-O3'-C3'	8.19	129.53	119.70
48	A2	1258	G	P-O3'-C3'	-8.19	109.87	119.70
48	A2	1255	C	P-O3'-C3'	-8.18	109.88	119.70
48	A2	2245	C	C3'-C2'-O2'	-8.18	89.58	113.30
48	A2	494	G	C2'-C3'-O3'	-8.17	91.52	109.50
48	A2	4407	U	P-O3'-C3'	-8.17	109.89	119.70
48	A2	2330	C	P-O3'-C3'	8.17	129.50	119.70
48	A2	4318	G	OP2-P-O3'	8.17	123.17	105.20
36	Ah	38	GLY	N-CA-C	8.15	133.48	113.10
48	A2	1579	G	P-O5'-C5'	-8.15	107.86	120.90
49	B1	1749	G	C4'-C3'-O3'	-8.15	92.28	109.40
48	A2	2683	C	C4'-C3'-O3'	-8.15	92.29	109.40
49	B1	742	U	C4'-C3'-O3'	-8.15	92.29	109.40
48	A2	2684	G	N9-C1'-C2'	-8.14	103.04	112.00
48	A2	3877	A	P-O5'-C5'	-8.14	107.88	120.90
48	A2	181	U	P-O3'-C3'	-8.13	109.94	119.70
47	Au	17	VAL	CA-CB-CG1	8.11	123.06	110.90
48	A2	3732	C	C5'-C4'-C3'	-8.11	103.03	116.00
48	A2	4593	G	P-O3'-C3'	8.11	129.43	119.70
49	B1	890	U	C2'-C3'-O3'	8.11	127.34	109.50
48	A2	736	G	C4'-C3'-O3'	-8.10	92.39	109.40
48	A2	3736	G	C4'-C3'-O3'	8.10	129.19	113.00
49	B1	866	U	C4'-C3'-O3'	8.08	129.17	113.00
49	B1	741	C	C5'-C4'-O4'	-8.07	99.41	109.10
48	A2	4017	A	P-O5'-C5'	-8.06	108.00	120.90
48	A2	4827	U	O4'-C1'-N1	-8.05	101.76	108.20
49	B1	1624	U	C5'-C4'-O4'	8.05	118.76	109.10
48	A2	4984	U	P-O3'-C3'	-8.03	110.06	119.70
49	B1	741	C	C2'-C3'-O3'	8.02	127.14	109.50
48	A2	4684	G	O4'-C1'-N9	8.01	114.61	108.20
48	A2	1256	G	O5'-C5'-C4'	-8.01	96.48	111.70
49	B1	368	U	C4'-C3'-O3'	-8.01	92.58	109.40
83	Bw	34	G	C2'-C3'-O3'	7.98	127.06	109.50
2	A4	112	U	OP2-P-O3'	7.98	122.76	105.20
45	Aq	112	ILE	CA-CB-CG1	7.97	126.14	111.00
1	A3	130	C	P-O3'-C3'	-7.96	110.15	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	1066	U	P-O3'-C3'	-7.96	110.15	119.70
48	A2	1741	G	C8-N9-C1'	7.96	137.34	127.00
48	A2	2793	C	O5'-C5'-C4'	7.95	126.81	111.70
48	A2	1251	G	P-O3'-C3'	7.95	129.24	119.70
49	B1	748	C	P-O5'-C5'	7.95	133.62	120.90
49	B1	1496	U	P-O3'-C3'	-7.95	110.16	119.70
49	B1	985	G	C3'-C2'-O2'	-7.95	90.25	113.30
1	A3	94	G	C5'-C4'-O4'	-7.94	99.57	109.10
13	AK	27	CYS	CA-CB-SG	7.94	128.29	114.00
48	A2	296	C	P-O3'-C3'	-7.93	110.18	119.70
49	B1	497	C	O3'-P-O5'	-7.93	88.93	104.00
48	A2	496	C	C4'-C3'-O3'	7.93	128.86	113.00
49	B1	1181	A	P-O3'-C3'	7.93	129.21	119.70
48	A2	1218	G	P-O3'-C3'	-7.92	110.20	119.70
48	A2	1741	G	C2'-C3'-O3'	7.92	126.92	109.50
49	B1	801	U	C4'-C3'-O3'	7.92	128.84	113.00
48	A2	4016	A	O3'-P-O5'	-7.92	88.96	104.00
49	B1	33	G	P-O3'-C3'	-7.91	110.21	119.70
49	B1	859	G	C4'-C3'-O3'	7.91	128.81	113.00
49	B1	1867	U	P-O3'-C3'	-7.90	110.22	119.70
49	B1	1825	A	P-O5'-C5'	-7.89	108.27	120.90
1	A3	129	C	OP2-P-O3'	7.89	122.56	105.20
1	A3	111	U	P-O3'-C3'	7.89	129.17	119.70
48	A2	3597	G	C2'-C3'-O3'	-7.89	92.14	109.50
49	B1	693	A	C2'-C3'-O3'	7.89	126.85	109.50
48	A2	4586	A	P-O3'-C3'	7.88	129.16	119.70
49	B1	1702	G	C1'-C2'-O2'	-7.87	86.98	110.60
48	A2	409	G	P-O3'-C3'	7.86	129.13	119.70
2	A4	9	C	P-O3'-C3'	7.86	129.13	119.70
48	A2	3736	G	O3'-P-O5'	-7.85	89.08	104.00
49	B1	745	C	C4'-C3'-O3'	-7.85	92.92	109.40
48	A2	228	U	C5'-C4'-C3'	-7.85	103.45	116.00
48	A2	1742	G	C4-N9-C1'	-7.82	116.33	126.50
48	A2	718	C	C1'-C2'-O2'	-7.81	87.17	110.60
49	B1	422	U	P-O3'-C3'	7.81	129.07	119.70
84	Bx	44	U	O3'-P-O5'	-7.79	89.19	104.00
47	Au	120	ILE	C-N-CD	-7.78	103.49	120.60
48	A2	1950	G	O4'-C1'-N9	7.78	114.42	108.20
49	B1	369	C	P-O5'-C5'	-7.77	108.47	120.90
49	B1	1783	C	O4'-C1'-N1	7.75	114.40	108.20
48	A2	3928	U	C4'-C3'-O3'	7.75	128.50	113.00
48	A2	1253	A	C4'-C3'-O3'	7.74	128.49	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	2324	G	C4'-C3'-O3'	-7.74	93.14	109.40
49	B1	802	A	C4'-C3'-O3'	-7.74	93.14	109.40
48	A2	4705	G	P-O3'-C3'	7.74	128.99	119.70
48	A2	1274	G	OP2-P-O3'	7.73	122.22	105.20
49	B1	1555	U	C5'-C4'-C3'	7.73	128.37	116.00
48	A2	2612	U	P-O3'-C3'	-7.73	110.42	119.70
49	B1	1224	G	P-O3'-C3'	7.72	128.96	119.70
48	A2	1752	A	O5'-P-OP1	-7.71	98.76	105.70
48	A2	2673	G	C1'-C2'-O2'	-7.71	87.48	110.60
48	A2	3743	U	C4'-C3'-O3'	-7.70	93.23	109.40
48	A2	3667	C	P-O3'-C3'	7.69	128.92	119.70
49	B1	627	U	P-O3'-C3'	-7.68	110.48	119.70
49	B1	886	A	C2'-C3'-O3'	7.68	126.41	109.50
48	A2	241	G	P-O3'-C3'	7.68	128.92	119.70
49	B1	740	C	O4'-C1'-N1	7.67	114.33	108.20
48	A2	138	C	P-O5'-C5'	7.67	133.16	120.90
49	B1	1620	A	P-O3'-C3'	7.66	128.90	119.70
48	A2	1761	U	P-O3'-C3'	-7.66	110.51	119.70
48	A2	509	C	P-O3'-C3'	-7.66	110.51	119.70
48	A2	1992	C	O4'-C1'-N1	7.66	114.32	108.20
49	B1	320	G	P-O5'-C5'	-7.65	108.66	120.90
49	B1	742	U	N1-C1'-C2'	7.65	123.95	114.00
49	B1	239	C	C5'-C4'-C3'	7.65	128.24	116.00
48	A2	661	G	P-O5'-C5'	7.65	133.13	120.90
48	A2	3850	G	P-O3'-C3'	7.64	128.87	119.70
49	B1	231	A	C5'-C4'-O4'	7.64	118.27	109.10
49	B1	1014	G	P-O3'-C3'	7.64	128.86	119.70
48	A2	3682	A	O4'-C4'-C3'	-7.63	96.37	104.00
49	B1	1453	C	C3'-C2'-O2'	-7.63	91.17	113.30
48	A2	9	C	O5'-P-OP1	-7.63	98.83	105.70
48	A2	1755	U	O5'-P-OP1	-7.62	98.84	105.70
48	A2	3731	A	O5'-P-OP2	-7.62	98.84	105.70
49	B1	306	C	N1-C1'-C2'	7.62	123.91	114.00
48	A2	204	G	P-O3'-C3'	7.62	128.84	119.70
49	B1	1785	C	O4'-C1'-N1	7.62	114.29	108.20
48	A2	322	A	C4'-C3'-O3'	-7.62	93.41	109.40
48	A2	737	A	P-O5'-C5'	7.62	133.09	120.90
49	B1	1287	A	O4'-C1'-N9	7.62	114.29	108.20
49	B1	1338	G	P-O3'-C3'	7.62	128.84	119.70
49	B1	14	C	O4'-C1'-N1	7.61	114.29	108.20
49	B1	869	A	O4'-C1'-N9	7.61	114.29	108.20
84	Bx	45	U	C5'-C4'-C3'	7.61	128.18	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	4606	G	P-O3'-C3'	7.60	128.82	119.70
48	A2	2600	A	P-O3'-C3'	-7.59	110.59	119.70
48	A2	3916	A	P-O3'-C3'	-7.58	110.61	119.70
48	A2	968	C	P-O5'-C5'	-7.58	108.78	120.90
49	B1	903	A	C5'-C4'-O4'	7.58	118.19	109.10
49	B1	689	U	C2'-C3'-O3'	-7.57	92.84	109.50
48	A2	482	G	P-O3'-C3'	-7.57	110.61	119.70
83	Bv	1	G	OP1-P-OP2	-7.57	108.25	119.60
49	B1	293	C	O4'-C1'-N1	-7.56	102.15	108.20
49	B1	688	U	O4'-C1'-N1	7.56	114.25	108.20
48	A2	1763	U	P-O3'-C3'	-7.56	110.63	119.70
49	B1	318	A	C4'-C3'-O3'	-7.55	93.53	109.40
48	A2	675	G	P-O3'-C3'	7.55	128.76	119.70
49	B1	1553	C	P-O5'-C5'	7.55	132.97	120.90
83	Bw	1	G	OP1-P-OP2	-7.54	108.29	119.60
48	A2	2872	U	P-O3'-C3'	-7.54	110.66	119.70
84	Bx	34	U	OP1-P-OP2	-7.53	108.30	119.60
47	Au	58	THR	CA-CB-OG1	7.53	124.82	109.00
48	A2	258	C	C2'-C3'-O3'	7.53	126.07	109.50
48	A2	289	A	C1'-C2'-O2'	-7.53	88.01	110.60
48	A2	912	C	O3'-P-O5'	-7.51	89.72	104.00
48	A2	965	G	O3'-P-O5'	-7.51	89.73	104.00
49	B1	238	C	C2'-C3'-O3'	-7.51	92.98	109.50
49	B1	741	C	P-O5'-C5'	-7.51	108.89	120.90
49	B1	1557	C	C2'-C3'-O3'	-7.51	92.99	109.50
1	A3	93	C	C4'-C3'-O3'	-7.50	93.65	109.40
2	A4	81	G	P-O3'-C3'	-7.50	110.70	119.70
48	A2	681	A	C2'-C3'-O3'	-7.49	93.01	109.50
48	A2	968	C	P-O3'-C3'	-7.49	110.71	119.70
48	A2	2457	C	P-O3'-C3'	-7.49	110.71	119.70
48	A2	1742	G	C8-N9-C1'	7.49	136.74	127.00
48	A2	4916	C	P-O3'-C3'	-7.48	110.72	119.70
48	A2	1743	G	O4'-C1'-N9	7.48	114.18	108.20
48	A2	49	U	C3'-C2'-O2'	-7.48	91.62	113.30
48	A2	2689	C	C5'-C4'-O4'	-7.48	100.13	109.10
48	A2	229	G	C5'-C4'-C3'	7.46	127.94	116.00
1	A3	123	U	O4'-C1'-N1	7.45	114.16	108.20
48	A2	4828	G	C1'-C2'-O2'	-7.45	88.24	110.60
48	A2	49	U	P-O3'-C3'	-7.45	110.76	119.70
49	B1	1620	A	C2'-C3'-O3'	-7.45	93.12	109.50
48	A2	4720	U	P-O3'-C3'	7.44	128.62	119.70
49	B1	1487	A	C4'-C3'-O3'	-7.44	93.78	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	494	G	O3'-P-O5'	7.43	118.12	104.00
2	A4	6	C	P-O3'-C3'	7.41	128.60	119.70
48	A2	191	C	C2'-C3'-O3'	7.40	125.78	109.50
48	A2	3877	A	C3'-C2'-O2'	-7.39	91.86	113.30
1	A3	13	G	O4'-C1'-N9	7.39	114.11	108.20
48	A2	2688	C	C2'-C3'-O3'	7.39	125.75	109.50
48	A2	3877	A	C5'-C4'-C3'	7.39	127.82	116.00
48	A2	4686	A	O5'-C5'-C4'	-7.38	97.67	111.70
48	A2	1615	G	P-O3'-C3'	7.38	128.55	119.70
49	B1	416	U	O3'-P-O5'	-7.38	89.98	104.00
49	B1	881	G	C2'-C3'-O3'	7.38	125.73	109.50
48	A2	3613	A	C5'-C4'-O4'	-7.37	100.25	109.10
49	B1	1623	A	O3'-P-O5'	-7.37	90.00	104.00
48	A2	2492	A	P-O3'-C3'	-7.37	110.86	119.70
48	A2	1433	C	OP2-P-O3'	7.36	121.39	105.20
49	B1	1389	C	P-O3'-C3'	7.36	128.53	119.70
49	B1	407	G	P-O3'-C3'	-7.36	110.87	119.70
48	A2	2425	C	P-O3'-C3'	7.36	128.53	119.70
49	B1	880	G	O4'-C1'-N9	7.35	114.08	108.20
49	B1	15	U	P-O3'-C3'	7.34	128.51	119.70
49	B1	289	G	P-O3'-C3'	-7.34	110.89	119.70
1	A3	94	G	P-O5'-C5'	-7.34	109.16	120.90
49	B1	876	C	C2'-C3'-O3'	7.34	125.65	109.50
48	A2	3590	G	O5'-P-OP2	-7.33	99.10	105.70
48	A2	959	C	C4'-C3'-O3'	7.31	127.63	113.00
45	Aq	109	ILE	CA-CB-CG1	7.31	124.89	111.00
1	A3	118	C	P-O3'-C3'	-7.31	110.93	119.70
48	A2	5007	G	N9-C1'-C2'	7.30	123.49	114.00
49	B1	745	C	C2'-C3'-O3'	7.30	125.55	109.50
49	B1	356	C	P-O3'-C3'	7.29	128.45	119.70
48	A2	2335	U	OP2-P-O3'	7.28	121.21	105.20
49	B1	1600	G	O4'-C1'-N9	7.27	114.02	108.20
48	A2	2673	G	C4'-C3'-O3'	-7.27	94.14	109.40
48	A2	4597	A	O4'-C1'-N9	7.26	114.01	108.20
48	A2	2700	G	P-O3'-C3'	-7.26	110.99	119.70
49	B1	892	U	C2'-C3'-O3'	7.26	125.47	109.50
48	A2	959	C	C5'-C4'-O4'	7.26	117.81	109.10
48	A2	736	G	P-O3'-C3'	-7.25	111.00	119.70
48	A2	676	G	O5'-P-OP2	7.25	119.40	110.70
49	B1	1621	U	P-O5'-C5'	-7.24	109.31	120.90
48	A2	4827	U	C4'-C3'-C2'	-7.24	95.36	102.60
45	Aq	37	LEU	CB-CG-CD1	7.23	123.29	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	2569	G	P-O3'-C3'	-7.23	111.03	119.70
49	B1	688	U	O5'-C5'-C4'	7.22	125.42	111.70
48	A2	4826	G	C3'-C2'-O2'	-7.22	92.37	113.30
49	B1	690	G	C5'-C4'-C3'	7.22	127.55	116.00
49	B1	915	G	O5'-C5'-C4'	7.20	125.39	111.70
48	A2	4715	U	C2'-C3'-O3'	-7.20	93.66	109.50
49	B1	361	U	O3'-P-O5'	7.20	117.68	104.00
49	B1	1526	G	P-O3'-C3'	-7.20	111.06	119.70
49	B1	1624	U	P-O5'-C5'	-7.20	109.38	120.90
48	A2	4841	C	P-O3'-C3'	7.20	128.34	119.70
48	A2	4717	G	O3'-P-O5'	-7.19	90.33	104.00
49	B1	396	U	P-O3'-C3'	-7.19	111.07	119.70
49	B1	1396	A	O4'-C1'-N9	7.19	113.95	108.20
48	A2	1202	G	O4'-C1'-N9	7.19	113.95	108.20
49	B1	790	C	O5'-P-OP1	-7.18	99.23	105.70
48	A2	1274	G	P-O3'-C3'	-7.18	111.09	119.70
48	A2	4980	U	OP2-P-O3'	7.17	120.98	105.20
49	B1	426	A	P-O3'-C3'	7.17	128.31	119.70
49	B1	799	U	N1-C1'-C2'	7.15	123.30	114.00
48	A2	4828	G	C3'-C2'-O2'	-7.15	92.56	113.30
48	A2	498	G	O4'-C1'-N9	7.14	113.92	108.20
48	A2	736	G	C1'-C2'-O2'	-7.14	89.17	110.60
49	B1	838	G	C5'-C4'-O4'	7.14	117.67	109.10
49	B1	368	U	O4'-C1'-N1	-7.14	102.49	108.20
48	A2	2245	C	O5'-P-OP2	-7.14	99.28	105.70
49	B1	809	A	P-O3'-C3'	-7.14	111.14	119.70
49	B1	737	G	O5'-P-OP2	-7.13	99.28	105.70
49	B1	183	G	O5'-P-OP2	7.13	119.26	110.70
49	B1	1105	G	C3'-C2'-O2'	-7.13	92.62	113.30
48	A2	286	G	C5'-C4'-O4'	7.13	117.65	109.10
48	A2	2245	C	O5'-P-OP1	-7.12	99.29	105.70
48	A2	4665	U	OP2-P-O3'	7.12	120.87	105.20
49	B1	1621	U	C4'-C3'-O3'	7.12	127.24	113.00
49	B1	358	C	P-O3'-C3'	-7.12	111.16	119.70
48	A2	3787	A	OP2-P-O3'	7.11	120.85	105.20
49	B1	841	G	O4'-C1'-N9	7.11	113.89	108.20
48	A2	3681	G	P-O3'-C3'	7.11	128.23	119.70
48	A2	1965	A	P-O3'-C3'	-7.11	111.17	119.70
49	B1	790	C	O5'-P-OP2	-7.11	99.30	105.70
48	A2	138	C	O4'-C4'-C3'	-7.10	96.90	104.00
48	A2	4685	A	O3'-P-O5'	7.09	117.47	104.00
84	Bx	46	U	C5'-C4'-C3'	-7.08	104.67	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	Bx	46	U	P-O5'-C5'	-7.08	109.58	120.90
2	A4	67	C	P-O3'-C3'	-7.08	111.21	119.70
83	Bv	34	G	O5'-P-OP2	-7.08	99.33	105.70
49	B1	737	G	O5'-P-OP1	-7.07	99.34	105.70
48	A2	3835	C	P-O3'-C3'	7.07	128.18	119.70
48	A2	2859	U	C2'-C3'-O3'	-7.07	93.95	109.50
49	B1	226	A	O4'-C1'-N9	-7.06	102.55	108.20
48	A2	3592	A	P-O3'-C3'	7.05	128.16	119.70
48	A2	1342	G	O4'-C4'-C3'	7.04	111.73	106.10
49	B1	1484	A	P-O3'-C3'	-7.04	111.25	119.70
48	A2	2245	C	P-O3'-C3'	-7.04	111.25	119.70
48	A2	3684	U	C5'-C4'-C3'	-7.04	104.74	116.00
48	A2	4722	G	P-O3'-C3'	-7.04	111.26	119.70
48	A2	4706	A	P-O3'-C3'	7.04	128.14	119.70
48	A2	2860	A	C2'-C3'-O3'	-7.03	94.05	109.50
48	A2	4596	U	O4'-C1'-N1	7.02	113.82	108.20
1	A3	150	C	OP2-P-O3'	7.02	120.65	105.20
49	B1	1557	C	O5'-C5'-C4'	-7.02	98.36	111.70
48	A2	3612	U	C5'-C4'-O4'	7.02	117.52	109.10
49	B1	852	G	P-O5'-C5'	-7.02	109.67	120.90
49	B1	871	U	O4'-C1'-N1	7.02	113.81	108.20
48	A2	4140	A	P-O3'-C3'	7.01	128.11	119.70
48	A2	43	U	C5'-C4'-C3'	7.01	127.22	116.00
48	A2	2617	G	C5'-C4'-C3'	7.01	127.21	116.00
49	B1	902	G	C4'-C3'-O3'	7.00	127.01	113.00
48	A2	2608	C	C4'-C3'-O3'	7.00	127.01	113.00
48	A2	1225	G	P-O5'-C5'	-7.00	109.70	120.90
48	A2	682	U	C5'-C4'-O4'	7.00	117.50	109.10
48	A2	699	G	O4'-C1'-N9	7.00	113.80	108.20
49	B1	1290	G	C5'-C4'-O4'	7.00	117.50	109.10
48	A2	1260	G	C5'-C4'-O4'	-6.99	100.71	109.10
49	B1	1454	A	O5'-C5'-C4'	6.99	124.98	111.70
48	A2	2325	C	C1'-C2'-O2'	-6.99	89.64	110.60
48	A2	50	C	C3'-C2'-O2'	-6.98	93.05	113.30
48	A2	961	C	C1'-C2'-O2'	6.98	131.55	110.60
49	B1	915	G	O4'-C1'-N9	6.98	113.78	108.20
48	A2	4459	U	OP2-P-O3'	6.98	120.55	105.20
48	A2	1071	C	P-O3'-C3'	-6.97	111.33	119.70
48	A2	2273	G	O4'-C1'-N9	6.97	113.78	108.20
48	A2	2480	C	OP2-P-O3'	6.97	120.54	105.20
48	A2	257	G	O5'-P-OP1	-6.97	99.43	105.70
1	A3	124	U	OP2-P-O3'	6.97	120.53	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	B1	370	G	O4'-C1'-N9	-6.97	102.62	108.20
48	A2	3612	U	O4'-C4'-C3'	6.96	111.67	106.10
48	A2	1271	G	P-O3'-C3'	6.96	128.05	119.70
48	A2	68	U	OP2-P-O3'	6.96	120.50	105.20
1	A3	80	A	O4'-C1'-N9	6.94	113.75	108.20
2	A4	15	C	C4'-C3'-O3'	6.94	126.88	113.00
48	A2	727	C	C2'-C3'-O3'	6.92	124.78	113.70
48	A2	1973	U	P-O3'-C3'	-6.92	111.39	119.70
48	A2	2325	C	P-O3'-C3'	6.92	128.01	119.70
49	B1	144	U	P-O3'-C3'	6.92	128.00	119.70
49	B1	738	C	P-O5'-C5'	-6.92	109.83	120.90
1	A3	150	C	OP1-P-O3'	-6.91	90.00	105.20
48	A2	131	C	O5'-P-OP2	-6.91	99.48	105.70
48	A2	2690	G	C4'-C3'-O3'	6.91	126.81	113.00
48	A2	2269	C	P-O3'-C3'	6.91	127.99	119.70
48	A2	4682	C	O3'-P-O5'	-6.90	90.89	104.00
49	B1	368	U	O5'-P-OP1	-6.90	99.49	105.70
48	A2	2458	G	P-O3'-C3'	-6.89	111.43	119.70
48	A2	356	A	P-O3'-C3'	-6.89	111.43	119.70
45	Aq	112	ILE	CG1-CB-CG2	-6.89	96.25	111.40
48	A2	1296	C	C1'-C2'-O2'	-6.88	89.95	110.60
48	A2	680	C	O4'-C4'-C3'	-6.88	97.12	104.00
49	B1	1284	A	C4'-C3'-O3'	-6.87	94.97	109.40
49	B1	692	G	P-O5'-C5'	6.87	131.88	120.90
48	A2	1589	C	P-O3'-C3'	6.85	127.92	119.70
48	A2	3605	G	O4'-C1'-N9	6.85	113.68	108.20
49	B1	1395	C	OP2-P-O3'	6.85	120.27	105.20
45	Aq	75	PRO	N-CA-CB	6.85	111.52	103.30
49	B1	891	G	P-O5'-C5'	-6.84	109.96	120.90
48	A2	257	G	N9-C1'-C2'	-6.84	104.48	112.00
49	B1	1555	U	C5'-C4'-O4'	6.84	117.30	109.10
48	A2	1880	G	P-O3'-C3'	6.83	127.90	119.70
48	A2	210	G	OP2-P-O3'	6.83	120.23	105.20
49	B1	656	G	C3'-C2'-O2'	-6.83	93.50	113.30
49	B1	1624	U	O5'-C5'-C4'	6.83	124.67	111.70
48	A2	3922	G	P-O3'-C3'	-6.82	111.51	119.70
48	A2	4045	U	P-O3'-C3'	-6.82	111.52	119.70
48	A2	463	C	C5'-C4'-O4'	-6.82	100.92	109.10
48	A2	2282	C	P-O3'-C3'	-6.81	111.52	119.70
48	A2	731	G	O3'-P-O5'	-6.81	91.06	104.00
48	A2	1061	A	P-O3'-C3'	-6.81	111.53	119.70
50	BA	113	GLN	N-CA-C	6.80	129.37	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	B1	847	A	C3'-C2'-O2'	-6.80	93.59	113.30
47	Au	48	ARG	NE-CZ-NH2	-6.79	116.91	120.30
49	B1	1447	G	O3'-P-O5'	6.78	116.88	104.00
2	A4	9	C	O4'-C1'-N1	6.78	113.62	108.20
49	B1	177	G	P-O3'-C3'	-6.78	111.56	119.70
49	B1	804	U	C5'-C4'-C3'	-6.78	105.15	116.00
48	A2	1741	G	C5'-C4'-O4'	-6.78	100.97	109.10
49	B1	738	C	C4'-C3'-O3'	-6.78	95.17	109.40
48	A2	3617	A	O4'-C1'-N9	-6.77	102.78	108.20
48	A2	1225	G	OP1-P-OP2	-6.77	109.44	119.60
48	A2	201	U	P-O3'-C3'	-6.77	111.58	119.70
49	B1	657	U	C3'-C2'-O2'	-6.77	93.67	113.30
48	A2	191	C	O5'-C5'-C4'	-6.77	98.84	111.70
48	A2	400	C	O3'-P-O5'	-6.77	91.14	104.00
48	A2	3669	G	P-O3'-C3'	-6.77	111.58	119.70
48	A2	1752	A	N9-C1'-C2'	-6.76	104.56	112.00
49	B1	638	C	O3'-P-O5'	6.76	116.85	104.00
48	A2	2820	G	O4'-C1'-N9	6.76	113.61	108.20
2	A4	35	U	P-O3'-C3'	-6.75	111.60	119.70
48	A2	4040	U	P-O3'-C3'	-6.75	111.60	119.70
45	Aq	87	GLU	C-N-CD	-6.75	105.75	120.60
48	A2	2747	C	C3'-C2'-O2'	-6.75	93.72	113.30
49	B1	1	U	O4'-C1'-N1	6.75	113.60	108.20
49	B1	1284	A	P-O5'-C5'	-6.75	110.10	120.90
49	B1	1785	C	P-O3'-C3'	-6.75	111.60	119.70
49	B1	689	U	O3'-P-O5'	-6.75	91.18	104.00
48	A2	320	C	P-O3'-C3'	6.74	127.79	119.70
48	A2	1849	A	P-O3'-C3'	-6.74	111.61	119.70
48	A2	4048	C	P-O3'-C3'	-6.74	111.61	119.70
48	A2	737	A	O5'-P-OP2	6.73	118.78	110.70
65	BP	68	PRO	C-N-CD	6.73	142.53	128.40
49	B1	308	G	C4'-C3'-O3'	-6.73	95.28	109.40
49	B1	1289	U	N1-C1'-C2'	6.72	122.74	114.00
48	A2	4714	U	C3'-C2'-O2'	-6.72	93.82	113.30
48	A2	712	G	O4'-C1'-N9	6.72	113.57	108.20
48	A2	2292	A	O4'-C1'-N9	6.72	113.57	108.20
49	B1	1745	A	P-O3'-C3'	6.71	127.76	119.70
49	B1	1777	G	N9-C1'-C2'	-6.71	104.62	112.00
1	A3	111	U	O3'-P-O5'	6.70	116.74	104.00
48	A2	912	C	OP2-P-O3'	6.70	119.95	105.20
48	A2	1974	C	O4'-C1'-N1	6.70	113.56	108.20
48	A2	3597	G	O5'-C5'-C4'	6.70	124.44	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	B1	1421	A	P-O3'-C3'	-6.70	111.66	119.70
48	A2	2860	A	C5'-C4'-O4'	6.69	117.13	109.10
49	B1	1785	C	C5'-C4'-C3'	-6.69	105.29	116.00
48	A2	506	U	P-O3'-C3'	-6.69	111.67	119.70
48	A2	3788	A	O4'-C1'-N9	-6.69	102.85	108.20
48	A2	4053	U	P-O3'-C3'	6.69	127.72	119.70
48	A2	5026	G	P-O3'-C3'	-6.69	111.67	119.70
48	A2	1053	G	O4'-C1'-N9	6.68	113.54	108.20
1	A3	124	U	OP1-P-O3'	-6.67	90.52	105.20
48	A2	464	A	O4'-C4'-C3'	-6.67	97.33	104.00
48	A2	3867	C	C4'-C3'-O3'	-6.67	95.39	109.40
48	A2	2534	G	O4'-C1'-N9	6.67	113.53	108.20
48	A2	1756	C	P-O5'-C5'	-6.67	110.23	120.90
48	A2	1970	G	P-O5'-C5'	6.66	131.56	120.90
49	B1	447	A	O3'-P-O5'	-6.66	91.34	104.00
48	A2	2745	A	C2'-C3'-O3'	6.65	124.34	113.70
48	A2	461	U	O5'-C5'-C4'	-6.65	99.07	111.70
48	A2	640	G	O4'-C1'-N9	6.64	113.51	108.20
48	A2	2688	C	C4'-C3'-O3'	-6.64	95.45	109.40
48	A2	1742	G	O4'-C1'-N9	6.64	113.51	108.20
48	A2	970	C	C4'-C3'-O3'	6.64	126.27	113.00
65	BP	72	LYS	C-N-CD	6.64	142.34	128.40
48	A2	1741	G	O5'-C5'-C4'	-6.63	99.10	111.70
49	B1	225	G	C2'-C3'-O3'	6.63	124.31	113.70
48	A2	111	C	C5'-C4'-C3'	6.63	126.60	116.00
48	A2	4660	C	P-O3'-C3'	6.63	127.65	119.70
48	A2	4891	C	P-O3'-C3'	-6.63	111.75	119.70
49	B1	1194	A	P-O3'-C3'	6.63	127.65	119.70
2	A4	63	C	P-O3'-C3'	-6.62	111.75	119.70
48	A2	1261	C	O5'-P-OP2	-6.62	99.74	105.70
48	A2	3916	A	O3'-P-O5'	-6.62	91.41	104.00
48	A2	1845	G	O4'-C1'-N9	6.61	113.49	108.20
48	A2	4839	U	P-O3'-C3'	6.61	127.63	119.70
49	B1	903	A	C2'-C3'-O3'	-6.60	94.97	109.50
48	A2	3588	G	C4'-C3'-O3'	6.60	126.20	113.00
48	A2	1420	C	P-O3'-C3'	-6.59	111.79	119.70
48	A2	4418	C	P-O3'-C3'	6.59	127.61	119.70
48	A2	4842	G	O4'-C1'-N9	6.59	113.47	108.20
49	B1	744	G	C5'-C4'-O4'	6.59	117.01	109.10
48	A2	2826	G	O4'-C1'-N9	6.59	113.47	108.20
48	A2	733	G	O4'-C1'-N9	6.58	113.47	108.20
48	A2	4158	G	P-O3'-C3'	6.58	127.60	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A3	102	G	P-O3'-C3'	-6.58	111.81	119.70
48	A2	682	U	O5'-C5'-C4'	6.58	124.19	111.70
49	B1	86	C	O4'-C1'-N1	6.57	113.46	108.20
48	A2	227	G	O4'-C1'-N9	-6.57	102.94	108.20
48	A2	2820	G	P-O3'-C3'	-6.57	111.82	119.70
48	A2	724	A	O3'-P-O5'	6.57	116.47	104.00
48	A2	1614	A	O4'-C1'-N9	6.57	113.45	108.20
48	A2	2246	U	C1'-C2'-O2'	-6.57	90.90	110.60
49	B1	446	G	P-O3'-C3'	6.57	127.58	119.70
49	B1	691	G	C4'-C3'-O3'	6.56	126.13	113.00
48	A2	502	G	O4'-C1'-N9	6.56	113.45	108.20
48	A2	4059	G	OP2-P-O3'	6.56	119.63	105.20
1	A3	108	A	O5'-P-OP2	-6.55	99.80	105.70
84	Bx	45	U	O4'-C4'-C3'	6.55	111.34	106.10
49	B1	237	C	P-O3'-C3'	6.55	127.56	119.70
49	B1	1867	U	O4'-C1'-N1	-6.55	102.96	108.20
49	B1	113	G	O4'-C1'-N9	-6.54	102.97	108.20
49	B1	848	U	C1'-C2'-O2'	-6.54	90.97	110.60
48	A2	3596	G	N9-C1'-C2'	-6.54	104.81	112.00
49	B1	533	A	C2'-C3'-O3'	-6.53	95.13	109.50
49	B1	1559	C	C4'-C3'-O3'	-6.53	95.69	109.40
48	A2	1260	G	O4'-C1'-N9	6.53	113.42	108.20
48	A2	3791	G	P-O5'-C5'	-6.53	110.45	120.90
49	B1	1701	C	P-O3'-C3'	6.53	127.53	119.70
49	B1	1337	C	O4'-C1'-N1	6.53	113.42	108.20
49	B1	32	U	OP2-P-O3'	6.52	119.55	105.20
49	B1	887	U	O4'-C1'-N1	6.52	113.42	108.20
49	B1	397	G	OP2-P-O3'	6.52	119.54	105.20
49	B1	976	G	C5'-C4'-O4'	6.52	116.92	109.10
48	A2	2750	G	OP2-P-O3'	6.52	119.54	105.20
49	B1	1080	A	OP2-P-O3'	6.52	119.54	105.20
76	Ba	97	PRO	C-N-CD	6.52	142.09	128.40
48	A2	724	A	P-O3'-C3'	6.52	127.52	119.70
48	A2	1732	G	P-O3'-C3'	-6.51	111.89	119.70
48	A2	4602	C	P-O3'-C3'	-6.51	111.89	119.70
49	B1	677	G	OP2-P-O3'	6.51	119.52	105.20
48	A2	214	C	P-O3'-C3'	-6.50	111.89	119.70
49	B1	351	G	P-O3'-C3'	-6.50	111.90	119.70
48	A2	153	G	C3'-C2'-O2'	-6.50	94.46	113.30
48	A2	963	G	P-O3'-C3'	-6.50	111.90	119.70
1	A3	126	C	O4'-C1'-N1	6.49	113.39	108.20
48	A2	2278	G	P-O3'-C3'	6.49	127.49	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	B1	231	A	O4'-C1'-N9	6.49	113.39	108.20
49	B1	690	G	O4'-C1'-N9	6.49	113.39	108.20
49	B1	209	A	P-O3'-C3'	-6.48	111.93	119.70
49	B1	418	A	P-O3'-C3'	6.48	127.47	119.70
49	B1	1285	G	C4'-C3'-O3'	-6.48	95.80	109.40
48	A2	462	U	O3'-P-O5'	6.47	116.30	104.00
49	B1	749	U	C4'-C3'-O3'	-6.47	95.81	109.40
1	A3	34	U	N1-C1'-C2'	6.47	122.41	114.00
48	A2	1707	U	O4'-C1'-N1	6.46	113.37	108.20
49	B1	609	U	P-O3'-C3'	-6.46	111.95	119.70
48	A2	1350	C	C2'-C3'-O3'	6.46	124.03	113.70
48	A2	1280	U	P-O3'-C3'	-6.46	111.95	119.70
48	A2	1058	G	OP2-P-O3'	6.45	119.40	105.20
48	A2	2492	A	OP2-P-O3'	6.45	119.40	105.20
48	A2	2685	G	O5'-P-OP2	-6.45	99.89	105.70
48	A2	3737	A	O4'-C1'-N9	6.45	113.36	108.20
48	A2	2285	G	O4'-C1'-N9	6.45	113.36	108.20
49	B1	977	C	O5'-P-OP2	6.45	118.44	110.70
48	A2	1995	C	P-O3'-C3'	-6.45	111.96	119.70
49	B1	1031	A	OP2-P-O3'	6.44	119.38	105.20
48	A2	702	A	P-O3'-C3'	6.44	127.43	119.70
48	A2	1269	C	O4'-C1'-N1	6.44	113.35	108.20
48	A2	1954	G	O4'-C1'-N9	6.44	113.35	108.20
48	A2	1225	G	P-O3'-C3'	6.44	127.42	119.70
49	B1	680	G	P-O3'-C3'	6.43	127.42	119.70
49	B1	843	C	P-O3'-C3'	6.43	127.41	119.70
49	B1	409	C	O3'-P-O5'	-6.43	91.79	104.00
45	Aq	59	THR	CA-CB-CG2	6.42	121.39	112.40
48	A2	224	A	C4'-C3'-O3'	6.42	125.85	113.00
48	A2	3613	A	P-O5'-C5'	-6.42	110.63	120.90
48	A2	42	A	C5'-C4'-C3'	-6.41	105.74	116.00
48	A2	4959	U	P-O3'-C3'	-6.41	112.01	119.70
49	B1	1254	C	P-O3'-C3'	-6.41	112.01	119.70
48	A2	153	G	O5'-P-OP1	-6.41	99.93	105.70
49	B1	503	C	P-O3'-C3'	-6.41	112.01	119.70
48	A2	657	C	O4'-C1'-N1	6.40	113.32	108.20
84	Bx	45	U	C2'-C3'-O3'	-6.40	95.42	109.50
48	A2	1952	C	O5'-P-OP2	6.39	118.37	110.70
48	A2	1525	G	OP2-P-O3'	6.39	119.26	105.20
48	A2	2823	A	O4'-C1'-N9	6.39	113.31	108.20
49	B1	803	C	C2'-C3'-O3'	6.38	123.91	113.70
48	A2	221	U	C1'-C2'-O2'	-6.38	91.47	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	4486	G	P-O3'-C3'	-6.38	112.05	119.70
49	B1	231	A	O4'-C4'-C3'	-6.38	97.62	104.00
48	A2	3737	A	P-O5'-C5'	6.37	131.10	120.90
48	A2	116	G	P-O3'-C3'	6.36	127.33	119.70
49	B1	534	G	P-O5'-C5'	6.36	131.07	120.90
49	B1	1750	C	O4'-C4'-C3'	6.36	111.19	106.10
13	AK	2	PRO	CA-N-CD	-6.36	102.60	111.50
48	A2	4682	C	P-O3'-C3'	-6.36	112.07	119.70
48	A2	4695	C	P-O3'-C3'	6.36	127.33	119.70
48	A2	5007	G	O4'-C1'-N9	-6.36	103.12	108.20
49	B1	1312	G	P-O3'-C3'	6.36	127.33	119.70
48	A2	1974	C	P-O3'-C3'	-6.35	112.08	119.70
13	AK	25	PRO	N-CA-CB	6.35	110.92	103.30
49	B1	1415	C	P-O3'-C3'	-6.35	112.08	119.70
48	A2	3596	G	C4-N9-C1'	6.34	134.75	126.50
48	A2	191	C	C1'-C2'-O2'	-6.34	91.57	110.60
2	A4	79	U	O3'-P-O5'	6.34	116.04	104.00
48	A2	230	U	P-O3'-C3'	6.34	127.30	119.70
48	A2	1952	C	C2'-C3'-O3'	6.34	123.84	113.70
48	A2	400	C	OP2-P-O3'	6.33	119.13	105.20
49	B1	187	G	O4'-C1'-N9	6.33	113.27	108.20
48	A2	2690	G	O3'-P-O5'	6.33	116.03	104.00
48	A2	49	U	O5'-P-OP2	-6.33	100.00	105.70
49	B1	687	C	C4'-C3'-O3'	6.33	125.66	113.00
48	A2	1498	G	P-O5'-C5'	-6.33	110.78	120.90
48	A2	221	U	C2'-C3'-O3'	-6.32	95.59	109.50
48	A2	1308	C	C4'-C3'-O3'	-6.32	96.13	109.40
48	A2	2684	G	C4-N9-C1'	-6.32	118.29	126.50
49	B1	802	A	C2'-C3'-O3'	6.32	123.80	113.70
48	A2	225	C	O4'-C4'-C3'	-6.31	97.69	104.00
49	B1	742	U	P-O5'-C5'	-6.31	110.81	120.90
45	Aq	7	PRO	CA-N-CD	-6.30	102.67	111.50
48	A2	967	U	O3'-P-O5'	6.30	115.98	104.00
49	B1	791	C	C4'-C3'-O3'	-6.30	96.17	109.40
49	B1	370	G	C3'-C2'-O2'	-6.30	95.03	113.30
45	Aq	88	PRO	N-CA-CB	6.30	110.86	103.30
49	B1	861	A	C4'-C3'-O3'	-6.30	96.18	109.40
48	A2	893	C	P-O3'-C3'	-6.29	112.15	119.70
49	B1	1069	U	P-O3'-C3'	6.29	127.25	119.70
48	A2	496	C	O5'-C5'-C4'	-6.29	99.75	111.70
48	A2	405	G	O4'-C1'-N9	6.29	113.23	108.20
49	B1	356	C	O5'-P-OP1	6.29	118.24	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	2059	C	P-O3'-C3'	-6.28	112.16	119.70
48	A2	323	A	P-O5'-C5'	-6.28	110.85	120.90
48	A2	1226	C	O4'-C4'-C3'	-6.28	97.72	104.00
48	A2	2751	C	OP2-P-O3'	6.28	119.02	105.20
48	A2	50	C	O5'-C5'-C4'	-6.28	99.77	111.70
49	B1	1777	G	P-O5'-C5'	-6.28	110.86	120.90
49	B1	1290	G	P-O5'-C5'	6.28	130.94	120.90
66	BQ	43	GLU	C-N-CD	6.28	141.58	128.40
1	A3	36	G	C4'-C3'-O3'	-6.27	96.23	109.40
48	A2	300	A	P-O3'-C3'	6.26	127.22	119.70
49	B1	114	G	OP1-P-O3'	-6.26	91.42	105.20
48	A2	718	C	P-O3'-C3'	-6.26	112.19	119.70
49	B1	1825	A	C4'-C3'-O3'	6.26	125.52	113.00
49	B1	887	U	P-O5'-C5'	6.26	130.91	120.90
48	A2	640	G	P-O3'-C3'	-6.25	112.20	119.70
49	B1	1126	G	P-O3'-C3'	-6.25	112.20	119.70
48	A2	4895	C	C4'-C3'-O3'	-6.25	96.28	109.40
48	A2	4977	A	O4'-C1'-N9	6.25	113.20	108.20
49	B1	907	G	C5'-C4'-O4'	6.25	116.60	109.10
48	A2	4467	C	P-O3'-C3'	-6.25	112.20	119.70
48	A2	4317	G	O4'-C1'-N9	6.24	113.19	108.20
49	B1	985	G	O5'-P-OP1	-6.24	100.09	105.70
48	A2	1249	G	O4'-C1'-N9	6.23	113.19	108.20
48	A2	681	A	O4'-C4'-C3'	-6.23	97.77	104.00
48	A2	968	C	C2'-C3'-O3'	-6.23	95.79	109.50
48	A2	2680	U	P-O3'-C3'	-6.23	112.22	119.70
48	A2	4171	G	P-O3'-C3'	-6.23	112.22	119.70
48	A2	212	C	OP2-P-O3'	6.23	118.90	105.20
48	A2	16	G	O4'-C1'-N9	6.23	113.18	108.20
48	A2	183	G	O4'-C1'-N9	6.22	113.18	108.20
49	B1	900	C	C4'-C3'-O3'	-6.22	96.33	109.40
48	A2	2245	C	C4'-C3'-O3'	-6.22	96.34	109.40
48	A2	2285	G	P-O3'-C3'	6.21	127.16	119.70
1	A3	144	U	P-O3'-C3'	-6.21	112.25	119.70
2	A4	43	U	P-O3'-C3'	6.21	127.15	119.70
48	A2	681	A	C5'-C4'-O4'	6.21	116.55	109.10
48	A2	746	C	P-O3'-C3'	-6.21	112.25	119.70
48	A2	2324	G	P-O3'-C3'	6.21	127.15	119.70
49	B1	1784	G	C5'-C4'-C3'	-6.21	106.07	116.00
49	B1	874	G	C5'-C4'-O4'	6.20	116.54	109.10
48	A2	1197	C	P-O5'-C5'	6.20	130.82	120.90
48	A2	3619	A	O4'-C1'-N9	6.20	113.16	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	4410	G	P-O3'-C3'	6.20	127.14	119.70
49	B1	1289	U	C2'-C3'-O3'	-6.20	95.86	109.50
48	A2	1850	G	C1'-C2'-O2'	-6.19	92.02	110.60
48	A2	4717	G	C2'-C3'-O3'	6.19	123.61	113.70
48	A2	2794	A	C4'-C3'-O3'	-6.19	96.40	109.40
48	A2	62	A	O3'-P-O5'	-6.19	92.24	104.00
48	A2	104	G	P-O3'-C3'	-6.19	112.28	119.70
49	B1	1106	C	C5'-C4'-C3'	6.19	125.90	116.00
48	A2	242	C	P-O5'-C5'	-6.19	111.00	120.90
48	A2	3817	C	O4'-C1'-N1	6.19	113.15	108.20
48	A2	2689	C	N1-C1'-C2'	-6.18	105.20	112.00
65	BP	67	ALA	C-N-CD	6.18	141.39	128.40
48	A2	2618	U	C4'-C3'-O3'	-6.18	96.42	109.40
48	A2	5006	A	P-O3'-C3'	-6.18	112.29	119.70
48	A2	1252	G	P-O5'-C5'	-6.17	111.03	120.90
48	A2	2747	C	C4'-C3'-O3'	-6.17	96.45	109.40
48	A2	2673	G	C2'-C3'-O3'	-6.16	95.94	109.50
34	Af	59	THR	C-N-CD	6.16	141.34	128.40
48	A2	477	G	P-O3'-C3'	-6.16	112.31	119.70
48	A2	1194	G	O3'-P-O5'	6.16	115.71	104.00
48	A2	1265	G	C4'-C3'-O3'	-6.16	96.46	109.40
49	B1	370	G	C4'-C3'-O3'	6.15	125.30	113.00
5	AC	304	ALA	C-N-CD	6.15	141.31	128.40
49	B1	306	C	O4'-C4'-C3'	6.15	111.02	106.10
49	B1	1254	C	O4'-C1'-N1	6.15	113.12	108.20
49	B1	1288	U	P-O3'-C3'	-6.15	112.32	119.70
48	A2	212	C	OP1-P-O3'	-6.15	91.68	105.20
48	A2	4617	A	OP2-P-O3'	6.15	118.72	105.20
48	A2	5004	U	C1'-C2'-O2'	-6.14	92.17	110.60
48	A2	909	C	P-O3'-C3'	-6.14	112.33	119.70
48	A2	3771	A	C4'-C3'-O3'	6.14	125.27	113.00
48	A2	681	A	C4'-C3'-O3'	6.13	125.27	113.00
48	A2	57	G	C4'-C3'-O3'	-6.13	96.53	109.40
49	B1	1287	A	P-O5'-C5'	-6.13	111.09	120.90
49	B1	231	A	C2'-C3'-O3'	-6.13	96.02	109.50
48	A2	3596	G	C8-N9-C1'	-6.12	119.05	127.00
49	B1	1176	G	O4'-C1'-N9	6.12	113.09	108.20
48	A2	4725	U	C4'-C3'-O3'	-6.11	96.56	109.40
48	A2	2304	C	P-O3'-C3'	-6.11	112.36	119.70
49	B1	895	G	C5'-C4'-O4'	6.11	116.43	109.10
48	A2	1296	C	C2'-C3'-O3'	6.11	123.47	113.70
48	A2	4015	G	P-O3'-C3'	-6.11	112.38	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	960	G	O5'-P-OP1	6.10	118.02	110.70
33	Ae	5	ARG	C-N-CD	6.10	141.21	128.40
48	A2	4907	G	O3'-P-O5'	6.10	115.59	104.00
49	B1	91	A	O4'-C1'-N9	6.10	113.08	108.20
45	Aq	7	PRO	N-CA-CB	6.10	110.62	103.30
49	B1	110	U	OP2-P-O3'	6.09	118.61	105.20
48	A2	308	G	C3'-C2'-O2'	-6.09	95.64	113.30
49	B1	898	U	O5'-C5'-C4'	6.09	123.28	111.70
2	A4	114	U	OP2-P-O3'	6.09	118.60	105.20
48	A2	4017	A	C5'-C4'-C3'	6.09	125.74	116.00
49	B1	639	C	O5'-C5'-C4'	-6.08	100.14	111.70
48	A2	4925	A	O4'-C1'-N9	6.08	113.06	108.20
49	B1	1675	A	O4'-C1'-N9	6.08	113.06	108.20
49	B1	1481	G	O3'-P-O5'	6.07	115.54	104.00
48	A2	403	G	P-O3'-C3'	-6.07	112.41	119.70
48	A2	683	U	C5'-C4'-O4'	6.07	116.39	109.10
61	BL	33	LEU	C-N-CD	6.07	141.15	128.40
49	B1	1105	G	P-O5'-C5'	6.07	130.61	120.90
48	A2	1433	C	O3'-P-O5'	-6.07	92.47	104.00
48	A2	3597	G	O4'-C1'-N9	6.07	113.05	108.20
49	B1	1285	G	N9-C1'-C2'	-6.06	105.33	112.00
13	AK	73	PRO	N-CA-CB	6.06	110.58	103.30
1	A3	117	C	P-O3'-C3'	-6.06	112.43	119.70
48	A2	744	C	O4'-C1'-N1	6.06	113.05	108.20
70	BU	52	GLY	C-N-CD	6.06	141.12	128.40
48	A2	5025	U	OP1-P-O3'	6.05	118.52	105.20
13	AK	2	PRO	N-CA-CB	6.05	110.56	103.30
48	A2	508	U	C2'-C3'-O3'	6.05	123.38	113.70
48	A2	680	C	N1-C1'-C2'	-6.05	105.34	112.00
49	B1	322	C	C4'-C3'-O3'	-6.05	96.69	109.40
56	BG	173	ALA	C-N-CD	6.05	141.10	128.40
48	A2	2328	A	OP2-P-O3'	6.05	118.50	105.20
57	BH	101	LEU	C-N-CD	6.05	141.10	128.40
84	Bx	45	U	P-O5'-C5'	-6.04	111.23	120.90
49	B1	1285	G	C2'-C3'-O3'	-6.04	96.20	109.50
49	B1	918	U	P-O3'-C3'	-6.04	112.45	119.70
48	A2	967	U	C5'-C4'-O4'	6.04	116.34	109.10
49	B1	1777	G	C4'-C3'-O3'	-6.03	96.74	109.40
19	AQ	17	GLU	C-N-CD	6.03	141.05	128.40
49	B1	1700	C	C1'-C2'-O2'	-6.03	92.53	110.60
48	A2	3727	A	O5'-C5'-C4'	-6.02	100.25	111.70
48	A2	290	A	O4'-C1'-N9	-6.02	103.38	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	AK	108	PRO	N-CA-CB	6.02	110.52	103.30
28	AZ	36	ARG	C-N-CD	6.02	141.04	128.40
48	A2	1741	G	O5'-P-OP1	-6.02	100.28	105.70
49	B1	1826	G	C2'-C3'-O3'	6.02	123.33	113.70
48	A2	2690	G	P-O5'-C5'	-6.01	111.28	120.90
49	B1	370	G	C3'-C2'-C1'	-6.01	96.69	101.50
59	BJ	169	ARG	C-N-CD	6.01	141.03	128.40
49	B1	306	C	C3'-C2'-O2'	-6.01	95.86	113.30
48	A2	1586	G	OP2-P-O3'	6.01	118.43	105.20
49	B1	1278	A	OP2-P-O3'	6.00	118.41	105.20
13	AK	25	PRO	N-CD-CG	6.00	112.21	103.20
48	A2	968	C	O4'-C1'-N1	6.00	113.00	108.20
49	B1	1288	U	N1-C1'-C2'	6.00	121.80	114.00
48	A2	2794	A	C2'-C3'-O3'	5.99	123.29	113.70
14	AL	133	ALA	C-N-CD	5.99	140.98	128.40
48	A2	85	G	O4'-C1'-N9	5.99	112.99	108.20
48	A2	1845	G	P-O3'-C3'	-5.99	112.51	119.70
48	A2	2798	U	OP2-P-O3'	5.99	118.37	105.20
1	A3	34	U	P-O3'-C3'	5.98	126.88	119.70
48	A2	234	G	P-O3'-C3'	-5.98	112.52	119.70
2	A4	15	C	P-O5'-C5'	5.98	130.47	120.90
48	A2	1265	G	C2'-C3'-O3'	5.98	123.27	113.70
48	A2	4085	C	C4'-C3'-O3'	5.98	124.96	113.00
1	A3	111	U	C1'-C2'-O2'	-5.98	92.66	110.60
49	B1	793	G	O5'-C5'-C4'	-5.98	100.35	111.70
49	B1	976	G	P-O5'-C5'	5.97	130.46	120.90
48	A2	940	C	P-O5'-C5'	-5.97	111.35	120.90
48	A2	1992	C	P-O5'-C5'	5.97	130.44	120.90
48	A2	131	C	O5'-P-OP1	5.96	117.86	110.70
1	A3	153	C	O4'-C1'-N1	5.96	112.97	108.20
48	A2	279	G	O4'-C1'-N9	5.96	112.97	108.20
48	A2	959	C	C4'-C3'-C2'	-5.96	96.64	102.60
49	B1	1497	G	P-O5'-C5'	-5.96	111.37	120.90
49	B1	113	G	OP2-P-O3'	5.95	118.30	105.20
48	A2	4056	G	P-O3'-C3'	-5.94	112.57	119.70
49	B1	1287	A	C5'-C4'-O4'	5.94	116.23	109.10
48	A2	3731	A	N9-C1'-C2'	5.93	121.71	114.00
48	A2	1847	U	P-O3'-C3'	5.93	126.82	119.70
48	A2	4622	G	P-O3'-C3'	-5.93	112.58	119.70
48	A2	3790	G	C5'-C4'-O4'	5.93	116.22	109.10
48	A2	2690	G	C8-N9-C1'	5.92	134.70	127.00
48	A2	180	C	O3'-P-O5'	5.92	115.25	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	481	G	OP2-P-O3'	5.92	118.23	105.20
48	A2	4058	C	P-O3'-C3'	5.92	126.81	119.70
48	A2	680	C	C5'-C4'-C3'	-5.92	106.53	116.00
49	B1	319	C	O3'-P-O5'	-5.92	92.75	104.00
48	A2	663	C	O4'-C1'-N1	5.92	112.93	108.20
48	A2	933	C	O4'-C1'-N1	5.92	112.94	108.20
2	A4	75	G	C2'-C3'-O3'	-5.92	96.48	109.50
45	Aq	31	LYS	CB-CG-CD	5.91	126.97	111.60
48	A2	1352	C	P-O5'-C5'	5.91	130.36	120.90
48	A2	2673	G	C3'-C2'-O2'	-5.91	96.15	113.30
48	A2	3589	C	C4'-C3'-O3'	-5.91	96.99	109.40
48	A2	48	G	C4'-C3'-O3'	5.91	124.81	113.00
48	A2	229	G	C3'-C2'-O2'	-5.90	96.18	113.30
48	A2	965	G	C4'-C3'-O3'	-5.90	97.01	109.40
48	A2	1973	U	O4'-C1'-N1	-5.89	103.49	108.20
48	A2	221	U	P-O3'-C3'	-5.89	112.63	119.70
48	A2	1764	U	OP2-P-O3'	5.89	118.16	105.20
2	A4	115	A	P-O3'-C3'	-5.88	112.64	119.70
48	A2	1198	C	P-O5'-C5'	-5.88	111.50	120.90
48	A2	2685	G	O3'-P-O5'	5.88	115.16	104.00
45	Aq	89	PRO	N-CA-CB	5.87	110.35	103.30
49	B1	1286	G	P-O5'-C5'	5.87	130.29	120.90
48	A2	238	G	O3'-P-O5'	5.87	115.14	104.00
49	B1	887	U	N1-C1'-C2'	5.86	121.62	114.00
29	Aa	28	HIS	C-N-CD	5.86	140.71	128.40
49	B1	1125	C	P-O3'-C3'	-5.86	112.67	119.70
10	AH	99	PHE	C-N-CD	5.85	140.69	128.40
48	A2	1295	A	C1'-C2'-O2'	-5.85	93.04	110.60
48	A2	3683	A	O3'-P-O5'	-5.85	92.88	104.00
48	A2	50	C	O4'-C4'-C3'	-5.85	98.15	104.00
48	A2	1751	G	C4'-C3'-O3'	5.85	124.69	113.00
49	B1	803	C	O5'-C5'-C4'	-5.84	100.60	111.70
48	A2	1273	G	O4'-C1'-N9	5.84	112.87	108.20
48	A2	2246	U	C3'-C2'-O2'	-5.84	96.37	113.30
49	B1	1557	C	P-O5'-C5'	5.84	130.24	120.90
45	Aq	39	PRO	N-CA-CB	5.83	110.30	103.30
48	A2	485	G	O4'-C1'-N9	5.83	112.86	108.20
49	B1	202	G	P-O3'-C3'	-5.83	112.71	119.70
49	B1	975	G	C4'-C3'-O3'	-5.83	97.16	109.40
48	A2	248	C	P-O3'-C3'	-5.83	112.71	119.70
49	B1	398	A	P-O3'-C3'	-5.82	112.72	119.70
48	A2	138	C	N1-C1'-C2'	-5.82	105.60	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	AC	50	GLN	C-N-CD	5.81	140.61	128.40
48	A2	4708	C	O4'-C1'-N1	5.81	112.85	108.20
48	A2	3576	C	O4'-C1'-N1	5.81	112.85	108.20
49	B1	841	G	O4'-C4'-C3'	-5.81	98.19	104.00
48	A2	928	C	P-O3'-C3'	-5.81	112.73	119.70
48	A2	1742	G	P-O5'-C5'	-5.81	111.61	120.90
2	A4	70	G	O4'-C1'-N9	5.80	112.84	108.20
48	A2	5005	C	C2'-C3'-O3'	-5.80	96.73	109.50
48	A2	1200	G	P-O3'-C3'	5.80	126.66	119.70
48	A2	1918	C	O4'-C1'-N1	5.80	112.84	108.20
45	Aq	59	THR	CA-CB-OG1	-5.80	96.82	109.00
48	A2	193	C	P-O5'-C5'	-5.80	111.62	120.90
48	A2	3666	U	O4'-C1'-N1	5.80	112.84	108.20
1	A3	37	A	O4'-C1'-N9	-5.80	103.56	108.20
48	A2	3737	A	C5'-C4'-O4'	5.79	116.05	109.10
55	BF	107	ASN	C-N-CD	5.79	140.57	128.40
48	A2	718	C	O5'-P-OP1	5.79	117.65	110.70
48	A2	4924	A	O3'-P-O5'	-5.79	93.00	104.00
71	BV	13	VAL	C-N-CD	5.79	140.56	128.40
48	A2	2282	C	OP2-P-O3'	5.79	117.93	105.20
48	A2	2302	C	P-O3'-C3'	-5.79	112.75	119.70
49	B1	1105	G	O5'-P-OP2	5.79	117.64	110.70
1	A3	10	G	C5'-C4'-C3'	5.78	125.25	116.00
2	A4	3	C	O5'-C5'-C4'	-5.78	100.71	111.70
48	A2	222	G	O4'-C1'-N9	5.78	112.83	108.20
48	A2	2449	C	O4'-C1'-N1	-5.78	103.58	108.20
49	B1	306	C	P-O3'-C3'	-5.78	112.76	119.70
45	Aq	34	PRO	N-CA-CB	5.78	110.23	103.30
14	AL	11	LYS	C-N-CD	5.77	140.52	128.40
48	A2	4633	C	OP2-P-O3'	5.77	117.90	105.20
49	B1	306	C	C4'-C3'-O3'	5.77	124.54	113.00
14	AL	53	GLY	C-N-CD	5.77	140.52	128.40
48	A2	737	A	C2'-C3'-O3'	5.77	122.93	113.70
83	Bv	73	A	C3'-C2'-O2'	-5.77	96.57	113.30
48	A2	1191	G	P-O3'-C3'	5.77	126.62	119.70
5	AC	224	ILE	C-N-CD	5.77	140.51	128.40
48	A2	66	A	C3'-C2'-O2'	-5.77	96.58	113.30
48	A2	4533	A	P-O5'-C5'	-5.77	111.67	120.90
2	A4	47	G	P-O5'-C5'	-5.76	111.68	120.90
48	A2	1283	G	OP2-P-O3'	5.76	117.87	105.20
49	B1	239	C	C2'-C3'-O3'	-5.76	96.83	109.50
49	B1	460	A	OP2-P-O3'	5.76	117.87	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	3590	G	C3'-C2'-O2'	-5.76	96.60	113.30
48	A2	3795	A	P-O3'-C3'	5.76	126.61	119.70
48	A2	710	C	P-O3'-C3'	5.75	126.61	119.70
49	B1	1558	C	P-O3'-C3'	5.75	126.60	119.70
48	A2	3596	G	C4'-C3'-O3'	5.75	124.50	113.00
48	A2	1297	C	P-O5'-C5'	-5.75	111.70	120.90
48	A2	66	A	C2'-C3'-O3'	-5.75	96.86	109.50
49	B1	871	U	N1-C1'-C2'	5.75	121.47	114.00
2	A4	83	A	P-O3'-C3'	5.74	126.59	119.70
48	A2	43	U	P-O5'-C5'	-5.74	111.71	120.90
67	BR	121	GLN	C-N-CD	5.74	140.45	128.40
2	A4	113	G	P-O3'-C3'	-5.74	112.81	119.70
48	A2	717	G	C2'-C3'-O3'	5.74	122.88	113.70
48	A2	1193	C	OP2-P-O3'	5.74	117.82	105.20
48	A2	1308	C	P-O5'-C5'	-5.74	111.72	120.90
49	B1	746	C	C5'-C4'-C3'	-5.74	106.82	116.00
48	A2	931	A	N9-C1'-C2'	5.73	121.45	114.00
48	A2	18	C	P-O3'-C3'	5.73	126.57	119.70
49	B1	802	A	O5'-C5'-C4'	-5.73	100.82	111.70
67	BR	99	ASP	C-N-CD	5.73	140.43	128.40
48	A2	1351	A	P-O3'-C3'	-5.73	112.83	119.70
13	AK	79	LEU	C-N-CD	5.72	140.42	128.40
48	A2	4139	C	O4'-C1'-N1	5.72	112.78	108.20
49	B1	1475	G	OP2-P-O3'	5.72	117.79	105.20
48	A2	4010	C	P-O3'-C3'	5.72	126.56	119.70
48	A2	4989	G	P-O3'-C3'	5.72	126.57	119.70
1	A3	34	U	O5'-C5'-C4'	-5.72	100.84	111.70
48	A2	1317	A	O4'-C1'-N9	5.72	112.77	108.20
49	B1	1444	U	O5'-C5'-C4'	-5.72	100.84	111.70
49	B1	986	G	N9-C1'-C2'	-5.71	105.72	112.00
1	A3	127	U	O4'-C1'-N1	5.71	112.77	108.20
48	A2	464	A	O5'-C5'-C4'	-5.71	100.85	111.70
48	A2	1739	U	N1-C1'-C2'	-5.71	105.72	112.00
48	A2	221	U	P-O5'-C5'	-5.71	111.77	120.90
48	A2	932	U	N1-C1'-C2'	5.71	121.42	114.00
48	A2	1644	C	O3'-P-O5'	5.71	114.85	104.00
49	B1	39	A	P-O3'-C3'	5.71	126.55	119.70
48	A2	959	C	C1'-C2'-O2'	-5.71	93.48	110.60
48	A2	1771	C	O3'-P-O5'	5.71	114.84	104.00
48	A2	4597	A	C4'-C3'-O3'	-5.71	97.42	109.40
48	A2	1287	C	P-O3'-C3'	-5.71	112.85	119.70
19	AQ	155	ALA	C-N-CD	5.70	140.38	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	14	C	P-O3'-C3'	5.70	126.54	119.70
48	A2	908	C	P-O5'-C5'	5.70	130.02	120.90
48	A2	2269	C	OP2-P-O3'	5.70	117.74	105.20
48	A2	4704	G	O4'-C1'-N9	5.70	112.76	108.20
49	B1	56	G	P-O3'-C3'	5.70	126.54	119.70
48	A2	656	C	O4'-C1'-N1	5.70	112.76	108.20
48	A2	4599	G	O4'-C1'-N9	5.70	112.76	108.20
49	B1	112	U	O3'-P-O5'	5.70	114.82	104.00
49	B1	558	G	OP2-P-O3'	5.70	117.73	105.20
48	A2	3877	A	C4'-C3'-O3'	-5.69	97.44	109.40
67	BR	41	ILE	C-N-CD	5.69	140.35	128.40
48	A2	4462	U	P-O3'-C3'	-5.69	112.87	119.70
48	A2	507	U	O3'-P-O5'	5.69	114.80	104.00
21	AS	139	ARG	C-N-CD	5.68	140.34	128.40
48	A2	4606	G	O4'-C1'-N9	5.68	112.74	108.20
1	A3	34	U	C1'-C2'-O2'	5.67	127.62	110.60
73	BX	61	GLN	C-N-CD	5.67	140.31	128.40
48	A2	3597	G	C5'-C4'-C3'	5.67	125.06	116.00
19	AQ	72	LEU	C-N-CD	5.66	140.29	128.40
48	A2	1756	C	P-O3'-C3'	-5.66	112.90	119.70
50	BA	104	THR	C-N-CD	5.66	140.29	128.40
48	A2	3731	A	C2'-C3'-O3'	5.66	122.75	113.70
14	AL	130	LYS	C-N-CD	5.66	140.28	128.40
49	B1	416	U	OP2-P-O3'	5.66	117.64	105.20
48	A2	1712	U	OP2-P-O3'	5.66	117.64	105.20
2	A4	28	C	P-O3'-C3'	5.65	126.48	119.70
49	B1	29	G	OP2-P-O3'	5.65	117.62	105.20
49	B1	1289	U	P-O3'-C3'	-5.65	112.92	119.70
48	A2	1632	A	P-O5'-C5'	-5.64	111.87	120.90
48	A2	1244	G	O4'-C1'-N9	5.64	112.71	108.20
48	A2	58	G	O5'-C5'-C4'	-5.64	100.99	111.70
48	A2	4319	G	OP2-P-O3'	5.64	117.60	105.20
48	A2	150	G	C1'-O4'-C4'	-5.63	105.39	109.90
48	A2	2686	U	O5'-C5'-C4'	5.63	122.41	111.70
49	B1	601	G	P-O3'-C3'	5.63	126.46	119.70
48	A2	225	C	O4'-C1'-N1	5.63	112.71	108.20
48	A2	4997	U	P-O3'-C3'	5.63	126.46	119.70
49	B1	338	G	P-O3'-C3'	-5.63	112.95	119.70
49	B1	793	G	O4'-C1'-N9	5.63	112.70	108.20
1	A3	126	C	O3'-P-O5'	5.63	114.69	104.00
48	A2	673	C	O3'-P-O5'	5.63	114.69	104.00
48	A2	697	C	P-O3'-C3'	-5.62	112.95	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	B1	354	U	P-O3'-C3'	-5.62	112.96	119.70
49	B1	746	C	C2'-C3'-O3'	5.62	122.69	113.70
48	A2	1773	U	O4'-C1'-N1	5.62	112.69	108.20
48	A2	2680	U	O4'-C1'-N1	5.62	112.69	108.20
48	A2	2299	G	C2'-C3'-O3'	5.62	122.68	113.70
49	B1	792	C	C4'-C3'-O3'	5.61	124.23	113.00
61	BL	13	GLN	C-N-CD	5.61	140.19	128.40
48	A2	112	C	C3'-C2'-O2'	-5.61	97.03	113.30
49	B1	1553	C	O4'-C1'-N1	5.61	112.69	108.20
48	A2	309	G	C2'-C3'-O3'	5.61	122.67	113.70
48	A2	112	C	O5'-C5'-C4'	5.61	122.36	111.70
13	AK	73	PRO	N-CD-CG	5.61	111.61	103.20
49	B1	450	C	O5'-P-OP2	5.61	117.43	110.70
48	A2	1744	C	P-O5'-C5'	-5.60	111.93	120.90
48	A2	2270	G	P-O3'-C3'	-5.60	112.98	119.70
6	AD	20	PHE	CB-CG-CD2	-5.60	116.88	120.80
47	Au	41	TYR	CB-CG-CD2	-5.60	117.64	121.00
48	A2	4718	C	C4'-C3'-O3'	5.60	124.19	113.00
1	A3	85	U	C4'-C3'-O3'	-5.60	97.65	109.40
48	A2	168	U	O4'-C1'-N1	5.59	112.68	108.20
48	A2	654	G	O4'-C1'-N9	5.59	112.67	108.20
49	B1	898	U	P-O5'-C5'	-5.59	111.95	120.90
48	A2	1777	A	O4'-C1'-N9	5.59	112.67	108.20
49	B1	114	G	O3'-P-O5'	5.59	114.62	104.00
48	A2	1415	G	P-O3'-C3'	-5.59	112.99	119.70
48	A2	66	A	C5'-C4'-O4'	5.59	115.80	109.10
48	A2	1059	C	O4'-C1'-N1	5.59	112.67	108.20
47	Au	59	PRO	CA-N-CD	-5.58	103.68	111.50
48	A2	3925	A	P-O3'-C3'	5.58	126.39	119.70
49	B1	744	G	C4'-C3'-C2'	-5.58	97.03	102.60
49	B1	1337	C	P-O3'-C3'	5.58	126.39	119.70
48	A2	1727	G	O4'-C1'-N9	5.57	112.66	108.20
53	BD	79	PHE	C-N-CD	5.57	140.10	128.40
38	Aj	83	THR	C-N-CD	5.57	140.10	128.40
48	A2	3877	A	P-O3'-C3'	5.57	126.39	119.70
48	A2	4041	U	OP2-P-O3'	5.57	117.46	105.20
48	A2	4896	A	O5'-C5'-C4'	-5.57	101.12	111.70
48	A2	660	C	C4'-C3'-O3'	-5.57	97.70	109.40
48	A2	1878	A	O3'-P-O5'	-5.57	93.42	104.00
48	A2	4326	G	O4'-C1'-N9	5.57	112.66	108.20
49	B1	836	G	C5'-C4'-O4'	-5.57	102.42	109.10
7	AE	121	VAL	C-N-CD	5.57	140.09	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
63	BN	81	ALA	C-N-CD	5.57	140.09	128.40
48	A2	4514	U	C2'-C3'-O3'	5.56	122.60	113.70
48	A2	5	A	O3'-P-O5'	5.56	114.56	104.00
48	A2	701	G	P-O3'-C3'	5.56	126.37	119.70
48	A2	732	C	OP2-P-O3'	5.56	117.43	105.20
49	B1	306	C	C4'-C3'-C2'	-5.56	97.04	102.60
48	A2	219	C	O4'-C1'-N1	5.55	112.64	108.20
48	A2	4617	A	OP1-P-O3'	-5.55	92.98	105.20
49	B1	1154	U	C4'-C3'-O3'	-5.55	97.73	109.40
49	B1	1444	U	C4'-C3'-O3'	5.55	124.10	113.00
48	A2	2688	C	O5'-C5'-C4'	-5.54	101.17	111.70
49	B1	239	C	O4'-C1'-N1	5.54	112.63	108.20
48	A2	1711	A	O3'-P-O5'	-5.54	93.47	104.00
68	BS	73	ASN	C-N-CD	5.54	140.03	128.40
48	A2	727	C	P-O5'-C5'	-5.54	112.04	120.90
48	A2	1937	A	O4'-C1'-N9	5.54	112.63	108.20
48	A2	939	G	O5'-C5'-C4'	-5.53	101.19	111.70
48	A2	3818	C	P-O3'-C3'	-5.53	113.06	119.70
48	A2	251	G	P-O3'-C3'	5.53	126.34	119.70
49	B1	691	G	P-O5'-C5'	5.53	129.75	120.90
48	A2	447	G	C4'-C3'-O3'	5.53	124.05	113.00
49	B1	1447	G	O5'-C5'-C4'	-5.53	101.20	111.70
49	B1	1575	G	O4'-C1'-N9	5.53	112.62	108.20
48	A2	43	U	N1-C1'-C2'	-5.52	105.92	112.00
48	A2	1299	G	P-O3'-C3'	-5.52	113.08	119.70
2	A4	2	U	O3'-P-O5'	5.52	114.48	104.00
48	A2	934	C	OP2-P-O3'	5.52	117.34	105.20
48	A2	1743	G	P-O3'-C3'	-5.52	113.08	119.70
48	A2	4599	G	P-O3'-C3'	-5.52	113.08	119.70
48	A2	966	C	C2'-C3'-O3'	-5.52	97.36	109.50
48	A2	2687	U	C4'-C3'-O3'	-5.52	97.82	109.40
48	A2	3597	G	C4'-C3'-O3'	-5.51	97.82	109.40
1	A3	129	C	OP1-P-O3'	-5.51	93.08	105.20
1	A3	103	A	C4'-C3'-O3'	5.51	124.02	113.00
49	B1	1486	A	O4'-C1'-N9	5.51	112.61	108.20
49	B1	182	C	O4'-C1'-N1	5.50	112.60	108.20
48	A2	728	C	O4'-C1'-N1	5.50	112.60	108.20
45	Aq	30	PRO	N-CA-CB	5.50	109.90	103.30
48	A2	50	C	N1-C1'-C2'	-5.50	105.95	112.00
49	B1	238	C	O4'-C1'-N1	5.50	112.60	108.20
49	B1	1551	U	O4'-C1'-N1	5.50	112.60	108.20
49	B1	1645	C	O3'-P-O5'	5.50	114.45	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	1857	U	P-O3'-C3'	-5.50	113.10	119.70
48	A2	1919	C	O3'-P-O5'	-5.50	93.56	104.00
48	A2	3629	C	P-O3'-C3'	-5.50	113.11	119.70
48	A2	3739	U	N1-C1'-C2'	-5.50	105.95	112.00
48	A2	286	G	O4'-C1'-N9	-5.49	103.81	108.20
48	A2	1890	G	O4'-C1'-N9	5.49	112.59	108.20
48	A2	4987	C	O4'-C1'-N1	5.49	112.59	108.20
48	A2	919	A	OP2-P-O3'	5.49	117.27	105.20
49	B1	903	A	O5'-C5'-C4'	5.49	122.12	111.70
54	BE	82	TYR	C-N-CD	5.49	139.92	128.40
48	A2	5019	A	OP2-P-O3'	5.48	117.26	105.20
48	A2	3687	C	OP2-P-O3'	5.48	117.26	105.20
1	A3	33	G	C2'-C3'-O3'	-5.48	97.44	109.50
48	A2	2684	G	C1'-C2'-O2'	-5.48	94.17	110.60
48	A2	671	C	OP2-P-O3'	5.47	117.24	105.20
48	A2	301	A	O4'-C1'-N9	5.47	112.58	108.20
48	A2	1428	U	P-O3'-C3'	-5.47	113.13	119.70
48	A2	230	U	C5'-C4'-O4'	-5.47	102.53	109.10
48	A2	5005	C	C4'-C3'-O3'	5.47	123.94	113.00
49	B1	882	U	O4'-C1'-N1	5.47	112.58	108.20
48	A2	1743	G	O5'-P-OP1	5.47	117.26	110.70
49	B1	875	A	C4'-C3'-O3'	-5.47	97.92	109.40
48	A2	910	C	OP2-P-O3'	5.47	117.22	105.20
49	B1	743	U	O4'-C1'-N1	5.47	112.57	108.20
49	B1	1623	A	N9-C1'-C2'	5.47	121.11	114.00
48	A2	2256	C	C4'-C3'-O3'	-5.46	97.92	109.40
49	B1	887	U	O5'-C5'-C4'	-5.46	101.32	111.70
48	A2	149	U	O4'-C1'-N1	5.46	112.57	108.20
48	A2	1255	C	O5'-P-OP1	-5.46	100.79	105.70
7	AE	127	SER	N-CA-C	5.46	125.73	111.00
48	A2	1741	G	C1'-C2'-O2'	-5.46	94.23	110.60
49	B1	34	U	P-O3'-C3'	5.46	126.25	119.70
48	A2	1757	A	C5'-C4'-C3'	5.45	124.72	116.00
48	A2	1255	C	O5'-P-OP2	5.45	117.24	110.70
49	B1	881	G	O4'-C4'-C3'	5.45	110.46	106.10
48	A2	1799	U	O3'-P-O5'	5.45	114.36	104.00
49	B1	839	C	O5'-C5'-C4'	-5.45	101.34	111.70
49	B1	1599	U	O4'-C1'-N1	-5.45	103.84	108.20
49	B1	189	U	OP2-P-O3'	5.45	117.19	105.20
49	B1	321	C	P-O3'-C3'	5.45	126.24	119.70
48	A2	480	C	OP1-P-O3'	5.45	117.18	105.20
48	A2	4685	A	C3'-C2'-O2'	-5.45	97.51	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	3744	U	C4'-C3'-O3'	5.44	123.88	113.00
48	A2	4600	U	O3'-P-O5'	5.44	114.34	104.00
48	A2	5005	C	C5'-C4'-O4'	5.44	115.63	109.10
49	B1	1555	U	N1-C1'-C2'	5.44	121.07	114.00
48	A2	1753	U	P-O5'-C5'	-5.44	112.20	120.90
48	A2	1851	C	OP2-P-O3'	5.44	117.16	105.20
48	A2	3738	C	O5'-C5'-C4'	-5.44	101.37	111.70
48	A2	4726	A	C4'-C3'-O3'	5.44	123.87	113.00
49	B1	871	U	C4'-C3'-O3'	5.44	123.87	113.00
49	B1	1702	G	N9-C1'-C2'	-5.43	106.03	112.00
48	A2	2525	G	P-O3'-C3'	-5.43	113.19	119.70
48	A2	4726	A	C1'-C2'-O2'	-5.43	94.32	110.60
47	Au	48	ARG	NE-CZ-NH1	5.43	123.01	120.30
49	B1	1485	U	OP2-P-O3'	5.43	117.14	105.20
48	A2	746	C	O4'-C1'-N1	5.42	112.54	108.20
48	A2	656	C	OP2-P-O3'	5.42	117.13	105.20
48	A2	1337	A	O4'-C1'-N9	-5.42	103.86	108.20
48	A2	1990	A	O4'-C4'-C3'	-5.42	98.58	104.00
48	A2	1970	G	O4'-C1'-N9	5.42	112.53	108.20
48	A2	2282	C	O3'-P-O5'	-5.42	93.71	104.00
49	B1	1175	G	P-O3'-C3'	-5.41	113.20	119.70
48	A2	1425	C	P-O3'-C3'	-5.41	113.20	119.70
50	BA	110	ASN	C-N-CA	5.41	135.23	121.70
79	Bd	40	ARG	C-N-CA	-5.41	108.17	121.70
48	A2	2284	U	OP2-P-O3'	5.41	117.10	105.20
48	A2	3790	G	C2'-C3'-O3'	-5.41	97.60	109.50
49	B1	1580	A	O4'-C1'-N9	5.41	112.53	108.20
48	A2	137	G	N9-C1'-C2'	-5.41	106.05	112.00
49	B1	1475	G	P-O3'-C3'	-5.41	113.21	119.70
48	A2	4120	C	P-O3'-C3'	5.41	126.19	119.70
48	A2	892	C	P-O3'-C3'	-5.41	113.21	119.70
48	A2	1754	C	N1-C1'-C2'	-5.41	106.05	112.00
48	A2	1756	C	C4'-C3'-O3'	-5.41	98.05	109.40
48	A2	4039	U	O4'-C1'-N1	5.41	112.53	108.20
48	A2	4095	C	OP2-P-O3'	5.40	117.09	105.20
48	A2	2420	C	O4'-C1'-N1	5.40	112.52	108.20
49	B1	1287	A	O5'-C5'-C4'	5.40	121.96	111.70
1	A3	33	G	N9-C1'-C2'	-5.40	106.06	112.00
48	A2	192	C	C4'-C3'-O3'	-5.40	98.06	109.40
3	AA	247	ARG	N-CA-CB	-5.40	100.88	110.60
45	Aq	39	PRO	N-CD-CG	5.40	111.30	103.20
49	B1	1445	U	C5'-C4'-C3'	5.40	124.64	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	1711	A	OP2-P-O3'	5.39	117.07	105.20
48	A2	5005	C	O4'-C1'-N1	-5.39	103.88	108.20
48	A2	3930	U	O4'-C4'-C3'	-5.39	98.61	104.00
48	A2	4974	A	P-O3'-C3'	5.39	126.17	119.70
48	A2	290	A	O4'-C4'-C3'	5.39	110.41	106.10
49	B1	742	U	P-O3'-C3'	5.39	126.17	119.70
48	A2	4014	U	O4'-C1'-N1	5.38	112.51	108.20
48	A2	85	G	O5'-P-OP2	-5.38	100.86	105.70
48	A2	919	A	P-O3'-C3'	5.38	126.15	119.70
2	A4	22	A	P-O3'-C3'	5.37	126.15	119.70
48	A2	3668	U	P-O3'-C3'	-5.37	113.25	119.70
48	A2	3877	A	C1'-C2'-O2'	-5.37	94.48	110.60
48	A2	1333	C	P-O3'-C3'	-5.37	113.26	119.70
45	Aq	71	ILE	CA-CB-CG2	-5.37	100.17	110.90
48	A2	2251	C	O5'-C5'-C4'	-5.37	101.50	111.70
1	A3	110	U	C3'-C2'-O2'	-5.36	97.75	113.30
48	A2	931	A	C2'-C3'-O3'	-5.36	97.70	109.50
48	A2	138	C	C4'-C3'-O3'	-5.36	98.16	109.40
48	A2	1763	U	OP2-P-O3'	5.36	116.98	105.20
48	A2	2692	C	C5'-C4'-C3'	-5.35	107.43	116.00
47	Au	60	ARG	C-N-CD	5.35	139.64	128.40
49	B1	356	C	C3'-C2'-O2'	-5.35	97.78	113.30
48	A2	1254	G	O4'-C4'-C3'	-5.35	98.65	104.00
49	B1	1806	A	O4'-C1'-N9	5.35	112.48	108.20
48	A2	1920	A	P-O5'-C5'	5.35	129.46	120.90
48	A2	189	G	O4'-C1'-N9	5.35	112.48	108.20
13	AK	24	TYR	CB-CG-CD1	5.34	124.21	121.00
49	B1	428	U	C4'-C3'-O3'	-5.34	98.18	109.40
2	A4	60	G	P-O3'-C3'	-5.34	113.29	119.70
48	A2	24	G	P-O3'-C3'	5.34	126.11	119.70
48	A2	350	G	P-O3'-C3'	-5.34	113.29	119.70
48	A2	2457	C	OP2-P-O3'	5.34	116.95	105.20
48	A2	4461	G	OP2-P-O3'	5.34	116.94	105.20
49	B1	534	G	C5'-C4'-C3'	-5.34	107.46	116.00
49	B1	6	G	P-O3'-C3'	5.33	126.10	119.70
49	B1	320	G	O5'-C5'-C4'	5.33	121.84	111.70
49	B1	796	G	O4'-C4'-C3'	5.33	110.37	106.10
48	A2	4840	U	O4'-C1'-N1	5.33	112.47	108.20
49	B1	1278	A	P-O3'-C3'	5.33	126.10	119.70
48	A2	502	G	P-O3'-C3'	5.33	126.10	119.70
2	A4	117	G	O4'-C1'-N9	5.33	112.46	108.20
48	A2	1284	C	OP2-P-O3'	5.33	116.92	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	B1	620	G	C1'-O4'-C4'	-5.33	105.64	109.90
48	A2	1615	G	OP2-P-O3'	5.33	116.92	105.20
48	A2	1877	A	O5'-C5'-C4'	-5.33	101.58	111.70
48	A2	437	G	P-O3'-C3'	5.33	126.09	119.70
48	A2	699	G	P-O3'-C3'	-5.33	113.31	119.70
48	A2	2701	G	O3'-P-O5'	-5.33	93.88	104.00
48	A2	5020	G	C3'-C2'-C1'	-5.33	97.24	101.50
49	B1	321	C	C2'-C3'-O3'	-5.33	97.78	109.50
49	B1	802	A	N9-C1'-C2'	-5.32	106.14	112.00
2	A4	112	U	O3'-P-O5'	-5.32	93.89	104.00
48	A2	2690	G	C2'-C3'-O3'	5.32	122.21	113.70
48	A2	3732	C	P-O5'-C5'	-5.32	112.39	120.90
48	A2	3930	U	O4'-C1'-N1	5.32	112.45	108.20
49	B1	915	G	C2'-C3'-O3'	-5.32	97.80	109.50
49	B1	1129	G	O4'-C1'-N9	5.32	112.45	108.20
45	Aq	81	ILE	CA-CB-CG2	5.32	121.53	110.90
48	A2	1966	G	P-O3'-C3'	5.32	126.08	119.70
49	B1	301	A	P-O3'-C3'	-5.32	113.32	119.70
48	A2	1714	C	P-O3'-C3'	-5.31	113.33	119.70
48	A2	76	A	P-O3'-C3'	5.31	126.07	119.70
48	A2	4647	U	P-O3'-C3'	-5.31	113.33	119.70
79	Bd	21	CYS	CA-CB-SG	5.31	123.56	114.00
7	AE	108	LYS	C-N-CA	-5.31	108.43	121.70
2	A4	43	U	OP2-P-O3'	-5.30	93.53	105.20
48	A2	1992	C	O4'-C4'-C3'	-5.30	98.69	104.00
48	A2	4727	G	N9-C1'-C2'	-5.30	106.17	112.00
49	B1	848	U	C2'-C3'-O3'	5.30	122.19	113.70
47	Au	191	VAL	CA-CB-CG1	5.30	118.85	110.90
48	A2	672	G	OP2-P-O3'	5.30	116.86	105.20
48	A2	4599	G	O3'-P-O5'	-5.30	93.93	104.00
45	Aq	28	LEU	CB-CG-CD1	5.30	120.01	111.00
48	A2	194	A	O5'-P-OP1	-5.30	100.93	105.70
48	A2	4586	A	C1'-O4'-C4'	-5.30	105.66	109.90
49	B1	737	G	N9-C1'-C2'	-5.30	106.17	112.00
48	A2	289	A	C3'-C2'-O2'	-5.29	97.95	113.30
48	A2	2304	C	O4'-C1'-N1	5.29	112.43	108.20
48	A2	2377	U	OP2-P-O3'	5.29	116.84	105.20
48	A2	4726	A	C5'-C4'-C3'	5.29	124.47	116.00
48	A2	382	A	P-O5'-C5'	5.29	129.36	120.90
48	A2	3930	U	O5'-C5'-C4'	-5.29	101.66	111.70
48	A2	112	C	C1'-C2'-O2'	5.29	126.46	110.60
48	A2	2784	C	P-O3'-C3'	5.29	126.04	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	185	G	O3'-P-O5'	5.28	114.04	104.00
48	A2	4993	U	P-O3'-C3'	-5.28	113.36	119.70
48	A2	357	A	O5'-C5'-C4'	-5.28	101.66	111.70
48	A2	3618	A	O4'-C1'-N9	5.28	112.42	108.20
49	B1	663	C	OP2-P-O3'	5.27	116.80	105.20
14	AL	177	LYS	N-CA-C	5.27	125.24	111.00
48	A2	220	G	C4'-C3'-O3'	-5.27	98.33	109.40
48	A2	464	A	O4'-C1'-N9	5.27	112.42	108.20
48	A2	2693	G	P-O5'-C5'	-5.27	112.46	120.90
48	A2	1420	C	C4'-C3'-O3'	5.27	123.54	113.00
48	A2	4038	U	O4'-C1'-N1	5.27	112.42	108.20
48	A2	957	G	C5'-C4'-C3'	5.27	124.43	116.00
48	A2	638	G	O4'-C1'-N9	5.27	112.41	108.20
48	A2	1755	U	N1-C1'-C2'	-5.26	106.21	112.00
48	A2	3590	G	C4'-C3'-O3'	5.26	123.52	113.00
48	A2	676	G	O5'-P-OP1	-5.26	100.97	105.70
49	B1	744	G	C2'-C3'-O3'	-5.26	97.93	109.50
2	A4	48	G	P-O3'-C3'	-5.26	113.39	119.70
48	A2	2860	A	P-O5'-C5'	-5.26	112.49	120.90
48	A2	4666	C	OP2-P-O3'	5.26	116.76	105.20
49	B1	72	C	O3'-P-O5'	-5.26	94.01	104.00
49	B1	335	G	P-O3'-C3'	-5.25	113.39	119.70
48	A2	3789	U	O3'-P-O5'	-5.25	94.02	104.00
49	B1	920	A	P-O3'-C3'	5.25	126.00	119.70
48	A2	735	G	C2'-C3'-O3'	5.25	122.10	113.70
48	A2	2733	G	P-O3'-C3'	-5.25	113.40	119.70
49	B1	238	C	C5'-C4'-O4'	5.25	115.40	109.10
48	A2	1273	G	OP2-P-O3'	5.25	116.75	105.20
48	A2	4085	C	C3'-C2'-O2'	-5.25	98.07	113.30
48	A2	120	A	P-O5'-C5'	-5.25	112.50	120.90
48	A2	348	U	P-O3'-C3'	5.25	126.00	119.70
48	A2	200	U	OP2-P-O3'	5.25	116.74	105.20
48	A2	895	G	O4'-C1'-N9	5.24	112.39	108.20
48	A2	1421	U	O4'-C4'-C3'	-5.24	98.76	104.00
48	A2	5025	U	P-O3'-C3'	-5.24	113.41	119.70
2	A4	70	G	OP2-P-O3'	5.24	116.73	105.20
47	Au	187	VAL	CA-CB-CG2	5.24	118.76	110.90
48	A2	938	G	P-O3'-C3'	-5.24	113.41	119.70
48	A2	3588	G	P-O3'-C3'	-5.24	113.41	119.70
48	A2	65	A	O3'-P-O5'	-5.24	94.05	104.00
49	B1	880	G	O4'-C4'-C3'	-5.24	98.76	104.00
48	A2	1743	G	C4-N9-C1'	-5.23	119.70	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	948	G	O4'-C1'-N9	5.23	112.39	108.20
48	A2	1300	U	OP2-P-O3'	5.23	116.71	105.20
49	B1	45	A	P-O3'-C3'	-5.23	113.43	119.70
48	A2	650	C	OP2-P-O3'	5.22	116.69	105.20
48	A2	2750	G	O5'-C5'-C4'	-5.22	101.78	111.70
49	B1	1598	G	P-O5'-C5'	5.22	129.25	120.90
48	A2	905	G	C2'-C3'-O3'	5.22	122.05	113.70
48	A2	651	C	O3'-P-O5'	-5.22	94.08	104.00
48	A2	3683	A	P-O5'-C5'	5.22	129.25	120.90
48	A2	3877	A	O5'-C5'-C4'	5.22	121.61	111.70
48	A2	1799	U	O4'-C1'-N1	5.21	112.37	108.20
48	A2	1805	G	O4'-C1'-N9	5.21	112.37	108.20
48	A2	4123	G	O3'-P-O5'	5.21	113.90	104.00
2	A4	60	G	O4'-C1'-N9	5.21	112.37	108.20
48	A2	2608	C	P-O3'-C3'	-5.21	113.45	119.70
49	B1	111	A	OP2-P-O3'	5.21	116.66	105.20
49	B1	836	G	O3'-P-O5'	5.21	113.89	104.00
25	AW	89	ASP	CB-CG-OD2	5.20	122.98	118.30
28	AZ	91	LEU	N-CA-C	-5.20	96.96	111.00
48	A2	227	G	C2'-C3'-O3'	-5.20	98.06	109.50
48	A2	2830	G	O3'-P-O5'	5.20	113.88	104.00
47	Au	43	PRO	N-CA-CB	5.20	109.54	103.30
48	A2	2325	C	C2'-C3'-O3'	-5.20	98.07	109.50
49	B1	882	U	O5'-C5'-C4'	-5.19	101.83	111.70
50	BA	110	ASN	O-C-N	5.19	131.01	122.70
2	A4	4	U	P-O3'-C3'	-5.19	113.47	119.70
48	A2	503	A	OP2-P-O3'	5.19	116.62	105.20
49	B1	1124	C	P-O3'-C3'	-5.19	113.47	119.70
48	A2	1757	A	C4'-C3'-O3'	5.19	123.38	113.00
48	A2	3623	A	OP2-P-O3'	5.19	116.61	105.20
48	A2	959	C	O4'-C4'-C3'	-5.19	98.81	104.00
49	B1	1702	G	O4'-C4'-C3'	-5.18	98.82	104.00
1	A3	93	C	O5'-P-OP1	-5.18	101.04	105.70
48	A2	308	G	O5'-P-OP1	5.18	116.92	110.70
48	A2	1850	G	O4'-C1'-N9	-5.18	104.06	108.20
49	B1	1624	U	O5'-P-OP1	5.18	116.91	110.70
48	A2	2728	C	P-O3'-C3'	5.17	125.91	119.70
2	A4	60	G	O3'-P-O5'	-5.17	94.17	104.00
49	B1	907	G	O5'-C5'-C4'	5.17	121.53	111.70
48	A2	1284	C	O4'-C1'-N1	5.17	112.34	108.20
49	B1	1388	A	OP2-P-O3'	5.17	116.58	105.20
48	A2	2747	C	O3'-P-O5'	-5.17	94.18	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A4	39	C	OP2-P-O3'	5.17	116.57	105.20
48	A2	165	C	O4'-C1'-N1	5.17	112.33	108.20
48	A2	287	G	C1'-C2'-O2'	5.17	126.11	110.60
48	A2	1968	C	O4'-C1'-N1	5.17	112.33	108.20
48	A2	4694	G	OP2-P-O3'	5.17	116.57	105.20
49	B1	70	G	O4'-C1'-N9	5.17	112.33	108.20
49	B1	191	A	P-O3'-C3'	5.17	125.90	119.70
84	Bx	45	U	P-O3'-C3'	-5.17	113.50	119.70
48	A2	1755	U	O4'-C1'-N1	5.17	112.33	108.20
48	A2	1743	G	C8-N9-C1'	5.16	133.71	127.00
48	A2	1805	G	C1'-O4'-C4'	-5.16	105.77	109.90
49	B1	83	A	O4'-C1'-N9	5.16	112.33	108.20
49	B1	369	C	C5'-C4'-C3'	-5.16	107.74	116.00
48	A2	1944	C	P-O3'-C3'	-5.16	113.51	119.70
49	B1	38	A	OP2-P-O3'	5.15	116.54	105.20
48	A2	191	C	C5'-C4'-O4'	5.15	115.28	109.10
48	A2	2750	G	O3'-P-O5'	-5.15	94.21	104.00
48	A2	3604	C	OP2-P-O3'	5.15	116.52	105.20
7	AE	208	ILE	C-N-CD	5.14	139.20	128.40
47	Au	121	PRO	N-CA-CB	5.14	109.47	103.30
48	A2	1259	C	O3'-P-O5'	-5.14	94.23	104.00
48	A2	486	U	P-O3'-C3'	5.14	125.87	119.70
48	A2	1359	C	P-O3'-C3'	-5.14	113.53	119.70
48	A2	1957	G	OP2-P-O3'	5.14	116.51	105.20
48	A2	4826	G	C4'-C3'-O3'	-5.14	98.61	109.40
49	B1	357	C	C5'-C4'-C3'	5.14	124.22	116.00
20	AR	72	LYS	C-N-CA	5.14	133.09	122.30
84	Bx	43	U	N1-C1'-C2'	5.14	120.68	114.00
48	A2	3590	G	N9-C1'-C2'	5.14	120.68	114.00
45	Aq	129	ILE	CB-CG1-CD1	5.13	128.28	113.90
48	A2	726	G	P-O3'-C3'	-5.13	113.54	119.70
48	A2	2702	U	P-O3'-C3'	5.13	125.86	119.70
49	B1	871	U	C2'-C3'-O3'	-5.13	98.20	109.50
48	A2	2793	C	C4'-C3'-C2'	5.13	107.73	102.60
13	AK	11	SER	CA-CB-OG	5.13	125.05	111.20
48	A2	3629	C	O4'-C1'-N1	5.13	112.30	108.20
48	A2	3697	A	O3'-P-O5'	5.13	113.75	104.00
83	Bv	34	G	O5'-P-OP1	5.13	116.86	110.70
48	A2	15	A	OP2-P-O3'	5.12	116.47	105.20
48	A2	1841	U	O3'-P-O5'	5.12	113.73	104.00
76	Ba	97	PRO	CA-N-CD	-5.12	104.34	111.50
49	B1	688	U	N1-C1'-C2'	-5.12	106.37	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	68	U	O5'-P-OP2	-5.11	101.10	105.70
48	A2	1944	C	OP2-P-O3'	5.11	116.45	105.20
48	A2	4061	G	O4'-C1'-N9	5.11	112.29	108.20
48	A2	3876	A	C5'-C4'-O4'	5.11	115.23	109.10
49	B1	1104	G	P-O3'-C3'	-5.11	113.57	119.70
49	B1	801	U	O5'-C5'-C4'	-5.11	101.99	111.70
48	A2	919	A	O3'-P-O5'	-5.11	94.30	104.00
49	B1	930	C	P-O3'-C3'	-5.11	113.57	119.70
48	A2	1971	A	OP2-P-O3'	5.10	116.43	105.20
48	A2	2736	A	O3'-P-O5'	-5.10	94.30	104.00
48	A2	2781	C	OP2-P-O3'	5.10	116.43	105.20
49	B1	1279	C	P-O3'-C3'	5.10	125.82	119.70
48	A2	481	G	P-O3'-C3'	-5.10	113.58	119.70
49	B1	1701	C	C1'-C2'-O2'	-5.10	95.30	110.60
34	Af	107	PRO	CA-N-CD	-5.10	104.36	111.50
49	B1	897	U	O3'-P-O5'	-5.10	94.31	104.00
49	B1	1558	C	C4'-C3'-O3'	5.10	123.19	113.00
48	A2	703	C	P-O3'-C3'	-5.09	113.59	119.70
47	Au	94	ASN	CA-CB-CG	5.09	124.60	113.40
49	B1	915	G	O4'-C4'-C3'	-5.09	98.91	104.00
48	A2	71	C	C1'-C2'-O2'	-5.08	95.34	110.60
48	A2	949	C	P-O3'-C3'	5.08	125.80	119.70
49	B1	231	A	O5'-C5'-C4'	5.08	121.36	111.70
48	A2	3789	U	C4'-C3'-O3'	-5.08	98.73	109.40
48	A2	3597	G	C5'-C4'-O4'	5.08	115.20	109.10
49	B1	93	U	P-O3'-C3'	5.08	125.80	119.70
48	A2	4827	U	O3'-P-O5'	5.07	113.64	104.00
48	A2	7	C	C1'-C2'-O2'	5.07	125.81	110.60
48	A2	1709	U	P-O3'-C3'	5.07	125.79	119.70
48	A2	2860	A	O5'-C5'-C4'	5.07	121.33	111.70
48	A2	3588	G	C2'-C3'-O3'	-5.07	98.35	109.50
48	A2	4924	A	OP2-P-O3'	5.07	116.35	105.20
48	A2	3578	U	O5'-C5'-C4'	-5.06	102.08	111.70
49	B1	889	U	O4'-C1'-N1	5.06	112.25	108.20
49	B1	890	U	P-O3'-C3'	5.06	125.78	119.70
48	A2	2325	C	C5'-C4'-C3'	5.06	124.10	116.00
11	AI	39	LYS	N-CA-CB	-5.06	101.49	110.60
48	A2	2428	A	O4'-C1'-N9	5.06	112.25	108.20
48	A2	639	G	P-O3'-C3'	-5.06	113.63	119.70
49	B1	1284	A	P-O3'-C3'	5.06	125.77	119.70
49	B1	893	U	O5'-C5'-C4'	-5.06	102.09	111.70
48	A2	1277	A	O4'-C1'-N9	5.05	112.24	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	2539	C	P-O5'-C5'	-5.05	112.81	120.90
48	A2	3612	U	O3'-P-O5'	-5.05	94.40	104.00
49	B1	1153	C	C4'-C3'-O3'	5.05	123.11	113.00
49	B1	1389	C	O3'-P-O5'	5.05	113.60	104.00
66	BQ	44	PRO	CA-N-CD	-5.05	104.43	111.50
49	B1	691	G	O3'-P-O5'	5.05	113.60	104.00
49	B1	744	G	O4'-C1'-C2'	-5.05	100.75	105.80
48	A2	2422	G	OP2-P-O3'	5.05	116.31	105.20
49	B1	1679	A	O5'-C5'-C4'	-5.05	102.11	111.70
1	A3	135	C	OP2-P-O3'	5.05	116.30	105.20
48	A2	1752	A	P-O5'-C5'	5.05	128.97	120.90
48	A2	3586	G	O4'-C1'-N9	-5.05	104.16	108.20
49	B1	181	A	O3'-P-O5'	-5.05	94.41	104.00
49	B1	1080	A	O3'-P-O5'	-5.05	94.41	104.00
6	AD	20	PHE	CB-CG-CD1	5.04	124.33	120.80
48	A2	58	G	C2'-C3'-O3'	-5.04	98.40	109.50
49	B1	74	G	O4'-C1'-N9	5.04	112.23	108.20
13	AK	30	VAL	CA-CB-CG1	5.04	118.46	110.90
49	B1	898	U	C5'-C4'-O4'	5.04	115.15	109.10
48	A2	4406	C	O3'-P-O5'	-5.04	94.43	104.00
48	A2	309	G	N9-C1'-C2'	5.04	120.55	114.00
13	AK	108	PRO	N-CD-CG	5.03	110.75	103.20
48	A2	4685	A	O5'-P-OP1	5.03	116.74	110.70
49	B1	1555	U	O4'-C4'-C3'	5.03	110.13	106.10
49	B1	293	C	OP2-P-O3'	5.03	116.27	105.20
79	Bd	8	TRP	N-CA-CB	-5.03	101.55	110.60
48	A2	415	C	P-O3'-C3'	-5.03	113.67	119.70
48	A2	1297	C	C5'-C4'-O4'	5.03	115.14	109.10
48	A2	2064	C	C4'-C3'-O3'	5.03	123.06	113.00
2	A4	105	C	O4'-C1'-N1	5.03	112.22	108.20
48	A2	2674	A	C5'-C4'-O4'	5.03	115.13	109.10
49	B1	750	C	N1-C1'-C2'	5.03	120.53	114.00
49	B1	1754	G	C2'-C3'-O3'	5.03	121.74	113.70
48	A2	2697	U	P-O3'-C3'	5.02	125.72	119.70
49	B1	306	C	C5'-C4'-C3'	-5.02	107.97	116.00
49	B1	367	U	C2'-C3'-O3'	-5.02	98.45	109.50
49	B1	370	G	P-O3'-C3'	5.02	125.72	119.70
49	B1	1484	A	OP2-P-O3'	5.02	116.25	105.20
48	A2	349	A	O4'-C1'-N9	5.02	112.21	108.20
48	A2	967	U	N1-C1'-C2'	5.02	120.52	114.00
48	A2	2422	G	O3'-P-O5'	-5.02	94.47	104.00
48	A2	408	C	O4'-C1'-N1	5.01	112.21	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	736	G	C3'-C2'-O2'	5.01	127.84	113.30
49	B1	307	G	C1'-C2'-O2'	-5.01	95.56	110.60
49	B1	308	G	N9-C1'-C2'	5.01	120.52	114.00
49	B1	1105	G	C5'-C4'-C3'	5.01	124.02	116.00
48	A2	4904	U	P-O3'-C3'	5.01	125.72	119.70
49	B1	321	C	C4'-C3'-O3'	5.01	123.02	113.00
48	A2	381	G	C2'-C3'-O3'	-5.01	98.48	109.50
13	AK	2	PRO	N-CD-CG	5.00	110.70	103.20
48	A2	230	U	C3'-C2'-C1'	-5.00	97.50	101.50
49	B1	1553	C	O4'-C4'-C3'	-5.00	99.00	104.00
48	A2	1429	C	O5'-C5'-C4'	-5.00	102.20	111.70
48	A2	4716	G	O5'-P-OP1	5.00	116.70	110.70

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
48	A2	131	C	C3'
48	A2	137	G	C3'
49	B1	1289	U	C4'

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
48	A2	1741	G	Sidechain
48	A2	2690	G	Sidechain
48	A2	3596	G	Sidechain
4	AB	295	ASP	Peptide
4	AB	296	GLY	Peptide
4	AB	297	LYS	Peptide
5	AC	98	GLY	Peptide
5	AC	99	GLY	Peptide
7	AE	108	LYS	Mainchain
8	AF	161	LYS	Peptide
8	AF	163	ASN	Peptide
10	AH	4	ILE	Peptide
10	AH	5	LEU	Peptide
10	AH	8	GLN	Peptide
13	AK	32	ALA	Peptide
13	AK	34	ASN	Peptide
13	AK	35	VAL	Peptide
14	AL	132	SER	Peptide
14	AL	133	ALA	Peptide

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Mol	Chain	Res	Type	Group
14	AL	134	PRO	Peptide
14	AL	135	LYS	Peptide
14	AL	136	LYS	Peptide
14	AL	138	ASP	Peptide
39	Ak	14	THR	Mainchain
54	BE	91	SER	Peptide
54	BE	92	ILE	Peptide
54	BE	93	GLU	Peptide
54	BE	94	LYS	Peptide
54	BE	95	THR	Peptide
54	BE	97	GLU	Peptide
63	BN	28	LEU	Peptide
63	BN	29	THR	Peptide
64	BO	138	ASP	Peptide
64	BO	139	SER	Peptide
65	BP	46	ASN	Peptide
65	BP	47	ARG	Peptide
65	BP	48	GLY	Peptide
65	BP	49	LEU	Peptide
65	BP	50	ARG	Peptide
65	BP	66	GLU	Peptide
65	BP	67	ALA	Peptide
65	BP	68	PRO	Peptide
65	BP	71	GLU	Peptide
65	BP	72	LYS	Peptide
65	BP	73	PRO	Peptide
66	BQ	13	PHE	Peptide
66	BQ	14	GLY	Peptide
66	BQ	15	ARG	Peptide
66	BQ	48	GLN	Peptide
66	BQ	51	LEU	Peptide
66	BQ	74	GLY	Peptide
72	BW	100	GLY	Peptide
72	BW	101	PHE	Peptide
72	BW	99	PHE	Peptide
76	Ba	97	PRO	Peptide
79	Bd	39	CYS	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
3	AA	250/257 (97%)	237 (95%)	7 (3%)	6 (2%)	5 30
4	AB	392/403 (97%)	370 (94%)	10 (3%)	12 (3%)	3 26
5	AC	361/427 (84%)	333 (92%)	13 (4%)	15 (4%)	2 19
6	AD	292/297 (98%)	270 (92%)	14 (5%)	8 (3%)	4 28
7	AE	192/288 (67%)	161 (84%)	12 (6%)	19 (10%)	0 6
8	AF	232/248 (94%)	213 (92%)	10 (4%)	9 (4%)	2 21
9	AG	232/266 (87%)	217 (94%)	10 (4%)	5 (2%)	5 31
10	AH	189/192 (98%)	175 (93%)	8 (4%)	6 (3%)	3 25
11	AI	204/214 (95%)	192 (94%)	7 (3%)	5 (2%)	4 29
12	AJ	167/178 (94%)	154 (92%)	7 (4%)	6 (4%)	3 22
13	AK	107/317 (34%)	34 (32%)	37 (35%)	36 (34%)	0 0
14	AL	203/211 (96%)	175 (86%)	14 (7%)	14 (7%)	1 10
15	AM	137/215 (64%)	127 (93%)	5 (4%)	5 (4%)	3 22
16	AN	201/204 (98%)	193 (96%)	6 (3%)	2 (1%)	13 46
17	AO	193/203 (95%)	187 (97%)	3 (2%)	3 (2%)	8 38
18	AP	151/184 (82%)	147 (97%)	4 (3%)	0	100 100
19	AQ	185/188 (98%)	163 (88%)	10 (5%)	12 (6%)	1 12
20	AR	179/196 (91%)	171 (96%)	4 (2%)	4 (2%)	5 31
21	AS	173/176 (98%)	156 (90%)	11 (6%)	6 (4%)	3 24
22	AT	155/160 (97%)	144 (93%)	6 (4%)	5 (3%)	3 25
23	AU	97/128 (76%)	81 (84%)	7 (7%)	9 (9%)	0 7
24	AV	127/140 (91%)	125 (98%)	2 (2%)	0	100 100
25	AW	119/157 (76%)	96 (81%)	18 (15%)	5 (4%)	2 19
26	AX	115/156 (74%)	113 (98%)	2 (2%)	0	100 100
27	AY	125/145 (86%)	119 (95%)	2 (2%)	4 (3%)	3 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
28	AZ	132/136 (97%)	118 (89%)	6 (4%)	8 (6%)	1 13
29	Aa	145/148 (98%)	135 (93%)	6 (4%)	4 (3%)	4 27
30	Ab	66/159 (42%)	57 (86%)	5 (8%)	4 (6%)	1 13
31	Ac	101/115 (88%)	97 (96%)	2 (2%)	2 (2%)	6 33
32	Ad	104/125 (83%)	99 (95%)	3 (3%)	2 (2%)	6 34
33	Ae	127/135 (94%)	116 (91%)	6 (5%)	5 (4%)	2 21
34	Af	107/110 (97%)	93 (87%)	5 (5%)	9 (8%)	0 8
35	Ag	112/117 (96%)	107 (96%)	3 (3%)	2 (2%)	7 35
36	Ah	120/123 (98%)	112 (93%)	2 (2%)	6 (5%)	1 16
37	Ai	95/105 (90%)	83 (87%)	7 (7%)	5 (5%)	1 14
38	Aj	82/97 (84%)	69 (84%)	7 (8%)	6 (7%)	1 9
39	Ak	67/70 (96%)	50 (75%)	7 (10%)	10 (15%)	0 3
40	Al	48/51 (94%)	47 (98%)	1 (2%)	0	100 100
41	Am	48/128 (38%)	44 (92%)	3 (6%)	1 (2%)	5 32
42	An	23/25 (92%)	23 (100%)	0	0	100 100
43	Ao	103/106 (97%)	94 (91%)	5 (5%)	4 (4%)	2 21
44	Ap	89/92 (97%)	84 (94%)	3 (3%)	2 (2%)	5 31
45	Aq	136/165 (82%)	40 (29%)	47 (35%)	49 (36%)	0 0
46	At	120/137 (88%)	107 (89%)	10 (8%)	3 (2%)	4 29
47	Au	215/217 (99%)	185 (86%)	20 (9%)	10 (5%)	2 17
50	BA	213/295 (72%)	197 (92%)	12 (6%)	4 (2%)	6 34
51	BB	210/264 (80%)	180 (86%)	12 (6%)	18 (9%)	0 7
52	BC	220/293 (75%)	204 (93%)	7 (3%)	9 (4%)	2 20
53	BD	218/243 (90%)	201 (92%)	10 (5%)	7 (3%)	3 25
54	BE	255/263 (97%)	230 (90%)	14 (6%)	11 (4%)	2 19
55	BF	188/204 (92%)	163 (87%)	15 (8%)	10 (5%)	1 14
56	BG	230/249 (92%)	211 (92%)	11 (5%)	8 (4%)	3 24
57	BH	181/194 (93%)	169 (93%)	8 (4%)	4 (2%)	5 31
58	BI	205/208 (99%)	175 (85%)	20 (10%)	10 (5%)	2 16
59	BJ	177/194 (91%)	137 (77%)	28 (16%)	12 (7%)	1 11
60	BK	96/165 (58%)	84 (88%)	7 (7%)	5 (5%)	1 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
61	BL	151/158 (96%)	133 (88%)	11 (7%)	7 (5%)	2 18
62	BM	118/132 (89%)	113 (96%)	1 (1%)	4 (3%)	3 24
63	BN	147/151 (97%)	126 (86%)	13 (9%)	8 (5%)	1 14
64	BO	134/151 (89%)	113 (84%)	11 (8%)	10 (8%)	1 9
65	BP	118/145 (81%)	100 (85%)	9 (8%)	9 (8%)	1 9
66	BQ	137/146 (94%)	120 (88%)	10 (7%)	7 (5%)	1 16
67	BR	123/135 (91%)	106 (86%)	9 (7%)	8 (6%)	1 12
68	BS	137/152 (90%)	125 (91%)	7 (5%)	5 (4%)	3 22
69	BT	141/145 (97%)	131 (93%)	6 (4%)	4 (3%)	4 27
70	BU	95/119 (80%)	91 (96%)	2 (2%)	2 (2%)	5 32
71	BV	79/83 (95%)	77 (98%)	2 (2%)	0	100 100
72	BW	127/130 (98%)	120 (94%)	3 (2%)	4 (3%)	3 26
73	BX	137/143 (96%)	124 (90%)	8 (6%)	5 (4%)	3 22
74	BY	123/133 (92%)	116 (94%)	6 (5%)	1 (1%)	16 51
75	BZ	84/125 (67%)	80 (95%)	1 (1%)	3 (4%)	3 22
76	Ba	95/115 (83%)	87 (92%)	7 (7%)	1 (1%)	12 45
77	Bb	78/84 (93%)	72 (92%)	4 (5%)	2 (3%)	4 28
78	Bc	60/69 (87%)	57 (95%)	1 (2%)	2 (3%)	3 25
79	Bd	49/56 (88%)	42 (86%)	4 (8%)	3 (6%)	1 13
80	Be	53/59 (90%)	49 (92%)	2 (4%)	2 (4%)	2 21
81	Bf	71/156 (46%)	63 (89%)	7 (10%)	1 (1%)	9 40
82	Bg	312/317 (98%)	292 (94%)	12 (4%)	8 (3%)	4 28
All	All	11580/13387 (86%)	10401 (90%)	657 (6%)	522 (4%)	3 18

All (522) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AA	138	SER
3	AA	144	LYS
3	AA	197	PRO
4	AB	189	THR
4	AB	356	LYS
5	AC	149	GLU
5	AC	151	PRO

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Mol	Chain	Res	Type
5	AC	304	ALA
6	AD	6	VAL
6	AD	231	VAL
6	AD	290	ALA
6	AD	291	GLN
7	AE	96	VAL
7	AE	107	VAL
7	AE	110	ARG
7	AE	111	LYS
7	AE	128	HIS
7	AE	158	ARG
7	AE	185	PRO
7	AE	187	ARG
7	AE	230	GLY
7	AE	284	HIS
8	AF	166	ARG
8	AF	170	THR
8	AF	222	LYS
9	AG	162	ASP
11	AI	24	ARG
11	AI	113	THR
12	AJ	12	MET
12	AJ	54	ARG
13	AK	30	VAL
13	AK	32	ALA
13	AK	35	VAL
13	AK	48	ARG
13	AK	64	ALA
13	AK	72	ASN
13	AK	78	LEU
13	AK	85	ASN
13	AK	88	PHE
13	AK	102	LEU
13	AK	104	ALA
14	AL	47	ALA
14	AL	139	SER
14	AL	140	SER
14	AL	145	LYS
14	AL	156	PRO
14	AL	173	GLU
14	AL	178	ALA
14	AL	179	PHE

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Mol	Chain	Res	Type
15	AM	21	ALA
15	AM	44	GLN
17	AO	184	ASN
19	AQ	4	ASP
19	AQ	13	VAL
19	AQ	16	LYS
19	AQ	98	LEU
19	AQ	161	SER
20	AR	24	LEU
20	AR	61	ALA
20	AR	113	LYS
22	AT	32	ARG
22	AT	53	PRO
23	AU	48	LYS
23	AU	55	ASN
25	AW	61	LYS
25	AW	82	ILE
27	AY	67	ILE
28	AZ	93	LYS
28	AZ	95	VAL
28	AZ	100	VAL
29	Aa	24	LYS
29	Aa	82	VAL
29	Aa	93	ASN
29	Aa	95	THR
31	Ac	104	ILE
31	Ac	107	SER
32	Ad	20	VAL
34	Af	59	THR
34	Af	61	GLY
34	Af	62	GLY
34	Af	63	LYS
34	Af	106	TYR
34	Af	107	PRO
35	Ag	44	SER
36	Ah	10	ARG
37	Ai	18	THR
37	Ai	65	LYS
38	Aj	32	SER
38	Aj	79	ARG
38	Aj	82	THR
39	Ak	17	ARG

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Mol	Chain	Res	Type
39	Ak	19	ASP
39	Ak	38	CYS
43	Ao	76	ASN
45	Aq	10	ILE
45	Aq	17	CYS
45	Aq	25	THR
45	Aq	31	LYS
45	Aq	35	LEU
45	Aq	38	SER
45	Aq	39	PRO
45	Aq	49	ALA
45	Aq	58	ILE
45	Aq	75	PRO
45	Aq	77	ALA
45	Aq	78	SER
45	Aq	88	PRO
45	Aq	90	ARG
45	Aq	104	ILE
45	Aq	106	PHE
45	Aq	112	ILE
45	Aq	113	ALA
45	Aq	124	GLU
45	Aq	141	CYS
47	Au	5	VAL
47	Au	59	PRO
47	Au	60	ARG
50	BA	206	ASP
51	BB	39	PHE
51	BB	40	ASN
51	BB	51	ARG
51	BB	71	LEU
51	BB	73	ASP
52	BC	65	LYS
53	BD	213	PRO
53	BD	217	ILE
53	BD	218	LEU
54	BE	92	ILE
54	BE	93	GLU
54	BE	101	LEU
54	BE	113	ARG
54	BE	151	ASP
55	BF	40	ALA

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Mol	Chain	Res	Type
55	BF	121	PRO
55	BF	129	GLY
56	BG	43	GLU
57	BH	115	LYS
57	BH	116	ARG
58	BI	133	GLU
58	BI	155	ASN
58	BI	193	LYS
59	BJ	4	ALA
59	BJ	91	LYS
59	BJ	156	HIS
59	BJ	165	TYR
59	BJ	170	PRO
60	BK	28	HIS
61	BL	29	GLY
62	BM	129	LYS
63	BN	23	PRO
63	BN	25	TRP
63	BN	62	GLN
64	BO	90	ILE
64	BO	139	SER
64	BO	141	ARG
64	BO	146	ARG
65	BP	48	GLY
65	BP	68	PRO
65	BP	101	THR
65	BP	126	VAL
66	BQ	51	LEU
66	BQ	52	LEU
67	BR	3	ARG
67	BR	4	VAL
67	BR	5	ARG
67	BR	95	ILE
67	BR	115	SER
68	BS	78	LYS
68	BS	134	GLN
69	BT	37	VAL
72	BW	98	GLN
72	BW	99	PHE
72	BW	101	PHE
73	BX	136	GLY
73	BX	139	GLU

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Mol	Chain	Res	Type
76	Ba	97	PRO
77	Bb	41	TYR
78	Bc	38	THR
79	Bd	11	PRO
79	Bd	12	ARG
79	Bd	25	SER
81	Bf	87	THR
82	Bg	49	GLU
4	AB	5	LYS
4	AB	18	PRO
4	AB	175	GLN
5	AC	91	ALA
5	AC	218	ILE
5	AC	223	ASN
5	AC	323	ARG
6	AD	20	PHE
6	AD	266	TRP
7	AE	283	PRO
8	AF	165	LYS
8	AF	185	ILE
8	AF	224	THR
9	AG	41	ILE
9	AG	131	LYS
10	AH	4	ILE
10	AH	116	ASN
10	AH	117	PHE
11	AI	111	LEU
11	AI	116	ARG
12	AJ	151	ILE
13	AK	15	LEU
13	AK	37	SER
13	AK	39	GLN
13	AK	40	MET
13	AK	52	VAL
13	AK	55	MET
13	AK	68	HIS
13	AK	84	GLY
14	AL	138	ASP
14	AL	155	MET
15	AM	104	MET
17	AO	198	THR
19	AQ	19	LYS

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Mol	Chain	Res	Type
19	AQ	104	ARG
21	AS	5	GLY
21	AS	86	SER
21	AS	145	PHE
22	AT	81	LYS
23	AU	53	ALA
25	AW	81	ALA
27	AY	43	ASN
27	AY	65	GLN
28	AZ	32	GLY
28	AZ	102	ARG
30	Ab	26	SER
30	Ab	51	LYS
33	Ae	4	LEU
35	Ag	46	CYS
36	Ah	9	LEU
36	Ah	96	ASN
36	Ah	122	LYS
38	Aj	81	GLY
39	Ak	14	THR
39	Ak	20	ALA
43	Ao	29	GLY
45	Aq	14	TYR
45	Aq	21	GLU
45	Aq	41	LYS
45	Aq	55	GLY
45	Aq	60	VAL
45	Aq	66	ASN
45	Aq	69	ALA
45	Aq	71	ILE
45	Aq	91	ASP
45	Aq	117	ARG
45	Aq	140	GLY
47	Au	197	ASN
51	BB	37	ALA
52	BC	63	VAL
52	BC	103	LYS
52	BC	174	ILE
54	BE	98	HIS
55	BF	34	SER
55	BF	183	GLY
56	BG	88	ARG

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Mol	Chain	Res	Type
56	BG	165	GLU
57	BH	109	ARG
57	BH	148	LEU
58	BI	159	SER
59	BJ	3	VAL
59	BJ	131	ARG
60	BK	41	PRO
61	BL	14	PRO
61	BL	15	THR
63	BN	20	ARG
63	BN	24	THR
63	BN	31	ASP
63	BN	107	LYS
64	BO	19	PRO
64	BO	21	VAL
64	BO	91	THR
65	BP	51	ARG
65	BP	116	LEU
65	BP	130	ARG
66	BQ	15	ARG
66	BQ	53	GLU
66	BQ	144	SER
67	BR	113	SER
68	BS	93	GLY
70	BU	67	LYS
72	BW	84	LYS
73	BX	107	ARG
73	BX	116	PRO
75	BZ	104	ARG
78	Bc	33	GLU
80	Be	32	ALA
82	Bg	126	ASP
3	AA	229	ALA
4	AB	281	ASN
4	AB	292	LEU
5	AC	95	MET
5	AC	194	GLY
5	AC	222	ARG
7	AE	108	LYS
7	AE	109	LEU
7	AE	122	PRO
7	AE	126	LEU

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Mol	Chain	Res	Type
7	AE	131	LYS
7	AE	132	PRO
9	AG	32	PHE
9	AG	133	PRO
10	AH	175	PHE
12	AJ	58	ARG
13	AK	14	PHE
13	AK	25	PRO
13	AK	33	ASP
13	AK	34	ASN
13	AK	62	ARG
13	AK	70	GLU
13	AK	83	ARG
13	AK	103	LEU
13	AK	105	ASN
13	AK	107	VAL
14	AL	158	ARG
15	AM	5	ARG
16	AN	94	PHE
16	AN	145	ASN
19	AQ	160	HIS
21	AS	88	SER
22	AT	127	GLN
23	AU	33	ILE
23	AU	51	GLY
28	AZ	22	LYS
28	AZ	103	ASP
32	Ad	95	ASP
33	Ae	19	LYS
37	Ai	17	VAL
39	Ak	11	PHE
39	Ak	18	LYS
41	Am	79	GLU
43	Ao	31	ASP
44	Ap	12	GLY
45	Aq	15	LEU
45	Aq	54	LYS
45	Aq	70	GLN
45	Aq	86	LYS
45	Aq	95	GLN
45	Aq	131	GLU
47	Au	22	GLN

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Mol	Chain	Res	Type
47	Au	126	PRO
51	BB	70	SER
51	BB	76	ASN
51	BB	82	ARG
51	BB	119	THR
51	BB	207	LEU
51	BB	213	ARG
52	BC	171	GLY
52	BC	261	PHE
53	BD	75	LYS
55	BF	37	ASP
55	BF	80	GLY
58	BI	85	ALA
58	BI	171	LEU
59	BJ	101	LYS
59	BJ	121	LYS
59	BJ	122	SER
61	BL	11	GLN
61	BL	12	LYS
64	BO	89	GLY
67	BR	122	PRO
69	BT	28	LEU
69	BT	32	GLU
73	BX	41	PHE
75	BZ	40	VAL
75	BZ	78	LYS
82	Bg	146	SER
82	Bg	171	ASP
82	Bg	255	SER
82	Bg	284	PRO
3	AA	180	LEU
3	AA	250	LYS
4	AB	17	LEU
5	AC	52	TYR
5	AC	73	VAL
6	AD	44	TYR
7	AE	119	GLU
10	AH	7	ASN
10	AH	8	GLN
11	AI	103	LEU
12	AJ	111	GLU
13	AK	66	ARG

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Mol	Chain	Res	Type
14	AL	133	ALA
15	AM	33	GLN
20	AR	53	LYS
21	AS	3	ALA
21	AS	7	LEU
23	AU	101	ARG
28	AZ	60	LYS
33	Ae	3	ALA
34	Af	41	PHE
39	Ak	6	GLU
43	Ao	49	GLY
44	Ap	19	GLY
45	Aq	89	PRO
45	Aq	92	ARG
45	Aq	120	SER
45	Aq	122	ALA
46	At	21	ASN
47	Au	40	ASN
47	Au	58	THR
47	Au	70	ASP
50	BA	6	ASP
51	BB	23	ASP
51	BB	179	ASN
51	BB	209	ASP
52	BC	135	GLY
52	BC	176	LYS
53	BD	83	SER
54	BE	171	ASN
56	BG	47	GLY
56	BG	106	LEU
58	BI	127	ALA
58	BI	158	ILE
59	BJ	36	GLY
59	BJ	104	ASP
60	BK	32	HIS
61	BL	21	LYS
62	BM	102	LYS
65	BP	67	ALA
66	BQ	44	PRO
68	BS	79	ILE
5	AC	305	PRO
7	AE	234	ASP

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Mol	Chain	Res	Type
8	AF	160	GLY
13	AK	71	ASN
13	AK	98	ILE
13	AK	108	PRO
19	AQ	38	ARG
23	AU	35	ASP
23	AU	59	GLY
25	AW	69	LYS
30	Ab	25	ARG
30	Ab	46	ALA
33	Ae	5	ARG
34	Af	58	VAL
34	Af	60	PRO
36	Ah	7	ARG
36	Ah	87	LYS
37	Ai	19	LYS
38	Aj	80	GLU
45	Aq	98	ILE
45	Aq	121	LEU
45	Aq	136	ALA
53	BD	76	ARG
53	BD	113	LEU
54	BE	203	GLY
55	BF	92	ILE
56	BG	115	LYS
56	BG	135	PRO
58	BI	24	LYS
61	BL	34	PRO
63	BN	22	VAL
65	BP	49	LEU
66	BQ	143	LYS
68	BS	133	GLY
70	BU	53	PRO
74	BY	59	GLY
80	Be	9	ALA
4	AB	3	HIS
4	AB	293	ILE
4	AB	298	LEU
4	AB	326	VAL
6	AD	260	GLU
8	AF	163	ASN
13	AK	49	GLY

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Mol	Chain	Res	Type
13	AK	53	VAL
13	AK	99	ARG
14	AL	135	LYS
17	AO	186	GLU
19	AQ	157	GLY
25	AW	103	ALA
37	Ai	21	VAL
39	Ak	15	ALA
39	Ak	60	LEU
45	Aq	85	LEU
47	Au	172	VAL
50	BA	95	GLY
50	BA	193	HIS
51	BB	69	VAL
51	BB	132	GLY
51	BB	210	VAL
54	BE	91	SER
55	BF	185	SER
58	BI	192	GLY
64	BO	140	THR
69	BT	51	ASN
77	Bb	62	VAL
19	AQ	5	ILE
19	AQ	159	PRO
45	Aq	23	GLY
45	Aq	64	ILE
55	BF	41	VAL
60	BK	86	PRO
82	Bg	61	GLY
5	AC	70	GLY
5	AC	98	GLY
8	AF	197	VAL
23	AU	47	ILE
27	AY	70	VAL
45	Aq	102	GLY
45	Aq	132	ILE
52	BC	61	MET
60	BK	3	MET
62	BM	30	GLY
82	Bg	190	GLY
12	AJ	175	LEU
33	Ae	8	VAL

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Mol	Chain	Res	Type
46	At	28	GLU
54	BE	153	VAL
56	BG	108	VAL
14	AL	48	PRO
22	AT	126	VAL
46	At	122	LYS
54	BE	102	VAL
38	Aj	84	PRO
62	BM	115	GLY
64	BO	145	GLY
67	BR	88	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	AA	194/199 (98%)	185 (95%)	9 (5%)	23 52
4	AB	343/349 (98%)	323 (94%)	20 (6%)	17 44
5	AC	302/348 (87%)	278 (92%)	24 (8%)	10 34
6	AD	248/250 (99%)	229 (92%)	19 (8%)	10 34
7	AE	174/252 (69%)	127 (73%)	47 (27%)	0 2
8	AF	203/215 (94%)	193 (95%)	10 (5%)	21 50
9	AG	199/223 (89%)	192 (96%)	7 (4%)	31 59
10	AH	170/171 (99%)	160 (94%)	10 (6%)	16 44
11	AI	178/181 (98%)	174 (98%)	4 (2%)	47 70
12	AJ	142/149 (95%)	138 (97%)	4 (3%)	38 65
13	AK	95/258 (37%)	70 (74%)	25 (26%)	0 3
14	AL	171/177 (97%)	156 (91%)	15 (9%)	8 31
15	AM	118/161 (73%)	104 (88%)	14 (12%)	4 21
16	AN	171/172 (99%)	163 (95%)	8 (5%)	22 51
17	AO	168/174 (97%)	164 (98%)	4 (2%)	44 68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	AP	134/163 (82%)	123 (92%)	11 (8%)	9 33
19	AQ	164/165 (99%)	144 (88%)	20 (12%)	4 20
20	AR	160/175 (91%)	145 (91%)	15 (9%)	7 29
21	AS	156/157 (99%)	149 (96%)	7 (4%)	23 53
22	AT	138/140 (99%)	126 (91%)	12 (9%)	8 31
23	AU	89/115 (77%)	78 (88%)	11 (12%)	4 20
24	AV	100/107 (94%)	98 (98%)	2 (2%)	50 72
25	AW	100/126 (79%)	94 (94%)	6 (6%)	16 43
26	AX	105/133 (79%)	95 (90%)	10 (10%)	7 28
27	AY	119/135 (88%)	109 (92%)	10 (8%)	9 32
28	AZ	117/118 (99%)	100 (86%)	17 (14%)	2 15
29	Aa	120/121 (99%)	110 (92%)	10 (8%)	9 32
30	Ab	58/126 (46%)	54 (93%)	4 (7%)	13 39
31	Ac	88/97 (91%)	85 (97%)	3 (3%)	32 60
32	Ad	97/110 (88%)	96 (99%)	1 (1%)	73 84
33	Ae	115/121 (95%)	114 (99%)	1 (1%)	75 86
34	Af	88/89 (99%)	85 (97%)	3 (3%)	32 60
35	Ag	98/100 (98%)	93 (95%)	5 (5%)	20 48
36	Ah	109/110 (99%)	96 (88%)	13 (12%)	4 21
37	Ai	83/89 (93%)	80 (96%)	3 (4%)	30 59
38	Aj	71/80 (89%)	65 (92%)	6 (8%)	8 32
39	Ak	64/65 (98%)	46 (72%)	18 (28%)	0 2
40	Al	47/48 (98%)	44 (94%)	3 (6%)	14 41
41	Am	46/116 (40%)	45 (98%)	1 (2%)	47 70
42	An	24/24 (100%)	23 (96%)	1 (4%)	25 54
43	Ao	93/94 (99%)	85 (91%)	8 (9%)	8 32
44	Ap	74/75 (99%)	71 (96%)	3 (4%)	26 55
45	Aq	114/137 (83%)	90 (79%)	24 (21%)	1 5
46	At	106/121 (88%)	88 (83%)	18 (17%)	1 10
47	Au	196/196 (100%)	180 (92%)	16 (8%)	9 33
50	BA	180/243 (74%)	165 (92%)	15 (8%)	9 32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
51	BB	193/231 (84%)	177 (92%)	16 (8%)	9 32
52	BC	188/225 (84%)	177 (94%)	11 (6%)	16 44
53	BD	183/202 (91%)	175 (96%)	8 (4%)	24 53
54	BE	220/225 (98%)	213 (97%)	7 (3%)	34 62
55	BF	160/170 (94%)	155 (97%)	5 (3%)	35 63
56	BG	202/218 (93%)	177 (88%)	25 (12%)	4 20
57	BH	164/174 (94%)	160 (98%)	4 (2%)	44 68
58	BI	179/180 (99%)	175 (98%)	4 (2%)	47 70
59	BJ	160/168 (95%)	151 (94%)	9 (6%)	17 45
60	BK	89/136 (65%)	83 (93%)	6 (7%)	13 40
61	BL	138/142 (97%)	134 (97%)	4 (3%)	37 64
62	BM	102/108 (94%)	101 (99%)	1 (1%)	73 84
63	BN	130/131 (99%)	122 (94%)	8 (6%)	15 42
64	BO	106/119 (89%)	99 (93%)	7 (7%)	14 41
65	BP	109/130 (84%)	93 (85%)	16 (15%)	2 15
66	BQ	115/121 (95%)	102 (89%)	13 (11%)	4 22
67	BR	113/122 (93%)	97 (86%)	16 (14%)	2 16
68	BS	121/132 (92%)	106 (88%)	15 (12%)	4 20
69	BT	113/115 (98%)	102 (90%)	11 (10%)	6 27
70	BU	90/107 (84%)	85 (94%)	5 (6%)	17 45
71	BV	65/67 (97%)	59 (91%)	6 (9%)	7 29
72	BW	112/113 (99%)	108 (96%)	4 (4%)	30 59
73	BX	111/115 (96%)	101 (91%)	10 (9%)	8 30
74	BY	107/115 (93%)	103 (96%)	4 (4%)	29 58
75	BZ	75/103 (73%)	57 (76%)	18 (24%)	0 3
76	Ba	84/98 (86%)	75 (89%)	9 (11%)	5 24
77	Bb	72/76 (95%)	72 (100%)	0	100 100
78	Bc	55/62 (89%)	52 (94%)	3 (6%)	18 46
79	Bd	45/49 (92%)	40 (89%)	5 (11%)	5 23
80	Be	44/48 (92%)	38 (86%)	6 (14%)	3 17
81	Bf	66/140 (47%)	65 (98%)	1 (2%)	60 77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
82	Bg	272/275 (99%)	268 (98%)	4 (2%)	60 77
All	All	10112/11392 (89%)	9354 (92%)	758 (8%)	14 35

All (758) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	AA	10	LYS
3	AA	20	VAL
3	AA	58	LEU
3	AA	63	PHE
3	AA	72	ARG
3	AA	93	LYS
3	AA	226	ARG
3	AA	227	ARG
3	AA	228	ASP
4	AB	17	LEU
4	AB	24	ARG
4	AB	42	HIS
4	AB	46	PHE
4	AB	103	LYS
4	AB	109	HIS
4	AB	130	PHE
4	AB	189	THR
4	AB	192	GLU
4	AB	226	LYS
4	AB	258	HIS
4	AB	274	TYR
4	AB	292	LEU
4	AB	294	LYS
4	AB	297	LYS
4	AB	299	ILE
4	AB	325	GLU
4	AB	351	LEU
4	AB	354	GLN
4	AB	394	LYS
5	AC	52	TYR
5	AC	56	GLU
5	AC	57	LEU
5	AC	67	TRP
5	AC	89	GLN
5	AC	92	PHE
5	AC	95	MET

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Mol	Chain	Res	Type
5	AC	97	ARG
5	AC	107	THR
5	AC	162	LYS
5	AC	202	ILE
5	AC	204	ARG
5	AC	205	ARG
5	AC	208	CYS
5	AC	209	ILE
5	AC	211	TYR
5	AC	213	GLU
5	AC	215	ASN
5	AC	218	ILE
5	AC	221	PHE
5	AC	222	ARG
5	AC	229	LEU
5	AC	230	LEU
5	AC	287	THR
6	AD	4	VAL
6	AD	6	VAL
6	AD	10	LYS
6	AD	12	TYR
6	AD	20	PHE
6	AD	25	GLU
6	AD	69	ILE
6	AD	197	LYS
6	AD	198	HIS
6	AD	216	GLU
6	AD	225	GLN
6	AD	227	ILE
6	AD	229	ASN
6	AD	232	THR
6	AD	234	ASP
6	AD	235	MET
6	AD	236	MET
6	AD	265	ARG
6	AD	268	ARG
7	AE	100	LYS
7	AE	105	ARG
7	AE	106	VAL
7	AE	108	LYS
7	AE	109	LEU
7	AE	110	ARG

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Mol	Chain	Res	Type
7	AE	111	LYS
7	AE	114	ARG
7	AE	115	TYR
7	AE	116	TYR
7	AE	118	THR
7	AE	121	VAL
7	AE	123	ARG
7	AE	124	LYS
7	AE	125	LEU
7	AE	126	LEU
7	AE	131	LYS
7	AE	138	ARG
7	AE	140	LEU
7	AE	141	ARG
7	AE	167	GLN
7	AE	173	LEU
7	AE	186	LEU
7	AE	187	ARG
7	AE	188	ARG
7	AE	189	THR
7	AE	201	ILE
7	AE	203	ILE
7	AE	207	LYS
7	AE	210	LYS
7	AE	211	HIS
7	AE	212	LEU
7	AE	213	THR
7	AE	216	TYR
7	AE	218	LYS
7	AE	220	LYS
7	AE	222	LEU
7	AE	223	ARG
7	AE	224	LYS
7	AE	228	GLN
7	AE	237	LYS
7	AE	239	LYS
7	AE	241	GLU
7	AE	278	THR
7	AE	279	ASN
7	AE	282	TYR
7	AE	285	LYS
8	AF	19	LYS

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Mol	Chain	Res	Type
8	AF	86	GLU
8	AF	88	LYS
8	AF	161	LYS
8	AF	165	LYS
8	AF	166	ARG
8	AF	182	TYR
8	AF	220	MET
8	AF	221	LYS
8	AF	222	LYS
9	AG	84	THR
9	AG	97	LYS
9	AG	110	LYS
9	AG	121	LYS
9	AG	136	LEU
9	AG	159	HIS
9	AG	162	ASP
10	AH	5	LEU
10	AH	8	GLN
10	AH	20	LEU
10	AH	60	TRP
10	AH	63	ASN
10	AH	96	TYR
10	AH	107	GLU
10	AH	108	ASN
10	AH	111	LEU
10	AH	134	CYS
11	AI	3	ARG
11	AI	48	LEU
11	AI	51	HIS
11	AI	74	LYS
12	AJ	33	LEU
12	AJ	64	ARG
12	AJ	159	LYS
12	AJ	175	LEU
13	AK	4	GLU
13	AK	13	TYR
13	AK	14	PHE
13	AK	20	LEU
13	AK	21	LEU
13	AK	24	TYR
13	AK	25	PRO
13	AK	28	PHE

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Mol	Chain	Res	Type
13	AK	30	VAL
13	AK	35	VAL
13	AK	42	GLN
13	AK	53	VAL
13	AK	54	LEU
13	AK	55	MET
13	AK	60	MET
13	AK	69	LEU
13	AK	73	PRO
13	AK	76	GLU
13	AK	78	LEU
13	AK	85	ASN
13	AK	90	PHE
13	AK	99	ARG
13	AK	102	LEU
13	AK	105	ASN
13	AK	108	PRO
14	AL	55	ILE
14	AL	56	ARG
14	AL	81	LEU
14	AL	126	LEU
14	AL	129	ARG
14	AL	130	LYS
14	AL	135	LYS
14	AL	151	THR
14	AL	155	MET
14	AL	159	ASN
14	AL	167	ARG
14	AL	173	GLU
14	AL	174	LYS
14	AL	175	ASN
14	AL	177	LYS
15	AM	6	PHE
15	AM	43	THR
15	AM	44	GLN
15	AM	46	ARG
15	AM	47	ARG
15	AM	50	MET
15	AM	79	LYS
15	AM	93	LYS
15	AM	94	LYS
15	AM	99	GLU

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Mol	Chain	Res	Type
15	AM	100	ARG
15	AM	103	LYS
15	AM	114	LYS
15	AM	132	LYS
16	AN	19	MET
16	AN	38	ARG
16	AN	108	ARG
16	AN	113	LEU
16	AN	124	ASP
16	AN	148	THR
16	AN	151	ILE
16	AN	183	THR
17	AO	25	LYS
17	AO	61	ARG
17	AO	92	THR
17	AO	148	LYS
18	AP	4	TYR
18	AP	10	ASN
18	AP	13	LYS
18	AP	22	LEU
18	AP	41	ILE
18	AP	47	TYR
18	AP	48	LEU
18	AP	49	LYS
18	AP	69	ARG
18	AP	75	GLN
18	AP	94	MET
19	AQ	6	ARG
19	AQ	8	ASN
19	AQ	9	LYS
19	AQ	11	ARG
19	AQ	13	VAL
19	AQ	15	ARG
19	AQ	16	LYS
19	AQ	37	ARG
19	AQ	48	LEU
19	AQ	63	LEU
19	AQ	75	ARG
19	AQ	76	GLU
19	AQ	92	VAL
19	AQ	98	LEU
19	AQ	99	LYS

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Mol	Chain	Res	Type
19	AQ	154	LYS
19	AQ	158	THR
19	AQ	170	LYS
19	AQ	175	GLU
19	AQ	176	ARG
20	AR	22	VAL
20	AR	24	LEU
20	AR	25	ASP
20	AR	27	ASN
20	AR	28	GLU
20	AR	62	ARG
20	AR	70	ARG
20	AR	71	ARG
20	AR	72	LYS
20	AR	74	ARG
20	AR	114	LYS
20	AR	132	PHE
20	AR	138	LEU
20	AR	170	ARG
20	AR	172	ARG
21	AS	1	MET
21	AS	7	LEU
21	AS	27	LEU
21	AS	52	LYS
21	AS	84	TYR
21	AS	136	LYS
21	AS	139	ARG
22	AT	2	THR
22	AT	17	ARG
22	AT	102	ARG
22	AT	106	LEU
22	AT	110	LYS
22	AT	113	ASP
22	AT	118	GLU
22	AT	121	GLU
22	AT	125	TRP
22	AT	128	LEU
22	AT	143	THR
22	AT	158	PHE
23	AU	50	ASN
23	AU	52	LYS
23	AU	55	ASN

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Mol	Chain	Res	Type
23	AU	56	LEU
23	AU	60	VAL
23	AU	65	ARG
23	AU	97	ARG
23	AU	99	TRP
23	AU	113	ARG
23	AU	115	PHE
23	AU	116	GLN
24	AV	48	ARG
24	AV	49	LEU
25	AW	50	ASN
25	AW	60	LYS
25	AW	63	GLN
25	AW	66	GLU
25	AW	68	GLN
25	AW	79	GLN
26	AX	54	LEU
26	AX	55	ARG
26	AX	77	ILE
26	AX	114	LYS
26	AX	115	LYS
26	AX	117	TYR
26	AX	118	ASP
26	AX	119	ILE
26	AX	120	ASP
26	AX	129	ARG
27	AY	1	MET
27	AY	4	ASN
27	AY	8	THR
27	AY	36	LYS
27	AY	40	GLN
27	AY	41	LYS
27	AY	42	TYR
27	AY	45	ARG
27	AY	49	ILE
27	AY	122	LYS
28	AZ	5	MET
28	AZ	31	ASP
28	AZ	36	ARG
28	AZ	51	ARG
28	AZ	59	LYS
28	AZ	60	LYS

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Mol	Chain	Res	Type
28	AZ	61	LYS
28	AZ	91	LEU
28	AZ	93	LYS
28	AZ	98	LYS
28	AZ	99	ASP
28	AZ	109	LYS
28	AZ	112	ARG
28	AZ	122	TYR
28	AZ	123	LYS
28	AZ	126	LYS
28	AZ	128	LYS
29	Aa	25	HIS
29	Aa	27	LYS
29	Aa	28	HIS
29	Aa	47	LYS
29	Aa	61	TYR
29	Aa	87	ARG
29	Aa	92	LYS
29	Aa	94	LYS
29	Aa	116	LYS
29	Aa	132	ARG
30	Ab	32	LEU
30	Ab	33	LYS
30	Ab	54	LEU
30	Ab	55	LYS
31	Ac	17	ARG
31	Ac	42	LYS
31	Ac	44	LYS
32	Ad	77	ILE
33	Ae	50	LYS
34	Af	106	TYR
34	Af	107	PRO
34	Af	110	ILE
35	Ag	5	LEU
35	Ag	21	ARG
35	Ag	22	LEU
35	Ag	32	TYR
35	Ag	60	ARG
36	Ah	14	LYS
36	Ah	31	LEU
36	Ah	35	LYS
36	Ah	37	THR

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Mol	Chain	Res	Type
36	Ah	48	ARG
36	Ah	49	VAL
36	Ah	51	ARG
36	Ah	66	LYS
36	Ah	79	LYS
36	Ah	91	MET
36	Ah	92	ARG
36	Ah	107	GLN
36	Ah	111	GLU
37	Ai	25	ARG
37	Ai	28	ARG
37	Ai	76	ARG
38	Aj	11	ARG
38	Aj	17	THR
38	Aj	19	CYS
38	Aj	20	ARG
38	Aj	36	LYS
38	Aj	37	CYS
39	Ak	12	LEU
39	Ak	13	LEU
39	Ak	17	ARG
39	Ak	18	LYS
39	Ak	19	ASP
39	Ak	21	LYS
39	Ak	22	SER
39	Ak	27	LYS
39	Ak	38	CYS
39	Ak	39	SER
39	Ak	40	ARG
39	Ak	41	TYR
39	Ak	54	GLU
39	Ak	55	LYS
39	Ak	56	LEU
39	Ak	57	LYS
39	Ak	59	SER
39	Ak	60	LEU
40	Al	13	LEU
40	Al	21	ARG
40	Al	28	ARG
41	Am	127	VAL
42	An	16	LYS
43	Ao	40	ARG

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Mol	Chain	Res	Type
43	Ao	42	ASP
43	Ao	43	ARG
43	Ao	97	LYS
43	Ao	98	LYS
43	Ao	102	GLN
43	Ao	103	VAL
43	Ao	105	GLN
44	Ap	28	LYS
44	Ap	62	LYS
44	Ap	84	ARG
45	Aq	9	GLU
45	Aq	21	GLU
45	Aq	22	VAL
45	Aq	28	LEU
45	Aq	30	PRO
45	Aq	31	LYS
45	Aq	35	LEU
45	Aq	37	LEU
45	Aq	39	PRO
45	Aq	46	ILE
45	Aq	50	THR
45	Aq	57	ARG
45	Aq	58	ILE
45	Aq	59	THR
45	Aq	75	PRO
45	Aq	81	ILE
45	Aq	85	LEU
45	Aq	97	ASN
45	Aq	104	ILE
45	Aq	109	ILE
45	Aq	111	ASN
45	Aq	125	LEU
45	Aq	128	THR
45	Aq	143	VAL
46	At	13	CYS
46	At	16	PHE
46	At	18	ILE
46	At	38	PHE
46	At	41	ASN
46	At	56	ASP
46	At	65	LYS
46	At	67	ARG

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Mol	Chain	Res	Type
46	At	68	SER
46	At	70	GLN
46	At	71	ARG
46	At	79	ARG
46	At	80	THR
46	At	83	ASN
46	At	87	ARG
46	At	89	THR
46	At	106	LEU
46	At	117	ILE
47	Au	17	VAL
47	Au	28	PHE
47	Au	29	LEU
47	Au	41	TYR
47	Au	58	THR
47	Au	59	PRO
47	Au	71	GLN
47	Au	94	ASN
47	Au	121	PRO
47	Au	180	VAL
47	Au	185	LEU
47	Au	188	ASN
47	Au	194	LEU
47	Au	198	TRP
47	Au	210	MET
47	Au	214	GLN
50	BA	12	GLU
50	BA	25	LEU
50	BA	34	MET
50	BA	36	GLN
50	BA	40	LYS
50	BA	41	ARG
50	BA	94	THR
50	BA	104	THR
50	BA	112	ILE
50	BA	116	PHE
50	BA	132	GLN
50	BA	142	LEU
50	BA	201	LEU
50	BA	202	TYR
50	BA	206	ASP
51	BB	75	GLN

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Mol	Chain	Res	Type
51	BB	79	VAL
51	BB	81	PHE
51	BB	116	LYS
51	BB	117	TRP
51	BB	135	LEU
51	BB	137	LEU
51	BB	174	ARG
51	BB	175	GLU
51	BB	177	GLN
51	BB	179	ASN
51	BB	182	LYS
51	BB	183	GLU
51	BB	184	VAL
51	BB	187	LYS
51	BB	218	LEU
52	BC	98	LEU
52	BC	102	LEU
52	BC	116	THR
52	BC	121	ARG
52	BC	123	ARG
52	BC	134	ASN
52	BC	160	LEU
52	BC	166	ARG
52	BC	167	ARG
52	BC	200	ARG
52	BC	209	VAL
53	BD	12	VAL
53	BD	18	LYS
53	BD	26	THR
53	BD	55	THR
53	BD	66	ILE
53	BD	113	LEU
53	BD	162	ASP
53	BD	216	GLU
54	BE	37	LYS
54	BE	75	LYS
54	BE	94	LYS
54	BE	129	ILE
54	BE	153	VAL
54	BE	212	ASP
54	BE	238	LEU
55	BF	23	TRP

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Mol	Chain	Res	Type
55	BF	89	THR
55	BF	107	ASN
55	BF	130	ARG
55	BF	133	THR
56	BG	53	SER
56	BG	147	LEU
56	BG	164	LYS
56	BG	172	LYS
56	BG	179	LEU
56	BG	195	LYS
56	BG	197	GLN
56	BG	199	THR
56	BG	200	LYS
56	BG	201	LYS
56	BG	202	ASN
56	BG	204	GLU
56	BG	205	GLU
56	BG	212	LEU
56	BG	215	LYS
56	BG	216	ARG
56	BG	217	MET
56	BG	218	LYS
56	BG	222	GLU
56	BG	224	ARG
56	BG	226	GLU
56	BG	227	GLN
56	BG	230	LYS
56	BG	231	ARG
56	BG	232	ARG
57	BH	15	LYS
57	BH	76	GLN
57	BH	135	PHE
57	BH	152	ARG
58	BI	19	LYS
58	BI	52	ASN
58	BI	58	LEU
58	BI	139	LYS
59	BJ	30	LYS
59	BJ	47	LYS
59	BJ	49	THR
59	BJ	50	LEU
59	BJ	54	ARG

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Mol	Chain	Res	Type
59	BJ	55	LYS
59	BJ	131	ARG
59	BJ	139	LYS
59	BJ	140	GLN
60	BK	3	MET
60	BK	29	MET
60	BK	32	HIS
60	BK	70	TYR
60	BK	72	THR
60	BK	96	ARG
61	BL	24	LEU
61	BL	27	GLU
61	BL	54	THR
61	BL	151	THR
62	BM	88	TRP
63	BN	25	TRP
63	BN	26	LEU
63	BN	40	LEU
63	BN	42	LYS
63	BN	54	LEU
63	BN	58	HIS
63	BN	76	LYS
63	BN	78	LYS
64	BO	45	THR
64	BO	75	MET
64	BO	76	LEU
64	BO	79	GLN
64	BO	83	GLN
64	BO	105	THR
64	BO	138	ASP
65	BP	12	PHE
65	BP	29	SER
65	BP	30	TYR
65	BP	33	LEU
65	BP	36	LEU
65	BP	49	LEU
65	BP	51	ARG
65	BP	52	LYS
65	BP	66	GLU
65	BP	71	GLU
65	BP	72	LYS
65	BP	83	MET

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Mol	Chain	Res	Type
65	BP	85	ILE
65	BP	86	LEU
65	BP	90	VAL
65	BP	130	ARG
66	BQ	11	GLN
66	BQ	17	LYS
66	BQ	25	CYS
66	BQ	37	ARG
66	BQ	39	LEU
66	BQ	45	ARG
66	BQ	46	THR
66	BQ	47	LEU
66	BQ	50	LYS
66	BQ	51	LEU
66	BQ	69	ARG
66	BQ	105	LYS
66	BQ	146	ARG
67	BR	4	VAL
67	BR	5	ARG
67	BR	6	THR
67	BR	10	LYS
67	BR	11	LYS
67	BR	17	ILE
67	BR	20	TYR
67	BR	35	CYS
67	BR	36	GLU
67	BR	38	ILE
67	BR	41	ILE
67	BR	91	LEU
67	BR	94	GLU
67	BR	99	ASP
67	BR	118	GLN
67	BR	126	MET
68	BS	13	LEU
68	BS	14	ARG
68	BS	16	LEU
68	BS	17	ASN
68	BS	23	ARG
68	BS	45	LEU
68	BS	47	LYS
68	BS	49	ASP
68	BS	52	LEU

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Mol	Chain	Res	Type
68	BS	53	THR
68	BS	59	LEU
68	BS	60	THR
68	BS	63	GLU
68	BS	75	ARG
68	BS	116	LYS
69	BT	5	THR
69	BT	7	LYS
69	BT	34	VAL
69	BT	39	LEU
69	BT	41	LYS
69	BT	42	HIS
69	BT	44	GLU
69	BT	62	ARG
69	BT	94	ARG
69	BT	116	ASP
69	BT	123	LEU
70	BU	20	ILE
70	BU	22	ILE
70	BU	47	ASN
70	BU	55	ARG
70	BU	56	MET
71	BV	12	TYR
71	BV	34	MET
71	BV	41	LYS
71	BV	45	ARG
71	BV	50	PHE
71	BV	81	LYS
72	BW	3	ARG
72	BW	4	MET
72	BW	56	HIS
72	BW	97	ARG
73	BX	9	THR
73	BX	17	ARG
73	BX	54	LYS
73	BX	60	LYS
73	BX	63	ASN
73	BX	134	TYR
73	BX	135	LYS
73	BX	137	LYS
73	BX	138	LYS
73	BX	139	GLU

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Mol	Chain	Res	Type
74	BY	29	HIS
74	BY	93	ARG
74	BY	102	THR
74	BY	122	LYS
75	BZ	34	LYS
75	BZ	44	LEU
75	BZ	50	PHE
75	BZ	55	TYR
75	BZ	60	LYS
75	BZ	61	GLU
75	BZ	65	TYR
75	BZ	66	LYS
75	BZ	67	LEU
75	BZ	75	GLU
75	BZ	77	LEU
75	BZ	83	LEU
75	BZ	85	ARG
75	BZ	88	LEU
75	BZ	92	LEU
75	BZ	96	LEU
75	BZ	98	LYS
75	BZ	102	LYS
76	Ba	15	ARG
76	Ba	38	LYS
76	Ba	39	PHE
76	Ba	40	VAL
76	Ba	42	ARG
76	Ba	80	HIS
76	Ba	82	LYS
76	Ba	93	LYS
76	Ba	95	ARG
78	Bc	9	ILE
78	Bc	21	THR
78	Bc	33	GLU
79	Bd	24	CYS
79	Bd	30	LEU
79	Bd	31	ILE
79	Bd	40	ARG
79	Bd	41	GLN
80	Be	6	LEU
80	Be	18	LYS
80	Be	28	LYS

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Mol	Chain	Res	Type
80	Be	35	ARG
80	Be	46	VAL
80	Be	52	LYS
81	Bf	89	LYS
82	Bg	24	THR
82	Bg	94	THR
82	Bg	195	LEU
82	Bg	255	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (196) such sidechains are listed below:

Mol	Chain	Res	Type
3	AA	95	GLN
3	AA	132	ASN
3	AA	187	HIS
3	AA	209	HIS
3	AA	216	HIS
4	AB	55	HIS
4	AB	158	GLN
4	AB	167	GLN
4	AB	179	HIS
4	AB	186	ASN
4	AB	245	HIS
4	AB	322	HIS
5	AC	48	ASN
5	AC	50	GLN
5	AC	187	GLN
5	AC	198	ASN
5	AC	212	ASN
5	AC	223	ASN
5	AC	286	ASN
5	AC	362	GLN
6	AD	9	ASN
6	AD	63	GLN
6	AD	191	ASN
6	AD	229	ASN
6	AD	244	HIS
7	AE	167	GLN
7	AE	191	GLN
7	AE	268	GLN
7	AE	279	ASN
8	AF	80	ASN

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Mol	Chain	Res	Type
8	AF	131	ASN
8	AF	226	HIS
9	AG	82	GLN
9	AG	195	HIS
10	AH	8	GLN
10	AH	102	ASN
10	AH	108	ASN
10	AH	163	GLN
11	AI	14	ASN
11	AI	59	GLN
11	AI	147	HIS
11	AI	213	HIS
12	AJ	42	GLN
12	AJ	46	GLN
12	AJ	112	HIS
12	AJ	168	GLN
13	AK	85	ASN
14	AL	15	HIS
14	AL	175	ASN
15	AM	20	HIS
15	AM	70	GLN
15	AM	83	ASN
15	AM	125	ASN
16	AN	37	HIS
16	AN	87	HIS
16	AN	145	ASN
16	AN	201	HIS
17	AO	42	ASN
17	AO	63	ASN
17	AO	96	GLN
18	AP	10	ASN
18	AP	93	HIS
18	AP	120	ASN
19	AQ	8	ASN
19	AQ	40	ASN
19	AQ	45	GLN
19	AQ	162	HIS
20	AR	118	HIS
21	AS	77	ASN
21	AS	156	HIS
21	AS	162	GLN
22	AT	3	ASN

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Mol	Chain	Res	Type
23	AU	50	ASN
23	AU	116	GLN
24	AV	101	ASN
24	AV	135	ASN
25	AW	63	GLN
26	AX	93	ASN
27	AY	4	ASN
27	AY	86	GLN
28	AZ	40	HIS
29	Aa	25	HIS
29	Aa	39	HIS
29	Aa	49	HIS
29	Aa	60	HIS
29	Aa	85	GLN
29	Aa	89	ASN
30	Ab	6	ASN
30	Ab	12	GLN
30	Ab	60	ASN
31	Ac	15	ASN
32	Ad	79	ASN
33	Ae	24	GLN
33	Ae	34	ASN
34	Af	65	ASN
34	Af	99	HIS
35	Ag	110	GLN
36	Ah	63	GLN
38	Aj	66	HIS
40	Al	19	GLN
40	Al	20	ASN
40	Al	33	ASN
41	Am	87	GLN
43	Ao	3	ASN
43	Ao	18	HIS
43	Ao	36	GLN
43	Ao	45	GLN
43	Ao	51	GLN
43	Ao	102	GLN
45	Aq	70	GLN
45	Aq	103	ASN
46	At	4	HIS
46	At	6	GLN
46	At	21	ASN

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Mol	Chain	Res	Type
46	At	41	ASN
46	At	70	GLN
46	At	95	HIS
46	At	100	ASN
46	At	121	GLN
47	Au	143	ASN
50	BA	111	GLN
50	BA	169	HIS
51	BB	75	GLN
51	BB	118	GLN
51	BB	177	GLN
51	BB	179	ASN
51	BB	186	ASN
52	BC	115	GLN
52	BC	134	ASN
52	BC	178	HIS
52	BC	235	ASN
53	BD	74	GLN
54	BE	216	ASN
55	BF	65	GLN
55	BF	82	ASN
55	BF	83	ASN
55	BF	95	HIS
55	BF	107	ASN
55	BF	203	ASN
56	BG	65	GLN
56	BG	70	HIS
56	BG	146	ASN
56	BG	225	GLN
57	BH	114	GLN
58	BI	44	HIS
58	BI	88	ASN
59	BJ	75	ASN
59	BJ	111	GLN
59	BJ	125	HIS
60	BK	28	HIS
61	BL	13	GLN
63	BN	5	HIS
64	BO	20	GLN
64	BO	79	GLN
64	BO	83	GLN
64	BO	113	GLN

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Mol	Chain	Res	Type
65	BP	35	GLN
65	BP	41	GLN
65	BP	79	HIS
65	BP	104	GLN
66	BQ	11	GLN
66	BQ	24	HIS
66	BQ	77	HIS
66	BQ	80	GLN
66	BQ	86	GLN
66	BQ	142	GLN
68	BS	17	ASN
68	BS	19	ASN
68	BS	42	HIS
68	BS	73	ASN
68	BS	125	HIS
69	BT	42	HIS
70	BU	81	GLN
70	BU	92	HIS
70	BU	100	GLN
71	BV	29	HIS
72	BW	15	ASN
72	BW	16	ASN
72	BW	24	GLN
72	BW	44	HIS
72	BW	56	HIS
72	BW	70	ASN
73	BX	16	HIS
73	BX	127	ASN
74	BY	89	HIS
74	BY	94	HIS
75	BZ	106	GLN
76	Ba	19	GLN
76	Ba	25	ASN
78	Bc	7	GLN
78	Bc	29	GLN
79	Bd	41	GLN
80	Be	39	ASN
82	Bg	26	GLN
82	Bg	56	GLN
82	Bg	226	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A3	156/194 (80%)	28 (17%)	4 (2%)
2	A4	118/121 (97%)	23 (19%)	1 (0%)
48	A2	3600/5029 (71%)	695 (19%)	48 (1%)
49	B1	1701/1869 (91%)	290 (17%)	19 (1%)
83	Bv	75/76 (98%)	38 (50%)	0
83	Bw	75/76 (98%)	34 (45%)	0
84	Bx	27/28 (96%)	18 (66%)	0
All	All	5752/7393 (77%)	1126 (19%)	72 (1%)

All (1126) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A3	2	G
1	A3	12	G
1	A3	16	G
1	A3	35	C
1	A3	59	A
1	A3	63	U
1	A3	72	A
1	A3	80	A
1	A3	81	C
1	A3	82	A
1	A3	87	G
1	A3	105	C
1	A3	108	A
1	A3	109	C
1	A3	110	U
1	A3	111	U
1	A3	112	G
1	A3	121	G
1	A3	122	G
1	A3	123	U
1	A3	124	U
1	A3	126	C
1	A3	128	C
1	A3	129	C
1	A3	130	C
1	A3	135	C
1	A3	148	A
1	A3	151	G
2	A4	12	U
2	A4	13	A
2	A4	14	C

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Mol	Chain	Res	Type
2	A4	16	A
2	A4	22	A
2	A4	23	A
2	A4	25	G
2	A4	27	G
2	A4	33	U
2	A4	34	C
2	A4	49	A
2	A4	53	U
2	A4	54	A
2	A4	57	C
2	A4	64	G
2	A4	66	G
2	A4	74	A
2	A4	103	A
2	A4	104	C
2	A4	107	G
2	A4	110	G
2	A4	118	C
2	A4	119	U
48	A2	4	G
48	A2	6	C
48	A2	10	A
48	A2	25	A
48	A2	28	C
48	A2	30	C
48	A2	32	G
48	A2	33	A
48	A2	39	A
48	A2	42	A
48	A2	48	G
48	A2	49	U
48	A2	59	A
48	A2	64	A
48	A2	65	A
48	A2	68	U
48	A2	71	C
48	A2	72	C
48	A2	73	A
48	A2	74	G
48	A2	84	A
48	A2	85	G

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Mol	Chain	Res	Type
48	A2	91	G
48	A2	96	U
48	A2	101	A
48	A2	116	G
48	A2	119	G
48	A2	128	C
48	A2	131	C
48	A2	132	G
48	A2	133	C
48	A2	134	G
48	A2	135	G
48	A2	136	G
48	A2	141	G
48	A2	143	G
48	A2	149	U
48	A2	157	G
48	A2	169	C
48	A2	174	G
48	A2	175	C
48	A2	181	U
48	A2	182	C
48	A2	183	G
48	A2	184	U
48	A2	185	G
48	A2	195	A
48	A2	196	G
48	A2	197	U
48	A2	201	U
48	A2	206	U
48	A2	212	C
48	A2	213	C
48	A2	214	C
48	A2	215	A
48	A2	222	G
48	A2	227	G
48	A2	228	U
48	A2	234	G
48	A2	253	G
48	A2	256	C
48	A2	260	C
48	A2	285	U
48	A2	286	G

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Mol	Chain	Res	Type
48	A2	289	A
48	A2	291	U
48	A2	300	A
48	A2	304	G
48	A2	308	G
48	A2	309	G
48	A2	310	U
48	A2	311	A
48	A2	320	C
48	A2	334	C
48	A2	341	A
48	A2	349	A
48	A2	351	U
48	A2	364	U
48	A2	367	G
48	A2	370	A
48	A2	375	U
48	A2	380	A
48	A2	381	G
48	A2	397	G
48	A2	407	G
48	A2	411	G
48	A2	425	G
48	A2	426	U
48	A2	444	G
48	A2	446	A
48	A2	448	U
48	A2	449	C
48	A2	457	A
48	A2	459	G
48	A2	460	A
48	A2	476	G
48	A2	479	C
48	A2	482	G
48	A2	492	C
48	A2	493	G
48	A2	494	G
48	A2	497	C
48	A2	498	G
48	A2	504	U
48	A2	505	C
48	A2	509	C

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Mol	Chain	Res	Type
48	A2	513	C
48	A2	515	C
48	A2	633	U
48	A2	634	C
48	A2	635	G
48	A2	638	G
48	A2	639	G
48	A2	641	G
48	A2	643	A
48	A2	649	C
48	A2	674	C
48	A2	676	G
48	A2	677	G
48	A2	678	C
48	A2	679	G
48	A2	689	G
48	A2	692	G
48	A2	693	U
48	A2	694	G
48	A2	695	C
48	A2	702	A
48	A2	720	G
48	A2	721	G
48	A2	724	A
48	A2	731	G
48	A2	733	G
48	A2	735	G
48	A2	736	G
48	A2	738	A
48	A2	739	G
48	A2	741	U
48	A2	901	U
48	A2	902	A
48	A2	903	C
48	A2	904	A
48	A2	905	G
48	A2	906	C
48	A2	909	C
48	A2	913	G
48	A2	914	G
48	A2	917	G
48	A2	918	C

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Mol	Chain	Res	Type
48	A2	919	A
48	A2	920	G
48	A2	921	C
48	A2	923	C
48	A2	924	U
48	A2	925	C
48	A2	926	G
48	A2	927	C
48	A2	929	G
48	A2	932	U
48	A2	933	C
48	A2	942	G
48	A2	943	A
48	A2	944	G
48	A2	947	A
48	A2	949	C
48	A2	950	G
48	A2	951	A
48	A2	953	A
48	A2	955	C
48	A2	956	C
48	A2	960	G
48	A2	965	G
48	A2	967	U
48	A2	969	U
48	A2	1055	C
48	A2	1058	G
48	A2	1059	C
48	A2	1065	C
48	A2	1067	C
48	A2	1084	C
48	A2	1085	U
48	A2	1087	C
48	A2	1147	G
48	A2	1149	G
48	A2	1150	C
48	A2	1152	G
48	A2	1156	G
48	A2	1159	C
48	A2	1161	G
48	A2	1162	U
48	A2	1163	C

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Mol	Chain	Res	Type
48	A2	1164	C
48	A2	1165	C
48	A2	1167	A
48	A2	1192	U
48	A2	1193	C
48	A2	1196	G
48	A2	1201	G
48	A2	1220	C
48	A2	1221	A
48	A2	1222	C
48	A2	1223	G
48	A2	1249	G
48	A2	1250	C
48	A2	1257	A
48	A2	1267	G
48	A2	1268	U
48	A2	1269	C
48	A2	1270	G
48	A2	1271	G
48	A2	1277	A
48	A2	1278	C
48	A2	1309	A
48	A2	1320	A
48	A2	1337	A
48	A2	1341	G
48	A2	1343	G
48	A2	1348	C
48	A2	1349	G
48	A2	1351	A
48	A2	1362	C
48	A2	1370	A
48	A2	1374	A
48	A2	1380	A
48	A2	1381	A
48	A2	1391	G
48	A2	1392	C
48	A2	1393	U
48	A2	1394	C
48	A2	1395	G
48	A2	1403	A
48	A2	1408	G
48	A2	1426	A

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Mol	Chain	Res	Type
48	A2	1428	U
48	A2	1430	C
48	A2	1431	G
48	A2	1432	C
48	A2	1460	C
48	A2	1463	C
48	A2	1464	G
48	A2	1465	C
48	A2	1466	G
48	A2	1467	C
48	A2	1480	G
48	A2	1483	C
48	A2	1485	A
48	A2	1499	G
48	A2	1500	A
48	A2	1501	C
48	A2	1507	A
48	A2	1516	A
48	A2	1548	C
48	A2	1560	U
48	A2	1573	U
48	A2	1578	U
48	A2	1581	A
48	A2	1589	C
48	A2	1595	A
48	A2	1606	G
48	A2	1607	G
48	A2	1613	A
48	A2	1620	A
48	A2	1623	G
48	A2	1636	G
48	A2	1643	C
48	A2	1659	U
48	A2	1678	C
48	A2	1679	G
48	A2	1702	C
48	A2	1713	C
48	A2	1721	G
48	A2	1723	G
48	A2	1737	C
48	A2	1739	U
48	A2	1745	C

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Mol	Chain	Res	Type
48	A2	1746	G
48	A2	1747	A
48	A2	1748	A
48	A2	1751	G
48	A2	1769	A
48	A2	1776	A
48	A2	1784	A
48	A2	1785	G
48	A2	1786	A
48	A2	1803	G
48	A2	1814	G
48	A2	1815	U
48	A2	1816	G
48	A2	1817	G
48	A2	1818	A
48	A2	1823	G
48	A2	1833	U
48	A2	1834	G
48	A2	1835	G
48	A2	1836	G
48	A2	1844	U
48	A2	1860	C
48	A2	1862	C
48	A2	1873	A
48	A2	1876	G
48	A2	1889	A
48	A2	1893	G
48	A2	1896	C
48	A2	1902	C
48	A2	1903	G
48	A2	1921	G
48	A2	1928	U
48	A2	1929	G
48	A2	1932	G
48	A2	1939	A
48	A2	1940	U
48	A2	1941	A
48	A2	1942	G
48	A2	1943	A
48	A2	1945	A
48	A2	1956	G
48	A2	1961	U

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Mol	Chain	Res	Type
48	A2	1963	G
48	A2	1964	A
48	A2	1965	A
48	A2	1968	C
48	A2	1972	A
48	A2	1973	U
48	A2	1978	U
48	A2	1980	A
48	A2	1983	A
48	A2	1984	G
48	A2	2004	C
48	A2	2005	G
48	A2	2006	A
48	A2	2007	A
48	A2	2008	U
48	A2	2011	A
48	A2	2025	U
48	A2	2029	U
48	A2	2037	G
48	A2	2044	G
48	A2	2050	A
48	A2	2057	G
48	A2	2246	U
48	A2	2247	A
48	A2	2279	A
48	A2	2280	G
48	A2	2285	G
48	A2	2301	G
48	A2	2312	G
48	A2	2324	G
48	A2	2327	G
48	A2	2330	C
48	A2	2331	U
48	A2	2339	A
48	A2	2340	G
48	A2	2356	C
48	A2	2357	G
48	A2	2358	A
48	A2	2373	G
48	A2	2374	A
48	A2	2377	U
48	A2	2385	G

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Mol	Chain	Res	Type
48	A2	2389	C
48	A2	2400	G
48	A2	2401	C
48	A2	2419	U
48	A2	2423	U
48	A2	2426	U
48	A2	2429	G
48	A2	2449	C
48	A2	2450	G
48	A2	2467	C
48	A2	2468	C
48	A2	2469	U
48	A2	2482	G
48	A2	2485	G
48	A2	2486	A
48	A2	2490	A
48	A2	2492	A
48	A2	2498	U
48	A2	2515	A
48	A2	2516	A
48	A2	2522	A
48	A2	2523	G
48	A2	2524	U
48	A2	2525	G
48	A2	2528	G
48	A2	2531	G
48	A2	2534	G
48	A2	2565	G
48	A2	2580	A
48	A2	2584	G
48	A2	2595	C
48	A2	2606	C
48	A2	2619	G
48	A2	2620	A
48	A2	2632	C
48	A2	2637	G
48	A2	2638	A
48	A2	2639	A
48	A2	2648	C
48	A2	2651	C
48	A2	2665	G
48	A2	2666	U

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Mol	Chain	Res	Type
48	A2	2667	G
48	A2	2673	G
48	A2	2675	A
48	A2	2676	A
48	A2	2683	C
48	A2	2684	G
48	A2	2690	G
48	A2	2691	G
48	A2	2700	G
48	A2	2704	A
48	A2	2705	G
48	A2	2706	C
48	A2	2713	U
48	A2	2719	U
48	A2	2720	U
48	A2	2723	A
48	A2	2739	G
48	A2	2741	G
48	A2	2742	U
48	A2	2744	A
48	A2	2751	C
48	A2	2755	G
48	A2	2766	A
48	A2	2767	U
48	A2	2769	U
48	A2	2773	C
48	A2	2776	C
48	A2	2785	A
48	A2	2786	A
48	A2	2805	U
48	A2	2806	G
48	A2	2834	G
48	A2	2852	U
48	A2	2853	U
48	A2	2854	C
48	A2	2859	U
48	A2	2870	U
48	A2	2871	C
48	A2	2880	G
48	A2	3572	C
48	A2	3577	U
48	A2	3586	G

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Mol	Chain	Res	Type
48	A2	3587	U
48	A2	3591	G
48	A2	3595	A
48	A2	3596	G
48	A2	3606	A
48	A2	3624	A
48	A2	3633	A
48	A2	3645	G
48	A2	3657	G
48	A2	3663	A
48	A2	3681	G
48	A2	3683	A
48	A2	3688	A
48	A2	3694	A
48	A2	3699	A
48	A2	3707	A
48	A2	3711	G
48	A2	3719	A
48	A2	3724	G
48	A2	3731	A
48	A2	3733	U
48	A2	3741	U
48	A2	3748	G
48	A2	3751	G
48	A2	3754	A
48	A2	3781	C
48	A2	3782	G
48	A2	3785	U
48	A2	3788	A
48	A2	3789	U
48	A2	3795	A
48	A2	3797	C
48	A2	3798	G
48	A2	3799	A
48	A2	3811	U
48	A2	3813	C
48	A2	3814	C
48	A2	3825	C
48	A2	3838	A
48	A2	3847	A
48	A2	3848	A
48	A2	3850	G

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Mol	Chain	Res	Type
48	A2	3852	G
48	A2	3860	G
48	A2	3866	G
48	A2	3872	A
48	A2	3875	G
48	A2	3876	A
48	A2	3878	G
48	A2	3879	A
48	A2	3886	U
48	A2	3889	G
48	A2	3890	C
48	A2	3909	G
48	A2	3926	G
48	A2	3927	G
48	A2	3928	U
48	A2	3935	U
48	A2	3936	A
48	A2	3943	A
48	A2	3944	G
48	A2	4015	G
48	A2	4019	U
48	A2	4020	A
48	A2	4025	U
48	A2	4026	A
48	A2	4027	C
48	A2	4029	C
48	A2	4033	U
48	A2	4035	G
48	A2	4046	G
48	A2	4065	G
48	A2	4066	C
48	A2	4067	G
48	A2	4068	A
48	A2	4073	G
48	A2	4074	A
48	A2	4076	G
48	A2	4078	G
48	A2	4079	C
48	A2	4081	C
48	A2	4087	U
48	A2	4088	C
48	A2	4089	U

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Mol	Chain	Res	Type
48	A2	4105	C
48	A2	4106	C
48	A2	4108	G
48	A2	4109	G
48	A2	4110	C
48	A2	4118	G
48	A2	4120	C
48	A2	4126	C
48	A2	4132	A
48	A2	4133	C
48	A2	4145	G
48	A2	4146	G
48	A2	4153	G
48	A2	4157	G
48	A2	4159	G
48	A2	4165	A
48	A2	4176	A
48	A2	4191	U
48	A2	4195	A
48	A2	4213	A
48	A2	4216	G
48	A2	4228	G
48	A2	4230	A
48	A2	4234	G
48	A2	4235	A
48	A2	4242	A
48	A2	4243	A
48	A2	4252	U
48	A2	4253	G
48	A2	4266	A
48	A2	4267	G
48	A2	4276	C
48	A2	4291	G
48	A2	4292	G
48	A2	4294	C
48	A2	4301	A
48	A2	4307	C
48	A2	4316	U
48	A2	4332	G
48	A2	4333	G
48	A2	4334	U
48	A2	4338	A

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Mol	Chain	Res	Type
48	A2	4339	G
48	A2	4340	A
48	A2	4341	A
48	A2	4342	A
48	A2	4349	C
48	A2	4356	A
48	A2	4360	C
48	A2	4361	U
48	A2	4382	U
48	A2	4384	A
48	A2	4386	A
48	A2	4399	U
48	A2	4426	A
48	A2	4428	C
48	A2	4436	A
48	A2	4437	G
48	A2	4438	C
48	A2	4439	A
48	A2	4448	C
48	A2	4459	U
48	A2	4462	U
48	A2	4474	U
48	A2	4475	A
48	A2	4477	G
48	A2	4481	C
48	A2	4482	G
48	A2	4485	A
48	A2	4486	G
48	A2	4502	C
48	A2	4510	A
48	A2	4545	C
48	A2	4546	A
48	A2	4551	A
48	A2	4552	A
48	A2	4570	G
48	A2	4579	G
48	A2	4589	U
48	A2	4596	U
48	A2	4598	U
48	A2	4599	G
48	A2	4614	G
48	A2	4618	A

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Mol	Chain	Res	Type
48	A2	4620	G
48	A2	4621	G
48	A2	4632	C
48	A2	4633	C
48	A2	4640	G
48	A2	4641	G
48	A2	4662	A
48	A2	4679	A
48	A2	4693	G
48	A2	4694	G
48	A2	4695	C
48	A2	4696	A
48	A2	4697	G
48	A2	4700	C
48	A2	4702	G
48	A2	4703	C
48	A2	4704	G
48	A2	4705	G
48	A2	4714	U
48	A2	4715	U
48	A2	4726	A
48	A2	4730	G
48	A2	4731	G
48	A2	4732	U
48	A2	4826	G
48	A2	4827	U
48	A2	4828	G
48	A2	4829	C
48	A2	4831	G
48	A2	4832	A
48	A2	4833	G
48	A2	4834	U
48	A2	4840	U
48	A2	4841	C
48	A2	4847	G
48	A2	4852	A
48	A2	4853	C
48	A2	4854	G
48	A2	4855	G
48	A2	4856	G
48	A2	4858	C
48	A2	4859	G

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Mol	Chain	Res	Type
48	A2	4861	G
48	A2	4865	G
48	A2	4866	G
48	A2	4867	A
48	A2	4868	A
48	A2	4869	A
48	A2	4870	G
48	A2	4871	G
48	A2	4880	C
48	A2	4882	C
48	A2	4885	G
48	A2	4886	C
48	A2	4887	C
48	A2	4888	C
48	A2	4895	C
48	A2	4899	G
48	A2	4902	C
48	A2	4907	G
48	A2	4908	U
48	A2	4909	G
48	A2	4910	G
48	A2	4934	U
48	A2	4937	A
48	A2	4947	U
48	A2	4950	G
48	A2	4971	C
48	A2	4975	G
48	A2	4977	A
48	A2	4982	C
48	A2	4984	U
48	A2	4985	C
48	A2	4986	G
48	A2	4989	G
48	A2	4999	G
48	A2	5008	C
48	A2	5011	U
48	A2	5012	C
48	A2	5016	A
48	A2	5019	A
48	A2	5020	G
48	A2	5023	U
48	A2	5026	G

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Mol	Chain	Res	Type
48	A2	5028	C
49	B1	4	C
49	B1	17	C
49	B1	33	G
49	B1	41	G
49	B1	44	U
49	B1	46	A
49	B1	67	C
49	B1	71	G
49	B1	72	C
49	B1	73	C
49	B1	75	G
49	B1	76	U
49	B1	77	A
49	B1	78	C
49	B1	103	A
49	B1	113	G
49	B1	114	G
49	B1	115	U
49	B1	142	C
49	B1	143	U
49	B1	146	G
49	B1	155	G
49	B1	157	U
49	B1	158	A
49	B1	161	U
49	B1	162	C
49	B1	170	A
49	B1	172	U
49	B1	174	C
49	B1	175	A
49	B1	181	A
49	B1	183	G
49	B1	209	A
49	B1	211	G
49	B1	228	C
49	B1	229	A
49	B1	230	A
49	B1	283	G
49	B1	284	C
49	B1	285	U
49	B1	286	U

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Mol	Chain	Res	Type
49	B1	287	U
49	B1	292	A
49	B1	296	U
49	B1	306	C
49	B1	313	A
49	B1	314	U
49	B1	315	C
49	B1	318	A
49	B1	325	C
49	B1	327	G
49	B1	328	U
49	B1	329	G
49	B1	331	C
49	B1	332	G
49	B1	333	G
49	B1	363	A
49	B1	364	A
49	B1	370	G
49	B1	385	G
49	B1	386	C
49	B1	391	C
49	B1	407	G
49	B1	408	A
49	B1	409	C
49	B1	417	C
49	B1	426	A
49	B1	427	U
49	B1	439	A
49	B1	448	A
49	B1	450	C
49	B1	463	C
49	B1	464	A
49	B1	465	A
49	B1	466	G
49	B1	469	A
49	B1	472	C
49	B1	476	A
49	B1	482	G
49	B1	485	A
49	B1	486	A
49	B1	487	U
49	B1	489	A

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Mol	Chain	Res	Type
49	B1	492	C
49	B1	493	A
49	B1	509	G
49	B1	522	A
49	B1	525	A
49	B1	526	A
49	B1	529	A
49	B1	533	A
49	B1	536	A
49	B1	541	U
49	B1	542	U
49	B1	544	G
49	B1	545	A
49	B1	546	G
49	B1	547	G
49	B1	548	C
49	B1	554	A
49	B1	559	G
49	B1	560	A
49	B1	561	A
49	B1	562	U
49	B1	563	G
49	B1	588	G
49	B1	590	A
49	B1	591	U
49	B1	592	C
49	B1	605	A
49	B1	606	G
49	B1	607	U
49	B1	608	C
49	B1	614	C
49	B1	629	A
49	B1	630	U
49	B1	635	G
49	B1	636	C
49	B1	643	A
49	B1	644	G
49	B1	645	C
49	B1	651	U
49	B1	660	C
49	B1	668	A
49	B1	669	A

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Mol	Chain	Res	Type
49	B1	671	A
49	B1	672	A
49	B1	673	G
49	B1	675	U
49	B1	681	U
49	B1	684	G
49	B1	696	G
49	B1	748	C
49	B1	750	C
49	B1	797	C
49	B1	798	G
49	B1	800	U
49	B1	808	A
49	B1	834	C
49	B1	847	A
49	B1	858	A
49	B1	869	A
49	B1	870	A
49	B1	911	C
49	B1	913	A
49	B1	914	U
49	B1	916	A
49	B1	917	U
49	B1	919	A
49	B1	920	A
49	B1	925	G
49	B1	929	G
49	B1	933	G
49	B1	943	U
49	B1	956	G
49	B1	960	U
49	B1	969	U
49	B1	987	A
49	B1	989	C
49	B1	990	A
49	B1	1001	A
49	B1	1008	A
49	B1	1025	U
49	B1	1044	G
49	B1	1045	U
49	B1	1048	G
49	B1	1055	A

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Mol	Chain	Res	Type
49	B1	1061	U
49	B1	1066	U
49	B1	1083	A
49	B1	1085	C
49	B1	1109	C
49	B1	1110	G
49	B1	1114	U
49	B1	1115	U
49	B1	1116	C
49	B1	1117	C
49	B1	1119	A
49	B1	1120	U
49	B1	1121	G
49	B1	1123	C
49	B1	1139	C
49	B1	1140	G
49	B1	1148	A
49	B1	1149	A
49	B1	1150	A
49	B1	1199	A
49	B1	1207	G
49	B1	1215	C
49	B1	1224	G
49	B1	1242	U
49	B1	1243	U
49	B1	1251	A
49	B1	1256	G
49	B1	1257	G
49	B1	1258	A
49	B1	1259	A
49	B1	1261	C
49	B1	1274	G
49	B1	1275	G
49	B1	1286	G
49	B1	1288	U
49	B1	1301	A
49	B1	1302	G
49	B1	1303	C
49	B1	1311	C
49	B1	1330	G
49	B1	1332	A
49	B1	1344	A

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Mol	Chain	Res	Type
49	B1	1345	G
49	B1	1348	G
49	B1	1354	G
49	B1	1371	U
49	B1	1372	U
49	B1	1378	A
49	B1	1380	C
49	B1	1381	G
49	B1	1396	A
49	B1	1399	C
49	B1	1409	A
49	B1	1411	G
49	B1	1416	C
49	B1	1418	C
49	B1	1419	C
49	B1	1420	G
49	B1	1439	A
49	B1	1442	U
49	B1	1462	U
49	B1	1463	U
49	B1	1476	A
49	B1	1477	U
49	B1	1478	U
49	B1	1489	A
49	B1	1495	G
49	B1	1498	A
49	B1	1519	U
49	B1	1520	G
49	B1	1521	C
49	B1	1522	A
49	B1	1525	C
49	B1	1531	A
49	B1	1533	A
49	B1	1543	U
49	B1	1548	G
49	B1	1551	U
49	B1	1580	A
49	B1	1586	U
49	B1	1601	A
49	B1	1602	U
49	B1	1604	G
49	B1	1606	G

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Mol	Chain	Res	Type
49	B1	1620	A
49	B1	1622	U
49	B1	1623	A
49	B1	1638	G
49	B1	1654	G
49	B1	1660	C
49	B1	1661	A
49	B1	1662	U
49	B1	1663	A
49	B1	1665	G
49	B1	1668	U
49	B1	1671	G
49	B1	1673	U
49	B1	1683	C
49	B1	1721	U
49	B1	1742	C
49	B1	1751	C
49	B1	1757	G
49	B1	1776	G
49	B1	1780	G
49	B1	1782	G
49	B1	1793	A
49	B1	1829	G
49	B1	1831	A
49	B1	1834	A
49	B1	1835	A
49	B1	1838	U
49	B1	1839	U
49	B1	1841	C
49	B1	1849	G
49	B1	1851	A
49	B1	1852	C
49	B1	1861	G
49	B1	1862	G
49	B1	1864	U
49	B1	1865	C
49	B1	1866	A
49	B1	1867	U
49	B1	1869	A
83	Bv	2	C
83	Bv	7	A
83	Bv	8	U

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Mol	Chain	Res	Type
83	Bv	9	A
83	Bv	11	C
83	Bv	13	C
83	Bv	17	C
83	Bv	18	G
83	Bv	19	G
83	Bv	20	U
83	Bv	24	G
83	Bv	25	C
83	Bv	26	A
83	Bv	31	A
83	Bv	33	U
83	Bv	37	A
83	Bv	38	A
83	Bv	39	U
83	Bv	41	C
83	Bv	42	C
83	Bv	43	C
83	Bv	44	G
83	Bv	45	U
83	Bv	46	G
83	Bv	48	C
83	Bv	51	U
83	Bv	53	G
83	Bv	54	U
83	Bv	58	A
83	Bv	60	U
83	Bv	61	C
83	Bv	63	G
83	Bv	66	U
83	Bv	69	G
83	Bv	71	G
83	Bv	72	C
83	Bv	75	C
83	Bv	76	A
83	Bw	2	C
83	Bw	3	C
83	Bw	5	G
83	Bw	6	G
83	Bw	7	A
83	Bw	9	A
83	Bw	10	G

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Mol	Chain	Res	Type
83	Bw	16	U
83	Bw	17	C
83	Bw	18	G
83	Bw	19	G
83	Bw	20	U
83	Bw	21	A
83	Bw	26	A
83	Bw	32	U
83	Bw	36	A
83	Bw	40	C
83	Bw	41	C
83	Bw	46	G
83	Bw	47	U
83	Bw	48	C
83	Bw	50	U
83	Bw	52	G
83	Bw	53	G
83	Bw	54	U
83	Bw	55	U
83	Bw	58	A
83	Bw	59	U
83	Bw	65	G
83	Bw	66	U
83	Bw	68	C
83	Bw	71	G
83	Bw	75	C
83	Bw	76	A
84	Bx	35	U
84	Bx	36	U
84	Bx	37	U
84	Bx	38	U
84	Bx	39	U
84	Bx	40	U
84	Bx	41	U
84	Bx	42	U
84	Bx	49	U
84	Bx	51	U
84	Bx	52	U
84	Bx	53	U
84	Bx	54	U
84	Bx	55	U
84	Bx	56	U

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Mol	Chain	Res	Type
84	Bx	57	U
84	Bx	58	U
84	Bx	61	U

All (72) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A3	34	U
1	A3	81	C
1	A3	108	A
1	A3	110	U
2	A4	13	A
48	A2	31	U
48	A2	70	A
48	A2	71	C
48	A2	84	A
48	A2	135	G
48	A2	227	G
48	A2	229	G
48	A2	230	U
48	A2	309	G
48	A2	738	A
48	A2	740	G
48	A2	901	U
48	A2	902	A
48	A2	958	U
48	A2	959	C
48	A2	1161	G
48	A2	1162	U
48	A2	1342	G
48	A2	1379	G
48	A2	1402	G
48	A2	1500	A
48	A2	1559	G
48	A2	1785	G
48	A2	1816	G
48	A2	1943	A
48	A2	2005	G
48	A2	2006	A
48	A2	2485	G
48	A2	2508	A
48	A2	2684	G

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Mol	Chain	Res	Type
48	A2	2743	A
48	A2	3595	A
48	A2	3798	G
48	A2	3799	A
48	A2	3814	C
48	A2	4026	A
48	A2	4107	C
48	A2	4242	A
48	A2	4596	U
48	A2	4597	A
48	A2	4661	U
48	A2	4714	U
48	A2	4828	G
48	A2	4832	A
48	A2	4865	G
48	A2	4870	G
48	A2	4907	G
48	A2	4946	U
49	B1	180	G
49	B1	226	A
49	B1	227	U
49	B1	229	A
49	B1	283	G
49	B1	286	U
49	B1	369	C
49	B1	546	G
49	B1	547	G
49	B1	560	A
49	B1	561	A
49	B1	683	G
49	B1	797	C
49	B1	869	A
49	B1	1287	A
49	B1	1289	U
49	B1	1398	G
49	B1	1555	U
49	B1	1756	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 331 ligands modelled in this entry, 331 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (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
49	B1	8
48	A2	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B1	842:C	O3'	843:C	P	1.85
1	B1	558:G	O3'	559:G	P	1.84
1	B1	497:C	O3'	498:C	P	1.83
1	B1	72:C	O3'	73:C	P	1.82
1	B1	1253:A	O3'	1254:C	P	1.82
1	A2	1716:G	O3'	1717:U	P	1.80
1	B1	1420:G	O3'	1421:A	P	1.80
1	A2	1057:G	O3'	1058:G	P	1.76
1	A2	1249:G	O3'	1250:C	P	1.76
1	B1	683:G	O3'	684:G	P	1.76
1	B1	351:G	O3'	352:U	P	1.75

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A2	2689:C	O3'	2690:G	P	1.37
1	A2	3612:U	O3'	3613:A	P	1.35

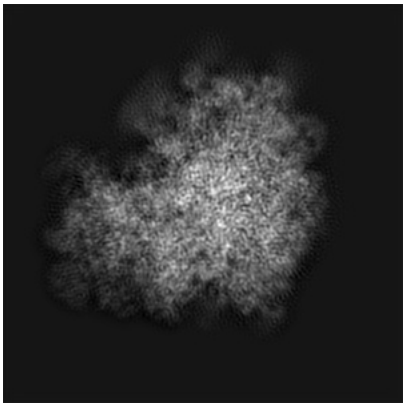
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2875. These allow visual inspection of the internal detail of the map and identification of artifacts.

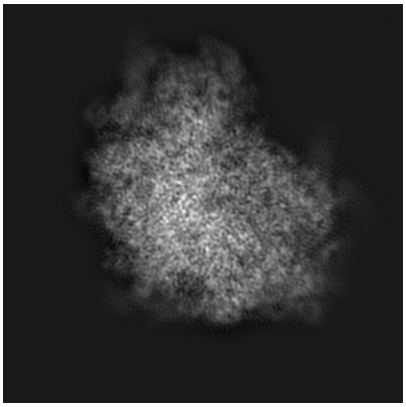
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

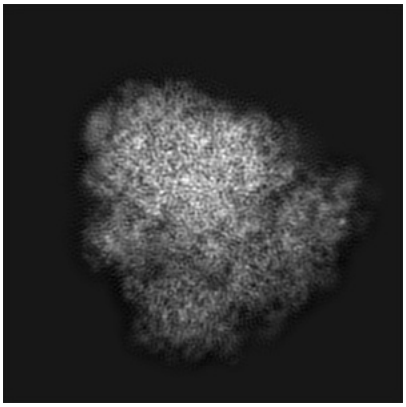
6.1.1 Primary map



X



Y

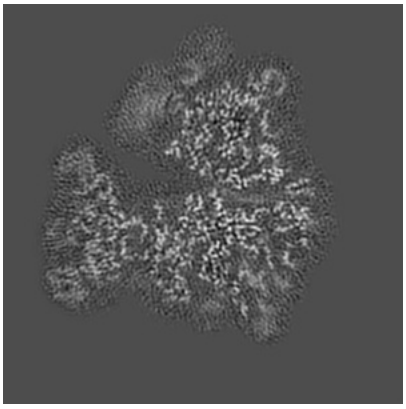


Z

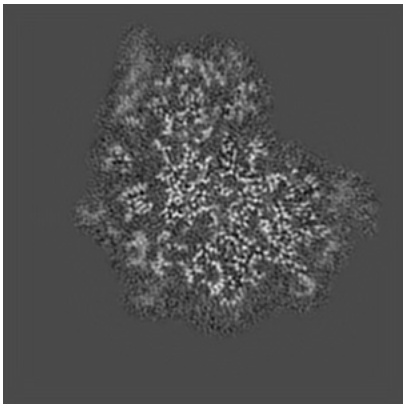
The images above show the map projected in three orthogonal directions.

6.2 Central slices

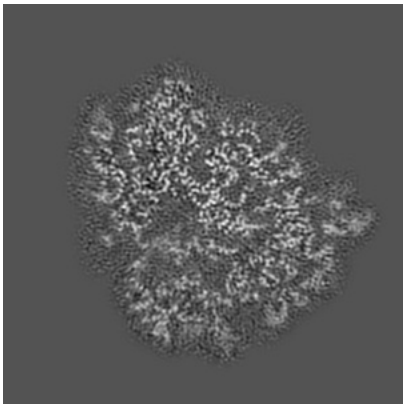
6.2.1 Primary map



X Index: 200



Y Index: 200

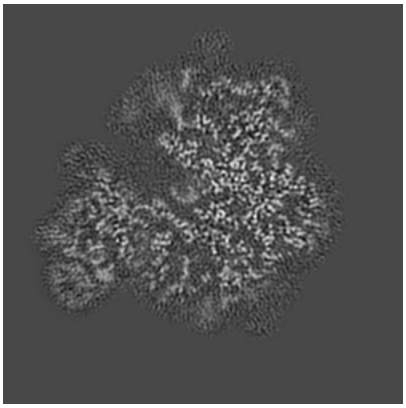


Z Index: 200

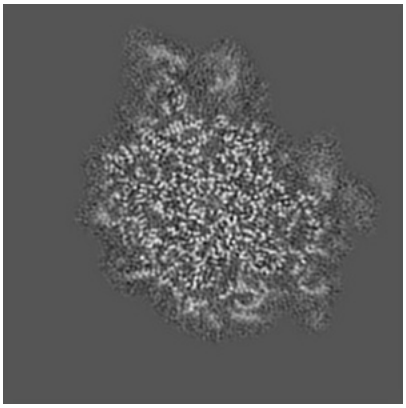
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

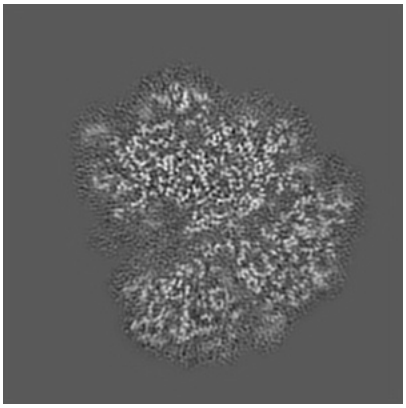
6.3.1 Primary map



X Index: 186



Y Index: 220

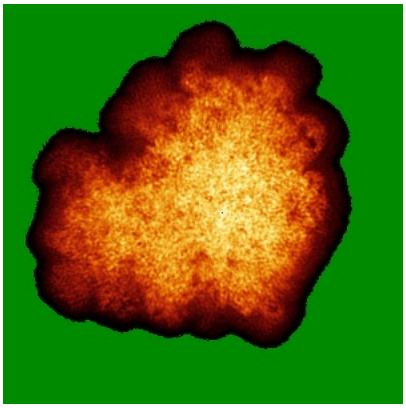


Z Index: 184

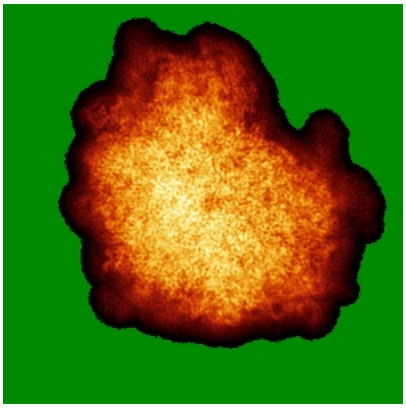
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

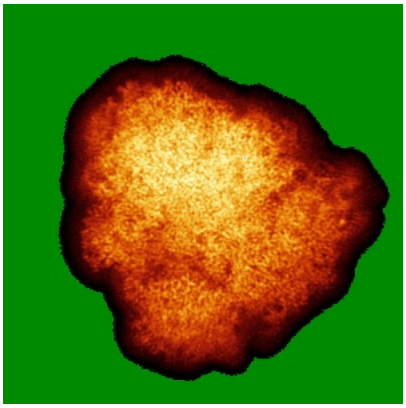
6.4.1 Primary map



X



Y

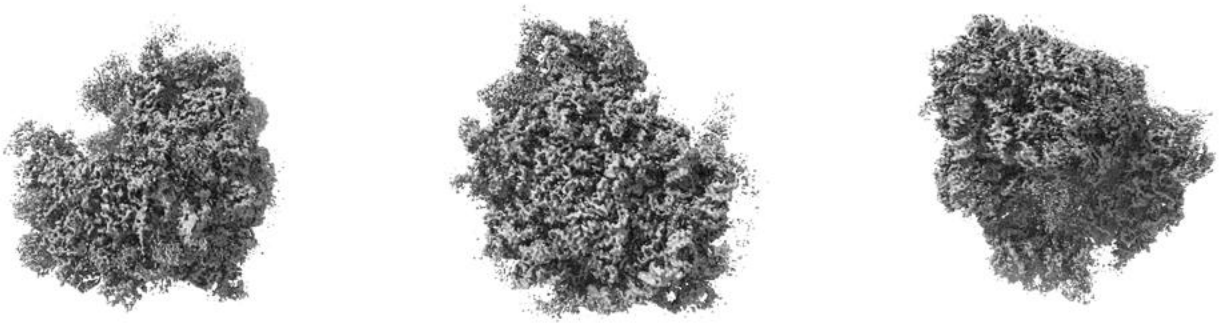


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

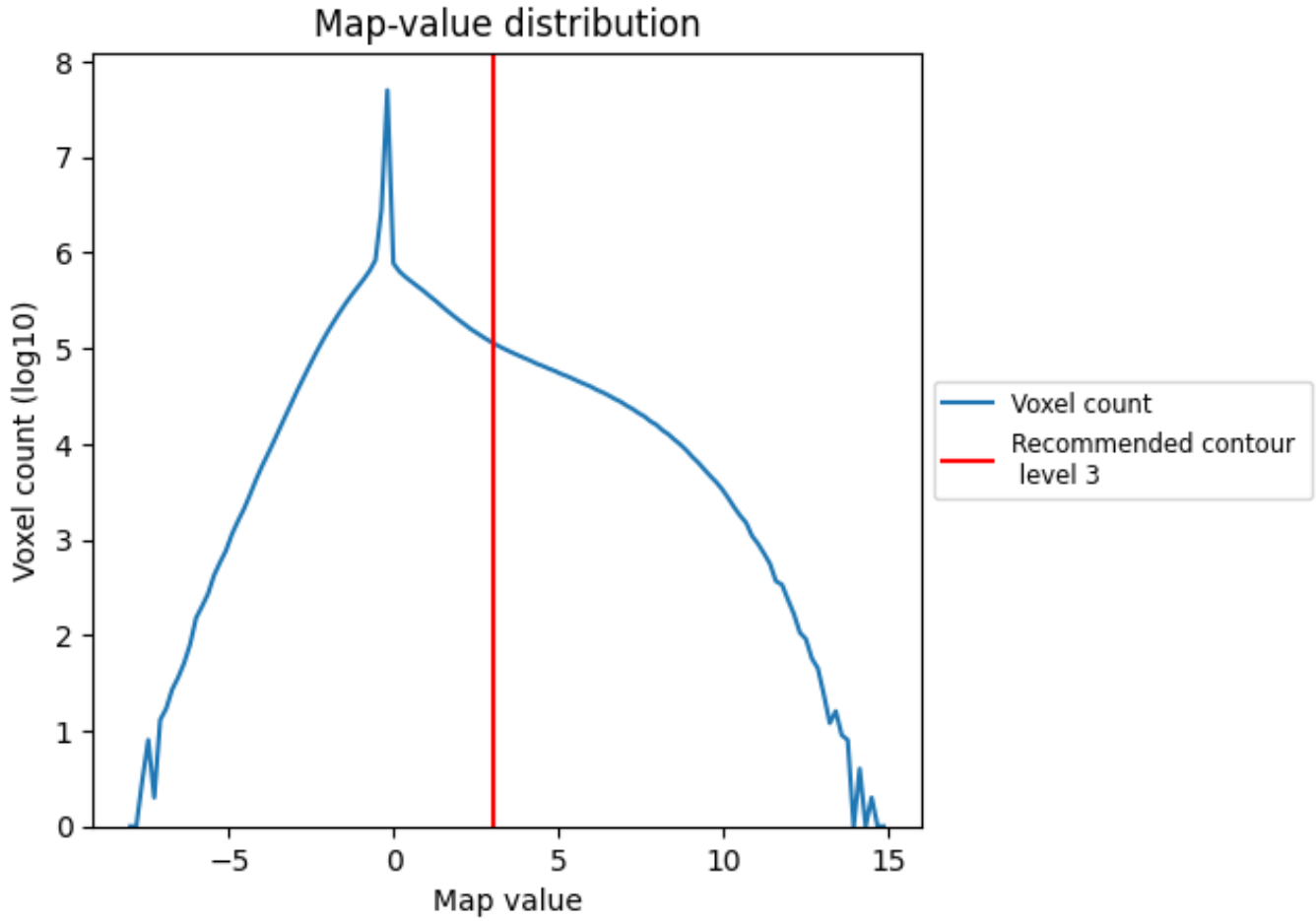
6.6 Mask visualisation (i)

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

7 Map analysis

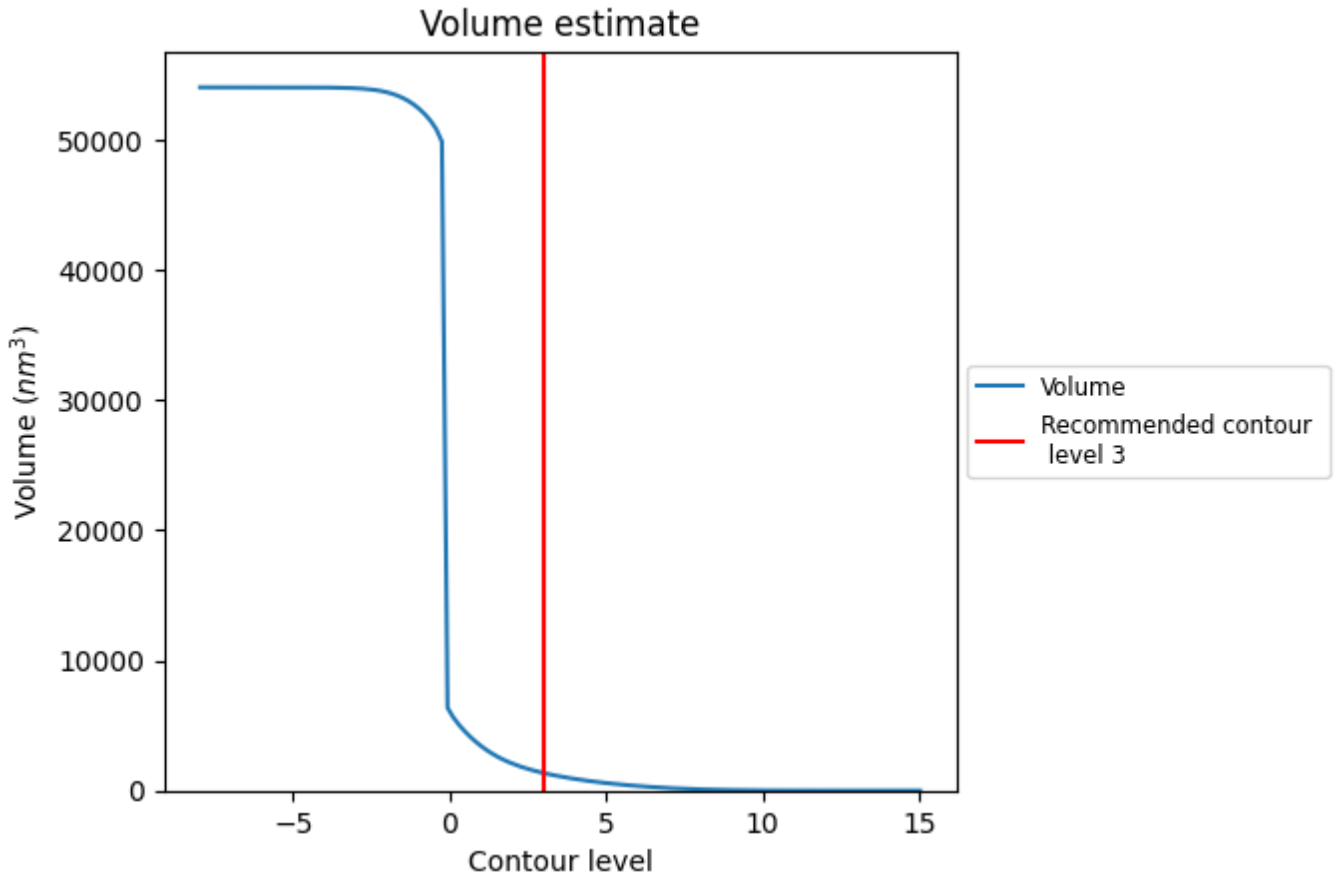
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

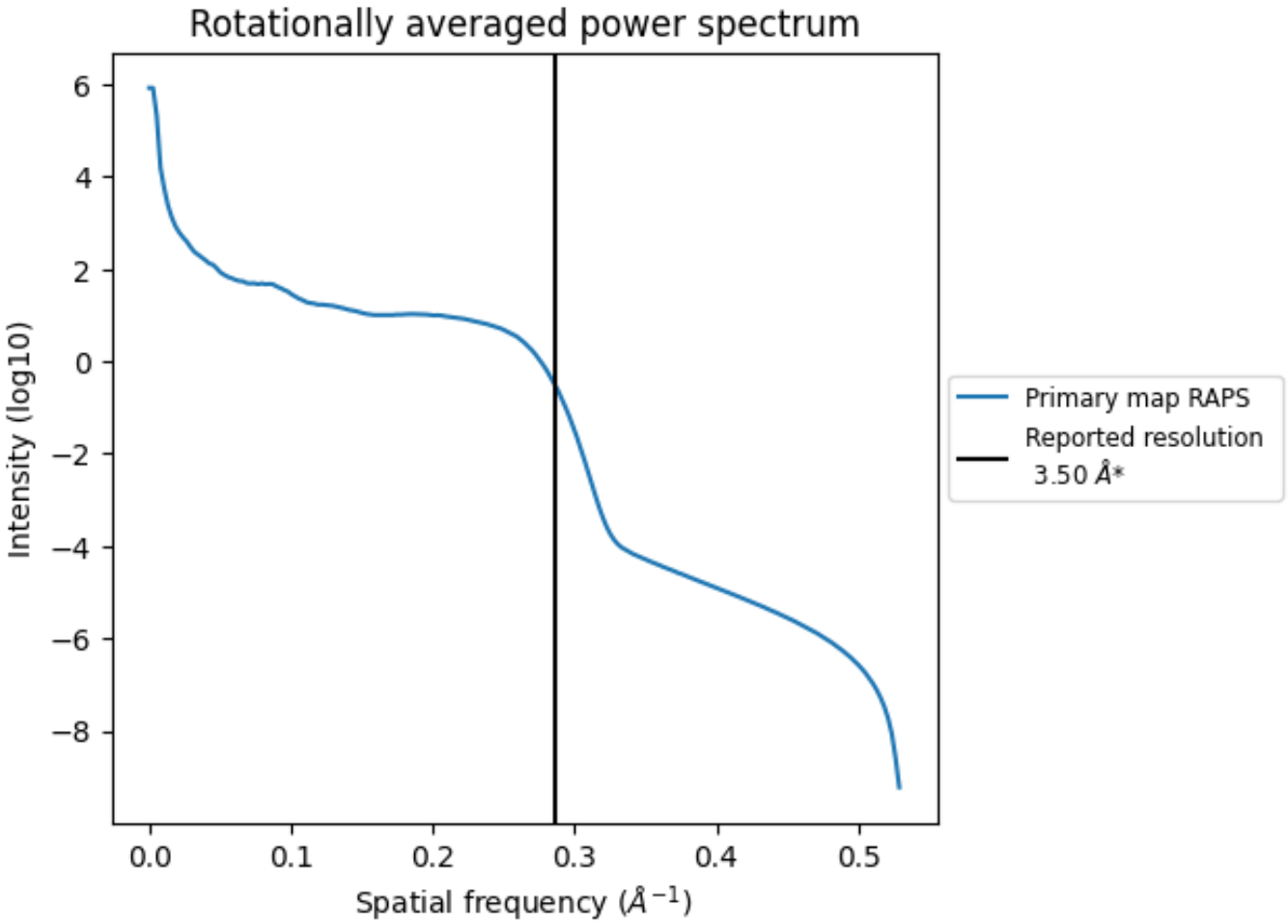
7.2 Volume estimate



The volume at the recommended contour level is 1346 nm^3; this corresponds to an approximate mass of 1216 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 0.286 Å^{-1}

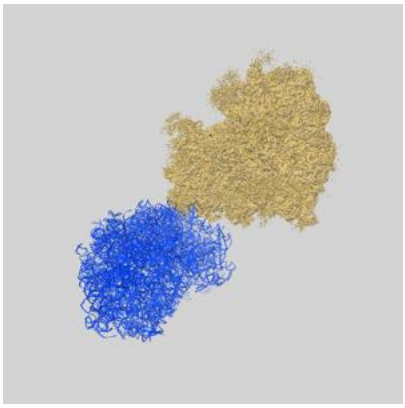
8 Fourier-Shell correlation

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

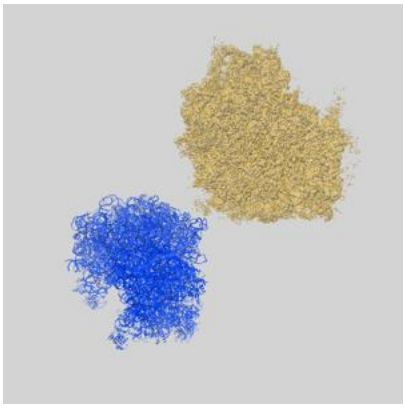
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2875 and PDB model 5AJ0. Per-residue inclusion information can be found in section 3 on page 21.

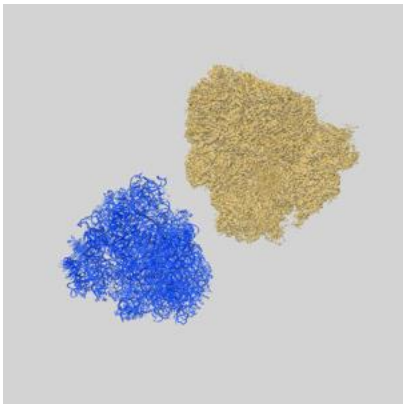
9.1 Map-model overlay



X



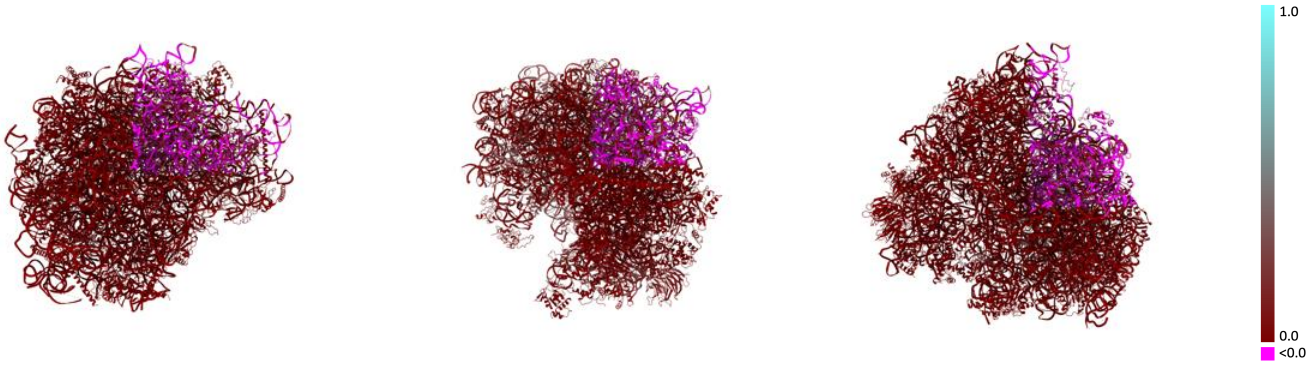
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0 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.

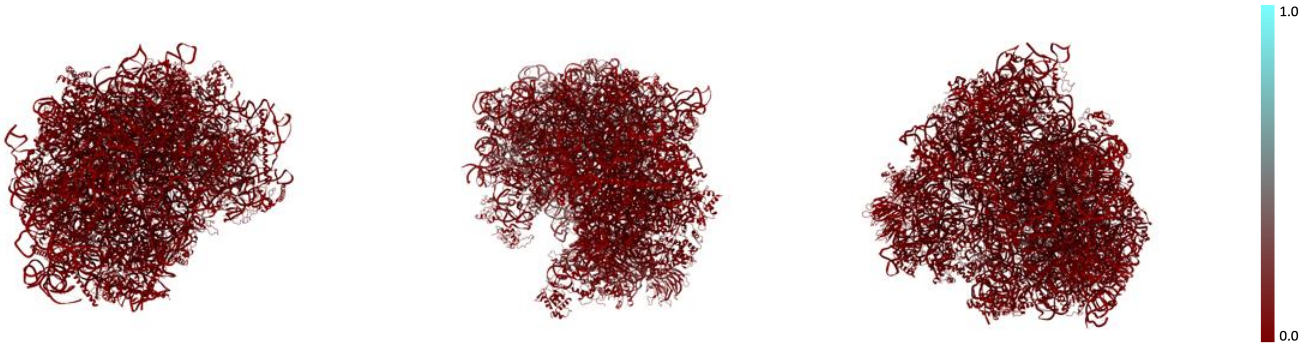
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

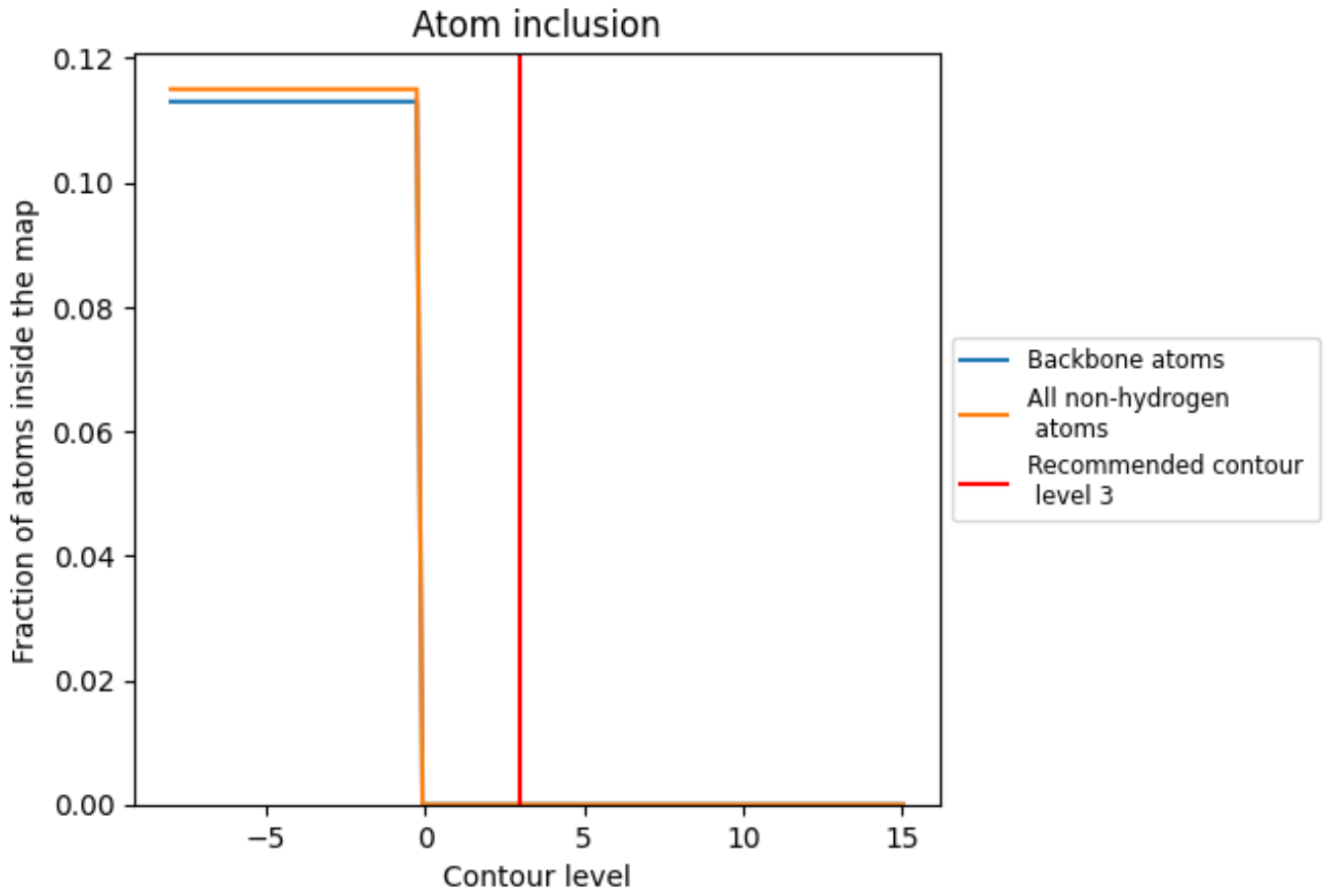
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (3).

9.4 Atom inclusion (i)



At the recommended contour level, 0% of all backbone atoms, 0% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0000	0.0000
A2	0.0000	0.0000
A3	0.0000	0.0030
A4	0.0000	0.0000
AA	0.0000	0.0010
AB	0.0000	0.0000
AC	0.0000	0.0000
AD	0.0000	0.0000
AE	0.0000	0.0000
AF	0.0000	0.0000
AG	0.0000	-0.0010
AH	0.0000	0.0000
AI	0.0000	0.0000
AJ	0.0000	0.0000
AK	0.0000	0.0000
AL	0.0000	0.0000
AM	0.0000	0.0000
AN	0.0000	0.0000
AO	0.0000	0.0000
AP	0.0000	0.0010
AQ	0.0000	0.0000
AR	0.0000	0.0150
AS	0.0000	0.0000
AT	0.0000	0.0000
AU	0.0000	-0.0210
AV	0.0000	0.0000
AW	0.0000	0.0000
AX	0.0000	0.0020
AY	0.0000	0.0000
AZ	0.0000	0.0050
Aa	0.0000	0.0000
Ab	0.0000	0.0000
Ac	0.0000	-0.0080
Ad	0.0000	0.0000
Ae	0.0000	0.0000

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Chain	Atom inclusion	Q-score
Af	0.0000	0.0000
Ag	0.0000	0.0190
Ah	0.0000	0.0000
Ai	0.0000	0.0000
Aj	0.0000	-0.0050
Ak	0.0000	0.0040
Al	0.0000	0.0220
Am	0.0000	0.0000
An	0.0000	0.0000
Ao	0.0000	0.0000
Ap	0.0000	-0.0110
Aq	0.0000	0.0000
At	0.0000	0.0000
Au	0.0000	0.0000
B1	0.0000	0.0000
BA	0.0000	0.0000
BB	0.0000	0.0000
BC	0.0000	0.0000
BD	0.0000	0.0000
BE	0.0000	0.0000
BF	0.0000	0.0000
BG	0.0000	0.0000
BH	0.0000	0.0000
BI	0.0000	0.0150
BJ	0.0000	0.0000
BK	0.0000	0.0000
BL	0.0000	0.0040
BM	0.0000	0.0000
BN	0.0000	0.0010
BO	0.0000	0.0000
BP	0.0000	0.0000
BQ	0.0000	0.0000
BR	0.0000	0.0000
BS	0.0000	0.0000
BT	0.0000	0.0000
BU	0.0000	0.0000
BV	0.0000	0.0000
BW	0.0000	0.0000
BX	0.0000	0.0000
BY	0.0000	0.0000
BZ	0.0000	0.0000
Ba	0.0000	0.0000

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Chain	Atom inclusion	Q-score
Bb	0.0000	0.0000
Bc	0.0000	0.0000
Bd	0.0000	0.0000
Be	0.0000	0.0000
Bf	0.0000	0.0000
Bg	0.0000	0.0000
Bv	0.0000	0.0000
Bw	0.0000	0.0000
Bx	0.0000	0.0000
By	0.0000	0.0210