



Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 02:09 am GMT

PDB ID : 4UJC
EMDB ID : EMD-2683
Title : mammalian 80S HCV-IRES initiation complex with eIF5B POST-like state
Authors : Yamamoto, H.; Unbehaun, A.; Loerke, J.; Behrmann, E.; Marianne, C.;
Burger, J.; Mielke, T.; Spahn, C.M.T.
Deposited on : 2014-06-18
Resolution : 9.50 Å(reported)
Based on initial model : 4CXC

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:

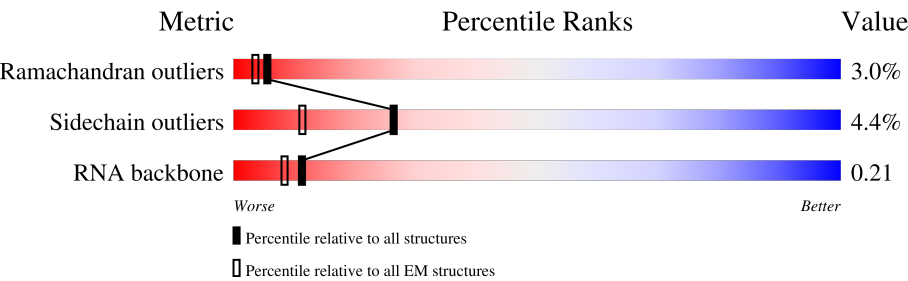
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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 9.50 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	76	<div><div>12%</div><div>67%</div><div>32%</div><div>.</div></div>
2	AB	627	<div><div>62%</div><div>85%</div><div>10%</div><div>..</div></div>
3	AC	504	<div><div>19%</div><div>15%</div><div>21%</div><div>12%</div><div>48%</div></div>
4	A2	5025	<div><div>30%</div><div>41%</div><div>.</div><div>28%</div></div>
5	A3	194	<div><div>38%</div><div>41%</div><div>.</div><div>19%</div></div>
6	A4	121	<div><div>40%</div><div>56%</div><div>..</div></div>
7	BA	257	<div><div>12%</div><div>93%</div><div>..</div></div>
8	BB	403	<div><div>8%</div><div>90%</div><div>7%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
9	BC	427	
10	BD	297	
11	BE	158	
12	BF	248	
13	BG	266	
14	BH	192	
15	BI	214	
16	BJ	178	
17	BL	211	
18	BM	215	
19	BN	204	
20	BO	203	
21	BP	184	
22	BQ	188	
23	BR	196	
24	BS	176	
25	BT	160	
26	BU	128	
27	BV	140	
28	BW	157	
29	BX	156	
30	BY	145	
31	BZ	136	
32	Ba	148	
33	Bb	159	

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Mol	Chain	Length	Quality of chain
34	Bc	115	
35	Bd	125	
36	Be	135	
37	Bf	110	
38	Bg	117	
39	Bh	123	
40	Bi	105	
41	Bj	97	
42	Bk	70	
43	Bl	51	
44	Bm	128	
45	Bn	25	
46	Bo	106	
47	Bp	92	
48	Bt	137	
49	Bu	210	
50	C1	1869	
51	CA	263	
52	CB	264	
53	CC	293	
54	CD	243	
55	CE	263	
56	CF	204	
57	CG	249	
58	CH	194	

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Mol	Chain	Length	Quality of chain
59	CI	208	
60	CJ	194	
61	CK	165	
62	CL	158	
63	CM	132	
64	CN	151	
65	CO	151	
66	CP	145	
67	CQ	146	
68	CR	135	
69	CS	152	
70	CT	145	
71	CU	119	
72	CV	83	
73	CW	130	
74	CX	143	
75	CY	133	
76	CZ	125	
77	Ca	115	
78	Cb	84	
79	Cc	69	
80	Cd	56	
81	Ce	59	
82	Cf	156	
83	Cg	317	

2 Entry composition [i](#)

There are 85 unique types of molecules in this entry. The entry contains 223911 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 TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

- Molecule 2 is a protein called EIF5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	611	Total	C	N	O	S	0	0
			4846	3084	834	906	22		

- Molecule 3 is a RNA chain called HCV-IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	261	Total	C	N	O	P	0	0
			5574	2485	1001	1828	260		

- Molecule 4 is a RNA chain called 28S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A2	3616	Total	C	N	O	P	0	0
			77488	34508	14153	25212	3615		

- Molecule 5 is a RNA chain called 5.8S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A3	157	Total	C	N	O	P	0	0
			3334	1489	587	1102	156		

- Molecule 6 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A4	119	Total	C	N	O	P	0	0
			2538	1132	454	834	118		

- Molecule 7 is a protein called 60S RIBOSOMAL PROTEIN L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BA	247	Total	C	N	O	S	0	1
			1888	1183	388	311	6		

- Molecule 8 is a protein called 60S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BB	396	Total	C	N	O	S	0	1
			3190	2030	601	545	14		

- Molecule 9 is a protein called 60S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BC	364	Total	C	N	O	S	0	1
			2889	1817	578	480	14		

- Molecule 10 is a protein called 60S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BD	290	Total	C	N	O	S	0	0
			2362	1489	431	428	14		

- Molecule 11 is a protein called 60S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BE	158	Total	C	N	O		0	0
			1287	834	238	215			

- Molecule 12 is a protein called 60S RIBOSOMAL PROTEIN L7.

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

- Molecule 13 is a protein called 60S RIBOSOMAL PROTEIN L7A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BG	235	Total	C	N	O	S	0	1
			1881	1197	363	317	4		

- Molecule 14 is a protein called 60S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BH	192	Total	C	N	O	S	0	0
			1536	965	286	279	6		

- Molecule 15 is a protein called 60S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BI	196	Total	C	N	O	S	0	0
			1605	1022	308	263	12		

- Molecule 16 is a protein called 60S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BJ	170	Total	C	N	O	S	0	0
			1363	861	254	242	6		

- Molecule 17 is a protein called 60S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BL	200	Total	C	N	O	S	0	1
			1617	1013	335	265	4		

- Molecule 18 is a protein called 60S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BM	140	Total	C	N	O	S	0	1
			1139	730	219	183	7		

- Molecule 19 is a protein called 60S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BN	204	Total	C	N	O	S	0	0
			1709	1077	360	267	5		

- Molecule 20 is a protein called 60S RIBOSOMAL PROTEIN L13A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BO	196	Total	C	N	O	S	0	1
			1607	1034	316	252	5		

- Molecule 21 is a protein called 60S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BP	153	Total	C	N	O	S	0	1
			1234	771	241	213	9		

- Molecule 22 is a protein called 60S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BQ	184	Total	C	N	O	S	0	0
			1494	933	311	245	5		

- Molecule 23 is a protein called 60S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BR	183	Total	C	N	O	S	0	1
			1526	943	331	242	10		

- Molecule 24 is a protein called 60S RIBOSOMAL PROTEIN L18A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BS	173	Total	C	N	O	S	0	0
			1439	916	280	233	10		

- Molecule 25 is a protein called 60S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BT	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 26 is a protein called 60S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BU	102	Total	C	N	O	S	0	1
			827	529	146	150	2		

- Molecule 27 is a protein called 60S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BV	128	Total	C	N	O	S	0	0
			964	610	181	168	5		

- Molecule 28 is a protein called 60S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BW	64	Total	C	N	O	S	0	1
			529	337	104	85	3		

- Molecule 29 is a protein called 60S RIBOSOMAL PROTEIN L23A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BX	119	Total	C	N	O	S	0	0
			976	624	183	168	1		

- Molecule 30 is a protein called 60S RIBOSOMAL PROTEIN L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BY	128	Total	C	N	O	S	0	1
			1065	668	217	177	3		

- Molecule 31 is a protein called 60S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BZ	136	Total	C	N	O	S	0	0
			1115	719	209	183	4		

- Molecule 32 is a protein called 60S RIBOSOMAL PROTEIN L27A.

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

- Molecule 33 is a protein called 60S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Bb	69	Total	C	N	O	S	0	1
			560	344	123	90	3		

- Molecule 34 is a protein called 60S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Bc	104	Total	C	N	O	S	0	1
			802	508	142	145	7		

- Molecule 35 is a protein called 60S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Bd	109	Total	C	N	O	S	0	0
			905	570	174	159	2		

- Molecule 36 is a protein called 60S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Be	128	Total	C	N	O	S	0	1
			1053	664	219	165	5		

- Molecule 37 is a protein called 60S RIBOSOMAL PROTEIN L35A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Bf	107	Total	C	N	O	S	0	0
			866	550	172	141	3		

- Molecule 38 is a protein called 60S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Bg	115	Total	C	N	O	S	0	1
			907	566	188	147	6		

- Molecule 39 is a protein called 60S RIBOSOMAL PROTEIN UL29.

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

- Molecule 40 is a protein called 60S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Bi	97	Total	C	N	O	S	0	1
			783	488	168	122	5		

- Molecule 41 is a protein called 60S RIBOSOMAL PROTEIN L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Bj	85	Total	C	N	O	S	0	1
			690	423	153	109	5		

- Molecule 42 is a protein called 60S RIBOSOMAL PROTEIN L38.

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

- Molecule 43 is a protein called 60S RIBOSOMAL PROTEIN L39.

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

- Molecule 44 is a protein called UBIQUITIN-60S RIBOSOMAL PROTEIN L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Bm	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 45 is a protein called 60S RIBOSOMAL PROTEIN L41.

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

- Molecule 46 is a protein called 60S RIBOSOMAL PROTEIN L36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Bo	106	Total	C	N	O	S	0	0
			871	547	176	141	7		

- Molecule 47 is a protein called 60S RIBOSOMAL PROTEIN L37A.

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

- Molecule 48 is a protein called 60S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Bt	130	Total	C	N	O	S	0	1
			1043	646	220	172	5		

- Molecule 49 is a protein called 60S RIBOSOMAL PROTEIN L10A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Bu	210	Total	C	N	O	S	0	0
			1622	990	278	348	6		

- Molecule 50 is a RNA chain called 18S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	C1	1742	Total	C	N	O	P	0	0
			37159	16589	6665	12164	1741		

- Molecule 51 is a protein called 40S RIBOSOMAL PROTEIN US2.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	CA	218	Total	C	N	O	S	0	0
			1719	1091	301	319	8		

- Molecule 52 is a protein called 40S RIBOSOMAL PROTEIN ES1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	CB	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 53 is a protein called 40S RIBOSOMAL PROTEIN US5.

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

- Molecule 54 is a protein called 40S RIBOSOMAL PROTEIN US3.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	CD	212	Total	C	N	O	S	0	0
			1646	1050	299	290	7		

- Molecule 55 is a protein called 40S RIBOSOMAL PROTEIN ES4.

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

- Molecule 56 is a protein called 40S RIBOSOMAL PROTEIN US7.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	CF	188	Total	C	N	O	S	0	0
			1486	930	283	266	7		

- Molecule 57 is a protein called 40S RIBOSOMAL PROTEIN ES6.

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

- Molecule 58 is a protein called 40S RIBOSOMAL PROTEIN ES7.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	CH	191	Total	C	N	O	S	0	0
			1535	978	282	274	1		

- Molecule 59 is a protein called 40S RIBOSOMAL PROTEIN ES8.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	CI	207	Total	C	N	O	S	0	0
			1695	1064	334	292	5		

- Molecule 60 is a protein called 40S RIBOSOMAL PROTEIN US4.

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

- Molecule 61 is a protein called 40S RIBOSOMAL PROTEIN ES10.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	CK	94	Total	C	N	O	S	0	0
			791	519	138	129	5		

- Molecule 62 is a protein called 40S RIBOSOMAL PROTEIN US17.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	CL	146	Total	C	N	O	S	0	0
			1199	764	224	205	6		

- Molecule 63 is a protein called 40S RIBOSOMAL PROTEIN ES12.

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

- Molecule 64 is a protein called 40S RIBOSOMAL PROTEIN US15.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	CN	150	Total	C	N	O	S	0	0
			1207	773	229	204	1		

- Molecule 65 is a protein called 40S RIBOSOMAL PROTEIN US11.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	CO	137	Total	C	N	O	S	0	0
			1023	627	200	190	6		

- Molecule 66 is a protein called 40S RIBOSOMAL PROTEIN US19.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	CP	118	Total	C	N	O	S	0	0
			981	625	183	166	7		

- Molecule 67 is a protein called 40S RIBOSOMAL PROTEIN US9.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	CQ	139	Total	C	N	O	S	0	0
			1108	704	210	191	3		

- Molecule 68 is a protein called 40S RIBOSOMAL PROTEIN ES17.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	CR	109	Total	C	N	O	S	0	0
			893	561	170	159	3		

- Molecule 69 is a protein called 40S RIBOSOMAL PROTEIN US13.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	CS	142	Total	C	N	O	S	0	0
			1172	736	236	199	1		

- Molecule 70 is a protein called 40S RIBOSOMAL PROTEIN ES19.

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

- Molecule 71 is a protein called 40S RIBOSOMAL PROTEIN US10.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	CU	101	Total	C	N	O	S	0	0
			803	502	153	144	4		

- Molecule 72 is a protein called 40S RIBOSOMAL PROTEIN ES21.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	CV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 73 is a protein called 40S RIBOSOMAL PROTEIN US8.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	CW	129	Total	C	N	O	S	0	0
			1033	659	193	175	6		

- Molecule 74 is a protein called 40S RIBOSOMAL PROTEIN US12.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	CX	134	Total	C	N	O	S	0	0
			1046	663	205	176	2		

- Molecule 75 is a protein called 40S RIBOSOMAL PROTEIN ES24.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	CY	122	Total	C	N	O	S	0	0
			1002	635	196	166	5		

- Molecule 76 is a protein called 40S RIBOSOMAL PROTEIN ES25.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	CZ	76	Total	C	N	O	S	0	0
			605	387	112	105	1		

- Molecule 77 is a protein called 40S RIBOSOMAL PROTEIN ES26.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ca	96	Total	C	N	O	S	0	0
			767	476	159	127	5		

- Molecule 78 is a protein called 40S RIBOSOMAL PROTEIN ES27.

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

- Molecule 79 is a protein called 40S RIBOSOMAL PROTEIN ES28.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Cc	62	Total	C	N	O	S	0	0
			490	298	99	91	2		

- Molecule 80 is a protein called 40S RIBOSOMAL PROTEIN US14.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Cd	53	Total	C	N	O	S	0	0
			444	278	90	71	5		

- Molecule 81 is a protein called 40S RIBOSOMAL PROTEIN ES30.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Ce	51	Total	C	N	O	S	0	0
			412	258	90	63	1		

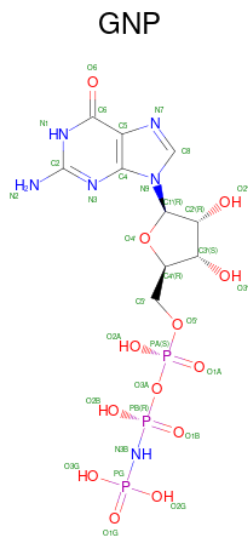
- Molecule 82 is a protein called 40S RIBOSOMAL PROTEIN ES31.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Cf	61	Total	C	N	O	S	0	0
			497	312	94	84	7		

- Molecule 83 is a protein called 40S RIBOSOMAL PROTEIN RACK1.

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

- Molecule 84 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



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

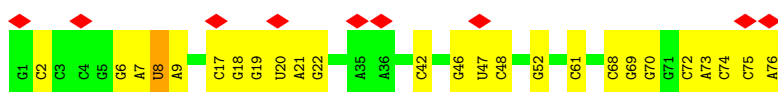
- Molecule 85 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
85	AB	1	Total Mg 1 1	0

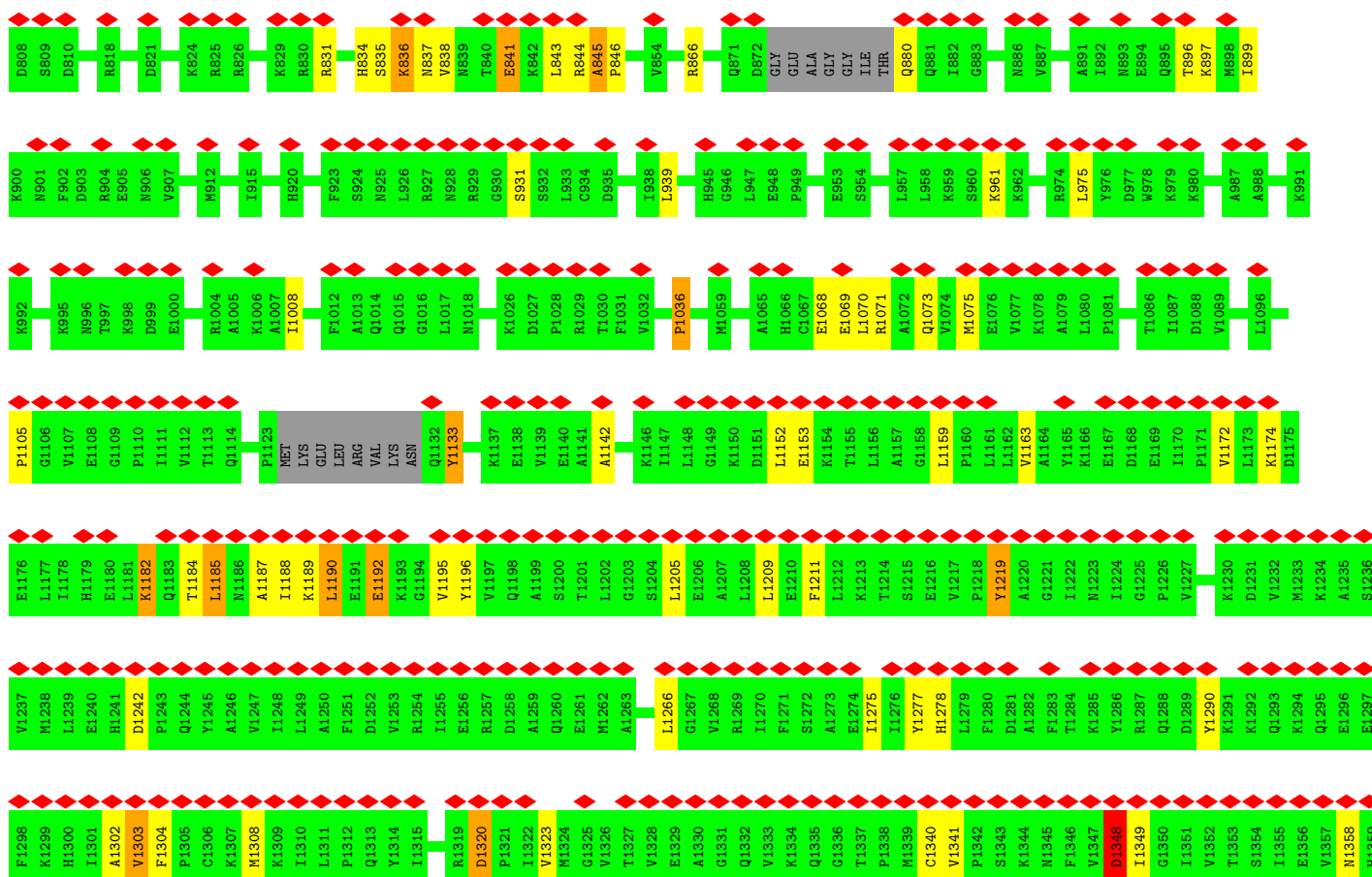
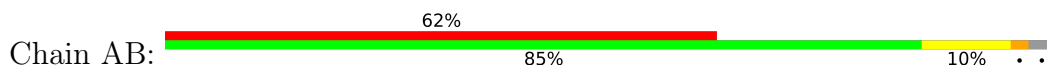
3 Residue-property plots

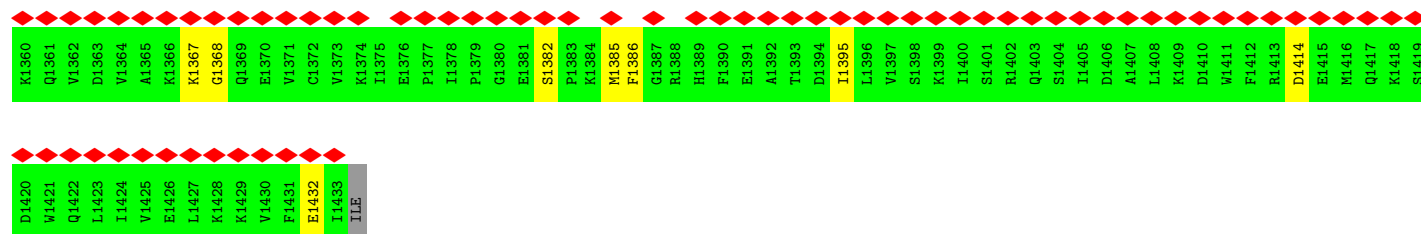
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

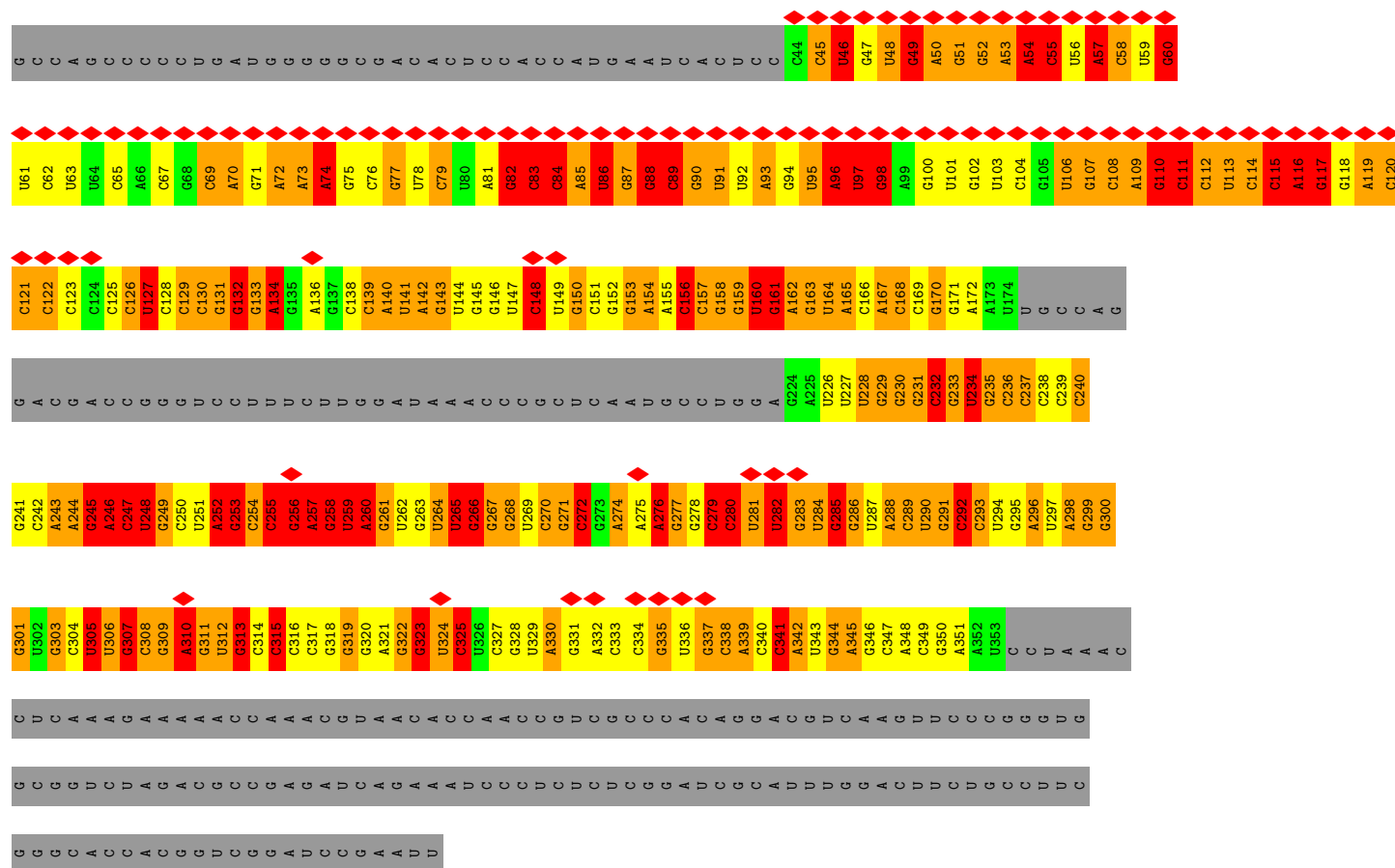


• Molecule 2: EIF5B

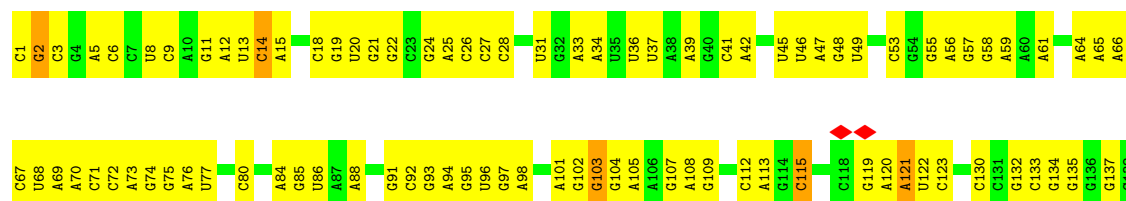


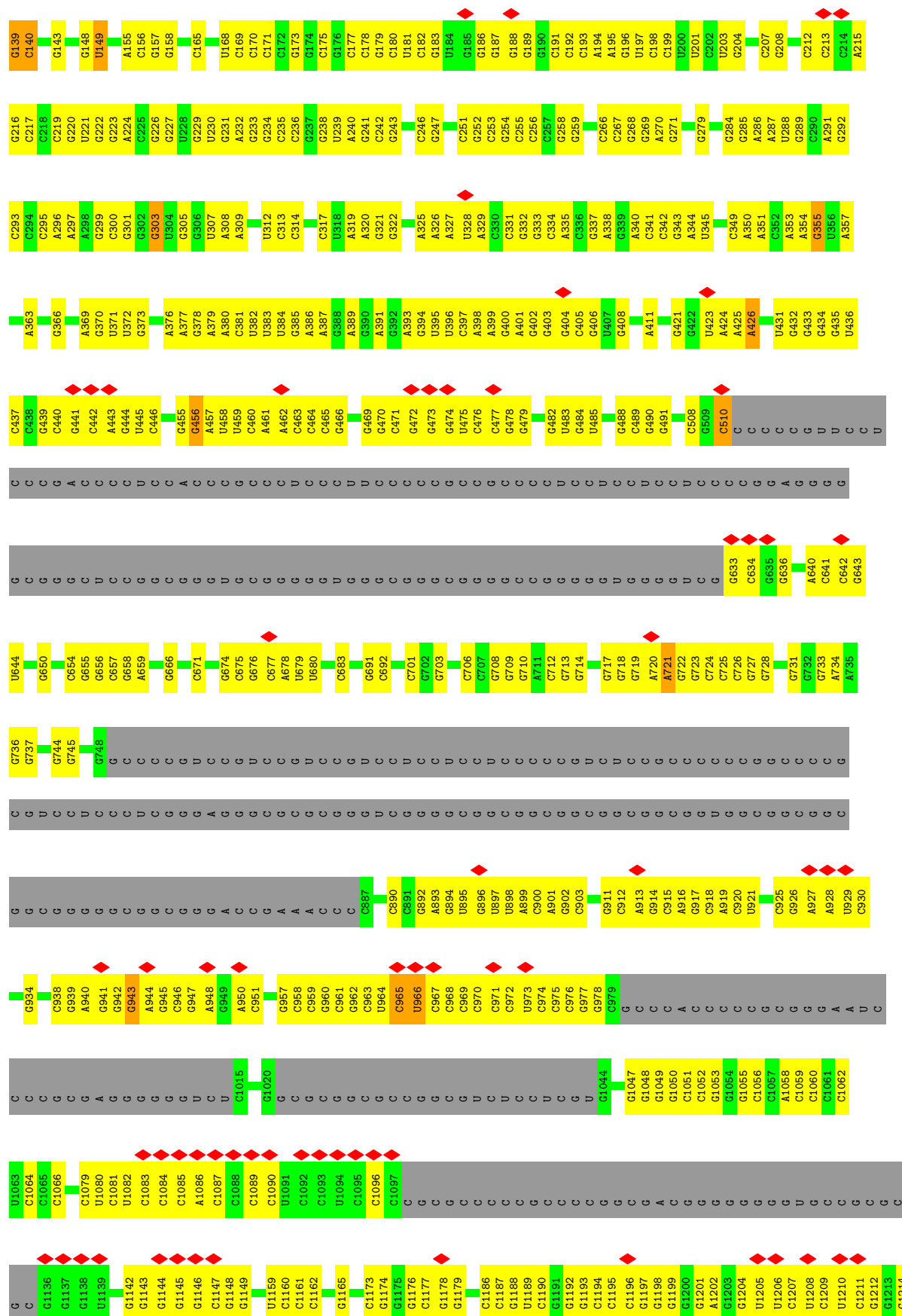


• Molecule 3: HCV-IRES



• Molecule 4: 28S RIBOSOMAL RNA

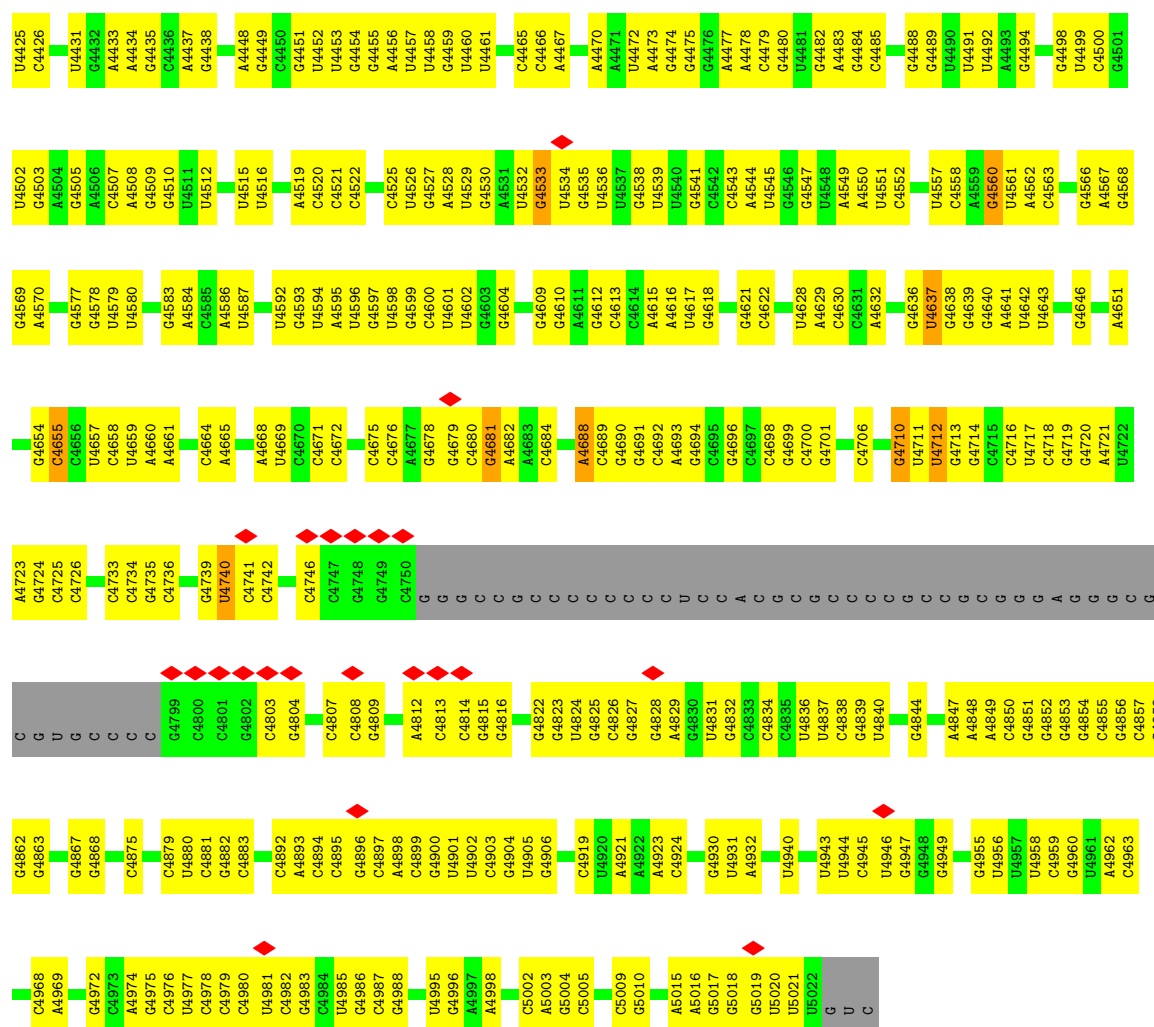




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C1216	C1288	C1367	G1452	C1530	G1608	G	A1744	G1813	U1883	A	G2024	A
A1218	C1289	A1368	U1452	G1531	A1609	G	A1745	G1814	U1884	A	A2025	A
C1219	G1291	A1368	U1452	A1531	A1610	G	A1746	A1815	U1885	U	G2026	G
G1220	C1292	A1372	G1454	A1533	A1611	C	C1747	U1816	A1886	C	G2027	C
C1221	C1293	G1373	C1455	A1537	G1612	C	G1748	G1817	C1887	C	G2028	C
G1222	C1294	G1374	G1458	A1537	A1613	C	A1749	C1818	C1891	G	C2029	G
C1223	U1297	U1375	G1459	G1540	A1614	C	U1752	G1819	C1892	G	G2030	G
G1224	U1299	A1377	C1459	G1540	U1615	G	C1753	A1820	C1893	A	C2031	A
C1225	U1300	A1378	C1460	A1541	A1616	A	A1754	G1821	G1894	C	U2032	C
C1229	U1301	G1384	C1461	A1542	A1617	C	A1755	G1822	U1895	C	G2033	U
C1232	G1302	G1388	C1462	A1543	U1618	C	C1756	C1825	G1896	C	G2034	C
G	A1303	G1388	C1463	A1544	C1619	C	U1757	G1826	G1897	C	A2035	C
A	A1304	G1389	C1464	C1545	G1620	A	C1758	G1829	C1898	C	G2036	G
A	A1305	U1390	C1465	U1548	C1623	C	U1759	G1832	C1899	C	C2037	C
G	A1306	U1391	G1467	G1549	U1628	C	U1760	G1833	G1900	U	U2039	U
A	C1307	G1392	G1468	G1550	A1629	C	U1761	C1834	U1901	A	G2040	A
G	G1308	C1393	G1471	G1553	G1630	C	A1766	C1835	G1902	C	G2041	G
A	A1313	C1398	G1475	G1554	U1631	C	A1767	A1836	G1903	G	G2042	C
G1238	A1314	C1398	A1476	G1555	A1632	C	C1768	U1839	A1912	A	G2043	G
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G1245	A1323	A1400	G1478	U1557	C1634	A	A1773	U1844	A1917	U	C2045	U
G1246	C1324	G1401	C1478	C1558	U1635	C	U1774	A1845	G1918	C	A2047	C
A1248	A1325	G1402	A1479	G1559	G1636	G	U1775	A1846	A1919	U	U2048	U
G1249	C1326	G1406	C1480	U1561	U1637	C1701	U1776	G1847	A1920	A	A2049	C
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A1254	G1333	C1412	C1484	G1571	C1644	U1706	A1781	U1706	G1926	C	C2052	C
G1255	A1334	C1416	A1487	G1572	A1648	U1709	G1782	A1852	G1929	C	G2056	C
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C1284	C1285	C1446	C1525	G1603	C1673	U1733	G1803	C1875	U	U	C	
C1285	U1361	C1446	C1525	G1604	U	U1734	U1804	G1876	C	C	C	
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						U1736	C1806	G1878	C	C	C	
						G1737	G1809	C1879	A	A	C	
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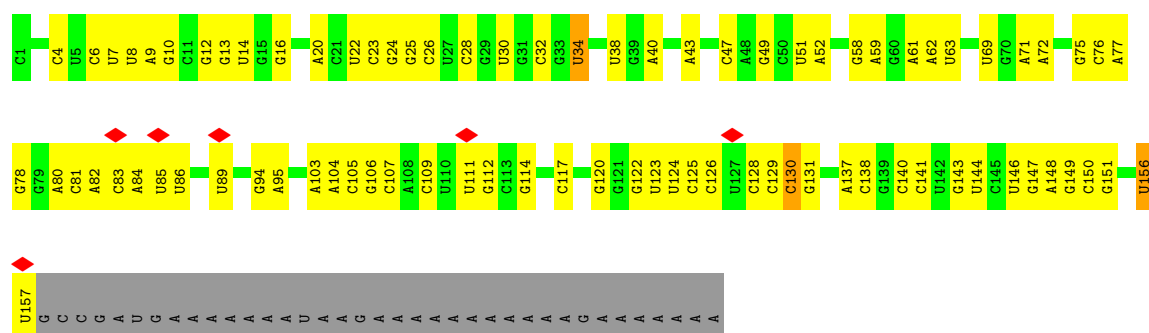
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A4357	A4211	C4122	C4047	C	C3917	C3847	G3761	U3678	U3600	U	G
C4358	C4212	U4123	G4050	G	A3918	G3848	G3762	G3679	G3601	C	A
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U4297	G4226	U4129	G4054	G	G3922	U3852	U3767	G3683	C3605	C	C
G4298	A4227	C4130	C4055	G	A3923	U3853	A3768	U3684	G	U	U
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U4302	G4229	U4135	G4057	G	G3925	G3855	U3770	U3610	C	C	C
U4303	A4231	C4136	G4058	U	G3926	C3856	U3771	A3611	C	C	C
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C4305	A4233	A4138	G4060	C	U3928	A3859	A3776	G	G	C	C
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C4315	A4240	U4151	G4071	C	G3935	G3869	U3787	A3631	C	C	C
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C4420	G4281	A4199	A4117	C	G	G	G	G	G	C	C
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C4422	A4283	G	C4042	C	G	G	G	G	G	C	C
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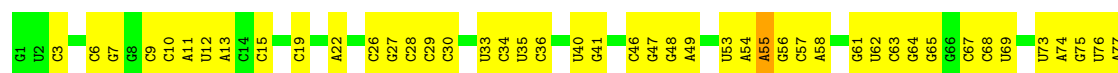
• Molecule 5: 5.8S RIBOSOMAL RNA

Chain A3: 38% 41% 19%



• Molecule 6: 5S RIBOSOMAL RNA

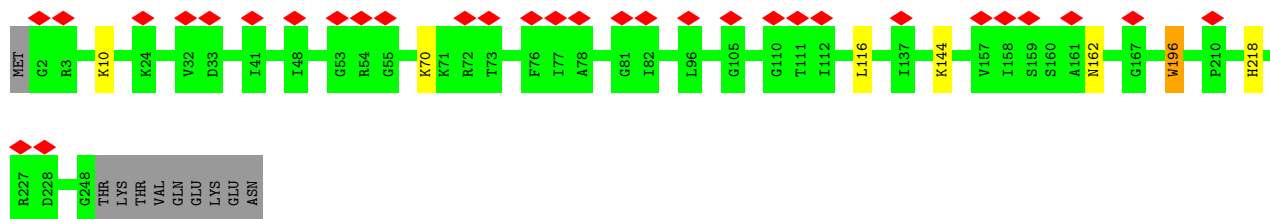
Chain A4: 40% 56% 4%





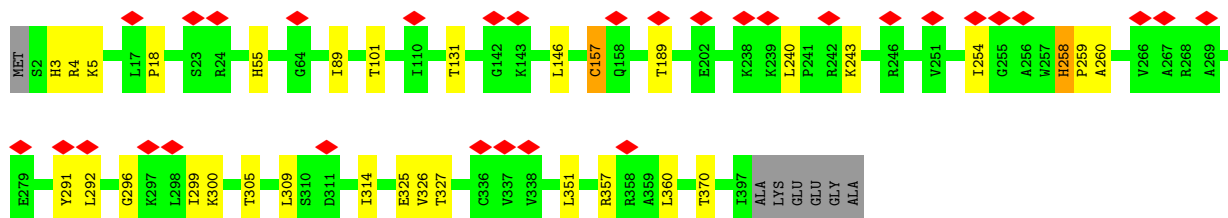
• Molecule 7: 60S RIBOSOMAL PROTEIN L8

Chain BA: 12% 93%



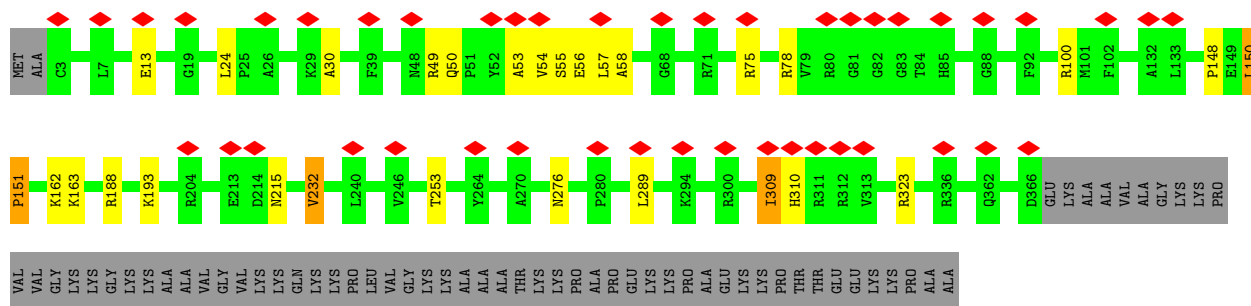
• Molecule 8: 60S RIBOSOMAL PROTEIN L3

Chain BB: 8% 90% 7%



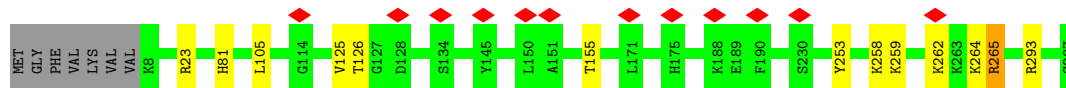
• Molecule 9: 60S RIBOSOMAL PROTEIN L4

Chain BC: 10% 78% 6% 15%



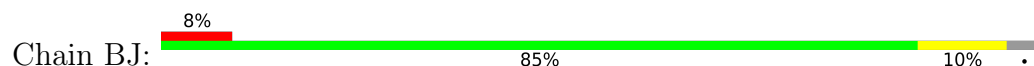
• Molecule 10: 60S RIBOSOMAL PROTEIN L5

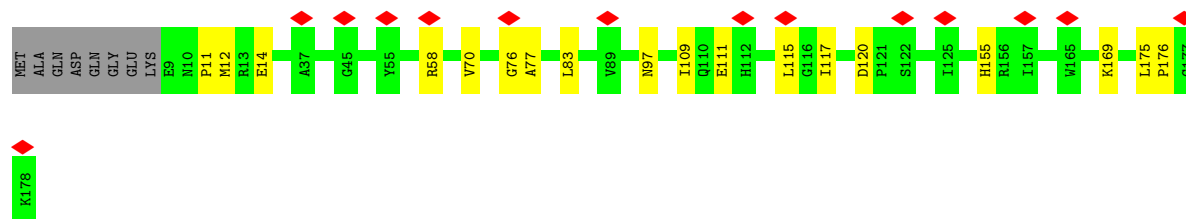
Chain BD: 1% 93%



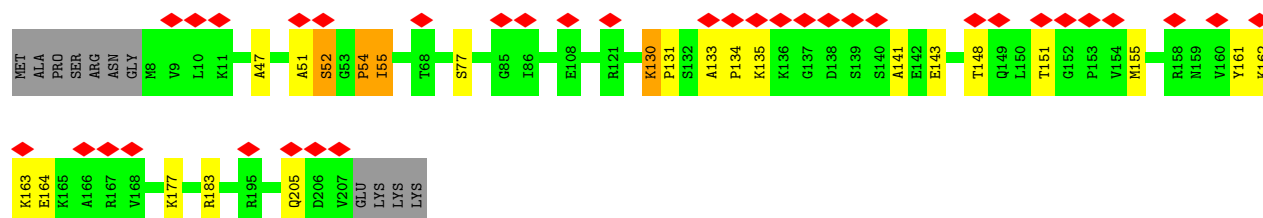
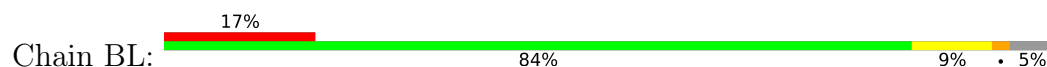
• Molecule 11: 60S RIBOSOMAL PROTEIN L6

Chain BE: 15% 91% 9%

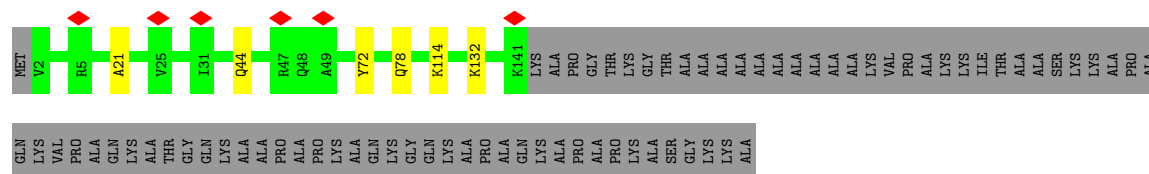




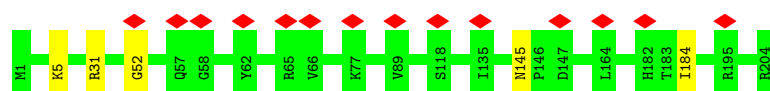
• Molecule 17: 60S RIBOSOMAL PROTEIN L13



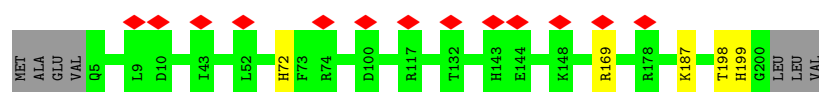
• Molecule 18: 60S RIBOSOMAL PROTEIN L14



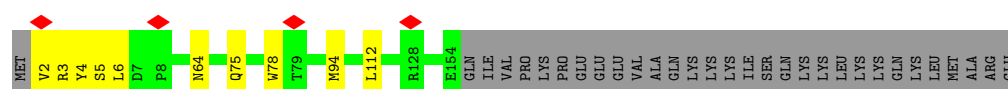
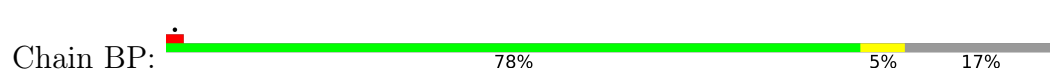
• Molecule 19: 60S RIBOSOMAL PROTEIN L15



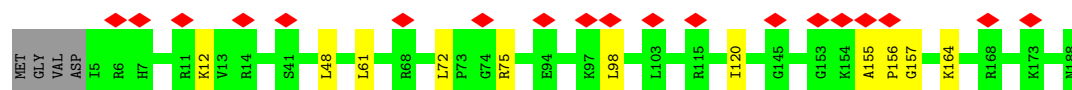
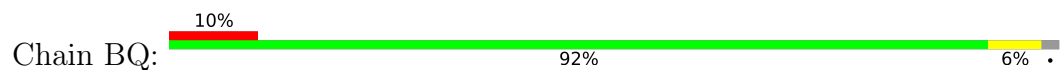
• Molecule 20: 60S RIBOSOMAL PROTEIN L13A



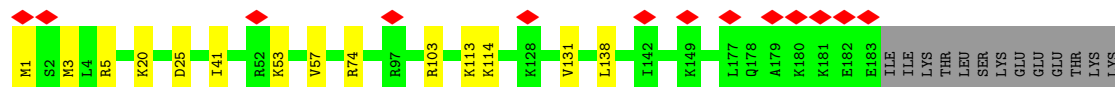
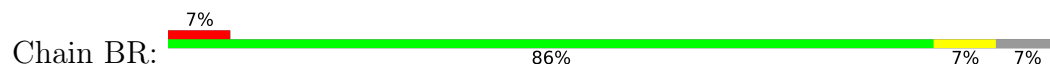
• Molecule 21: 60S RIBOSOMAL PROTEIN L17



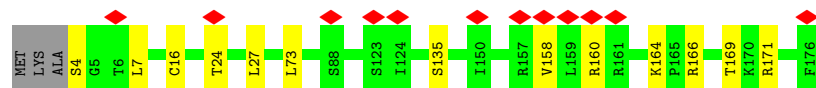
- Molecule 22: 60S RIBOSOMAL PROTEIN L18



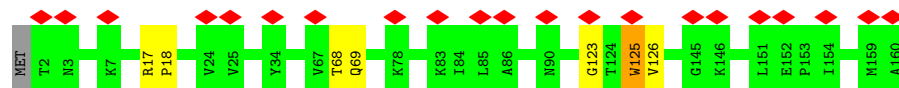
- Molecule 23: 60S RIBOSOMAL PROTEIN L19



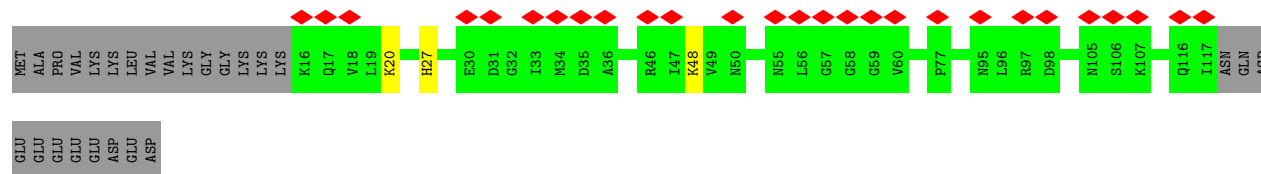
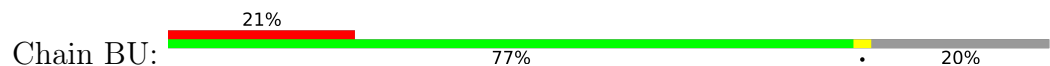
- Molecule 24: 60S RIBOSOMAL PROTEIN L18A



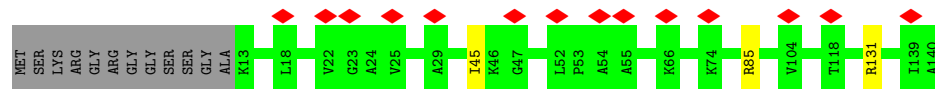
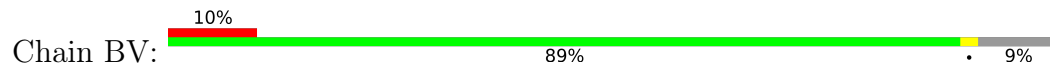
- Molecule 25: 60S RIBOSOMAL PROTEIN L21



- Molecule 26: 60S RIBOSOMAL PROTEIN L22

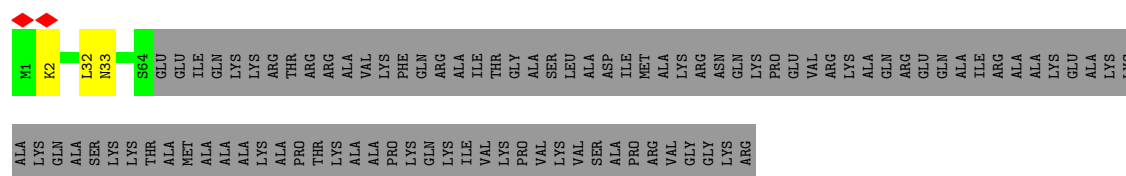


- Molecule 27: 60S RIBOSOMAL PROTEIN L23

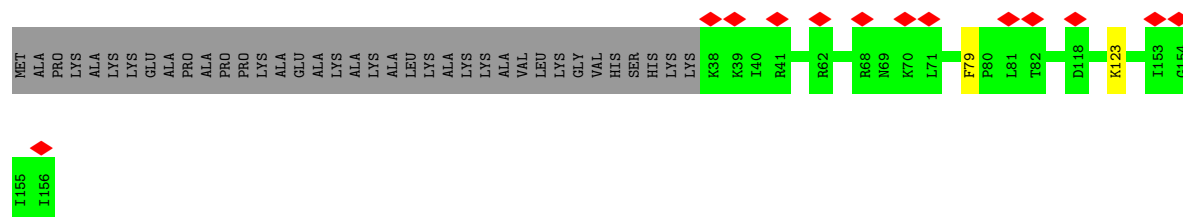
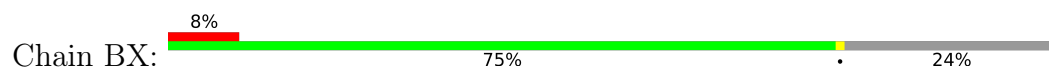


- Molecule 28: 60S RIBOSOMAL PROTEIN L24

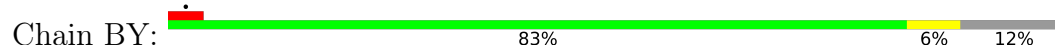




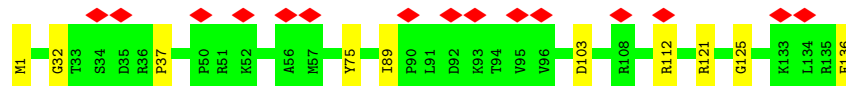
• Molecule 29: 60S RIBOSOMAL PROTEIN L23A



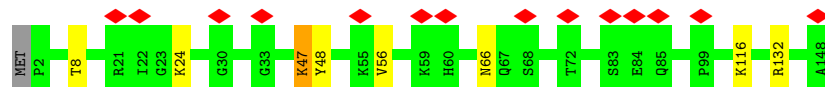
• Molecule 30: 60S RIBOSOMAL PROTEIN L26



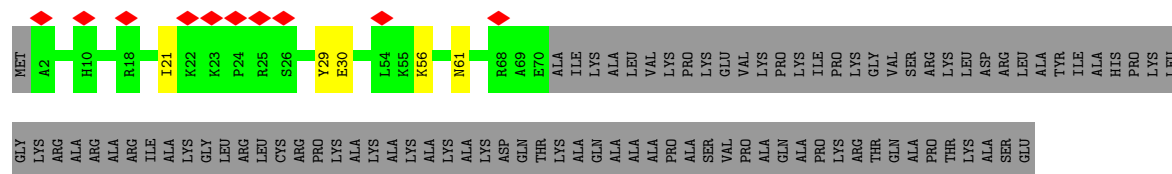
• Molecule 31: 60S RIBOSOMAL PROTEIN L27



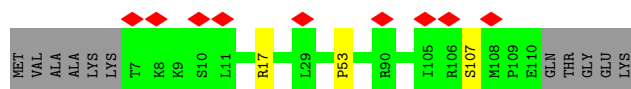
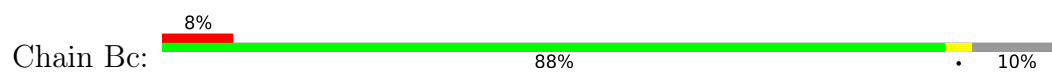
• Molecule 32: 60S RIBOSOMAL PROTEIN L27A



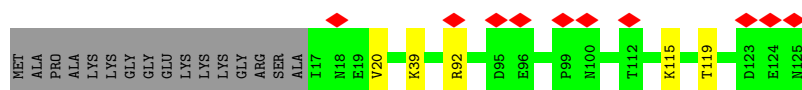
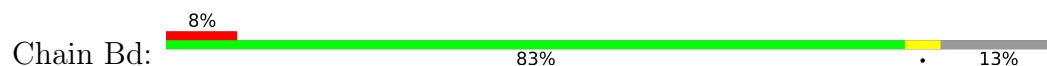
• Molecule 33: 60S RIBOSOMAL PROTEIN L29



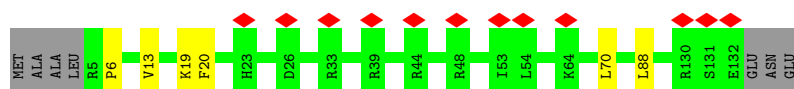
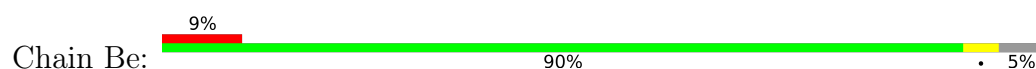
• Molecule 34: 60S RIBOSOMAL PROTEIN L30



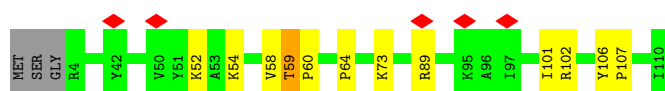
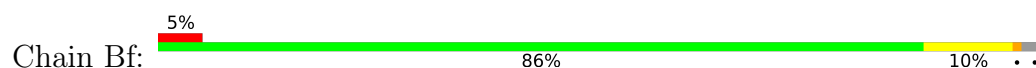
• Molecule 35: 60S RIBOSOMAL PROTEIN L31



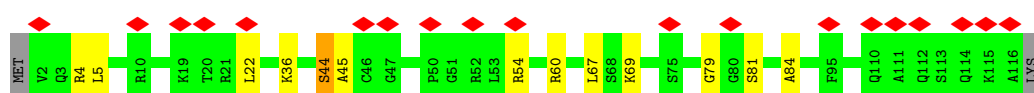
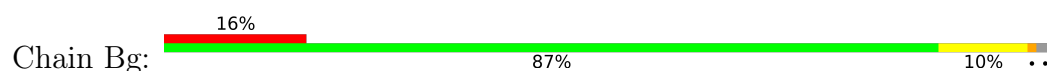
• Molecule 36: 60S RIBOSOMAL PROTEIN L32



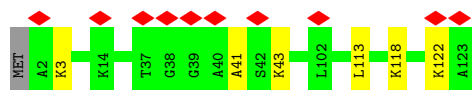
• Molecule 37: 60S RIBOSOMAL PROTEIN L35A



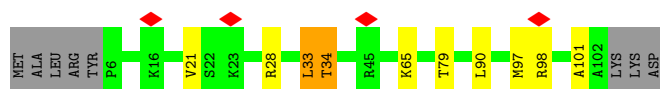
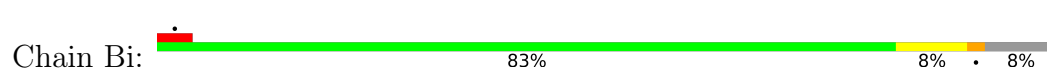
• Molecule 38: 60S RIBOSOMAL PROTEIN L34




• Molecule 39: 60S RIBOSOMAL PROTEIN UL29

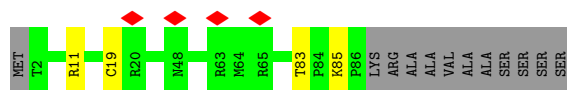


• Molecule 40: 60S RIBOSOMAL PROTEIN L36



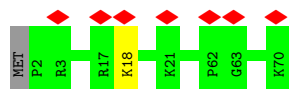
- Molecule 41: 60S RIBOSOMAL PROTEIN L37

Chain Bj:  84% 12%



- Molecule 42: 60S RIBOSOMAL PROTEIN L38

Chain Bk:  10% 97%



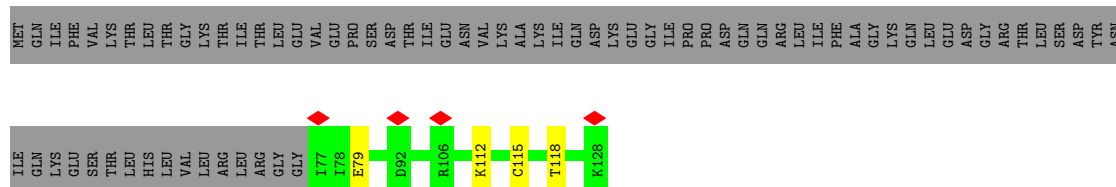
- Molecule 43: 60S RIBOSOMAL PROTEIN L39

Chain Bl:  8% 94%



- Molecule 44: UBIQUITIN-60S RIBOSOMAL PROTEIN L40

Chain Bm:  38% 59%



- Molecule 45: 60S RIBOSOMAL PROTEIN L41

Chain Bn:  100%

There are no outlier residues recorded for this chain.

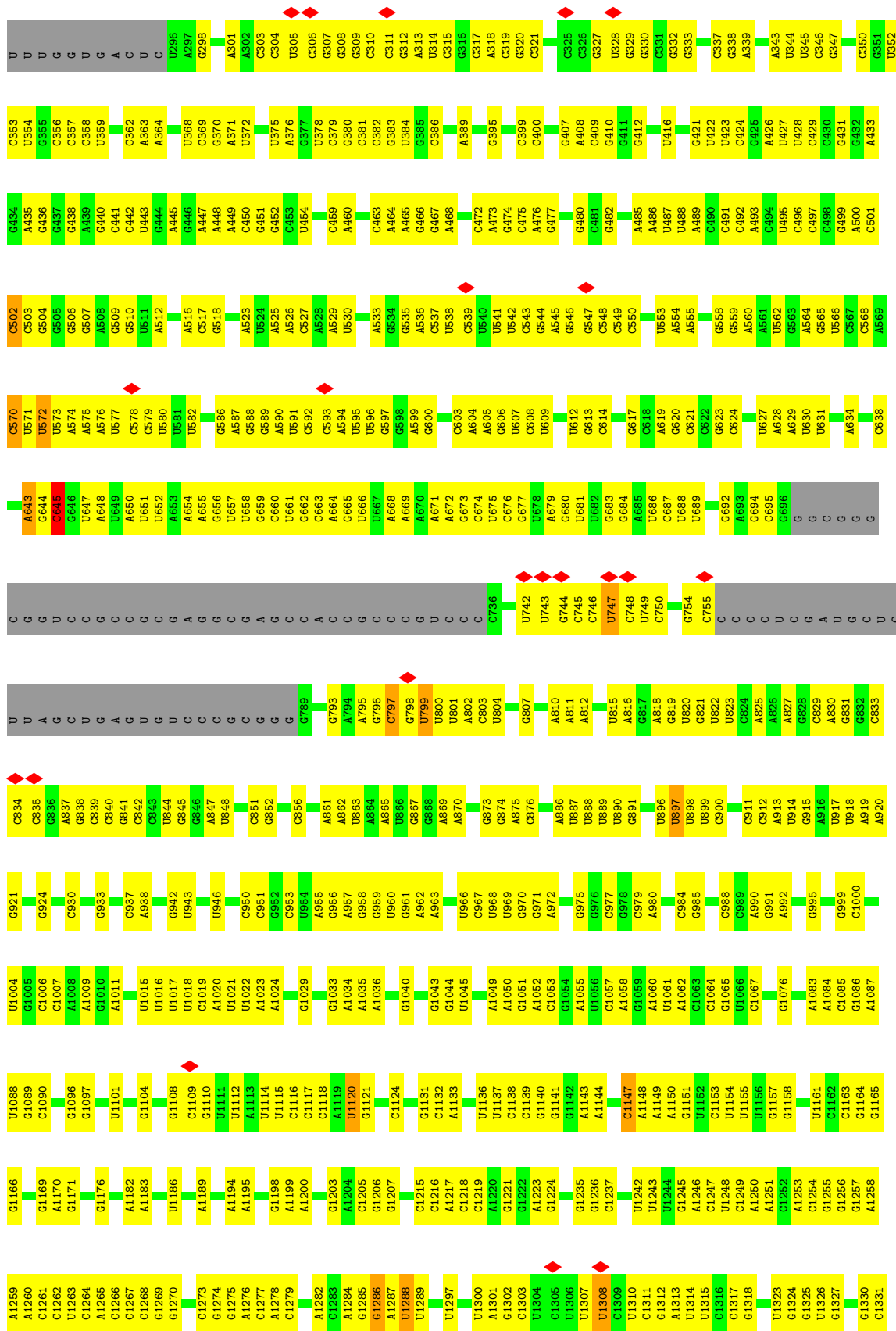
- Molecule 46: 60S RIBOSOMAL PROTEIN L36A

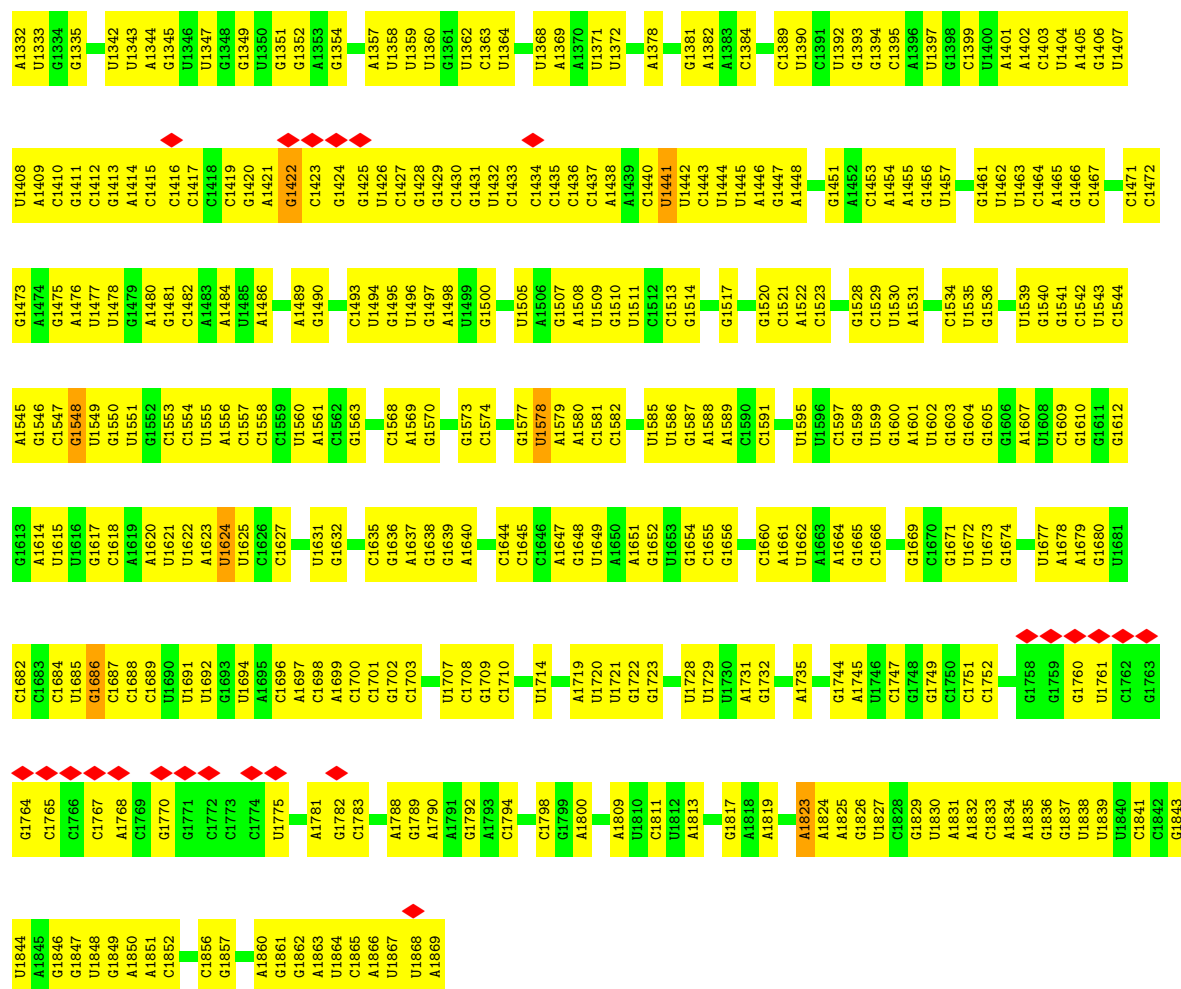
Chain Bo:  12% 93% 7%



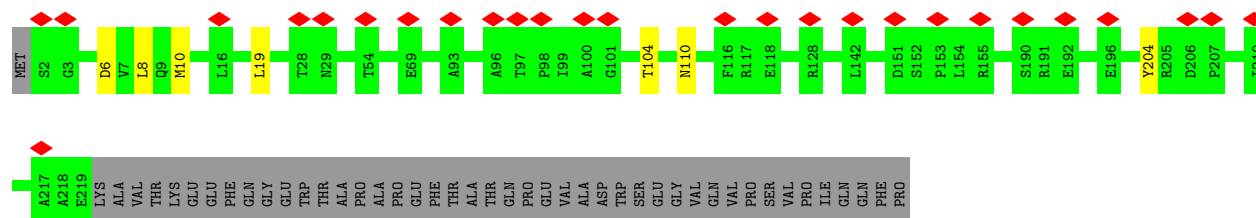
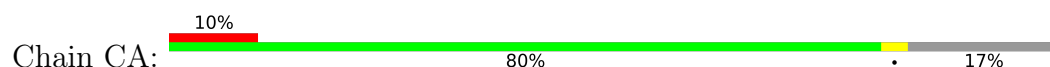
- Molecule 47: 60S RIBOSOMAL PROTEIN L37A

Chain Bp:  8% 93% 5%

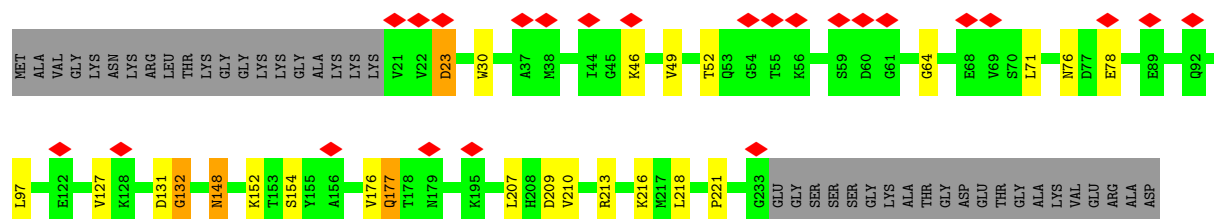
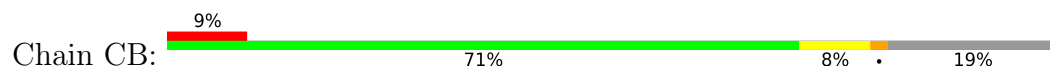


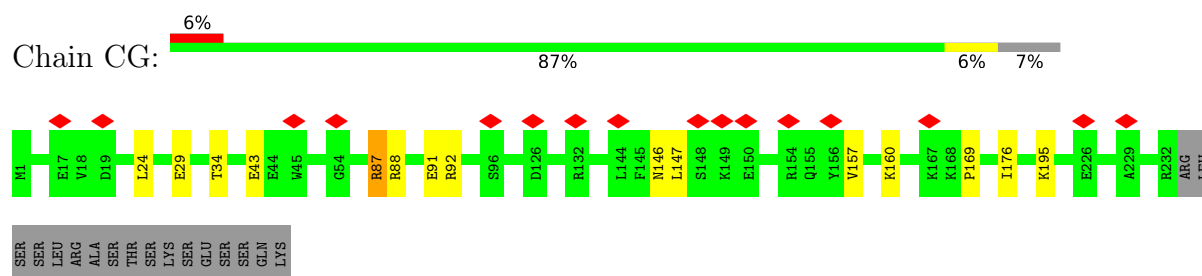


• Molecule 51: 40S RIBOSOMAL PROTEIN US2

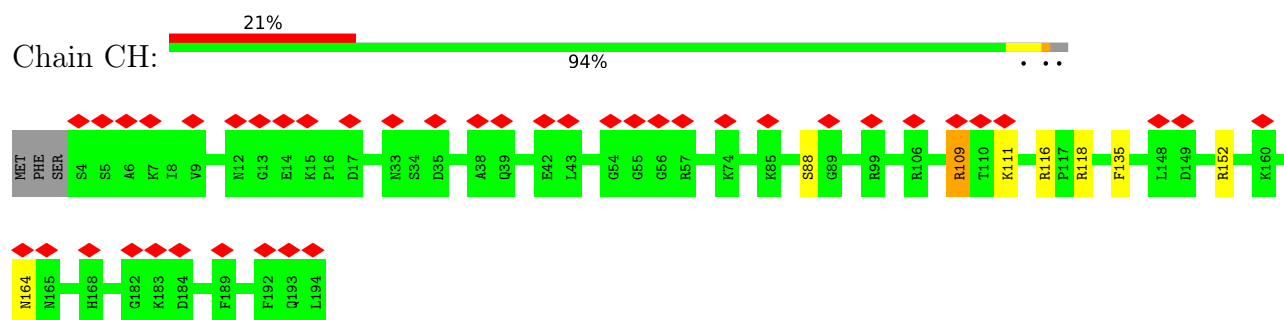


• Molecule 52: 40S RIBOSOMAL PROTEIN ES1

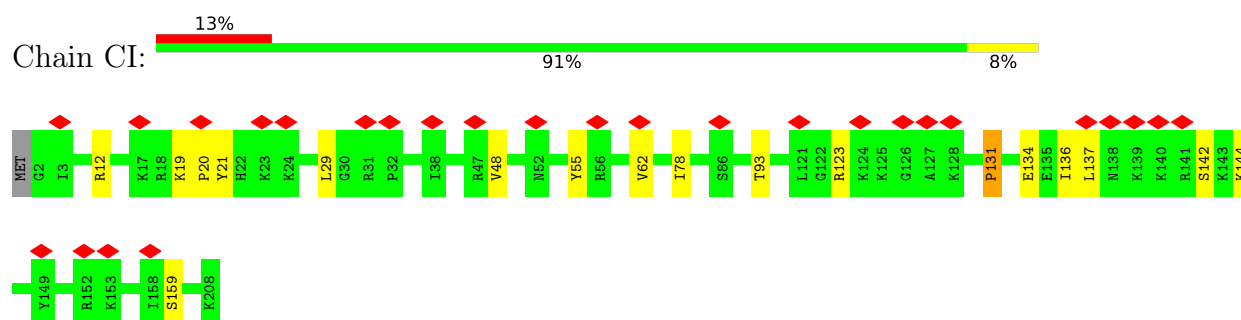




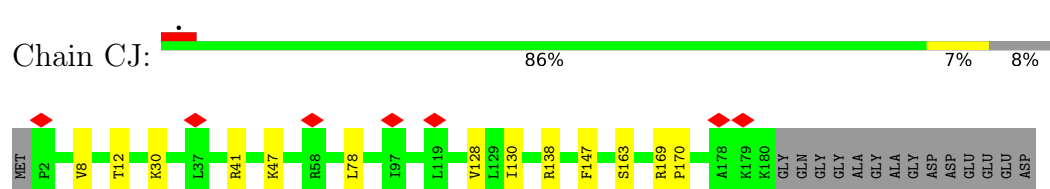
• Molecule 58: 40S RIBOSOMAL PROTEIN ES7



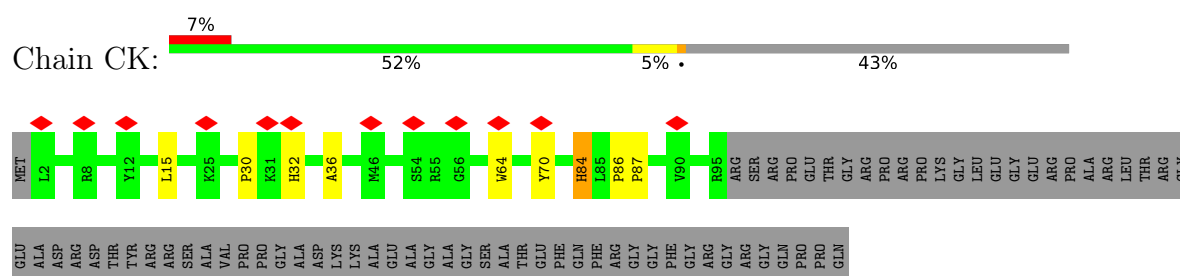
• Molecule 59: 40S RIBOSOMAL PROTEIN ES8



• Molecule 60: 40S RIBOSOMAL PROTEIN US4

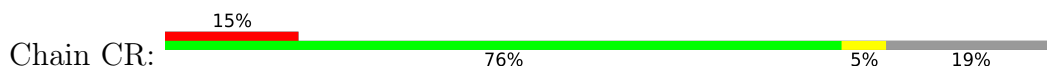


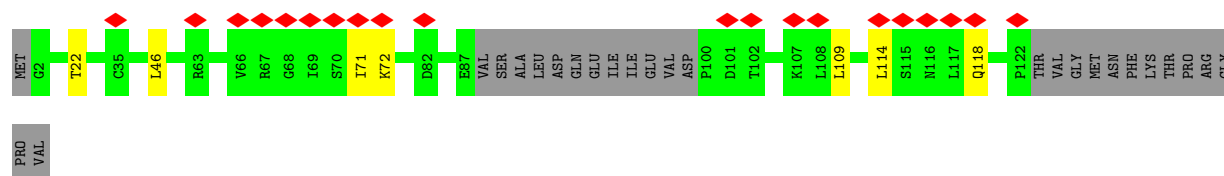
• Molecule 61: 40S RIBOSOMAL PROTEIN ES10



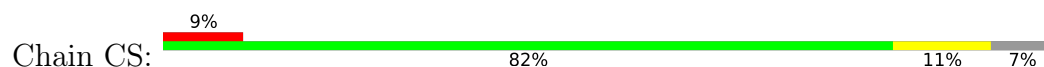
• Molecule 62: 40S RIBOSOMAL PROTEIN US17



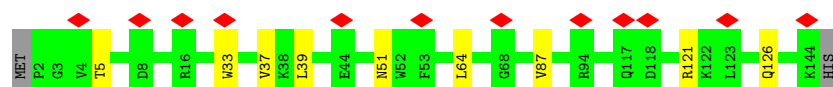




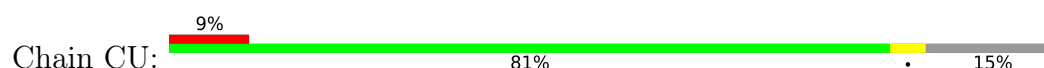
- Molecule 69: 40S RIBOSOMAL PROTEIN US13



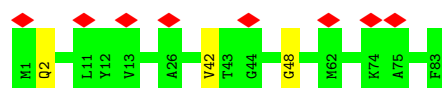
- Molecule 70: 40S RIBOSOMAL PROTEIN ES19



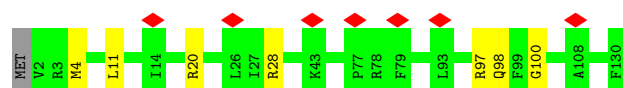
- Molecule 71: 40S RIBOSOMAL PROTEIN US10



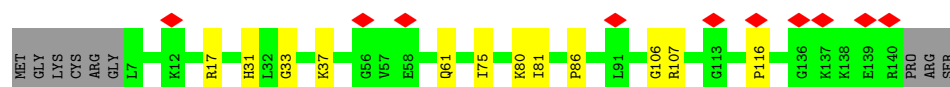
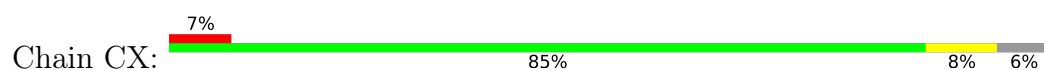
- Molecule 72: 40S RIBOSOMAL PROTEIN ES21




- Molecule 73: 40S RIBOSOMAL PROTEIN US8

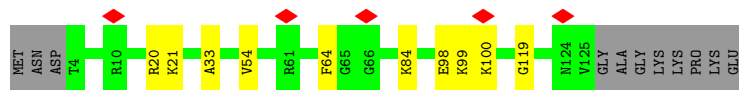


- Molecule 74: 40S RIBOSOMAL PROTEIN US12



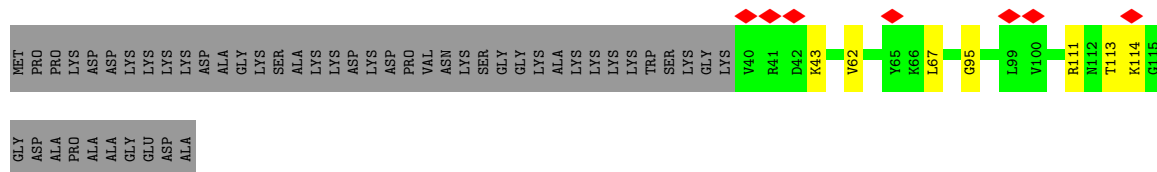
- Molecule 75: 40S RIBOSOMAL PROTEIN ES24

Chain CY: 




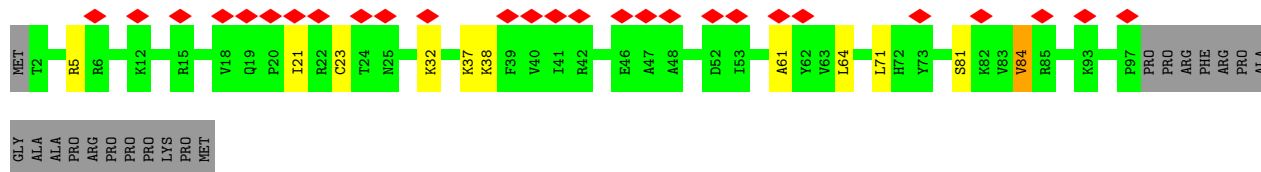
- Molecule 76: 40S RIBOSOMAL PROTEIN ES25

Chain CZ: 



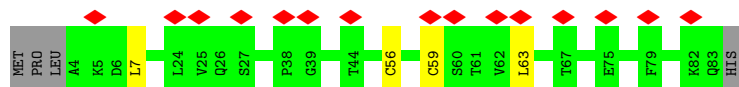
- Molecule 77: 40S RIBOSOMAL PROTEIN ES26

Chain Ca: 




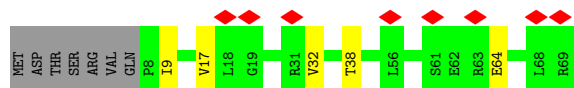
- Molecule 78: 40S RIBOSOMAL PROTEIN ES27

Chain Cb: 




- Molecule 79: 40S RIBOSOMAL PROTEIN ES28

Chain Cc: 

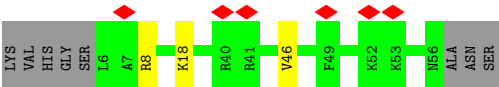
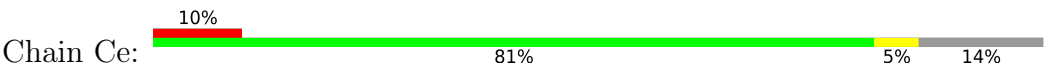


- Molecule 80: 40S RIBOSOMAL PROTEIN US14

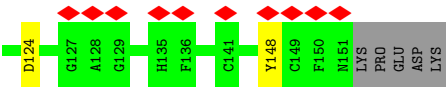
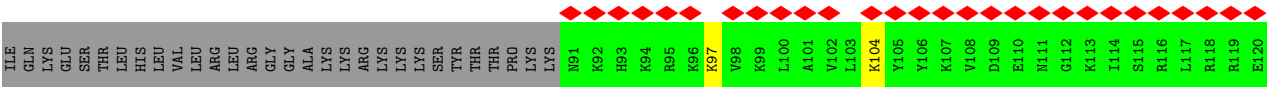
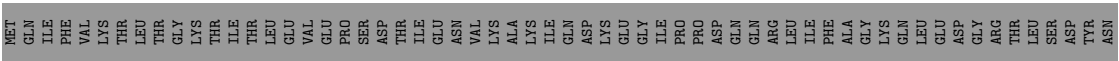
Chain Cd: 



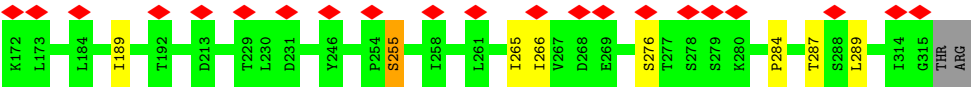
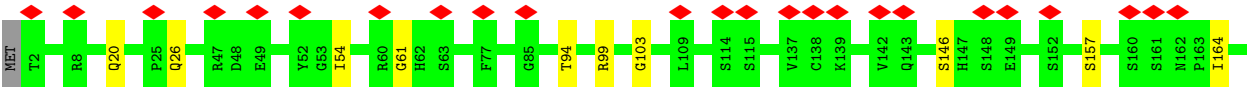
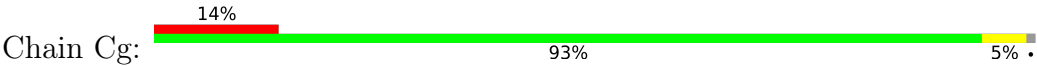
- Molecule 81: 40S RIBOSOMAL PROTEIN ES30



• Molecule 82: 40S RIBOSOMAL PROTEIN ES31



• Molecule 83: 40S RIBOSOMAL PROTEIN RACK1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	541570	Depositor
Resolution determination method	Not provided	
CTF correction method	CTFFIND3	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	194805	Depositor
Image detector	TVIPS TEMCAM-F416 (4k x 4k)	Depositor
Maximum map value	12450.331	Depositor
Minimum map value	-4370.861	Depositor
Average map value	-6.032	Depositor
Map value standard deviation	1022.400	Depositor
Recommended contour level	2700	Depositor
Map size (\AA)	453.6, 453.6, 453.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.26, 1.26, 1.26	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, GNP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.53	0/1809	1.02	17/2819 (0.6%)
2	AB	0.65	1/4926 (0.0%)	1.15	29/6641 (0.4%)
3	AC	1.52	10/6230 (0.2%)	2.37	535/9712 (5.5%)
4	A2	0.41	23/86672 (0.0%)	0.81	40/135198 (0.0%)
5	A3	0.36	0/3723	0.79	1/5800 (0.0%)
6	A4	0.38	0/2836	0.81	3/4421 (0.1%)
7	BA	0.44	0/1926	0.67	0/2583
8	BB	0.45	0/3258	0.73	2/4361 (0.0%)
9	BC	0.47	0/2943	0.73	0/3953
10	BD	0.49	2/2407 (0.1%)	0.70	1/3221 (0.0%)
11	BE	0.52	0/1312	0.73	0/1763
12	BF	0.45	0/1986	0.68	0/2644
13	BG	0.46	0/1914	0.72	0/2578
14	BH	0.43	0/1555	0.69	0/2089
15	BI	0.42	0/1643	0.67	0/2194
16	BJ	0.49	0/1386	0.71	0/1852
17	BL	0.53	2/1647 (0.1%)	0.73	3/2205 (0.1%)
18	BM	0.49	0/1162	0.70	0/1556
19	BN	0.43	0/1754	0.65	0/2348
20	BO	0.44	0/1639	0.69	0/2193
21	BP	0.44	0/1260	0.70	0/1691
22	BQ	0.45	0/1518	0.74	0/2026
23	BR	0.41	0/1542	0.64	0/2037
24	BS	0.44	0/1479	0.73	0/1985
25	BT	0.46	0/1326	0.71	0/1770
26	BU	0.47	0/841	0.71	0/1128
27	BV	0.43	0/978	0.63	0/1312
28	BW	0.43	0/542	0.59	0/722
29	BX	0.41	0/993	0.67	0/1334
30	BY	0.47	0/1082	0.72	1/1441 (0.1%)
31	BZ	0.47	0/1138	0.79	0/1517
32	Ba	0.45	0/1191	0.71	0/1591

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Bb	0.45	0/570	0.72	0/752
34	Bc	0.46	0/813	0.70	0/1091
35	Bd	0.45	0/920	0.67	0/1238
36	Be	0.45	0/1071	0.68	0/1428
37	Bf	0.50	0/885	0.81	0/1185
38	Bg	0.48	0/917	0.74	0/1222
39	Bh	0.38	0/1023	0.64	0/1351
40	Bi	0.43	0/793	0.75	0/1048
41	Bj	0.49	0/704	0.76	0/931
42	Bk	0.43	0/575	0.73	0/761
43	Bl	0.41	0/454	0.61	0/599
44	Bm	0.42	0/435	0.70	0/575
45	Bn	0.40	0/241	0.51	0/305
46	Bo	0.45	0/885	0.74	0/1166
47	Bp	0.40	0/718	0.61	0/953
48	Bt	0.48	0/1058	0.75	0/1416
49	Bu	0.45	0/1639	0.69	1/2222 (0.0%)
50	C1	0.37	2/41550 (0.0%)	0.80	6/64763 (0.0%)
51	CA	0.51	0/1756	0.68	0/2386
52	CB	0.51	0/1756	0.75	1/2350 (0.0%)
53	CC	0.42	0/1761	0.65	0/2379
54	CD	0.40	0/1672	0.66	0/2250
55	CE	0.47	0/2072	0.70	0/2793
56	CF	0.43	0/1507	0.74	0/2026
57	CG	0.48	0/1907	0.74	0/2538
58	CH	0.46	0/1558	0.74	1/2087 (0.0%)
59	CI	0.47	0/1724	0.72	0/2298
60	CJ	0.46	0/1520	0.77	0/2030
61	CK	0.48	0/815	0.68	0/1101
62	CL	0.45	0/1220	0.72	0/1633
63	CM	0.48	0/941	0.72	0/1264
64	CN	0.43	0/1231	0.73	1/1656 (0.1%)
65	CO	0.46	0/1036	0.71	0/1391
66	CP	0.43	0/1000	0.67	0/1335
67	CQ	0.43	0/1125	0.66	0/1506
68	CR	0.42	0/904	0.67	0/1208
69	CS	0.42	0/1190	0.68	0/1594
70	CT	0.44	0/1131	0.69	0/1515
71	CU	0.50	0/813	0.70	0/1092
72	CV	0.47	0/643	0.71	0/860
73	CW	0.44	0/1050	0.69	0/1406
74	CX	0.46	0/1063	0.70	0/1421
75	CY	0.45	0/1019	0.70	0/1354

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	CZ	0.46	0/611	0.71	0/820
77	Ca	0.48	0/778	0.75	1/1041 (0.1%)
78	Cb	0.48	0/637	0.68	0/854
79	Cc	0.46	0/492	0.74	0/657
80	Cd	0.51	0/454	0.76	0/603
81	Ce	0.45	0/417	0.69	0/548
82	Cf	0.53	0/507	0.84	1/673 (0.1%)
83	Cg	0.45	0/2497	0.67	0/3399
All	All	0.49	40/240676 (0.0%)	0.86	644/353759 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	14
3	AC	0	105
4	A2	0	35
5	A3	0	2
50	C1	0	24
All	All	0	180

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A2	1701	C	C5'-C4'	18.44	1.73	1.51
4	A2	1673	C	C3'-O3'	15.36	1.63	1.42
4	A2	1701	C	O5'-C5'	14.46	1.67	1.44
4	A2	1673	C	O3'-P	14.13	1.78	1.61
4	A2	1701	C	P-O5'	13.49	1.73	1.59
4	A2	1673	C	C5'-C4'	11.38	1.65	1.51
4	A2	1701	C	C4'-C3'	10.19	1.64	1.53
4	A2	1701	C	O3'-P	10.18	1.73	1.61
4	A2	1673	C	C4'-C3'	9.93	1.64	1.53
4	A2	1673	C	P-O5'	8.79	1.68	1.59
4	A2	1673	C	O5'-C5'	8.76	1.58	1.44
4	A2	943	G	C5-C6	-7.88	1.34	1.42
4	A2	1701	C	C3'-O3'	7.29	1.52	1.42
3	AC	338	C	N3-C4	-6.85	1.29	1.33
4	A2	2663	G	C6-O6	-6.75	1.18	1.24
3	AC	240	C	O3'-P	-6.63	1.53	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A2	1673	C	C2-N3	-6.51	1.30	1.35
50	C1	992	A	C6-N6	-6.23	1.28	1.33
4	A2	1481	G	C2-N2	-5.97	1.28	1.34
10	BD	264	LYS	N-CA	5.87	1.58	1.46
4	A2	1673	C	N3-C4	-5.73	1.29	1.33
4	A2	1701	C	C4'-O4'	5.50	1.52	1.45
3	AC	340	C	N3-C4	-5.50	1.30	1.33
17	BL	131	PRO	N-CD	5.45	1.55	1.47
3	AC	167	A	N3-C4	5.45	1.38	1.34
3	AC	83	C	N3-C4	-5.36	1.30	1.33
50	C1	1286	G	C2-N2	-5.35	1.29	1.34
17	BL	134	PRO	N-CD	5.31	1.55	1.47
4	A2	3924	G	C2-N2	-5.29	1.29	1.34
2	AB	846	PRO	N-CD	5.28	1.55	1.47
3	AC	288	A	P-O5'	5.25	1.65	1.59
3	AC	334	C	O5'-C5'	5.20	1.52	1.44
4	A2	1701	C	N1-C2	5.14	1.45	1.40
3	AC	237	C	C4-N4	-5.09	1.29	1.33
4	A2	1701	C	O4'-C1'	5.08	1.48	1.41
4	A2	456	G	C2-N2	-5.06	1.29	1.34
4	A2	4593	G	C2-N2	-5.04	1.29	1.34
3	AC	276	A	C4'-C3'	5.02	1.58	1.53
10	BD	265	ARG	N-CA	5.01	1.56	1.46
3	AC	85	A	N3-C4	5.00	1.37	1.34

All (644) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A2	1701	C	O4'-C4'-C3'	-15.17	88.83	104.00
2	AB	1133	TYR	CB-CG-CD2	-14.76	112.14	121.00
8	BB	258	HIS	C-N-CD	-13.97	89.87	120.60
1	AA	8	U	C5'-C4'-C3'	13.49	137.58	116.00
4	A2	1701	C	O4'-C1'-N1	12.28	118.02	108.20
3	AC	313	G	C5'-C4'-O4'	12.27	123.82	109.10
3	AC	276	A	C5-C6-N1	12.25	123.82	117.70
3	AC	276	A	O4'-C1'-N9	12.25	118.00	108.20
4	A2	1701	C	C4'-C3'-O3'	12.18	137.35	113.00
3	AC	259	U	O4'-C1'-N1	12.17	117.93	108.20
2	AB	1209	LEU	CB-CG-CD1	-11.98	90.64	111.00
3	AC	276	A	N1-C6-N6	-11.03	111.98	118.60
1	AA	6	G	C4'-C3'-O3'	10.84	134.69	113.00
3	AC	162	A	N1-C6-N6	-10.79	112.13	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A2	1701	C	C2'-C3'-O3'	-10.65	86.06	109.50
3	AC	255	C	O4'-C1'-N1	10.42	116.53	108.20
3	AC	298	A	N1-C6-N6	-10.41	112.35	118.60
3	AC	296	A	C5-C6-N1	10.37	122.88	117.70
3	AC	284	U	O4'-C1'-N1	10.35	116.48	108.20
3	AC	73	A	N1-C6-N6	-10.33	112.40	118.60
3	AC	57	A	N1-C6-N6	-10.19	112.49	118.60
3	AC	63	U	C4'-C3'-O3'	10.16	133.32	113.00
3	AC	271	G	O4'-C1'-N9	10.08	116.26	108.20
3	AC	330	A	P-O3'-C3'	9.96	131.66	119.70
3	AC	267	G	N1-C6-O6	-9.95	113.93	119.90
3	AC	312	U	C4'-C3'-C2'	-9.86	92.74	102.60
3	AC	50	A	N1-C6-N6	-9.68	112.79	118.60
3	AC	281	U	N3-C2-O2	-9.68	115.43	122.20
3	AC	93	A	N1-C6-N6	-9.60	112.84	118.60
3	AC	158	G	O4'-C1'-N9	9.57	115.85	108.20
3	AC	335	G	N1-C6-O6	-9.55	114.17	119.90
3	AC	287	U	O4'-C1'-N1	9.54	115.83	108.20
3	AC	232	C	O4'-C1'-N1	9.50	115.80	108.20
3	AC	275	A	N1-C6-N6	-9.47	112.92	118.60
3	AC	54	A	N1-C6-N6	-9.44	112.93	118.60
3	AC	116	A	N1-C6-N6	-9.40	112.96	118.60
3	AC	155	A	N1-C6-N6	-9.38	112.97	118.60
3	AC	266	G	N1-C6-O6	-9.37	114.28	119.90
3	AC	270	C	N3-C2-O2	-9.35	115.36	121.90
3	AC	337	G	N1-C6-O6	-9.30	114.32	119.90
3	AC	296	A	N1-C6-N6	-9.25	113.05	118.60
3	AC	282	U	O4'-C1'-N1	9.23	115.58	108.20
3	AC	231	G	O4'-C1'-N9	9.17	115.54	108.20
3	AC	276	A	C4'-C3'-C2'	-9.15	93.45	102.60
3	AC	72	A	N1-C6-N6	-9.03	113.19	118.60
3	AC	156	C	O4'-C1'-N1	8.97	115.38	108.20
3	AC	109	A	N1-C6-N6	-8.94	113.23	118.60
1	AA	8	U	P-O3'-C3'	8.87	130.34	119.70
3	AC	142	A	N1-C6-N6	-8.87	113.28	118.60
1	AA	74	C	C4'-C3'-O3'	8.84	130.68	113.00
3	AC	342	A	C5-C6-N1	8.84	122.12	117.70
3	AC	331	G	C5'-C4'-O4'	-8.82	98.52	109.10
3	AC	70	A	C5-C6-N1	8.76	122.08	117.70
3	AC	81	A	N1-C6-N6	-8.70	113.38	118.60
3	AC	119	A	C5-C6-N1	8.61	122.01	117.70
3	AC	51	G	N1-C6-O6	-8.61	114.73	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AC	345	A	C5-C6-N1	8.61	122.00	117.70
3	AC	85	A	N1-C6-N6	-8.59	113.45	118.60
3	AC	257	A	C5-C6-N1	8.58	121.99	117.70
3	AC	234	U	O4'-C1'-N1	8.57	115.06	108.20
3	AC	246	A	C5-C6-N1	8.56	121.98	117.70
3	AC	257	A	N1-C6-N6	-8.53	113.48	118.60
3	AC	161	G	O4'-C1'-N9	8.52	115.02	108.20
3	AC	82	G	N1-C6-O6	-8.47	114.81	119.90
3	AC	305	U	P-O3'-C3'	8.47	129.87	119.70
3	AC	344	G	N1-C6-O6	-8.46	114.82	119.90
3	AC	324	U	N3-C2-O2	-8.45	116.28	122.20
3	AC	299	G	N1-C6-O6	-8.40	114.86	119.90
3	AC	274	A	N1-C6-N6	-8.39	113.57	118.60
3	AC	256	G	N7-C8-N9	8.38	117.29	113.10
3	AC	340	C	N1-C2-O2	8.34	123.90	118.90
3	AC	145	G	N1-C6-O6	-8.32	114.91	119.90
3	AC	345	A	N1-C6-N6	-8.32	113.61	118.60
3	AC	298	A	C5-C6-N1	8.31	121.86	117.70
3	AC	96	A	N1-C6-N6	-8.31	113.61	118.60
3	AC	260	A	N1-C6-N6	-8.28	113.63	118.60
3	AC	126	C	N3-C2-O2	-8.27	116.11	121.90
3	AC	307	G	N1-C6-O6	-8.19	114.99	119.90
3	AC	155	A	O4'-C1'-N9	8.19	114.75	108.20
3	AC	235	G	N1-C6-O6	-8.15	115.01	119.90
1	AA	69	G	C4'-C3'-O3'	-8.11	92.37	109.40
3	AC	150	G	N1-C6-O6	-8.11	115.04	119.90
3	AC	256	G	C3'-C2'-C1'	8.10	107.98	101.50
3	AC	110	G	O4'-C1'-N9	8.07	114.66	108.20
3	AC	261	G	N1-C6-O6	-8.07	115.06	119.90
3	AC	119	A	N1-C6-N6	-8.06	113.76	118.60
3	AC	252	A	C5-C6-N1	8.04	121.72	117.70
3	AC	88	G	N1-C6-O6	-8.04	115.08	119.90
3	AC	340	C	N3-C2-O2	-8.03	116.28	121.90
4	A2	1673	C	C5'-C4'-O4'	-8.02	99.48	109.10
2	AB	1340	CYS	CA-CB-SG	-7.99	99.63	114.00
2	AB	1348	ASP	CB-CG-OD2	7.98	125.48	118.30
3	AC	239	C	N3-C2-O2	-7.97	116.32	121.90
3	AC	243	A	C5-C6-N1	7.96	121.68	117.70
3	AC	244	A	C5-C6-N1	7.96	121.68	117.70
3	AC	276	A	C2-N3-C4	7.94	114.57	110.60
3	AC	243	A	N1-C6-N6	-7.93	113.84	118.60
4	A2	1701	C	C5'-C4'-C3'	7.93	128.69	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AC	348	A	N1-C6-N6	-7.91	113.85	118.60
3	AC	140	A	O4'-C1'-N9	7.91	114.53	108.20
1	AA	72	C	C4'-C3'-O3'	7.91	128.81	113.00
3	AC	331	G	C2'-C3'-O3'	7.90	126.89	109.50
3	AC	75	G	N1-C6-O6	-7.88	115.17	119.90
3	AC	53	A	N1-C6-N6	-7.88	113.87	118.60
3	AC	74	A	N1-C6-N6	-7.87	113.88	118.60
3	AC	257	A	C4-C5-C6	-7.83	113.08	117.00
3	AC	348	A	C5-C6-N1	7.83	121.61	117.70
3	AC	81	A	C5-C6-N1	7.82	121.61	117.70
3	AC	272	C	O4'-C1'-N1	7.81	114.45	108.20
3	AC	106	U	N3-C2-O2	-7.80	116.74	122.20
3	AC	107	G	N1-C6-O6	-7.80	115.22	119.90
3	AC	240	C	N3-C2-O2	-7.76	116.47	121.90
3	AC	163	G	O4'-C1'-N9	7.75	114.40	108.20
3	AC	93	A	C5-C6-N1	7.74	121.57	117.70
3	AC	169	C	N3-C2-O2	-7.74	116.48	121.90
3	AC	271	G	C3'-C2'-C1'	7.70	107.66	101.50
3	AC	307	G	O4'-C1'-N9	7.67	114.33	108.20
3	AC	138	C	O4'-C1'-N1	7.64	114.32	108.20
3	AC	73	A	C4-C5-C6	-7.60	113.20	117.00
3	AC	120	C	N3-C2-O2	-7.57	116.60	121.90
3	AC	248	U	C5'-C4'-O4'	7.57	118.18	109.10
3	AC	83	C	O4'-C1'-N1	7.56	114.25	108.20
1	AA	69	G	C2'-C3'-O3'	7.55	126.11	109.50
3	AC	116	A	C5-C6-N1	7.54	121.47	117.70
2	AB	1348	ASP	CB-CG-OD1	-7.53	111.52	118.30
3	AC	310	A	N1-C6-N6	-7.53	114.08	118.60
3	AC	270	C	N1-C2-O2	7.53	123.42	118.90
3	AC	255	C	N3-C2-O2	-7.53	116.63	121.90
3	AC	54	A	C4-C5-C6	-7.52	113.24	117.00
3	AC	271	G	N1-C6-O6	-7.52	115.39	119.90
3	AC	73	A	C5-C6-N1	7.52	121.46	117.70
2	AB	1172	VAL	CG1-CB-CG2	-7.50	98.89	110.90
3	AC	258	G	N1-C6-O6	-7.50	115.40	119.90
3	AC	296	A	C4-C5-C6	-7.47	113.26	117.00
3	AC	300	G	N1-C6-O6	-7.47	115.42	119.90
3	AC	247	C	N3-C2-O2	-7.47	116.67	121.90
3	AC	110	G	N1-C6-O6	-7.45	115.43	119.90
3	AC	283	G	N1-C6-O6	-7.44	115.44	119.90
3	AC	346	G	N1-C6-O6	-7.42	115.45	119.90
3	AC	256	G	N1-C6-O6	-7.42	115.45	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AC	154	A	N1-C6-N6	-7.40	114.16	118.60
3	AC	146	G	N1-C6-O6	-7.39	115.46	119.90
3	AC	168	C	N3-C2-O2	-7.39	116.73	121.90
3	AC	334	C	P-O5'-C5'	7.39	132.72	120.90
3	AC	85	A	C5-C6-N1	7.38	121.39	117.70
3	AC	157	C	O4'-C1'-N1	7.36	114.09	108.20
3	AC	347	C	O4'-C1'-N1	7.34	114.07	108.20
3	AC	280	C	C6-N1-C2	-7.33	117.37	120.30
3	AC	315	C	N3-C2-O2	-7.32	116.77	121.90
3	AC	338	C	N3-C2-O2	-7.32	116.77	121.90
3	AC	299	G	O4'-C1'-N9	7.32	114.06	108.20
3	AC	338	C	N3-C4-C5	7.31	124.83	121.90
3	AC	70	A	N1-C6-N6	-7.31	114.22	118.60
3	AC	62	C	C4'-C3'-O3'	-7.26	94.16	109.40
3	AC	314	C	N3-C2-O2	-7.24	116.83	121.90
3	AC	57	A	C5-C6-N1	7.23	121.31	117.70
3	AC	266	G	P-O3'-C3'	7.21	128.35	119.70
3	AC	330	A	C4'-C3'-O3'	7.21	127.41	113.00
3	AC	238	C	N3-C2-O2	-7.20	116.86	121.90
3	AC	316	C	N3-C2-O2	-7.19	116.87	121.90
3	AC	154	A	C5-C6-N1	7.18	121.29	117.70
3	AC	324	U	O4'-C1'-N1	7.18	113.95	108.20
3	AC	317	C	N3-C2-O2	-7.18	116.87	121.90
3	AC	272	C	N3-C2-O2	-7.18	116.88	121.90
3	AC	142	A	C5-C6-N1	7.17	121.29	117.70
3	AC	133	G	O4'-C1'-N9	7.17	113.94	108.20
3	AC	256	G	C8-N9-C4	-7.16	103.53	106.40
3	AC	165	A	C5-C6-N1	7.16	121.28	117.70
4	A2	1673	C	O3'-P-O5'	7.16	117.60	104.00
3	AC	274	A	C5-C6-N1	7.15	121.27	117.70
3	AC	160	U	P-O3'-C3'	7.14	128.28	119.70
3	AC	163	G	N1-C6-O6	-7.14	115.62	119.90
3	AC	77	G	N1-C6-O6	-7.12	115.63	119.90
3	AC	243	A	C4-C5-C6	-7.11	113.44	117.00
3	AC	90	G	N1-C6-O6	-7.08	115.65	119.90
3	AC	250	C	N3-C2-O2	-7.08	116.94	121.90
4	A2	1673	C	C2-N1-C1'	-7.08	111.02	118.80
3	AC	275	A	C4-C5-C6	-7.04	113.48	117.00
3	AC	233	G	N1-C6-O6	-7.03	115.68	119.90
3	AC	338	C	N1-C2-O2	7.03	123.12	118.90
3	AC	313	G	O4'-C1'-N9	-6.99	102.61	108.20
5	A3	34	U	C3'-C2'-C1'	-6.99	95.91	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AC	252	A	N1-C6-N6	-6.98	114.41	118.60
3	AC	138	C	N3-C2-O2	-6.97	117.02	121.90
3	AC	147	U	O4'-C1'-N1	6.96	113.77	108.20
3	AC	321	A	C5-C6-N1	6.96	121.18	117.70
3	AC	309	G	O4'-C1'-N9	6.96	113.77	108.20
3	AC	126	C	C4'-C3'-C2'	-6.95	95.65	102.60
3	AC	231	G	N1-C6-O6	-6.94	115.74	119.90
3	AC	160	U	O4'-C1'-N1	6.88	113.70	108.20
3	AC	292	C	N3-C2-O2	-6.88	117.09	121.90
3	AC	171	G	N1-C6-O6	-6.87	115.78	119.90
3	AC	167	A	O4'-C1'-N9	6.86	113.69	108.20
3	AC	116	A	C4-C5-C6	-6.86	113.57	117.00
3	AC	332	A	C2'-C3'-O3'	6.86	124.68	113.70
3	AC	285	G	O4'-C1'-N9	6.85	113.68	108.20
3	AC	257	A	P-O3'-C3'	6.84	127.91	119.70
3	AC	289	C	N3-C2-O2	-6.84	117.11	121.90
3	AC	132	G	N1-C6-O6	-6.83	115.80	119.90
3	AC	275	A	C6-C5-N7	6.83	137.08	132.30
3	AC	166	C	N3-C2-O2	-6.82	117.13	121.90
3	AC	283	G	N3-C4-C5	-6.81	125.20	128.60
3	AC	342	A	N1-C6-N6	-6.80	114.52	118.60
3	AC	45	C	N3-C2-O2	-6.79	117.15	121.90
3	AC	249	G	N1-C6-O6	-6.76	115.84	119.90
3	AC	294	U	O4'-C1'-N1	6.76	113.61	108.20
3	AC	119	A	O4'-C1'-N9	6.75	113.60	108.20
3	AC	109	A	C5-C6-N1	6.75	121.07	117.70
3	AC	140	A	C4-C5-C6	-6.74	113.63	117.00
3	AC	339	A	C5-C6-N1	6.74	121.07	117.70
3	AC	117	G	N1-C6-O6	-6.73	115.86	119.90
3	AC	242	C	N3-C2-O2	-6.73	117.19	121.90
3	AC	233	G	O4'-C1'-N9	6.69	113.55	108.20
3	AC	255	C	N1-C2-O2	6.69	122.91	118.90
3	AC	81	A	C4-C5-C6	-6.68	113.66	117.00
3	AC	258	G	C3'-C2'-C1'	-6.67	96.16	101.50
2	AB	1152	LEU	CB-CG-CD1	-6.67	99.67	111.00
3	AC	97	U	O4'-C1'-N1	6.66	113.52	108.20
3	AC	228	U	O4'-C1'-N1	6.65	113.52	108.20
3	AC	259	U	C6-N1-C2	-6.65	117.01	121.00
3	AC	109	A	O4'-C1'-N9	6.64	113.51	108.20
3	AC	308	C	N3-C2-O2	-6.64	117.25	121.90
3	AC	76	C	O4'-C1'-N1	6.63	113.50	108.20
3	AC	49	G	N1-C6-O6	-6.62	115.93	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AC	306	U	O4'-C1'-N1	6.62	113.49	108.20
3	AC	131	G	N1-C6-O6	-6.61	115.93	119.90
3	AC	165	A	N1-C6-N6	-6.61	114.64	118.60
3	AC	82	G	O4'-C1'-N9	6.60	113.48	108.20
3	AC	327	C	N3-C2-O2	-6.59	117.29	121.90
3	AC	301	G	N1-C6-O6	-6.59	115.95	119.90
3	AC	108	C	N3-C2-O2	-6.58	117.29	121.90
3	AC	115	C	N3-C2-O2	-6.58	117.29	121.90
3	AC	164	U	N3-C2-O2	-6.58	117.59	122.20
3	AC	333	C	P-O3'-C3'	6.58	127.59	119.70
1	AA	9	A	P-O5'-C5'	6.55	131.39	120.90
3	AC	151	C	N3-C2-O2	-6.55	117.31	121.90
3	AC	139	C	N3-C2-O2	-6.55	117.32	121.90
3	AC	136	A	P-O3'-C3'	6.54	127.55	119.70
3	AC	74	A	C5-C6-N1	6.54	120.97	117.70
3	AC	56	U	N3-C2-O2	-6.53	117.63	122.20
2	AB	1323	VAL	CG1-CB-CG2	-6.53	100.46	110.90
3	AC	84	C	N3-C2-O2	-6.52	117.33	121.90
3	AC	133	G	N1-C6-O6	-6.51	116.00	119.90
3	AC	318	G	N1-C6-O6	-6.51	116.00	119.90
3	AC	333	C	C2'-C3'-O3'	-6.50	95.19	109.50
3	AC	271	G	C8-N9-C4	-6.50	103.80	106.40
3	AC	260	A	C5-C6-N1	6.49	120.94	117.70
3	AC	277	G	N1-C6-O6	-6.49	116.00	119.90
3	AC	252	A	P-O3'-C3'	6.49	127.48	119.70
3	AC	244	A	N1-C6-N6	-6.48	114.71	118.60
3	AC	170	G	N1-C6-O6	-6.48	116.01	119.90
3	AC	58	C	N3-C2-O2	-6.48	117.36	121.90
4	A2	1673	C	C5-C4-N4	6.48	124.73	120.20
3	AC	235	G	O4'-C1'-N9	6.47	113.38	108.20
3	AC	254	C	C3'-C2'-C1'	6.47	106.68	101.50
3	AC	234	U	C3'-C2'-C1'	6.47	106.68	101.50
3	AC	238	C	N1-C2-O2	6.47	122.78	118.90
3	AC	230	G	N1-C6-O6	-6.46	116.03	119.90
3	AC	127	U	N3-C2-O2	-6.46	117.68	122.20
3	AC	282	U	N3-C2-O2	-6.46	117.68	122.20
3	AC	254	C	N3-C2-O2	-6.46	117.38	121.90
3	AC	276	A	C4-C5-C6	-6.45	113.78	117.00
3	AC	140	A	C5-C6-N1	6.45	120.92	117.70
2	AB	1008	ILE	CG1-CB-CG2	-6.44	97.23	111.40
3	AC	162	A	C5-C6-N1	6.43	120.92	117.70
4	A2	139	G	C3'-C2'-C1'	-6.43	96.35	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AC	153	G	C5'-C4'-O4'	6.43	116.81	109.10
3	AC	298	A	C4-C5-C6	-6.42	113.79	117.00
4	A2	103	G	C3'-C2'-C1'	-6.42	96.37	101.50
3	AC	258	G	N9-C1'-C2'	6.42	122.34	114.00
3	AC	267	G	C5-C6-O6	6.41	132.45	128.60
3	AC	118	G	N1-C6-O6	-6.41	116.06	119.90
3	AC	275	A	O4'-C1'-N9	6.40	113.32	108.20
3	AC	107	G	N3-C4-C5	-6.40	125.40	128.60
3	AC	328	G	N1-C6-O6	-6.39	116.06	119.90
2	AB	1341	VAL	CG1-CB-CG2	-6.39	100.68	110.90
3	AC	109	A	C4-C5-C6	-6.39	113.81	117.00
3	AC	48	U	N3-C2-O2	-6.38	117.73	122.20
3	AC	130	C	N3-C2-O2	-6.38	117.43	121.90
3	AC	58	C	O4'-C1'-N1	6.37	113.30	108.20
2	AB	1211	PHE	CB-CG-CD1	-6.37	116.34	120.80
3	AC	69	C	N3-C2-O2	-6.37	117.44	121.90
3	AC	54	A	C5-C6-N1	6.34	120.87	117.70
3	AC	332	A	P-O3'-C3'	6.34	127.31	119.70
3	AC	237	C	N3-C2-O2	-6.33	117.47	121.90
3	AC	246	A	C4-C5-C6	-6.32	113.84	117.00
3	AC	330	A	O3'-P-O5'	-6.32	91.99	104.00
3	AC	86	U	C3'-C2'-C1'	-6.32	96.44	101.50
3	AC	126	C	C5'-C4'-O4'	6.32	116.68	109.10
3	AC	169	C	N1-C2-O2	6.32	122.69	118.90
3	AC	53	A	C5-C6-N1	6.32	120.86	117.70
3	AC	57	A	O4'-C1'-N9	6.31	113.25	108.20
3	AC	286	G	N1-C6-O6	-6.31	116.11	119.90
3	AC	258	G	C5-C6-N1	6.31	114.65	111.50
3	AC	319	G	N1-C6-O6	-6.30	116.12	119.90
3	AC	167	A	C5-C6-N1	6.30	120.85	117.70
3	AC	120	C	N1-C2-O2	6.29	122.68	118.90
3	AC	279	C	N3-C2-O2	-6.29	117.49	121.90
3	AC	290	U	P-O3'-C3'	6.29	127.25	119.70
4	A2	1673	C	N3-C4-N4	-6.29	113.60	118.00
3	AC	76	C	N3-C2-O2	-6.28	117.50	121.90
3	AC	153	G	N1-C6-O6	-6.27	116.14	119.90
3	AC	252	A	C4-C5-C6	-6.27	113.86	117.00
3	AC	341	C	N3-C4-C5	6.27	124.41	121.90
3	AC	315	C	C5'-C4'-O4'	6.27	116.62	109.10
3	AC	244	A	C4-C5-C6	-6.26	113.87	117.00
3	AC	258	G	C4'-C3'-C2'	-6.25	96.34	102.60
3	AC	155	A	C5-C6-N1	6.25	120.83	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AC	275	A	C5-C6-N1	6.25	120.83	117.70
4	A2	4688	A	C3'-C2'-C1'	-6.24	96.51	101.50
3	AC	111	C	O4'-C1'-N1	6.24	113.19	108.20
3	AC	239	C	N1-C2-O2	6.23	122.64	118.90
3	AC	98	G	O4'-C1'-N9	6.22	113.18	108.20
3	AC	278	G	O4'-C1'-N9	6.22	113.18	108.20
3	AC	285	G	N1-C6-O6	-6.22	116.17	119.90
3	AC	291	G	C5'-C4'-C3'	-6.22	106.04	116.00
3	AC	52	G	N1-C6-O6	-6.22	116.17	119.90
3	AC	86	U	O4'-C1'-N1	6.22	113.17	108.20
3	AC	228	U	C1'-O4'-C4'	-6.22	104.93	109.90
3	AC	89	C	N3-C2-O2	-6.21	117.55	121.90
3	AC	55	C	C6-N1-C2	-6.21	117.81	120.30
3	AC	152	G	N1-C6-O6	-6.20	116.18	119.90
3	AC	259	U	N3-C2-O2	-6.20	117.86	122.20
3	AC	292	C	O4'-C1'-N1	6.20	113.16	108.20
3	AC	320	G	N1-C6-O6	-6.19	116.19	119.90
3	AC	156	C	N3-C2-O2	-6.18	117.57	121.90
3	AC	50	A	C5-C6-N1	6.18	120.79	117.70
3	AC	234	U	N3-C2-O2	-6.18	117.88	122.20
3	AC	282	U	O5'-C5'-C4'	6.17	123.42	111.70
3	AC	95	U	O4'-C1'-N1	6.17	113.13	108.20
3	AC	70	A	C4-C5-C6	-6.16	113.92	117.00
3	AC	96	A	C5-C6-N1	6.14	120.77	117.70
3	AC	79	C	N3-C2-O2	-6.14	117.60	121.90
4	A2	1673	C	C4'-C3'-C2'	-6.13	96.47	102.60
3	AC	73	A	C6-C5-N7	6.13	136.59	132.30
3	AC	111	C	N3-C2-O2	-6.13	117.61	121.90
3	AC	276	A	C5'-C4'-O4'	-6.13	101.75	109.10
3	AC	276	A	P-O3'-C3'	6.12	127.05	119.70
3	AC	155	A	C4-C5-C6	-6.12	113.94	117.00
1	AA	7	A	P-O5'-C5'	6.11	130.68	120.90
4	A2	4560	G	C3'-C2'-C1'	-6.11	96.61	101.50
3	AC	114	C	N3-C2-O2	-6.11	117.62	121.90
3	AC	251	U	N3-C2-O2	-6.11	117.92	122.20
3	AC	314	C	O4'-C1'-N1	6.11	113.08	108.20
4	A2	1673	C	C4'-C3'-O3'	6.10	125.20	113.00
3	AC	142	A	C4-C5-C6	-6.10	113.95	117.00
4	A2	1673	C	C6-N1-C1'	6.10	128.12	120.80
3	AC	94	G	N1-C6-O6	-6.09	116.25	119.90
3	AC	94	G	O4'-C1'-C2'	-6.08	99.72	105.80
50	C1	502	C	C3'-C2'-C1'	-6.08	96.64	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AC	112	C	O4'-C1'-N1	6.07	113.06	108.20
2	AB	1275	ILE	CG1-CB-CG2	6.07	124.76	111.40
3	AC	305	U	N3-C2-O2	-6.07	117.95	122.20
3	AC	348	A	C4-C5-C6	-6.07	113.97	117.00
3	AC	281	U	O5'-C5'-C4'	6.07	123.22	111.70
3	AC	291	G	N1-C6-O6	-6.06	116.26	119.90
3	AC	74	A	O4'-C1'-N9	6.06	113.05	108.20
3	AC	129	C	N3-C2-O2	-6.06	117.66	121.90
3	AC	60	G	N1-C6-O6	-6.05	116.27	119.90
4	A2	1673	C	C5'-C4'-C3'	6.04	125.67	116.00
3	AC	150	G	C5'-C4'-O4'	6.04	116.35	109.10
3	AC	321	A	N1-C6-N6	-6.04	114.97	118.60
3	AC	340	C	N3-C4-C5	6.03	124.31	121.90
3	AC	86	U	N3-C2-O2	-6.02	117.98	122.20
3	AC	322	G	N1-C6-O6	-6.01	116.29	119.90
2	AB	1278	HIS	CG-CD2-NE2	6.01	120.61	109.20
3	AC	168	C	N1-C2-O2	5.99	122.50	118.90
3	AC	253	G	N1-C6-O6	-5.99	116.31	119.90
3	AC	333	C	N1-C1'-C2'	-5.98	105.42	112.00
3	AC	324	U	P-O3'-C3'	5.98	126.88	119.70
3	AC	84	C	N3-C4-C5	5.98	124.29	121.90
3	AC	171	G	O4'-C1'-N9	5.98	112.98	108.20
4	A2	683	C	C3'-C2'-C1'	-5.96	96.73	101.50
3	AC	112	C	N3-C2-O2	-5.96	117.73	121.90
3	AC	148	C	O4'-C1'-N1	5.96	112.96	108.20
3	AC	93	A	C4-C5-C6	-5.95	114.03	117.00
3	AC	343	U	N3-C2-O2	-5.94	118.04	122.20
3	AC	263	G	N1-C6-O6	-5.93	116.34	119.90
3	AC	314	C	C6-N1-C2	-5.90	117.94	120.30
3	AC	288	A	N1-C6-N6	-5.90	115.06	118.60
3	AC	98	G	N1-C6-O6	-5.89	116.36	119.90
3	AC	148	C	N1-C2-O2	5.89	122.44	118.90
3	AC	59	U	O4'-C1'-N1	5.88	112.90	108.20
3	AC	229	G	N1-C6-O6	-5.87	116.38	119.90
3	AC	119	A	C3'-C2'-C1'	-5.87	96.81	101.50
3	AC	256	G	N3-C4-C5	-5.86	125.67	128.60
3	AC	46	U	O4'-C1'-N1	5.86	112.89	108.20
3	AC	263	G	C5'-C4'-O4'	5.85	116.12	109.10
3	AC	254	C	O4'-C1'-N1	5.83	112.87	108.20
4	A2	1673	C	N1-C1'-C2'	5.83	121.58	114.00
3	AC	136	A	O4'-C1'-N9	5.83	112.86	108.20
3	AC	247	C	N1-C2-O2	5.83	122.40	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AC	72	A	C5-C6-N1	5.83	120.61	117.70
3	AC	304	C	N3-C2-O2	-5.82	117.83	121.90
1	AA	8	U	C4'-C3'-O3'	5.81	124.62	113.00
4	A2	3742	U	C3'-C2'-C1'	-5.81	96.86	101.50
3	AC	289	C	N1-C2-O2	5.80	122.38	118.90
3	AC	242	C	N1-C2-O2	5.79	122.37	118.90
4	A2	1942	A	N9-C1'-C2'	-5.79	105.63	112.00
3	AC	309	G	N1-C6-O6	-5.78	116.43	119.90
3	AC	347	C	N3-C2-O2	-5.78	117.86	121.90
3	AC	290	U	N3-C2-O2	-5.78	118.16	122.20
3	AC	260	A	C4-C5-C6	-5.77	114.11	117.00
3	AC	53	A	O4'-C1'-N9	5.77	112.81	108.20
3	AC	116	A	O4'-C1'-N9	5.76	112.81	108.20
3	AC	325	C	O4'-C1'-N1	5.75	112.80	108.20
3	AC	310	A	C5-C6-N1	5.74	120.57	117.70
3	AC	111	C	C3'-C2'-C1'	5.74	106.09	101.50
3	AC	148	C	N3-C2-O2	-5.74	117.88	121.90
3	AC	341	C	C3'-C2'-C1'	-5.74	96.91	101.50
2	AB	1320	ASP	CB-CA-C	5.73	121.87	110.40
10	BD	265	ARG	N-CA-C	5.73	126.47	111.00
4	A2	3677	C	C3'-C2'-C1'	-5.73	96.92	101.50
2	AB	975	LEU	CB-CG-CD1	-5.72	101.27	111.00
3	AC	115	C	O4'-C1'-N1	5.72	112.78	108.20
3	AC	168	C	O4'-C1'-N1	5.72	112.78	108.20
3	AC	55	C	N3-C2-O2	-5.72	117.89	121.90
3	AC	138	C	N1-C2-O2	5.71	122.33	118.90
3	AC	125	C	N3-C2-O2	-5.70	117.91	121.90
3	AC	119	A	C2-N3-C4	5.69	113.45	110.60
3	AC	113	U	C5-C6-N1	-5.69	119.85	122.70
3	AC	150	G	N3-C4-C5	-5.69	125.76	128.60
3	AC	322	G	C5-C6-N1	5.68	114.34	111.50
3	AC	53	A	C4-C5-C6	-5.68	114.16	117.00
2	AB	896	THR	OG1-CB-CG2	-5.66	96.97	110.00
1	AA	6	G	C2'-C3'-O3'	-5.66	97.05	109.50
3	AC	57	A	C4-C5-C6	-5.66	114.17	117.00
3	AC	240	C	O4'-C1'-N1	5.66	112.72	108.20
3	AC	249	G	C5'-C4'-O4'	5.66	115.89	109.10
3	AC	265	U	C5-C6-N1	-5.66	119.87	122.70
3	AC	293	C	N3-C2-O2	-5.66	117.94	121.90
3	AC	139	C	O4'-C1'-N1	5.65	112.72	108.20
3	AC	324	U	C3'-C2'-C1'	-5.65	96.98	101.50
3	AC	313	G	O3'-P-O5'	-5.64	93.28	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AC	245	G	C5'-C4'-O4'	5.64	115.87	109.10
4	A2	943	G	C5-C6-O6	-5.64	125.22	128.60
3	AC	255	C	C6-N1-C2	-5.64	118.05	120.30
50	C1	645	C	C3'-C2'-C1'	-5.64	96.99	101.50
3	AC	323	G	N1-C6-O6	-5.63	116.52	119.90
3	AC	299	G	C3'-C2'-C1'	5.63	106.00	101.50
3	AC	150	G	O4'-C1'-N9	5.63	112.70	108.20
3	AC	49	G	N3-C4-C5	-5.62	125.79	128.60
3	AC	324	U	C4'-C3'-C2'	-5.61	96.99	102.60
1	AA	73	A	P-O5'-C5'	-5.61	111.92	120.90
3	AC	281	U	N1-C1'-C2'	5.60	121.28	114.00
2	AB	1133	TYR	CD1-CG-CD2	5.59	124.05	117.90
2	AB	845	ALA	C-N-CD	5.59	140.14	128.40
3	AC	240	C	P-O3'-C3'	5.58	126.40	119.70
3	AC	145	G	C5-C6-N1	5.58	114.29	111.50
3	AC	120	C	C6-N1-C2	-5.58	118.07	120.30
3	AC	265	U	P-O3'-C3'	5.57	126.39	119.70
3	AC	344	G	C5-C6-N1	5.57	114.28	111.50
2	AB	1159	LEU	CB-CG-CD1	-5.57	101.54	111.00
3	AC	336	U	O4'-C1'-N1	5.56	112.65	108.20
3	AC	281	U	C5'-C4'-C3'	5.56	124.90	116.00
3	AC	143	G	N1-C6-O6	-5.56	116.56	119.90
3	AC	164	U	C4'-C3'-C2'	-5.55	97.05	102.60
3	AC	291	G	N3-C4-C5	-5.54	125.83	128.60
3	AC	265	U	N3-C2-O2	-5.54	118.32	122.20
50	C1	1441	U	C3'-C2'-C1'	-5.54	97.07	101.50
3	AC	250	C	N1-C2-O2	5.53	122.22	118.90
2	AB	1308	MET	CG-SD-CE	5.52	109.04	100.20
3	AC	87	G	N1-C6-O6	-5.52	116.59	119.90
3	AC	129	C	N1-C2-O2	5.52	122.21	118.90
3	AC	310	A	C4-C5-C6	-5.52	114.24	117.00
3	AC	303	G	C8-N9-C4	-5.51	104.19	106.40
4	A2	3868	G	C3'-C2'-C1'	-5.50	97.10	101.50
3	AC	340	C	N3-C4-N4	-5.50	114.15	118.00
3	AC	108	C	O4'-C1'-N1	5.50	112.60	108.20
3	AC	165	A	O4'-C1'-N9	5.50	112.60	108.20
3	AC	262	U	O4'-C1'-N1	5.50	112.60	108.20
3	AC	345	A	C4-C5-C6	-5.50	114.25	117.00
3	AC	134	A	C5-C6-N1	5.48	120.44	117.70
4	A2	1548	U	C3'-C2'-C1'	-5.48	97.12	101.50
4	A2	1703	G	O4'-C1'-C2'	-5.47	100.33	105.80
4	A2	2837	C	C3'-C2'-C1'	-5.47	97.12	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1133	TYR	CG-CD1-CE1	-5.46	116.93	121.30
17	BL	133	ALA	C-N-CD	5.46	139.88	128.40
3	AC	152	G	C5'-C4'-O4'	5.46	115.65	109.10
3	AC	315	C	C6-N1-C2	-5.45	118.12	120.30
3	AC	54	A	C6-C5-N7	5.45	136.11	132.30
3	AC	89	C	C3'-C2'-C1'	5.44	105.86	101.50
3	AC	284	U	N3-C2-O2	-5.44	118.39	122.20
3	AC	126	C	N3-C4-C5	5.44	124.08	121.90
1	AA	68	C	O3'-P-O5'	-5.43	93.67	104.00
3	AC	171	G	N9-C4-C5	5.43	107.57	105.40
3	AC	51	G	C6-C5-N7	5.43	133.66	130.40
1	AA	8	U	O5'-C5'-C4'	5.42	122.01	111.70
3	AC	241	G	C5'-C4'-O4'	5.41	115.59	109.10
3	AC	141	U	C5'-C4'-O4'	5.41	115.59	109.10
3	AC	171	G	C6-C5-N7	5.40	133.64	130.40
3	AC	116	A	C2-N3-C4	5.40	113.30	110.60
17	BL	130	LYS	C-N-CD	5.39	139.72	128.40
3	AC	53	A	C6-C5-N7	5.39	136.07	132.30
3	AC	254	C	N1-C2-O2	5.39	122.13	118.90
3	AC	233	G	C5-C6-N1	5.38	114.19	111.50
3	AC	281	U	C6-N1-C2	-5.37	117.78	121.00
3	AC	334	C	P-O3'-C3'	5.37	126.15	119.70
3	AC	167	A	N1-C6-N6	-5.37	115.38	118.60
64	CN	6	ALA	N-CA-C	-5.36	96.52	111.00
3	AC	281	U	N1-C2-N3	5.36	118.11	114.90
4	A2	4475	G	C3'-C2'-C1'	-5.36	97.22	101.50
3	AC	126	C	O4'-C1'-N1	5.36	112.48	108.20
6	A4	108	G	O4'-C4'-C3'	-5.35	98.65	104.00
3	AC	262	U	C5-C6-N1	-5.33	120.03	122.70
3	AC	244	A	C5'-C4'-O4'	5.33	115.49	109.10
3	AC	228	U	C5-C6-N1	-5.33	120.04	122.70
3	AC	109	A	C6-C5-N7	5.33	136.03	132.30
3	AC	74	A	C4-C5-C6	-5.32	114.34	117.00
3	AC	276	A	C6-N1-C2	-5.31	115.41	118.60
3	AC	267	G	O4'-C1'-N9	5.31	112.45	108.20
4	A2	4987	C	C3'-C2'-C1'	-5.30	97.26	101.50
3	AC	289	C	O4'-C1'-N1	5.30	112.44	108.20
3	AC	256	G	O4'-C1'-N9	5.30	112.44	108.20
58	CH	109	ARG	N-CA-CB	5.30	120.14	110.60
3	AC	126	C	N1-C2-O2	5.29	122.08	118.90
3	AC	279	C	O4'-C1'-N1	5.29	112.44	108.20
3	AC	158	G	N1-C6-O6	-5.29	116.72	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1133	TYR	CA-CB-CG	5.29	123.45	113.40
3	AC	337	G	C5-C6-O6	5.29	131.77	128.60
3	AC	240	C	N1-C2-O2	5.29	122.07	118.90
3	AC	268	G	N3-C2-N2	-5.28	116.20	119.90
4	A2	28	C	C3'-C2'-C1'	-5.27	97.28	101.50
52	CB	132	GLY	N-CA-C	5.27	126.27	113.10
4	A2	1672	U	C3'-C2'-C1'	-5.27	97.29	101.50
3	AC	84	C	C3'-C2'-C1'	5.26	105.71	101.50
3	AC	296	A	C3'-C2'-C1'	-5.26	97.29	101.50
3	AC	324	U	O4'-C1'-C2'	-5.26	100.54	105.80
3	AC	335	G	O4'-C1'-N9	5.26	112.41	108.20
3	AC	261	G	C5-C6-O6	5.26	131.75	128.60
3	AC	335	G	C5-C6-O6	5.26	131.75	128.60
6	A4	108	G	C5'-C4'-O4'	5.26	115.41	109.10
2	AB	961	LYS	CD-CE-NZ	5.25	123.78	111.70
4	A2	1432	A	C3'-C2'-C1'	-5.25	97.30	101.50
3	AC	314	C	N1-C2-O2	5.25	122.05	118.90
3	AC	122	C	N3-C2-O2	-5.25	118.23	121.90
50	C1	797	C	N1-C1'-C2'	-5.24	106.23	112.00
3	AC	317	C	O4'-C1'-N1	5.24	112.39	108.20
3	AC	268	G	C5'-C4'-C3'	-5.23	107.63	116.00
4	A2	355	G	C3'-C2'-C1'	-5.23	97.32	101.50
3	AC	50	A	C4-C5-C6	-5.23	114.39	117.00
3	AC	59	U	C5-C6-N1	-5.23	120.09	122.70
3	AC	278	G	N1-C6-O6	-5.22	116.77	119.90
50	C1	1422	G	C3'-C2'-C1'	-5.22	97.32	101.50
3	AC	315	C	N1-C2-O2	5.22	122.03	118.90
3	AC	114	C	N1-C2-O2	5.22	122.03	118.90
3	AC	92	U	C5-C6-N1	-5.21	120.09	122.70
3	AC	166	C	O4'-C1'-N1	5.21	112.37	108.20
3	AC	125	C	O3'-P-O5'	-5.21	94.11	104.00
3	AC	270	C	N3-C4-C5	5.21	123.98	121.90
3	AC	299	G	C5-C6-N1	5.20	114.10	111.50
3	AC	94	G	C3'-C2'-C1'	-5.20	97.34	101.50
3	AC	119	A	C4-C5-C6	-5.20	114.40	117.00
3	AC	228	U	N3-C2-O2	-5.20	118.56	122.20
3	AC	252	A	C2-N3-C4	5.19	113.20	110.60
3	AC	321	A	C4-C5-C6	-5.19	114.40	117.00
3	AC	337	G	N3-C4-C5	-5.19	126.00	128.60
3	AC	165	A	C4-C5-C6	-5.19	114.41	117.00
3	AC	120	C	O4'-C1'-C2'	-5.19	100.61	105.80
3	AC	327	C	O4'-C1'-N1	5.18	112.34	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	73	A	O3'-P-O5'	-5.18	94.16	104.00
3	AC	127	U	C1'-O4'-C4'	5.18	114.04	109.90
3	AC	309	G	N3-C2-N2	-5.17	116.28	119.90
3	AC	79	C	O4'-C1'-N1	5.17	112.33	108.20
3	AC	150	G	C5-C6-N1	5.17	114.08	111.50
3	AC	157	C	N3-C4-C5	5.16	123.96	121.90
3	AC	311	G	O4'-C1'-N9	5.16	112.33	108.20
3	AC	324	U	N1-C2-O2	5.16	126.41	122.80
2	AB	1152	LEU	CA-CB-CG	-5.15	103.45	115.30
3	AC	157	C	C3'-C2'-C1'	5.15	105.62	101.50
3	AC	141	U	N1-C2-N3	5.15	117.99	114.90
2	AB	1320	ASP	CB-CG-OD1	-5.15	113.67	118.30
3	AC	73	A	C3'-C2'-C1'	5.15	105.62	101.50
49	Bu	157	ARG	N-CA-CB	-5.14	101.34	110.60
3	AC	126	C	C6-N1-C2	-5.14	118.24	120.30
3	AC	69	C	N1-C2-O2	5.14	121.98	118.90
1	AA	70	G	O5'-C5'-C4'	-5.13	101.94	111.70
3	AC	323	G	P-O3'-C3'	5.13	125.86	119.70
3	AC	133	G	C3'-C2'-C1'	5.13	105.60	101.50
3	AC	70	A	C3'-C2'-C1'	5.12	105.60	101.50
3	AC	97	U	N3-C2-O2	-5.12	118.61	122.20
3	AC	283	G	C5-C6-N1	5.12	114.06	111.50
82	Cf	124	ASP	N-CA-C	-5.12	97.18	111.00
3	AC	79	C	N1-C2-O2	5.11	121.97	118.90
3	AC	116	A	C6-C5-N7	5.11	135.88	132.30
2	AB	1219	TYR	CB-CG-CD1	-5.11	117.93	121.00
3	AC	157	C	N3-C2-O2	-5.11	118.32	121.90
3	AC	83	C	N3-C4-C5	5.11	123.94	121.90
3	AC	346	G	C4'-C3'-C2'	-5.10	97.50	102.60
77	Ca	5	ARG	N-CA-CB	-5.10	101.42	110.60
4	A2	4467	A	C3'-C2'-C1'	-5.10	97.42	101.50
4	A2	1595	U	C3'-C2'-C1'	-5.10	97.42	101.50
3	AC	51	G	N3-C2-N2	-5.09	116.33	119.90
4	A2	303	G	C3'-C2'-C1'	-5.09	97.43	101.50
3	AC	49	G	C3'-C2'-C1'	5.09	105.57	101.50
3	AC	169	C	C3'-C2'-C1'	5.09	105.57	101.50
3	AC	171	G	C4-C5-N7	-5.09	108.76	110.80
3	AC	235	G	C5-C6-O6	5.09	131.65	128.60
3	AC	57	A	C3'-C2'-C1'	5.08	105.57	101.50
3	AC	298	A	O4'-C1'-N9	5.08	112.27	108.20
3	AC	45	C	O4'-C1'-N1	5.08	112.27	108.20
1	AA	75	C	O4'-C1'-N1	5.08	112.26	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AC	232	C	N3-C2-O2	-5.08	118.34	121.90
3	AC	233	G	N3-C2-N2	-5.08	116.34	119.90
3	AC	253	G	C8-N9-C4	-5.08	104.37	106.40
3	AC	257	A	C5'-C4'-O4'	-5.08	103.01	109.10
3	AC	335	G	C5-C6-N1	5.08	114.04	111.50
4	A2	14	C	OP2-P-O3'	5.08	116.37	105.20
3	AC	255	C	P-O3'-C3'	5.07	125.79	119.70
3	AC	294	U	C3'-C2'-C1'	5.07	105.56	101.50
3	AC	96	A	C3'-C2'-C1'	5.07	105.56	101.50
3	AC	49	G	C5-C6-N1	5.07	114.03	111.50
3	AC	331	G	O3'-P-O5'	-5.06	94.38	104.00
3	AC	277	G	C3'-C2'-C1'	5.06	105.55	101.50
3	AC	289	C	C6-N1-C2	-5.06	118.28	120.30
4	A2	4547	G	C3'-C2'-C1'	-5.06	97.45	101.50
6	A4	55	A	C3'-C2'-C1'	-5.06	97.45	101.50
17	BL	55	ILE	N-CA-C	-5.06	97.35	111.00
3	AC	85	A	C4-C5-C6	-5.05	114.47	117.00
8	BB	325	GLU	N-CA-C	5.05	124.65	111.00
30	BY	126	ARG	CB-CA-C	-5.05	100.29	110.40
3	AC	247	C	C5'-C4'-O4'	5.05	115.16	109.10
3	AC	317	C	N1-C2-O2	5.05	121.93	118.90
3	AC	264	U	C5-C6-N1	-5.04	120.18	122.70
3	AC	163	G	N3-C4-C5	-5.04	126.08	128.60
3	AC	249	G	C5-C6-N1	5.04	114.02	111.50
3	AC	51	G	C5-C6-O6	5.04	131.62	128.60
3	AC	266	G	C5-C6-N1	5.04	114.02	111.50
3	AC	88	G	C5-C6-N1	5.04	114.02	111.50
3	AC	318	G	C5'-C4'-O4'	5.03	115.14	109.10
50	C1	1147	C	C3'-C2'-C1'	-5.03	97.47	101.50
2	AB	1036	PRO	N-CA-CB	-5.03	97.07	102.60
2	AB	1275	ILE	CA-CB-CG1	-5.03	101.45	111.00
3	AC	237	C	N1-C2-O2	5.02	121.91	118.90
3	AC	69	C	C3'-C2'-C1'	5.02	105.52	101.50
3	AC	266	G	C5-C6-O6	5.02	131.61	128.60
3	AC	291	G	C3'-C2'-C1'	5.02	105.51	101.50
3	AC	310	A	C5'-C4'-O4'	5.02	115.12	109.10
3	AC	316	C	C5'-C4'-O4'	5.01	115.12	109.10
2	AB	1395	ILE	CA-CB-CG2	-5.01	100.88	110.90
3	AC	288	A	C5-C6-N1	5.01	120.20	117.70
4	A2	1217	C	OP1-P-O3'	5.01	116.22	105.20
3	AC	110	G	C5-C6-O6	5.00	131.60	128.60
3	AC	113	U	O4'-C1'-N1	5.00	112.20	108.20

There are no chirality outliers.

All (180) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A2	1	C	Sidechain
4	A2	115	C	Sidechain
4	A2	121	A	Sidechain
4	A2	1218	A	Sidechain
4	A2	1248	G	Sidechain
4	A2	1349	C	Sidechain
4	A2	140	C	Sidechain
4	A2	1481	G	Sidechain
4	A2	149	U	Sidechain
4	A2	1618	U	Sidechain
4	A2	1673	C	Sidechain
4	A2	2	G	Sidechain
4	A2	2064	G	Sidechain
4	A2	2246	G	Sidechain
4	A2	2274	U	Sidechain
4	A2	2294	G	Sidechain
4	A2	2338	G	Sidechain
4	A2	2354	C	Sidechain
4	A2	2570	C	Sidechain
4	A2	2581	C	Sidechain
4	A2	2624	A	Sidechain
4	A2	2795	C	Sidechain
4	A2	426	A	Sidechain
4	A2	4533	G	Sidechain
4	A2	4637	U	Sidechain
4	A2	4655	C	Sidechain
4	A2	4681	G	Sidechain
4	A2	4710	G	Sidechain
4	A2	4712	U	Sidechain
4	A2	4740	U	Sidechain
4	A2	510	C	Sidechain
4	A2	721	A	Sidechain
4	A2	902	G	Sidechain
4	A2	965	C	Sidechain
4	A2	966	U	Sidechain
5	A3	130	C	Sidechain
5	A3	156	U	Sidechain
2	AB	1105	PRO	Mainchain
2	AB	1133	TYR	Sidechain,Peptide
2	AB	1196	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	AB	1219	TYR	Sidechain
2	AB	1277	TYR	Sidechain
2	AB	1290	TYR	Sidechain
2	AB	1348	ASP	Mainchain,Peptide
2	AB	1385	MET	Peptide
2	AB	834	HIS	Peptide
2	AB	836	LYS	Peptide
2	AB	880	GLN	Mainchain
2	AB	899	ILE	Mainchain
3	AC	108	C	Sidechain
3	AC	109	A	Sidechain
3	AC	110	G	Sidechain
3	AC	111	C	Sidechain
3	AC	112	C	Sidechain
3	AC	113	U	Sidechain
3	AC	114	C	Sidechain
3	AC	115	C	Sidechain
3	AC	116	A	Sidechain
3	AC	117	G	Sidechain
3	AC	121	C	Sidechain
3	AC	122	C	Sidechain
3	AC	127	U	Sidechain
3	AC	128	C	Sidechain
3	AC	132	G	Sidechain
3	AC	134	A	Sidechain
3	AC	139	C	Sidechain
3	AC	143	G	Sidechain
3	AC	144	U	Sidechain
3	AC	148	C	Sidechain
3	AC	153	G	Sidechain
3	AC	156	C	Sidechain
3	AC	159	G	Sidechain
3	AC	160	U	Sidechain
3	AC	161	G	Sidechain
3	AC	162	A	Sidechain
3	AC	163	G	Sidechain
3	AC	232	C	Sidechain
3	AC	234	U	Sidechain
3	AC	236	C	Sidechain
3	AC	237	C	Sidechain
3	AC	240	C	Sidechain
3	AC	245	G	Sidechain

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Mol	Chain	Res	Type	Group
3	AC	246	A	Sidechain
3	AC	247	C	Sidechain
3	AC	248	U	Sidechain
3	AC	249	G	Sidechain
3	AC	252	A	Sidechain
3	AC	253	G	Sidechain
3	AC	254	C	Sidechain
3	AC	255	C	Sidechain
3	AC	256	G	Sidechain
3	AC	257	A	Sidechain
3	AC	258	G	Sidechain
3	AC	259	U	Sidechain
3	AC	260	A	Sidechain
3	AC	264	U	Sidechain
3	AC	265	U	Sidechain
3	AC	266	G	Sidechain
3	AC	269	U	Sidechain
3	AC	272	C	Sidechain
3	AC	274	A	Sidechain
3	AC	276	A	Sidechain
3	AC	279	C	Sidechain
3	AC	280	C	Sidechain
3	AC	281	U	Sidechain
3	AC	282	U	Sidechain
3	AC	283	G	Sidechain
3	AC	285	G	Sidechain
3	AC	286	G	Sidechain
3	AC	288	A	Sidechain
3	AC	292	C	Sidechain
3	AC	293	C	Sidechain
3	AC	303	G	Sidechain
3	AC	305	U	Sidechain
3	AC	307	G	Sidechain
3	AC	310	A	Sidechain
3	AC	313	G	Sidechain
3	AC	315	C	Sidechain
3	AC	323	G	Sidechain
3	AC	325	C	Sidechain
3	AC	335	G	Sidechain
3	AC	341	C	Sidechain
3	AC	46	U	Sidechain
3	AC	47	G	Sidechain

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Mol	Chain	Res	Type	Group
3	AC	48	U	Sidechain
3	AC	49	G	Sidechain
3	AC	50	A	Sidechain
3	AC	51	G	Sidechain
3	AC	52	G	Sidechain
3	AC	54	A	Sidechain
3	AC	55	C	Sidechain
3	AC	57	A	Sidechain
3	AC	58	C	Sidechain
3	AC	60	G	Sidechain
3	AC	69	C	Sidechain
3	AC	70	A	Sidechain
3	AC	71	G	Sidechain
3	AC	72	A	Sidechain
3	AC	73	A	Sidechain
3	AC	74	A	Sidechain
3	AC	78	U	Sidechain
3	AC	79	C	Sidechain
3	AC	82	G	Sidechain
3	AC	83	C	Sidechain
3	AC	84	C	Sidechain
3	AC	86	U	Sidechain
3	AC	87	G	Sidechain
3	AC	88	G	Sidechain
3	AC	89	C	Sidechain
3	AC	90	G	Sidechain
3	AC	91	U	Sidechain
3	AC	96	A	Sidechain
3	AC	97	U	Sidechain
3	AC	98	G	Sidechain
50	C1	111	A	Sidechain
50	C1	1120	U	Sidechain
50	C1	1288	U	Sidechain
50	C1	1308	U	Sidechain
50	C1	1414	A	Sidechain
50	C1	1548	G	Sidechain
50	C1	1578	U	Sidechain
50	C1	1624	U	Sidechain
50	C1	1686	G	Sidechain
50	C1	1823	A	Sidechain
50	C1	216	C	Sidechain
50	C1	235	A	Sidechain

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Mol	Chain	Res	Type	Group
50	C1	44	U	Sidechain
50	C1	570	C	Sidechain
50	C1	572	U	Sidechain
50	C1	643	A	Sidechain
50	C1	645	C	Sidechain
50	C1	747	U	Sidechain
50	C1	77	A	Sidechain
50	C1	799	U	Sidechain
50	C1	84	A	Sidechain
50	C1	867	G	Sidechain
50	C1	88	G	Sidechain
50	C1	897	U	Sidechain

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	
2	AB	605/627 (96%)	523 (86%)	50 (8%)	32 (5%)	1	15
7	BA	245/257 (95%)	236 (96%)	6 (2%)	3 (1%)	11	44
8	BB	394/403 (98%)	369 (94%)	11 (3%)	14 (4%)	3	20
9	BC	362/427 (85%)	338 (93%)	9 (2%)	15 (4%)	2	18
10	BD	288/297 (97%)	279 (97%)	4 (1%)	5 (2%)	7	37
11	BE	156/158 (99%)	141 (90%)	8 (5%)	7 (4%)	2	17
12	BF	232/248 (94%)	225 (97%)	3 (1%)	4 (2%)	7	37
13	BG	233/266 (88%)	217 (93%)	7 (3%)	9 (4%)	2	19
14	BH	190/192 (99%)	184 (97%)	3 (2%)	3 (2%)	8	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	BI	192/214 (90%)	187 (97%)	2 (1%)	3 (2%)	8	38
16	BJ	168/178 (94%)	153 (91%)	3 (2%)	12 (7%)	1	11
17	BL	198/211 (94%)	178 (90%)	9 (4%)	11 (6%)	1	14
18	BM	138/215 (64%)	132 (96%)	4 (3%)	2 (1%)	9	41
19	BN	202/204 (99%)	193 (96%)	6 (3%)	3 (2%)	8	40
20	BO	194/203 (96%)	187 (96%)	4 (2%)	3 (2%)	8	40
21	BP	151/184 (82%)	141 (93%)	7 (5%)	3 (2%)	6	32
22	BQ	182/188 (97%)	169 (93%)	7 (4%)	6 (3%)	3	21
23	BR	181/196 (92%)	175 (97%)	3 (2%)	3 (2%)	7	37
24	BS	171/176 (97%)	158 (92%)	7 (4%)	6 (4%)	3	20
25	BT	157/160 (98%)	150 (96%)	4 (2%)	3 (2%)	6	32
26	BU	100/128 (78%)	97 (97%)	3 (3%)	0	100	100
27	BV	126/140 (90%)	119 (94%)	5 (4%)	2 (2%)	8	38
28	BW	62/157 (40%)	61 (98%)	1 (2%)	0	100	100
29	BX	117/156 (75%)	113 (97%)	4 (3%)	0	100	100
30	BY	126/145 (87%)	119 (94%)	4 (3%)	3 (2%)	5	27
31	BZ	134/136 (98%)	125 (93%)	5 (4%)	4 (3%)	3	23
32	Ba	145/148 (98%)	134 (92%)	6 (4%)	5 (3%)	3	21
33	Bb	67/159 (42%)	60 (90%)	3 (4%)	4 (6%)	1	13
34	Bc	102/115 (89%)	99 (97%)	1 (1%)	2 (2%)	6	32
35	Bd	107/125 (86%)	103 (96%)	3 (3%)	1 (1%)	14	52
36	Be	126/135 (93%)	117 (93%)	6 (5%)	3 (2%)	5	27
37	Bf	105/110 (96%)	96 (91%)	4 (4%)	5 (5%)	2	16
38	Bg	113/117 (97%)	103 (91%)	6 (5%)	4 (4%)	3	20
39	Bh	120/123 (98%)	112 (93%)	5 (4%)	3 (2%)	4	26
40	Bi	95/105 (90%)	85 (90%)	4 (4%)	6 (6%)	1	13
41	Bj	83/97 (86%)	75 (90%)	6 (7%)	2 (2%)	5	27
42	Bk	67/70 (96%)	64 (96%)	2 (3%)	1 (2%)	8	40
43	Bl	48/51 (94%)	46 (96%)	1 (2%)	1 (2%)	5	30
44	Bm	50/128 (39%)	48 (96%)	1 (2%)	1 (2%)	6	32
45	Bn	23/25 (92%)	23 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	Bo	104/106 (98%)	98 (94%)	4 (4%)	2 (2%)	6	32
47	Bp	89/92 (97%)	83 (93%)	3 (3%)	3 (3%)	3	21
48	Bt	128/137 (93%)	112 (88%)	9 (7%)	7 (6%)	1	15
49	Bu	208/210 (99%)	199 (96%)	6 (3%)	3 (1%)	9	41
51	CA	216/263 (82%)	209 (97%)	5 (2%)	2 (1%)	14	52
52	CB	211/264 (80%)	176 (83%)	18 (8%)	17 (8%)	1	9
53	CC	220/293 (75%)	213 (97%)	2 (1%)	5 (2%)	5	28
54	CD	210/243 (86%)	201 (96%)	4 (2%)	5 (2%)	5	27
55	CE	255/263 (97%)	237 (93%)	13 (5%)	5 (2%)	6	32
56	CF	186/204 (91%)	163 (88%)	12 (6%)	11 (6%)	1	13
57	CG	230/249 (92%)	216 (94%)	5 (2%)	9 (4%)	2	19
58	CH	189/194 (97%)	178 (94%)	7 (4%)	4 (2%)	5	30
59	CI	205/208 (99%)	184 (90%)	14 (7%)	7 (3%)	3	21
60	CJ	177/194 (91%)	169 (96%)	5 (3%)	3 (2%)	7	37
61	CK	92/165 (56%)	84 (91%)	1 (1%)	7 (8%)	1	10
62	CL	144/158 (91%)	133 (92%)	5 (4%)	6 (4%)	2	17
63	CM	118/132 (89%)	111 (94%)	1 (1%)	6 (5%)	1	15
64	CN	148/151 (98%)	138 (93%)	5 (3%)	5 (3%)	3	21
65	CO	135/151 (89%)	129 (96%)	3 (2%)	3 (2%)	5	29
66	CP	116/145 (80%)	106 (91%)	5 (4%)	5 (4%)	2	17
67	CQ	137/146 (94%)	129 (94%)	6 (4%)	2 (2%)	8	40
68	CR	105/135 (78%)	99 (94%)	4 (4%)	2 (2%)	6	32
69	CS	140/152 (92%)	125 (89%)	7 (5%)	8 (6%)	1	14
70	CT	141/145 (97%)	135 (96%)	4 (3%)	2 (1%)	9	41
71	CU	99/119 (83%)	95 (96%)	3 (3%)	1 (1%)	13	49
72	CV	81/83 (98%)	78 (96%)	1 (1%)	2 (2%)	4	26
73	CW	127/130 (98%)	118 (93%)	7 (6%)	2 (2%)	8	38
74	CX	132/143 (92%)	120 (91%)	5 (4%)	7 (5%)	1	15
75	CY	120/133 (90%)	114 (95%)	2 (2%)	4 (3%)	3	21
76	CZ	74/125 (59%)	71 (96%)	0	3 (4%)	2	18
77	Ca	94/115 (82%)	85 (90%)	5 (5%)	4 (4%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
78	Cb	78/84 (93%)	70 (90%)	8 (10%)	0	100	100
79	Cc	60/69 (87%)	57 (95%)	1 (2%)	2 (3%)	3	21
80	Cd	51/56 (91%)	44 (86%)	7 (14%)	0	100	100
81	Ce	49/59 (83%)	43 (88%)	5 (10%)	1 (2%)	6	32
82	Cf	59/156 (38%)	53 (90%)	6 (10%)	0	100	100
83	Cg	312/317 (98%)	291 (93%)	14 (4%)	7 (2%)	5	29
All	All	11795/13363 (88%)	11000 (93%)	439 (4%)	356 (3%)	5	23

All (356) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	835	SER
2	AB	838	VAL
2	AB	843	LEU
2	AB	897	LYS
2	AB	931	SER
2	AB	1068	GLU
2	AB	1070	LEU
2	AB	1142	ALA
2	AB	1190	LEU
2	AB	1266	LEU
2	AB	1303	VAL
2	AB	1304	PHE
2	AB	1320	ASP
2	AB	1349	ILE
2	AB	1367	LYS
2	AB	1386	PHE
7	BA	144	LYS
7	BA	196	TRP
8	BB	4	ARG
8	BB	5	LYS
8	BB	157	CYS
8	BB	259	PRO
8	BB	260	ALA
8	BB	360	LEU
9	BC	50	GLN
9	BC	53	ALA
9	BC	54	VAL
9	BC	151	PRO
9	BC	309	ILE

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Mol	Chain	Res	Type
10	BD	258	LYS
11	BE	137	VAL
11	BE	183	ARG
11	BE	185	PRO
12	BF	222	LYS
13	BG	41	ILE
13	BG	42	GLY
13	BG	162	ASP
14	BH	4	ILE
14	BH	61	TRP
15	BI	189	ARG
16	BJ	11	PRO
16	BJ	14	GLU
16	BJ	77	ALA
16	BJ	155	HIS
16	BJ	175	LEU
17	BL	47	ALA
17	BL	52	SER
17	BL	54	PRO
17	BL	77	SER
17	BL	205	GLN
18	BM	21	ALA
19	BN	184	ILE
21	BP	3	ARG
21	BP	6	LEU
22	BQ	98	LEU
22	BQ	155	ALA
23	BR	131	VAL
24	BS	171	ARG
25	BT	18	PRO
30	BY	67	ILE
31	BZ	32	GLY
31	BZ	103	ASP
31	BZ	125	GLY
32	Ba	48	TYR
33	Bb	30	GLU
33	Bb	56	LYS
34	Bc	107	SER
36	Be	19	LYS
36	Be	20	PHE
37	Bf	60	PRO
37	Bf	64	PRO

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Mol	Chain	Res	Type
37	Bf	106	TYR
37	Bf	107	PRO
38	Bg	84	ALA
39	Bh	122	LYS
40	Bi	28	ARG
40	Bi	33	LEU
40	Bi	34	THR
41	Bj	11	ARG
41	Bj	85	LYS
42	Bk	18	LYS
43	Bl	4	HIS
48	Bt	44	ILE
48	Bt	61	VAL
48	Bt	76	SER
48	Bt	104	PRO
49	Bu	190	LYS
52	CB	76	ASN
52	CB	132	GLY
52	CB	148	ASN
52	CB	154	SER
52	CB	176	VAL
52	CB	177	GLN
52	CB	207	LEU
52	CB	221	PRO
53	CC	64	THR
53	CC	172	ASN
53	CC	176	LYS
54	CD	78	GLY
54	CD	199	GLY
55	CE	204	SER
55	CE	205	PHE
56	CF	20	PHE
56	CF	22	LYS
56	CF	40	ALA
56	CF	48	TYR
56	CF	80	GLY
56	CF	132	GLY
56	CF	185	SER
57	CG	43	GLU
57	CG	146	ASN
57	CG	147	LEU
57	CG	169	PRO

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Mol	Chain	Res	Type
58	CH	88	SER
58	CH	135	PHE
59	CI	123	ARG
59	CI	131	PRO
59	CI	134	GLU
59	CI	142	SER
59	CI	159	SER
61	CK	30	PRO
61	CK	32	HIS
61	CK	36	ALA
61	CK	84	HIS
61	CK	87	PRO
62	CL	8	ARG
62	CL	19	ASN
64	CN	7	PRO
64	CN	108	ASP
65	CO	100	THR
65	CO	146	ARG
66	CP	29	SER
66	CP	126	VAL
68	CR	72	LYS
69	CS	78	LYS
69	CS	79	ILE
69	CS	134	GLN
70	CT	37	VAL
71	CU	52	GLY
72	CV	42	VAL
73	CW	100	GLY
74	CX	61	GLN
74	CX	106	GLY
74	CX	107	ARG
74	CX	116	PRO
75	CY	33	ALA
75	CY	98	GLU
76	CZ	95	GLY
83	Cg	255	SER
83	Cg	284	PRO
2	AB	841	GLU
2	AB	1153	GLU
2	AB	1185	LEU
2	AB	1195	VAL
2	AB	1432	GLU

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Mol	Chain	Res	Type
8	BB	299	ILE
8	BB	309	LEU
8	BB	357	ARG
9	BC	55	SER
9	BC	58	ALA
9	BC	148	PRO
9	BC	276	ASN
12	BF	166	ARG
12	BF	170	THR
13	BG	84	THR
14	BH	190	ALA
15	BI	41	ALA
15	BI	194	GLY
16	BJ	97	ASN
16	BJ	117	ILE
17	BL	51	ALA
17	BL	143	GLU
17	BL	162	LYS
22	BQ	157	GLY
23	BR	113	LYS
27	BV	85	ARG
30	BY	84	ARG
32	Ba	47	LYS
32	Ba	66	ASN
32	Ba	116	LYS
38	Bg	44	SER
38	Bg	45	ALA
46	Bo	34	TYR
47	Bp	12	GLY
51	CA	6	ASP
52	CB	52	THR
52	CB	78	GLU
52	CB	127	VAL
52	CB	209	ASP
53	CC	174	ILE
54	CD	81	GLU
55	CE	231	GLY
55	CE	243	GLY
56	CF	34	SER
56	CF	56	TYR
57	CG	87	ARG
57	CG	157	VAL

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Mol	Chain	Res	Type
58	CH	164	ASN
61	CK	64	TRP
62	CL	119	ASP
63	CM	30	GLY
63	CM	60	MET
63	CM	106	CYS
63	CM	107	SER
64	CN	143	SER
68	CR	114	LEU
69	CS	24	ARG
69	CS	31	THR
69	CS	90	VAL
69	CS	92	ASP
72	CV	48	GLY
77	Ca	61	ALA
83	Cg	276	SER
2	AB	1302	ALA
2	AB	1414	ASP
8	BB	292	LEU
8	BB	296	GLY
9	BC	57	LEU
9	BC	75	ARG
9	BC	150	LEU
10	BD	265	ARG
11	BE	135	GLN
11	BE	265	PRO
13	BG	161	VAL
13	BG	163	PRO
16	BJ	111	GLU
17	BL	141	ALA
17	BL	161	TYR
17	BL	177	LYS
20	BO	72	HIS
20	BO	198	THR
20	BO	199	HIS
21	BP	5	SER
22	BQ	12	LYS
24	BS	135	SER
30	BY	123	ALA
31	BZ	37	PRO
33	Bb	29	TYR
39	Bh	41	ALA

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Mol	Chain	Res	Type
40	Bi	101	ALA
44	Bm	79	GLU
47	Bp	51	ALA
49	Bu	3	GLN
52	CB	49	VAL
52	CB	213	ARG
54	CD	142	LEU
55	CE	203	GLY
56	CF	79	HIS
57	CG	91	GLU
57	CG	92	ARG
58	CH	109	ARG
62	CL	7	GLU
63	CM	102	LYS
64	CN	3	ARG
67	CQ	17	LYS
67	CQ	74	GLY
74	CX	33	GLY
74	CX	86	PRO
75	CY	64	PHE
76	CZ	113	THR
77	Ca	81	SER
79	Cc	38	THR
2	AB	1187	ALA
2	AB	1348	ASP
2	AB	1358	ASN
7	BA	70	LYS
10	BD	253	TYR
11	BE	227	HIS
13	BG	44	ASP
16	BJ	120	ASP
16	BJ	176	PRO
18	BM	44	GLN
19	BN	145	ASN
22	BQ	164	LYS
24	BS	16	CYS
24	BS	158	VAL
24	BS	160	ARG
25	BT	125	TRP
34	Bc	53	PRO
39	Bh	3	LYS
48	Bt	79	ARG

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Mol	Chain	Res	Type
48	Bt	89	THR
64	CN	62	GLN
66	CP	39	ALA
73	CW	28	ARG
74	CX	75	ILE
75	CY	119	GLY
79	Cc	64	GLU
83	Cg	146	SER
2	AB	845	ALA
2	AB	1182	LYS
2	AB	1192	GLU
2	AB	1242	ASP
8	BB	189	THR
9	BC	30	ALA
9	BC	56	GLU
13	BG	134	PRO
22	BQ	156	PRO
24	BS	164	LYS
48	Bt	45	HIS
49	Bu	39	PRO
53	CC	261	PHE
57	CG	88	ARG
60	CJ	138	ARG
60	CJ	169	ARG
62	CL	115	PRO
66	CP	28	MET
66	CP	125	PRO
70	CT	51	ASN
76	CZ	114	LYS
77	Ca	38	LYS
81	Ce	8	ARG
8	BB	326	VAL
10	BD	125	VAL
10	BD	259	LYS
12	BF	184	ILE
16	BJ	58	ARG
16	BJ	76	GLY
23	BR	53	LYS
25	BT	123	GLY
32	Ba	24	LYS
33	Bb	21	ILE
37	Bf	59	THR

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Mol	Chain	Res	Type
40	Bi	21	VAL
40	Bi	65	LYS
51	CA	104	THR
52	CB	23	ASP
52	CB	210	VAL
56	CF	131	ALA
59	CI	12	ARG
69	CS	6	PRO
77	Ca	84	VAL
13	BG	30	PRO
38	Bg	79	GLY
47	Bp	19	GLY
52	CB	64	GLY
60	CJ	170	PRO
61	CK	86	PRO
2	AB	1368	GLY
2	AB	1382	SER
59	CI	20	PRO
62	CL	29	GLY
63	CM	100	PRO
83	Cg	103	GLY
8	BB	18	PRO
9	BC	232	VAL
11	BE	144	ILE
35	Bd	20	VAL
65	CO	53	ILE
83	Cg	61	GLY
19	BN	52	GLY
46	Bo	101	GLY
83	Cg	265	ILE
27	BV	45	ILE
36	Be	6	PRO
54	CD	63	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	540/552 (98%)	517 (96%)	23 (4%)	25	46
7	BA	189/199 (95%)	184 (97%)	5 (3%)	41	59
8	BB	344/349 (99%)	326 (95%)	18 (5%)	19	40
9	BC	302/348 (87%)	284 (94%)	18 (6%)	16	37
10	BD	244/250 (98%)	237 (97%)	7 (3%)	37	56
11	BE	143/143 (100%)	135 (94%)	8 (6%)	17	38
12	BF	203/215 (94%)	196 (97%)	7 (3%)	32	51
13	BG	199/223 (89%)	192 (96%)	7 (4%)	31	51
14	BH	171/171 (100%)	164 (96%)	7 (4%)	26	47
15	BI	170/181 (94%)	161 (95%)	9 (5%)	19	40
16	BJ	143/149 (96%)	137 (96%)	6 (4%)	25	46
17	BL	167/177 (94%)	156 (93%)	11 (7%)	14	34
18	BM	118/161 (73%)	114 (97%)	4 (3%)	32	51
19	BN	172/172 (100%)	170 (99%)	2 (1%)	67	78
20	BO	168/174 (97%)	166 (99%)	2 (1%)	67	78
21	BP	133/163 (82%)	126 (95%)	7 (5%)	19	40
22	BQ	162/165 (98%)	157 (97%)	5 (3%)	35	54
23	BR	161/175 (92%)	150 (93%)	11 (7%)	13	34
24	BS	155/157 (99%)	148 (96%)	7 (4%)	23	45
25	BT	139/140 (99%)	134 (96%)	5 (4%)	30	50
26	BU	91/115 (79%)	88 (97%)	3 (3%)	33	52
27	BV	100/107 (94%)	99 (99%)	1 (1%)	73	82
28	BW	55/126 (44%)	52 (94%)	3 (6%)	18	39
29	BX	107/133 (80%)	105 (98%)	2 (2%)	52	69
30	BY	119/135 (88%)	115 (97%)	4 (3%)	32	51
31	BZ	118/118 (100%)	112 (95%)	6 (5%)	20	41
32	Ba	120/121 (99%)	116 (97%)	4 (3%)	33	52
33	Bb	58/126 (46%)	57 (98%)	1 (2%)	56	72
34	Bc	88/97 (91%)	87 (99%)	1 (1%)	70	80
35	Bd	100/110 (91%)	96 (96%)	4 (4%)	27	47
36	Be	115/121 (95%)	112 (97%)	3 (3%)	41	59
37	Bf	87/89 (98%)	79 (91%)	8 (9%)	7	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	Bg	98/100 (98%)	88 (90%)	10 (10%)	6	20
39	Bh	109/110 (99%)	106 (97%)	3 (3%)	38	57
40	Bi	82/89 (92%)	76 (93%)	6 (7%)	11	31
41	Bj	71/80 (89%)	69 (97%)	2 (3%)	38	57
42	Bk	64/65 (98%)	64 (100%)	0	100	100
43	Bl	47/48 (98%)	46 (98%)	1 (2%)	48	66
44	Bm	48/116 (41%)	45 (94%)	3 (6%)	15	36
45	Bn	24/24 (100%)	24 (100%)	0	100	100
46	Bo	94/94 (100%)	89 (95%)	5 (5%)	19	40
47	Bp	74/75 (99%)	72 (97%)	2 (3%)	40	58
48	Bt	113/121 (93%)	106 (94%)	7 (6%)	15	36
49	Bu	177/177 (100%)	163 (92%)	14 (8%)	10	29
51	CA	181/219 (83%)	176 (97%)	5 (3%)	38	57
52	CB	194/231 (84%)	183 (94%)	11 (6%)	17	38
53	CC	188/225 (84%)	181 (96%)	7 (4%)	29	49
54	CD	175/202 (87%)	166 (95%)	9 (5%)	20	41
55	CE	220/225 (98%)	208 (94%)	12 (6%)	18	39
56	CF	158/170 (93%)	151 (96%)	7 (4%)	24	45
57	CG	202/218 (93%)	195 (96%)	7 (4%)	31	51
58	CH	171/174 (98%)	167 (98%)	4 (2%)	45	64
59	CI	179/180 (99%)	167 (93%)	12 (7%)	13	34
60	CJ	160/168 (95%)	150 (94%)	10 (6%)	15	36
61	CK	85/136 (62%)	82 (96%)	3 (4%)	31	51
62	CL	133/142 (94%)	131 (98%)	2 (2%)	60	75
63	CM	102/108 (94%)	96 (94%)	6 (6%)	16	37
64	CN	130/131 (99%)	128 (98%)	2 (2%)	60	75
65	CO	107/119 (90%)	100 (94%)	7 (6%)	14	35
66	CP	107/130 (82%)	102 (95%)	5 (5%)	22	44
67	CQ	115/121 (95%)	111 (96%)	4 (4%)	31	51
68	CR	99/122 (81%)	94 (95%)	5 (5%)	20	41
69	CS	123/132 (93%)	114 (93%)	9 (7%)	11	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	CT	113/115 (98%)	106 (94%)	7 (6%)	15	36
71	CU	93/107 (87%)	89 (96%)	4 (4%)	25	46
72	CV	67/67 (100%)	66 (98%)	1 (2%)	60	75
73	CW	112/113 (99%)	107 (96%)	5 (4%)	23	45
74	CX	108/115 (94%)	103 (95%)	5 (5%)	23	44
75	CY	107/115 (93%)	101 (94%)	6 (6%)	17	38
76	CZ	67/103 (65%)	63 (94%)	4 (6%)	16	37
77	Ca	83/98 (85%)	76 (92%)	7 (8%)	9	27
78	Cb	72/76 (95%)	68 (94%)	4 (6%)	17	38
79	Cc	55/62 (89%)	52 (94%)	3 (6%)	18	39
80	Cd	47/49 (96%)	43 (92%)	4 (8%)	8	27
81	Ce	42/48 (88%)	40 (95%)	2 (5%)	21	43
82	Cf	54/140 (39%)	51 (94%)	3 (6%)	17	38
83	Cg	272/275 (99%)	260 (96%)	12 (4%)	24	45
All	All	10303/11397 (90%)	9847 (96%)	456 (4%)	26	45

All (456) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	831	ARG
2	AB	836	LYS
2	AB	837	ASN
2	AB	841	GLU
2	AB	844	ARG
2	AB	866	ARG
2	AB	939	LEU
2	AB	1036	PRO
2	AB	1069	GLU
2	AB	1071	ARG
2	AB	1073	GLN
2	AB	1075	MET
2	AB	1163	VAL
2	AB	1174	LYS
2	AB	1182	LYS
2	AB	1184	THR
2	AB	1185	LEU
2	AB	1188	ILE

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Mol	Chain	Res	Type
2	AB	1189	LYS
2	AB	1190	LEU
2	AB	1192	GLU
2	AB	1205	LEU
2	AB	1303	VAL
7	BA	10	LYS
7	BA	116	LEU
7	BA	162	ASN
7	BA	196	TRP
7	BA	218	HIS
8	BB	3	HIS
8	BB	55	HIS
8	BB	89	ILE
8	BB	101	THR
8	BB	131	THR
8	BB	146	LEU
8	BB	157	CYS
8	BB	240	LEU
8	BB	243	LYS
8	BB	254	ILE
8	BB	258	HIS
8	BB	291	TYR
8	BB	300	LYS
8	BB	305	THR
8	BB	314	ILE
8	BB	327	THR
8	BB	351	LEU
8	BB	370	THR
9	BC	13	GLU
9	BC	24	LEU
9	BC	49	ARG
9	BC	78	ARG
9	BC	100	ARG
9	BC	150	LEU
9	BC	151	PRO
9	BC	162	LYS
9	BC	163	LYS
9	BC	188	ARG
9	BC	193	LYS
9	BC	215	ASN
9	BC	232	VAL
9	BC	253	THR

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Mol	Chain	Res	Type
9	BC	289	LEU
9	BC	309	ILE
9	BC	310	HIS
9	BC	323	ARG
10	BD	23	ARG
10	BD	81	HIS
10	BD	105	LEU
10	BD	126	THR
10	BD	155	THR
10	BD	262	LYS
10	BD	293	ARG
11	BE	162	VAL
11	BE	172	LEU
11	BE	188	ARG
11	BE	189	THR
11	BE	197	THR
11	BE	212	LEU
11	BE	217	PHE
11	BE	278	THR
12	BF	15	PRO
12	BF	32	ARG
12	BF	34	ARG
12	BF	37	PHE
12	BF	44	LYS
12	BF	199	LYS
12	BF	226	HIS
13	BG	34	LYS
13	BG	46	GLN
13	BG	55	VAL
13	BG	81	ASN
13	BG	162	ASP
13	BG	163	PRO
13	BG	218	LEU
14	BH	2	LYS
14	BH	20	LEU
14	BH	41	ILE
14	BH	45	LEU
14	BH	71	ARG
14	BH	129	ARG
14	BH	188	GLN
15	BI	33	ILE
15	BI	39	LYS

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Mol	Chain	Res	Type
15	BI	52	MET
15	BI	53	VAL
15	BI	96	VAL
15	BI	163	GLN
15	BI	166	HIS
15	BI	174	THR
15	BI	200	ILE
16	BJ	12	MET
16	BJ	70	VAL
16	BJ	83	LEU
16	BJ	109	ILE
16	BJ	115	LEU
16	BJ	169	LYS
17	BL	52	SER
17	BL	54	PRO
17	BL	55	ILE
17	BL	130	LYS
17	BL	135	LYS
17	BL	148	THR
17	BL	151	THR
17	BL	155	MET
17	BL	163	LYS
17	BL	164	GLU
17	BL	183	ARG
18	BM	72	TYR
18	BM	78	GLN
18	BM	114	LYS
18	BM	132	LYS
19	BN	5	LYS
19	BN	31	ARG
20	BO	169	ARG
20	BO	187	LYS
21	BP	2	VAL
21	BP	4	TYR
21	BP	64	ASN
21	BP	75	GLN
21	BP	78	TRP
21	BP	94	MET
21	BP	112	LEU
22	BQ	48	LEU
22	BQ	61	LEU
22	BQ	72	LEU

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Mol	Chain	Res	Type
22	BQ	75	ARG
22	BQ	120	ILE
23	BR	1	MET
23	BR	3	MET
23	BR	5	ARG
23	BR	20	LYS
23	BR	25	ASP
23	BR	41	ILE
23	BR	57	VAL
23	BR	74	ARG
23	BR	103	ARG
23	BR	114	LYS
23	BR	138	LEU
24	BS	4	SER
24	BS	7	LEU
24	BS	24	THR
24	BS	27	LEU
24	BS	73	LEU
24	BS	166	ARG
24	BS	169	THR
25	BT	17	ARG
25	BT	68	THR
25	BT	69	GLN
25	BT	125	TRP
25	BT	126	VAL
26	BU	20	LYS
26	BU	27	HIS
26	BU	48	LYS
27	BV	131	ARG
28	BW	2	LYS
28	BW	32	LEU
28	BW	33	ASN
29	BX	79	PHE
29	BX	123	LYS
30	BY	8	THR
30	BY	36	LYS
30	BY	70	VAL
30	BY	115	ARG
31	BZ	1	MET
31	BZ	75	TYR
31	BZ	89	ILE
31	BZ	112	ARG

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Mol	Chain	Res	Type
31	BZ	121	ARG
31	BZ	136	PHE
32	Ba	8	THR
32	Ba	47	LYS
32	Ba	56	VAL
32	Ba	132	ARG
33	Bb	61	ASN
34	Bc	17	ARG
35	Bd	39	LYS
35	Bd	92	ARG
35	Bd	115	LYS
35	Bd	119	THR
36	Be	13	VAL
36	Be	70	LEU
36	Be	88	LEU
37	Bf	52	LYS
37	Bf	54	LYS
37	Bf	58	VAL
37	Bf	59	THR
37	Bf	73	LYS
37	Bf	89	ARG
37	Bf	101	ILE
37	Bf	102	ARG
38	Bg	4	ARG
38	Bg	5	LEU
38	Bg	22	LEU
38	Bg	36	LYS
38	Bg	44	SER
38	Bg	54	ARG
38	Bg	60	ARG
38	Bg	67	LEU
38	Bg	69	LYS
38	Bg	81	SER
39	Bh	43	LYS
39	Bh	113	LEU
39	Bh	118	LYS
40	Bi	33	LEU
40	Bi	34	THR
40	Bi	79	THR
40	Bi	90	LEU
40	Bi	97	MET
40	Bi	98	ARG

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Mol	Chain	Res	Type
41	Bj	19	CYS
41	Bj	83	THR
43	Bl	5	LYS
44	Bm	112	LYS
44	Bm	115	CYS
44	Bm	118	THR
46	Bo	32	SER
46	Bo	83	LEU
46	Bo	93	LEU
46	Bo	99	ARG
46	Bo	100	LYS
47	Bp	29	ILE
47	Bp	52	VAL
48	Bt	4	HIS
48	Bt	18	ILE
48	Bt	20	ARG
48	Bt	61	VAL
48	Bt	76	SER
48	Bt	77	TYR
48	Bt	81	THR
49	Bu	21	PHE
49	Bu	24	THR
49	Bu	30	ASN
49	Bu	53	THR
49	Bu	57	THR
49	Bu	60	VAL
49	Bu	101	THR
49	Bu	110	LEU
49	Bu	145	MET
49	Bu	156	ARG
49	Bu	190	LYS
49	Bu	193	LEU
49	Bu	197	THR
49	Bu	210	VAL
51	CA	8	LEU
51	CA	10	MET
51	CA	19	LEU
51	CA	110	ASN
51	CA	204	TYR
52	CB	23	ASP
52	CB	30	TRP
52	CB	46	LYS

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Mol	Chain	Res	Type
52	CB	71	LEU
52	CB	97	LEU
52	CB	131	ASP
52	CB	148	ASN
52	CB	152	LYS
52	CB	177	GLN
52	CB	216	LYS
52	CB	218	LEU
53	CC	89	LYS
53	CC	137	VAL
53	CC	205	VAL
53	CC	209	VAL
53	CC	240	THR
53	CC	252	THR
53	CC	256	TRP
54	CD	5	ILE
54	CD	16	ILE
54	CD	42	THR
54	CD	66	ILE
54	CD	93	THR
54	CD	150	MET
54	CD	162	ASP
54	CD	193	ASP
54	CD	211	VAL
55	CE	23	LEU
55	CE	37	LYS
55	CE	51	ARG
55	CE	95	THR
55	CE	114	ILE
55	CE	115	THR
55	CE	128	LYS
55	CE	136	ILE
55	CE	148	ARG
55	CE	166	THR
55	CE	189	LEU
55	CE	205	PHE
56	CF	47	LYS
56	CF	63	LYS
56	CF	68	ILE
56	CF	72	LEU
56	CF	103	LEU
56	CF	135	ARG

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Mol	Chain	Res	Type
56	CF	195	GLU
57	CG	24	LEU
57	CG	29	GLU
57	CG	34	THR
57	CG	87	ARG
57	CG	160	LYS
57	CG	176	ILE
57	CG	195	LYS
58	CH	111	LYS
58	CH	116	ARG
58	CH	118	ARG
58	CH	152	ARG
59	CI	19	LYS
59	CI	21	TYR
59	CI	29	LEU
59	CI	48	VAL
59	CI	55	TYR
59	CI	62	VAL
59	CI	78	ILE
59	CI	93	THR
59	CI	131	PRO
59	CI	136	ILE
59	CI	137	LEU
59	CI	144	LYS
60	CJ	8	VAL
60	CJ	12	THR
60	CJ	30	LYS
60	CJ	41	ARG
60	CJ	47	LYS
60	CJ	78	LEU
60	CJ	128	VAL
60	CJ	130	ILE
60	CJ	147	PHE
60	CJ	163	SER
61	CK	15	LEU
61	CK	70	TYR
61	CK	84	HIS
62	CL	17	PHE
62	CL	69	ARG
63	CM	52	LEU
63	CM	83	LYS
63	CM	88	TRP

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Mol	Chain	Res	Type
63	CM	106	CYS
63	CM	107	SER
63	CM	117	GLU
64	CN	7	PRO
64	CN	80	LEU
65	CO	45	THR
65	CO	63	LYS
65	CO	100	THR
65	CO	105	THR
65	CO	129	ILE
65	CO	132	VAL
65	CO	140	THR
66	CP	16	THR
66	CP	29	SER
66	CP	40	ARG
66	CP	44	ARG
66	CP	74	GLU
67	CQ	39	LEU
67	CQ	43	GLU
67	CQ	72	VAL
67	CQ	105	LYS
68	CR	22	THR
68	CR	46	LEU
68	CR	71	ILE
68	CR	109	LEU
68	CR	118	GLN
69	CS	3	LEU
69	CS	5	ILE
69	CS	8	LYS
69	CS	23	ARG
69	CS	25	LYS
69	CS	45	LEU
69	CS	60	THR
69	CS	99	LEU
69	CS	139	THR
70	CT	5	THR
70	CT	33	TRP
70	CT	39	LEU
70	CT	64	LEU
70	CT	87	VAL
70	CT	121	ARG
70	CT	126	GLN

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Mol	Chain	Res	Type
71	CU	24	LEU
71	CU	59	LYS
71	CU	61	LEU
71	CU	115	THR
72	CV	2	GLN
73	CW	4	MET
73	CW	11	LEU
73	CW	20	ARG
73	CW	97	ARG
73	CW	98	GLN
74	CX	17	ARG
74	CX	31	HIS
74	CX	37	LYS
74	CX	80	LYS
74	CX	81	ILE
75	CY	20	ARG
75	CY	21	LYS
75	CY	54	VAL
75	CY	84	LYS
75	CY	99	LYS
75	CY	100	LYS
76	CZ	43	LYS
76	CZ	62	VAL
76	CZ	67	LEU
76	CZ	111	ARG
77	Ca	21	ILE
77	Ca	23	CYS
77	Ca	32	LYS
77	Ca	37	LYS
77	Ca	64	LEU
77	Ca	71	LEU
77	Ca	84	VAL
78	Cb	7	LEU
78	Cb	56	CYS
78	Cb	59	CYS
78	Cb	63	LEU
79	Cc	9	ILE
79	Cc	17	VAL
79	Cc	32	VAL
80	Cd	28	HIS
80	Cd	40	ARG
80	Cd	44	ARG

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Mol	Chain	Res	Type
80	Cd	48	LYS
81	Ce	18	LYS
81	Ce	46	VAL
82	Cf	97	LYS
82	Cf	104	LYS
82	Cf	148	TYR
83	Cg	20	GLN
83	Cg	26	GLN
83	Cg	54	ILE
83	Cg	94	THR
83	Cg	99	ARG
83	Cg	157	SER
83	Cg	164	ILE
83	Cg	189	ILE
83	Cg	255	SER
83	Cg	266	ILE
83	Cg	287	THR
83	Cg	289	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (227) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	853	HIS
2	AB	881	GLN
2	AB	895	GLN
2	AB	906	ASN
2	AB	928	ASN
2	AB	950	GLN
2	AB	1015	GLN
2	AB	1073	GLN
2	AB	1132	GLN
2	AB	1179	HIS
2	AB	1278	HIS
2	AB	1335	GLN
2	AB	1389	HIS
2	AB	1403	GLN
2	AB	1417	GLN
7	BA	50	HIS
7	BA	97	ASN
7	BA	132	ASN
7	BA	209	HIS
8	BB	25	HIS

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Mol	Chain	Res	Type
8	BB	167	GLN
8	BB	175	GLN
8	BB	208	ASN
8	BB	213	GLN
8	BB	271	GLN
8	BB	328	ASN
8	BB	354	GLN
9	BC	43	ASN
9	BC	50	GLN
9	BC	187	GLN
9	BC	329	ASN
9	BC	347	HIS
9	BC	362	GLN
10	BD	191	ASN
10	BD	195	HIS
10	BD	244	HIS
10	BD	291	GLN
11	BE	135	GLN
11	BE	182	ASN
11	BE	205	ASN
11	BE	211	HIS
11	BE	228	GLN
11	BE	256	GLN
11	BE	279	ASN
12	BF	80	ASN
12	BF	116	GLN
12	BF	131	ASN
12	BF	151	ASN
13	BG	66	GLN
13	BG	108	GLN
14	BH	15	ASN
14	BH	162	GLN
15	BI	14	ASN
15	BI	51	HIS
15	BI	59	GLN
15	BI	144	ASN
16	BJ	97	ASN
16	BJ	112	HIS
16	BJ	167	GLN
16	BJ	168	GLN
17	BL	19	GLN
17	BL	27	ASN

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Mol	Chain	Res	Type
17	BL	149	GLN
18	BM	20	HIS
18	BM	33	GLN
18	BM	131	GLN
19	BN	139	HIS
19	BN	158	HIS
19	BN	181	HIS
19	BN	201	HIS
20	BO	180	GLN
21	BP	25	HIS
21	BP	54	GLN
21	BP	64	ASN
21	BP	120	ASN
22	BQ	40	ASN
22	BQ	45	GLN
23	BR	39	GLN
23	BR	40	GLN
23	BR	118	HIS
23	BR	141	HIS
24	BS	91	HIS
24	BS	117	HIS
24	BS	122	HIS
24	BS	125	GLN
24	BS	156	HIS
24	BS	173	ASN
25	BT	69	GLN
25	BT	127	GLN
25	BT	131	GLN
25	BT	139	HIS
25	BT	144	ASN
26	BU	17	GLN
26	BU	44	GLN
26	BU	116	GLN
27	BV	36	ASN
27	BV	84	GLN
27	BV	135	ASN
28	BW	48	GLN
28	BW	63	GLN
29	BX	93	ASN
29	BX	107	HIS
29	BX	111	GLN
29	BX	125	ASN

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Mol	Chain	Res	Type
30	BY	66	GLN
30	BY	72	GLN
30	BY	91	ASN
31	BZ	132	GLN
32	Ba	17	HIS
32	Ba	40	HIS
32	Ba	67	GLN
32	Ba	74	ASN
32	Ba	93	ASN
33	Bb	19	ASN
33	Bb	42	ASN
33	Bb	50	ASN
33	Bb	60	ASN
34	Bc	15	ASN
35	Bd	125	ASN
37	Bf	21	GLN
37	Bf	65	ASN
38	Bg	3	GLN
38	Bg	100	GLN
38	Bg	112	GLN
39	Bh	62	ASN
39	Bh	101	ASN
40	Bi	36	HIS
40	Bi	80	HIS
41	Bj	30	GLN
42	Bk	28	ASN
44	Bm	87	GLN
44	Bm	90	ASN
45	Bn	22	GLN
46	Bo	45	GLN
46	Bo	51	GLN
46	Bo	102	GLN
48	Bt	23	GLN
49	Bu	3	GLN
49	Bu	55	GLN
49	Bu	194	ASN
51	CA	50	ASN
51	CA	110	ASN
51	CA	215	GLN
52	CB	40	ASN
52	CB	53	GLN
52	CB	149	GLN

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Mol	Chain	Res	Type
52	CB	157	GLN
52	CB	160	GLN
52	CB	177	GLN
53	CC	267	GLN
54	CD	4	GLN
54	CD	56	GLN
54	CD	57	ASN
54	CD	101	GLN
54	CD	179	GLN
55	CE	36	HIS
55	CE	138	HIS
55	CE	188	ASN
55	CE	216	ASN
55	CE	230	ASN
56	CF	29	GLN
56	CF	82	ASN
56	CF	95	HIS
56	CF	107	ASN
56	CF	110	GLN
56	CF	114	ASN
56	CF	165	ASN
56	CF	203	ASN
57	CG	65	GLN
57	CG	81	HIS
57	CG	105	ASN
58	CH	25	GLN
58	CH	76	GLN
58	CH	97	GLN
58	CH	112	ASN
59	CI	22	HIS
60	CJ	124	HIS
60	CJ	143	ASN
61	CK	44	HIS
61	CK	84	HIS
62	CL	5	GLN
62	CL	112	HIS
63	CM	19	GLN
64	CN	105	ASN
65	CO	32	HIS
65	CO	43	HIS
65	CO	113	GLN
66	CP	35	GLN

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Mol	Chain	Res	Type
66	CP	104	GLN
67	CQ	11	GLN
67	CQ	48	GLN
67	CQ	80	GLN
67	CQ	86	GLN
68	CR	62	GLN
69	CS	19	ASN
69	CS	73	ASN
69	CS	85	ASN
69	CS	87	GLN
70	CT	63	HIS
70	CT	126	GLN
71	CU	100	GLN
72	CV	2	GLN
73	CW	24	GLN
73	CW	82	GLN
73	CW	113	HIS
74	CX	61	GLN
74	CX	73	GLN
74	CX	77	ASN
74	CX	97	ASN
75	CY	19	GLN
75	CY	22	GLN
75	CY	29	HIS
76	CZ	103	HIS
77	Ca	19	GLN
78	Cb	49	HIS
79	Cc	45	ASN
80	Cd	5	GLN
80	Cd	16	GLN
80	Cd	26	ASN
80	Cd	41	GLN
81	Ce	22	GLN
81	Ce	44	ASN
83	Cg	20	GLN
83	Cg	26	GLN
83	Cg	64	HIS
83	Cg	117	ASN
83	Cg	196	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	75/76 (98%)	14 (18%)	1 (1%)
3	AC	259/504 (51%)	135 (52%)	40 (15%)
4	A2	3605/5025 (71%)	2041 (56%)	325 (9%)
5	A3	156/194 (80%)	82 (52%)	6 (3%)
50	C1	1738/1869 (92%)	1038 (59%)	151 (8%)
6	A4	118/121 (97%)	68 (57%)	9 (7%)
All	All	5951/7789 (76%)	3378 (56%)	532 (8%)

All (3378) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	C
1	AA	17	C
1	AA	18	G
1	AA	19	G
1	AA	20	U
1	AA	21	A
1	AA	22	G
1	AA	42	C
1	AA	46	G
1	AA	47	U
1	AA	48	C
1	AA	52	G
1	AA	61	C
1	AA	76	A
3	AC	45	C
3	AC	46	U
3	AC	49	G
3	AC	53	A
3	AC	54	A
3	AC	55	C
3	AC	57	A
3	AC	60	G
3	AC	61	U
3	AC	65	C
3	AC	67	C
3	AC	74	A
3	AC	77	G
3	AC	82	G
3	AC	83	C
3	AC	84	C
3	AC	85	A
3	AC	86	U

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Mol	Chain	Res	Type
3	AC	88	G
3	AC	89	C
3	AC	91	U
3	AC	93	A
3	AC	96	A
3	AC	97	U
3	AC	98	G
3	AC	100	G
3	AC	101	U
3	AC	102	G
3	AC	103	U
3	AC	104	C
3	AC	106	U
3	AC	107	G
3	AC	110	G
3	AC	111	C
3	AC	115	C
3	AC	116	A
3	AC	117	G
3	AC	119	A
3	AC	120	C
3	AC	121	C
3	AC	123	C
3	AC	127	U
3	AC	129	C
3	AC	130	C
3	AC	131	G
3	AC	133	G
3	AC	134	A
3	AC	140	A
3	AC	141	U
3	AC	142	A
3	AC	148	C
3	AC	149	U
3	AC	150	G
3	AC	154	A
3	AC	157	C
3	AC	158	G
3	AC	159	G
3	AC	161	G
3	AC	164	U
3	AC	165	A

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Mol	Chain	Res	Type
3	AC	167	A
3	AC	168	C
3	AC	170	G
3	AC	172	A
3	AC	226	U
3	AC	227	U
3	AC	228	U
3	AC	229	G
3	AC	231	G
3	AC	232	C
3	AC	233	G
3	AC	234	U
3	AC	235	G
3	AC	236	C
3	AC	243	A
3	AC	244	A
3	AC	245	G
3	AC	246	A
3	AC	247	C
3	AC	248	U
3	AC	252	A
3	AC	253	G
3	AC	255	C
3	AC	256	G
3	AC	257	A
3	AC	258	G
3	AC	259	U
3	AC	260	A
3	AC	261	G
3	AC	266	G
3	AC	267	G
3	AC	268	G
3	AC	270	C
3	AC	271	G
3	AC	272	C
3	AC	276	A
3	AC	277	G
3	AC	279	C
3	AC	280	C
3	AC	282	U
3	AC	284	U
3	AC	285	G

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Mol	Chain	Res	Type
3	AC	289	C
3	AC	291	G
3	AC	292	C
3	AC	295	G
3	AC	296	A
3	AC	297	U
3	AC	298	A
3	AC	299	G
3	AC	300	G
3	AC	305	U
3	AC	306	U
3	AC	307	G
3	AC	308	C
3	AC	310	A
3	AC	311	G
3	AC	312	U
3	AC	313	G
3	AC	315	C
3	AC	319	G
3	AC	322	G
3	AC	324	U
3	AC	325	C
3	AC	329	U
3	AC	330	A
3	AC	337	G
3	AC	338	C
3	AC	339	A
3	AC	341	C
3	AC	342	A
3	AC	344	G
3	AC	345	A
3	AC	350	G
3	AC	351	A
4	A2	2	G
4	A2	3	C
4	A2	5	A
4	A2	6	C
4	A2	8	U
4	A2	9	C
4	A2	11	G
4	A2	12	A
4	A2	13	U

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Mol	Chain	Res	Type
4	A2	14	C
4	A2	15	A
4	A2	18	C
4	A2	19	G
4	A2	20	U
4	A2	21	G
4	A2	22	G
4	A2	24	G
4	A2	25	A
4	A2	26	C
4	A2	27	C
4	A2	31	U
4	A2	33	A
4	A2	34	A
4	A2	36	U
4	A2	37	U
4	A2	39	A
4	A2	41	C
4	A2	42	A
4	A2	45	U
4	A2	46	U
4	A2	47	A
4	A2	48	G
4	A2	49	U
4	A2	53	C
4	A2	55	G
4	A2	56	A
4	A2	57	G
4	A2	58	G
4	A2	59	A
4	A2	61	A
4	A2	64	A
4	A2	65	A
4	A2	66	A
4	A2	67	C
4	A2	68	U
4	A2	69	A
4	A2	70	A
4	A2	71	C
4	A2	72	C
4	A2	73	A
4	A2	74	G

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Mol	Chain	Res	Type
4	A2	75	G
4	A2	76	A
4	A2	77	U
4	A2	80	C
4	A2	84	A
4	A2	85	G
4	A2	86	U
4	A2	88	A
4	A2	91	G
4	A2	92	C
4	A2	93	G
4	A2	94	A
4	A2	95	G
4	A2	96	U
4	A2	97	G
4	A2	98	A
4	A2	101	A
4	A2	102	G
4	A2	103	G
4	A2	104	G
4	A2	105	A
4	A2	107	G
4	A2	108	A
4	A2	109	G
4	A2	112	C
4	A2	113	A
4	A2	115	C
4	A2	119	G
4	A2	120	A
4	A2	121	A
4	A2	122	U
4	A2	123	C
4	A2	130	C
4	A2	132	G
4	A2	133	C
4	A2	134	G
4	A2	135	G
4	A2	137	G
4	A2	139	G
4	A2	140	C
4	A2	143	G
4	A2	148	G

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Mol	Chain	Res	Type
4	A2	149	U
4	A2	155	A
4	A2	156	C
4	A2	157	G
4	A2	158	G
4	A2	165	C
4	A2	168	U
4	A2	169	C
4	A2	170	C
4	A2	171	C
4	A2	173	G
4	A2	175	C
4	A2	177	C
4	A2	178	C
4	A2	179	G
4	A2	180	C
4	A2	181	U
4	A2	182	C
4	A2	183	G
4	A2	186	G
4	A2	187	G
4	A2	188	G
4	A2	189	G
4	A2	191	C
4	A2	193	C
4	A2	194	A
4	A2	195	A
4	A2	196	G
4	A2	197	U
4	A2	198	C
4	A2	199	C
4	A2	201	U
4	A2	203	U
4	A2	204	G
4	A2	207	C
4	A2	208	G
4	A2	212	C
4	A2	213	C
4	A2	215	A
4	A2	216	G
4	A2	217	C
4	A2	219	C

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Mol	Chain	Res	Type
4	A2	220	G
4	A2	221	U
4	A2	222	G
4	A2	223	G
4	A2	224	A
4	A2	226	G
4	A2	227	G
4	A2	229	G
4	A2	230	U
4	A2	231	G
4	A2	232	A
4	A2	233	G
4	A2	234	G
4	A2	235	C
4	A2	236	C
4	A2	238	G
4	A2	239	U
4	A2	240	A
4	A2	241	G
4	A2	242	C
4	A2	243	G
4	A2	246	C
4	A2	247	G
4	A2	251	C
4	A2	252	G
4	A2	253	C
4	A2	254	G
4	A2	255	C
4	A2	256	C
4	A2	258	G
4	A2	259	G
4	A2	266	C
4	A2	267	C
4	A2	268	G
4	A2	269	G
4	A2	270	A
4	A2	271	G
4	A2	279	G
4	A2	284	G
4	A2	285	G
4	A2	286	A
4	A2	287	A

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Mol	Chain	Res	Type
4	A2	288	U
4	A2	289	G
4	A2	291	A
4	A2	292	G
4	A2	293	C
4	A2	295	C
4	A2	296	A
4	A2	297	A
4	A2	299	G
4	A2	300	C
4	A2	301	G
4	A2	303	G
4	A2	305	G
4	A2	307	U
4	A2	308	A
4	A2	309	A
4	A2	312	U
4	A2	313	C
4	A2	314	C
4	A2	317	C
4	A2	319	A
4	A2	320	A
4	A2	321	G
4	A2	322	G
4	A2	325	A
4	A2	326	A
4	A2	327	A
4	A2	328	U
4	A2	329	A
4	A2	331	C
4	A2	332	G
4	A2	333	G
4	A2	334	C
4	A2	335	A
4	A2	337	G
4	A2	338	A
4	A2	340	A
4	A2	341	C
4	A2	342	C
4	A2	343	G
4	A2	344	A
4	A2	345	U

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Mol	Chain	Res	Type
4	A2	349	C
4	A2	350	A
4	A2	351	A
4	A2	353	A
4	A2	354	A
4	A2	355	G
4	A2	357	A
4	A2	363	A
4	A2	366	G
4	A2	369	A
4	A2	370	G
4	A2	372	U
4	A2	373	G
4	A2	376	A
4	A2	377	A
4	A2	378	G
4	A2	379	A
4	A2	380	A
4	A2	381	C
4	A2	382	U
4	A2	383	U
4	A2	384	U
4	A2	385	G
4	A2	386	A
4	A2	387	A
4	A2	389	A
4	A2	391	A
4	A2	393	A
4	A2	394	G
4	A2	395	U
4	A2	396	U
4	A2	397	C
4	A2	398	A
4	A2	399	A
4	A2	400	G
4	A2	401	A
4	A2	402	G
4	A2	403	G
4	A2	404	G
4	A2	405	C
4	A2	406	G
4	A2	408	G

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Mol	Chain	Res	Type
4	A2	411	A
4	A2	421	G
4	A2	423	U
4	A2	424	A
4	A2	425	A
4	A2	426	A
4	A2	431	U
4	A2	432	G
4	A2	433	G
4	A2	434	G
4	A2	435	G
4	A2	436	U
4	A2	437	C
4	A2	439	G
4	A2	440	C
4	A2	441	G
4	A2	442	C
4	A2	443	A
4	A2	444	G
4	A2	445	U
4	A2	446	C
4	A2	455	G
4	A2	456	G
4	A2	457	A
4	A2	458	U
4	A2	459	U
4	A2	460	C
4	A2	461	A
4	A2	462	A
4	A2	463	C
4	A2	464	C
4	A2	465	C
4	A2	466	G
4	A2	469	G
4	A2	470	G
4	A2	471	C
4	A2	472	G
4	A2	473	G
4	A2	474	G
4	A2	475	U
4	A2	476	C
4	A2	477	C

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Mol	Chain	Res	Type
4	A2	478	G
4	A2	479	G
4	A2	482	G
4	A2	483	U
4	A2	484	G
4	A2	485	U
4	A2	488	G
4	A2	489	C
4	A2	490	G
4	A2	491	G
4	A2	508	C
4	A2	510	C
4	A2	634	C
4	A2	636	G
4	A2	640	A
4	A2	641	C
4	A2	642	C
4	A2	643	G
4	A2	644	U
4	A2	650	G
4	A2	654	C
4	A2	655	G
4	A2	656	G
4	A2	657	C
4	A2	658	G
4	A2	659	A
4	A2	666	G
4	A2	671	C
4	A2	674	G
4	A2	675	C
4	A2	676	G
4	A2	677	C
4	A2	678	A
4	A2	679	U
4	A2	680	U
4	A2	691	G
4	A2	692	C
4	A2	701	C
4	A2	703	G
4	A2	706	C
4	A2	708	G
4	A2	709	G

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Mol	Chain	Res	Type
4	A2	710	G
4	A2	712	C
4	A2	713	G
4	A2	714	G
4	A2	717	G
4	A2	718	G
4	A2	719	G
4	A2	720	A
4	A2	721	A
4	A2	722	G
4	A2	723	G
4	A2	724	C
4	A2	725	C
4	A2	726	C
4	A2	727	G
4	A2	728	G
4	A2	731	G
4	A2	733	G
4	A2	734	A
4	A2	736	G
4	A2	737	G
4	A2	744	G
4	A2	745	G
4	A2	890	C
4	A2	892	G
4	A2	893	A
4	A2	894	G
4	A2	895	U
4	A2	896	G
4	A2	897	U
4	A2	898	U
4	A2	899	A
4	A2	900	C
4	A2	901	A
4	A2	903	C
4	A2	911	G
4	A2	912	C
4	A2	913	A
4	A2	914	G
4	A2	915	C
4	A2	916	A
4	A2	917	G

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Mol	Chain	Res	Type
4	A2	918	C
4	A2	919	A
4	A2	920	C
4	A2	921	U
4	A2	925	C
4	A2	926	G
4	A2	927	A
4	A2	928	A
4	A2	929	U
4	A2	930	C
4	A2	934	G
4	A2	938	C
4	A2	939	G
4	A2	940	A
4	A2	941	G
4	A2	942	G
4	A2	943	G
4	A2	944	A
4	A2	945	G
4	A2	946	C
4	A2	947	G
4	A2	948	A
4	A2	950	A
4	A2	951	C
4	A2	957	G
4	A2	958	C
4	A2	959	C
4	A2	960	G
4	A2	961	C
4	A2	962	G
4	A2	963	C
4	A2	964	U
4	A2	965	C
4	A2	966	U
4	A2	967	C
4	A2	968	C
4	A2	969	C
4	A2	970	C
4	A2	971	C
4	A2	972	C
4	A2	973	U
4	A2	974	C

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Mol	Chain	Res	Type
4	A2	975	C
4	A2	976	C
4	A2	977	G
4	A2	978	G
4	A2	1047	G
4	A2	1048	G
4	A2	1049	G
4	A2	1050	G
4	A2	1051	C
4	A2	1052	C
4	A2	1053	G
4	A2	1055	G
4	A2	1056	C
4	A2	1058	A
4	A2	1059	C
4	A2	1060	C
4	A2	1062	C
4	A2	1064	C
4	A2	1066	C
4	A2	1079	C
4	A2	1080	U
4	A2	1081	C
4	A2	1082	U
4	A2	1083	C
4	A2	1084	C
4	A2	1085	C
4	A2	1086	A
4	A2	1087	C
4	A2	1089	C
4	A2	1090	C
4	A2	1096	C
4	A2	1142	G
4	A2	1143	G
4	A2	1144	G
4	A2	1145	G
4	A2	1146	G
4	A2	1147	C
4	A2	1148	G
4	A2	1149	G
4	A2	1159	U
4	A2	1160	C
4	A2	1161	C

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Mol	Chain	Res	Type
4	A2	1162	C
4	A2	1165	G
4	A2	1173	C
4	A2	1174	G
4	A2	1176	G
4	A2	1177	C
4	A2	1178	G
4	A2	1179	G
4	A2	1186	C
4	A2	1187	C
4	A2	1188	G
4	A2	1189	U
4	A2	1190	C
4	A2	1192	G
4	A2	1193	G
4	A2	1194	C
4	A2	1195	C
4	A2	1196	C
4	A2	1197	G
4	A2	1198	G
4	A2	1199	G
4	A2	1201	G
4	A2	1202	A
4	A2	1204	G
4	A2	1205	U
4	A2	1206	U
4	A2	1207	C
4	A2	1208	U
4	A2	1209	C
4	A2	1210	U
4	A2	1212	G
4	A2	1214	G
4	A2	1215	G
4	A2	1216	C
4	A2	1217	C
4	A2	1218	A
4	A2	1219	C
4	A2	1220	G
4	A2	1221	C
4	A2	1223	C
4	A2	1224	G
4	A2	1225	C

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Mol	Chain	Res	Type
4	A2	1242	G
4	A2	1245	G
4	A2	1246	G
4	A2	1247	C
4	A2	1248	G
4	A2	1249	G
4	A2	1250	A
4	A2	1251	G
4	A2	1254	A
4	A2	1255	G
4	A2	1256	C
4	A2	1258	C
4	A2	1259	A
4	A2	1262	G
4	A2	1263	G
4	A2	1264	G
4	A2	1267	G
4	A2	1268	G
4	A2	1273	G
4	A2	1274	A
4	A2	1276	G
4	A2	1277	U
4	A2	1279	G
4	A2	1280	G
4	A2	1281	C
4	A2	1282	U
4	A2	1283	A
4	A2	1284	C
4	A2	1285	C
4	A2	1287	A
4	A2	1289	C
4	A2	1290	C
4	A2	1292	A
4	A2	1293	C
4	A2	1294	C
4	A2	1297	U
4	A2	1299	U
4	A2	1300	U
4	A2	1301	G
4	A2	1302	A
4	A2	1303	A
4	A2	1305	C

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Mol	Chain	Res	Type
4	A2	1306	A
4	A2	1308	G
4	A2	1313	A
4	A2	1314	A
4	A2	1318	G
4	A2	1323	A
4	A2	1324	C
4	A2	1326	C
4	A2	1329	G
4	A2	1332	C
4	A2	1334	A
4	A2	1336	U
4	A2	1337	C
4	A2	1338	G
4	A2	1339	G
4	A2	1340	G
4	A2	1341	G
4	A2	1349	C
4	A2	1350	G
4	A2	1351	A
4	A2	1354	G
4	A2	1356	C
4	A2	1357	G
4	A2	1358	C
4	A2	1359	C
4	A2	1360	G
4	A2	1361	U
4	A2	1366	C
4	A2	1367	A
4	A2	1368	A
4	A2	1372	A
4	A2	1374	G
4	A2	1376	G
4	A2	1377	A
4	A2	1378	A
4	A2	1384	G
4	A2	1388	G
4	A2	1389	C
4	A2	1390	U
4	A2	1392	G
4	A2	1393	C
4	A2	1398	C

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Mol	Chain	Res	Type
4	A2	1399	G
4	A2	1400	A
4	A2	1401	G
4	A2	1402	G
4	A2	1406	G
4	A2	1409	C
4	A2	1410	C
4	A2	1412	G
4	A2	1416	C
4	A2	1417	C
4	A2	1418	U
4	A2	1419	C
4	A2	1420	U
4	A2	1421	C
4	A2	1422	C
4	A2	1423	A
4	A2	1424	G
4	A2	1426	C
4	A2	1428	G
4	A2	1433	G
4	A2	1434	G
4	A2	1436	G
4	A2	1438	A
4	A2	1444	G
4	A2	1445	G
4	A2	1446	C
4	A2	1449	G
4	A2	1452	U
4	A2	1454	G
4	A2	1455	C
4	A2	1459	C
4	A2	1460	C
4	A2	1461	G
4	A2	1463	G
4	A2	1464	C
4	A2	1465	C
4	A2	1466	G
4	A2	1467	G
4	A2	1468	G
4	A2	1471	G
4	A2	1476	A
4	A2	1477	G

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Mol	Chain	Res	Type
4	A2	1478	C
4	A2	1479	A
4	A2	1480	C
4	A2	1481	G
4	A2	1482	A
4	A2	1483	G
4	A2	1484	C
4	A2	1487	A
4	A2	1488	C
4	A2	1493	U
4	A2	1495	G
4	A2	1498	C
4	A2	1499	C
4	A2	1500	C
4	A2	1502	A
4	A2	1503	A
4	A2	1504	A
4	A2	1505	G
4	A2	1513	A
4	A2	1518	G
4	A2	1520	C
4	A2	1521	U
4	A2	1522	G
4	A2	1523	G
4	A2	1524	G
4	A2	1526	A
4	A2	1530	C
4	A2	1531	G
4	A2	1532	A
4	A2	1533	A
4	A2	1537	A
4	A2	1540	G
4	A2	1541	G
4	A2	1542	A
4	A2	1543	A
4	A2	1544	A
4	A2	1545	C
4	A2	1550	G
4	A2	1553	G
4	A2	1554	A
4	A2	1555	G
4	A2	1556	G

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Mol	Chain	Res	Type
4	A2	1557	U
4	A2	1558	C
4	A2	1561	U
4	A2	1567	U
4	A2	1570	U
4	A2	1571	G
4	A2	1572	A
4	A2	1573	C
4	A2	1574	G
4	A2	1575	U
4	A2	1576	G
4	A2	1580	A
4	A2	1582	C
4	A2	1583	G
4	A2	1585	U
4	A2	1590	C
4	A2	1591	G
4	A2	1593	C
4	A2	1595	U
4	A2	1596	G
4	A2	1597	G
4	A2	1599	U
4	A2	1600	A
4	A2	1603	G
4	A2	1604	G
4	A2	1607	C
4	A2	1609	A
4	A2	1610	A
4	A2	1611	A
4	A2	1612	G
4	A2	1613	A
4	A2	1614	C
4	A2	1615	U
4	A2	1616	A
4	A2	1617	A
4	A2	1620	G
4	A2	1623	C
4	A2	1629	A
4	A2	1630	G
4	A2	1631	U
4	A2	1633	G
4	A2	1635	U

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Mol	Chain	Res	Type
4	A2	1637	G
4	A2	1639	U
4	A2	1640	C
4	A2	1644	C
4	A2	1648	A
4	A2	1649	G
4	A2	1650	U
4	A2	1651	U
4	A2	1653	C
4	A2	1654	C
4	A2	1655	C
4	A2	1656	U
4	A2	1657	C
4	A2	1658	A
4	A2	1659	G
4	A2	1660	G
4	A2	1661	A
4	A2	1663	A
4	A2	1666	U
4	A2	1667	G
4	A2	1669	C
4	A2	1671	C
4	A2	1672	U
4	A2	1673	C
4	A2	1701	C
4	A2	1703	G
4	A2	1704	U
4	A2	1706	U
4	A2	1709	U
4	A2	1710	C
4	A2	1711	C
4	A2	1712	G
4	A2	1713	G
4	A2	1714	U
4	A2	1715	A
4	A2	1719	C
4	A2	1721	A
4	A2	1725	A
4	A2	1726	U
4	A2	1727	U
4	A2	1729	G
4	A2	1730	A

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Mol	Chain	Res	Type
4	A2	1732	G
4	A2	1733	U
4	A2	1734	C
4	A2	1736	U
4	A2	1737	G
4	A2	1743	G
4	A2	1744	A
4	A2	1745	A
4	A2	1746	A
4	A2	1747	C
4	A2	1749	A
4	A2	1752	U
4	A2	1754	A
4	A2	1755	A
4	A2	1757	C
4	A2	1758	U
4	A2	1759	A
4	A2	1760	U
4	A2	1761	U
4	A2	1766	A
4	A2	1768	C
4	A2	1772	A
4	A2	1773	A
4	A2	1775	U
4	A2	1779	U
4	A2	1780	A
4	A2	1781	A
4	A2	1783	A
4	A2	1784	A
4	A2	1785	G
4	A2	1786	C
4	A2	1787	C
4	A2	1789	G
4	A2	1790	G
4	A2	1792	U
4	A2	1793	C
4	A2	1794	G
4	A2	1795	C
4	A2	1796	U
4	A2	1797	G
4	A2	1798	G
4	A2	1799	C

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Mol	Chain	Res	Type
4	A2	1800	G
4	A2	1801	U
4	A2	1802	G
4	A2	1804	A
4	A2	1805	G
4	A2	1806	C
4	A2	1809	G
4	A2	1810	G
4	A2	1811	G
4	A2	1813	G
4	A2	1815	A
4	A2	1816	A
4	A2	1818	G
4	A2	1820	G
4	A2	1821	A
4	A2	1822	G
4	A2	1825	C
4	A2	1829	G
4	A2	1832	G
4	A2	1833	G
4	A2	1835	C
4	A2	1836	A
4	A2	1839	U
4	A2	1840	U
4	A2	1844	U
4	A2	1845	A
4	A2	1846	A
4	A2	1847	G
4	A2	1848	C
4	A2	1849	A
4	A2	1852	A
4	A2	1853	C
4	A2	1855	G
4	A2	1856	G
4	A2	1857	C
4	A2	1859	C
4	A2	1860	U
4	A2	1861	G
4	A2	1865	G
4	A2	1867	U
4	A2	1868	G
4	A2	1869	A

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Mol	Chain	Res	Type
4	A2	1870	A
4	A2	1871	C
4	A2	1873	G
4	A2	1874	A
4	A2	1875	A
4	A2	1876	C
4	A2	1877	G
4	A2	1879	C
4	A2	1880	G
4	A2	1881	G
4	A2	1883	U
4	A2	1884	U
4	A2	1885	A
4	A2	1886	A
4	A2	1891	C
4	A2	1893	C
4	A2	1894	G
4	A2	1895	A
4	A2	1896	U
4	A2	1897	G
4	A2	1898	C
4	A2	1899	C
4	A2	1900	G
4	A2	1901	A
4	A2	1903	G
4	A2	1911	G
4	A2	1912	A
4	A2	1917	A
4	A2	1918	G
4	A2	1919	A
4	A2	1920	A
4	A2	1924	G
4	A2	1925	U
4	A2	1926	G
4	A2	1929	G
4	A2	1930	G
4	A2	1931	U
4	A2	1935	U
4	A2	1936	A
4	A2	1939	G
4	A2	1941	C
4	A2	1942	A

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Mol	Chain	Res	Type
4	A2	2000	C
4	A2	2001	C
4	A2	2002	G
4	A2	2004	A
4	A2	2005	U
4	A2	2006	C
4	A2	2007	A
4	A2	2009	C
4	A2	2010	U
4	A2	2011	A
4	A2	2012	G
4	A2	2013	C
4	A2	2014	C
4	A2	2016	U
4	A2	2020	A
4	A2	2022	U
4	A2	2023	G
4	A2	2024	G
4	A2	2025	A
4	A2	2026	U
4	A2	2027	G
4	A2	2029	C
4	A2	2030	G
4	A2	2031	C
4	A2	2032	U
4	A2	2033	G
4	A2	2035	A
4	A2	2037	C
4	A2	2039	U
4	A2	2040	C
4	A2	2041	G
4	A2	2042	G
4	A2	2043	G
4	A2	2044	C
4	A2	2046	C
4	A2	2047	A
4	A2	2048	U
4	A2	2049	A
4	A2	2050	C
4	A2	2052	C
4	A2	2056	C
4	A2	2057	G

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Mol	Chain	Res	Type
4	A2	2061	C
4	A2	2062	C
4	A2	2064	G
4	A2	2251	G
4	A2	2254	G
4	A2	2255	A
4	A2	2257	U
4	A2	2258	A
4	A2	2259	G
4	A2	2260	G
4	A2	2263	G
4	A2	2264	G
4	A2	2265	C
4	A2	2266	C
4	A2	2267	G
4	A2	2268	C
4	A2	2269	U
4	A2	2270	G
4	A2	2271	C
4	A2	2273	G
4	A2	2274	U
4	A2	2275	G
4	A2	2276	A
4	A2	2277	G
4	A2	2279	C
4	A2	2280	U
4	A2	2282	G
4	A2	2283	A
4	A2	2284	A
4	A2	2288	U
4	A2	2289	A
4	A2	2290	G
4	A2	2293	C
4	A2	2294	G
4	A2	2295	C
4	A2	2296	G
4	A2	2297	G
4	A2	2298	G
4	A2	2301	C
4	A2	2302	G
4	A2	2304	G
4	A2	2306	G

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Mol	Chain	Res	Type
4	A2	2307	G
4	A2	2308	A
4	A2	2309	G
4	A2	2310	G
4	A2	2311	C
4	A2	2315	C
4	A2	2320	G
4	A2	2321	U
4	A2	2322	G
4	A2	2325	G
4	A2	2326	A
4	A2	2328	C
4	A2	2329	U
4	A2	2331	G
4	A2	2332	G
4	A2	2333	U
4	A2	2334	G
4	A2	2337	A
4	A2	2344	A
4	A2	2345	A
4	A2	2346	U
4	A2	2347	A
4	A2	2348	U
4	A2	2351	A
4	A2	2353	A
4	A2	2354	C
4	A2	2355	G
4	A2	2358	A
4	A2	2359	A
4	A2	2360	C
4	A2	2361	U
4	A2	2362	U
4	A2	2367	G
4	A2	2368	G
4	A2	2369	C
4	A2	2370	C
4	A2	2371	G
4	A2	2372	A
4	A2	2373	A
4	A2	2374	G
4	A2	2376	G
4	A2	2379	G

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Mol	Chain	Res	Type
4	A2	2380	A
4	A2	2381	A
4	A2	2384	G
4	A2	2385	U
4	A2	2386	U
4	A2	2387	C
4	A2	2388	C
4	A2	2392	U
4	A2	2393	G
4	A2	2394	A
4	A2	2395	A
4	A2	2396	C
4	A2	2397	A
4	A2	2398	G
4	A2	2399	C
4	A2	2400	A
4	A2	2402	U
4	A2	2403	U
4	A2	2405	A
4	A2	2407	C
4	A2	2411	G
4	A2	2412	G
4	A2	2414	C
4	A2	2415	A
4	A2	2416	G
4	A2	2418	C
4	A2	2421	U
4	A2	2424	U
4	A2	2426	A
4	A2	2427	G
4	A2	2429	G
4	A2	2430	A
4	A2	2431	U
4	A2	2433	G
4	A2	2435	C
4	A2	2436	G
4	A2	2437	A
4	A2	2440	G
4	A2	2442	C
4	A2	2443	G
4	A2	2444	U
4	A2	2445	U

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Mol	Chain	Res	Type
4	A2	2446	C
4	A2	2447	C
4	A2	2448	G
4	A2	2449	A
4	A2	2450	A
4	A2	2451	G
4	A2	2452	G
4	A2	2453	G
4	A2	2455	C
4	A2	2456	G
4	A2	2457	G
4	A2	2458	G
4	A2	2462	U
4	A2	2463	G
4	A2	2464	G
4	A2	2465	C
4	A2	2466	C
4	A2	2467	U
4	A2	2468	C
4	A2	2469	C
4	A2	2477	U
4	A2	2479	G
4	A2	2480	G
4	A2	2481	C
4	A2	2482	C
4	A2	2483	G
4	A2	2484	A
4	A2	2486	C
4	A2	2490	A
4	A2	2492	G
4	A2	2494	A
4	A2	2496	U
4	A2	2499	G
4	A2	2502	U
4	A2	2503	C
4	A2	2504	A
4	A2	2507	U
4	A2	2508	C
4	A2	2509	C
4	A2	2510	C
4	A2	2511	C
4	A2	2519	G

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Mol	Chain	Res	Type
4	A2	2521	G
4	A2	2524	G
4	A2	2525	C
4	A2	2526	G
4	A2	2527	G
4	A2	2528	A
4	A2	2529	G
4	A2	2531	U
4	A2	2532	G
4	A2	2537	C
4	A2	2538	C
4	A2	2544	G
4	A2	2548	C
4	A2	2549	C
4	A2	2550	A
4	A2	2552	U
4	A2	2553	G
4	A2	2554	C
4	A2	2556	G
4	A2	2557	U
4	A2	2559	A
4	A2	2560	C
4	A2	2561	G
4	A2	2562	C
4	A2	2563	G
4	A2	2564	A
4	A2	2565	C
4	A2	2566	C
4	A2	2567	G
4	A2	2574	G
4	A2	2575	A
4	A2	2576	G
4	A2	2577	A
4	A2	2578	A
4	A2	2579	G
4	A2	2582	G
4	A2	2587	G
4	A2	2588	A
4	A2	2589	G
4	A2	2590	C
4	A2	2592	C
4	A2	2593	C

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Mol	Chain	Res	Type
4	A2	2594	G
4	A2	2596	G
4	A2	2597	G
4	A2	2598	A
4	A2	2599	G
4	A2	2601	G
4	A2	2602	U
4	A2	2603	U
4	A2	2604	C
4	A2	2607	U
4	A2	2608	U
4	A2	2609	U
4	A2	2613	U
4	A2	2624	A
4	A2	2625	G
4	A2	2627	G
4	A2	2628	C
4	A2	2629	G
4	A2	2630	C
4	A2	2631	C
4	A2	2632	C
4	A2	2633	U
4	A2	2635	G
4	A2	2636	A
4	A2	2639	G
4	A2	2641	G
4	A2	2642	U
4	A2	2646	C
4	A2	2647	C
4	A2	2648	C
4	A2	2651	A
4	A2	2652	G
4	A2	2653	A
4	A2	2654	G
4	A2	2658	G
4	A2	2661	C
4	A2	2663	G
4	A2	2664	U
4	A2	2665	G
4	A2	2666	C
4	A2	2669	U
4	A2	2671	G

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Mol	Chain	Res	Type
4	A2	2672	A
4	A2	2673	A
4	A2	2674	A
4	A2	2676	C
4	A2	2677	G
4	A2	2678	U
4	A2	2682	G
4	A2	2683	G
4	A2	2684	U
4	A2	2685	U
4	A2	2686	C
4	A2	2687	C
4	A2	2689	G
4	A2	2692	G
4	A2	2696	C
4	A2	2698	G
4	A2	2700	U
4	A2	2701	G
4	A2	2702	A
4	A2	2703	G
4	A2	2704	C
4	A2	2705	U
4	A2	2706	C
4	A2	2707	U
4	A2	2709	G
4	A2	2710	C
4	A2	2711	U
4	A2	2715	C
4	A2	2716	C
4	A2	2717	U
4	A2	2718	U
4	A2	2719	G
4	A2	2720	A
4	A2	2729	G
4	A2	2731	G
4	A2	2732	A
4	A2	2733	G
4	A2	2734	A
4	A2	2735	G
4	A2	2736	G
4	A2	2739	G
4	A2	2740	U

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Mol	Chain	Res	Type
4	A2	2741	A
4	A2	2742	A
4	A2	2745	C
4	A2	2746	U
4	A2	2750	G
4	A2	2751	C
4	A2	2752	C
4	A2	2755	G
4	A2	2759	U
4	A2	2761	C
4	A2	2762	C
4	A2	2764	A
4	A2	2765	U
4	A2	2766	A
4	A2	2767	U
4	A2	2771	C
4	A2	2772	A
4	A2	2774	C
4	A2	2775	A
4	A2	2778	U
4	A2	2780	U
4	A2	2782	C
4	A2	2783	A
4	A2	2789	A
4	A2	2791	C
4	A2	2792	A
4	A2	2794	C
4	A2	2796	U
4	A2	2801	C
4	A2	2802	A
4	A2	2803	U
4	A2	2804	G
4	A2	2805	U
4	A2	2806	U
4	A2	2807	G
4	A2	2810	A
4	A2	2811	C
4	A2	2812	A
4	A2	2815	G
4	A2	2817	A
4	A2	2818	G
4	A2	2823	G

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Mol	Chain	Res	Type
4	A2	2826	A
4	A2	2827	A
4	A2	2828	G
4	A2	2831	G
4	A2	2832	G
4	A2	2833	C
4	A2	2835	A
4	A2	2837	C
4	A2	2839	G
4	A2	2840	G
4	A2	2843	C
4	A2	2844	C
4	A2	2845	G
4	A2	2846	U
4	A2	2847	A
4	A2	2848	A
4	A2	2852	C
4	A2	2853	G
4	A2	2854	G
4	A2	2857	U
4	A2	2858	A
4	A2	2860	G
4	A2	2861	G
4	A2	2863	U
4	A2	2864	U
4	A2	2867	C
4	A2	2868	U
4	A2	2869	C
4	A2	2871	A
4	A2	2873	G
4	A2	2877	U
4	A2	2878	G
4	A2	2879	G
4	A2	3567	C
4	A2	3568	A
4	A2	3570	C
4	A2	3574	C
4	A2	3575	U
4	A2	3578	G
4	A2	3579	A
4	A2	3583	G
4	A2	3584	G

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Mol	Chain	Res	Type
4	A2	3585	U
4	A2	3586	G
4	A2	3587	C
4	A2	3588	G
4	A2	3590	A
4	A2	3594	G
4	A2	3595	G
4	A2	3597	G
4	A2	3599	A
4	A2	3600	U
4	A2	3602	C
4	A2	3603	G
4	A2	3604	A
4	A2	3605	C
4	A2	3610	U
4	A2	3611	A
4	A2	3612	A
4	A2	3613	U
4	A2	3617	A
4	A2	3618	A
4	A2	3619	C
4	A2	3622	A
4	A2	3624	C
4	A2	3626	U
4	A2	3627	C
4	A2	3631	A
4	A2	3634	G
4	A2	3635	C
4	A2	3636	C
4	A2	3641	G
4	A2	3642	C
4	A2	3643	G
4	A2	3646	U
4	A2	3649	U
4	A2	3650	G
4	A2	3651	A
4	A2	3652	C
4	A2	3653	G
4	A2	3654	C
4	A2	3655	G
4	A2	3657	U
4	A2	3658	G

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Mol	Chain	Res	Type
4	A2	3661	A
4	A2	3662	U
4	A2	3664	U
4	A2	3665	C
4	A2	3666	U
4	A2	3667	G
4	A2	3668	C
4	A2	3675	C
4	A2	3676	U
4	A2	3678	U
4	A2	3679	G
4	A2	3680	A
4	A2	3681	A
4	A2	3682	U
4	A2	3683	G
4	A2	3684	U
4	A2	3685	C
4	A2	3686	A
4	A2	3693	A
4	A2	3695	A
4	A2	3696	A
4	A2	3697	A
4	A2	3700	C
4	A2	3706	A
4	A2	3710	C
4	A2	3717	A
4	A2	3720	G
4	A2	3722	G
4	A2	3723	G
4	A2	3724	G
4	A2	3725	A
4	A2	3726	G
4	A2	3727	U
4	A2	3728	A
4	A2	3729	A
4	A2	3730	C
4	A2	3732	A
4	A2	3733	U
4	A2	3734	G
4	A2	3736	C
4	A2	3737	U
4	A2	3741	U

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Mol	Chain	Res	Type
4	A2	3743	A
4	A2	3744	A
4	A2	3746	G
4	A2	3749	G
4	A2	3750	C
4	A2	3751	C
4	A2	3753	A
4	A2	3754	A
4	A2	3755	U
4	A2	3756	G
4	A2	3759	U
4	A2	3761	G
4	A2	3764	A
4	A2	3765	U
4	A2	3767	U
4	A2	3768	A
4	A2	3769	A
4	A2	3770	U
4	A2	3771	U
4	A2	3772	A
4	A2	3776	A
4	A2	3778	G
4	A2	3779	C
4	A2	3780	G
4	A2	3781	C
4	A2	3782	A
4	A2	3786	A
4	A2	3787	U
4	A2	3788	G
4	A2	3792	G
4	A2	3793	A
4	A2	3797	A
4	A2	3798	G
4	A2	3799	A
4	A2	3800	U
4	A2	3801	U
4	A2	3802	C
4	A2	3803	C
4	A2	3807	U
4	A2	3808	G
4	A2	3809	U
4	A2	3814	A

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Mol	Chain	Res	Type
4	A2	3815	C
4	A2	3819	C
4	A2	3826	G
4	A2	3830	A
4	A2	3833	C
4	A2	3834	A
4	A2	3836	A
4	A2	3837	G
4	A2	3838	C
4	A2	3845	A
4	A2	3846	A
4	A2	3847	C
4	A2	3848	G
4	A2	3850	G
4	A2	3852	U
4	A2	3854	G
4	A2	3856	C
4	A2	3857	G
4	A2	3858	G
4	A2	3859	A
4	A2	3863	A
4	A2	3866	G
4	A2	3867	G
4	A2	3870	A
4	A2	3871	A
4	A2	3872	A
4	A2	3873	G
4	A2	3874	A
4	A2	3875	A
4	A2	3876	G
4	A2	3877	A
4	A2	3879	C
4	A2	3883	U
4	A2	3884	U
4	A2	3885	G
4	A2	3887	G
4	A2	3888	C
4	A2	3890	U
4	A2	3891	G
4	A2	3894	U
4	A2	3895	C
4	A2	3897	A

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Mol	Chain	Res	Type
4	A2	3898	G
4	A2	3905	A
4	A2	3907	G
4	A2	3908	G
4	A2	3910	G
4	A2	3912	A
4	A2	3913	G
4	A2	3919	U
4	A2	3922	G
4	A2	3923	A
4	A2	3924	G
4	A2	3925	G
4	A2	3926	U
4	A2	3927	G
4	A2	3931	A
4	A2	3933	U
4	A2	3934	A
4	A2	3936	G
4	A2	3938	G
4	A2	3941	A
4	A2	3942	G
4	A2	3943	G
4	A2	3945	C
4	A2	4007	G
4	A2	4008	C
4	A2	4009	C
4	A2	4011	G
4	A2	4012	U
4	A2	4015	A
4	A2	4018	A
4	A2	4024	A
4	A2	4025	C
4	A2	4026	U
4	A2	4027	C
4	A2	4029	G
4	A2	4032	C
4	A2	4033	G
4	A2	4041	A
4	A2	4044	G
4	A2	4045	A
4	A2	4046	C
4	A2	4047	C

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Mol	Chain	Res	Type
4	A2	4050	G
4	A2	4051	U
4	A2	4052	G
4	A2	4053	A
4	A2	4054	G
4	A2	4055	G
4	A2	4056	C
4	A2	4057	G
4	A2	4059	G
4	A2	4060	G
4	A2	4063	G
4	A2	4066	A
4	A2	4068	C
4	A2	4069	C
4	A2	4070	C
4	A2	4071	G
4	A2	4073	G
4	A2	4074	G
4	A2	4079	C
4	A2	4080	U
4	A2	4081	C
4	A2	4082	G
4	A2	4083	C
4	A2	4084	U
4	A2	4085	U
4	A2	4086	C
4	A2	4087	U
4	A2	4089	G
4	A2	4090	C
4	A2	4092	C
4	A2	4093	C
4	A2	4094	A
4	A2	4101	C
4	A2	4103	C
4	A2	4105	C
4	A2	4106	G
4	A2	4108	C
4	A2	4109	C
4	A2	4111	G
4	A2	4117	A
4	A2	4118	C
4	A2	4119	C

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Mol	Chain	Res	Type
4	A2	4120	C
4	A2	4121	G
4	A2	4122	C
4	A2	4123	U
4	A2	4124	C
4	A2	4126	G
4	A2	4129	G
4	A2	4130	A
4	A2	4131	C
4	A2	4135	G
4	A2	4137	C
4	A2	4138	A
4	A2	4142	G
4	A2	4143	G
4	A2	4144	G
4	A2	4145	G
4	A2	4151	G
4	A2	4155	G
4	A2	4156	G
4	A2	4159	C
4	A2	4163	A
4	A2	4164	C
4	A2	4165	A
4	A2	4166	C
4	A2	4168	U
4	A2	4174	A
4	A2	4175	C
4	A2	4176	G
4	A2	4177	G
4	A2	4179	A
4	A2	4180	A
4	A2	4181	C
4	A2	4182	G
4	A2	4185	G
4	A2	4186	G
4	A2	4187	U
4	A2	4188	G
4	A2	4189	U
4	A2	4190	C
4	A2	4191	C
4	A2	4192	U
4	A2	4193	A

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Mol	Chain	Res	Type
4	A2	4194	A
4	A2	4195	G
4	A2	4199	A
4	A2	4200	G
4	A2	4201	C
4	A2	4210	G
4	A2	4211	A
4	A2	4212	C
4	A2	4214	G
4	A2	4215	A
4	A2	4226	G
4	A2	4227	G
4	A2	4231	A
4	A2	4232	G
4	A2	4233	A
4	A2	4234	A
4	A2	4236	G
4	A2	4237	G
4	A2	4239	A
4	A2	4240	A
4	A2	4241	A
4	A2	4242	A
4	A2	4245	U
4	A2	4247	G
4	A2	4250	U
4	A2	4251	G
4	A2	4252	A
4	A2	4253	U
4	A2	4254	C
4	A2	4255	U
4	A2	4256	U
4	A2	4261	U
4	A2	4262	U
4	A2	4263	C
4	A2	4264	A
4	A2	4265	G
4	A2	4266	U
4	A2	4267	A
4	A2	4269	G
4	A2	4270	A
4	A2	4271	A
4	A2	4273	A

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Mol	Chain	Res	Type
4	A2	4276	G
4	A2	4277	A
4	A2	4279	C
4	A2	4280	G
4	A2	4283	A
4	A2	4286	G
4	A2	4287	C
4	A2	4288	G
4	A2	4289	G
4	A2	4290	G
4	A2	4291	G
4	A2	4292	C
4	A2	4293	C
4	A2	4297	C
4	A2	4298	G
4	A2	4301	C
4	A2	4303	U
4	A2	4304	U
4	A2	4305	C
4	A2	4306	U
4	A2	4308	A
4	A2	4309	C
4	A2	4313	U
4	A2	4314	U
4	A2	4315	G
4	A2	4316	G
4	A2	4317	G
4	A2	4319	U
4	A2	4321	U
4	A2	4324	G
4	A2	4326	A
4	A2	4327	G
4	A2	4328	G
4	A2	4329	A
4	A2	4331	G
4	A2	4333	G
4	A2	4335	C
4	A2	4336	A
4	A2	4337	G
4	A2	4338	A
4	A2	4339	A
4	A2	4341	A

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Mol	Chain	Res	Type
4	A2	4342	G
4	A2	4345	A
4	A2	4346	C
4	A2	4347	C
4	A2	4348	A
4	A2	4350	A
4	A2	4353	G
4	A2	4354	A
4	A2	4355	U
4	A2	4357	A
4	A2	4359	U
4	A2	4362	C
4	A2	4363	U
4	A2	4366	U
4	A2	4367	G
4	A2	4370	G
4	A2	4372	C
4	A2	4373	C
4	A2	4375	A
4	A2	4376	G
4	A2	4377	C
4	A2	4379	U
4	A2	4380	U
4	A2	4382	A
4	A2	4383	U
4	A2	4384	A
4	A2	4386	C
4	A2	4387	G
4	A2	4388	A
4	A2	4389	C
4	A2	4390	G
4	A2	4394	C
4	A2	4396	U
4	A2	4397	U
4	A2	4401	A
4	A2	4404	C
4	A2	4406	U
4	A2	4407	C
4	A2	4408	G
4	A2	4409	A
4	A2	4410	U
4	A2	4411	G

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Mol	Chain	Res	Type
4	A2	4412	U
4	A2	4413	C
4	A2	4415	G
4	A2	4416	C
4	A2	4420	U
4	A2	4421	C
4	A2	4422	C
4	A2	4423	U
4	A2	4424	A
4	A2	4425	U
4	A2	4426	C
4	A2	4431	U
4	A2	4433	A
4	A2	4434	A
4	A2	4435	G
4	A2	4437	A
4	A2	4438	G
4	A2	4448	A
4	A2	4449	G
4	A2	4451	G
4	A2	4452	U
4	A2	4453	U
4	A2	4454	G
4	A2	4455	G
4	A2	4456	A
4	A2	4457	U
4	A2	4458	U
4	A2	4459	G
4	A2	4460	U
4	A2	4461	U
4	A2	4465	C
4	A2	4466	C
4	A2	4470	A
4	A2	4472	U
4	A2	4473	A
4	A2	4474	G
4	A2	4477	A
4	A2	4478	A
4	A2	4479	C
4	A2	4480	G
4	A2	4482	G
4	A2	4483	A

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Mol	Chain	Res	Type
4	A2	4484	G
4	A2	4488	G
4	A2	4489	G
4	A2	4491	U
4	A2	4492	U
4	A2	4494	G
4	A2	4498	G
4	A2	4499	U
4	A2	4500	C
4	A2	4502	U
4	A2	4503	G
4	A2	4505	G
4	A2	4507	C
4	A2	4508	A
4	A2	4509	G
4	A2	4510	G
4	A2	4512	U
4	A2	4515	U
4	A2	4516	U
4	A2	4519	A
4	A2	4520	C
4	A2	4521	C
4	A2	4522	C
4	A2	4525	C
4	A2	4526	U
4	A2	4527	G
4	A2	4528	A
4	A2	4529	U
4	A2	4530	G
4	A2	4532	U
4	A2	4533	G
4	A2	4534	U
4	A2	4535	G
4	A2	4536	U
4	A2	4538	G
4	A2	4539	U
4	A2	4541	G
4	A2	4543	C
4	A2	4544	A
4	A2	4545	U
4	A2	4549	A
4	A2	4550	A

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Mol	Chain	Res	Type
4	A2	4551	U
4	A2	4552	C
4	A2	4557	U
4	A2	4558	C
4	A2	4560	G
4	A2	4561	U
4	A2	4562	A
4	A2	4563	C
4	A2	4566	G
4	A2	4567	A
4	A2	4568	G
4	A2	4569	G
4	A2	4570	A
4	A2	4577	G
4	A2	4578	G
4	A2	4579	U
4	A2	4580	U
4	A2	4583	G
4	A2	4584	A
4	A2	4586	A
4	A2	4587	U
4	A2	4592	U
4	A2	4594	U
4	A2	4595	A
4	A2	4596	U
4	A2	4597	G
4	A2	4598	U
4	A2	4599	G
4	A2	4600	C
4	A2	4601	U
4	A2	4602	U
4	A2	4604	G
4	A2	4609	G
4	A2	4610	G
4	A2	4612	G
4	A2	4613	C
4	A2	4615	A
4	A2	4616	A
4	A2	4617	U
4	A2	4618	G
4	A2	4621	G
4	A2	4622	C

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Mol	Chain	Res	Type
4	A2	4628	U
4	A2	4629	A
4	A2	4630	C
4	A2	4632	A
4	A2	4636	G
4	A2	4637	U
4	A2	4638	G
4	A2	4639	G
4	A2	4640	G
4	A2	4641	A
4	A2	4642	U
4	A2	4643	U
4	A2	4646	G
4	A2	4651	A
4	A2	4654	G
4	A2	4655	C
4	A2	4657	U
4	A2	4658	C
4	A2	4659	U
4	A2	4660	A
4	A2	4661	A
4	A2	4664	C
4	A2	4665	A
4	A2	4668	A
4	A2	4669	U
4	A2	4671	C
4	A2	4672	C
4	A2	4675	C
4	A2	4676	C
4	A2	4678	G
4	A2	4679	G
4	A2	4680	C
4	A2	4681	G
4	A2	4682	A
4	A2	4684	C
4	A2	4688	A
4	A2	4689	C
4	A2	4690	G
4	A2	4691	G
4	A2	4692	C
4	A2	4693	A
4	A2	4694	G

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Mol	Chain	Res	Type
4	A2	4696	G
4	A2	4698	C
4	A2	4699	G
4	A2	4700	C
4	A2	4701	G
4	A2	4706	C
4	A2	4710	G
4	A2	4711	U
4	A2	4712	U
4	A2	4713	G
4	A2	4714	G
4	A2	4716	C
4	A2	4718	C
4	A2	4719	G
4	A2	4720	G
4	A2	4721	A
4	A2	4723	A
4	A2	4724	G
4	A2	4725	C
4	A2	4726	C
4	A2	4733	C
4	A2	4734	C
4	A2	4735	G
4	A2	4736	C
4	A2	4739	G
4	A2	4740	U
4	A2	4741	C
4	A2	4742	C
4	A2	4746	C
4	A2	4803	C
4	A2	4804	G
4	A2	4807	C
4	A2	4808	C
4	A2	4809	G
4	A2	4812	A
4	A2	4813	C
4	A2	4814	C
4	A2	4815	G
4	A2	4816	G
4	A2	4822	G
4	A2	4824	U
4	A2	4825	G

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Mol	Chain	Res	Type
4	A2	4826	C
4	A2	4827	G
4	A2	4828	G
4	A2	4829	A
4	A2	4831	U
4	A2	4832	G
4	A2	4834	C
4	A2	4836	U
4	A2	4838	C
4	A2	4839	G
4	A2	4840	U
4	A2	4844	G
4	A2	4847	A
4	A2	4848	A
4	A2	4849	A
4	A2	4850	C
4	A2	4851	G
4	A2	4852	G
4	A2	4853	G
4	A2	4854	G
4	A2	4855	C
4	A2	4856	G
4	A2	4857	C
4	A2	4858	G
4	A2	4862	G
4	A2	4863	G
4	A2	4867	G
4	A2	4868	G
4	A2	4875	C
4	A2	4879	C
4	A2	4880	U
4	A2	4881	C
4	A2	4882	G
4	A2	4883	C
4	A2	4892	C
4	A2	4893	A
4	A2	4894	C
4	A2	4895	C
4	A2	4896	G
4	A2	4897	C
4	A2	4898	A
4	A2	4899	C

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Mol	Chain	Res	Type
4	A2	4900	G
4	A2	4901	U
4	A2	4902	U
4	A2	4903	C
4	A2	4904	G
4	A2	4905	U
4	A2	4906	G
4	A2	4919	C
4	A2	4921	A
4	A2	4923	A
4	A2	4924	C
4	A2	4930	G
4	A2	4931	U
4	A2	4932	A
4	A2	4940	U
4	A2	4943	U
4	A2	4944	U
4	A2	4945	C
4	A2	4946	U
4	A2	4947	G
4	A2	4949	G
4	A2	4955	G
4	A2	4956	U
4	A2	4958	U
4	A2	4959	C
4	A2	4960	G
4	A2	4962	A
4	A2	4963	C
4	A2	4968	C
4	A2	4969	A
4	A2	4972	G
4	A2	4974	A
4	A2	4975	G
4	A2	4976	C
4	A2	4978	C
4	A2	4979	C
4	A2	4980	C
4	A2	4981	U
4	A2	4982	C
4	A2	4983	G
4	A2	4985	U
4	A2	4986	G

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Mol	Chain	Res	Type
4	A2	4988	G
4	A2	4995	U
4	A2	4996	G
4	A2	4998	A
4	A2	5002	C
4	A2	5003	A
4	A2	5005	C
4	A2	5009	C
4	A2	5010	G
4	A2	5015	A
4	A2	5016	A
4	A2	5017	G
4	A2	5018	G
4	A2	5019	G
4	A2	5020	U
4	A2	5021	U
5	A3	4	C
5	A3	6	C
5	A3	7	U
5	A3	8	U
5	A3	9	A
5	A3	10	G
5	A3	12	G
5	A3	13	G
5	A3	14	U
5	A3	16	G
5	A3	20	A
5	A3	23	C
5	A3	24	G
5	A3	25	G
5	A3	26	C
5	A3	28	C
5	A3	30	U
5	A3	32	C
5	A3	34	U
5	A3	38	U
5	A3	40	A
5	A3	43	A
5	A3	47	C
5	A3	49	G
5	A3	51	U
5	A3	52	A

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Mol	Chain	Res	Type
5	A3	58	G
5	A3	59	A
5	A3	61	A
5	A3	62	A
5	A3	63	U
5	A3	69	U
5	A3	71	A
5	A3	72	A
5	A3	75	G
5	A3	76	C
5	A3	77	A
5	A3	78	G
5	A3	80	A
5	A3	81	C
5	A3	82	A
5	A3	83	C
5	A3	84	A
5	A3	85	U
5	A3	86	U
5	A3	89	U
5	A3	94	G
5	A3	95	A
5	A3	103	A
5	A3	104	A
5	A3	105	C
5	A3	106	G
5	A3	107	C
5	A3	109	C
5	A3	111	U
5	A3	112	G
5	A3	114	G
5	A3	117	C
5	A3	120	G
5	A3	122	G
5	A3	123	U
5	A3	124	U
5	A3	125	C
5	A3	126	C
5	A3	128	C
5	A3	129	C
5	A3	130	C
5	A3	131	G

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Mol	Chain	Res	Type
5	A3	137	A
5	A3	138	C
5	A3	140	C
5	A3	141	C
5	A3	143	G
5	A3	144	U
5	A3	146	U
5	A3	147	G
5	A3	148	A
5	A3	149	G
5	A3	150	C
5	A3	151	G
5	A3	156	U
5	A3	157	U
6	A4	3	C
6	A4	6	C
6	A4	7	G
6	A4	9	C
6	A4	10	C
6	A4	11	A
6	A4	12	U
6	A4	13	A
6	A4	15	C
6	A4	19	C
6	A4	22	A
6	A4	27	G
6	A4	28	C
6	A4	29	C
6	A4	30	C
6	A4	33	U
6	A4	34	C
6	A4	35	U
6	A4	36	C
6	A4	40	U
6	A4	41	G
6	A4	46	C
6	A4	47	G
6	A4	48	G
6	A4	49	A
6	A4	53	U
6	A4	54	A
6	A4	55	A

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Mol	Chain	Res	Type
6	A4	56	G
6	A4	57	C
6	A4	58	A
6	A4	61	G
6	A4	62	U
6	A4	63	C
6	A4	64	G
6	A4	65	G
6	A4	67	C
6	A4	68	C
6	A4	69	U
6	A4	73	U
6	A4	74	A
6	A4	75	G
6	A4	76	U
6	A4	77	A
6	A4	79	U
6	A4	81	G
6	A4	85	G
6	A4	86	G
6	A4	87	G
6	A4	89	G
6	A4	91	C
6	A4	94	C
6	A4	95	C
6	A4	96	U
6	A4	97	G
6	A4	99	G
6	A4	100	A
6	A4	101	A
6	A4	103	A
6	A4	105	C
6	A4	107	G
6	A4	108	G
6	A4	109	U
6	A4	110	G
6	A4	113	G
6	A4	116	G
6	A4	117	G
6	A4	118	C
50	C1	2	A
50	C1	3	C

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Mol	Chain	Res	Type
50	C1	4	C
50	C1	5	U
50	C1	6	G
50	C1	7	G
50	C1	8	U
50	C1	9	U
50	C1	15	U
50	C1	16	G
50	C1	17	C
50	C1	21	U
50	C1	22	A
50	C1	24	C
50	C1	25	A
50	C1	26	U
50	C1	30	C
50	C1	33	G
50	C1	39	A
50	C1	40	A
50	C1	41	G
50	C1	44	U
50	C1	45	A
50	C1	46	A
50	C1	47	G
50	C1	48	C
50	C1	50	A
50	C1	55	U
50	C1	56	G
50	C1	59	U
50	C1	60	A
50	C1	61	A
50	C1	62	G
50	C1	63	U
50	C1	64	A
50	C1	65	C
50	C1	66	G
50	C1	67	C
50	C1	68	A
50	C1	69	C
50	C1	70	G
50	C1	71	G
50	C1	72	C
50	C1	74	G

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Mol	Chain	Res	Type
50	C1	75	G
50	C1	76	U
50	C1	77	A
50	C1	78	C
50	C1	79	A
50	C1	80	G
50	C1	81	U
50	C1	82	G
50	C1	83	A
50	C1	84	A
50	C1	87	U
50	C1	98	C
50	C1	99	A
50	C1	101	U
50	C1	103	A
50	C1	104	A
50	C1	105	U
50	C1	106	C
50	C1	109	U
50	C1	110	U
50	C1	111	A
50	C1	112	U
50	C1	113	G
50	C1	114	G
50	C1	115	U
50	C1	116	U
50	C1	117	C
50	C1	118	C
50	C1	120	U
50	C1	121	U
50	C1	122	G
50	C1	123	G
50	C1	124	U
50	C1	125	C
50	C1	126	G
50	C1	127	C
50	C1	128	U
50	C1	129	C
50	C1	130	G
50	C1	131	C
50	C1	132	U
50	C1	133	C

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Mol	Chain	Res	Type
50	C1	134	C
50	C1	135	U
50	C1	136	C
50	C1	137	U
50	C1	138	C
50	C1	139	C
50	C1	140	C
50	C1	141	A
50	C1	142	C
50	C1	143	U
50	C1	144	U
50	C1	145	G
50	C1	146	G
50	C1	147	A
50	C1	150	A
50	C1	151	C
50	C1	152	U
50	C1	153	G
50	C1	158	A
50	C1	160	U
50	C1	161	U
50	C1	162	C
50	C1	163	U
50	C1	164	A
50	C1	166	A
50	C1	167	G
50	C1	168	C
50	C1	169	U
50	C1	171	A
50	C1	173	A
50	C1	174	C
50	C1	176	U
50	C1	179	C
50	C1	180	G
50	C1	181	A
50	C1	182	C
50	C1	183	G
50	C1	184	G
50	C1	185	G
50	C1	187	G
50	C1	193	C
50	C1	198	U

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Mol	Chain	Res	Type
50	C1	199	C
50	C1	200	G
50	C1	201	C
50	C1	202	G
50	C1	204	G
50	C1	205	G
50	C1	207	G
50	C1	208	G
50	C1	209	A
50	C1	210	U
50	C1	211	G
50	C1	213	G
50	C1	214	U
50	C1	215	G
50	C1	216	C
50	C1	217	A
50	C1	218	U
50	C1	219	U
50	C1	220	U
50	C1	225	G
50	C1	226	A
50	C1	227	U
50	C1	228	C
50	C1	229	A
50	C1	230	A
50	C1	233	C
50	C1	234	C
50	C1	235	A
50	C1	236	A
50	C1	237	C
50	C1	238	C
50	C1	239	C
50	C1	298	G
50	C1	301	A
50	C1	303	C
50	C1	304	C
50	C1	305	U
50	C1	306	C
50	C1	307	G
50	C1	308	G
50	C1	309	G
50	C1	310	C

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Mol	Chain	Res	Type
50	C1	311	C
50	C1	312	G
50	C1	313	A
50	C1	314	U
50	C1	315	C
50	C1	317	C
50	C1	318	A
50	C1	319	C
50	C1	320	G
50	C1	321	C
50	C1	327	G
50	C1	328	U
50	C1	329	G
50	C1	330	G
50	C1	332	G
50	C1	333	G
50	C1	337	C
50	C1	338	G
50	C1	339	A
50	C1	343	A
50	C1	344	U
50	C1	345	U
50	C1	346	C
50	C1	347	G
50	C1	350	C
50	C1	352	U
50	C1	353	C
50	C1	354	U
50	C1	356	C
50	C1	357	C
50	C1	358	C
50	C1	359	U
50	C1	362	C
50	C1	363	A
50	C1	364	A
50	C1	368	U
50	C1	369	C
50	C1	371	A
50	C1	372	U
50	C1	375	U
50	C1	376	A
50	C1	378	U

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Mol	Chain	Res	Type
50	C1	379	C
50	C1	380	G
50	C1	381	C
50	C1	382	C
50	C1	383	G
50	C1	384	U
50	C1	386	C
50	C1	389	A
50	C1	395	G
50	C1	399	C
50	C1	400	C
50	C1	407	G
50	C1	408	A
50	C1	409	C
50	C1	410	G
50	C1	412	G
50	C1	416	U
50	C1	421	G
50	C1	422	U
50	C1	423	U
50	C1	424	C
50	C1	426	A
50	C1	427	U
50	C1	429	C
50	C1	431	G
50	C1	433	A
50	C1	435	A
50	C1	436	G
50	C1	438	G
50	C1	440	G
50	C1	441	C
50	C1	442	C
50	C1	443	U
50	C1	445	A
50	C1	447	A
50	C1	448	A
50	C1	449	A
50	C1	450	C
50	C1	451	G
50	C1	452	G
50	C1	454	U
50	C1	459	C

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Mol	Chain	Res	Type
50	C1	460	A
50	C1	463	C
50	C1	464	A
50	C1	465	A
50	C1	466	G
50	C1	467	G
50	C1	468	A
50	C1	472	C
50	C1	473	A
50	C1	474	G
50	C1	475	C
50	C1	476	A
50	C1	477	G
50	C1	480	G
50	C1	482	G
50	C1	485	A
50	C1	487	U
50	C1	488	U
50	C1	489	A
50	C1	491	C
50	C1	492	C
50	C1	493	A
50	C1	495	U
50	C1	496	C
50	C1	497	C
50	C1	499	G
50	C1	500	A
50	C1	501	C
50	C1	502	C
50	C1	503	C
50	C1	504	G
50	C1	506	G
50	C1	507	G
50	C1	509	G
50	C1	510	G
50	C1	512	A
50	C1	516	A
50	C1	517	C
50	C1	518	G
50	C1	523	A
50	C1	525	A
50	C1	526	A

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Mol	Chain	Res	Type
50	C1	527	C
50	C1	529	A
50	C1	530	U
50	C1	533	A
50	C1	535	G
50	C1	536	A
50	C1	537	C
50	C1	538	U
50	C1	539	C
50	C1	541	U
50	C1	542	U
50	C1	543	C
50	C1	544	G
50	C1	545	A
50	C1	546	G
50	C1	547	G
50	C1	548	C
50	C1	549	C
50	C1	550	C
50	C1	553	U
50	C1	554	A
50	C1	555	A
50	C1	559	G
50	C1	560	A
50	C1	562	U
50	C1	564	A
50	C1	565	G
50	C1	566	U
50	C1	568	C
50	C1	570	C
50	C1	571	U
50	C1	572	U
50	C1	573	U
50	C1	574	A
50	C1	575	A
50	C1	576	A
50	C1	577	U
50	C1	578	C
50	C1	579	C
50	C1	580	U
50	C1	582	U
50	C1	586	G

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Mol	Chain	Res	Type
50	C1	587	A
50	C1	588	G
50	C1	589	G
50	C1	590	A
50	C1	591	U
50	C1	592	C
50	C1	593	C
50	C1	594	A
50	C1	595	U
50	C1	596	U
50	C1	597	G
50	C1	599	A
50	C1	600	G
50	C1	603	C
50	C1	604	A
50	C1	605	A
50	C1	606	G
50	C1	607	U
50	C1	608	C
50	C1	609	U
50	C1	612	U
50	C1	613	G
50	C1	614	C
50	C1	617	G
50	C1	619	A
50	C1	620	G
50	C1	621	C
50	C1	623	G
50	C1	624	C
50	C1	627	U
50	C1	628	A
50	C1	629	A
50	C1	630	U
50	C1	631	U
50	C1	634	A
50	C1	638	C
50	C1	643	A
50	C1	644	G
50	C1	645	C
50	C1	647	U
50	C1	648	A
50	C1	650	A

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Mol	Chain	Res	Type
50	C1	651	U
50	C1	652	U
50	C1	654	A
50	C1	655	A
50	C1	656	G
50	C1	657	U
50	C1	658	U
50	C1	659	G
50	C1	660	C
50	C1	661	U
50	C1	663	C
50	C1	664	A
50	C1	665	G
50	C1	666	U
50	C1	668	A
50	C1	669	A
50	C1	671	A
50	C1	672	A
50	C1	673	G
50	C1	674	C
50	C1	675	U
50	C1	676	C
50	C1	677	G
50	C1	679	A
50	C1	680	G
50	C1	681	U
50	C1	683	G
50	C1	684	G
50	C1	686	U
50	C1	688	U
50	C1	689	U
50	C1	692	G
50	C1	694	G
50	C1	695	C
50	C1	742	U
50	C1	743	U
50	C1	744	G
50	C1	745	C
50	C1	746	C
50	C1	747	U
50	C1	748	C
50	C1	749	U

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Mol	Chain	Res	Type
50	C1	750	C
50	C1	754	G
50	C1	755	C
50	C1	793	G
50	C1	795	A
50	C1	796	G
50	C1	797	C
50	C1	798	G
50	C1	799	U
50	C1	800	U
50	C1	801	U
50	C1	802	A
50	C1	803	C
50	C1	804	U
50	C1	807	G
50	C1	810	A
50	C1	812	A
50	C1	815	U
50	C1	816	A
50	C1	818	A
50	C1	819	G
50	C1	820	U
50	C1	821	G
50	C1	822	U
50	C1	823	U
50	C1	825	A
50	C1	827	A
50	C1	829	C
50	C1	830	A
50	C1	831	G
50	C1	834	C
50	C1	835	C
50	C1	837	A
50	C1	838	G
50	C1	839	C
50	C1	840	C
50	C1	841	G
50	C1	842	C
50	C1	844	U
50	C1	845	G
50	C1	847	A
50	C1	848	U

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Mol	Chain	Res	Type
50	C1	851	C
50	C1	852	G
50	C1	856	C
50	C1	861	A
50	C1	862	A
50	C1	863	U
50	C1	865	A
50	C1	869	A
50	C1	870	A
50	C1	873	G
50	C1	874	G
50	C1	875	A
50	C1	876	C
50	C1	886	A
50	C1	887	U
50	C1	888	U
50	C1	889	U
50	C1	890	U
50	C1	891	G
50	C1	896	U
50	C1	897	U
50	C1	898	U
50	C1	899	U
50	C1	900	C
50	C1	911	C
50	C1	912	C
50	C1	913	A
50	C1	914	U
50	C1	915	G
50	C1	917	U
50	C1	918	U
50	C1	919	A
50	C1	920	A
50	C1	921	G
50	C1	924	G
50	C1	930	C
50	C1	933	G
50	C1	937	C
50	C1	938	A
50	C1	942	G
50	C1	943	U
50	C1	946	U

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Mol	Chain	Res	Type
50	C1	950	C
50	C1	951	C
50	C1	953	C
50	C1	955	A
50	C1	956	G
50	C1	957	A
50	C1	958	G
50	C1	959	G
50	C1	960	U
50	C1	961	G
50	C1	962	A
50	C1	963	A
50	C1	966	U
50	C1	967	C
50	C1	968	U
50	C1	969	U
50	C1	970	G
50	C1	971	G
50	C1	972	A
50	C1	975	G
50	C1	977	C
50	C1	979	C
50	C1	980	A
50	C1	984	C
50	C1	985	G
50	C1	988	C
50	C1	990	A
50	C1	991	G
50	C1	995	G
50	C1	999	G
50	C1	1000	C
50	C1	1004	U
50	C1	1006	C
50	C1	1007	C
50	C1	1009	A
50	C1	1011	A
50	C1	1015	U
50	C1	1016	U
50	C1	1017	U
50	C1	1018	U
50	C1	1019	C
50	C1	1020	A

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Mol	Chain	Res	Type
50	C1	1021	U
50	C1	1022	U
50	C1	1023	A
50	C1	1024	A
50	C1	1029	G
50	C1	1033	G
50	C1	1034	A
50	C1	1035	A
50	C1	1036	A
50	C1	1040	G
50	C1	1044	G
50	C1	1045	U
50	C1	1049	A
50	C1	1050	A
50	C1	1051	G
50	C1	1052	A
50	C1	1053	C
50	C1	1055	A
50	C1	1057	C
50	C1	1058	A
50	C1	1060	A
50	C1	1061	U
50	C1	1062	A
50	C1	1064	C
50	C1	1065	G
50	C1	1067	C
50	C1	1076	G
50	C1	1083	A
50	C1	1084	A
50	C1	1085	C
50	C1	1086	G
50	C1	1087	A
50	C1	1088	U
50	C1	1089	G
50	C1	1090	C
50	C1	1096	G
50	C1	1097	G
50	C1	1101	U
50	C1	1104	G
50	C1	1108	G
50	C1	1109	C
50	C1	1110	G

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Mol	Chain	Res	Type
50	C1	1112	U
50	C1	1115	U
50	C1	1116	C
50	C1	1117	C
50	C1	1118	C
50	C1	1120	U
50	C1	1121	G
50	C1	1124	C
50	C1	1131	G
50	C1	1132	C
50	C1	1133	A
50	C1	1136	U
50	C1	1137	U
50	C1	1139	C
50	C1	1140	G
50	C1	1141	G
50	C1	1143	A
50	C1	1144	A
50	C1	1147	C
50	C1	1148	A
50	C1	1149	A
50	C1	1150	A
50	C1	1151	G
50	C1	1153	C
50	C1	1154	U
50	C1	1155	U
50	C1	1157	G
50	C1	1158	G
50	C1	1161	U
50	C1	1163	C
50	C1	1164	G
50	C1	1165	G
50	C1	1166	G
50	C1	1169	G
50	C1	1170	A
50	C1	1171	G
50	C1	1176	G
50	C1	1182	A
50	C1	1183	A
50	C1	1186	U
50	C1	1189	A
50	C1	1194	A

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Mol	Chain	Res	Type
50	C1	1195	A
50	C1	1198	G
50	C1	1199	A
50	C1	1200	A
50	C1	1203	G
50	C1	1205	C
50	C1	1206	G
50	C1	1207	G
50	C1	1215	C
50	C1	1216	C
50	C1	1217	A
50	C1	1218	C
50	C1	1219	C
50	C1	1221	G
50	C1	1223	A
50	C1	1224	G
50	C1	1235	G
50	C1	1236	G
50	C1	1237	C
50	C1	1242	U
50	C1	1243	U
50	C1	1245	G
50	C1	1246	A
50	C1	1247	C
50	C1	1248	U
50	C1	1249	C
50	C1	1251	A
50	C1	1253	A
50	C1	1254	C
50	C1	1255	G
50	C1	1256	G
50	C1	1257	G
50	C1	1258	A
50	C1	1259	A
50	C1	1260	A
50	C1	1261	C
50	C1	1262	C
50	C1	1263	U
50	C1	1264	C
50	C1	1265	A
50	C1	1266	C
50	C1	1267	C

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Mol	Chain	Res	Type
50	C1	1268	C
50	C1	1269	G
50	C1	1270	G
50	C1	1273	C
50	C1	1274	G
50	C1	1275	G
50	C1	1276	A
50	C1	1277	C
50	C1	1278	A
50	C1	1279	C
50	C1	1282	A
50	C1	1284	A
50	C1	1285	G
50	C1	1286	G
50	C1	1287	A
50	C1	1288	U
50	C1	1289	U
50	C1	1297	U
50	C1	1300	U
50	C1	1301	A
50	C1	1302	G
50	C1	1303	C
50	C1	1307	U
50	C1	1308	U
50	C1	1310	U
50	C1	1311	C
50	C1	1312	G
50	C1	1313	A
50	C1	1314	U
50	C1	1315	U
50	C1	1317	C
50	C1	1318	G
50	C1	1323	U
50	C1	1324	G
50	C1	1325	G
50	C1	1326	U
50	C1	1327	G
50	C1	1330	G
50	C1	1331	C
50	C1	1332	A
50	C1	1333	U
50	C1	1335	G

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Mol	Chain	Res	Type
50	C1	1343	U
50	C1	1344	A
50	C1	1345	G
50	C1	1347	U
50	C1	1349	G
50	C1	1351	G
50	C1	1352	G
50	C1	1354	G
50	C1	1357	A
50	C1	1358	U
50	C1	1359	U
50	C1	1360	U
50	C1	1363	C
50	C1	1364	U
50	C1	1368	U
50	C1	1369	A
50	C1	1371	U
50	C1	1372	U
50	C1	1378	A
50	C1	1381	G
50	C1	1382	A
50	C1	1384	C
50	C1	1389	C
50	C1	1390	U
50	C1	1392	U
50	C1	1393	G
50	C1	1394	G
50	C1	1395	C
50	C1	1397	U
50	C1	1399	C
50	C1	1401	A
50	C1	1402	A
50	C1	1403	C
50	C1	1404	U
50	C1	1405	A
50	C1	1406	G
50	C1	1407	U
50	C1	1408	U
50	C1	1409	A
50	C1	1410	C
50	C1	1411	G
50	C1	1412	C

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Mol	Chain	Res	Type
50	C1	1413	G
50	C1	1415	C
50	C1	1416	C
50	C1	1417	C
50	C1	1419	C
50	C1	1420	G
50	C1	1421	A
50	C1	1422	G
50	C1	1423	C
50	C1	1424	G
50	C1	1425	G
50	C1	1426	U
50	C1	1427	C
50	C1	1428	G
50	C1	1429	G
50	C1	1430	C
50	C1	1431	G
50	C1	1432	U
50	C1	1433	C
50	C1	1434	C
50	C1	1435	C
50	C1	1436	C
50	C1	1437	C
50	C1	1438	A
50	C1	1440	C
50	C1	1441	U
50	C1	1442	U
50	C1	1443	C
50	C1	1444	U
50	C1	1445	U
50	C1	1446	A
50	C1	1447	G
50	C1	1448	A
50	C1	1451	G
50	C1	1453	C
50	C1	1454	A
50	C1	1455	A
50	C1	1456	G
50	C1	1457	U
50	C1	1461	G
50	C1	1462	U
50	C1	1463	U

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Mol	Chain	Res	Type
50	C1	1464	C
50	C1	1465	A
50	C1	1466	G
50	C1	1467	C
50	C1	1471	C
50	C1	1472	C
50	C1	1473	G
50	C1	1475	G
50	C1	1476	A
50	C1	1477	U
50	C1	1478	U
50	C1	1480	A
50	C1	1481	G
50	C1	1482	C
50	C1	1484	A
50	C1	1486	A
50	C1	1489	A
50	C1	1490	G
50	C1	1493	C
50	C1	1494	U
50	C1	1495	G
50	C1	1496	U
50	C1	1498	A
50	C1	1500	G
50	C1	1505	U
50	C1	1507	G
50	C1	1508	A
50	C1	1509	U
50	C1	1510	G
50	C1	1511	U
50	C1	1513	C
50	C1	1514	G
50	C1	1517	G
50	C1	1520	G
50	C1	1521	C
50	C1	1522	A
50	C1	1523	C
50	C1	1528	G
50	C1	1529	C
50	C1	1530	U
50	C1	1531	A
50	C1	1535	U

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Mol	Chain	Res	Type
50	C1	1536	G
50	C1	1539	U
50	C1	1540	G
50	C1	1541	G
50	C1	1542	C
50	C1	1543	U
50	C1	1544	C
50	C1	1545	A
50	C1	1546	G
50	C1	1547	C
50	C1	1548	G
50	C1	1549	U
50	C1	1550	G
50	C1	1551	U
50	C1	1553	C
50	C1	1554	C
50	C1	1555	U
50	C1	1556	A
50	C1	1557	C
50	C1	1558	C
50	C1	1560	U
50	C1	1561	A
50	C1	1563	G
50	C1	1568	C
50	C1	1569	A
50	C1	1570	G
50	C1	1573	G
50	C1	1574	C
50	C1	1577	G
50	C1	1578	U
50	C1	1579	A
50	C1	1580	A
50	C1	1581	C
50	C1	1582	C
50	C1	1585	U
50	C1	1586	U
50	C1	1587	G
50	C1	1588	A
50	C1	1589	A
50	C1	1591	C
50	C1	1595	U
50	C1	1597	C

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Mol	Chain	Res	Type
50	C1	1598	G
50	C1	1599	U
50	C1	1600	G
50	C1	1601	A
50	C1	1602	U
50	C1	1603	G
50	C1	1604	G
50	C1	1605	G
50	C1	1607	A
50	C1	1609	C
50	C1	1610	G
50	C1	1612	G
50	C1	1614	A
50	C1	1615	U
50	C1	1617	G
50	C1	1618	C
50	C1	1620	A
50	C1	1621	U
50	C1	1622	U
50	C1	1623	A
50	C1	1624	U
50	C1	1625	U
50	C1	1627	C
50	C1	1631	U
50	C1	1632	G
50	C1	1635	C
50	C1	1636	G
50	C1	1637	A
50	C1	1638	G
50	C1	1639	G
50	C1	1640	A
50	C1	1644	C
50	C1	1645	C
50	C1	1647	A
50	C1	1648	G
50	C1	1649	U
50	C1	1651	A
50	C1	1652	G
50	C1	1654	G
50	C1	1655	C
50	C1	1656	G
50	C1	1660	C

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Mol	Chain	Res	Type
50	C1	1661	A
50	C1	1662	U
50	C1	1664	A
50	C1	1665	G
50	C1	1666	C
50	C1	1669	G
50	C1	1671	G
50	C1	1672	U
50	C1	1673	U
50	C1	1674	G
50	C1	1677	U
50	C1	1678	A
50	C1	1679	A
50	C1	1680	G
50	C1	1682	C
50	C1	1684	C
50	C1	1685	U
50	C1	1686	G
50	C1	1687	C
50	C1	1688	C
50	C1	1689	C
50	C1	1691	U
50	C1	1692	U
50	C1	1694	U
50	C1	1696	C
50	C1	1697	A
50	C1	1698	C
50	C1	1699	A
50	C1	1700	C
50	C1	1701	C
50	C1	1702	G
50	C1	1703	C
50	C1	1707	U
50	C1	1708	C
50	C1	1709	G
50	C1	1710	C
50	C1	1714	U
50	C1	1719	A
50	C1	1720	U
50	C1	1721	U
50	C1	1722	G
50	C1	1723	G

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Mol	Chain	Res	Type
50	C1	1728	U
50	C1	1729	U
50	C1	1731	A
50	C1	1732	G
50	C1	1735	A
50	C1	1744	G
50	C1	1745	A
50	C1	1747	C
50	C1	1749	G
50	C1	1751	C
50	C1	1752	C
50	C1	1760	G
50	C1	1761	U
50	C1	1764	G
50	C1	1765	C
50	C1	1767	C
50	C1	1768	A
50	C1	1770	G
50	C1	1775	U
50	C1	1781	A
50	C1	1782	G
50	C1	1783	C
50	C1	1788	A
50	C1	1789	G
50	C1	1790	A
50	C1	1792	G
50	C1	1794	C
50	C1	1798	C
50	C1	1800	A
50	C1	1809	A
50	C1	1811	C
50	C1	1813	A
50	C1	1817	G
50	C1	1819	A
50	C1	1823	A
50	C1	1824	A
50	C1	1825	A
50	C1	1826	G
50	C1	1827	U
50	C1	1829	G
50	C1	1831	A
50	C1	1832	A

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Mol	Chain	Res	Type
50	C1	1833	C
50	C1	1834	A
50	C1	1835	A
50	C1	1836	G
50	C1	1837	G
50	C1	1838	U
50	C1	1839	U
50	C1	1841	C
50	C1	1843	G
50	C1	1844	U
50	C1	1846	G
50	C1	1847	G
50	C1	1849	G
50	C1	1850	A
50	C1	1851	A
50	C1	1852	C
50	C1	1856	C
50	C1	1857	G
50	C1	1860	A
50	C1	1861	G
50	C1	1862	G
50	C1	1863	A
50	C1	1864	U
50	C1	1865	C
50	C1	1866	A
50	C1	1867	U
50	C1	1868	U
50	C1	1869	A

All (532) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	8	U
3	AC	83	C
3	AC	85	A
3	AC	95	U
3	AC	110	G
3	AC	119	A
3	AC	120	C
3	AC	126	C
3	AC	132	G
3	AC	133	G

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Mol	Chain	Res	Type
3	AC	140	A
3	AC	156	C
3	AC	158	G
3	AC	160	U
3	AC	161	G
3	AC	164	U
3	AC	167	A
3	AC	228	U
3	AC	230	G
3	AC	231	G
3	AC	232	C
3	AC	234	U
3	AC	252	A
3	AC	256	G
3	AC	257	A
3	AC	259	U
3	AC	265	U
3	AC	266	G
3	AC	271	G
3	AC	276	A
3	AC	284	U
3	AC	290	U
3	AC	291	G
3	AC	301	G
3	AC	305	U
3	AC	309	G
3	AC	323	G
3	AC	324	U
3	AC	344	G
3	AC	349	C
3	AC	350	G
4	A2	13	U
4	A2	14	C
4	A2	19	G
4	A2	48	G
4	A2	64	A
4	A2	69	A
4	A2	70	A
4	A2	96	U
4	A2	156	C
4	A2	181	U
4	A2	188	G

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Mol	Chain	Res	Type
4	A2	192	C
4	A2	193	C
4	A2	196	G
4	A2	207	C
4	A2	212	C
4	A2	215	A
4	A2	216	G
4	A2	221	U
4	A2	229	G
4	A2	266	C
4	A2	287	A
4	A2	292	G
4	A2	300	C
4	A2	328	U
4	A2	331	C
4	A2	333	G
4	A2	334	C
4	A2	342	C
4	A2	366	G
4	A2	371	U
4	A2	379	A
4	A2	381	C
4	A2	386	A
4	A2	398	A
4	A2	402	G
4	A2	424	A
4	A2	433	G
4	A2	441	G
4	A2	443	A
4	A2	444	G
4	A2	458	U
4	A2	459	U
4	A2	460	C
4	A2	461	A
4	A2	462	A
4	A2	473	G
4	A2	474	G
4	A2	477	C
4	A2	482	G
4	A2	633	G
4	A2	658	G
4	A2	717	G

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Mol	Chain	Res	Type
4	A2	718	G
4	A2	719	G
4	A2	720	A
4	A2	721	A
4	A2	727	G
4	A2	736	G
4	A2	897	U
4	A2	914	G
4	A2	916	A
4	A2	927	A
4	A2	928	A
4	A2	939	G
4	A2	941	G
4	A2	943	G
4	A2	944	A
4	A2	947	G
4	A2	957	G
4	A2	959	C
4	A2	967	C
4	A2	973	U
4	A2	974	C
4	A2	1082	U
4	A2	1147	C
4	A2	1177	C
4	A2	1193	G
4	A2	1196	C
4	A2	1197	G
4	A2	1204	G
4	A2	1205	U
4	A2	1207	C
4	A2	1208	U
4	A2	1209	C
4	A2	1211	C
4	A2	1216	C
4	A2	1217	C
4	A2	1218	A
4	A2	1219	C
4	A2	1249	G
4	A2	1280	G
4	A2	1282	U
4	A2	1293	C
4	A2	1299	U

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Mol	Chain	Res	Type
4	A2	1304	A
4	A2	1340	G
4	A2	1349	C
4	A2	1357	G
4	A2	1358	C
4	A2	1360	G
4	A2	1367	A
4	A2	1377	A
4	A2	1388	G
4	A2	1400	A
4	A2	1421	C
4	A2	1423	A
4	A2	1444	G
4	A2	1453	C
4	A2	1458	G
4	A2	1475	G
4	A2	1476	A
4	A2	1478	C
4	A2	1481	G
4	A2	1497	A
4	A2	1502	A
4	A2	1523	G
4	A2	1530	C
4	A2	1532	A
4	A2	1553	G
4	A2	1554	A
4	A2	1604	G
4	A2	1612	G
4	A2	1619	C
4	A2	1628	U
4	A2	1639	U
4	A2	1659	G
4	A2	1673	C
4	A2	1703	G
4	A2	1732	G
4	A2	1744	A
4	A2	1745	A
4	A2	1756	C
4	A2	1783	A
4	A2	1786	C
4	A2	1802	G
4	A2	1805	G

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Mol	Chain	Res	Type
4	A2	1836	A
4	A2	1846	A
4	A2	1855	G
4	A2	1859	C
4	A2	1860	U
4	A2	1868	G
4	A2	1870	A
4	A2	1874	A
4	A2	1883	U
4	A2	1885	A
4	A2	1900	G
4	A2	1916	C
4	A2	1918	G
4	A2	1924	G
4	A2	1930	G
4	A2	2000	C
4	A2	2003	A
4	A2	2006	C
4	A2	2009	C
4	A2	2011	A
4	A2	2023	G
4	A2	2024	G
4	A2	2034	G
4	A2	2046	C
4	A2	2048	U
4	A2	2270	G
4	A2	2294	G
4	A2	2309	G
4	A2	2310	G
4	A2	2324	A
4	A2	2333	U
4	A2	2347	A
4	A2	2348	U
4	A2	2358	A
4	A2	2360	C
4	A2	2369	C
4	A2	2371	G
4	A2	2373	A
4	A2	2375	U
4	A2	2394	A
4	A2	2395	A
4	A2	2396	C

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Mol	Chain	Res	Type
4	A2	2405	A
4	A2	2411	G
4	A2	2415	A
4	A2	2450	A
4	A2	2454	A
4	A2	2465	C
4	A2	2481	C
4	A2	2489	A
4	A2	2502	U
4	A2	2508	C
4	A2	2548	C
4	A2	2551	G
4	A2	2561	G
4	A2	2564	A
4	A2	2606	C
4	A2	2607	U
4	A2	2650	G
4	A2	2673	A
4	A2	2684	U
4	A2	2702	A
4	A2	2703	G
4	A2	2716	C
4	A2	2718	U
4	A2	2735	G
4	A2	2740	U
4	A2	2741	A
4	A2	2745	C
4	A2	2749	C
4	A2	2802	A
4	A2	2803	U
4	A2	2838	C
4	A2	3578	G
4	A2	3583	G
4	A2	3584	G
4	A2	3585	U
4	A2	3648	U
4	A2	3666	U
4	A2	3684	U
4	A2	3696	A
4	A2	3724	G
4	A2	3727	U
4	A2	3729	A

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Mol	Chain	Res	Type
4	A2	3733	U
4	A2	3743	A
4	A2	3753	A
4	A2	3754	A
4	A2	3769	A
4	A2	3770	U
4	A2	3802	C
4	A2	3821	A
4	A2	3845	A
4	A2	3865	C
4	A2	3866	G
4	A2	3873	G
4	A2	3876	G
4	A2	3887	G
4	A2	3907	G
4	A2	3926	U
4	A2	3933	U
4	A2	4017	U
4	A2	4033	G
4	A2	4043	U
4	A2	4044	G
4	A2	4081	C
4	A2	4083	C
4	A2	4084	U
4	A2	4085	U
4	A2	4088	G
4	A2	4091	G
4	A2	4105	C
4	A2	4117	A
4	A2	4122	C
4	A2	4130	A
4	A2	4155	G
4	A2	4181	C
4	A2	4211	A
4	A2	4226	G
4	A2	4236	G
4	A2	4252	A
4	A2	4254	C
4	A2	4292	C
4	A2	4336	A
4	A2	4338	A
4	A2	4354	A

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Mol	Chain	Res	Type
4	A2	4374	A
4	A2	4387	G
4	A2	4388	A
4	A2	4396	U
4	A2	4408	G
4	A2	4409	A
4	A2	4433	A
4	A2	4437	A
4	A2	4454	G
4	A2	4455	G
4	A2	4485	C
4	A2	4515	U
4	A2	4533	G
4	A2	4551	U
4	A2	4561	U
4	A2	4562	A
4	A2	4566	G
4	A2	4596	U
4	A2	4597	G
4	A2	4609	G
4	A2	4616	A
4	A2	4628	U
4	A2	4636	G
4	A2	4637	U
4	A2	4659	U
4	A2	4660	A
4	A2	4675	C
4	A2	4680	C
4	A2	4688	A
4	A2	4690	G
4	A2	4692	C
4	A2	4693	A
4	A2	4699	G
4	A2	4711	U
4	A2	4712	U
4	A2	4717	U
4	A2	4723	A
4	A2	4733	C
4	A2	4740	U
4	A2	4807	C
4	A2	4813	C
4	A2	4823	G

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Mol	Chain	Res	Type
4	A2	4824	U
4	A2	4825	G
4	A2	4827	G
4	A2	4837	U
4	A2	4847	A
4	A2	4848	A
4	A2	4849	A
4	A2	4854	G
4	A2	4862	G
4	A2	4867	G
4	A2	4895	C
4	A2	4930	G
4	A2	4943	U
4	A2	4944	U
4	A2	4977	U
4	A2	4978	C
4	A2	4980	C
4	A2	5002	C
4	A2	5004	G
4	A2	5019	G
5	A3	22	U
5	A3	71	A
5	A3	84	A
5	A3	105	C
5	A3	111	U
5	A3	125	C
6	A4	12	U
6	A4	26	C
6	A4	54	A
6	A4	63	C
6	A4	74	A
6	A4	75	G
6	A4	90	A
6	A4	108	G
6	A4	109	U
50	C1	24	C
50	C1	44	U
50	C1	61	A
50	C1	64	A
50	C1	66	G
50	C1	68	A
50	C1	77	A

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Mol	Chain	Res	Type
50	C1	78	C
50	C1	102	A
50	C1	111	A
50	C1	113	G
50	C1	124	U
50	C1	131	C
50	C1	136	C
50	C1	139	C
50	C1	140	C
50	C1	147	A
50	C1	162	C
50	C1	181	A
50	C1	183	G
50	C1	199	C
50	C1	200	G
50	C1	207	G
50	C1	209	A
50	C1	227	U
50	C1	304	C
50	C1	307	G
50	C1	308	G
50	C1	310	C
50	C1	312	G
50	C1	317	C
50	C1	319	C
50	C1	332	G
50	C1	338	G
50	C1	356	C
50	C1	363	A
50	C1	368	U
50	C1	370	G
50	C1	383	G
50	C1	399	C
50	C1	428	U
50	C1	448	A
50	C1	465	A
50	C1	475	C
50	C1	486	A
50	C1	487	U
50	C1	501	C
50	C1	544	G
50	C1	546	G

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Mol	Chain	Res	Type
50	C1	547	G
50	C1	558	G
50	C1	577	U
50	C1	578	C
50	C1	589	G
50	C1	590	A
50	C1	593	C
50	C1	604	A
50	C1	656	G
50	C1	662	G
50	C1	671	A
50	C1	687	C
50	C1	743	U
50	C1	799	U
50	C1	811	A
50	C1	821	G
50	C1	822	U
50	C1	833	C
50	C1	834	C
50	C1	840	C
50	C1	899	U
50	C1	913	A
50	C1	970	G
50	C1	971	G
50	C1	1015	U
50	C1	1016	U
50	C1	1020	A
50	C1	1021	U
50	C1	1043	G
50	C1	1060	A
50	C1	1088	U
50	C1	1108	G
50	C1	1114	U
50	C1	1115	U
50	C1	1138	C
50	C1	1150	A
50	C1	1164	G
50	C1	1198	G
50	C1	1215	C
50	C1	1242	U
50	C1	1247	C
50	C1	1250	A

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Mol	Chain	Res	Type
50	C1	1253	A
50	C1	1257	G
50	C1	1259	A
50	C1	1261	C
50	C1	1264	C
50	C1	1277	C
50	C1	1285	G
50	C1	1301	A
50	C1	1307	U
50	C1	1308	U
50	C1	1311	C
50	C1	1313	A
50	C1	1326	U
50	C1	1342	U
50	C1	1351	G
50	C1	1362	U
50	C1	1401	A
50	C1	1404	U
50	C1	1406	G
50	C1	1411	G
50	C1	1456	G
50	C1	1476	A
50	C1	1477	U
50	C1	1494	U
50	C1	1497	G
50	C1	1508	A
50	C1	1520	G
50	C1	1534	C
50	C1	1542	C
50	C1	1543	U
50	C1	1555	U
50	C1	1556	A
50	C1	1578	U
50	C1	1586	U
50	C1	1603	G
50	C1	1624	U
50	C1	1631	U
50	C1	1635	C
50	C1	1637	A
50	C1	1638	G
50	C1	1644	C
50	C1	1648	G

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Mol	Chain	Res	Type
50	C1	1654	G
50	C1	1655	C
50	C1	1673	U
50	C1	1697	A
50	C1	1698	C
50	C1	1700	C
50	C1	1721	U
50	C1	1781	A
50	C1	1823	A
50	C1	1824	A
50	C1	1830	U
50	C1	1833	C
50	C1	1834	A
50	C1	1836	G
50	C1	1848	U
50	C1	1860	A
50	C1	1862	G
50	C1	1867	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	GNP	AB	2434	85	29,34,34	2.16	8 (27%)	33,54,54	2.26	8 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	GNP	AB	2434	85	-	2/14/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	AB	2434	GNP	C2'-C1'	-6.47	1.43	1.53
84	AB	2434	GNP	C6-N1	5.33	1.42	1.33
84	AB	2434	GNP	C4-N3	2.90	1.40	1.35
84	AB	2434	GNP	PB-O3A	-2.62	1.55	1.59
84	AB	2434	GNP	PB-N3B	-2.48	1.56	1.63
84	AB	2434	GNP	C2-N1	2.41	1.39	1.35
84	AB	2434	GNP	C8-N7	-2.41	1.30	1.34
84	AB	2434	GNP	PG-N3B	-2.25	1.57	1.63

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	AB	2434	GNP	C5-C6-N1	-7.04	113.81	123.43
84	AB	2434	GNP	C2-N1-C6	5.18	124.16	115.93
84	AB	2434	GNP	N3-C2-N1	-3.57	122.46	127.22
84	AB	2434	GNP	O1B-PB-N3B	3.40	116.78	111.77
84	AB	2434	GNP	C4-C5-C6	-2.99	117.94	120.80
84	AB	2434	GNP	C1'-N9-C4	-2.75	121.81	126.64
84	AB	2434	GNP	O2G-PG-O1G	2.42	119.53	113.45
84	AB	2434	GNP	O3A-PB-N3B	2.21	112.71	106.59

There are no chirality outliers.

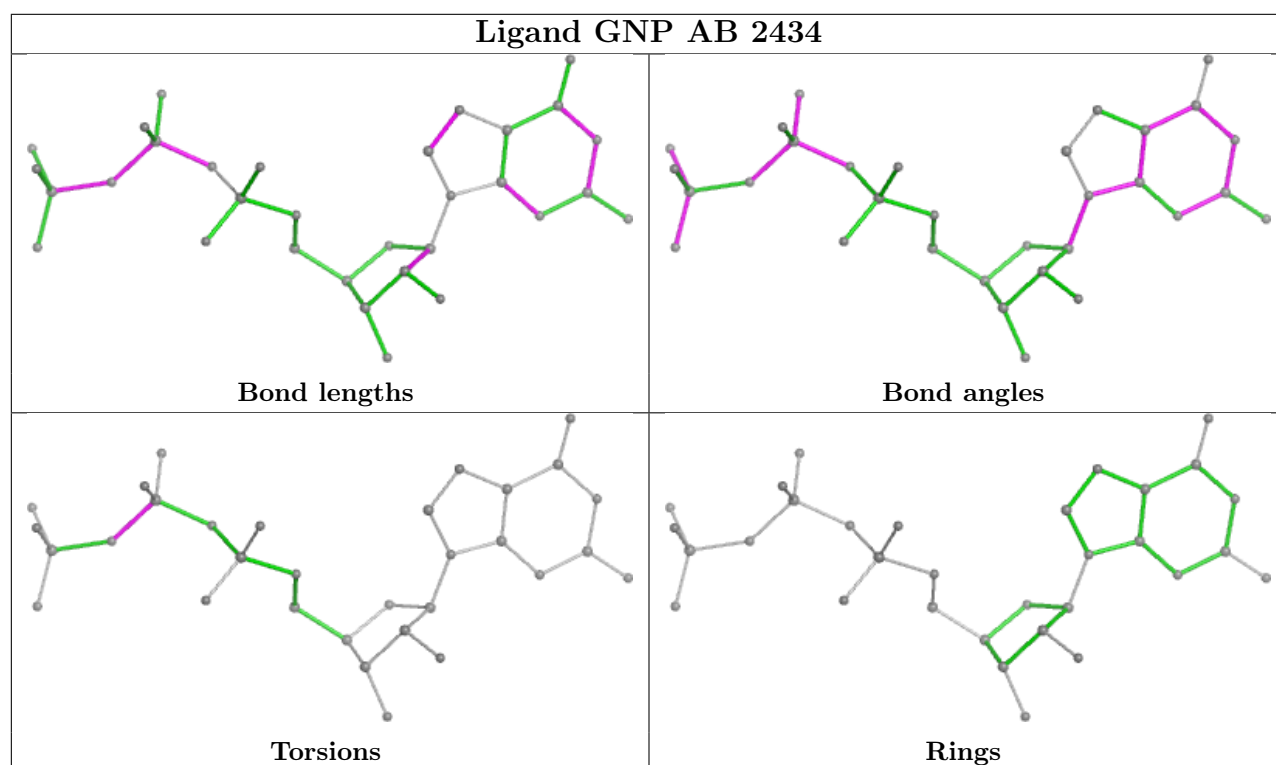
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
84	AB	2434	GNP	PG-N3B-PB-O1B
84	AB	2434	GNP	PG-N3B-PB-O3A

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

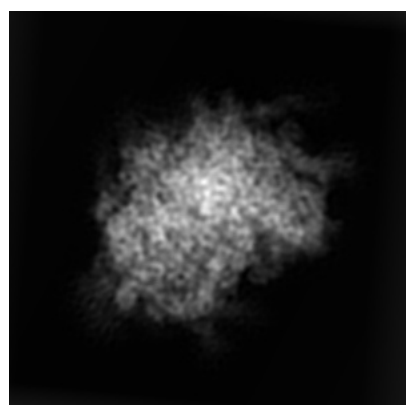
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2683. These allow visual inspection of the internal detail of the map and identification of artifacts.

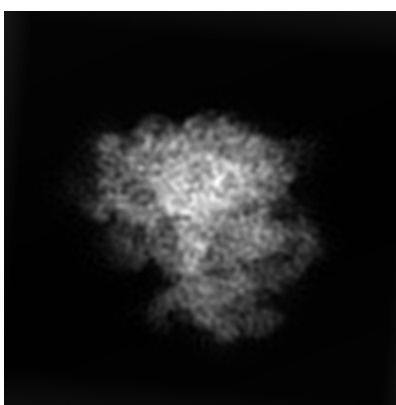
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

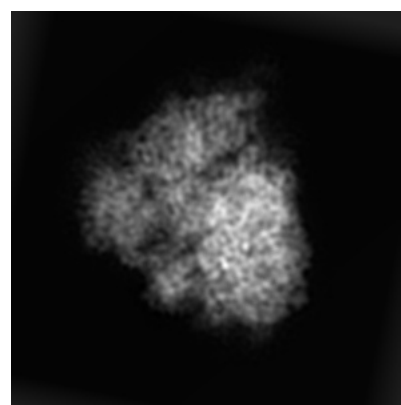
6.1.1 Primary map



X



Y

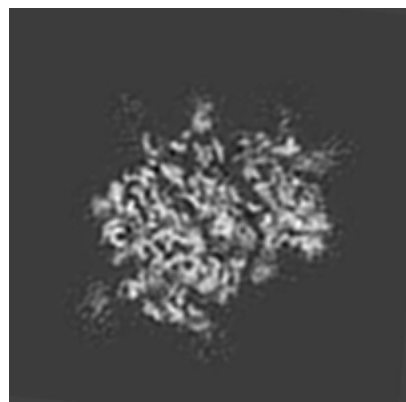


Z

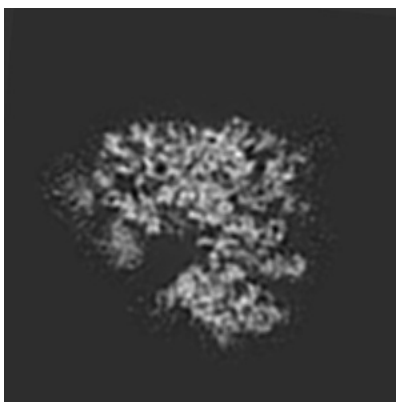
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

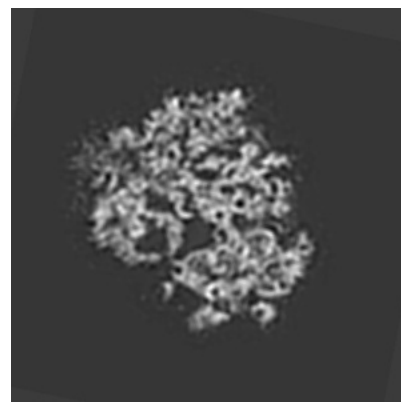
6.2.1 Primary map



X Index: 180



Y Index: 180

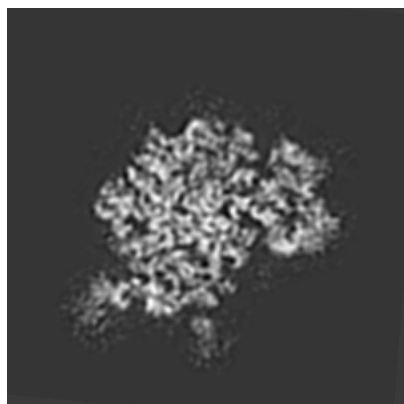


Z Index: 180

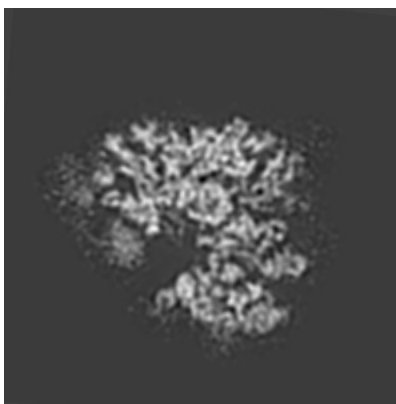
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

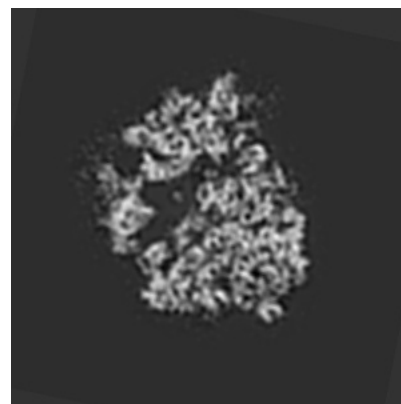
6.3.1 Primary map



X Index: 192



Y Index: 182

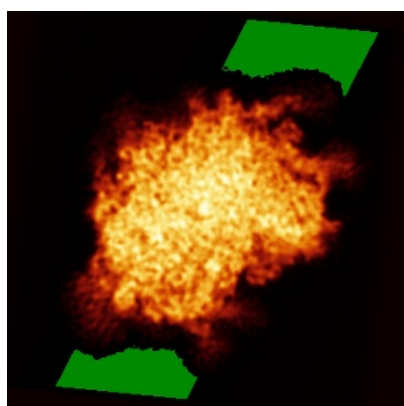


Z Index: 167

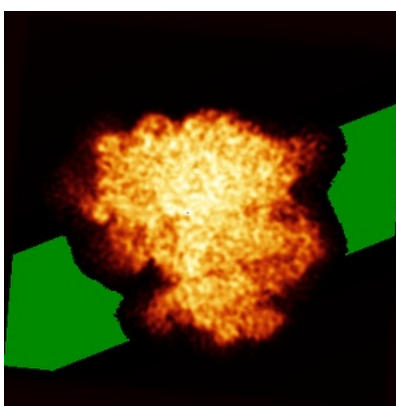
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

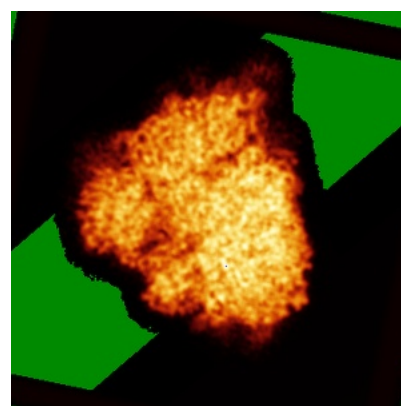
6.4.1 Primary map



X



Y

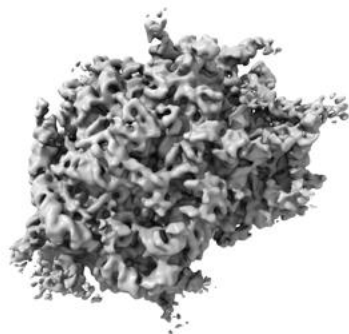


Z

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](#)

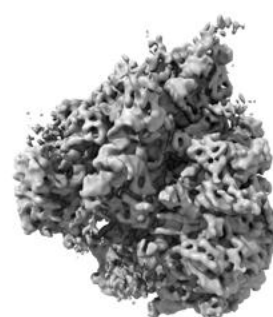
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2700.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

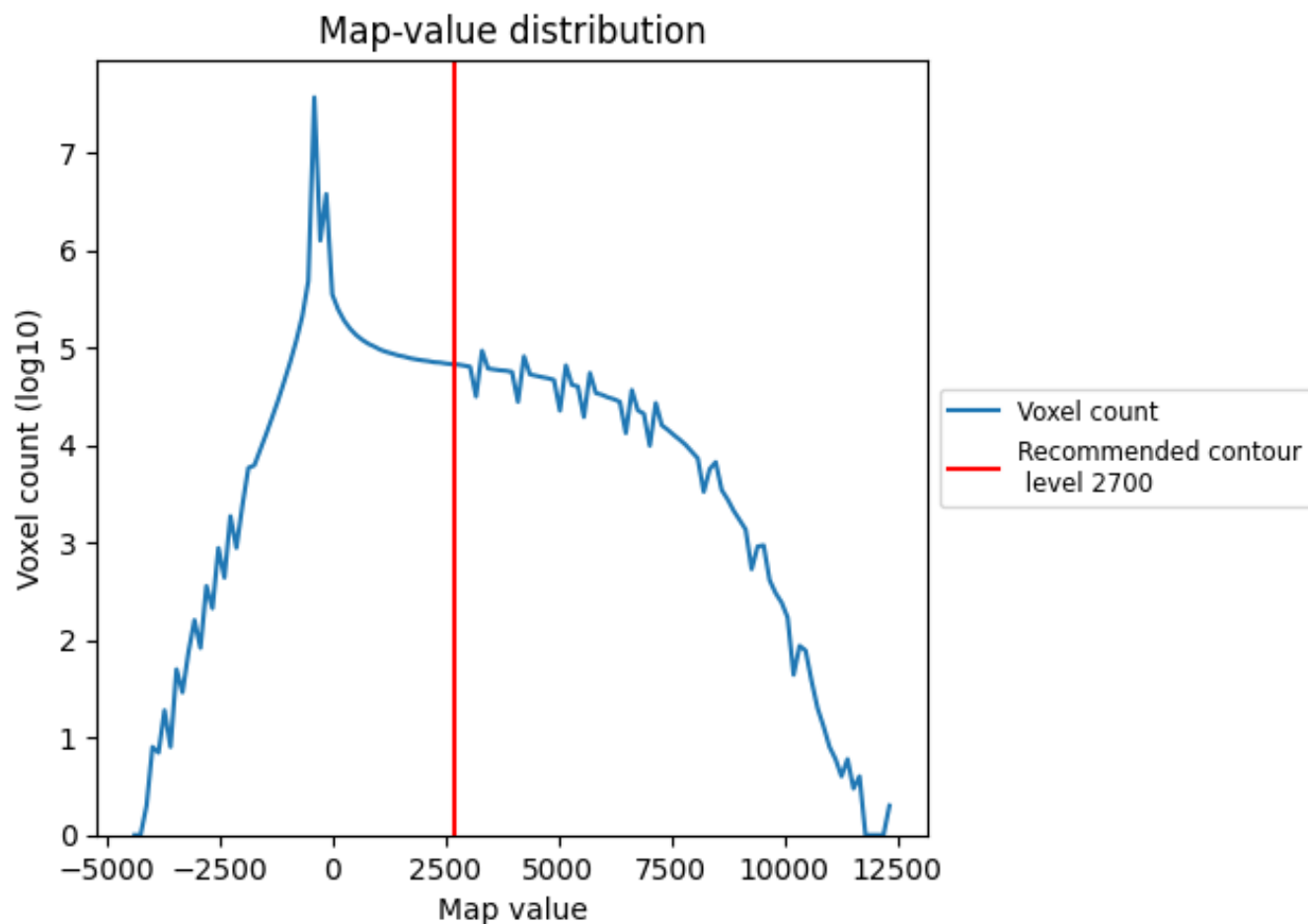
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

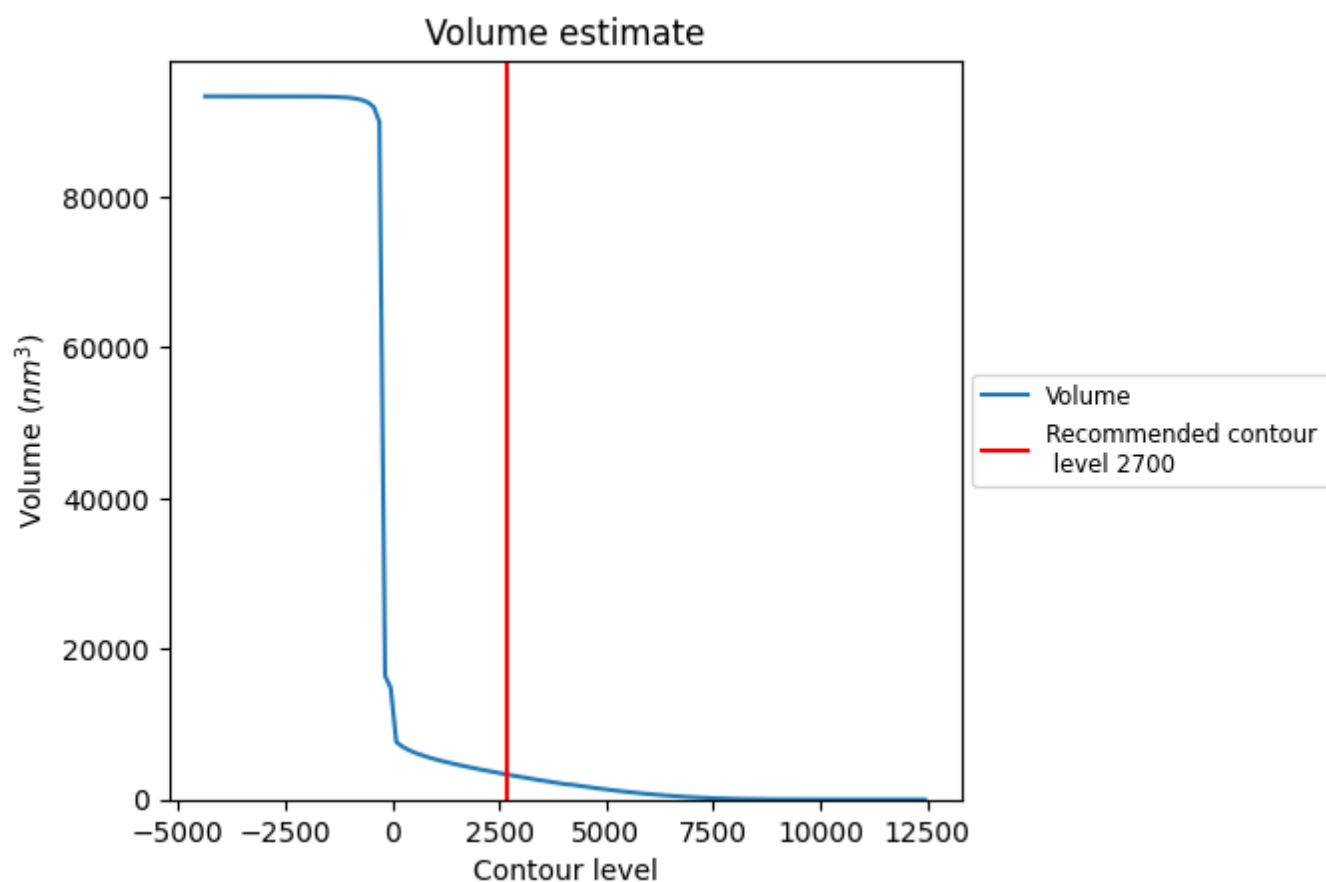
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

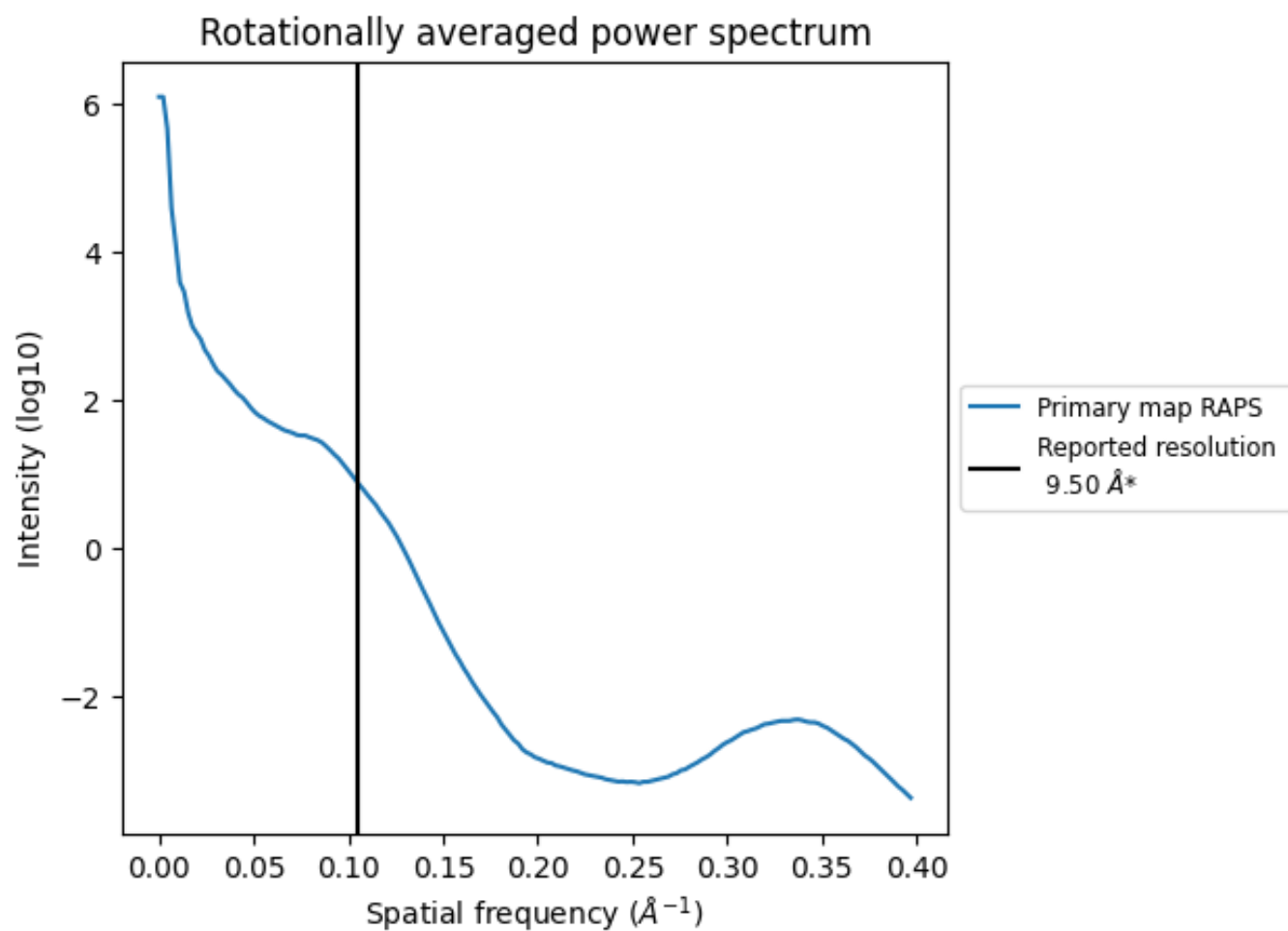
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3306 nm³; this corresponds to an approximate mass of 2986 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.105 Å⁻¹

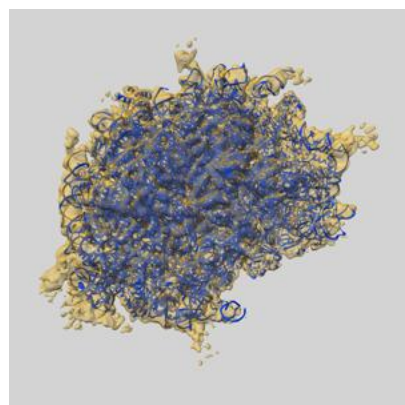
8 Fourier-Shell correlation

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

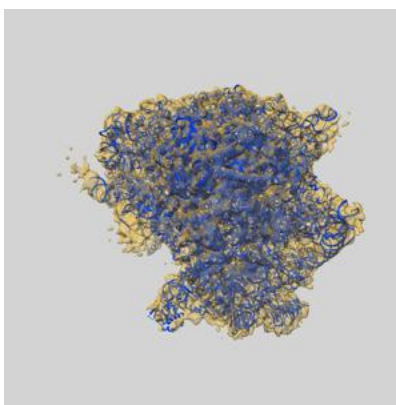
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2683 and PDB model 4UJC. Per-residue inclusion information can be found in [section 3](#) on [page 19](#).

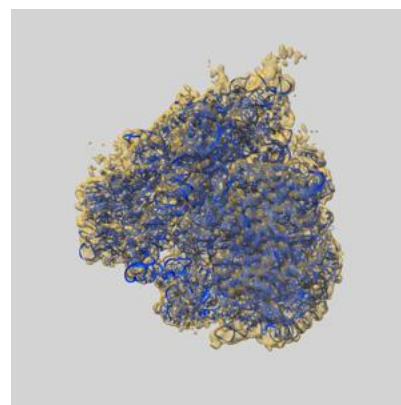
9.1 Map-model overlay [i](#)



X



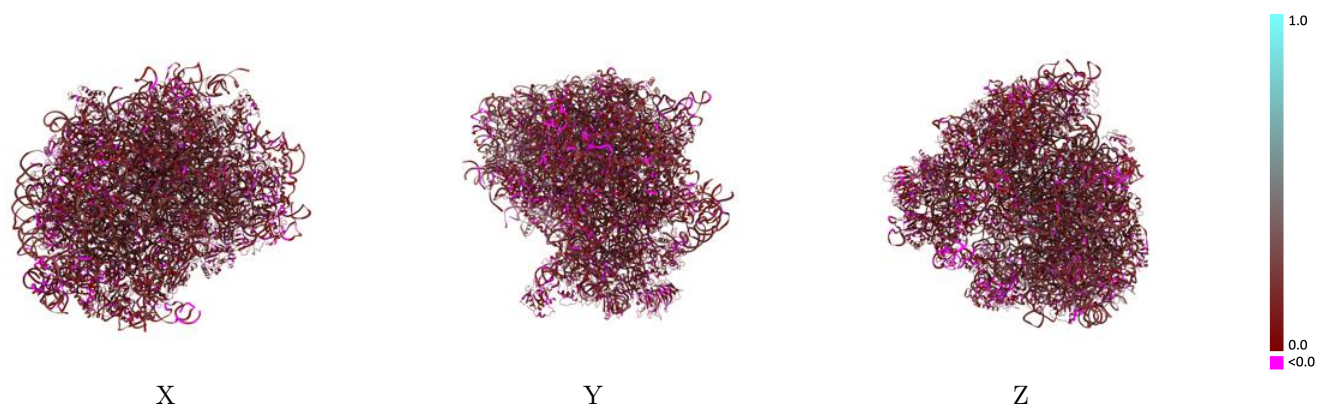
Y



Z

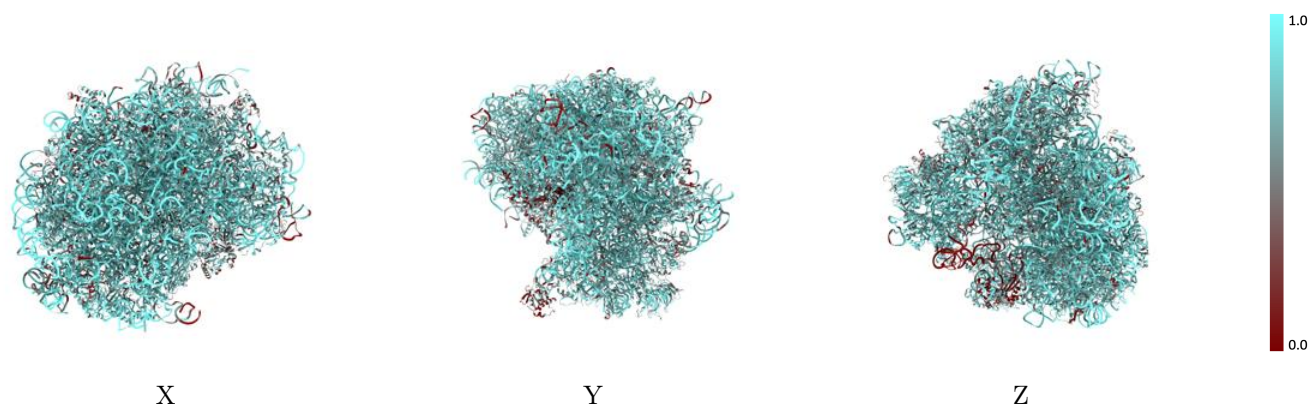
The images above show the 3D surface view of the map at the recommended contour level 2700.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



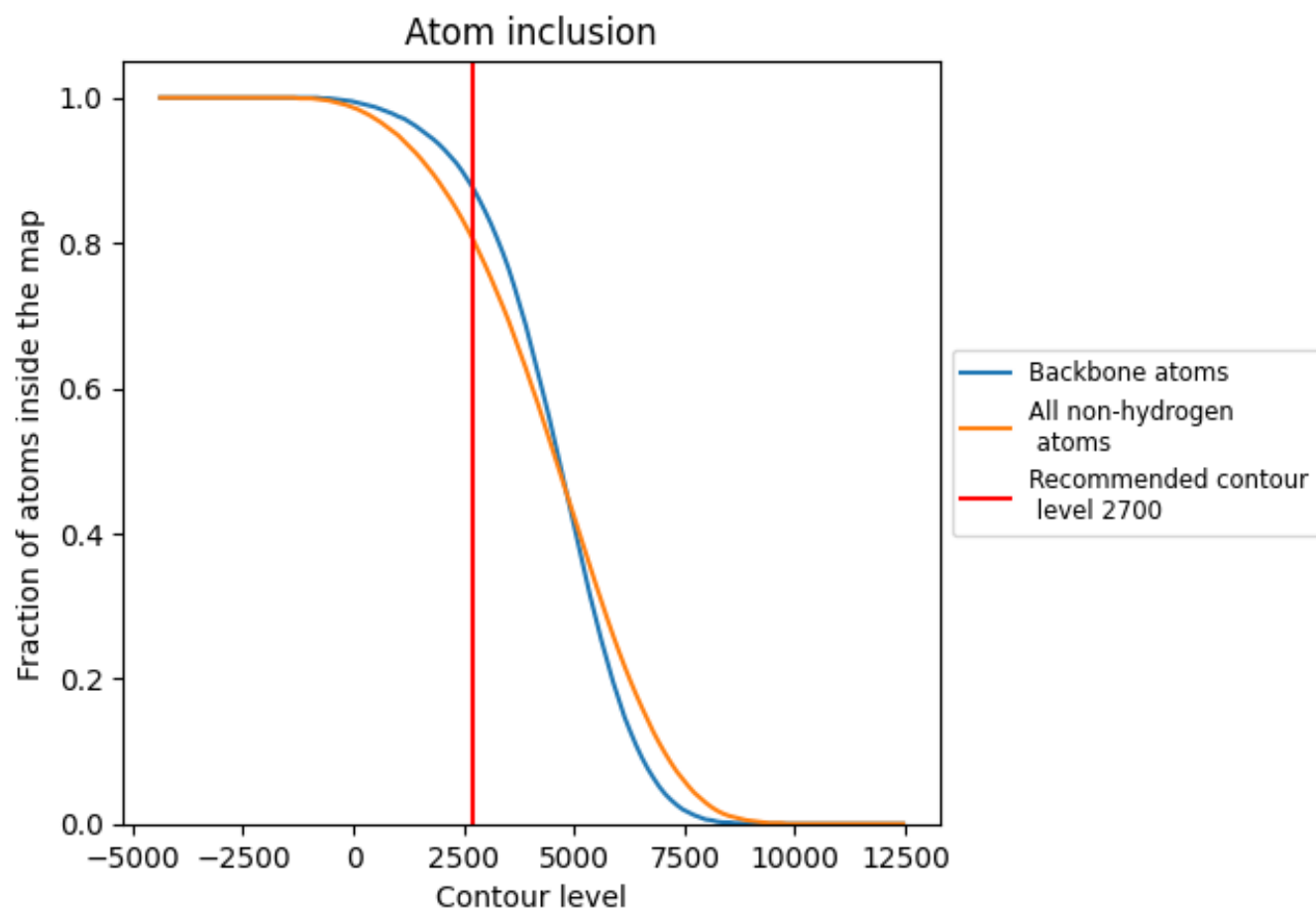
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2700).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 81% 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 (2700) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8060	 0.1400
A2	 0.9060	 0.1710
A3	 0.9320	 0.1780
A4	 0.9680	 0.1840
AA	 0.7430	 0.1320
AB	 0.3160	 0.0780
AC	 0.5430	 0.0940
BA	 0.6920	 0.1010
BB	 0.7540	 0.1020
BC	 0.7240	 0.0950
BD	 0.8020	 0.1160
BE	 0.6890	 0.1040
BF	 0.7250	 0.1010
BG	 0.6740	 0.1210
BH	 0.7570	 0.1210
BI	 0.7440	 0.1220
BJ	 0.7560	 0.0980
BL	 0.6860	 0.1040
BM	 0.8050	 0.1400
BN	 0.7750	 0.0860
BO	 0.7240	 0.1160
BP	 0.7990	 0.0960
BQ	 0.7080	 0.1120
BR	 0.7490	 0.1200
BS	 0.7280	 0.1100
BT	 0.7080	 0.1100
BU	 0.6070	 0.1230
BV	 0.6880	 0.1100
BW	 0.7880	 0.1160
BX	 0.7170	 0.1160
BY	 0.7960	 0.1030
BZ	 0.7170	 0.1140
Ba	 0.7360	 0.0960
Bb	 0.7130	 0.1000
Bc	 0.7190	 0.1300

















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Chain	Atom inclusion	Q-score
Bd	 0.7670	 0.1100
Be	 0.7450	 0.1190
Bf	 0.7440	 0.0770
Bg	 0.7090	 0.0940
Bh	 0.7430	 0.1200
Bi	 0.7420	 0.1290
Bj	 0.8140	 0.0930
Bk	 0.6930	 0.1150
Bl	 0.7590	 0.1200
Bm	 0.8240	 0.1110
Bn	 0.7310	 0.1120
Bo	 0.6940	 0.1080
Bp	 0.6930	 0.1200
Bt	 0.7010	 0.0830
Bu	 0.0870	 0.0300
C1	 0.9070	 0.1630
CA	 0.7260	 0.1290
CB	 0.7160	 0.1370
CC	 0.7200	 0.1190
CD	 0.6710	 0.1230
CE	 0.7520	 0.1130
CF	 0.7560	 0.1170
CG	 0.7610	 0.0990
CH	 0.5940	 0.1170
CI	 0.7240	 0.0950
CJ	 0.7500	 0.1110
CK	 0.7220	 0.0950
CL	 0.6920	 0.1140
CM	 0.3020	 0.0620
CN	 0.6650	 0.1120
CO	 0.7080	 0.1080
CP	 0.7370	 0.1200
CQ	 0.7570	 0.0990
CR	 0.6400	 0.1030
CS	 0.7330	 0.1030
CT	 0.8030	 0.1020
CU	 0.6780	 0.1020
CV	 0.7120	 0.1300
CW	 0.7350	 0.1170
CX	 0.7330	 0.1230
CY	 0.7880	 0.1010
CZ	 0.7150	 0.1280

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Chain	Atom inclusion	Q-score
Ca	 0.5990	 0.0860
Cb	 0.6720	 0.1070
Cc	 0.6680	 0.1080
Cd	 0.8150	 0.0830
Ce	 0.7050	 0.1180
Cf	 0.3500	 0.0560
Cg	 0.7470	 0.1030