



## Full wwPDB EM Validation Report ⓘ

Oct 22, 2024 – 02:19 PM EDT

PDB ID : 3JAJ  
EMDB ID : EMD-3037  
Title : Structure of the engaged state of the mammalian SRP-ribosome complex  
Authors : Voorhees, R.M.; Hegde, R.S.  
Deposited on : 2015-06-16  
Resolution : 3.75 Å(reported)  
Based on initial models : 1QB2, 1WGW, 1E8S, 4P3E, 3J7P, 3J7O, 1E80

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

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

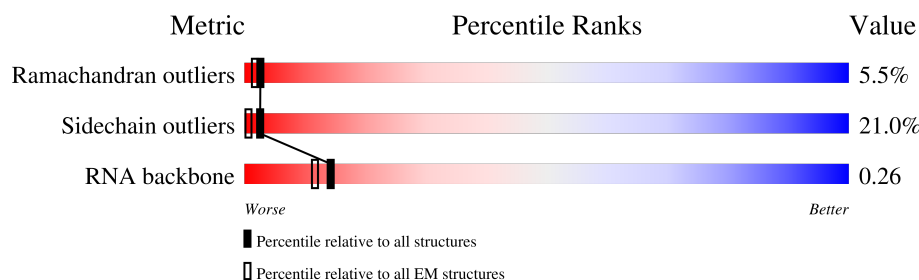
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.75 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.









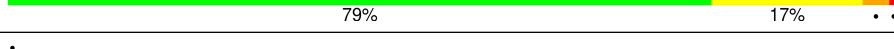
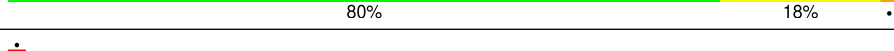
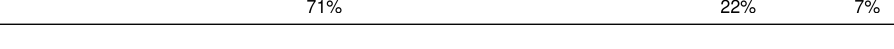
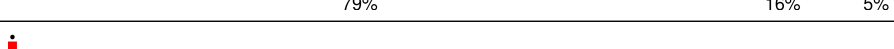
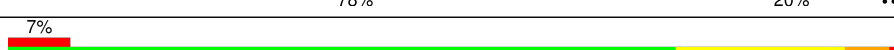

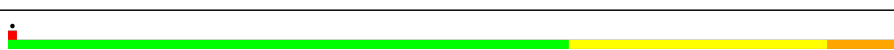

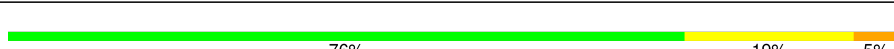





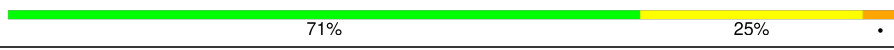
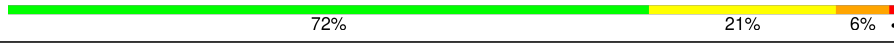
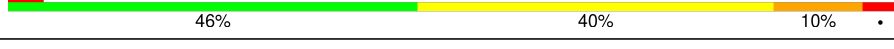


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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	A	244	
2	D	292	
3	G	238	
4	H	190	
5	J	170	
6	L	210	
7	M	138	
8	N	203	







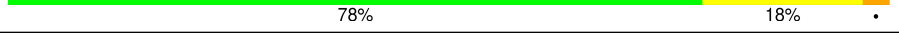




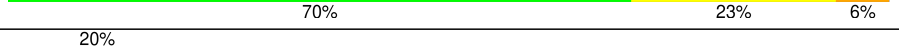



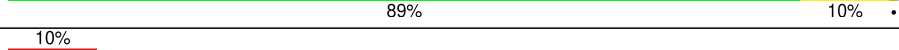



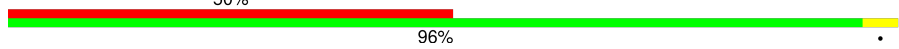

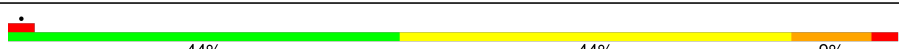


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Mol	Chain	Length	Quality of chain
9	O	201	
10	Q	187	
11	R	180	
12	S	175	
13	T	159	
14	U	99	
15	V	131	
16	X	119	
17	Y	134	
18	Z	135	
19	a	147	
20	b	75	
21	c	94	
22	d	107	
23	e	128	
24	f	109	
25	g	114	
26	h	122	
27	i	102	
28	k	69	
29	l	50	
30	m	52	
31	o	104	
32	5	3658	
33	7	120	

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Mol	Chain	Length	Quality of chain
34	8	156	
35	B	394	
36	C	367	
37	E	236	
38	F	225	
39	I	213	
40	P	153	
41	W	63	
42	j	86	
43	n	23	
44	p	91	
45	r	125	
46	K	163	
47	q	202	
48	z	426	
49	2	31	
50	3	76	
51	4	206	
52	9	105	
53	6	179	
54	S2	1742	
55	SA	208	
56	SB	213	
57	SC	218	
58	SE	262	

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Mol	Chain	Length	Quality of chain
59	SG	237	
60	SH	189	
61	SI	206	
62	SJ	185	
63	SL	152	
64	SN	149	
65	SO	136	
66	SV	82	
67	SW	129	
68	SX	141	
69	SY	126	
70	Sa	98	
71	Sb	83	
72	Se	57	
73	SD	227	
74	SF	191	
75	SK	98	
76	SM	124	
77	SP	96	
78	SQ	141	
79	SR	129	
80	SS	137	
81	ST	141	
82	SU	104	
83	SZ	75	

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Mol	Chain	Length	Quality of chain
84	Sc	64	
85	Sd	52	
86	Sf	71	
87	Sg	313	
88	S1	74	
89	S4	76	

## 2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 228197 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	244	Total	C	N	O	S	0	0
			1868	1171	382	309	6		

- Molecule 2 is a protein called Ribosomal protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	292	Total	C	N	O	S	0	0
			2380	1508	434	426	12		

- Molecule 3 is a protein called Ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	238	Total	C	N	O	S	0	0
			1912	1218	368	322	4		

- Molecule 4 is a protein called Ribosomal protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 5 is a protein called Ribosomal protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	170	Total	C	N	O	S	0	0
			1359	856	256	241	6		

- Molecule 6 is a protein called Ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	210	Total	C	N	O	S	0	0
			1703	1064	354	280	5		

- Molecule 7 is a protein called Ribosomal protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	138	Total	C	N	O	S	0	0
			1131	727	216	181	7		

- Molecule 8 is a protein called Ribosomal protein eL15.

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

- Molecule 9 is a protein called Ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	201	Total	C	N	O	S	0	0
			1651	1063	323	260	5		

- Molecule 10 is a protein called Ribosomal protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	187	Total	C	N	O	S	0	0
			1506	941	311	249	5		

- Molecule 11 is a protein called Ribosomal protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 12 is a protein called Ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S	175	Total	C	N	O	S	0	0
			1454	925	284	235	10		

- Molecule 13 is a protein called Ribosomal protein eL21.

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

- Molecule 14 is a protein called Ribosomal protein eL22.



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

- Molecule 15 is a protein called Ribosomal protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 16 is a protein called Ribosomal protein uL23.

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

- Molecule 17 is a protein called Ribosomal protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 18 is a protein called Ribosomal protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 19 is a protein called Ribosomal protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	147	Total	C	N	O	S	0	0
			1163	735	239	185	4		

- Molecule 20 is a protein called Ribosomal protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	75	Total	C	N	O	S	0	0
			610	378	130	99	3		

- Molecule 21 is a protein called Ribosomal protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	c	94	Total	C	N	O	S	0	0
			732	465	130	131	6		

- Molecule 22 is a protein called Ribosomal protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	d	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 23 is a protein called Ribosomal protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	e	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 24 is a protein called Ribosomal protein eL33.

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

- Molecule 25 is a protein called Ribosomal protein eL34.

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

- Molecule 26 is a protein called Ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	h	122	Total	C	N	O	S	0	0
			1015	642	205	167	1		

- Molecule 27 is a protein called Ribosomal protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	i	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 28 is a protein called Ribosomal protein eL38.

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

- Molecule 29 is a protein called Ribosomal protein eL39.

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

- Molecule 30 is a protein called Ribosomal protein eL40.

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

- Molecule 31 is a protein called Ribosomal protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	o	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 32 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	3658	Total	C	N	O	P	0	0
			78406	34911	14352	25486	3657		

- Molecule 33 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 34 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	8	156	Total	C	N	O	P	0	0
			3314	1480	585	1094	155		

- Molecule 35 is a protein called Ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	B	394	Total	C	N	O	S	0	0
			3147	2005	591	538	13		

- Molecule 36 is a protein called Ribosomal protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	C	367	Total	C	N	O	S	0	0
			2919	1836	582	486	15		

- Molecule 37 is a protein called Ribosomal protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	E	236	Total	C	N	O	S	0	0
			1904	1219	364	316	5		

- Molecule 38 is a protein called Ribosomal protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	F	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 39 is a protein called Ribosomal protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	I	213	Total	C	N	O	S	0	0
			1713	1083	331	284	15		

- Molecule 40 is a protein called Ribosomal protein uL22.

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

- Molecule 41 is a protein called Ribosomal protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	W	63	Total	C	N	O	S	0	0
			528	337	103	85	3		

- Molecule 42 is a protein called Ribosomal protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	86	Total	C	N	O	S	0	0
			706	436	155	110	5		

- Molecule 43 is a protein called Ribosomal protein eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	n	23	Total	C	N	O	S	0	0
			222	134	61	25	2		

- Molecule 44 is a protein called Ribosomal protein eL43.

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

- Molecule 45 is a protein called Ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	r	125	Total	C	N	O	S	0	0
			1001	622	206	168	5		

- Molecule 46 is a protein called Ribosomal protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	K	163	Total	C	N	O	S	0	0
			1238	773	230	230	5		

- Molecule 47 is a protein called Ribosomal protein uL10.

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

- Molecule 48 is a protein called SRP54.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	z	426	Total	C	N	O	S	0	0
			3241	2047	555	615	24		

- Molecule 49 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	2	31	Total	C	N	O	S	0	0
			233	167	32	32	2		

- Molecule 50 is a RNA chain called Val tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3	76	Total	C	N	O	P	0	0
			1616	723	290	528	75		

- Molecule 51 is a RNA chain called SRP 7S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	4	206	Total	C	N	O	P	6	0
			4551	2026	836	1477	212		

- Molecule 52 is a protein called SRP19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	9	105	Total	C	N	O	S	0	0
			844	534	152	152	6		

- Molecule 53 is a protein called SRP68.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	6	179	Total	C	N	O	S	0	0
			1497	939	280	271	7		

- Molecule 54 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	S2	1742	Total	C	N	O	P	0	0
			36900	16458	6595	12106	1741		

- Molecule 55 is a protein called Ribosomal protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SA	208	Total	C	N	O	S	0	0
			1642	1045	289	300	8		

- Molecule 56 is a protein called Ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SB	213	Total	C	N	O	S	0	0
			1725	1093	311	308	13		

- Molecule 57 is a protein called Ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SC	218	Total	C	N	O	S	0	0
			1690	1094	289	297	10		

- Molecule 58 is a protein called Ribosomal protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 59 is a protein called Ribosomal protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 60 is a protein called Ribosomal protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SH	189	Total	C	N	O	S	0	0
			1521	969	280	271	1		

- Molecule 61 is a protein called Ribosomal protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SI	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 62 is a protein called Ribosomal protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 63 is a protein called Ribosomal protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SL	152	Total	C	N	O	S	0	0
			1238	788	232	212	6		

- Molecule 64 is a protein called Ribosomal protein uS15.

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

- Molecule 65 is a protein called Ribosomal protein uS11.

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

- Molecule 66 is a protein called Ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SV	82	Total	C	N	O	S	0	0
			625	384	116	120	5		

- Molecule 67 is a protein called Ribosomal protein uS8.

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

- Molecule 68 is a protein called Ribosomal protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SX	141	Total	C	N	O	S	0	0
			1099	694	220	182	3		

- Molecule 69 is a protein called Ribosomal protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SY	126	Total	C	N	O	S	0	0
			1023	646	200	172	5		

- Molecule 70 is a protein called Ribosomal protein eS26.



Mol	Chain	Residues	Atoms					AltConf	Trace
70	Sa	98	Total	C	N	O	S	0	0
			781	486	161	129	5		

- Molecule 71 is a protein called Ribosomal protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Sb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 72 is a protein called Ribosomal protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Se	57	Total	C	N	O	S	0	0
			452	279	99	73	1		

- Molecule 73 is a protein called Ribosomal protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SD	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 74 is a protein called Ribosomal protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SF	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 75 is a protein called Ribosomal protein eS10.

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

- Molecule 76 is a protein called Ribosomal protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	SM	124	Total	C	N	O	S	0	0
			960	600	171	181	8		

- Molecule 77 is a protein called Ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	SP	96	Total	C	N	O	S	0	0
			805	506	158	135	6		

- Molecule 78 is a protein called Ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	SQ	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 79 is a protein called Ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	SR	129	Total	C	N	O	S	0	0
			1047	658	193	191	5		

- Molecule 80 is a protein called Ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	SS	137	Total	C	N	O	S	0	0
			1139	714	231	193	1		

- Molecule 81 is a protein called Ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	ST	141	Total	C	N	O	S	0	0
			1101	690	212	196	3		

- Molecule 82 is a protein called Ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	SU	104	Total	C	N	O	S	0	0
			818	513	153	148	4		

- Molecule 83 is a protein called Ribosomal protein es25.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	SZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 84 is a protein called Ribosomal protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Sc	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 85 is a protein called Ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Sd	52	Total	C	N	O	S	0	0
			434	273	87	69	5		

- Molecule 86 is a protein called Ribosomal protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Sf	71	Total	C	N	O	S	0	0
			581	367	109	98	7		

- Molecule 87 is a protein called Ribosomal protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	Sg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 88 is a protein called SRP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	S1	74	Total	C	N	O	S	0	0
			608	388	105	110	5		

- Molecule 89 is a protein called SRP14.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	S4	76	Total	C	N	O	S	0	0
			604	382	105	113	4		

- Molecule 90 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
90	D	1	Total	Mg	0
			1	1	
90	V	1	Total	Mg	0
			1	1	
90	g	1	Total	Mg	0
			1	1	

*Continued on next page...*

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Mol	Chain	Residues	Atoms		AltConf
90	5	116	Total 116	Mg 116	0
90	7	5	Total 5	Mg 5	0
90	8	6	Total 6	Mg 6	0
90	S2	36	Total 36	Mg 36	0

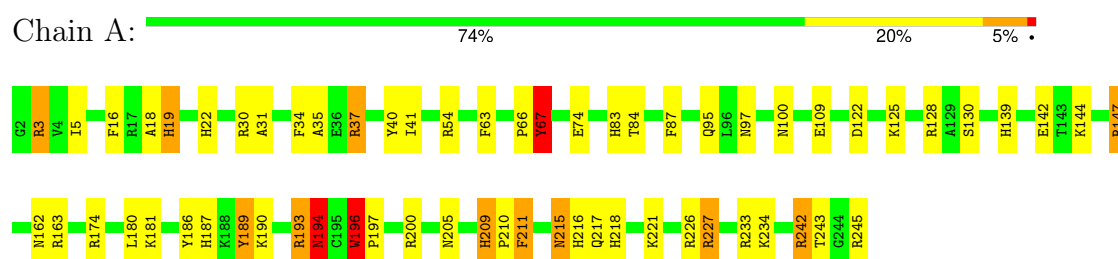
- Molecule 91 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
91	m	1	Total 1	Zn 1	0
91	o	1	Total 1	Zn 1	0
91	j	1	Total 1	Zn 1	0
91	Sa	1	Total 1	Zn 1	0

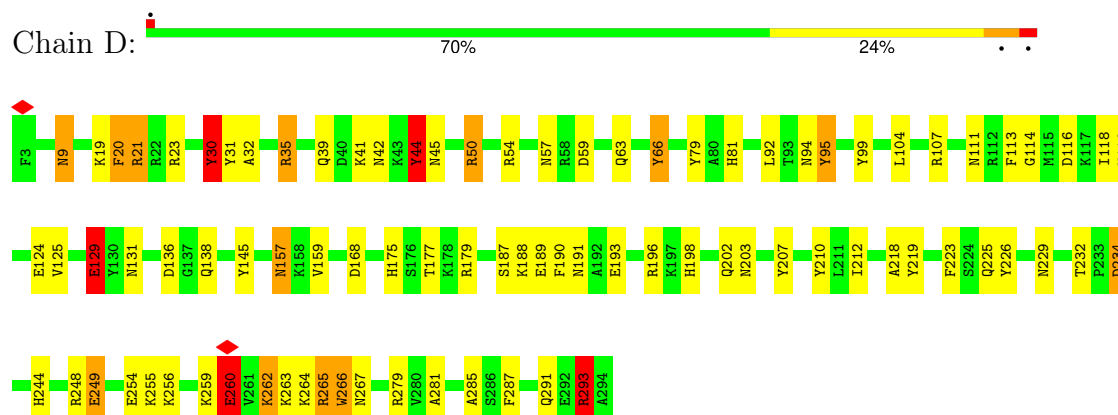
### 3 Residue-property plots [i](#)

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

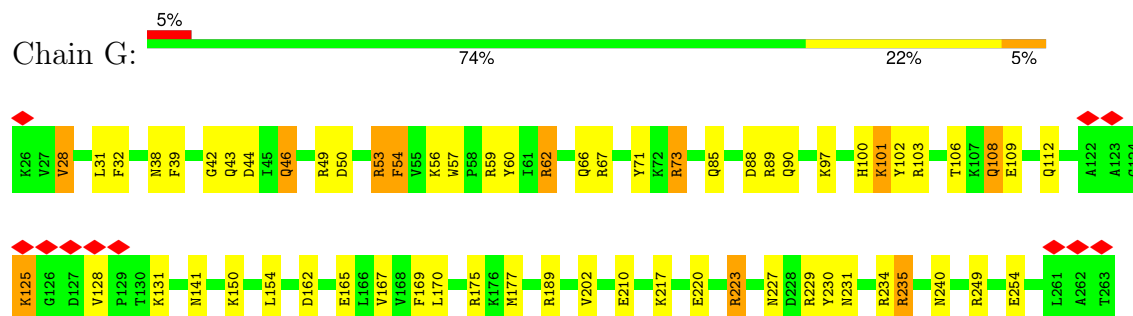
#### • Molecule 1: Ribosomal protein uL2




#### • Molecule 2: Ribosomal protein uL18

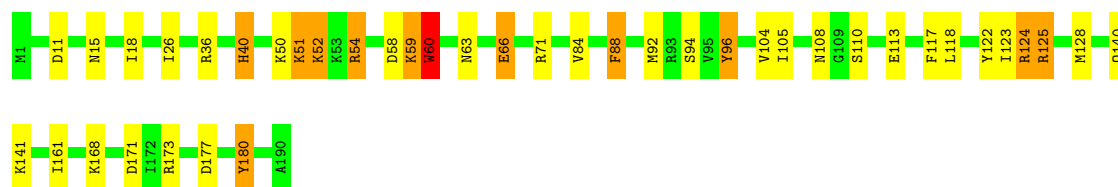


#### • Molecule 3: Ribosomal protein eL8



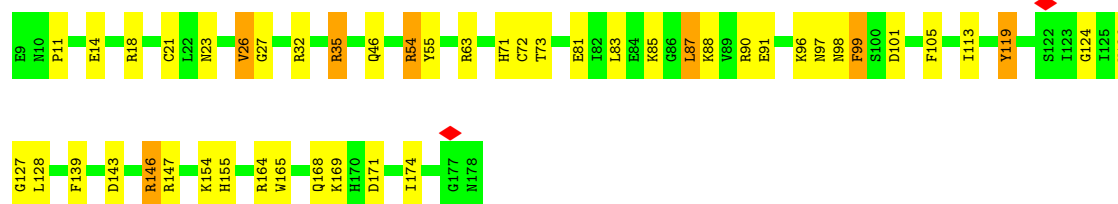
#### • Molecule 4: Ribosomal protein uL6

Chain H:  78% 15% 6% •



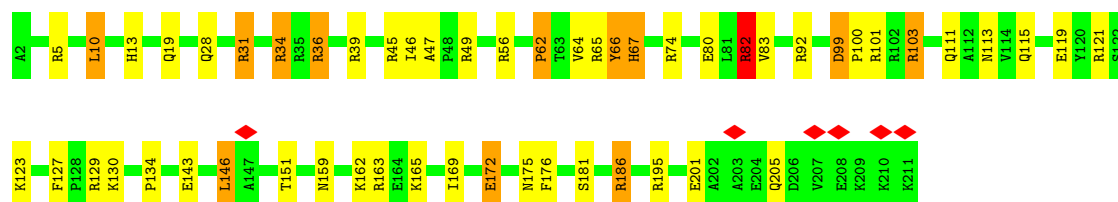
- Molecule 5: Ribosomal protein uL5

Chain J:  72% 24% •



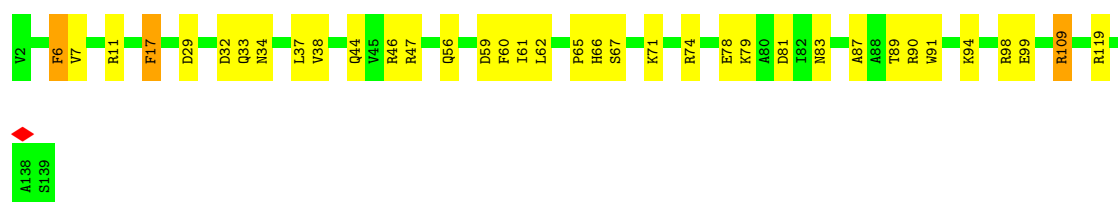
- Molecule 6: Ribosomal protein eL13

Chain L:  74% 20% 6% •



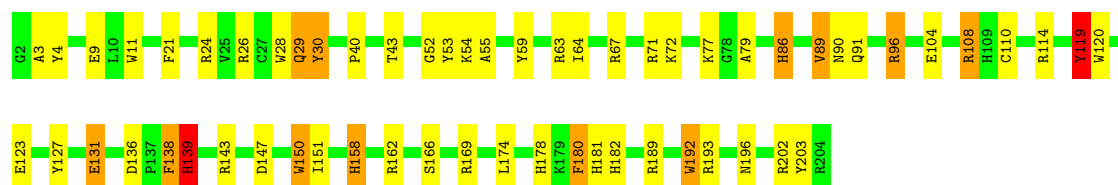
- Molecule 7: Ribosomal protein eL14

Chain M:  74% 24% •

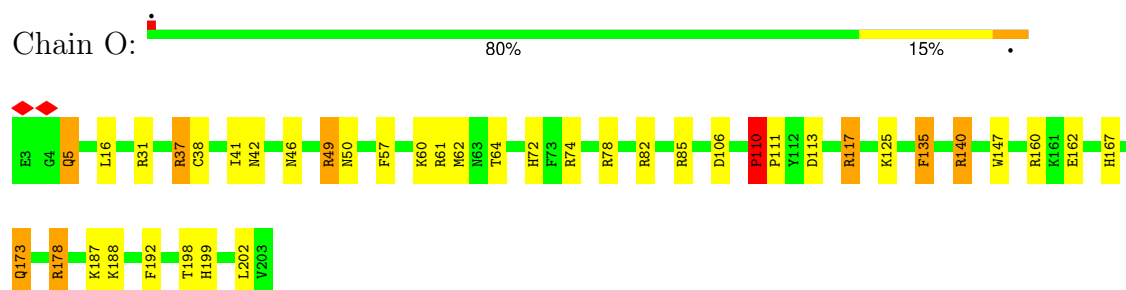


- Molecule 8: Ribosomal protein eL15

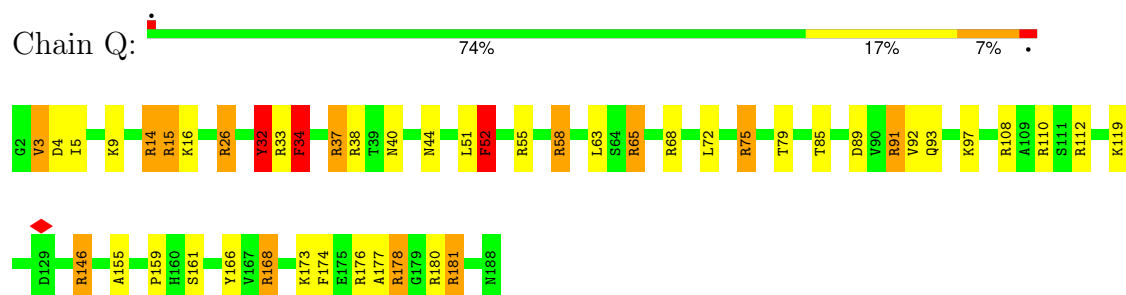
Chain N:  70% 23% 6% •



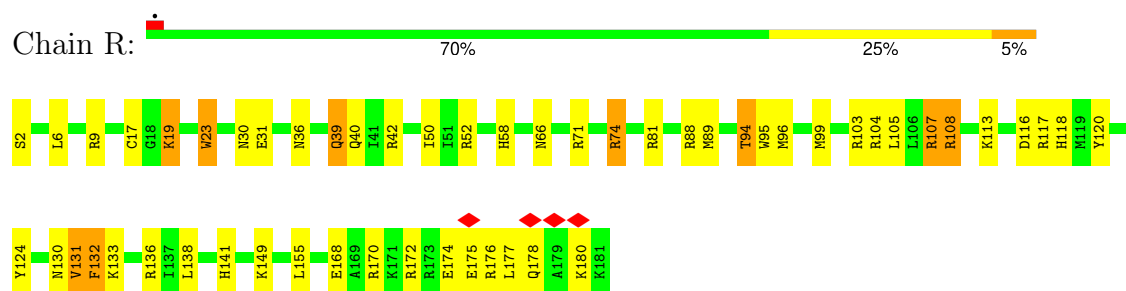
- Molecule 9: Ribosomal protein uL13



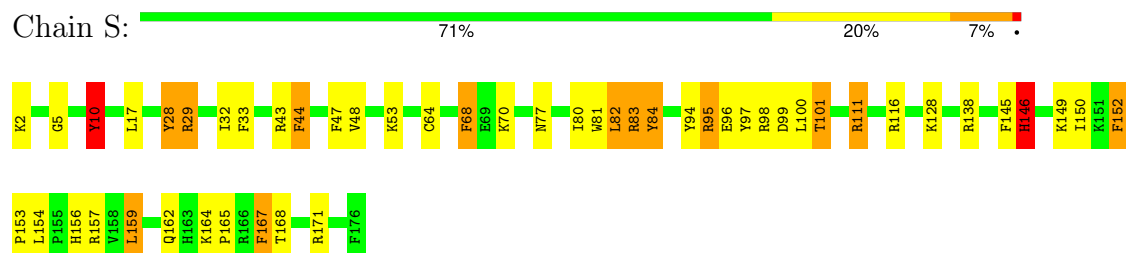
- Molecule 10: Ribosomal protein eL18



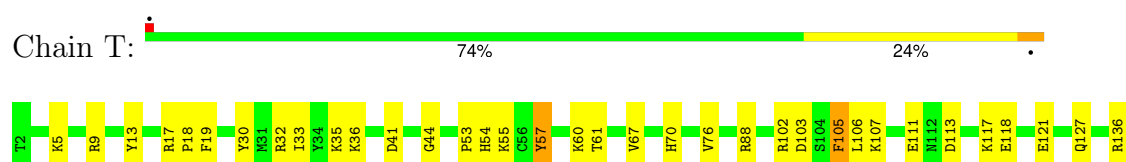
- Molecule 11: Ribosomal protein eL19

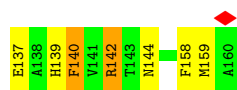


- Molecule 12: Ribosomal protein eL20



- Molecule 13: Ribosomal protein eL21





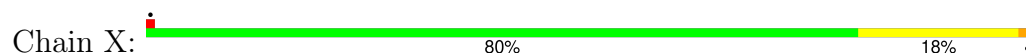
- Molecule 14: Ribosomal protein eL22



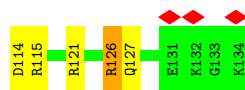
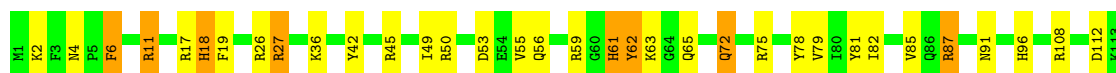
- Molecule 15: Ribosomal protein uL14



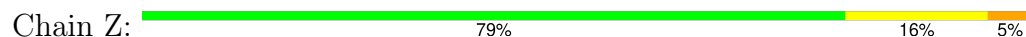
- Molecule 16: Ribosomal protein uL23



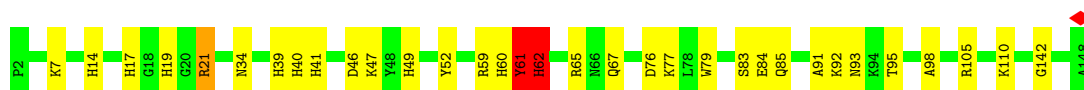
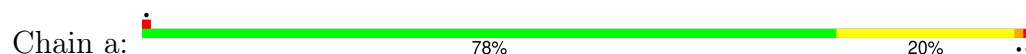
- Molecule 17: Ribosomal protein uL24



- Molecule 18: Ribosomal protein eL27

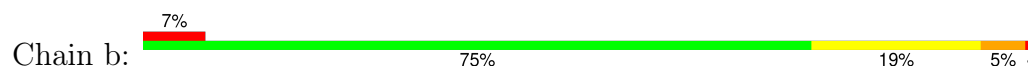


- Molecule 19: Ribosomal protein uL15





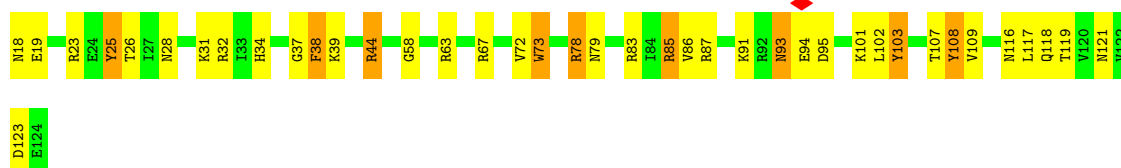
- Molecule 20: Ribosomal protein eL29



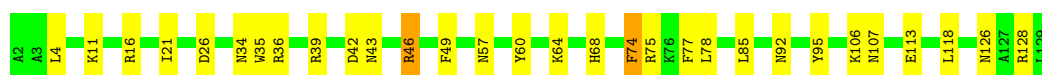
- Molecule 21: Ribosomal protein eL30



- Molecule 22: Ribosomal protein eL31



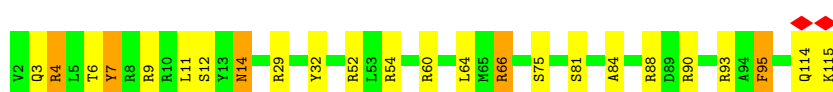
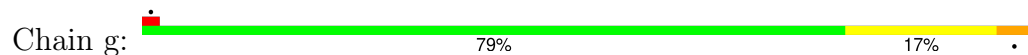
- Molecule 23: Ribosomal protein eL32



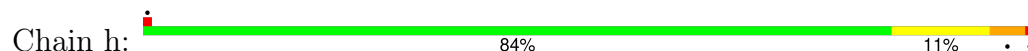
- Molecule 24: Ribosomal protein eL33



- Molecule 25: Ribosomal protein eL34



- Molecule 26: Ribosomal protein uL29

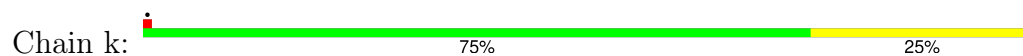




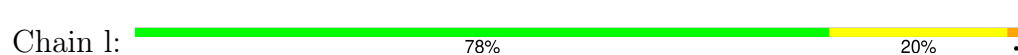
- Molecule 27: Ribosomal protein eL36



- Molecule 28: Ribosomal protein eL38



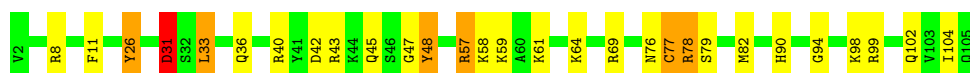
- Molecule 29: Ribosomal protein eL39



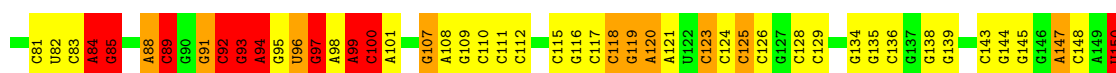
- Molecule 30: Ribosomal protein eL40

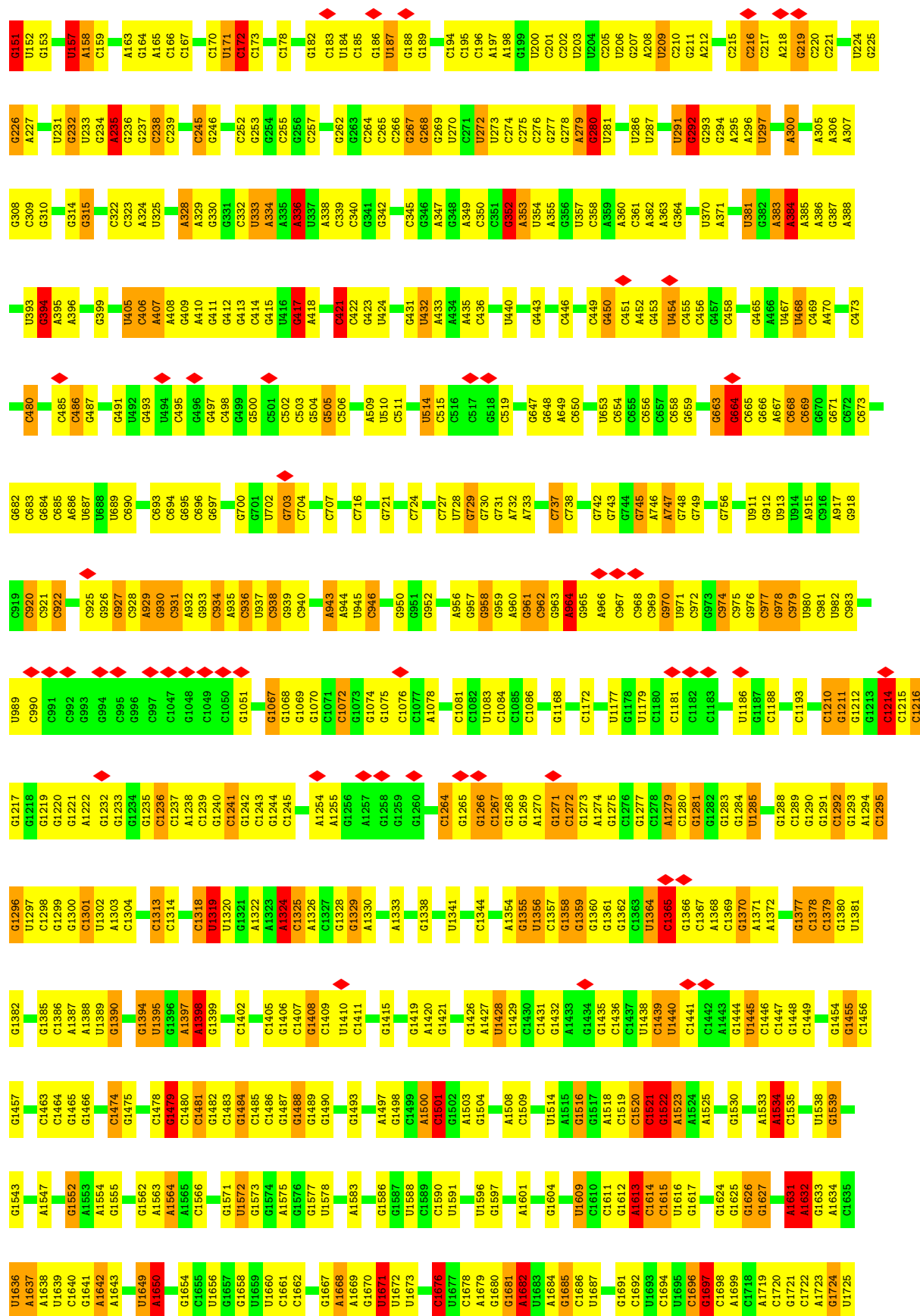


- Molecule 31: Ribosomal protein eL42

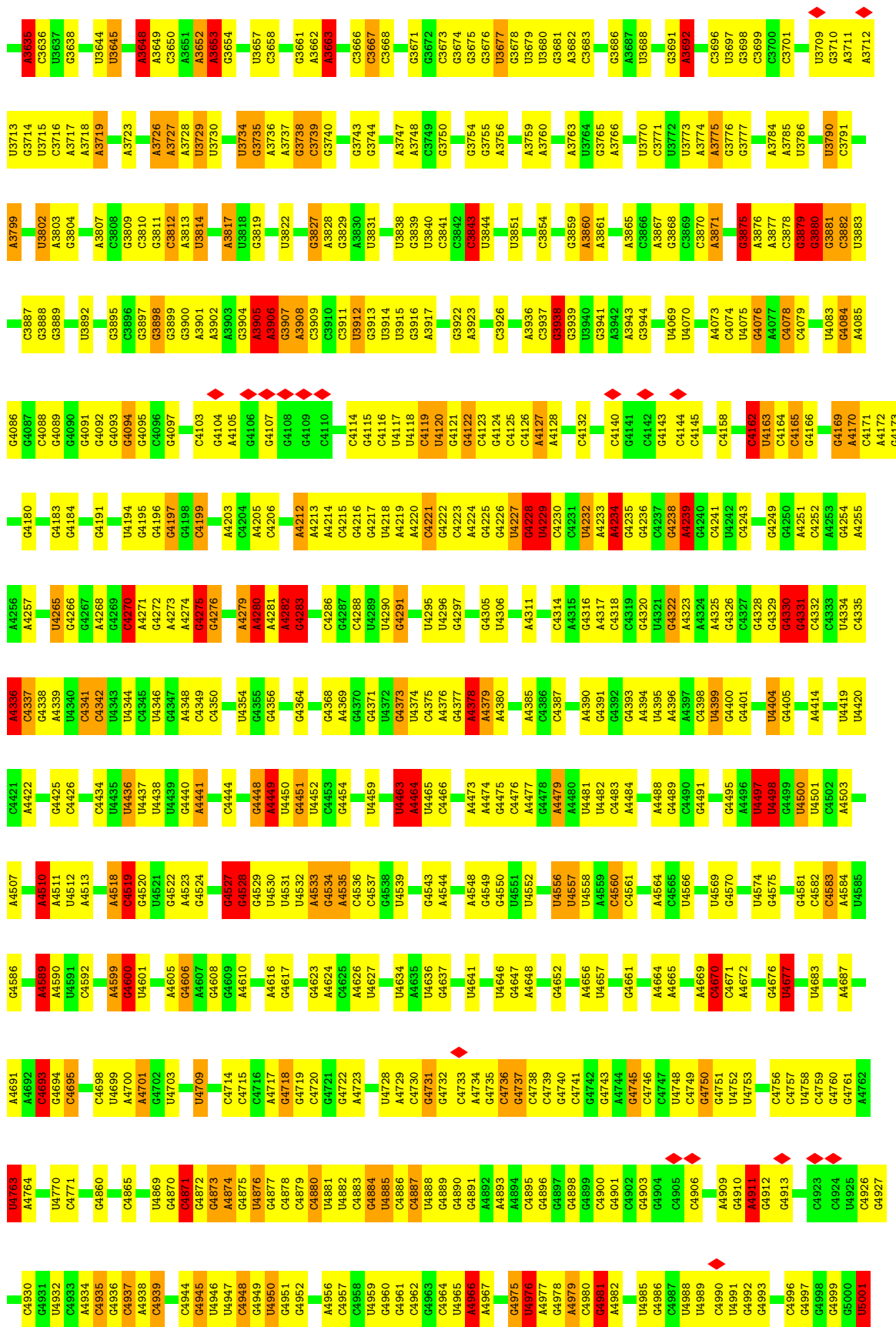


- Molecule 32: 28S ribosomal RNA





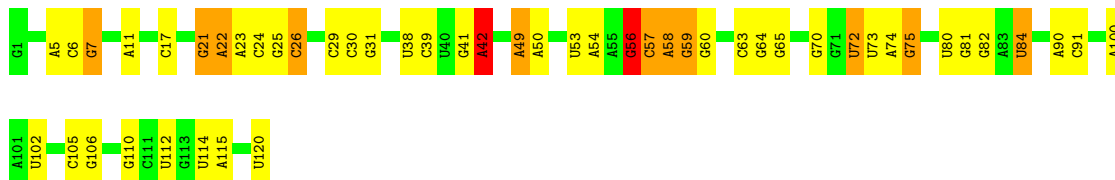






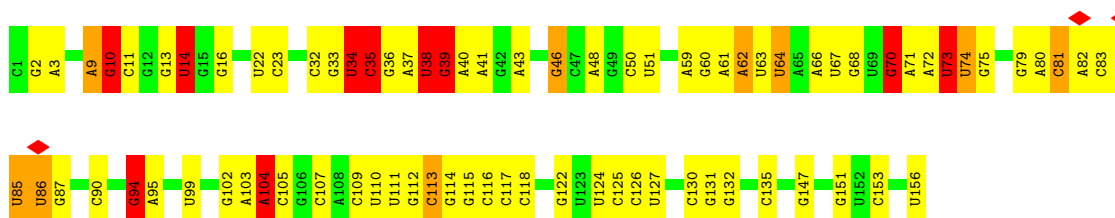
• Molecule 33: 5S ribosomal RNA

Chain 7: 58% 31% 9%



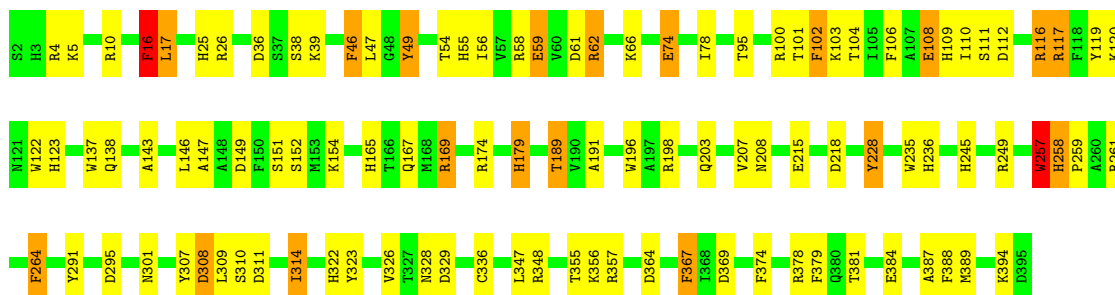
• Molecule 34: 5.8S ribosomal RNA

Chain 8: 48% 40% 6% 6%



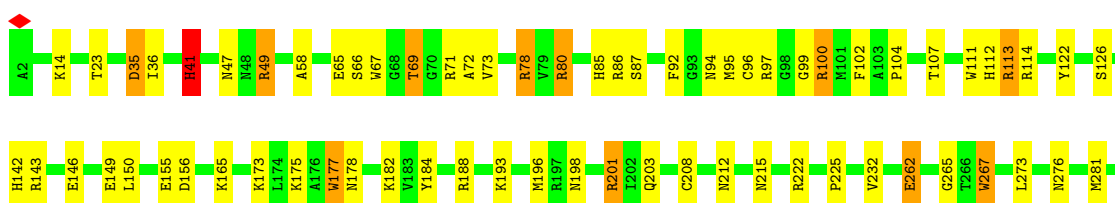
• Molecule 35: Ribosomal protein uL3

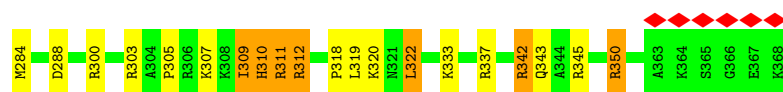
Chain B: 73% 22% 5%



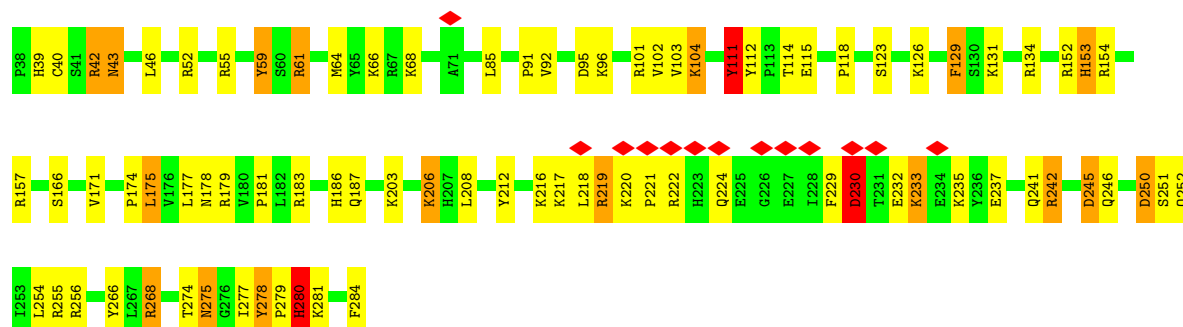
• Molecule 36: Ribosomal protein uL4

Chain C: 76% 19% 5%

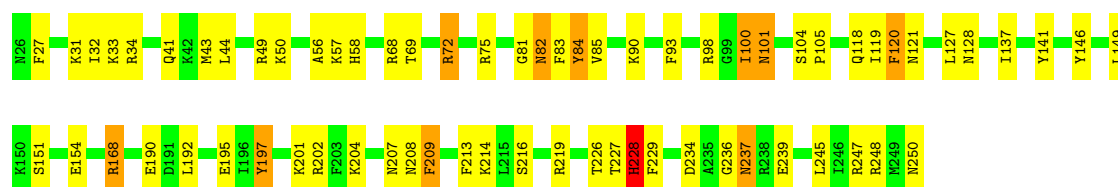




• Molecule 37: Ribosomal protein eL6



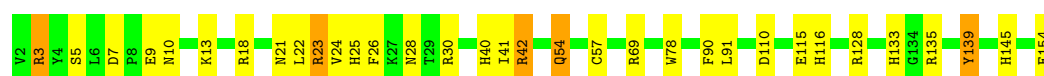
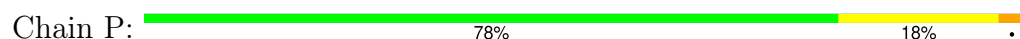
• Molecule 38: Ribosomal protein uL30



• Molecule 39: Ribosomal protein uL16



• Molecule 40: Ribosomal protein uL22



• Molecule 41: Ribosomal protein eL24

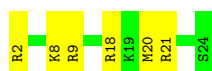




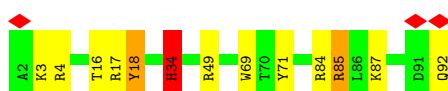
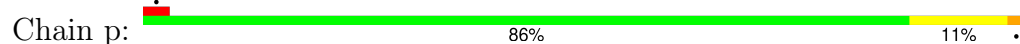
- Molecule 42: Ribosomal protein eL37



- Molecule 43: Ribosomal protein eL41



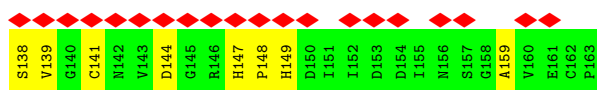
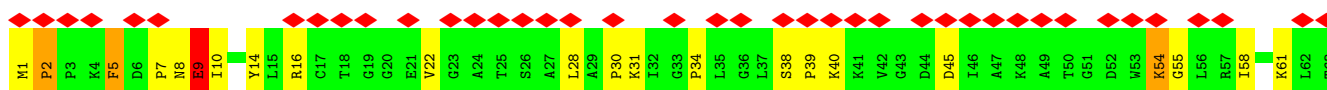
- Molecule 44: Ribosomal protein eL43



- Molecule 45: Ribosomal protein eL28



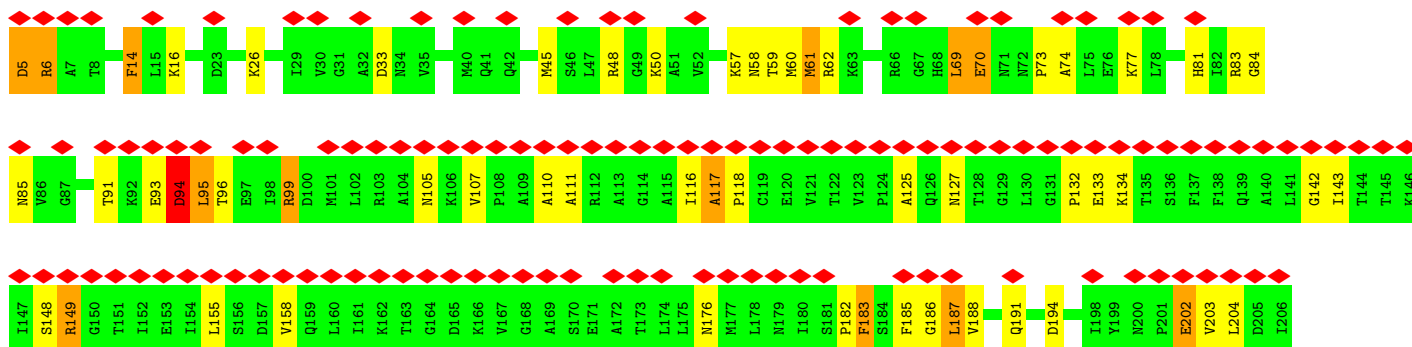
- Molecule 46: Ribosomal protein uL11



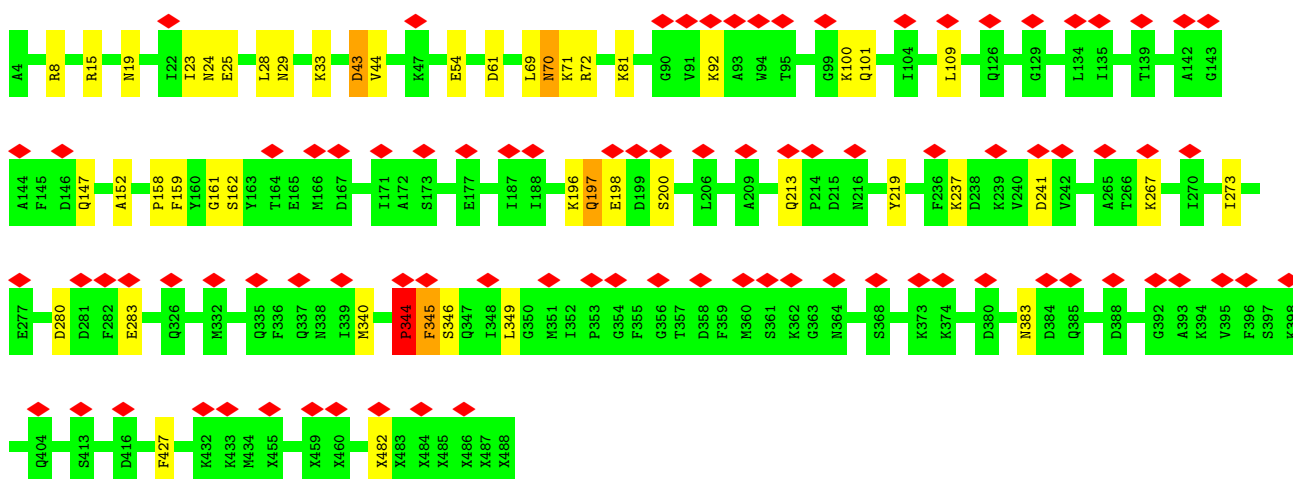
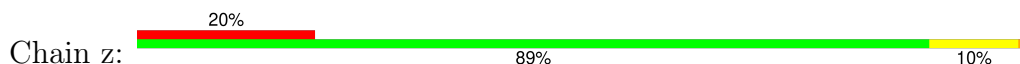
- Molecule 47: Ribosomal protein uL10



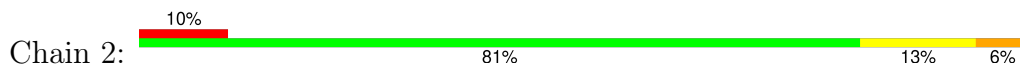




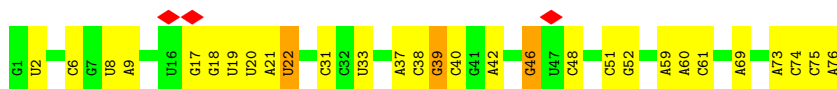
• Molecule 48: SRP54



• Molecule 49: Nascent chain

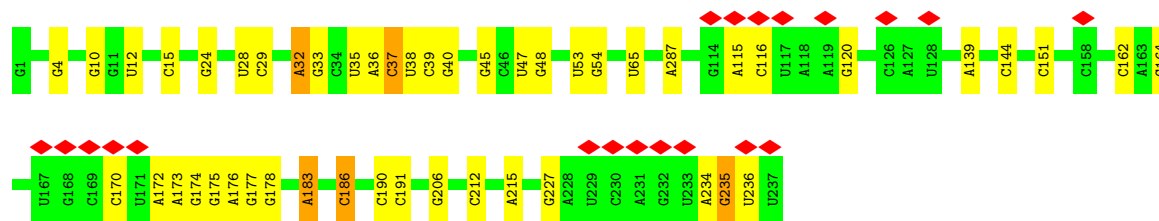


• Molecule 50: Val tRNA

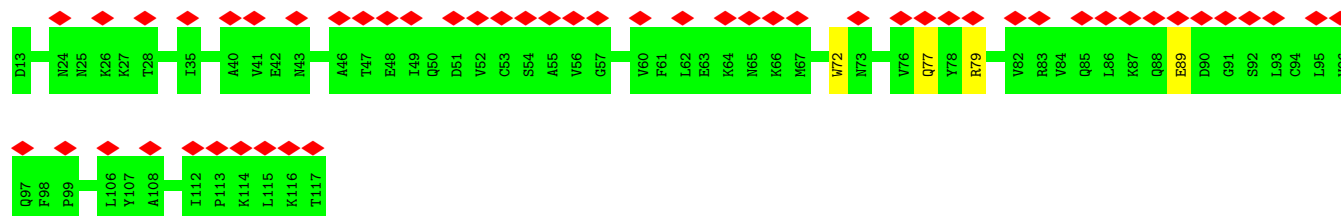


• Molecule 51: SRP 7S RNA

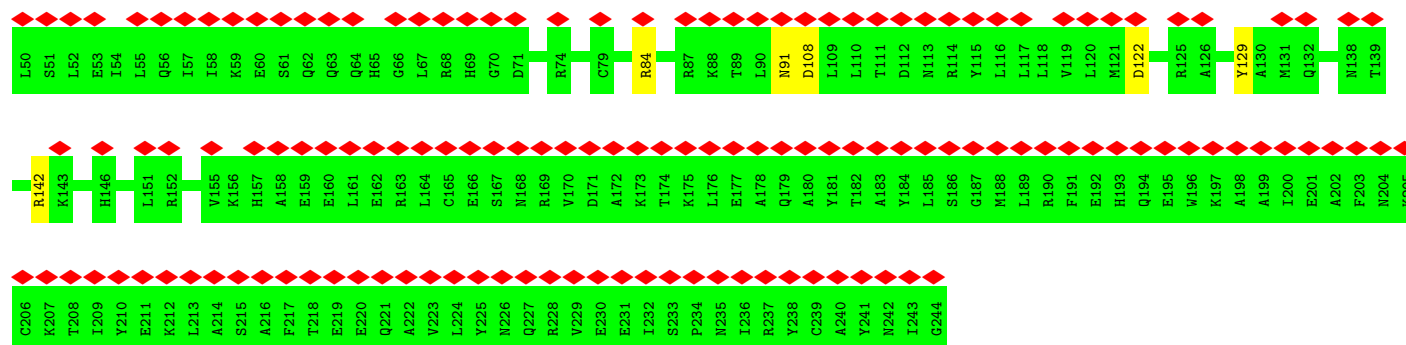
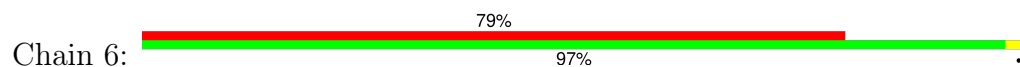




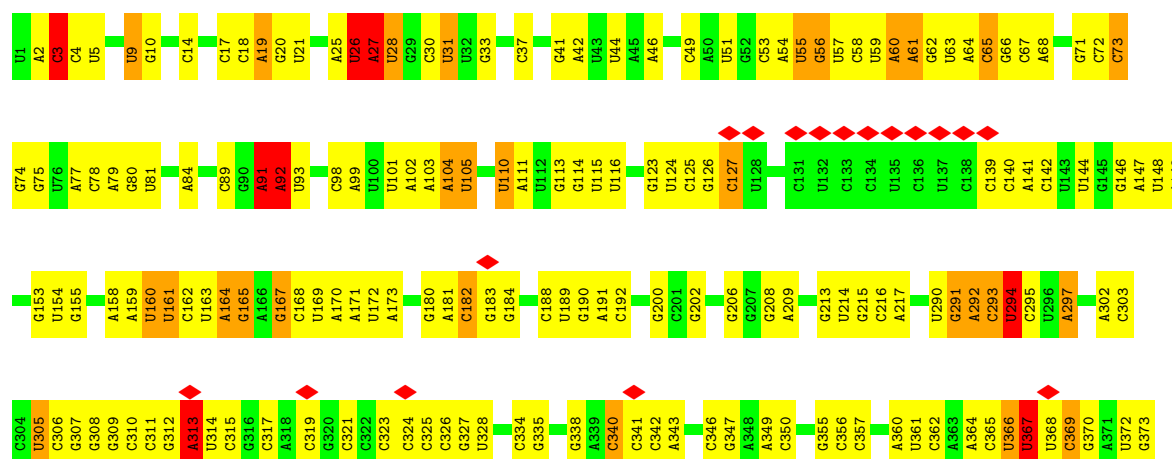
• Molecule 52: SRP19



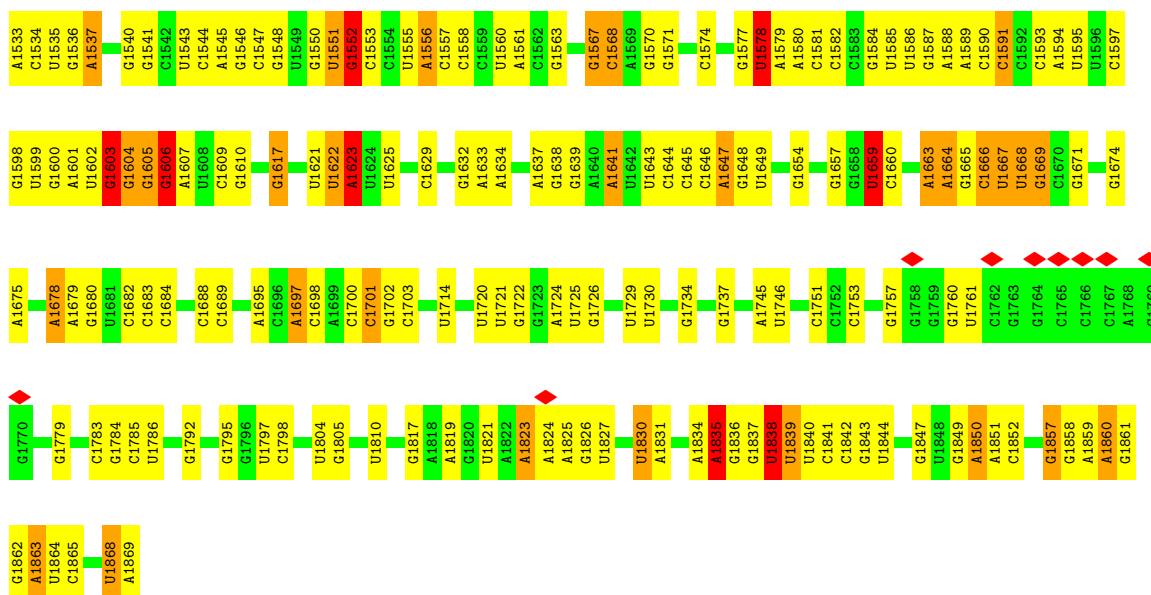
• Molecule 53: SRP68



• Molecule 54: 18S ribosomal RNA

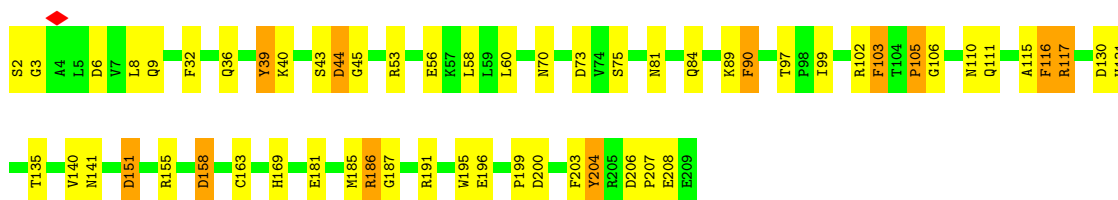






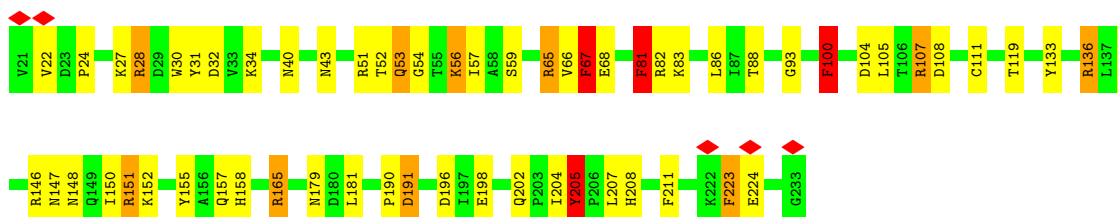
• Molecule 55: Ribosomal protein uS2

Chain SA: 72% 23% 5%



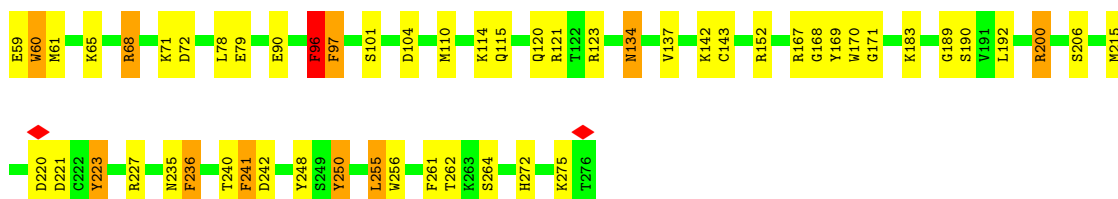
• Molecule 56: Ribosomal protein eS1

Chain SB: 71% 22% 5%

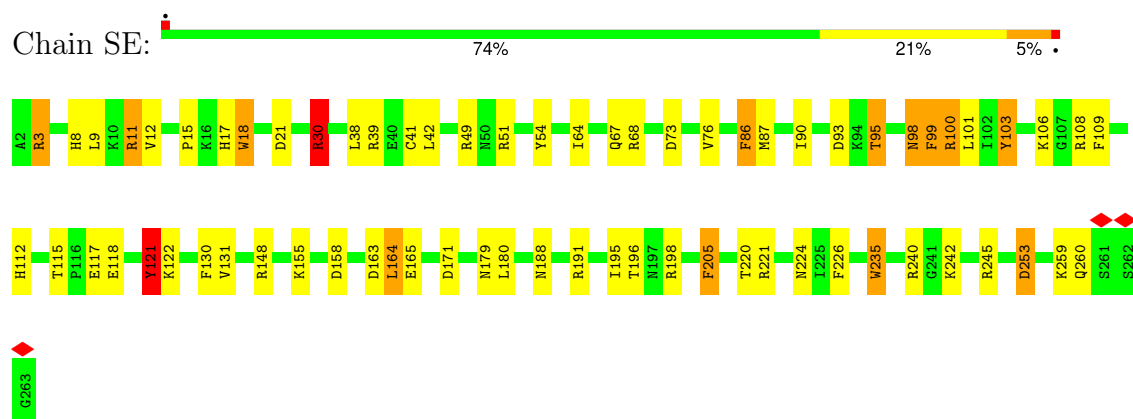


• Molecule 57: Ribosomal protein uS5

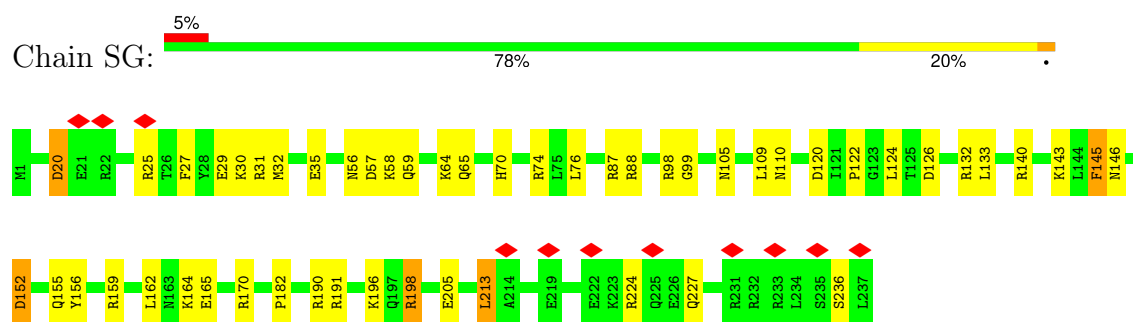
Chain SC: 75% 20% 5%



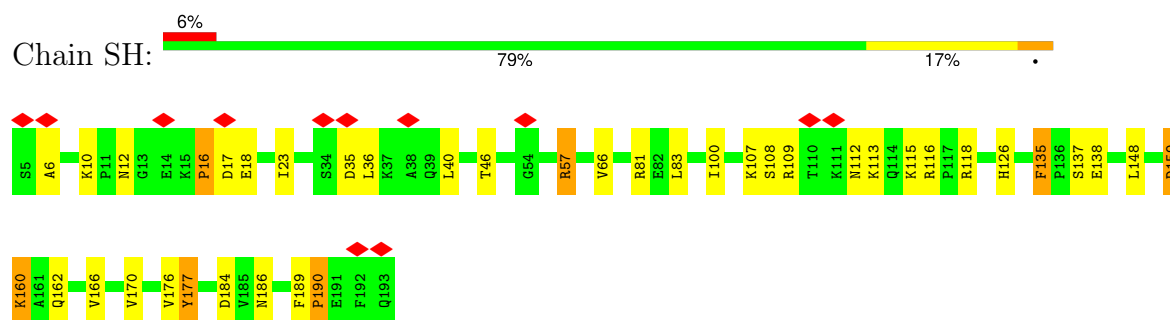
- Molecule 58: Ribosomal protein eS4



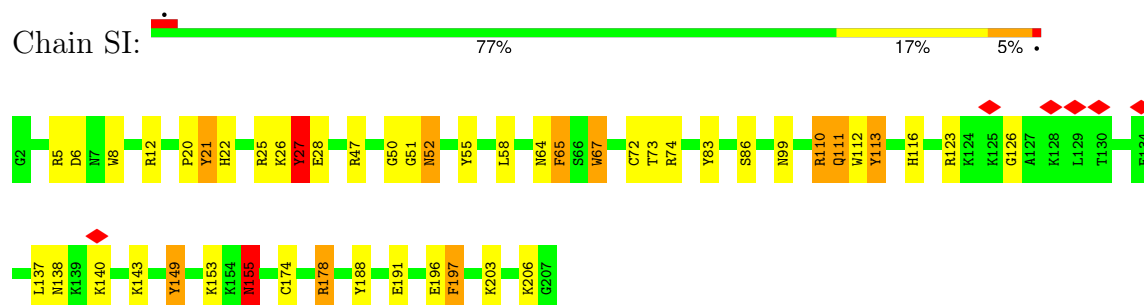
- Molecule 59: Ribosomal protein eS6



- Molecule 60: Ribosomal protein eS7

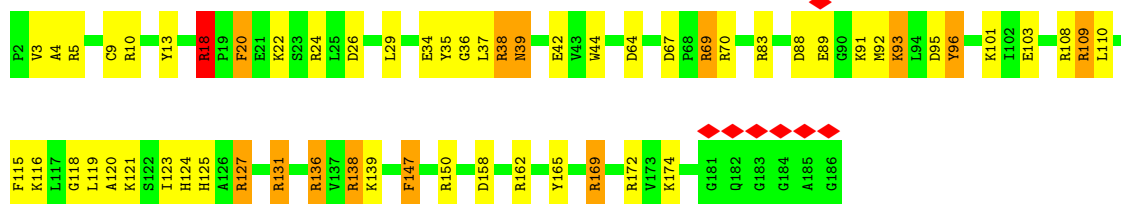


- Molecule 61: Ribosomal protein eS8




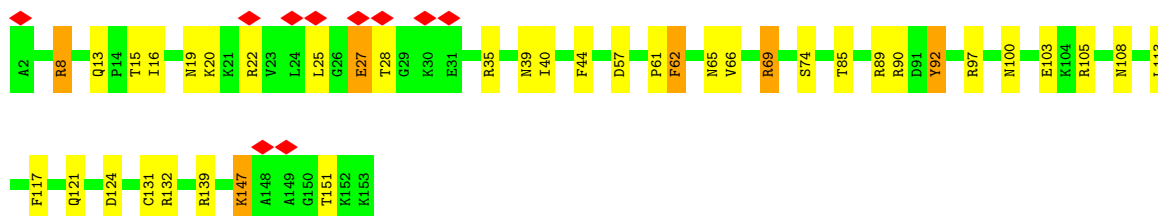
- Molecule 62: Ribosomal protein uS4

Chain SJ: 




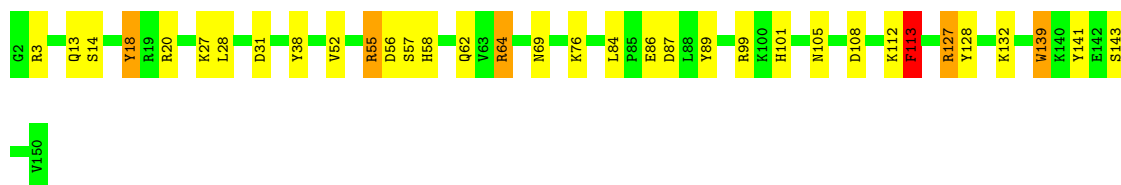
- Molecule 63: Ribosomal protein uS17

Chain SL: 



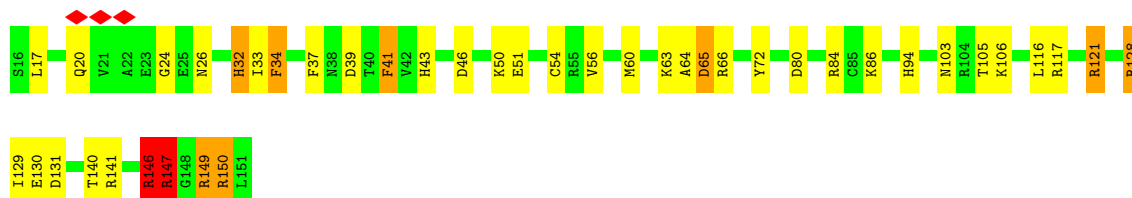
- Molecule 64: Ribosomal protein uS15

Chain SN: 



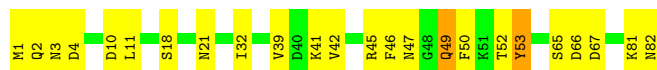
- Molecule 65: Ribosomal protein uS11

Chain SO: 




- Molecule 66: Ribosomal protein eS21

Chain SV: 




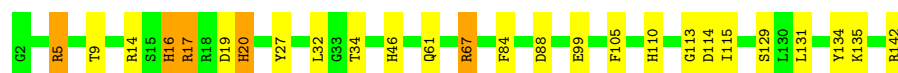
- Molecule 67: Ribosomal protein uS8

Chain SW:  76% 22%




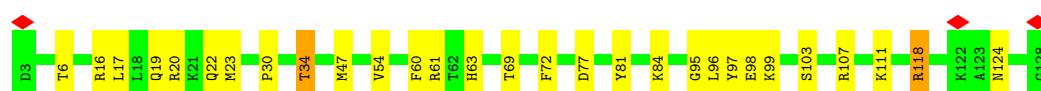
- Molecule 68: Ribosomal protein uS12

Chain SX:  82% 15%




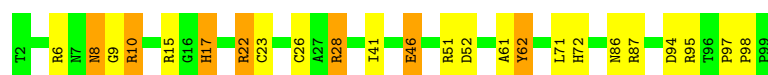
- Molecule 69: Ribosomal protein eS24

Chain SY:  77% 21%



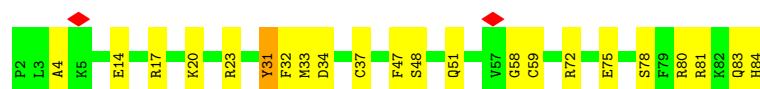
- Molecule 70: Ribosomal protein eS26

Chain Sa:  76% 17% 7%




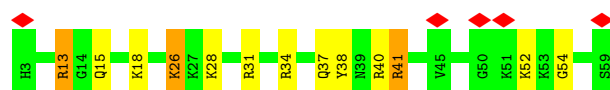
- Molecule 71: Ribosomal protein eS27

Chain Sb:  73% 25%




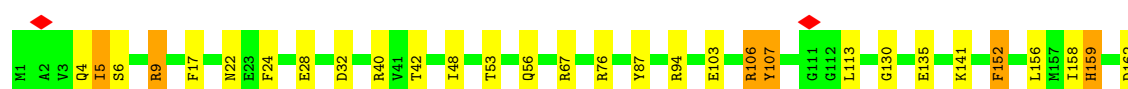
- Molecule 72: Ribosomal protein eS30

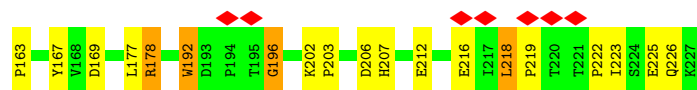
Chain Se:  9% 77% 18% 5%



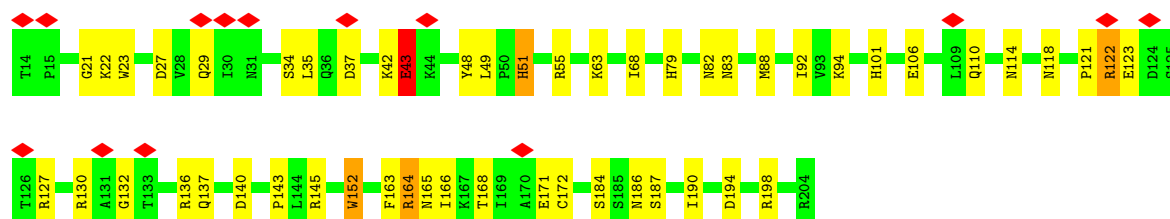
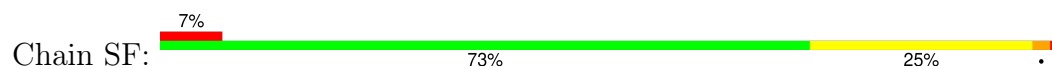
- Molecule 73: Ribosomal protein uS3

Chain SD:  78% 17%

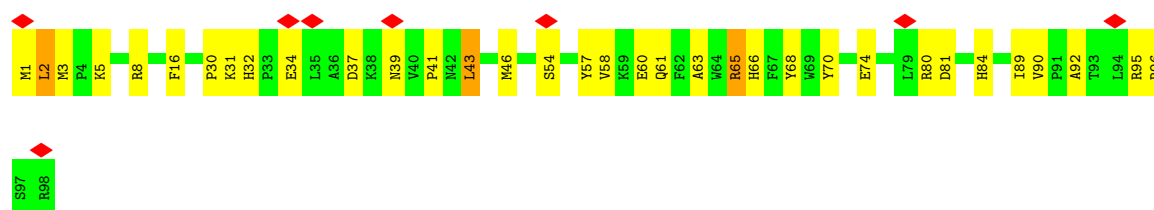




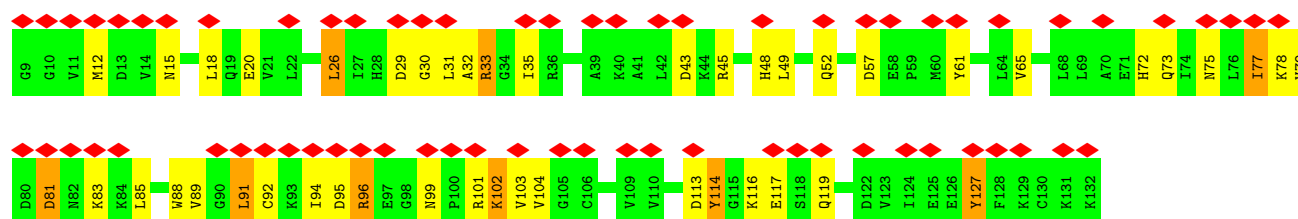
• Molecule 74: Ribosomal protein uS7



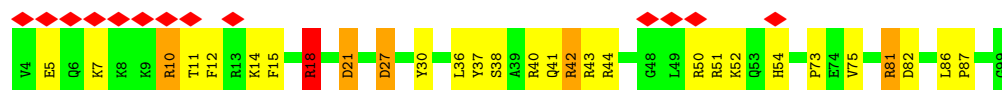
• Molecule 75: Ribosomal protein eS10



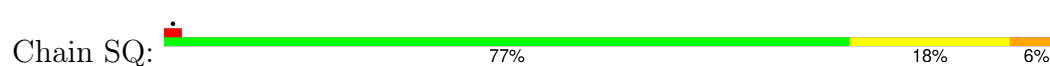
• Molecule 76: Ribosomal protein eS12



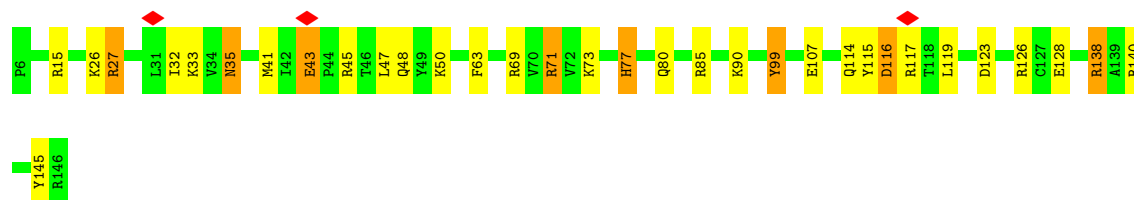
• Molecule 77: Ribosomal protein uS19



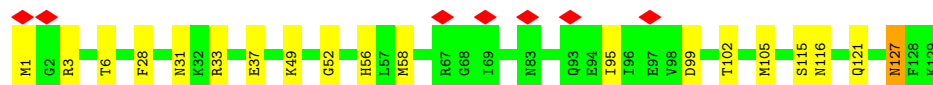
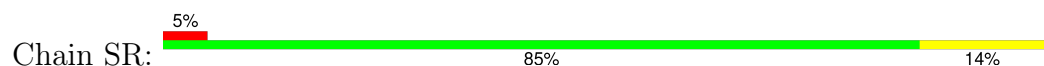
• Molecule 78: Ribosomal protein uS9



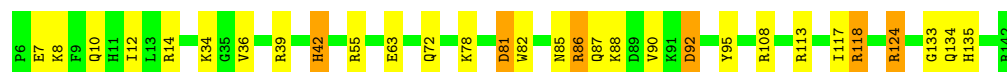
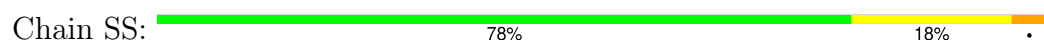




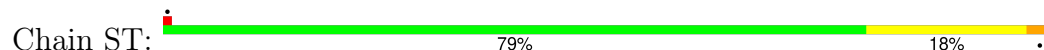
- Molecule 79: Ribosomal protein eS17



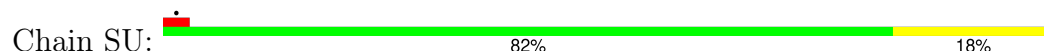
- Molecule 80: Ribosomal protein uS13



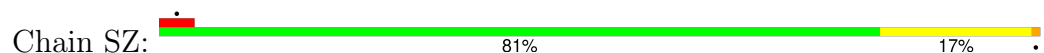
- Molecule 81: Ribosomal protein eS19



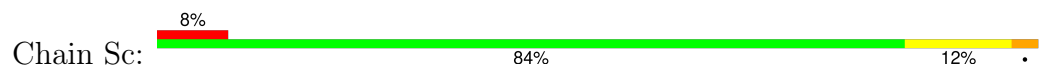
- Molecule 82: Ribosomal protein uS10

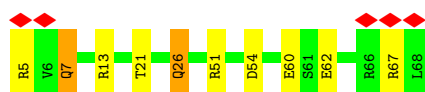


- Molecule 83: Ribosomal protein es25

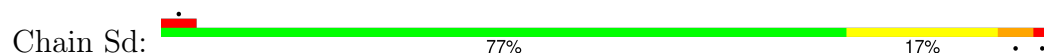


- Molecule 84: Ribosomal protein eS28

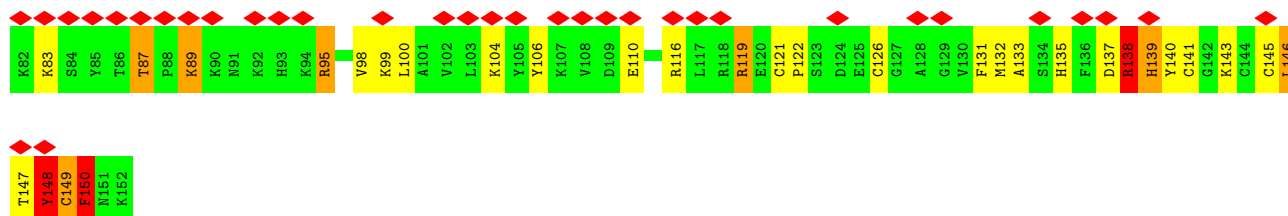




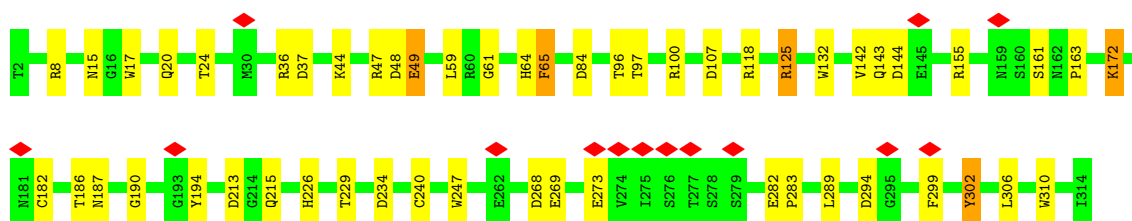
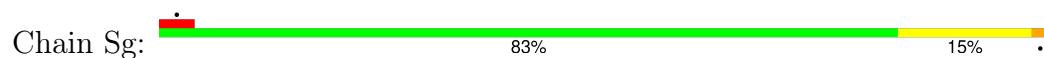
- Molecule 85: Ribosomal protein uS14



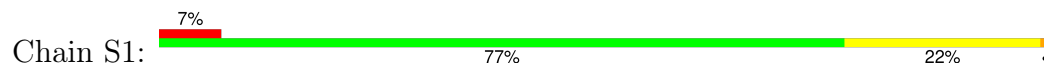
- Molecule 86: Ribosomal protein eS31



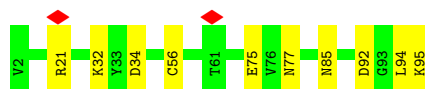
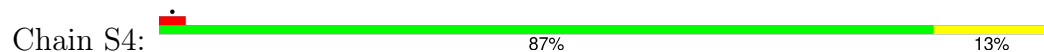
- Molecule 87: Ribosomal protein RACK1



- Molecule 88: SRP9



- Molecule 89: SRP14



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	52061	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	27	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.638	Depositor
Minimum map value	-0.471	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.05	Depositor
Map size ( $\text{\AA}$ )	562.8, 562.8, 562.8	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.3399999, 1.3399999, 1.3399999	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.70	1/1906 (0.1%)	1.25	19/2556 (0.7%)
2	D	0.67	2/2426 (0.1%)	1.17	25/3252 (0.8%)
3	G	0.78	8/1944 (0.4%)	1.10	14/2618 (0.5%)
4	H	0.77	2/1537 (0.1%)	1.10	10/2066 (0.5%)
5	J	0.69	2/1382 (0.1%)	1.09	15/1849 (0.8%)
6	L	0.68	3/1734 (0.2%)	1.05	7/2318 (0.3%)
7	M	0.63	1/1152 (0.1%)	1.10	5/1539 (0.3%)
8	N	0.72	3/1746 (0.2%)	1.25	11/2338 (0.5%)
9	O	0.63	2/1684 (0.1%)	1.08	11/2251 (0.5%)
10	Q	0.68	2/1530 (0.1%)	1.31	32/2041 (1.6%)
11	R	0.81	3/1524 (0.2%)	1.24	19/2013 (0.9%)
12	S	1.07	10/1493 (0.7%)	1.36	28/2002 (1.4%)
13	T	0.62	1/1326 (0.1%)	0.99	4/1770 (0.2%)
14	U	0.61	1/822 (0.1%)	0.99	2/1103 (0.2%)
15	V	0.57	0/993	0.98	2/1332 (0.2%)
16	X	0.56	0/993	0.95	3/1334 (0.2%)
17	Y	0.64	0/1132	1.17	12/1504 (0.8%)
18	Z	0.65	0/1130	1.14	8/1507 (0.5%)
19	a	0.66	0/1192	1.12	6/1591 (0.4%)
20	b	0.75	2/620 (0.3%)	1.17	7/819 (0.9%)
21	c	0.60	0/742	1.11	4/996 (0.4%)
22	d	0.69	2/903 (0.2%)	1.28	11/1216 (0.9%)
23	e	0.73	1/1071 (0.1%)	1.13	7/1429 (0.5%)
24	f	0.83	1/895 (0.1%)	1.28	10/1198 (0.8%)
25	g	0.59	0/916	1.14	8/1220 (0.7%)
26	h	0.55	0/1023	1.17	13/1350 (1.0%)
27	i	0.62	0/843	1.17	8/1115 (0.7%)
28	k	0.51	0/575	0.88	0/761
29	l	0.60	0/454	1.07	1/599 (0.2%)
30	m	0.47	0/435	0.95	1/575 (0.2%)
31	o	0.60	0/864	1.24	7/1140 (0.6%)
32	5	0.59	37/87703 (0.0%)	1.15	801/136805 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	7	0.52	0/2858	1.01	19/4455 (0.4%)
34	8	0.60	1/3701 (0.0%)	1.17	40/5766 (0.7%)
35	B	0.76	6/3214 (0.2%)	1.10	13/4308 (0.3%)
36	C	0.68	4/2973 (0.1%)	1.07	14/3990 (0.4%)
37	E	0.68	3/1941 (0.2%)	1.17	15/2601 (0.6%)
38	F	0.68	0/1905	1.17	13/2539 (0.5%)
39	I	0.59	1/1753 (0.1%)	1.05	8/2343 (0.3%)
40	P	0.77	3/1268 (0.2%)	1.15	12/1701 (0.7%)
41	W	0.73	0/541	1.17	3/720 (0.4%)
42	j	0.82	1/721 (0.1%)	1.31	12/953 (1.3%)
43	n	0.72	0/223	1.11	0/284
44	p	0.60	1/718 (0.1%)	1.00	4/953 (0.4%)
45	r	0.57	0/1017	1.05	4/1365 (0.3%)
46	K	0.76	2/1256 (0.2%)	1.17	6/1694 (0.4%)
47	q	0.73	2/1580 (0.1%)	0.93	5/2133 (0.2%)
48	z	0.92	7/3171 (0.2%)	0.95	10/4257 (0.2%)
49	2	0.50	0/234	0.99	1/317 (0.3%)
50	3	1.56	2/1804 (0.1%)	1.07	7/2805 (0.2%)
51	4	0.77	1/5090 (0.0%)	1.05	13/7936 (0.2%)
52	9	0.35	0/858	0.58	0/1156
53	6	0.29	0/1521	0.49	0/2039
54	S2	0.59	27/41241 (0.1%)	1.15	365/64249 (0.6%)
55	SA	0.63	1/1679 (0.1%)	1.05	10/2283 (0.4%)
56	SB	0.74	6/1753 (0.3%)	1.12	15/2350 (0.6%)
57	SC	0.69	1/1726 (0.1%)	1.05	14/2332 (0.6%)
58	SE	0.64	2/2118 (0.1%)	1.09	15/2849 (0.5%)
59	SG	0.69	4/1946 (0.2%)	1.05	8/2590 (0.3%)
60	SH	0.51	0/1544	0.94	5/2068 (0.2%)
61	SI	0.76	3/1715 (0.2%)	1.11	12/2287 (0.5%)
62	SJ	0.59	1/1550 (0.1%)	1.20	12/2069 (0.6%)
63	SL	0.66	1/1259 (0.1%)	1.05	4/1684 (0.2%)
64	SN	0.60	0/1226	1.05	7/1649 (0.4%)
65	SO	0.61	0/1029	1.23	13/1380 (0.9%)
66	SV	0.54	0/631	0.93	0/844
67	SW	0.65	1/1051 (0.1%)	1.04	6/1406 (0.4%)
68	SX	0.60	0/1118	1.06	9/1493 (0.6%)
69	SY	0.54	0/1040	0.94	0/1382
70	Sa	0.71	1/794 (0.1%)	1.17	6/1065 (0.6%)
71	Sb	0.48	0/665	0.90	1/891 (0.1%)
72	Se	0.50	0/458	0.97	3/602 (0.5%)
73	SD	0.60	1/1793 (0.1%)	1.01	5/2414 (0.2%)
74	SF	0.62	2/1531 (0.1%)	1.00	6/2059 (0.3%)
75	SK	0.58	0/851	1.01	5/1147 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	SM	0.69	0/970	1.05	6/1300 (0.5%)
77	SP	0.87	2/816 (0.2%)	1.19	10/1084 (0.9%)
78	SQ	0.51	0/1142	1.08	12/1528 (0.8%)
79	SR	0.50	0/1060	0.73	0/1421
80	SS	0.46	0/1157	0.99	5/1548 (0.3%)
81	ST	0.61	1/1119 (0.1%)	1.05	3/1499 (0.2%)
82	SU	0.52	0/828	0.92	0/1112
83	SZ	0.47	0/604	0.84	0/810
84	Sc	0.57	2/507 (0.4%)	0.75	0/677
85	Sd	0.66	0/445	1.12	2/589 (0.3%)
86	Sf	0.96	3/593 (0.5%)	1.61	15/786 (1.9%)
87	Sg	0.56	0/2493	0.85	3/3394 (0.1%)
88	S1	1.04	4/619 (0.6%)	0.90	1/832 (0.1%)
89	S4	0.88	2/608 (0.3%)	0.77	0/809
All	All	0.64	183/244716 (0.1%)	1.12	1888/359004 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
2	D	0	9
3	G	0	4
4	H	0	2
5	J	0	2
6	L	0	4
7	M	0	3
8	N	0	9
9	O	0	4
10	Q	0	5
11	R	0	7
12	S	0	8
13	T	0	2
15	V	0	3
16	X	0	2
17	Y	0	3
18	Z	0	1
19	a	0	6
20	b	0	2
21	c	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
22	d	0	5
23	e	0	1
24	f	0	2
25	g	0	2
26	h	0	1
27	i	0	3
28	k	0	1
30	m	0	1
31	o	0	3
32	5	0	175
33	7	0	2
34	8	0	11
35	B	0	12
36	C	0	4
37	E	0	16
38	F	0	8
39	I	0	3
40	P	0	4
41	W	0	1
42	j	0	4
44	p	0	2
45	r	0	3
46	K	0	10
47	q	0	8
48	z	0	7
49	2	0	1
54	S2	0	59
55	SA	0	5
56	SB	0	7
57	SC	0	7
58	SE	0	6
59	SG	0	1
60	SH	0	2
61	SI	0	9
62	SJ	0	3
63	SL	0	3
64	SN	0	5
65	SO	0	1
66	SV	0	3
67	SW	0	3
68	SX	0	2
69	SY	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
70	Sa	0	3
71	Sb	0	1
73	SD	0	3
74	SF	0	4
75	SK	0	1
76	SM	0	2
77	SP	0	3
78	SQ	0	1
80	SS	0	1
81	ST	0	2
82	SU	0	1
83	SZ	0	1
85	Sd	0	3
86	Sf	0	4
87	Sg	0	3
88	S1	0	4
All	All	0	529

All (183) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	3	31	C	O3'-P	-62.24	0.86	1.61
51	4	183	A	O3'-P	-44.16	1.08	1.61
32	5	1823	G	O3'-P	35.59	2.03	1.61
48	z	340	MET	C-N	22.92	1.86	1.34
48	z	345	PHE	C-N	-18.40	0.91	1.34
4	H	66	GLU	CD-OE1	18.38	1.45	1.25
12	S	96	GLU	CD-OE1	17.58	1.45	1.25
48	z	25	GLU	CD-OE2	16.69	1.44	1.25
50	3	39	G	O3'-P	-15.04	1.43	1.61
89	S4	75	GLU	CD-OE1	15.04	1.42	1.25
48	z	25	GLU	CD-OE1	14.70	1.41	1.25
11	R	149	LYS	C-N	14.54	1.67	1.34
77	SP	21	ASP	CG-OD1	13.73	1.56	1.25
35	B	59	GLU	CD-OE2	13.66	1.40	1.25
59	SG	35	GLU	CD-OE1	13.65	1.40	1.25
12	S	96	GLU	CD-OE2	13.63	1.40	1.25
88	S1	8	GLU	CD-OE1	13.55	1.40	1.25
3	G	54	PHE	CB-CG	-12.51	1.30	1.51
47	q	93	GLU	CD-OE1	12.47	1.39	1.25
5	J	14	GLU	CD-OE1	12.01	1.38	1.25
6	L	119	GLU	CD-OE1	11.70	1.38	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	S	81	TRP	CB-CG	-11.64	1.29	1.50
88	S1	44	ASP	CG-OD2	11.45	1.51	1.25
57	SC	90	GLU	CD-OE1	10.83	1.37	1.25
4	H	66	GLU	CD-OE2	10.68	1.37	1.25
61	SI	99	ASN	CG-OD1	10.66	1.47	1.24
89	S4	75	GLU	CD-OE2	10.61	1.37	1.25
48	z	198	GLU	CD-OE2	10.43	1.37	1.25
54	S2	1292	C	O3'-P	10.07	1.73	1.61
46	K	9	GLU	C-N	-9.96	1.11	1.34
88	S1	8	GLU	CD-OE2	9.90	1.36	1.25
11	R	95	TRP	CB-CG	-9.90	1.32	1.50
24	f	6	TRP	CB-CG	-9.73	1.32	1.50
48	z	198	GLU	CD-OE1	9.71	1.36	1.25
35	B	215	GLU	CD-OE1	9.29	1.35	1.25
12	S	81	TRP	CA-CB	9.25	1.74	1.53
61	SI	99	ASN	CG-ND2	9.22	1.55	1.32
56	SB	224	GLU	CD-OE2	9.15	1.35	1.25
36	C	35	ASP	CG-OD1	9.06	1.46	1.25
54	S2	1309	C	O3'-P	8.97	1.72	1.61
54	S2	1290	G	O3'-P	8.95	1.71	1.61
77	SP	21	ASP	CG-OD2	8.70	1.45	1.25
3	G	109	GLU	CD-OE2	8.67	1.35	1.25
74	SF	127	ARG	CZ-NH1	8.51	1.44	1.33
63	SL	27	GLU	CD-OE2	8.43	1.34	1.25
36	C	35	ASP	CB-CG	8.41	1.69	1.51
20	b	16	TRP	CB-CG	-8.40	1.35	1.50
40	P	139	TYR	CB-CG	-8.35	1.39	1.51
54	S2	1291	A	O3'-P	7.96	1.70	1.61
88	S1	44	ASP	CG-OD1	7.73	1.43	1.25
59	SG	205	GLU	CD-OE2	7.64	1.34	1.25
37	E	278	TYR	CB-CG	-7.53	1.40	1.51
35	B	74	GLU	CD-OE1	7.42	1.33	1.25
40	P	139	TYR	CA-CB	7.28	1.70	1.53
32	5	4390	A	O3'-P	-7.28	1.52	1.61
32	5	964	A	O3'-P	7.26	1.69	1.61
32	5	4497	U	O3'-P	7.24	1.69	1.61
37	E	278	TYR	CA-CB	7.24	1.69	1.53
59	SG	35	GLU	CD-OE2	7.23	1.33	1.25
5	J	14	GLU	CD-OE2	7.16	1.33	1.25
32	5	514	U	O3'-P	7.10	1.69	1.61
3	G	109	GLU	CG-CD	7.06	1.62	1.51
32	5	1887	G	O3'-P	6.99	1.69	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	54	PHE	N-CA	6.97	1.60	1.46
3	G	46	GLN	CD-NE2	6.94	1.50	1.32
3	G	57	TRP	CB-CG	-6.93	1.37	1.50
84	Sc	26	GLN	CD-OE1	6.74	1.38	1.24
70	Sa	46	GLU	CD-OE1	6.74	1.33	1.25
54	S2	1838	U	O3'-P	6.71	1.69	1.61
8	N	119	TYR	CB-CG	-6.70	1.41	1.51
32	5	3729	U	C4-O4	-6.69	1.18	1.23
58	SE	121	TYR	CB-CG	-6.69	1.41	1.51
54	S2	409	C	O3'-P	6.65	1.69	1.61
54	S2	662	G	O3'-P	6.63	1.69	1.61
6	L	119	GLU	CD-OE2	6.54	1.32	1.25
3	G	54	PHE	CA-CB	6.53	1.68	1.53
12	S	10	TYR	CB-CG	-6.50	1.41	1.51
32	5	2362	U	O3'-P	6.50	1.69	1.61
32	5	1669	A	O3'-P	-6.47	1.53	1.61
11	R	132	PHE	CB-CG	-6.45	1.40	1.51
32	5	1365	C	O3'-P	6.44	1.68	1.61
46	K	2	PRO	CA-C	6.43	1.65	1.52
10	Q	34	PHE	CA-CB	6.39	1.68	1.53
42	j	49	TRP	CB-CG	-6.37	1.38	1.50
32	5	1364	U	O3'-P	6.34	1.68	1.61
32	5	171	U	O3'-P	-6.34	1.53	1.61
59	SG	205	GLU	CD-OE1	6.30	1.32	1.25
48	z	54	GLU	CD-OE2	6.28	1.32	1.25
13	T	111	GLU	CD-OE1	6.25	1.32	1.25
55	SA	151	ASP	CB-CG	6.25	1.64	1.51
74	SF	152	TRP	CB-CG	-6.24	1.39	1.50
32	5	1632	A	O3'-P	6.23	1.68	1.61
32	5	2037	C	C2-O2	-6.23	1.18	1.24
12	S	10	TYR	CA-CB	6.22	1.67	1.53
32	5	2278	G	O3'-P	6.21	1.68	1.61
32	5	3652	A	O3'-P	6.15	1.68	1.61
32	5	3905	A	O3'-P	6.14	1.68	1.61
35	B	257	TRP	CA-CB	6.12	1.67	1.53
54	S2	1378	A	O3'-P	6.10	1.68	1.61
32	5	1522	G	O3'-P	6.08	1.68	1.61
39	I	171	TRP	CB-CG	-6.08	1.39	1.50
54	S2	1623	A	O3'-P	6.06	1.68	1.61
32	5	45	U	O3'-P	-6.05	1.53	1.61
56	SB	198	GLU	CG-CD	6.00	1.60	1.51
86	Sf	146	LEU	CA-CB	5.98	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	SI	27	TYR	CB-CG	-5.97	1.42	1.51
32	5	3635	A	O3'-P	5.95	1.68	1.61
32	5	4464	A	O3'-P	5.93	1.68	1.61
32	5	2268	A	O3'-P	5.92	1.68	1.61
2	D	44	TYR	CA-CB	5.90	1.67	1.53
67	SW	49	GLU	CD-OE1	5.90	1.32	1.25
32	5	2459	G	O3'-P	5.90	1.68	1.61
54	S2	1207	G	O3'-P	-5.86	1.54	1.61
32	5	1883	G	O3'-P	-5.85	1.54	1.61
54	S2	999	G	O3'-P	5.85	1.68	1.61
36	C	262	GLU	CD-OE2	5.85	1.32	1.25
73	SD	192	TRP	CB-CG	5.78	1.60	1.50
54	S2	294	U	O3'-P	5.77	1.68	1.61
81	ST	33	TRP	CA-CB	5.75	1.66	1.53
56	SB	157	GLN	CD-OE1	5.73	1.36	1.24
58	SE	18	TRP	CA-CB	5.73	1.66	1.53
36	C	111	TRP	CB-CG	-5.72	1.40	1.50
84	Sc	26	GLN	CD-NE2	5.71	1.47	1.32
32	5	1756	U	C4-O4	-5.68	1.19	1.23
56	SB	205	TYR	CB-CG	-5.67	1.43	1.51
54	S2	639	C	O3'-P	-5.64	1.54	1.61
47	q	93	GLU	CD-OE2	5.63	1.31	1.25
54	S2	876	C	O3'-P	5.63	1.68	1.61
7	M	6	PHE	CB-CG	-5.61	1.41	1.51
32	5	1946	G	O3'-P	5.61	1.67	1.61
12	S	152	PHE	CB-CG	-5.59	1.41	1.51
54	S2	9	U	O3'-P	5.56	1.67	1.61
12	S	33	PHE	CB-CG	-5.51	1.42	1.51
56	SB	81	PHE	CB-CG	-5.51	1.42	1.51
12	S	94	TYR	CE1-CZ	-5.51	1.31	1.38
54	S2	1473	G	O3'-P	5.51	1.67	1.61
23	e	35	TRP	CB-CG	-5.49	1.40	1.50
32	5	2520	C	O3'-P	-5.47	1.54	1.61
8	N	119	TYR	CA-CB	5.45	1.66	1.53
32	5	1681	G	O3'-P	5.43	1.67	1.61
20	b	16	TRP	CA-CB	5.42	1.65	1.53
32	5	4566	U	O3'-P	-5.42	1.54	1.61
32	5	1301	C	O3'-P	5.40	1.67	1.61
54	S2	427	U	O5'-C5'	5.37	1.53	1.44
44	p	18	TYR	CB-CG	-5.37	1.43	1.51
14	U	99	TRP	CB-CG	-5.36	1.40	1.50
32	5	3875	G	O3'-P	5.36	1.67	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	SB	198	GLU	CD-OE2	5.34	1.31	1.25
32	5	85	G	O3'-P	5.33	1.67	1.61
54	S2	92	A	O3'-P	5.31	1.67	1.61
3	G	53	ARG	CA-C	5.30	1.66	1.52
9	O	173	GLN	CD-OE1	5.28	1.35	1.24
6	L	31	ARG	CZ-NH2	5.24	1.39	1.33
22	d	108	TYR	CB-CG	-5.22	1.43	1.51
32	5	3653	A	O3'-P	5.22	1.67	1.61
54	S2	1170	A	O3'-P	-5.21	1.54	1.61
54	S2	1341	C	O3'-P	5.20	1.67	1.61
54	S2	1293	A	O3'-P	5.20	1.67	1.61
54	S2	1839	U	O3'-P	5.20	1.67	1.61
32	5	2034	G	O3'-P	5.20	1.67	1.61
32	5	2253	A	O3'-P	5.19	1.67	1.61
86	Sf	149	CYS	N-CA	5.19	1.56	1.46
54	S2	1659	U	O3'-P	5.19	1.67	1.61
8	N	120	TRP	CE3-CZ3	-5.19	1.29	1.38
10	Q	34	PHE	CB-CG	-5.17	1.42	1.51
40	P	139	TYR	CD1-CE1	-5.17	1.31	1.39
54	S2	426	A	O3'-P	5.17	1.67	1.61
1	A	211	PHE	CB-CG	-5.17	1.42	1.51
86	Sf	150	PHE	CB-CG	5.16	1.60	1.51
32	5	2667	C	O3'-P	-5.15	1.54	1.61
62	SJ	34	GLU	CG-CD	5.14	1.59	1.51
34	8	73	U	O3'-P	5.12	1.67	1.61
35	B	257	TRP	CE3-CZ3	-5.11	1.29	1.38
54	S2	440	G	O3'-P	-5.10	1.55	1.61
9	O	162	GLU	CD-OE1	5.10	1.31	1.25
2	D	95	TYR	CA-CB	5.08	1.65	1.53
54	S2	427	U	C5'-C4'	5.06	1.57	1.51
32	5	1609	U	O3'-P	5.06	1.67	1.61
54	S2	1370	A	O3'-P	5.05	1.67	1.61
35	B	367	PHE	CB-CG	-5.05	1.42	1.51
22	d	25	TYR	CB-CG	-5.03	1.44	1.51
12	S	29	ARG	CA-CB	5.03	1.65	1.53
37	E	250	ASP	CG-OD2	5.02	1.36	1.25

All (1888) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	3	38	C	P-O3'-C3'	-20.63	94.95	119.70
48	z	340	MET	O-C-N	19.47	153.86	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	3	31	C	O3'-P-O5'	-18.73	68.40	104.00
48	z	340	MET	C-N-CA	-18.61	75.16	121.70
86	Sf	146	LEU	CA-CB-CG	16.39	153.01	115.30
48	z	340	MET	CA-C-N	-16.04	81.91	117.20
54	S2	3	C	N1-C1'-C2'	15.72	134.44	114.00
54	S2	1838	U	N1-C1'-C2'	14.63	133.02	114.00
32	5	1501	C	N1-C1'-C2'	14.21	132.48	114.00
54	S2	92	A	N9-C1'-C2'	13.95	132.13	114.00
32	5	1501	C	O4'-C1'-N1	12.75	118.40	108.20
32	5	1697	G	N9-C1'-C2'	12.65	130.45	114.00
54	S2	367	U	N1-C1'-C2'	-12.62	97.60	114.00
54	S2	294	U	N1-C1'-C2'	12.60	130.38	114.00
32	5	2396	A	N9-C1'-C2'	12.07	129.69	114.00
1	A	67	TYR	CA-CB-CG	12.04	136.27	113.40
70	Sa	28	ARG	NE-CZ-NH1	12.03	126.31	120.30
54	S2	428	U	N1-C1'-C2'	11.81	129.36	114.00
54	S2	1835	A	N9-C1'-C2'	11.76	129.29	114.00
32	5	336	A	O4'-C1'-N9	11.76	117.60	108.20
54	S2	447	A	O4'-C1'-N9	11.74	117.59	108.20
32	5	2513	A	N9-C1'-C2'	11.64	129.13	114.00
32	5	1	C	N1-C1'-C2'	11.61	129.09	114.00
48	z	345	PHE	C-N-CA	11.60	150.71	121.70
3	G	54	PHE	CB-CG-CD1	-11.57	112.70	120.80
32	5	2361	G	N9-C1'-C2'	-11.49	99.06	114.00
54	S2	1063	C	N1-C1'-C2'	-11.45	99.11	114.00
32	5	664	G	O4'-C1'-N9	11.38	117.30	108.20
54	S2	1452	A	N9-C1'-C2'	11.37	128.78	114.00
32	5	2046	G	O4'-C1'-N9	11.27	117.22	108.20
51	4	186	C	O3'-P-O5'	-11.25	82.62	104.00
32	5	151	G	N9-C1'-C2'	-11.22	99.41	114.00
32	5	5040	U	N1-C1'-C2'	11.22	128.59	114.00
32	5	336	A	C8-N9-C1'	-11.09	107.73	127.70
32	5	1370	G	N9-C1'-C2'	11.05	128.36	114.00
32	5	4234	A	N9-C1'-C2'	11.03	128.34	114.00
32	5	2268	A	N9-C1'-C2'	11.02	128.33	114.00
54	S2	1247	C	N1-C1'-C2'	11.01	128.31	114.00
1	A	3	ARG	NE-CZ-NH1	11.00	125.80	120.30
32	5	2438	A	N9-C1'-C2'	-10.97	99.74	114.00
54	S2	1823	A	N9-C1'-C2'	10.88	128.15	114.00
32	5	1938	C	N1-C1'-C2'	10.87	128.13	114.00
32	5	2586	G	N9-C1'-C2'	10.78	128.01	114.00
32	5	4911	A	O4'-C1'-N9	10.72	116.78	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	4693	C	O4'-C1'-N1	-10.70	99.64	108.20
11	R	132	PHE	CB-CA-C	10.66	131.72	110.40
32	5	2436	U	N1-C1'-C2'	10.62	127.81	114.00
32	5	2806	A	N9-C1'-C2'	-10.61	100.21	114.00
32	5	4373	G	N9-C1'-C2'	10.59	127.77	114.00
37	E	278	TYR	CA-CB-CG	-10.56	93.34	113.40
32	5	4871	C	N1-C1'-C2'	10.48	127.63	114.00
32	5	2389	A	C2'-C3'-O3'	10.45	132.49	109.50
32	5	2394	G	N9-C1'-C2'	-10.42	100.46	114.00
32	5	4275	G	N9-C1'-C2'	-10.40	100.47	114.00
34	8	70	G	N9-C1'-C2'	-10.40	100.47	114.00
32	5	2553	A	N9-C1'-C2'	10.34	127.44	114.00
33	7	56	G	N9-C1'-C2'	10.32	127.42	114.00
26	h	93	ARG	NE-CZ-NH1	10.30	125.45	120.30
32	5	4162	C	N1-C1'-C2'	10.27	127.35	114.00
12	S	81	TRP	CA-CB-CG	-10.24	94.24	113.70
54	S2	1088	U	N1-C1'-C2'	10.21	127.27	114.00
32	5	2465	C	N1-C1'-C2'	10.20	127.26	114.00
32	5	280	G	O4'-C1'-N9	10.14	116.31	108.20
32	5	30	C	N1-C1'-C2'	10.13	127.17	114.00
32	5	4163	U	C4'-C3'-O3'	10.12	133.25	113.00
54	S2	421	G	N9-C1'-C2'	10.12	127.15	114.00
77	SP	21	ASP	CB-CG-OD1	-10.11	109.20	118.30
32	5	3938	G	N9-C1'-C2'	10.09	127.11	114.00
86	Sf	119	ARG	NE-CZ-NH1	10.07	125.34	120.30
54	S2	437	G	N9-C1'-C2'	10.07	127.09	114.00
34	8	85	U	C2'-C3'-O3'	10.04	131.59	109.50
34	8	14	U	N1-C1'-C2'	10.01	127.02	114.00
3	G	54	PHE	CB-CG-CD2	-10.00	113.80	120.80
54	S2	1552	G	C2'-C3'-O3'	9.99	131.49	109.50
10	Q	34	PHE	N-CA-CB	9.97	128.56	110.60
65	SO	146	ARG	NE-CZ-NH2	-9.97	115.32	120.30
11	R	108	ARG	NE-CZ-NH1	9.92	125.26	120.30
22	d	85	ARG	NE-CZ-NH1	9.89	125.25	120.30
54	S2	1408	U	N1-C1'-C2'	9.88	126.84	114.00
62	SJ	127	ARG	NE-CZ-NH1	9.86	125.23	120.30
32	5	4528	G	C2'-C3'-O3'	9.83	131.13	109.50
32	5	1398	A	N9-C1'-C2'	9.80	126.75	114.00
32	5	1474	C	C2'-C3'-O3'	9.78	131.01	109.50
19	a	79	TRP	CA-CB-CG	-9.77	95.14	113.70
42	j	11	ARG	NE-CZ-NH2	-9.75	115.42	120.30
86	Sf	143	LYS	CD-CE-NZ	9.75	134.12	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	S	81	TRP	CB-CA-C	9.74	129.89	110.40
32	5	4464	A	O4'-C1'-N9	-9.74	100.40	108.20
62	SJ	131	ARG	NE-CZ-NH2	-9.73	115.43	120.30
32	5	4404	U	N1-C1'-C2'	-9.72	101.31	112.00
32	5	5043	A	N9-C1'-C2'	9.72	126.64	114.00
42	j	66	HIS	N-CA-CB	9.72	128.09	110.60
54	S2	833	C	C2'-C3'-O3'	9.71	130.85	109.50
10	Q	37	ARG	NE-CZ-NH2	9.69	125.15	120.30
32	5	3938	G	O4'-C1'-N9	-9.69	100.45	108.20
32	5	4693	C	N1-C1'-C2'	9.65	126.54	114.00
78	SQ	71	ARG	NE-CZ-NH1	9.63	125.11	120.30
22	d	44	ARG	NE-CZ-NH1	9.63	125.11	120.30
20	b	44	ARG	NE-CZ-NH1	9.60	125.10	120.30
46	K	9	GLU	O-C-N	-9.58	107.37	122.70
31	o	78	ARG	NE-CZ-NH2	9.57	125.09	120.30
37	E	278	TYR	CB-CA-C	9.56	129.51	110.40
32	5	93	G	N9-C1'-C2'	9.55	126.42	114.00
32	5	2666	U	N1-C1'-C2'	-9.54	101.51	112.00
32	5	1974	U	N1-C1'-C2'	9.53	126.39	114.00
32	5	2446	C	N1-C1'-C2'	9.52	126.38	114.00
22	d	25	TYR	CA-CB-CG	-9.50	95.35	113.40
32	5	31	U	N1-C1'-C2'	9.49	126.34	114.00
27	i	85	ARG	NE-CZ-NH1	9.47	125.04	120.30
32	5	2087	C	N1-C1'-C2'	-9.47	101.59	112.00
4	H	54	ARG	NE-CZ-NH1	9.42	125.01	120.30
54	S2	666	U	N1-C1'-C2'	9.40	126.22	114.00
8	N	131	GLU	CA-CB-CG	9.39	134.07	113.40
61	SI	197	PHE	N-CA-CB	9.39	127.51	110.60
32	5	1815	G	N9-C1'-C2'	9.39	126.21	114.00
32	5	4221	C	N1-C1'-C2'	-9.39	101.67	112.00
9	O	135	PHE	N-CA-C	9.37	136.30	111.00
7	M	109	ARG	NE-CZ-NH2	9.32	124.96	120.30
55	SA	117	ARG	NE-CZ-NH1	9.32	124.96	120.30
32	5	2851	G	N9-C1'-C2'	-9.30	101.77	112.00
32	5	4265	U	N1-C1'-C2'	9.29	126.08	114.00
32	5	1211	G	C2'-C3'-O3'	9.27	129.89	109.50
54	S2	1249	C	N1-C1'-C2'	-9.27	101.80	112.00
54	S2	313	A	O4'-C1'-N9	9.25	115.60	108.20
54	S2	1838	U	O4'-C1'-N1	-9.24	100.81	108.20
32	5	2511	A	C4'-C3'-O3'	-9.22	90.04	109.40
32	5	974	C	C2'-C3'-O3'	9.22	129.78	109.50
77	SP	81	ARG	NE-CZ-NH1	9.22	124.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	S2	631	U	N1-C1'-C2'	9.20	125.95	114.00
32	5	3790	U	N1-C1'-C2'	9.19	125.94	114.00
11	R	132	PHE	N-CA-C	-9.16	86.26	111.00
32	5	1853	G	N9-C1'-C2'	-9.15	101.93	112.00
5	J	54	ARG	NE-CZ-NH1	9.14	124.87	120.30
3	G	235	ARG	NE-CZ-NH1	9.12	124.86	120.30
32	5	4228	G	N9-C1'-C2'	-9.09	102.00	112.00
11	R	132	PHE	CB-CG-CD1	-9.09	114.44	120.80
62	SJ	69	ARG	NE-CZ-NH2	9.08	124.84	120.30
32	5	1379	C	O4'-C1'-N1	9.07	115.45	108.20
3	G	57	TRP	CA-CB-CG	-9.04	96.53	113.70
25	g	66	ARG	NE-CZ-NH1	9.03	124.81	120.30
54	S2	73	C	O4'-C1'-N1	9.03	115.42	108.20
32	5	5046	U	C2'-C3'-O3'	9.02	129.34	109.50
17	Y	87	ARG	NE-CZ-NH2	9.01	124.81	120.30
32	5	1358	G	C4'-C3'-O3'	9.01	131.02	113.00
54	S2	1429	G	C2'-C3'-O3'	9.01	129.31	109.50
7	M	6	PHE	CB-CG-CD2	-9.00	114.50	120.80
87	Sg	125	ARG	NE-CZ-NH2	-8.99	115.80	120.30
32	5	1324	A	N9-C1'-C2'	8.97	125.67	114.00
32	5	1214	C	N1-C1'-C2'	8.97	125.66	114.00
57	SC	200	ARG	NE-CZ-NH2	8.96	124.78	120.30
58	SE	103	TYR	CA-CB-CG	8.94	130.39	113.40
32	5	1296	G	O4'-C1'-N9	8.93	115.34	108.20
32	5	62	A	N9-C1'-C2'	8.91	125.58	114.00
67	SW	57	ARG	NE-CZ-NH1	8.91	124.76	120.30
54	S2	1292	C	C4'-C3'-O3'	8.91	130.81	113.00
80	SS	86	ARG	NE-CZ-NH1	-8.86	115.87	120.30
65	SO	147	ARG	CA-CB-CG	8.81	132.79	113.40
54	S2	1313	A	N9-C1'-C2'	8.81	125.45	114.00
32	5	315	G	O4'-C1'-N9	8.80	115.24	108.20
24	f	36	ARG	NE-CZ-NH1	8.79	124.69	120.30
32	5	1668	A	N9-C1'-C2'	8.79	125.43	114.00
5	J	35	ARG	NE-CZ-NH1	8.78	124.69	120.30
32	5	514	U	N1-C1'-C2'	-8.77	102.35	112.00
32	5	1887	G	N9-C1'-C2'	-8.75	102.37	112.00
54	S2	1419	C	C2'-C3'-O3'	8.75	128.75	109.50
44	p	85	ARG	NE-CZ-NH1	8.74	124.67	120.30
18	Z	36	ARG	NE-CZ-NH1	8.74	124.67	120.30
32	5	336	A	C1'-O4'-C4'	-8.74	102.91	109.90
19	a	62	HIS	N-CA-CB	8.73	126.32	110.60
81	ST	62	ARG	NE-CZ-NH2	8.73	124.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	SS	124	ARG	NE-CZ-NH1	8.72	124.66	120.30
68	SX	27	TYR	CA-CB-CG	8.72	129.96	113.40
78	SQ	138	ARG	NE-CZ-NH1	8.71	124.66	120.30
32	5	3683	C	N1-C1'-C2'	8.70	125.30	114.00
32	5	3906	A	N9-C1'-C2'	-8.70	102.44	112.00
32	5	3908	A	N9-C1'-C2'	8.69	125.29	114.00
32	5	150	U	O4'-C1'-N1	8.68	115.15	108.20
40	P	3	ARG	NE-CZ-NH1	8.68	124.64	120.30
32	5	2263	A	O4'-C1'-N9	-8.67	101.26	108.20
2	D	265	ARG	NE-CZ-NH1	8.67	124.64	120.30
64	SN	18	TYR	N-CA-CB	8.66	126.19	110.60
17	Y	75	ARG	CG-CD-NE	8.63	129.93	111.80
32	5	72	C	O4'-C1'-N1	8.60	115.08	108.20
54	S2	399	C	N1-C1'-C2'	-8.59	102.55	112.00
34	8	81	C	O4'-C1'-N1	8.58	115.07	108.20
54	S2	747	U	C2'-C3'-O3'	8.58	128.37	109.50
32	5	1916	G	N9-C1'-C2'	8.56	125.14	114.00
32	5	2406	G	N9-C1'-C2'	-8.56	102.58	112.00
32	5	4880	C	N1-C1'-C2'	8.55	125.11	114.00
39	I	171	TRP	CA-CB-CG	-8.55	97.46	113.70
32	5	1534	A	O4'-C1'-N9	-8.54	101.37	108.20
32	5	336	A	C4-N9-C1'	8.54	141.66	126.30
32	5	3868	G	N9-C1'-C2'	-8.51	102.64	112.00
32	5	292	G	N9-C1'-C2'	8.50	125.05	114.00
32	5	962	C	N1-C1'-C2'	8.50	125.05	114.00
54	S2	1623	A	C2'-C3'-O3'	8.50	128.19	109.50
54	S2	448	A	N9-C1'-C2'	-8.49	102.66	112.00
32	5	92	C	N1-C1'-C2'	-8.48	102.67	112.00
32	5	118	C	C2'-C3'-O3'	8.45	128.10	109.50
32	5	1631	A	O4'-C1'-N9	-8.45	101.44	108.20
32	5	1637	A	N9-C1'-C2'	-8.45	102.70	112.00
32	5	42	A	O4'-C1'-N9	8.45	114.96	108.20
32	5	4464	A	C2'-C3'-O3'	8.45	128.08	109.50
8	N	180	PHE	CB-CA-C	8.44	127.28	110.40
12	S	28	TYR	CB-CG-CD1	8.43	126.06	121.00
32	5	2796	G	N9-C1'-C2'	8.42	124.95	114.00
32	5	2398	U	C2'-C3'-O3'	8.42	128.02	109.50
32	5	5001	U	N1-C1'-C2'	8.42	124.94	114.00
32	5	4234	A	O4'-C1'-N9	-8.41	101.47	108.20
65	SO	146	ARG	NE-CZ-NH1	8.40	124.50	120.30
32	5	1325	C	N1-C1'-C2'	8.39	124.91	114.00
54	S2	596	U	N1-C1'-C2'	8.39	124.91	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	4194	U	N1-C1'-C2'	-8.38	102.78	112.00
32	5	3879	G	N9-C1'-C2'	-8.38	102.78	112.00
54	S2	1114	U	N1-C1'-C2'	8.37	124.88	114.00
54	S2	1578	U	N1-C1'-C2'	8.37	124.88	114.00
54	S2	91	A	N9-C1'-C2'	-8.36	102.80	112.00
32	5	4280	A	N9-C1'-C2'	-8.36	102.80	112.00
9	O	140	ARG	NE-CZ-NH2	8.36	124.48	120.30
21	c	56	ARG	NE-CZ-NH1	8.36	124.48	120.30
32	5	4280	A	C2'-C3'-O3'	8.36	127.89	109.50
32	5	292	G	O4'-C1'-N9	-8.35	101.52	108.20
32	5	1329	G	C2'-C3'-O3'	8.34	127.85	109.50
17	Y	126	ARG	NE-CZ-NH1	8.33	124.46	120.30
32	5	3790	U	O4'-C1'-N1	-8.31	101.55	108.20
56	SB	107	ARG	NE-CZ-NH1	8.30	124.45	120.30
32	5	4119	C	C2'-C3'-O3'	8.30	127.76	109.50
54	S2	956	G	N9-C1'-C2'	8.30	124.79	114.00
32	5	668	C	C2'-C3'-O3'	8.29	127.75	109.50
32	5	2280	G	N9-C1'-C2'	8.29	124.78	114.00
32	5	1946	G	N9-C1'-C2'	-8.29	102.88	112.00
54	S2	645	C	N1-C1'-C2'	-8.29	102.88	112.00
54	S2	604	A	C2'-C3'-O3'	8.28	127.72	109.50
32	5	1356	U	C2'-C3'-O3'	8.28	127.71	109.50
32	5	4464	A	C5'-C4'-O4'	8.27	119.02	109.10
32	5	977	C	C2'-C3'-O3'	8.26	127.67	109.50
32	5	2848	G	N9-C1'-C2'	-8.22	102.96	112.00
32	5	1481	C	C2'-C3'-O3'	8.22	127.58	109.50
32	5	1522	G	N9-C1'-C2'	-8.21	102.97	112.00
32	5	1890	G	N9-C1'-C2'	-8.21	102.97	112.00
32	5	2124	G	C2'-C3'-O3'	8.20	127.53	109.50
32	5	964	A	C4'-C3'-O3'	8.17	129.35	113.00
16	X	73	HIS	CB-CA-C	8.17	126.74	110.40
32	5	157	U	O4'-C1'-N1	8.17	114.74	108.20
32	5	4885	U	C2'-C3'-O3'	8.17	127.48	109.50
54	S2	1167	G	N9-C1'-C2'	8.17	124.62	114.00
22	d	25	TYR	CB-CA-C	8.17	126.73	110.40
32	5	5040	U	C4'-C3'-O3'	-8.15	92.28	109.40
56	SB	205	TYR	CA-CB-CG	-8.15	97.92	113.40
32	5	1685	G	N9-C1'-C2'	8.14	124.59	114.00
32	5	157	U	N1-C1'-C2'	-8.14	103.05	112.00
19	a	79	TRP	CB-CA-C	8.14	126.67	110.40
32	5	72	C	C1'-O4'-C4'	-8.14	103.39	109.90
32	5	2046	G	C1'-O4'-C4'	-8.14	103.39	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	8	34	U	C4'-C3'-O3'	-8.14	92.31	109.40
74	SF	127	ARG	NE-CZ-NH2	-8.13	116.23	120.30
32	5	1805	A	N9-C1'-C2'	8.13	124.57	114.00
32	5	1650	A	C4-N9-C1'	-8.13	111.67	126.30
58	SE	30	ARG	NE-CZ-NH1	8.13	124.36	120.30
32	5	1272	C	O4'-C1'-N1	8.12	114.70	108.20
36	C	78	ARG	NE-CZ-NH1	8.12	124.36	120.30
54	S2	1352	G	C2'-C3'-O3'	8.12	127.36	109.50
32	5	1881	C	N1-C1'-C2'	8.11	124.55	114.00
68	SX	5	ARG	NE-CZ-NH2	8.11	124.36	120.30
32	5	2271	C	N1-C1'-C2'	8.11	124.54	114.00
32	5	4163	U	N1-C1'-C2'	-8.10	103.09	112.00
50	3	31	C	OP2-P-O3'	8.09	122.99	105.20
77	SP	10	ARG	NE-CZ-NH1	8.07	124.34	120.30
54	S2	1519	U	N1-C1'-C2'	8.06	124.48	114.00
54	S2	1225	U	N1-C1'-C2'	-8.06	103.14	112.00
32	5	172	C	O4'-C1'-N1	8.05	114.64	108.20
32	5	4464	A	N9-C1'-C2'	8.05	124.46	114.00
32	5	3635	A	N9-C1'-C2'	-8.05	103.15	112.00
32	5	3905	A	C2'-C3'-O3'	8.04	127.20	109.50
54	S2	73	C	N1-C1'-C2'	8.04	124.46	114.00
32	5	187	U	C2'-C3'-O3'	8.04	127.19	109.50
41	W	44	ARG	NE-CZ-NH1	8.04	124.32	120.30
32	5	1365	C	N1-C1'-C2'	8.04	124.45	114.00
32	5	2394	G	O4'-C1'-N9	8.03	114.62	108.20
37	E	268	ARG	NE-CZ-NH1	8.03	124.31	120.30
64	SN	18	TYR	CA-CB-CG	-8.02	98.16	113.40
39	I	4	ARG	CG-CD-NE	-8.01	94.98	111.80
54	S2	798	A	C2'-C3'-O3'	7.99	127.08	109.50
25	g	9	ARG	CG-CD-NE	-7.99	95.03	111.80
32	5	1279	A	C2'-C3'-O3'	7.98	127.06	109.50
32	5	2790	U	N1-C1'-C2'	7.97	124.36	114.00
32	5	3880	G	N9-C1'-C2'	7.96	124.35	114.00
32	5	3735	G	C2'-C3'-O3'	7.96	127.01	109.50
12	S	10	TYR	CA-CB-CG	-7.96	98.28	113.40
32	5	88	A	N9-C1'-C2'	7.95	124.34	114.00
32	5	4693	C	C2'-C3'-O3'	7.95	126.98	109.50
58	SE	86	PHE	N-CA-CB	7.94	124.90	110.60
4	H	125	ARG	NE-CZ-NH1	7.94	124.27	120.30
32	5	4169	G	N9-C1'-C2'	7.92	124.30	114.00
54	S2	662	G	N9-C1'-C2'	7.91	124.29	114.00
32	5	5066	U	N1-C1'-C2'	7.91	124.28	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	4379	A	N9-C1'-C2'	-7.91	103.31	112.00
32	5	219	G	O5'-P-OP2	-7.90	98.59	105.70
1	A	242	ARG	NE-CZ-NH1	7.90	124.25	120.30
32	5	53	C	C2'-C3'-O3'	7.89	126.86	109.50
32	5	1552	G	N9-C1'-C2'	-7.89	103.32	112.00
32	5	5006	U	N1-C1'-C2'	-7.88	103.33	112.00
32	5	4911	A	C1'-O4'-C4'	-7.88	103.60	109.90
32	5	1379	C	N1-C1'-C2'	7.87	124.24	114.00
54	S2	1394	G	C2'-C3'-O3'	7.87	126.82	109.50
56	SB	165	ARG	NE-CZ-NH2	7.87	124.23	120.30
34	8	35	C	N1-C1'-C2'	7.86	124.22	114.00
86	Sf	138	ARG	NE-CZ-NH1	7.86	124.23	120.30
32	5	1359	G	C2'-C3'-O3'	7.85	126.77	109.50
32	5	2282	A	N9-C1'-C2'	7.85	124.20	114.00
32	5	2369	U	N1-C1'-C2'	-7.83	103.39	112.00
77	SP	18	ARG	NE-CZ-NH1	7.83	124.22	120.30
68	SX	20	HIS	CB-CA-C	7.83	126.05	110.40
32	5	1930	U	N1-C1'-C2'	7.82	124.17	114.00
32	5	1521	C	N1-C1'-C2'	-7.82	103.40	112.00
54	S2	92	A	O4'-C1'-N9	-7.81	101.95	108.20
32	5	29	G	N9-C1'-C2'	7.81	124.16	114.00
34	8	38	U	O4'-C1'-N1	7.81	114.45	108.20
1	A	193	ARG	CG-CD-NE	-7.80	95.41	111.80
32	5	978	G	C2'-C3'-O3'	7.80	126.67	109.50
32	5	2658	G	N9-C1'-C2'	-7.80	103.42	112.00
3	G	53	ARG	NE-CZ-NH2	-7.80	116.40	120.30
32	5	4693	C	C5'-C4'-O4'	7.78	118.44	109.10
32	5	1379	C	C1'-O4'-C4'	-7.77	103.68	109.90
32	5	4463	U	N1-C1'-C2'	-7.77	103.46	112.00
54	S2	1668	U	N1-C1'-C2'	7.76	124.09	114.00
54	S2	41	G	N9-C1'-C2'	-7.76	103.47	112.00
58	SE	86	PHE	CB-CG-CD1	-7.76	115.37	120.80
32	5	3625	G	C2'-C3'-O3'	7.75	126.55	109.50
27	i	39	PHE	N-CA-CB	7.75	124.55	110.60
32	5	54	G	N9-C1'-C2'	-7.74	103.48	112.00
32	5	350	C	N1-C1'-C2'	7.74	124.06	114.00
32	5	2046	G	C2'-C3'-O3'	7.74	126.52	109.50
32	5	4498	U	N1-C1'-C2'	-7.74	103.49	112.00
32	5	4718	G	N9-C1'-C2'	-7.74	103.49	112.00
32	5	4976	U	O4'-C1'-N1	-7.74	102.01	108.20
32	5	1455	G	C2'-C3'-O3'	7.73	126.52	109.50
33	7	72	U	C2'-C3'-O3'	7.72	126.49	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	S2	110	U	C2'-C3'-O3'	7.72	126.48	109.50
54	S2	1407	U	N1-C1'-C2'	7.72	124.03	114.00
76	SM	127	TYR	CA-CB-CG	7.70	128.03	113.40
17	Y	27	ARG	NE-CZ-NH2	7.70	124.15	120.30
32	5	2119	C	O4'-C1'-N1	7.69	114.35	108.20
32	5	1649	U	N1-C1'-C2'	7.69	124.00	114.00
54	S2	1168	G	N9-C1'-C2'	7.69	124.00	114.00
47	q	99	ARG	CG-CD-NE	7.68	127.93	111.80
32	5	2263	A	C5'-C4'-O4'	7.68	118.32	109.10
46	K	9	GLU	C-N-CA	7.68	140.90	121.70
54	S2	1194	A	N9-C1'-C2'	-7.68	103.56	112.00
11	R	149	LYS	C-N-CA	-7.67	102.54	121.70
32	5	352	G	N9-C1'-C2'	-7.66	103.57	112.00
76	SM	33	ARG	NE-CZ-NH1	7.66	124.13	120.30
32	5	353	A	N9-C1'-C2'	-7.66	103.58	112.00
54	S2	1697	A	C4-N9-C1'	7.65	140.08	126.30
32	5	3663	A	O4'-C1'-N9	-7.65	102.08	108.20
32	5	5056	A	N9-C1'-C2'	7.65	123.94	114.00
54	S2	662	G	O4'-C1'-N9	-7.64	102.08	108.20
2	D	54	ARG	CG-CD-NE	-7.64	95.76	111.80
54	S2	825	A	N9-C1'-C2'	7.63	123.92	114.00
10	Q	75	ARG	NE-CZ-NH1	7.63	124.12	120.30
54	S2	1109	C	O4'-C1'-N1	7.63	114.31	108.20
54	S2	642	U	N1-C1'-C2'	-7.63	103.61	112.00
62	SJ	131	ARG	NE-CZ-NH1	7.63	124.11	120.30
32	5	4737	G	N9-C1'-C2'	7.62	123.91	114.00
54	S2	1606	G	N9-C1'-C2'	-7.62	103.61	112.00
32	5	2082	G	N9-C1'-C2'	7.62	123.91	114.00
32	5	300	A	C4-N9-C1'	7.62	140.02	126.30
56	SB	82	ARG	CG-CD-NE	-7.62	95.80	111.80
32	5	42	A	C1'-O4'-C4'	-7.62	103.81	109.90
54	S2	313	A	C1'-O4'-C4'	-7.61	103.81	109.90
54	S2	1419	C	O5'-P-OP2	-7.60	98.86	105.70
54	S2	1697	A	C8-N9-C1'	-7.60	114.03	127.70
40	P	23	ARG	NE-CZ-NH1	7.59	124.09	120.30
61	SI	197	PHE	CB-CA-C	-7.59	95.22	110.40
7	M	17	PHE	CB-CG-CD2	7.59	126.11	120.80
32	5	2827	G	O4'-C1'-N9	-7.58	102.14	108.20
32	5	2246	C	C2'-C3'-O3'	7.58	126.17	109.50
32	5	958	G	C2'-C3'-O3'	7.57	126.16	109.50
32	5	33	A	N9-C1'-C2'	7.57	123.84	114.00
32	5	664	G	C1'-O4'-C4'	-7.57	103.84	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	315	G	C1'-O4'-C4'	-7.57	103.84	109.90
54	S2	1395	C	C2'-C3'-O3'	7.57	126.15	109.50
19	a	34	ASN	CB-CA-C	7.56	125.52	110.40
54	S2	1842	C	N1-C1'-C2'	7.56	123.83	114.00
26	h	89	ARG	NE-CZ-NH1	7.55	124.07	120.30
32	5	946	C	O4'-C1'-N1	7.54	114.24	108.20
26	h	117	ARG	CG-CD-NE	-7.54	95.96	111.80
32	5	3843	C	N1-C1'-C2'	7.54	123.81	114.00
8	N	139	HIS	N-CA-CB	7.54	124.17	110.60
32	5	58	G	N9-C1'-C2'	7.54	123.80	114.00
54	S2	3	C	O4'-C1'-N1	7.53	114.22	108.20
10	Q	26	ARG	NE-CZ-NH2	-7.52	116.54	120.30
32	5	1	C	C5'-C4'-O4'	7.52	118.13	109.10
32	5	4876	U	N1-C1'-C2'	7.52	123.77	114.00
32	5	3817	A	N9-C1'-C2'	7.52	123.77	114.00
32	5	94	A	N9-C1'-C2'	7.51	123.77	114.00
40	P	139	TYR	CB-CG-CD1	-7.51	116.49	121.00
51	4	37	C	C2'-C3'-O3'	7.50	126.01	109.50
39	I	171	TRP	N-CA-CB	7.50	124.10	110.60
32	5	1292	C	C2'-C3'-O3'	7.50	125.99	109.50
32	5	1534	A	N9-C1'-C2'	7.50	123.75	114.00
54	S2	427	U	C5'-C4'-O4'	7.49	118.09	109.10
65	SO	121	ARG	NE-CZ-NH1	7.49	124.05	120.30
32	5	454	U	C2'-C3'-O3'	7.49	125.97	109.50
32	5	3735	G	C4'-C3'-O3'	-7.49	93.68	109.40
74	SF	51	HIS	N-CA-CB	7.48	124.06	110.60
32	5	300	A	C8-N9-C1'	-7.47	114.25	127.70
75	SK	68	TYR	CA-CB-CG	-7.46	99.22	113.40
54	S2	1109	C	N1-C1'-C2'	7.46	123.70	114.00
32	5	4371	G	O4'-C1'-N9	7.46	114.17	108.20
54	S2	1603	G	N9-C1'-C2'	7.46	123.69	114.00
1	A	37	ARG	NE-CZ-NH2	-7.45	116.57	120.30
36	C	35	ASP	CB-CG-OD1	7.45	125.00	118.30
32	5	3875	G	N9-C1'-C2'	-7.45	103.81	112.00
70	Sa	22	ARG	NE-CZ-NH2	-7.44	116.58	120.30
32	5	147	A	N9-C1'-C2'	7.44	123.67	114.00
32	5	4723	A	C4-N9-C1'	7.44	139.69	126.30
34	8	81	C	C1'-O4'-C4'	-7.44	103.95	109.90
34	8	104	A	O4'-C1'-N9	-7.44	102.25	108.20
32	5	4497	U	N1-C1'-C2'	-7.44	103.82	112.00
32	5	235	A	N9-C1'-C2'	-7.43	103.82	112.00
54	S2	1433	C	C4'-C3'-O3'	7.43	127.87	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	44	TYR	CB-CA-C	7.43	125.26	110.40
3	G	53	ARG	CA-CB-CG	7.43	129.75	113.40
54	S2	1623	A	N9-C1'-C2'	-7.43	103.83	112.00
32	5	209	U	C4'-C3'-O3'	7.42	127.84	113.00
32	5	2797	C	N1-C1'-C2'	-7.42	103.84	112.00
32	5	2517	A	N9-C1'-C2'	7.41	123.64	114.00
32	5	332	C	N1-C1'-C2'	7.41	123.64	114.00
32	5	3882	C	N1-C1'-C2'	7.41	123.63	114.00
54	S2	822	U	N1-C1'-C2'	7.41	123.63	114.00
32	5	1676	C	C1'-C2'-O2'	-7.40	88.40	110.60
54	S2	821	G	O4'-C1'-N9	-7.40	102.28	108.20
54	S2	161	U	N1-C1'-C2'	7.40	123.61	114.00
54	S2	829	C	N1-C1'-C2'	-7.39	103.87	112.00
34	8	94	G	O4'-C1'-N9	-7.38	102.29	108.20
54	S2	1221	G	N9-C1'-C2'	7.37	123.58	114.00
54	S2	31	U	N1-C1'-C2'	7.37	123.58	114.00
58	SE	18	TRP	CB-CA-C	7.36	125.12	110.40
32	5	2553	A	O4'-C1'-N9	7.36	114.09	108.20
54	S2	30	C	N1-C1'-C2'	7.36	123.56	114.00
57	SC	170	TRP	CA-CB-CG	-7.36	99.72	113.70
32	5	1319	U	N1-C1'-C2'	-7.34	103.92	112.00
54	S2	55	U	N1-C1'-C2'	7.34	123.55	114.00
32	5	1642	A	C4'-C3'-O3'	-7.34	93.98	109.40
1	A	189	TYR	CA-CB-CG	7.33	127.34	113.40
54	S2	447	A	C1'-O4'-C4'	-7.33	104.04	109.90
54	S2	968	U	N1-C1'-C2'	-7.32	103.95	112.00
4	H	60	TRP	CB-CA-C	7.32	125.03	110.40
32	5	84	A	O4'-C1'-N9	-7.32	102.34	108.20
32	5	1214	C	O4'-C1'-N1	-7.32	102.35	108.20
32	5	1894	C	N1-C1'-C2'	7.32	123.51	114.00
32	5	4120	U	N1-C1'-C2'	-7.31	103.95	112.00
32	5	4272	G	N9-C1'-C2'	7.31	123.50	114.00
58	SE	3	ARG	NE-CZ-NH1	7.31	123.95	120.30
54	S2	1085	C	N1-C1'-C2'	7.30	123.49	114.00
32	5	4282	A	N9-C1'-C2'	7.30	123.49	114.00
2	D	35	ARG	NE-CZ-NH1	7.29	123.95	120.30
32	5	4723	A	C8-N9-C1'	-7.29	114.57	127.70
74	SF	122	ARG	NE-CZ-NH1	7.29	123.95	120.30
32	5	85	G	O4'-C1'-N9	7.29	114.03	108.20
32	5	4336	A	N9-C1'-C2'	-7.28	103.99	112.00
34	8	73	U	N1-C1'-C2'	-7.28	104.00	112.00
32	5	3677	U	N1-C1'-C2'	7.27	123.45	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	54	G	C2'-C3'-O3'	7.26	125.48	109.50
32	5	1364	U	C2'-C3'-O3'	7.26	125.48	109.50
32	5	432	U	N1-C1'-C2'	-7.26	104.02	112.00
54	S2	746	C	C2'-C3'-O3'	7.26	125.47	109.50
54	S2	532	C	C2'-C3'-O3'	7.24	125.43	109.50
42	j	11	ARG	NE-CZ-NH1	7.24	123.92	120.30
32	5	3905	A	N9-C1'-C2'	-7.23	104.04	112.00
32	5	1377	G	C2'-C3'-O3'	7.23	125.40	109.50
86	Sf	146	LEU	CB-CG-CD1	7.23	123.29	111.00
32	5	1500	A	C4'-C3'-O3'	7.22	127.44	113.00
32	5	4600	G	N9-C1'-C2'	-7.22	104.06	112.00
38	F	120	PHE	CB-CA-C	7.22	124.84	110.40
5	J	119	TYR	CA-CB-CG	7.21	127.11	113.40
32	5	2597	G	N9-C1'-C2'	7.21	123.37	114.00
54	S2	1059	G	N9-C1'-C2'	7.21	123.37	114.00
54	S2	1452	A	C2'-C3'-O3'	7.21	125.36	109.50
19	a	61	TYR	CB-CA-C	7.20	124.80	110.40
56	SB	28	ARG	NE-CZ-NH1	7.20	123.90	120.30
61	SI	55	TYR	CA-CB-CG	-7.20	99.73	113.40
54	S2	1341	C	N1-C1'-C2'	7.19	123.35	114.00
86	Sf	95	ARG	NE-CZ-NH1	7.19	123.90	120.30
32	5	394	G	N9-C1'-C2'	-7.19	104.09	112.00
32	5	406	C	C2'-C3'-O3'	7.19	125.31	109.50
34	8	86	U	O4'-C1'-C2'	-7.18	98.62	105.80
8	N	131	GLU	CB-CA-C	7.18	124.76	110.40
32	5	2511	A	O4'-C1'-N9	-7.18	102.46	108.20
20	b	7	HIS	CB-CA-C	-7.18	96.05	110.40
54	S2	1701	C	N1-C1'-C2'	7.17	123.33	114.00
32	5	125	C	C2'-C3'-O3'	7.15	125.24	109.50
12	S	157	ARG	CG-CD-NE	7.15	126.81	111.80
32	5	2511	A	C2'-C3'-O3'	7.15	125.23	109.50
32	5	171	U	C4'-C3'-O3'	-7.14	94.40	109.40
32	5	4279	A	N9-C1'-C2'	-7.14	104.14	112.00
32	5	1650	A	O4'-C1'-N9	-7.14	102.48	108.20
65	SO	147	ARG	CG-CD-NE	-7.14	96.80	111.80
32	5	929	A	N9-C1'-C2'	-7.13	104.15	112.00
12	S	29	ARG	CG-CD-NE	-7.13	96.82	111.80
54	S2	594	A	N9-C1'-C2'	-7.13	104.15	112.00
17	Y	78	TYR	CB-CA-C	7.13	124.66	110.40
40	P	42	ARG	NE-CZ-NH1	7.13	123.87	120.30
54	S2	1567	G	O4'-C1'-N9	7.13	113.90	108.20
54	S2	1664	A	C2'-C3'-O3'	7.13	125.18	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	SL	62	PHE	CB-CA-C	7.12	124.65	110.40
32	5	514	U	C2'-C3'-O3'	7.12	125.16	109.50
32	5	1893	C	N1-C1'-C2'	7.12	123.25	114.00
54	S2	91	A	C2'-C3'-O3'	7.12	125.16	109.50
54	S2	165	G	O4'-C1'-N9	7.12	113.90	108.20
32	5	52	G	C2'-C3'-O3'	7.12	125.16	109.50
38	F	58	HIS	CB-CA-C	-7.11	96.18	110.40
54	S2	841	G	O4'-C1'-C2'	-7.11	98.69	105.80
54	S2	1082	A	N9-C1'-C2'	7.10	123.23	114.00
32	5	226	G	N9-C1'-C2'	-7.10	104.19	112.00
26	h	78	TYR	CA-CB-CG	-7.10	99.92	113.40
32	5	4979	A	N9-C1'-C2'	7.09	123.22	114.00
54	S2	427	U	N1-C1'-C2'	7.09	123.21	114.00
32	5	4966	A	N9-C1'-C2'	7.08	123.21	114.00
32	5	3883	U	N1-C1'-C2'	7.08	123.20	114.00
32	5	2695	A	C2'-C3'-O3'	7.08	125.07	109.50
32	5	4945	G	O5'-P-OP1	-7.08	99.33	105.70
31	o	57	ARG	NE-CZ-NH1	7.07	123.84	120.30
35	B	367	PHE	CB-CG-CD1	-7.07	115.85	120.80
32	5	4518	A	O5'-P-OP2	-7.07	99.33	105.70
32	5	1067	G	C2'-C3'-O3'	7.07	125.05	109.50
54	S2	980	A	C2'-C3'-O3'	7.07	125.05	109.50
32	5	1992	U	N1-C1'-C2'	7.07	123.19	114.00
32	5	3653	A	N9-C1'-C2'	-7.06	104.23	112.00
1	A	211	PHE	CB-CA-C	7.06	124.51	110.40
54	S2	349	A	C2'-C3'-O3'	7.06	125.03	109.50
32	5	267	G	C2'-C3'-O3'	7.05	125.01	109.50
32	5	1534	A	C5'-C4'-O4'	7.04	117.55	109.10
36	C	41	HIS	N-CA-CB	7.04	123.28	110.60
18	Z	38	TYR	N-CA-C	-7.04	92.00	111.00
18	Z	75	TYR	CA-CB-CG	7.03	126.76	113.40
54	S2	1556	A	N9-C1'-C2'	7.03	123.14	114.00
27	i	39	PHE	CB-CG-CD1	-7.02	115.88	120.80
54	S2	957	A	N9-C1'-C2'	7.02	123.13	114.00
9	O	178	ARG	NE-CZ-NH1	7.02	123.81	120.30
12	S	167	PHE	CB-CG-CD1	-7.01	115.89	120.80
32	5	5061	A	C2'-C3'-O3'	7.01	124.93	109.50
32	5	1398	A	O4'-C1'-N9	7.01	113.81	108.20
54	S2	1293	A	C4'-C3'-O3'	7.01	127.02	113.00
32	5	3692	A	C2'-C3'-O3'	7.01	124.91	109.50
32	5	2443	G	N9-C1'-C2'	7.00	123.10	114.00
36	C	311	ARG	NE-CZ-NH2	-7.00	116.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	157	U	C1'-O4'-C4'	-7.00	104.30	109.90
32	5	2546	G	C4'-C3'-O3'	7.00	127.00	113.00
12	S	167	PHE	CB-CG-CD2	7.00	125.70	120.80
32	5	3729	U	C2'-C3'-O3'	6.99	124.88	113.70
32	5	2632	U	N1-C1'-C2'	6.99	123.08	114.00
32	5	4497	U	C2'-C3'-O3'	6.99	124.88	113.70
32	5	279	A	C4'-C3'-O3'	-6.98	94.74	109.40
32	5	3691	G	N9-C1'-C2'	6.98	123.08	114.00
32	5	4378	A	O4'-C1'-N9	6.98	113.79	108.20
54	S2	845	G	N9-C1'-C2'	6.98	123.08	114.00
54	S2	1453	C	O4'-C1'-N1	6.98	113.78	108.20
32	5	48	G	C2'-C3'-O3'	6.98	124.87	113.70
32	5	97	G	N9-C1'-C2'	-6.98	104.32	112.00
54	S2	1529	C	N1-C1'-C2'	6.97	123.07	114.00
16	X	48	ARG	NE-CZ-NH2	-6.97	116.81	120.30
32	5	1998	A	N9-C1'-C2'	6.97	123.06	114.00
32	5	2581	A	N9-C1'-C2'	6.97	123.06	114.00
32	5	3692	A	N9-C1'-C2'	-6.96	104.34	112.00
54	S2	631	U	O4'-C1'-N1	-6.96	102.63	108.20
54	S2	1114	U	O4'-C1'-N1	6.96	113.77	108.20
32	5	84	A	N9-C1'-C2'	6.96	123.04	114.00
32	5	4599	A	N9-C1'-C2'	6.95	123.04	114.00
32	5	4986	G	N9-C1'-C2'	6.95	123.04	114.00
40	P	139	TYR	CA-CB-CG	-6.95	100.19	113.40
54	S2	1350	U	C2'-C3'-O3'	6.95	124.83	113.70
32	5	3667	C	C2'-C3'-O3'	6.94	124.81	113.70
26	h	119	PHE	CB-CA-C	-6.94	96.52	110.40
8	N	143	ARG	CG-CD-NE	-6.93	97.24	111.80
32	5	1355	G	N9-C1'-C2'	6.92	123.00	114.00
58	SE	103	TYR	CB-CG-CD1	-6.92	116.84	121.00
10	Q	91	ARG	NE-CZ-NH2	6.92	123.76	120.30
32	5	2054	U	C1'-O4'-C4'	-6.92	104.36	109.90
32	5	2319	C	N1-C1'-C2'	6.92	123.00	114.00
32	5	2463	G	N9-C1'-C2'	6.92	122.99	114.00
32	5	3739	C	O4'-C1'-C2'	-6.91	98.89	105.80
55	SA	103	PHE	N-CA-CB	6.91	123.03	110.60
32	5	1937	C	N1-C1'-C2'	6.90	122.97	114.00
34	8	94	G	C2'-C3'-O3'	6.89	124.73	113.70
32	5	100	C	N1-C1'-C2'	-6.88	104.43	112.00
32	5	747	A	C2'-C3'-O3'	6.88	124.71	113.70
32	5	4238	G	N9-C1'-C2'	-6.88	104.44	112.00
32	5	4589	A	O4'-C1'-N9	-6.87	102.71	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	SM	33	ARG	CG-CD-NE	6.87	126.22	111.80
32	5	4510	A	O4'-C1'-N9	-6.86	102.71	108.20
45	r	45	HIS	N-CA-CB	-6.86	98.25	110.60
34	8	38	U	C1'-O4'-C4'	-6.86	104.41	109.90
11	R	95	TRP	N-CA-CB	6.86	122.94	110.60
54	S2	1567	G	C1'-O4'-C4'	-6.85	104.42	109.90
10	Q	33	ARG	CA-CB-CG	6.85	128.47	113.40
54	S2	393	U	O4'-C1'-N1	6.85	113.68	108.20
12	S	29	ARG	CA-CB-CG	6.85	128.46	113.40
32	5	53	C	N1-C1'-C2'	-6.84	104.47	112.00
32	5	2623	A	C4-N9-C1'	6.84	138.62	126.30
54	S2	1114	U	C1'-O4'-C4'	-6.84	104.43	109.90
32	5	979	C	C2'-C3'-O3'	6.83	124.63	113.70
32	5	235	A	O4'-C1'-N9	6.83	113.67	108.20
36	C	80	ARG	NE-CZ-NH1	6.83	123.72	120.30
34	8	79	G	N9-C1'-C2'	6.83	122.88	114.00
32	5	2467	U	N1-C1'-C2'	-6.83	104.49	112.00
65	SO	149	ARG	NE-CZ-NH1	6.82	123.71	120.30
33	7	84	U	N1-C1'-C2'	6.81	122.85	114.00
34	8	66	A	N9-C1'-C2'	6.81	122.85	114.00
54	S2	1144	A	C4-N9-C1'	6.81	138.56	126.30
32	5	1501	C	C1'-O4'-C4'	-6.81	104.45	109.90
32	5	4170	A	N9-C1'-C2'	6.81	122.85	114.00
32	5	2270	G	N9-C1'-C2'	6.80	122.84	114.00
32	5	486	C	C2'-C3'-O3'	6.80	124.58	113.70
32	5	2081	C	N1-C1'-C2'	6.80	122.84	114.00
24	f	4	ARG	CA-CB-CG	6.79	128.34	113.40
32	5	43	U	C5'-C4'-O4'	6.79	117.25	109.10
9	O	49	ARG	CG-CD-NE	-6.79	97.55	111.80
6	L	34	ARG	NE-CZ-NH1	6.79	123.69	120.30
32	5	514	U	C5'-C4'-O4'	6.78	117.24	109.10
32	5	100	C	C2'-C3'-O3'	6.78	124.55	113.70
32	5	4224	A	N9-C1'-C2'	-6.78	104.54	112.00
54	S2	965	U	N1-C1'-C2'	6.77	122.80	114.00
32	5	2307	A	N9-C1'-C2'	6.77	122.80	114.00
59	SG	156	TYR	CA-CB-CG	-6.76	100.55	113.40
32	5	450	G	N9-C1'-C2'	-6.76	104.56	112.00
60	SH	177	TYR	N-CA-CB	6.76	122.77	110.60
12	S	83	ARG	CG-CD-NE	6.76	125.99	111.80
54	S2	1850	A	N9-C1'-C2'	6.76	122.78	114.00
54	S2	924	G	N9-C1'-C2'	-6.75	104.57	112.00
10	Q	58	ARG	NE-CZ-NH1	6.74	123.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	SA	117	ARG	NE-CZ-NH2	-6.74	116.93	120.30
32	5	1934	A	N9-C1'-C2'	-6.74	104.59	112.00
32	5	4950	U	N1-C1'-C2'	6.74	122.76	114.00
32	5	2588	C	C4'-C3'-O3'	6.73	126.47	113.00
32	5	1614	C	C2'-C3'-O3'	6.73	124.47	113.70
54	S2	1552	G	N9-C1'-C2'	-6.73	104.60	112.00
25	g	4	ARG	NE-CZ-NH2	-6.72	116.94	120.30
32	5	3775	A	N9-C1'-C2'	6.72	122.74	114.00
70	Sa	10	ARG	N-CA-C	-6.72	92.87	111.00
54	S2	1293	A	N9-C1'-C2'	6.71	122.73	114.00
54	S2	1401	A	C2'-C3'-O3'	6.71	124.44	113.70
1	A	37	ARG	NE-CZ-NH1	6.71	123.65	120.30
32	5	4238	G	C2'-C3'-O3'	6.70	124.42	113.70
54	S2	1150	A	N9-C1'-C2'	6.70	122.72	114.00
32	5	1789	C	N1-C1'-C2'	6.70	122.71	114.00
54	S2	1144	A	C8-N9-C1'	-6.70	115.64	127.70
32	5	4911	A	O5'-P-OP2	-6.69	99.68	105.70
51	4	186	C	OP2-P-O3'	6.69	119.92	105.20
54	S2	964	A	N9-C1'-C2'	6.69	122.69	114.00
54	S2	1678	A	N9-C1'-C2'	-6.69	104.64	112.00
34	8	13	G	N9-C1'-C2'	6.68	122.68	114.00
7	M	17	PHE	CB-CG-CD1	-6.67	116.13	120.80
32	5	3648	A	C1'-O4'-C4'	-6.67	104.56	109.90
3	G	62	ARG	NE-CZ-NH2	-6.67	116.97	120.30
32	5	43	U	N1-C1'-C2'	-6.67	104.67	112.00
18	Z	21	ARG	NE-CZ-NH1	6.66	123.63	120.30
32	5	2623	A	C8-N9-C1'	-6.66	115.71	127.70
32	5	1671	U	O4'-C1'-C2'	-6.65	99.15	105.80
32	5	3799	A	N9-C1'-C2'	6.65	122.65	114.00
77	SP	42	ARG	NE-CZ-NH2	-6.65	116.97	120.30
32	5	1440	U	C2'-C3'-O3'	6.65	124.34	113.70
32	5	1586	G	N9-C1'-C2'	6.65	122.65	114.00
65	SO	150	ARG	NE-CZ-NH2	6.65	123.63	120.30
32	5	3912	U	C1'-C2'-O2'	-6.65	90.65	110.60
32	5	2649	G	N9-C1'-C2'	6.65	122.64	114.00
32	5	1564	A	N9-C1'-C2'	6.64	122.64	114.00
32	5	4449	A	N9-C1'-C2'	-6.64	104.69	112.00
57	SC	241	PHE	N-CA-CB	6.64	122.56	110.60
32	5	920	C	C5'-C4'-O4'	6.64	117.06	109.10
32	5	291	U	N1-C1'-C2'	6.63	122.62	114.00
32	5	89	C	N1-C1'-C2'	6.63	122.62	114.00
27	i	4	ARG	NE-CZ-NH1	6.63	123.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	1740	C	N1-C1'-C2'	-6.63	104.71	112.00
32	5	4510	A	N9-C1'-C2'	6.63	122.61	114.00
54	S2	426	A	O4'-C1'-N9	6.62	113.50	108.20
32	5	1867	A	N9-C1'-C2'	6.62	122.60	114.00
62	SJ	138	ARG	NE-CZ-NH1	6.62	123.61	120.30
25	g	14	ASN	N-CA-CB	6.61	122.50	110.60
33	7	58	A	C2'-C3'-O3'	6.61	124.28	113.70
32	5	1479	G	N9-C1'-C2'	6.61	122.59	114.00
32	5	1390	G	N9-C1'-C2'	-6.60	104.74	112.00
54	S2	1591	C	C2'-C3'-O3'	6.60	124.27	113.70
86	Sf	148	TYR	CA-CB-CG	6.60	125.94	113.40
32	5	5044	A	N9-C1'-C2'	6.59	122.57	114.00
65	SO	41	PHE	CB-CG-CD1	6.58	125.41	120.80
26	h	78	TYR	CB-CA-C	6.58	123.56	110.40
32	5	4589	A	N9-C1'-C2'	6.58	122.56	114.00
34	8	68	G	N9-C1'-C2'	6.58	122.56	114.00
23	e	35	TRP	CA-CB-CG	-6.58	101.20	113.70
32	5	3611	A	N9-C1'-C2'	6.58	122.55	114.00
35	B	169	ARG	NE-CZ-NH1	6.58	123.59	120.30
32	5	292	G	C4-N9-C1'	-6.57	117.95	126.50
54	S2	1190	A	N9-C1'-C2'	6.57	122.55	114.00
61	SI	197	PHE	CB-CG-CD2	-6.57	116.20	120.80
1	A	34	PHE	N-CA-CB	6.57	122.43	110.60
54	S2	65	C	O4'-C1'-N1	6.57	113.45	108.20
32	5	384	A	N9-C1'-C2'	6.56	122.53	114.00
32	5	2317	C	N1-C1'-C2'	6.56	122.52	114.00
58	SE	121	TYR	CA-CB-CG	-6.55	100.95	113.40
25	g	66	ARG	NE-CZ-NH2	-6.55	117.02	120.30
32	5	171	U	N1-C1'-C2'	6.55	122.52	114.00
32	5	1631	A	C4'-C3'-O3'	-6.55	95.65	109.40
54	S2	385	G	N9-C1'-C2'	6.55	122.52	114.00
39	I	98	ARG	NE-CZ-NH2	6.55	123.57	120.30
32	5	1523	A	O5'-P-OP1	-6.55	99.81	105.70
32	5	1573	G	N9-C1'-C2'	6.54	122.51	114.00
23	e	46	ARG	NE-CZ-NH1	6.54	123.57	120.30
32	5	417	G	O4'-C1'-N9	6.54	113.43	108.20
32	5	421	C	N1-C1'-C2'	-6.54	104.81	112.00
32	5	1886	G	N9-C1'-C2'	-6.54	104.81	112.00
32	5	4976	U	C5'-C4'-O4'	6.53	116.94	109.10
40	P	54	GLN	CA-CB-CG	6.53	127.77	113.40
32	5	4341	C	N1-C1'-C2'	-6.53	104.82	112.00
48	z	344	PRO	O-C-N	-6.53	112.26	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	SJ	24	ARG	NE-CZ-NH1	6.52	123.56	120.30
64	SN	139	TRP	CA-CB-CG	6.52	126.09	113.70
32	5	4291	G	N9-C1'-C2'	6.52	122.47	114.00
32	5	2675	G	N9-C1'-C2'	-6.52	104.83	112.00
3	G	57	TRP	CB-CA-C	6.51	123.43	110.40
47	q	99	ARG	NE-CZ-NH1	6.51	123.56	120.30
32	5	1378	C	N1-C1'-C2'	6.51	122.46	114.00
37	E	278	TYR	CB-CG-CD2	-6.51	117.09	121.00
54	S2	850	C	N1-C1'-C2'	6.51	122.46	114.00
54	S2	454	U	N1-C1'-C2'	6.51	122.46	114.00
32	5	3723	A	C4-N9-C1'	6.50	138.01	126.30
54	S2	732	U	C2'-C3'-O3'	6.50	124.10	113.70
32	5	280	G	C1'-O4'-C4'	-6.50	104.70	109.90
32	5	4887	C	C2'-C3'-O3'	6.50	124.10	113.70
54	S2	919	A	C4'-C3'-O3'	6.49	125.99	113.00
32	5	1484	G	O4'-C4'-C3'	-6.49	97.51	104.00
54	S2	1868	U	N1-C1'-C2'	6.49	122.43	114.00
2	D	210	TYR	N-CA-CB	6.49	122.27	110.60
32	5	3827	G	N9-C1'-C2'	-6.49	104.87	112.00
51	4	186	C	C2-N1-C1'	6.49	125.94	118.80
32	5	4326	G	N9-C1'-C2'	6.48	122.42	114.00
16	X	48	ARG	NE-CZ-NH1	6.48	123.54	120.30
32	5	4871	C	O4'-C1'-N1	-6.48	103.02	108.20
32	5	4978	G	N9-C1'-C2'	6.48	122.42	114.00
32	5	1521	C	C2'-C3'-O3'	6.47	124.06	113.70
32	5	1658	G	N9-C1'-C2'	6.47	122.42	114.00
54	S2	26	U	C2'-C3'-O3'	6.47	124.06	113.70
8	N	150	TRP	CA-CB-CG	6.47	125.99	113.70
32	5	1882	U	O5'-P-OP1	-6.47	99.88	105.70
32	5	216	C	C2'-C3'-O3'	6.47	124.05	113.70
32	5	1932	A	N9-C1'-C2'	6.46	122.40	114.00
32	5	3871	A	N9-C1'-C2'	6.46	122.40	114.00
32	5	4500	U	O5'-P-OP1	-6.46	99.89	105.70
54	S2	666	U	C6-N1-C1'	-6.46	112.15	121.20
75	SK	2	LEU	CA-CB-CG	6.46	130.16	115.30
57	SC	236	PHE	N-CA-CB	6.45	122.20	110.60
54	S2	1394	G	O4'-C1'-C2'	-6.45	99.35	105.80
12	S	77	ASN	CB-CA-C	6.44	123.29	110.40
32	5	4378	A	N9-C1'-C2'	6.44	122.37	114.00
54	S2	1374	C	N1-C1'-C2'	6.44	122.37	114.00
54	S2	381	C	O4'-C1'-N1	-6.44	103.05	108.20
54	S2	1309	C	C4'-C3'-O3'	6.44	125.88	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	50	C	N1-C1'-C2'	6.44	122.37	114.00
62	SJ	147	PHE	CB-CG-CD1	6.44	125.31	120.80
46	K	95	GLN	N-CA-C	-6.43	93.64	111.00
54	S2	1292	C	P-O5'-C5'	6.43	131.19	120.90
32	5	2116	C	C2'-C3'-O3'	6.42	123.97	113.70
32	5	1696	C	C2'-C3'-O3'	6.42	123.97	113.70
68	SX	16	HIS	N-CA-CB	6.42	122.15	110.60
32	5	4556	U	O4'-C1'-N1	6.41	113.33	108.20
54	S2	426	A	C4'-C3'-O3'	6.41	125.82	113.00
22	d	85	ARG	NE-CZ-NH2	-6.40	117.10	120.30
54	S2	19	A	C2'-C3'-O3'	6.40	123.93	113.70
32	5	964	A	N9-C1'-C2'	-6.39	104.97	112.00
54	S2	968	U	C4'-C3'-O3'	6.39	125.79	113.00
32	5	4331	G	N9-C1'-C2'	-6.39	104.97	112.00
70	Sa	22	ARG	CG-CD-NE	-6.39	98.38	111.80
46	K	9	GLU	CA-C-N	6.39	131.25	117.20
2	D	198	HIS	CB-CA-C	6.38	123.16	110.40
32	5	4338	G	N9-C1'-C2'	-6.38	104.98	112.00
32	5	4731	G	O4'-C1'-N9	6.38	113.31	108.20
32	5	245	C	C2'-C3'-O3'	6.38	123.91	113.70
54	S2	841	G	N9-C1'-C2'	-6.38	104.98	112.00
32	5	4981	G	N9-C1'-C2'	-6.38	104.99	112.00
54	S2	393	U	O4'-C1'-C2'	-6.38	99.42	105.80
68	SX	67	ARG	NE-CZ-NH2	6.38	123.49	120.30
80	SS	86	ARG	NE-CZ-NH2	6.38	123.49	120.30
32	5	1379	C	C5'-C4'-O4'	6.37	116.75	109.10
78	SQ	85	ARG	NE-CZ-NH1	6.37	123.48	120.30
54	S2	666	U	C2-N1-C1'	6.37	125.34	117.70
54	S2	1857	G	N9-C1'-C2'	-6.37	105.00	112.00
77	SP	81	ARG	NE-CZ-NH2	-6.36	117.12	120.30
32	5	3723	A	C8-N9-C1'	-6.36	116.25	127.70
32	5	46	U	N1-C1'-C2'	6.35	122.26	114.00
39	I	139	ARG	CG-CD-NE	6.35	125.14	111.80
5	J	99	PHE	CB-CA-C	6.35	123.09	110.40
38	F	141	TYR	CA-CB-CG	6.35	125.46	113.40
32	5	2874	U	O4'-C1'-N1	-6.34	103.12	108.20
32	5	4076	G	N9-C1'-C2'	-6.34	105.02	112.00
1	A	211	PHE	CB-CG-CD2	-6.34	116.36	120.80
32	5	2118	G	C4'-C3'-O3'	6.34	125.67	113.00
32	5	4378	A	C1'-O4'-C4'	-6.33	104.83	109.90
32	5	1211	G	N9-C1'-C2'	-6.33	105.03	112.00
9	O	117	ARG	NE-CZ-NH1	6.33	123.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	4560	C	O4'-C1'-N1	-6.33	103.14	108.20
5	J	119	TYR	CB-CG-CD1	6.32	124.79	121.00
17	Y	6	PHE	CB-CA-C	6.32	123.04	110.40
37	E	59	TYR	N-CA-C	-6.32	93.93	111.00
59	SG	25	ARG	CG-CD-NE	-6.32	98.54	111.80
54	S2	1667	U	N1-C1'-C2'	6.31	122.21	114.00
32	5	2769	U	N1-C1'-C2'	-6.31	105.06	112.00
54	S2	1142	G	C2'-C3'-O3'	6.31	123.79	113.70
56	SB	165	ARG	CG-CD-NE	6.31	125.05	111.80
67	SW	44	HIS	CB-CA-C	6.30	123.01	110.40
50	3	46	G	N9-C1'-C2'	6.30	122.19	114.00
54	S2	9	U	C2'-C3'-O3'	6.30	123.78	113.70
74	SF	165	ASN	N-CA-CB	6.30	121.94	110.60
32	5	1887	G	C2'-C3'-O3'	6.29	123.77	113.70
32	5	2632	U	C2-N1-C1'	6.29	125.25	117.70
32	5	1211	G	C4'-C3'-O3'	6.29	125.58	113.00
32	5	4122	G	C2'-C3'-O3'	6.29	123.76	113.70
22	d	108	TYR	CA-CB-CG	-6.29	101.45	113.40
32	5	2075	G	C2'-C3'-O3'	6.28	123.75	113.70
2	D	210	TYR	CA-CB-CG	-6.28	101.47	113.40
32	5	1370	G	C1'-O4'-C4'	-6.28	104.88	109.90
59	SG	145	PHE	CB-CG-CD1	6.28	125.19	120.80
8	N	192	TRP	CA-CB-CG	6.28	125.62	113.70
32	5	4583	C	N1-C1'-C2'	-6.28	105.10	112.00
51	4	164	G	N3-C4-C5	6.27	131.74	128.60
54	S2	427	U	O4'-C1'-N1	-6.27	103.18	108.20
32	5	2470	C	O4'-C1'-C2'	-6.27	99.53	105.80
54	S2	340	C	C2'-C3'-O3'	6.27	123.73	113.70
32	5	2348	G	O4'-C1'-N9	-6.27	103.19	108.20
42	j	27	TYR	CA-CB-CG	-6.26	101.50	113.40
54	S2	104	A	C2'-C3'-O3'	6.26	123.72	113.70
9	O	106	ASP	CB-CG-OD1	-6.26	112.67	118.30
26	h	93	ARG	NE-CZ-NH2	-6.26	117.17	120.30
32	5	2529	A	C1'-O4'-C4'	-6.26	104.89	109.90
54	S2	1063	C	C1'-C2'-O2'	6.25	129.36	110.60
54	S2	9	U	N1-C1'-C2'	-6.25	105.12	112.00
32	5	3938	G	C5'-C4'-O4'	6.25	116.60	109.10
32	5	5022	U	C2'-C3'-O3'	6.25	123.70	113.70
51	4	235	G	P-O3'-C3'	6.25	127.20	119.70
85	Sd	46	TYR	CA-CB-CG	-6.25	101.53	113.40
32	5	1216	C	C2'-C3'-O3'	6.25	123.69	113.70
11	R	88	ARG	NE-CZ-NH1	6.24	123.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	S2	1584	G	N9-C1'-C2'	6.24	122.12	114.00
32	5	1613	A	C8-N9-C1'	-6.24	116.47	127.70
23	e	60	TYR	CB-CA-C	6.24	122.87	110.40
32	5	2827	G	N9-C1'-C2'	6.24	122.11	114.00
72	Se	38	TYR	CA-CB-CG	6.24	125.25	113.40
34	8	94	G	C5'-C4'-O4'	6.23	116.58	109.10
18	Z	75	TYR	CB-CG-CD2	6.23	124.74	121.00
32	5	3879	G	O4'-C1'-N9	6.23	113.18	108.20
32	5	2038	U	N1-C1'-C2'	6.23	122.09	114.00
54	S2	426	A	N9-C1'-C2'	-6.23	105.15	112.00
32	5	1210	C	N1-C1'-C2'	6.22	122.09	114.00
32	5	1615	C	N1-C1'-C2'	-6.22	105.16	112.00
32	5	2683	C	C2'-C3'-O3'	6.22	123.65	113.70
32	5	1285	U	O4'-C1'-N1	6.22	113.17	108.20
32	5	3648	A	O4'-C1'-N9	6.22	113.17	108.20
9	O	110	PRO	C-N-CD	-6.21	106.93	120.60
2	D	35	ARG	CG-CD-NE	6.21	124.85	111.80
32	5	1650	A	C8-N9-C1'	6.21	138.88	127.70
1	A	3	ARG	NE-CZ-NH2	-6.21	117.20	120.30
10	Q	33	ARG	NE-CZ-NH2	-6.21	117.20	120.30
10	Q	52	PHE	N-CA-C	6.21	127.76	111.00
36	C	267	TRP	CA-CB-CG	6.20	125.49	113.70
32	5	407	A	N9-C1'-C2'	-6.20	105.18	112.00
32	5	1631	A	N9-C1'-C2'	6.20	122.06	114.00
32	5	3727	A	N9-C1'-C2'	6.20	122.06	114.00
54	S2	1123	C	O4'-C1'-C2'	-6.20	99.60	105.80
21	c	90	ARG	CA-CB-CG	6.20	127.03	113.40
78	SQ	27	ARG	NE-CZ-NH1	6.20	123.40	120.30
54	S2	967	C	N1-C1'-C2'	-6.19	105.19	112.00
51	4	186	C	C6-N1-C1'	-6.19	113.37	120.80
54	S2	1226	G	N9-C1'-C2'	-6.19	105.19	112.00
58	SE	11	ARG	NE-CZ-NH2	6.19	123.39	120.30
2	D	293	ARG	NE-CZ-NH1	6.19	123.39	120.30
54	S2	26	U	O4'-C1'-C2'	-6.19	99.61	105.80
11	R	74	ARG	NE-CZ-NH2	6.18	123.39	120.30
32	5	2395	A	C2'-C3'-O3'	6.18	123.59	113.70
32	5	3739	C	C2'-C3'-O3'	6.18	123.59	113.70
18	Z	75	TYR	CB-CG-CD1	-6.18	117.29	121.00
54	S2	1246	A	N9-C1'-C2'	-6.17	105.21	112.00
25	g	14	ASN	N-CA-C	-6.17	94.34	111.00
32	5	2675	G	C5'-C4'-O4'	6.17	116.50	109.10
32	5	970	G	N9-C1'-C2'	6.17	122.02	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	2325	C	O4'-C1'-C2'	-6.17	99.64	105.80
32	5	505	G	C2'-C3'-O3'	6.16	123.55	113.70
32	5	1575	A	N9-C1'-C2'	6.15	122.00	114.00
32	5	2673	G	O4'-C1'-C2'	-6.15	99.65	105.80
60	SH	57	ARG	NE-CZ-NH1	-6.15	117.22	120.30
61	SI	178	ARG	NE-CZ-NH1	6.15	123.38	120.30
24	f	51	TYR	CA-CB-CG	6.15	125.08	113.40
12	S	28	TYR	CA-CB-CG	6.14	125.07	113.40
54	S2	983	A	C8-N9-C1'	-6.14	116.64	127.70
32	5	150	U	C1'-O4'-C4'	-6.14	104.99	109.90
32	5	1626	G	N9-C1'-C2'	-6.14	105.25	112.00
54	S2	1223	A	N9-C1'-C2'	-6.14	105.25	112.00
54	S2	1669	G	N9-C1'-C2'	6.14	121.98	114.00
32	5	123	C	C2'-C3'-O3'	6.13	123.51	113.70
32	5	1295	C	N1-C1'-C2'	6.13	121.97	114.00
32	5	4519	C	C2'-C3'-O3'	6.13	123.51	113.70
54	S2	1859	A	C8-N9-C1'	-6.13	116.67	127.70
32	5	1613	A	C4-N9-C1'	6.13	137.33	126.30
36	C	312	ARG	CG-CD-NE	-6.13	98.93	111.80
54	S2	71	G	N9-C1'-C2'	6.13	121.97	114.00
54	S2	400	C	N1-C1'-C2'	-6.13	105.26	112.00
32	5	514	U	C4'-C3'-C2'	-6.12	96.48	102.60
22	d	78	ARG	NE-CZ-NH1	6.12	123.36	120.30
32	5	40	G	N9-C1'-C2'	6.12	121.95	114.00
32	5	2403	A	N9-C1'-C2'	6.11	121.94	114.00
32	5	4276	G	N9-C1'-C2'	-6.11	105.28	112.00
80	SS	42	HIS	N-CA-CB	6.11	121.59	110.60
54	S2	417	C	C2'-C3'-O3'	6.11	123.47	113.70
54	S2	1603	G	O4'-C1'-N9	-6.11	103.31	108.20
32	5	938	C	N1-C1'-C2'	6.10	121.94	114.00
32	5	3843	C	O4'-C1'-N1	-6.10	103.32	108.20
38	F	168	ARG	NE-CZ-NH1	6.10	123.35	120.30
59	SG	156	TYR	CB-CA-C	6.10	122.60	110.40
32	5	2448	G	N9-C1'-C2'	6.10	121.93	114.00
32	5	215	C	C2'-C3'-O3'	6.09	123.45	113.70
12	S	28	TYR	CB-CG-CD2	-6.09	117.35	121.00
32	5	4342	C	C2'-C3'-O3'	6.09	123.44	113.70
32	5	1359	G	N9-C1'-C2'	6.09	121.91	114.00
32	5	314	G	N9-C1'-C2'	-6.08	105.31	112.00
67	SW	46	TYR	CA-CB-CG	-6.08	101.84	113.40
32	5	4745	G	N9-C1'-C2'	6.08	121.91	114.00
78	SQ	85	ARG	NE-CZ-NH2	-6.08	117.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	1479	G	C1'-C2'-O2'	-6.08	92.37	110.60
54	S2	1577	G	N9-C1'-C2'	6.08	121.90	114.00
54	S2	617	G	N9-C1'-C2'	-6.08	105.32	112.00
32	5	1382	G	N9-C1'-C2'	6.07	121.90	114.00
32	5	1724	G	O4'-C4'-C3'	-6.07	97.93	104.00
32	5	4400	G	N9-C1'-C2'	-6.07	105.32	112.00
54	S2	532	C	O5'-P-OP1	6.07	117.99	110.70
61	SI	51	GLY	N-CA-C	-6.07	97.92	113.10
32	5	2529	A	O4'-C1'-N9	6.07	113.06	108.20
32	5	2118	G	O4'-C4'-C3'	-6.07	97.93	104.00
32	5	2851	G	C2'-C3'-O3'	6.07	123.41	113.70
54	S2	1622	U	O4'-C1'-N1	-6.07	103.35	108.20
86	Sf	138	ARG	CG-CD-NE	6.06	124.53	111.80
32	5	4127	A	O4'-C1'-N9	6.06	113.05	108.20
64	SN	113	PHE	CB-CA-C	-6.06	98.28	110.40
34	8	34	U	C5'-C4'-O4'	6.05	116.36	109.10
32	5	4731	G	N9-C1'-C2'	6.05	121.87	114.00
54	S2	1663	A	N9-C1'-C2'	-6.05	105.34	112.00
42	j	56	ARG	CG-CD-NE	6.05	124.51	111.80
10	Q	15	ARG	NE-CZ-NH2	-6.05	117.28	120.30
54	S2	912	C	C2'-C3'-O3'	6.05	123.38	113.70
54	S2	1242	U	N1-C1'-C2'	6.05	121.86	114.00
32	5	4199	C	O4'-C1'-C2'	-6.05	99.75	105.80
78	SQ	99	TYR	CA-CB-CG	6.05	124.89	113.40
54	S2	824	C	N1-C1'-C2'	6.04	121.86	114.00
32	5	2858	A	O4'-C1'-N9	-6.04	103.37	108.20
54	S2	1835	A	O4'-C1'-N9	-6.04	103.37	108.20
32	5	119	G	O4'-C4'-C3'	-6.03	97.97	104.00
32	5	4527	G	N9-C1'-C2'	-6.03	105.37	112.00
54	S2	1339	U	N1-C1'-C2'	-6.03	105.37	112.00
32	5	55	G	N9-C1'-C2'	-6.03	105.37	112.00
54	S2	470	G	C5'-C4'-O4'	6.03	116.33	109.10
2	D	50	ARG	NE-CZ-NH2	6.02	123.31	120.30
32	5	1632	A	N9-C1'-C2'	-6.02	105.38	112.00
35	B	117	ARG	NE-CZ-NH2	-6.02	117.29	120.30
54	S2	680	G	N9-C1'-C2'	6.02	121.83	114.00
54	S2	160	U	C2'-C3'-O3'	6.02	123.33	113.70
73	SD	152	PHE	CB-CG-CD1	-6.02	116.59	120.80
32	5	158	A	N9-C1'-C2'	-6.01	105.39	112.00
54	S2	1643	U	N1-C1'-C2'	6.01	121.82	114.00
54	S2	382	C	N1-C1'-C2'	6.01	121.82	114.00
12	S	146	HIS	N-CA-C	6.01	127.23	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	5062	G	P-O5'-C5'	6.01	130.52	120.90
54	S2	1440	C	C5'-C4'-O4'	6.01	116.31	109.10
32	5	927	G	O4'-C1'-N9	6.01	113.01	108.20
32	5	4197	G	N9-C1'-C2'	-6.01	105.39	112.00
42	j	71	TYR	CA-CB-CG	6.00	124.81	113.40
35	B	169	ARG	CG-CD-NE	6.00	124.40	111.80
85	Sd	46	TYR	CB-CA-C	6.00	122.40	110.40
54	S2	1378	A	O4'-C1'-N9	-6.00	103.40	108.20
24	f	19	ARG	CA-CB-CG	6.00	126.60	113.40
32	5	4448	G	N9-C1'-C2'	6.00	121.80	114.00
54	S2	1292	C	C4'-C3'-C2'	-6.00	96.60	102.60
32	5	292	G	O4'-C4'-C3'	-6.00	98.00	104.00
35	B	62	ARG	NE-CZ-NH1	6.00	123.30	120.30
32	5	297	U	N1-C1'-C2'	-5.99	105.41	112.00
54	S2	983	A	C4-N9-C1'	5.99	137.08	126.30
54	S2	1378	A	O4'-C4'-C3'	-5.99	98.01	104.00
38	F	237	ASN	N-CA-CB	5.99	121.38	110.60
20	b	6	ASN	CB-CA-C	5.99	122.37	110.40
54	S2	291	G	C4'-C3'-O3'	-5.99	96.83	109.40
41	W	55	TYR	CB-CG-CD1	5.98	124.59	121.00
54	S2	622	C	N1-C1'-C2'	-5.98	105.42	112.00
32	5	4527	G	O4'-C1'-N9	5.98	112.99	108.20
10	Q	26	ARG	NE-CZ-NH1	5.98	123.29	120.30
27	i	28	ARG	CG-CD-NE	-5.98	99.24	111.80
32	5	4736	C	N1-C1'-C2'	5.98	121.78	114.00
57	SC	223	TYR	CB-CG-CD1	-5.98	117.41	121.00
25	g	66	ARG	CG-CD-NE	5.98	124.36	111.80
32	5	29	G	C8-N9-C1'	-5.98	119.23	127.00
31	o	26	TYR	CB-CG-CD1	5.98	124.58	121.00
32	5	2613	C	C2'-C3'-O3'	5.98	123.26	113.70
32	5	4481	U	N1-C1'-C2'	5.97	121.77	114.00
37	E	219	ARG	NE-CZ-NH1	5.97	123.29	120.30
32	5	4078	C	N1-C1'-C2'	-5.97	105.43	112.00
32	5	2305	U	O4'-C1'-N1	-5.97	103.42	108.20
54	S2	1480	A	N9-C1'-C2'	5.97	121.76	114.00
32	5	3726	A	N9-C1'-C2'	5.97	121.76	114.00
32	5	4948	C	C2'-C3'-O3'	5.96	123.24	113.70
26	h	89	ARG	CG-CD-NE	5.96	124.31	111.80
54	S2	1367	U	C2'-C3'-O3'	5.96	123.23	113.70
3	G	53	ARG	CG-CD-NE	-5.95	99.30	111.80
32	5	85	G	O4'-C1'-C2'	-5.95	99.85	105.80
32	5	1484	G	O4'-C1'-N9	-5.95	103.44	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	2666	U	C4'-C3'-C2'	-5.95	96.65	102.60
32	5	4084	G	C2'-C3'-O3'	5.95	123.22	113.70
32	5	1601	A	N9-C1'-C2'	-5.95	105.46	112.00
31	o	48	TYR	CB-CA-C	5.94	122.29	110.40
37	E	179	ARG	NE-CZ-NH1	5.94	123.27	120.30
26	h	119	PHE	CB-CG-CD2	-5.94	116.64	120.80
32	5	3738	G	N9-C1'-C2'	-5.94	105.47	112.00
24	f	4	ARG	N-CA-CB	5.94	121.29	110.60
32	5	964	A	C5'-C4'-O4'	-5.94	101.97	109.10
42	j	8	PHE	CB-CA-C	5.94	122.27	110.40
32	5	2321	G	N9-C1'-C2'	5.93	121.72	114.00
32	5	423	G	C5'-C4'-O4'	5.93	116.22	109.10
56	SB	67	PHE	N-CA-CB	-5.93	99.93	110.60
1	A	209	HIS	N-CA-CB	5.93	121.27	110.60
32	5	4519	C	O4'-C4'-C3'	-5.93	98.07	104.00
54	S2	366	U	N1-C1'-C2'	-5.93	105.48	112.00
32	5	1	C	C5'-C4'-C3'	5.92	125.48	116.00
54	S2	603	C	N1-C1'-C2'	-5.92	105.48	112.00
65	SO	34	PHE	CB-CG-CD1	5.92	124.95	120.80
37	E	242	ARG	NE-CZ-NH1	5.92	123.26	120.30
6	L	103	ARG	NE-CZ-NH2	-5.92	117.34	120.30
37	E	111	TYR	N-CA-CB	5.92	121.26	110.60
32	5	1672	U	C2-N1-C1'	5.92	124.80	117.70
2	D	20	PHE	CB-CA-C	5.92	122.24	110.40
19	a	21	ARG	NE-CZ-NH2	5.92	123.26	120.30
32	5	1631	A	C5'-C4'-O4'	5.92	116.20	109.10
54	S2	399	C	C3'-C2'-C1'	5.92	106.23	101.50
59	SG	213	LEU	CA-CB-CG	5.92	128.91	115.30
34	8	135	C	N1-C1'-C2'	5.92	121.69	114.00
32	5	669	C	O4'-C1'-N1	5.91	112.93	108.20
62	SJ	20	PHE	CB-CG-CD1	5.91	124.94	120.80
32	5	1292	C	N1-C1'-C2'	5.90	121.67	114.00
54	S2	426	A	C4'-C3'-C2'	-5.89	96.70	102.60
32	5	4600	G	O4'-C1'-N9	5.89	112.91	108.20
54	S2	798	A	N9-C1'-C2'	-5.89	105.52	112.00
54	S2	1326	U	N1-C1'-C2'	5.89	121.66	114.00
36	C	78	ARG	NE-CZ-NH2	-5.88	117.36	120.30
54	S2	1291	A	P-O3'-C3'	5.88	126.76	119.70
60	SH	57	ARG	NE-CZ-NH2	5.88	123.24	120.30
32	5	2673	G	C1'-O4'-C4'	-5.88	105.20	109.90
54	S2	797	C	O4'-C1'-N1	5.87	112.90	108.20
46	K	2	PRO	C-N-CD	5.87	140.72	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	2344	U	N1-C1'-C2'	5.87	121.63	114.00
32	5	209	U	N1-C1'-C2'	-5.87	105.55	112.00
54	S2	863	U	N1-C1'-C2'	5.86	121.62	114.00
54	S2	1859	A	C4-N9-C1'	5.86	136.85	126.30
54	S2	1863	A	N9-C1'-C2'	5.86	121.62	114.00
54	S2	842	C	N1-C1'-C2'	5.86	121.61	114.00
29	1	45	ARG	CG-CD-NE	-5.86	99.50	111.80
32	5	2450	G	N9-C1'-C2'	-5.86	105.56	112.00
32	5	1361	G	C2'-C3'-O3'	5.85	123.07	113.70
34	8	74	U	O4'-C1'-C2'	-5.85	99.95	105.80
34	8	10	G	N9-C1'-C2'	-5.85	105.56	112.00
32	5	1359	G	C4'-C3'-O3'	-5.85	97.12	109.40
32	5	4266	G	N9-C1'-C2'	-5.85	105.57	112.00
32	5	2324	C	C2'-C3'-O3'	5.85	123.06	113.70
44	p	34	HIS	CB-CA-C	5.85	122.09	110.40
54	S2	426	A	O4'-C4'-C3'	-5.85	98.15	104.00
18	Z	36	ARG	CG-CD-NE	5.85	124.08	111.80
32	5	1487	G	C2'-C3'-O3'	5.84	123.05	113.70
57	SC	241	PHE	CB-CG-CD2	-5.84	116.71	120.80
32	5	4528	G	O4'-C1'-C2'	-5.84	99.96	105.80
32	5	4873	G	N9-C1'-C2'	5.84	121.59	114.00
32	5	4911	A	C4-N9-C1'	-5.84	115.79	126.30
54	S2	1536	G	N9-C1'-C2'	-5.84	105.57	112.00
32	5	36	U	C2'-C3'-O3'	5.83	123.04	113.70
54	S2	3	C	C1'-O4'-C4'	-5.83	105.23	109.90
34	8	104	A	N9-C1'-C2'	5.83	121.58	114.00
75	SK	57	TYR	CA-CB-CG	-5.83	102.31	113.40
32	5	2515	G	N9-C1'-C2'	-5.83	105.58	112.00
54	S2	660	C	N1-C1'-C2'	-5.83	105.59	112.00
54	S2	1022	U	O4'-C1'-N1	5.83	112.86	108.20
12	S	84	TYR	CB-CG-CD1	5.83	124.50	121.00
34	8	72	A	N9-C1'-C2'	-5.83	105.59	112.00
57	SC	250	TYR	CA-CB-CG	-5.83	102.33	113.40
32	5	4212	A	N9-C1'-C2'	5.83	121.57	114.00
32	5	4944	C	N1-C1'-C2'	5.82	121.57	114.00
61	SI	67	TRP	N-CA-CB	5.82	121.08	110.60
32	5	2782	U	C4'-C3'-O3'	5.82	124.64	113.00
12	S	81	TRP	N-CA-C	-5.82	95.29	111.00
73	SD	106	ARG	NE-CZ-NH2	-5.82	117.39	120.30
32	5	25	A	N9-C1'-C2'	5.82	121.56	114.00
32	5	1428	U	C2'-C3'-O3'	5.82	123.00	113.70
32	5	2323	C	C2'-C3'-O3'	5.82	123.00	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	3686	G	N9-C1'-C2'	-5.82	105.60	112.00
4	H	54	ARG	NE-CZ-NH2	-5.81	117.39	120.30
32	5	1887	G	C4'-C3'-C2'	-5.81	96.79	102.60
38	F	209	PHE	N-CA-CB	5.81	121.06	110.60
54	S2	1551	U	C2'-C3'-O3'	5.81	122.99	113.70
32	5	934	C	O4'-C1'-N1	-5.80	103.56	108.20
64	SN	55	ARG	NE-CZ-NH1	5.80	123.20	120.30
65	SO	147	ARG	NE-CZ-NH2	-5.80	117.40	120.30
32	5	5048	A	C2'-C3'-O3'	5.80	122.98	113.70
54	S2	1522	A	C5'-C4'-O4'	5.80	116.06	109.10
14	U	97	ARG	NE-CZ-NH1	5.80	123.20	120.30
10	Q	33	ARG	CB-CG-CD	5.80	126.67	111.60
10	Q	38	ARG	NE-CZ-NH2	-5.80	117.40	120.30
9	O	117	ARG	NE-CZ-NH2	-5.79	117.40	120.30
12	S	83	ARG	NE-CZ-NH2	5.79	123.19	120.30
38	F	98	ARG	NE-CZ-NH2	-5.79	117.41	120.30
5	J	99	PHE	CB-CG-CD2	-5.79	116.75	120.80
11	R	74	ARG	NE-CZ-NH1	-5.79	117.41	120.30
32	5	1236	C	C2'-C3'-O3'	5.78	122.95	113.70
32	5	3870	C	N1-C1'-C2'	5.78	121.52	114.00
33	7	75	G	O4'-C1'-N9	5.78	112.83	108.20
32	5	74	G	N9-C1'-C2'	5.78	121.52	114.00
32	5	232	G	N9-C1'-C2'	-5.78	105.64	112.00
33	7	26	C	N1-C1'-C2'	-5.78	105.64	112.00
32	5	1930	U	O4'-C1'-N1	-5.78	103.58	108.20
54	S2	647	U	O4'-C1'-C2'	-5.78	100.02	105.80
54	S2	855	G	N9-C1'-C2'	-5.78	105.64	112.00
9	O	37	ARG	NE-CZ-NH1	5.78	123.19	120.30
34	8	41	A	N9-C1'-C2'	-5.78	105.64	112.00
32	5	99	A	C2'-C3'-O3'	5.78	122.94	113.70
86	Sf	146	LEU	CB-CA-C	5.78	121.17	110.20
61	SI	55	TYR	CB-CA-C	5.77	121.94	110.40
32	5	4232	U	N1-C1'-C2'	5.77	121.50	114.00
32	5	4519	C	O4'-C1'-N1	5.77	112.81	108.20
54	S2	1851	A	N9-C1'-C2'	5.76	121.50	114.00
54	S2	1368	U	C4'-C3'-O3'	5.76	124.53	113.00
12	S	111	ARG	CB-CG-CD	5.76	126.57	111.60
37	E	250	ASP	CB-CA-C	5.76	121.92	110.40
32	5	3938	G	C4'-C3'-O3'	-5.76	97.31	109.40
3	G	235	ARG	NE-CZ-NH2	-5.76	117.42	120.30
32	5	1697	G	C3'-C2'-C1'	-5.76	96.89	101.50
54	S2	14	C	N1-C1'-C2'	5.75	121.48	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Q	176	ARG	CG-CD-NE	-5.75	99.72	111.80
54	S2	1319	U	N1-C1'-C2'	5.75	121.48	114.00
77	SP	42	ARG	NE-CZ-NH1	5.75	123.18	120.30
32	5	4165	C	O4'-C1'-C2'	-5.75	100.05	105.80
54	S2	294	U	O4'-C1'-N1	-5.75	103.60	108.20
54	S2	381	C	C5'-C4'-O4'	5.75	116.00	109.10
32	5	1822	U	N1-C1'-C2'	5.75	121.47	114.00
31	o	31	ASP	CB-CA-C	5.75	121.89	110.40
26	h	109	ARG	CG-CD-NE	5.74	123.86	111.80
32	5	2077	C	C2'-C3'-O3'	5.74	122.89	113.70
4	H	124	ARG	NE-CZ-NH2	-5.74	117.43	120.30
35	B	49	TYR	CA-CB-CG	5.74	124.31	113.40
48	z	159	PHE	CB-CG-CD1	-5.74	116.78	120.80
86	Sf	119	ARG	NE-CZ-NH2	-5.74	117.43	120.30
55	SA	155	ARG	CG-CD-NE	-5.74	99.75	111.80
32	5	1318	C	N1-C1'-C2'	-5.74	105.69	112.00
32	5	3663	A	N9-C1'-C2'	5.74	121.45	114.00
38	F	197	TYR	N-CA-CB	5.73	120.92	110.60
56	SB	67	PHE	CB-CG-CD2	-5.73	116.79	120.80
10	Q	181	ARG	CA-CB-CG	5.73	126.01	113.40
15	V	98	PHE	CB-CG-CD1	-5.73	116.79	120.80
32	5	2119	C	C1'-O4'-C4'	-5.73	105.31	109.90
68	SX	14	ARG	NE-CZ-NH1	5.73	123.17	120.30
33	7	59	G	N9-C1'-C2'	-5.73	105.70	112.00
32	5	4909	A	C1'-O4'-C4'	-5.73	105.32	109.90
32	5	930	G	C4'-C3'-O3'	5.72	124.45	113.00
54	S2	1647	A	N9-C1'-C2'	5.72	121.44	114.00
9	O	37	ARG	NE-CZ-NH2	-5.72	117.44	120.30
35	B	137	TRP	CA-CB-CG	-5.72	102.83	113.70
54	S2	1141	G	C2'-C3'-O3'	5.72	122.86	113.70
17	Y	87	ARG	CG-CD-NE	5.72	123.81	111.80
32	5	1394	G	N9-C1'-C2'	5.72	121.44	114.00
2	D	248	ARG	NE-CZ-NH2	-5.72	117.44	120.30
32	5	1632	A	O4'-C1'-N9	5.72	112.78	108.20
6	L	34	ARG	NE-CZ-NH2	-5.72	117.44	120.30
32	5	4270	C	C2'-C3'-O3'	5.72	122.84	113.70
37	E	275	ASN	N-CA-CB	5.71	120.89	110.60
54	S2	1136	U	N1-C1'-C2'	5.71	121.42	114.00
32	5	964	A	O4'-C1'-C2'	-5.71	100.09	105.80
32	5	3653	A	O5'-P-OP1	-5.71	100.56	105.70
54	S2	1315	U	C2'-C3'-O3'	5.71	122.83	113.70
54	S2	293	C	N1-C1'-C2'	5.70	121.41	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	S2	65	C	C1'-O4'-C4'	-5.70	105.34	109.90
54	S2	1291	A	C5'-C4'-O4'	5.70	115.94	109.10
34	8	64	U	C5'-C4'-O4'	5.70	115.94	109.10
32	5	4534	G	N9-C1'-C2'	-5.70	105.73	112.00
45	r	107	ARG	NE-CZ-NH1	5.70	123.15	120.30
54	S2	918	U	N1-C1'-C2'	5.70	121.41	114.00
32	5	3802	U	C1'-O4'-C4'	-5.69	105.35	109.90
54	S2	1085	C	O4'-C1'-N1	-5.69	103.65	108.20
54	S2	1171	G	O4'-C1'-N9	5.69	112.75	108.20
3	G	235	ARG	CG-CD-NE	5.69	123.75	111.80
8	N	108	ARG	CG-CD-NE	-5.69	99.85	111.80
32	5	1667	G	C2'-C3'-O3'	5.69	122.80	113.70
54	S2	60	A	C1'-C2'-O2'	-5.69	93.54	110.60
54	S2	305	U	C2'-C3'-O3'	5.68	122.79	113.70
64	SN	113	PHE	N-CA-CB	5.68	120.83	110.60
26	h	119	PHE	CB-CG-CD1	5.68	124.78	120.80
54	S2	920	A	N9-C1'-C2'	5.68	121.38	114.00
54	S2	1291	A	C3'-C2'-C1'	5.68	106.04	101.50
61	SI	110	ARG	NE-CZ-NH1	5.68	123.14	120.30
32	5	1241	C	C2'-C3'-O3'	5.68	122.78	113.70
26	h	109	ARG	NE-CZ-NH1	5.67	123.14	120.30
32	5	4937	C	N1-C1'-C2'	5.67	121.37	114.00
42	j	27	TYR	N-CA-CB	5.67	120.81	110.60
34	8	39	G	N9-C1'-C2'	-5.67	105.77	112.00
73	SD	9	ARG	NE-CZ-NH1	5.67	123.14	120.30
54	S2	482	G	N9-C1'-C2'	-5.67	105.77	112.00
54	S2	1659	U	C4'-C3'-C2'	-5.67	96.93	102.60
54	S2	28	U	N1-C1'-C2'	5.66	121.36	114.00
54	S2	1021	U	N1-C1'-C2'	5.66	121.36	114.00
20	b	41	ARG	CG-CD-NE	-5.66	99.92	111.80
54	S2	1341	C	O4'-C1'-N1	-5.66	103.68	108.20
33	7	7	G	C5'-C4'-O4'	5.65	115.89	109.10
32	5	2070	U	N1-C1'-C2'	5.65	121.35	114.00
54	S2	1198	G	C2'-C3'-O3'	5.65	122.74	113.70
2	D	50	ARG	NE-CZ-NH1	-5.65	117.47	120.30
50	3	22	U	N1-C1'-C2'	5.65	121.35	114.00
40	P	139	TYR	CB-CA-C	5.65	121.70	110.40
32	5	2464	C	N1-C1'-C2'	5.65	121.34	114.00
32	5	2057	A	N9-C1'-C2'	5.64	121.34	114.00
34	8	81	C	N1-C1'-C2'	5.64	121.34	114.00
59	SG	213	LEU	CB-CG-CD1	5.64	120.60	111.00
54	S2	1459	G	C2'-C3'-O3'	5.64	122.73	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	Sa	17	HIS	N-CA-CB	5.64	120.76	110.60
24	f	42	TYR	CA-CB-CG	-5.64	102.69	113.40
38	F	239	GLU	CA-CB-CG	5.64	125.80	113.40
76	SM	26	LEU	CA-CB-CG	5.64	128.26	115.30
54	S2	963	A	N9-C1'-C2'	5.63	121.33	114.00
35	B	116	ARG	CG-CD-NE	5.63	123.63	111.80
54	S2	182	C	C2'-C3'-O3'	5.63	122.71	113.70
32	5	443	G	N9-C1'-C2'	5.63	121.32	114.00
54	S2	1378	A	N9-C1'-C2'	5.63	121.32	114.00
23	e	46	ARG	NE-CZ-NH2	-5.63	117.49	120.30
32	5	4399	U	N1-C1'-C2'	-5.63	105.81	112.00
73	SD	107	TYR	CA-CB-CG	5.63	124.09	113.40
32	5	328	A	C1'-O4'-C4'	-5.62	105.40	109.90
32	5	2311	C	N1-C1'-C2'	-5.62	105.81	112.00
54	S2	1622	U	N1-C1'-C2'	5.62	121.31	114.00
54	S2	1438	A	N9-C1'-C2'	5.62	121.31	114.00
58	SE	103	TYR	CB-CG-CD2	5.62	124.37	121.00
32	5	2745	A	N9-C1'-C2'	5.62	121.31	114.00
32	5	1408	G	N9-C1'-C2'	-5.62	105.82	112.00
50	3	38	C	O3'-P-O5'	-5.62	93.33	104.00
54	S2	413	G	N9-C1'-C2'	5.62	121.30	114.00
58	SE	99	PHE	CB-CG-CD1	5.62	124.73	120.80
11	R	107	ARG	NE-CZ-NH1	5.62	123.11	120.30
32	5	1676	C	N1-C1'-C2'	5.62	121.30	114.00
32	5	72	C	C5'-C4'-O4'	5.61	115.84	109.10
54	S2	165	G	C1'-O4'-C4'	-5.61	105.41	109.90
32	5	2827	G	O4'-C4'-C3'	-5.61	98.39	104.00
54	S2	1373	C	N1-C1'-C2'	5.61	121.30	114.00
32	5	236	G	N9-C1'-C2'	5.61	121.29	114.00
32	5	4451	G	N9-C1'-C2'	5.61	121.29	114.00
32	5	3734	U	N1-C1'-C2'	5.61	121.29	114.00
54	S2	797	C	O4'-C1'-C2'	-5.61	100.19	105.80
54	S2	1834	A	N9-C1'-C2'	5.61	121.29	114.00
32	5	4874	A	O4'-C1'-C2'	-5.60	100.20	105.80
54	S2	1567	G	N9-C1'-C2'	5.60	121.29	114.00
54	S2	452	G	N9-C1'-C2'	5.60	121.28	114.00
32	5	1	C	C1'-O4'-C4'	-5.60	105.42	109.90
39	I	94	PHE	CB-CG-CD2	-5.59	116.88	120.80
54	S2	617	G	C2'-C3'-O3'	5.59	122.65	113.70
8	N	21	PHE	N-CA-CB	5.59	120.66	110.60
32	5	2092	G	N9-C1'-C2'	5.59	121.27	114.00
27	i	26	HIS	N-CA-CB	5.59	120.66	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	S2	797	C	C1'-O4'-C4'	-5.59	105.43	109.90
11	R	52	ARG	NE-CZ-NH1	5.58	123.09	120.30
57	SC	170	TRP	N-CA-CB	5.58	120.65	110.60
47	q	14	PHE	CB-CG-CD1	5.58	124.71	120.80
32	5	2632	U	C6-N1-C1'	-5.58	113.39	121.20
40	P	3	ARG	CG-CD-NE	5.58	123.52	111.80
32	5	2039	G	N9-C1'-C2'	5.58	121.25	114.00
32	5	4280	A	C4'-C3'-C2'	-5.58	97.02	102.60
32	5	4518	A	O5'-P-OP1	5.58	117.39	110.70
12	S	95	ARG	NE-CZ-NH1	5.58	123.09	120.30
32	5	1072	C	N1-C1'-C2'	5.58	121.25	114.00
22	d	25	TYR	CB-CG-CD1	-5.57	117.66	121.00
47	q	99	ARG	NE-CZ-NH2	-5.57	117.52	120.30
13	T	13	TYR	N-CA-CB	-5.57	100.58	110.60
32	5	943	A	N9-C1'-C2'	-5.57	105.88	112.00
32	5	1650	A	O4'-C4'-C3'	-5.57	98.43	104.00
24	f	36	ARG	NE-CZ-NH2	-5.57	117.52	120.30
32	5	1572	U	N1-C1'-C2'	5.57	121.23	114.00
35	B	102	PHE	CB-CA-C	-5.57	99.27	110.40
51	4	164	G	N3-C4-N9	-5.57	122.66	126.00
32	5	1	C	O4'-C1'-N1	5.56	112.65	108.20
32	5	172	C	O4'-C1'-C2'	-5.56	100.24	105.80
32	5	422	C	C2'-C3'-O3'	5.56	122.60	113.70
11	R	52	ARG	NE-CZ-NH2	-5.56	117.52	120.30
21	c	89	TYR	CA-CB-CG	5.56	123.96	113.40
61	SI	113	TYR	CB-CG-CD2	-5.56	117.67	121.00
34	8	62	A	C8-N9-C1'	5.55	137.70	127.70
32	5	1449	C	C2'-C3'-O3'	5.55	122.58	113.70
32	5	4464	A	C8-N9-C1'	-5.55	117.71	127.70
54	S2	844	U	C1'-O4'-C4'	-5.55	105.46	109.90
81	ST	62	ARG	NE-CZ-NH1	-5.55	117.53	120.30
54	S2	1838	U	O4'-C4'-C3'	-5.55	98.45	104.00
32	5	4283	G	O4'-C1'-C2'	-5.55	100.25	105.80
25	g	90	ARG	CG-CD-NE	-5.54	100.16	111.80
32	5	2091	C	N1-C1'-C2'	5.54	121.21	114.00
32	5	2509	C	C1'-C2'-O2'	-5.54	93.97	110.60
51	4	186	C	O4'-C1'-N1	5.54	112.64	108.20
12	S	82	LEU	CA-CB-CG	5.54	128.04	115.30
32	5	2474	G	C2'-C3'-O3'	5.54	122.56	113.70
32	5	92	C	C3'-C2'-C1'	5.54	105.93	101.50
32	5	1682	A	C8-N9-C1'	-5.54	117.73	127.70
17	Y	72	GLN	CA-CB-CG	5.54	125.58	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	4479	A	N9-C1'-C2'	-5.53	105.91	112.00
48	z	219	TYR	CA-CB-CG	5.53	123.91	113.40
63	SL	92	TYR	CA-CB-CG	5.53	123.91	113.40
54	S2	366	U	C2'-C3'-O3'	5.53	122.55	113.70
54	S2	1442	U	O4'-C1'-C2'	-5.53	100.27	105.80
59	SG	145	PHE	CB-CG-CD2	-5.53	116.93	120.80
62	SJ	136	ARG	NE-CZ-NH1	5.53	123.06	120.30
32	5	55	G	C5'-C4'-O4'	5.53	115.73	109.10
32	5	334	A	N9-C1'-C2'	5.53	121.18	114.00
32	5	1325	C	O4'-C1'-N1	-5.53	103.78	108.20
32	5	153	G	C5'-C4'-O4'	5.52	115.73	109.10
54	S2	1292	C	C5'-C4'-C3'	5.52	124.84	116.00
32	5	1539	G	N9-C1'-C2'	-5.52	105.93	112.00
32	5	2554	U	C2'-C3'-O3'	5.52	122.53	113.70
32	5	1901	C	N1-C1'-C2'	5.52	121.17	114.00
48	z	197	GLN	N-CA-C	5.52	125.90	111.00
65	SO	72	TYR	CA-CB-CG	5.52	123.88	113.40
32	5	1787	A	N9-C1'-C2'	5.52	121.17	114.00
32	5	2643	G	C2'-C3'-O3'	5.51	122.52	113.70
54	S2	27	A	C5'-C4'-O4'	5.51	115.72	109.10
32	5	977	C	C5'-C4'-O4'	5.51	115.71	109.10
32	5	3814	U	N1-C1'-C2'	5.51	121.17	114.00
59	SG	198	ARG	NE-CZ-NH1	5.51	123.06	120.30
32	5	4076	G	C1'-O4'-C4'	-5.51	105.50	109.90
54	S2	1036	A	N9-C1'-C2'	-5.51	105.94	112.00
7	M	6	PHE	CB-CA-C	5.50	121.41	110.40
34	8	102	G	N9-C1'-C2'	5.50	121.15	114.00
87	Sg	132	TRP	CA-CB-CG	-5.50	103.25	113.70
32	5	4935	C	C2'-C3'-O3'	5.50	122.50	113.70
54	S2	655	A	N9-C1'-C2'	5.50	121.15	114.00
78	SQ	126	ARG	NE-CZ-NH2	5.50	123.05	120.30
12	S	152	PHE	CB-CG-CD2	-5.50	116.95	120.80
32	5	328	A	O4'-C1'-N9	5.50	112.60	108.20
32	5	215	C	C4'-C3'-O3'	-5.50	97.86	109.40
32	5	1447	C	C1'-O4'-C4'	-5.49	105.50	109.90
68	SX	14	ARG	NE-CZ-NH2	-5.49	117.55	120.30
54	S2	303	C	N1-C1'-C2'	5.49	121.14	114.00
13	T	57	TYR	CA-CB-CG	5.49	123.83	113.40
32	5	2325	C	C2'-C3'-O3'	5.49	122.48	113.70
38	F	58	HIS	N-CA-CB	5.49	120.48	110.60
32	5	2858	A	C4'-C3'-O3'	-5.49	97.88	109.40
54	S2	1088	U	O4'-C1'-N1	-5.49	103.81	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	e	36	ARG	NE-CZ-NH1	-5.48	117.56	120.30
32	5	2754	G	N9-C1'-C2'	-5.48	105.97	112.00
26	h	119	PHE	N-CA-CB	5.48	120.47	110.60
32	5	85	G	N9-C1'-C2'	-5.48	105.97	112.00
32	5	2305	U	N1-C1'-C2'	5.48	121.12	114.00
32	5	2666	U	C2'-C3'-O3'	5.48	122.47	113.70
32	5	2852	U	C4'-C3'-O3'	5.48	123.96	113.00
2	D	248	ARG	NE-CZ-NH1	5.48	123.04	120.30
32	5	1615	C	C2'-C3'-O3'	5.48	122.46	113.70
32	5	4665	A	N9-C1'-C2'	-5.48	105.98	112.00
12	S	10	TYR	CB-CA-C	5.47	121.35	110.40
32	5	1319	U	C2'-C3'-O3'	5.47	122.46	113.70
54	S2	1512	C	N1-C1'-C2'	5.47	121.12	114.00
32	5	1539	G	C2'-C3'-O3'	5.47	122.46	113.70
32	5	3645	U	N1-C1'-C2'	5.47	121.11	114.00
54	S2	415	A	C4-N9-C1'	-5.47	116.45	126.30
32	5	268	G	C2'-C3'-O3'	5.47	122.45	113.70
32	5	5016	A	C1'-O4'-C4'	-5.47	105.52	109.90
12	S	96	GLU	OE1-CD-OE2	5.47	129.86	123.30
32	5	977	C	C4'-C3'-C2'	-5.47	97.13	102.60
54	S2	1617	G	N9-C1'-C2'	-5.47	105.98	112.00
32	5	4199	C	C4'-C3'-O3'	5.47	123.94	113.00
32	5	3804	G	N9-C1'-C2'	-5.47	105.99	112.00
33	7	21	G	N9-C1'-C2'	5.47	121.11	114.00
54	S2	292	A	C2'-C3'-O3'	5.47	122.45	113.70
10	Q	26	ARG	CG-CD-NE	-5.46	100.33	111.80
10	Q	174	PHE	CB-CA-C	5.46	121.32	110.40
32	5	307	A	N9-C1'-C2'	5.46	121.10	114.00
32	5	4346	U	N1-C1'-C2'	5.46	121.10	114.00
32	5	4701	A	C8-N9-C1'	-5.46	117.88	127.70
54	S2	975	G	C5'-C4'-O4'	5.46	115.65	109.10
54	S2	1292	C	C5'-C4'-O4'	5.46	115.65	109.10
24	f	51	TYR	CB-CG-CD2	-5.46	117.73	121.00
32	5	1279	A	N9-C1'-C2'	5.46	121.09	114.00
32	5	3879	G	O4'-C1'-C2'	-5.46	100.34	105.80
32	5	1891	A	N9-C1'-C2'	5.45	121.09	114.00
32	5	2854	G	N9-C1'-C2'	-5.45	106.00	112.00
20	b	44	ARG	NE-CZ-NH2	-5.45	117.58	120.30
37	E	154	ARG	NE-CZ-NH1	5.45	123.03	120.30
57	SC	200	ARG	CG-CD-NE	5.45	123.24	111.80
32	5	2395	A	N9-C1'-C2'	-5.45	106.01	112.00
54	S2	1860	A	C3'-C2'-C1'	5.45	105.86	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	S2	385	G	O4'-C1'-N9	-5.44	103.84	108.20
11	R	108	ARG	NE-CZ-NH2	-5.44	117.58	120.30
32	5	4328	G	N9-C1'-C2'	-5.44	106.02	112.00
2	D	249	GLU	CA-CB-CG	5.44	125.36	113.40
3	G	223	ARG	NE-CZ-NH1	5.44	123.02	120.30
32	5	3812	C	C2'-C3'-O3'	5.44	122.40	113.70
32	5	4944	C	O4'-C1'-N1	-5.44	103.85	108.20
32	5	100	C	C5'-C4'-O4'	5.44	115.62	109.10
32	5	235	A	C1'-O4'-C4'	-5.43	105.55	109.90
12	S	43	ARG	NE-CZ-NH2	5.43	123.02	120.30
54	S2	1045	U	O4'-C1'-C2'	-5.43	100.37	105.80
86	Sf	146	LEU	N-CA-C	-5.43	96.33	111.00
4	H	180	TYR	CA-CB-CG	5.43	123.72	113.40
58	SE	253	ASP	CB-CG-OD1	5.43	123.19	118.30
54	S2	1860	A	N9-C1'-C2'	-5.43	106.03	112.00
57	SC	200	ARG	NE-CZ-NH1	-5.43	117.58	120.30
5	J	146	ARG	NE-CZ-NH1	-5.43	117.59	120.30
32	5	1975	G	O4'-C1'-N9	-5.43	103.86	108.20
34	8	62	A	C4-N9-C1'	-5.43	116.53	126.30
3	G	53	ARG	NE-CZ-NH1	5.43	123.01	120.30
5	J	35	ARG	CG-CD-NE	5.43	123.20	111.80
10	Q	75	ARG	NE-CZ-NH2	-5.43	117.59	120.30
32	5	1588	U	N1-C1'-C2'	5.43	121.05	114.00
44	p	18	TYR	CB-CG-CD2	-5.43	117.75	121.00
54	S2	807	G	N9-C1'-C2'	5.43	121.06	114.00
32	5	2275	G	C2'-C3'-O3'	5.42	122.38	113.70
54	S2	1123	C	O5'-P-OP1	-5.42	100.82	105.70
65	SO	34	PHE	CB-CG-CD2	-5.42	117.00	120.80
54	S2	415	A	C8-N9-C1'	5.42	137.46	127.70
54	S2	426	A	O5'-P-OP1	-5.42	100.82	105.70
32	5	2054	U	N1-C1'-C2'	5.42	121.04	114.00
11	R	9	ARG	NE-CZ-NH1	5.42	123.01	120.30
32	5	1660	U	N1-C1'-C2'	-5.42	106.04	112.00
54	S2	1376	A	C2'-C3'-O3'	5.42	122.36	113.70
77	SP	42	ARG	CA-CB-CG	5.42	125.31	113.40
32	5	1439	C	O4'-C1'-C2'	-5.41	100.39	105.80
54	S2	457	C	C2'-C3'-O3'	5.41	122.36	113.70
32	5	4677	U	N1-C1'-C2'	-5.41	106.05	112.00
32	5	1395	U	N1-C1'-C2'	5.41	121.03	114.00
32	5	2536	A	C2'-C3'-O3'	5.41	122.36	113.70
32	5	4320	G	N9-C1'-C2'	5.41	121.03	114.00
54	S2	427	U	P-O5'-C5'	5.41	129.56	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	Sa	28	ARG	NE-CZ-NH2	-5.41	117.60	120.30
12	S	44	PHE	N-CA-CB	5.41	120.33	110.60
32	5	745	G	N9-C1'-C2'	5.41	121.03	114.00
42	j	43	ARG	CG-CD-NE	5.41	123.15	111.80
34	8	85	U	P-O3'-C3'	5.40	126.19	119.70
54	S2	369	C	N1-C1'-C2'	5.40	121.02	114.00
75	SK	57	TYR	CB-CA-C	5.40	121.21	110.40
32	5	4557	U	N1-C1'-C2'	5.40	121.02	114.00
54	S2	800	U	O4'-C4'-C3'	-5.40	98.60	104.00
54	S2	28	U	C4'-C3'-O3'	5.40	123.80	113.00
2	D	30	TYR	CB-CA-C	5.40	121.19	110.40
32	5	663	G	C4'-C3'-O3'	5.40	123.79	113.00
32	5	1616	U	O4'-C1'-C2'	-5.40	100.40	105.80
37	E	278	TYR	N-CA-C	-5.40	96.43	111.00
32	5	4325	A	N9-C1'-C2'	5.40	121.02	114.00
32	5	4451	G	C4'-C3'-O3'	5.40	123.79	113.00
54	S2	73	C	C1'-O4'-C4'	-5.40	105.58	109.90
54	S2	1292	C	O4'-C4'-C3'	-5.40	98.60	104.00
9	O	140	ARG	NE-CZ-NH1	-5.39	117.60	120.30
10	Q	14	ARG	NE-CZ-NH1	5.39	123.00	120.30
32	5	238	C	N1-C1'-C2'	5.39	121.01	114.00
32	5	4731	G	C1'-O4'-C4'	-5.39	105.58	109.90
33	7	29	C	N1-C1'-C2'	5.39	121.01	114.00
81	ST	33	TRP	CB-CA-C	5.39	121.19	110.40
56	SB	165	ARG	CD-NE-CZ	5.39	131.15	123.60
37	E	42	ARG	N-CA-C	5.39	125.54	111.00
54	S2	1839	U	C2-N1-C1'	5.39	124.17	117.70
32	5	2056	G	N9-C1'-C2'	-5.38	106.08	112.00
32	5	2746	A	N9-C1'-C2'	5.38	121.00	114.00
36	C	67	TRP	CA-CB-CG	5.38	123.93	113.70
62	SJ	109	ARG	NE-CZ-NH1	5.38	122.99	120.30
32	5	4078	C	C2'-C3'-O3'	5.38	122.30	113.70
10	Q	65	ARG	NE-CZ-NH1	5.37	122.99	120.30
34	8	34	U	O4'-C1'-N1	-5.37	103.90	108.20
54	S2	149	A	N9-C1'-C2'	5.37	120.98	114.00
54	S2	105	U	C2'-C3'-O3'	5.37	122.29	113.70
72	Se	41	ARG	NE-CZ-NH1	5.37	122.98	120.30
86	Sf	133	ALA	N-CA-C	5.37	125.49	111.00
32	5	4330	G	N9-C1'-C2'	-5.37	106.10	112.00
2	D	31	TYR	N-CA-C	-5.36	96.52	111.00
32	5	2256	C	N1-C1'-C2'	5.36	120.97	114.00
12	S	97	TYR	CA-CB-CG	-5.36	103.21	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	S2	1092	G	C2'-C3'-O3'	5.36	122.28	113.70
32	5	2272	C	C1'-C2'-O2'	-5.36	94.52	110.60
51	4	15	C	N1-C1'-C2'	-5.36	106.10	112.00
32	5	4398	C	C2'-C3'-O3'	5.36	122.27	113.70
32	5	4909	A	O4'-C1'-N9	5.36	112.49	108.20
33	7	42	A	O4'-C1'-C2'	-5.36	100.44	105.80
32	5	1847	C	N1-C1'-C2'	5.36	120.96	114.00
62	SJ	38	ARG	NE-CZ-NH2	-5.36	117.62	120.30
4	H	125	ARG	CG-CD-NE	5.35	123.04	111.80
10	Q	15	ARG	NE-CZ-NH1	5.35	122.97	120.30
77	SP	18	ARG	NE-CZ-NH2	-5.35	117.63	120.30
32	5	4683	U	N1-C1'-C2'	5.35	120.95	114.00
55	SA	39	TYR	CA-CB-CG	5.35	123.56	113.40
55	SA	117	ARG	CG-CD-NE	5.35	123.03	111.80
32	5	922	C	C2'-C3'-O3'	5.34	122.25	113.70
32	5	2008	U	O4'-C4'-C3'	-5.34	98.66	104.00
32	5	3663	A	O4'-C4'-C3'	-5.34	98.66	104.00
5	J	147	ARG	NE-CZ-NH2	-5.34	117.63	120.30
54	S2	980	A	C4-N9-C1'	5.34	135.91	126.30
54	S2	1671	G	N9-C1'-C2'	5.34	120.94	114.00
10	Q	176	ARG	NE-CZ-NH2	-5.34	117.63	120.30
32	5	2250	C	P-O5'-C5'	5.34	129.44	120.90
54	S2	654	A	N9-C1'-C2'	-5.34	106.13	112.00
54	S2	1146	C	N1-C1'-C2'	5.34	120.94	114.00
32	5	1642	A	C2'-C3'-O3'	5.34	122.24	113.70
32	5	3723	A	C5-C6-N6	-5.34	119.43	123.70
32	5	4533	A	N9-C1'-C2'	-5.34	106.13	112.00
47	q	99	ARG	CD-NE-CZ	5.34	131.07	123.60
32	5	4463	U	O4'-C1'-N1	5.33	112.47	108.20
4	H	96	TYR	CA-CB-CG	5.33	123.53	113.40
32	5	5047	C	O5'-P-OP2	-5.33	100.90	105.70
32	5	1264	C	C2'-C3'-O3'	5.33	122.22	113.70
32	5	2075	G	N9-C1'-C2'	-5.33	106.14	112.00
35	B	228	TYR	CB-CG-CD1	5.33	124.20	121.00
57	SC	96	PHE	N-CA-CB	5.33	120.19	110.60
32	5	729	G	N9-C1'-C2'	5.33	120.92	114.00
32	5	4497	U	C4'-C3'-C2'	-5.33	97.27	102.60
32	5	2323	C	N1-C1'-C2'	-5.33	106.14	112.00
32	5	4750	G	N9-C1'-C2'	-5.33	106.14	112.00
21	c	56	ARG	NE-CZ-NH2	-5.32	117.64	120.30
24	f	22	ARG	NE-CZ-NH1	5.32	122.96	120.30
40	P	3	ARG	NE-CZ-NH2	-5.32	117.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	140	PHE	CB-CA-C	-5.32	99.76	110.40
32	5	381	U	N1-C1'-C2'	5.32	120.91	114.00
32	5	4227	U	C2'-C3'-O3'	5.32	122.21	113.70
32	5	1880	G	N9-C1'-C2'	5.32	120.91	114.00
32	5	2088	A	N9-C1'-C2'	-5.32	106.15	112.00
54	S2	1641	A	N9-C1'-C2'	5.32	120.91	114.00
10	Q	180	ARG	NE-CZ-NH2	5.31	122.96	120.30
15	V	96	LEU	CA-CB-CG	5.31	127.52	115.30
32	5	1484	G	C4-N9-C1'	-5.31	119.59	126.50
32	5	2424	G	N9-C1'-C2'	5.31	120.91	114.00
10	Q	34	PHE	CB-CG-CD2	-5.31	117.08	120.80
32	5	1313	C	O4'-C1'-N1	-5.31	103.95	108.20
32	5	2689	C	O4'-C1'-C2'	-5.31	100.49	105.80
45	r	107	ARG	NE-CZ-NH2	-5.31	117.64	120.30
5	J	54	ARG	NE-CZ-NH2	-5.31	117.65	120.30
12	S	157	ARG	NE-CZ-NH2	-5.31	117.65	120.30
54	S2	167	G	N9-C1'-C2'	5.31	120.90	114.00
17	Y	61	HIS	N-CA-CB	5.31	120.15	110.60
10	Q	33	ARG	N-CA-C	-5.30	96.68	111.00
32	5	2361	G	O4'-C1'-N9	5.30	112.44	108.20
40	P	42	ARG	CG-CD-NE	5.30	122.94	111.80
76	SM	127	TYR	CB-CG-CD1	5.30	124.18	121.00
32	5	2436	U	O4'-C1'-N1	-5.30	103.96	108.20
32	5	2858	A	N9-C1'-C2'	5.30	120.89	114.00
86	Sf	148	TYR	C-N-CA	5.30	134.95	121.70
10	Q	75	ARG	CG-CD-NE	5.30	122.93	111.80
11	R	103	ARG	NE-CZ-NH2	-5.30	117.65	120.30
23	e	74	PHE	CB-CG-CD1	-5.30	117.09	120.80
58	SE	103	TYR	N-CA-CB	5.30	120.14	110.60
1	A	193	ARG	NE-CZ-NH2	-5.30	117.65	120.30
76	SM	26	LEU	CB-CG-CD2	5.30	120.01	111.00
51	4	162	C	N3-C4-C5	-5.30	119.78	121.90
23	e	75	ARG	CG-CD-NE	-5.29	100.68	111.80
32	5	405	U	C2'-C3'-O3'	5.29	122.17	113.70
57	SC	97	PHE	CB-CG-CD2	-5.29	117.09	120.80
17	Y	26	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	A	189	TYR	N-CA-CB	5.29	120.13	110.60
2	D	226	TYR	CA-CB-CG	-5.29	103.34	113.40
32	5	1211	G	O4'-C1'-C2'	-5.29	100.51	105.80
40	P	25	HIS	CB-CA-C	5.29	120.98	110.40
54	S2	1666	C	N1-C1'-C2'	5.29	120.88	114.00
20	b	41	ARG	NE-CZ-NH2	-5.29	117.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	936	C	N1-C1'-C2'	-5.29	106.18	112.00
33	7	114	U	N1-C1'-C2'	5.29	120.88	114.00
32	5	3905	A	O4'-C4'-C3'	-5.29	98.71	104.00
32	5	2316	G	N9-C1'-C2'	5.29	120.87	114.00
55	SA	116	PHE	CB-CG-CD1	5.29	124.50	120.80
35	B	179	HIS	CB-CA-C	5.28	120.97	110.40
54	S2	428	U	O4'-C1'-N1	-5.28	103.97	108.20
67	SW	97	ARG	NE-CZ-NH1	5.28	122.94	120.30
54	S2	843	C	N1-C1'-C2'	5.28	120.86	114.00
54	S2	1093	A	C5'-C4'-O4'	5.28	115.44	109.10
5	J	32	ARG	NE-CZ-NH2	-5.28	117.66	120.30
32	5	88	A	C1'-C2'-O2'	-5.28	94.77	110.60
32	5	333	U	N1-C1'-C2'	5.28	120.86	114.00
32	5	2889	G	N9-C1'-C2'	5.28	120.86	114.00
32	5	2117	G	C1'-O4'-C4'	-5.28	105.68	109.90
54	S2	957	A	C4'-C3'-O3'	-5.27	98.33	109.40
32	5	279	A	N9-C1'-C2'	5.27	120.85	114.00
32	5	4234	A	C2'-C3'-O3'	5.27	122.14	113.70
34	8	73	U	C2'-C3'-O3'	5.27	122.14	113.70
32	5	2733	C	C2'-C3'-O3'	5.27	122.13	113.70
54	S2	1453	C	C4'-C3'-O3'	5.27	123.54	113.00
22	d	73	TRP	N-CA-CB	-5.27	101.12	110.60
32	5	4763	U	O4'-C1'-N1	5.27	112.42	108.20
54	S2	457	C	N1-C1'-C2'	-5.27	106.21	112.00
8	N	96	ARG	NE-CZ-NH2	5.26	122.93	120.30
31	o	78	ARG	NE-CZ-NH1	-5.26	117.67	120.30
32	5	737	C	C2'-C3'-O3'	5.26	122.12	113.70
32	5	4761	G	N9-C1'-C2'	5.26	120.84	114.00
48	z	109	LEU	CA-CB-CG	5.26	127.40	115.30
64	SN	64	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	D	157	ASN	CB-CA-C	5.26	120.92	110.40
54	S2	1568	C	N1-C1'-C2'	5.26	120.84	114.00
32	5	1445	U	C2'-C3'-O3'	5.26	122.11	113.70
32	5	480	C	C2'-C3'-O3'	5.26	122.11	113.70
77	SP	42	ARG	CG-CD-NE	-5.25	100.76	111.80
55	SA	158	ASP	CB-CG-OD2	5.25	123.03	118.30
60	SH	118	ARG	NE-CZ-NH2	-5.25	117.67	120.30
63	SL	105	ARG	NE-CZ-NH1	5.25	122.93	120.30
32	5	703	G	C1'-O4'-C4'	-5.25	105.70	109.90
32	5	4695	C	N1-C1'-C2'	5.25	120.83	114.00
13	T	105	PHE	CB-CA-C	5.25	120.90	110.40
49	2	123	PHE	CB-CG-CD1	-5.25	117.13	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	2545	U	C5'-C4'-O4'	5.25	115.39	109.10
54	S2	367	U	C1'-C2'-O2'	5.25	126.34	110.60
65	SO	147	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	147	ARG	NE-CZ-NH1	5.24	122.92	120.30
32	5	2753	G	C2'-C3'-O3'	5.24	122.09	113.70
32	5	2745	A	C1'-C2'-O2'	-5.24	94.88	110.60
54	S2	1605	G	C2'-C3'-O3'	5.24	122.08	113.70
75	SK	68	TYR	CB-CA-C	5.24	120.88	110.40
6	L	186	ARG	CG-CD-NE	-5.24	100.80	111.80
10	Q	33	ARG	N-CA-CB	5.24	120.03	110.60
24	f	51	TYR	CB-CG-CD1	5.24	124.14	121.00
2	D	66	TYR	CA-CB-CG	5.24	123.35	113.40
32	5	2665	U	C2'-C3'-O3'	5.24	122.08	113.70
54	S2	1080	A	O4'-C1'-N9	5.24	112.39	108.20
54	S2	1420	G	C2'-C3'-O3'	5.24	122.08	113.70
54	S2	1675	A	N9-C1'-C2'	-5.23	106.24	112.00
32	5	210	C	N1-C1'-C2'	5.23	120.80	114.00
50	3	38	C	OP1-P-O3'	5.23	116.71	105.20
61	SI	197	PHE	N-CA-C	-5.23	96.87	111.00
32	5	1852	U	N1-C1'-C2'	-5.23	106.25	112.00
32	5	2089	G	O4'-C1'-N9	5.23	112.38	108.20
32	5	4723	A	C5'-C4'-O4'	5.23	115.38	109.10
32	5	2665	U	N1-C1'-C2'	-5.23	106.25	112.00
4	H	88	PHE	CB-CG-CD2	-5.23	117.14	120.80
1	A	189	TYR	CB-CG-CD2	-5.22	117.86	121.00
32	5	2737	C	N1-C1'-C2'	5.22	120.79	114.00
17	Y	87	ARG	NE-CZ-NH1	-5.22	117.69	120.30
32	5	2725	A	N9-C1'-C2'	5.22	120.79	114.00
54	S2	1522	A	O4'-C4'-C3'	-5.22	98.78	104.00
72	Se	13	ARG	NE-CZ-NH1	5.22	122.91	120.30
32	5	1484	G	N9-C1'-C2'	5.22	120.78	114.00
32	5	2089	G	C1'-O4'-C4'	-5.22	105.72	109.90
32	5	2586	G	O4'-C1'-N9	5.22	112.38	108.20
54	S2	651	U	N1-C1'-C2'	5.22	120.79	114.00
32	5	1697	G	O4'-C1'-N9	5.22	112.38	108.20
54	S2	1395	C	O4'-C1'-C2'	-5.22	100.58	105.80
67	SW	57	ARG	NE-CZ-NH2	-5.22	117.69	120.30
78	SQ	71	ARG	CG-CD-NE	5.22	122.76	111.80
54	S2	297	A	N9-C1'-C2'	-5.22	106.26	112.00
18	Z	38	TYR	CB-CA-C	5.21	120.83	110.40
68	SX	67	ARG	NE-CZ-NH1	-5.21	117.69	120.30
2	D	145	TYR	CB-CA-C	5.21	120.82	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	2741	U	N1-C1'-C2'	5.21	120.77	114.00
56	SB	136	ARG	NE-CZ-NH2	5.21	122.90	120.30
32	5	1266	G	C2'-C3'-O3'	5.21	122.03	113.70
32	5	1885	G	C4'-C3'-O3'	5.21	123.41	113.00
58	SE	18	TRP	CA-CB-CG	-5.21	103.81	113.70
32	5	5043	A	C1'-C2'-O2'	-5.20	94.99	110.60
42	j	66	HIS	CA-CB-CG	-5.20	104.75	113.60
57	SC	68	ARG	NE-CZ-NH1	5.20	122.90	120.30
32	5	272	U	N1-C1'-C2'	5.20	120.76	114.00
32	5	4966	A	C8-N9-C1'	-5.20	118.34	127.70
35	B	257	TRP	N-CA-CB	5.20	119.96	110.60
42	j	27	TYR	CB-CG-CD1	-5.20	117.88	121.00
54	S2	1225	U	C2'-C3'-O3'	5.20	122.02	113.70
32	5	4701	A	C4-N9-C1'	5.20	135.66	126.30
36	C	201	ARG	NE-CZ-NH1	5.20	122.90	120.30
51	4	183	A	P-O3'-C3'	-5.20	113.46	119.70
32	5	2328	G	C1'-C2'-O2'	-5.20	95.01	110.60
32	5	4322	G	C2'-C3'-O3'	5.20	122.01	113.70
36	C	100	ARG	NE-CZ-NH1	5.20	122.90	120.30
54	S2	1049	A	C1'-O4'-C4'	-5.19	105.75	109.90
32	5	393	U	N1-C1'-C2'	-5.19	106.29	112.00
32	5	468	U	N1-C1'-C2'	5.19	120.75	114.00
54	S2	1522	A	N9-C1'-C2'	-5.19	106.29	112.00
1	A	227	ARG	NE-CZ-NH1	5.19	122.89	120.30
2	D	145	TYR	CA-CB-CG	-5.19	103.54	113.40
32	5	4709	U	C5'-C4'-O4'	5.19	115.32	109.10
33	7	5	A	N9-C1'-C2'	-5.19	106.30	112.00
5	J	147	ARG	NE-CZ-NH1	5.18	122.89	120.30
32	5	2056	G	O4'-C1'-N9	5.18	112.35	108.20
34	8	46	G	N9-C1'-C2'	5.18	120.74	114.00
54	S2	631	U	C2'-C3'-O3'	5.18	122.00	113.70
5	J	32	ARG	NE-CZ-NH1	5.18	122.89	120.30
32	5	1296	G	C1'-O4'-C4'	-5.18	105.75	109.90
32	5	4234	A	C4-N9-C1'	-5.18	116.97	126.30
44	p	85	ARG	CG-CD-NE	5.18	122.69	111.80
32	5	4556	U	C1'-O4'-C4'	-5.18	105.76	109.90
32	5	4280	A	C5'-C4'-O4'	5.18	115.31	109.10
54	S2	980	A	C8-N9-C1'	-5.18	118.38	127.70
32	5	4337	C	N1-C1'-C2'	5.17	120.73	114.00
11	R	155	LEU	CA-CB-CG	5.17	127.20	115.30
32	5	4670	C	O4'-C1'-N1	-5.17	104.06	108.20
32	5	96	U	C2'-C3'-O3'	5.17	121.97	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	I	119	PHE	CB-CG-CD1	5.17	124.42	120.80
32	5	1733	G	N9-C1'-C2'	-5.17	106.31	112.00
27	i	41	ARG	NE-CZ-NH1	5.17	122.88	120.30
32	5	3908	A	C3'-C2'-C1'	-5.17	97.37	101.50
36	C	35	ASP	CB-CG-OD2	-5.17	113.65	118.30
55	SA	204	TYR	CB-CG-CD1	5.17	124.10	121.00
56	SB	100	PHE	N-CA-CB	5.17	119.90	110.60
32	5	1609	U	C2'-C3'-O3'	5.17	121.96	113.70
46	K	55	GLY	N-CA-C	-5.17	100.19	113.10
32	5	2077	C	N1-C1'-C2'	-5.16	106.32	112.00
32	5	4589	A	O4'-C4'-C3'	-5.16	98.84	104.00
54	S2	1386	A	C2'-C3'-O3'	5.16	121.96	113.70
17	Y	87	ARG	CD-NE-CZ	5.16	130.82	123.60
32	5	219	G	O4'-C1'-C2'	-5.16	100.64	105.80
32	5	2360	A	N9-C1'-C2'	5.16	120.70	114.00
54	S2	600	G	N9-C1'-C2'	5.16	120.71	114.00
54	S2	645	C	C2'-C3'-O3'	5.16	121.95	113.70
32	5	1365	C	P-O3'-C3'	5.16	125.89	119.70
32	5	1793	A	C2'-C3'-O3'	5.16	121.95	113.70
32	5	2080	U	N1-C1'-C2'	5.16	120.70	114.00
56	SB	82	ARG	N-CA-C	5.15	124.92	111.00
54	S2	61	A	C4'-C3'-O3'	-5.15	98.58	109.40
54	S2	844	U	O4'-C1'-N1	5.15	112.32	108.20
11	R	95	TRP	N-CA-C	-5.15	97.09	111.00
32	5	2802	C	N1-C1'-C2'	-5.15	106.33	112.00
32	5	961	G	C4'-C3'-O3'	5.15	123.30	113.00
54	S2	1292	C	P-O3'-C3'	5.15	125.88	119.70
2	D	44	TYR	CA-CB-CG	-5.15	103.62	113.40
32	5	4270	C	C5'-C4'-O4'	5.15	115.28	109.10
33	7	6	C	N1-C1'-C2'	-5.15	106.34	112.00
38	F	100	ILE	CG1-CB-CG2	5.15	122.72	111.40
32	5	58	G	O4'-C1'-N9	-5.15	104.08	108.20
32	5	4229	U	O4'-C1'-C2'	-5.15	100.65	105.80
45	r	45	HIS	CB-CA-C	-5.15	100.11	110.40
54	S2	1823	A	C2'-C3'-O3'	5.15	121.93	113.70
20	b	16	TRP	CB-CA-C	5.14	120.69	110.40
32	5	3898	G	C2'-C3'-O3'	5.14	121.93	113.70
54	S2	638	C	N1-C1'-C2'	5.14	120.69	114.00
32	5	931	C	N1-C1'-C2'	5.14	120.69	114.00
54	S2	165	G	O4'-C4'-C3'	-5.14	98.86	104.00
32	5	1832	C	C2'-C3'-O3'	5.14	121.92	113.70
42	j	11	ARG	CG-CD-NE	-5.14	101.00	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	SB	107	ARG	NE-CZ-NH2	-5.14	117.73	120.30
6	L	36	ARG	NE-CZ-NH1	5.14	122.87	120.30
32	5	5005	G	N9-C1'-C2'	-5.14	106.35	112.00
37	E	129	PHE	CB-CG-CD1	5.14	124.40	120.80
54	S2	1525	C	C2'-C3'-O3'	5.14	121.92	113.70
32	5	1444	G	N9-C1'-C2'	5.14	120.68	114.00
54	S2	957	A	C2'-C3'-O3'	5.14	121.92	113.70
62	SJ	127	ARG	NE-CZ-NH2	-5.14	117.73	120.30
10	Q	181	ARG	CG-CD-NE	-5.13	101.03	111.80
54	S2	603	C	C4'-C3'-O3'	5.13	123.26	113.00
74	SF	48	TYR	CA-CB-CG	5.13	123.15	113.40
63	SL	62	PHE	CB-CG-CD2	-5.13	117.21	120.80
2	D	175	HIS	N-CA-C	-5.12	97.16	111.00
32	5	4441	A	C2'-C3'-O3'	5.12	121.90	113.70
54	S2	1142	G	C4'-C3'-C2'	-5.12	97.47	102.60
55	SA	90	PHE	N-CA-CB	5.12	119.82	110.60
3	G	73	ARG	NE-CZ-NH1	5.12	122.86	120.30
5	J	146	ARG	NE-CZ-NH2	5.12	122.86	120.30
6	L	82	ARG	NE-CZ-NH2	-5.12	117.74	120.30
10	Q	168	ARG	NE-CZ-NH1	5.12	122.86	120.30
32	5	21	G	C4'-C3'-O3'	5.12	123.24	113.00
32	5	1520	C	C2'-C3'-O3'	5.12	121.89	113.70
33	7	57	C	C2'-C3'-O3'	5.12	121.90	113.70
54	S2	1391	C	C2'-C3'-O3'	5.12	121.89	113.70
32	5	1947	U	C4'-C3'-O3'	5.12	123.24	113.00
61	SI	28	GLU	N-CA-C	-5.12	97.18	111.00
32	5	5002	U	N1-C1'-C2'	5.12	120.65	114.00
32	5	107	G	N9-C1'-C2'	-5.12	106.37	112.00
32	5	1447	C	O4'-C1'-N1	5.12	112.29	108.20
54	S2	619	A	C3'-C2'-C1'	-5.12	97.41	101.50
8	N	143	ARG	NE-CZ-NH2	-5.11	117.74	120.30
32	5	209	U	O4'-C1'-N1	5.11	112.29	108.20
32	5	1365	C	O4'-C1'-N1	-5.11	104.11	108.20
32	5	4239	A	C2'-C3'-O3'	5.11	121.88	113.70
32	5	4884	G	O4'-C1'-C2'	-5.11	100.69	105.80
32	5	2782	U	P-O3'-C3'	5.11	125.83	119.70
32	5	3727	A	C1'-C2'-O2'	-5.11	95.27	110.60
33	7	22	A	C1'-O4'-C4'	-5.11	105.81	109.90
51	4	32	A	N9-C1'-C2'	-5.11	106.38	112.00
56	SB	81	PHE	CB-CG-CD1	-5.11	117.22	120.80
71	Sb	31	TYR	CA-CB-CG	5.11	123.11	113.40
32	5	514	U	C4'-C3'-O3'	5.11	123.21	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	2787	A	O5'-P-OP1	5.11	116.83	110.70
54	S2	446	G	N9-C1'-C2'	-5.11	106.38	112.00
74	SF	152	TRP	N-CA-CB	5.11	119.79	110.60
32	5	148	C	N1-C1'-C2'	5.11	120.64	114.00
78	SQ	71	ARG	CD-NE-CZ	5.10	130.75	123.60
86	Sf	138	ARG	CD-NE-CZ	5.10	130.75	123.60
1	A	194	ASN	N-CA-CB	5.10	119.78	110.60
22	d	44	ARG	NE-CZ-NH2	-5.10	117.75	120.30
32	5	1341	U	N1-C1'-C2'	5.10	120.63	114.00
32	5	4463	U	O4'-C1'-C2'	-5.10	100.70	105.80
36	C	143	ARG	NE-CZ-NH2	-5.10	117.75	120.30
54	S2	1481	G	N9-C1'-C2'	5.10	120.63	114.00
32	5	394	G	C4'-C3'-C2'	-5.10	97.50	102.60
32	5	3719	A	C2'-C3'-O3'	5.10	121.85	113.70
31	o	42	ASP	N-CA-CB	5.09	119.77	110.60
32	5	1271	G	C4'-C3'-O3'	5.09	123.18	113.00
32	5	2127	C	N1-C1'-C2'	5.09	120.62	114.00
54	S2	943	U	C5'-C4'-O4'	5.09	115.21	109.10
54	S2	1703	C	N1-C1'-C2'	-5.09	106.40	112.00
54	S2	1097	G	C2'-C3'-O3'	5.09	121.84	113.70
10	Q	33	ARG	CG-CD-NE	-5.08	101.12	111.80
32	5	338	A	C2'-C3'-O3'	5.08	121.83	113.70
33	7	81	G	C2'-C3'-O3'	5.08	121.83	113.70
32	5	1267	C	N1-C1'-C2'	5.08	120.61	114.00
32	5	3740	G	O4'-C1'-C2'	-5.08	100.72	105.80
35	B	117	ARG	CG-CD-NE	-5.08	101.13	111.80
33	7	49	A	N9-C1'-C2'	-5.08	106.41	112.00
54	S2	839	C	N1-C1'-C2'	5.08	120.60	114.00
54	S2	1149	A	N9-C1'-C2'	-5.08	106.41	112.00
54	S2	1036	A	C2'-C3'-O3'	5.08	121.83	113.70
11	R	108	ARG	CG-CD-NE	5.08	122.46	111.80
54	S2	381	C	P-O5'-C5'	5.08	129.02	120.90
57	SC	68	ARG	CG-CD-NE	5.08	122.46	111.80
68	SX	17	ARG	CG-CD-NE	-5.08	101.14	111.80
78	SQ	71	ARG	NE-CZ-NH2	-5.07	117.77	120.30
87	Sg	302	TYR	CB-CG-CD2	-5.07	117.96	121.00
32	5	2586	G	C3'-C2'-C1'	-5.07	97.45	101.50
54	S2	798	A	C4'-C3'-C2'	-5.07	97.53	102.60
54	S2	56	G	N9-C1'-C2'	5.06	120.58	114.00
54	S2	646	G	C2'-C3'-O3'	5.06	121.80	113.70
32	5	1488	G	C2'-C3'-O3'	5.06	121.80	113.70
32	5	4911	A	N9-C1'-C2'	-5.06	106.43	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	2264	C	C2'-C3'-O3'	5.06	121.80	113.70
41	W	8	PHE	CB-CA-C	5.06	120.52	110.40
54	S2	1404	U	C4'-C3'-O3'	-5.06	98.77	109.40
54	S2	1604	G	C2'-C3'-O3'	5.06	121.80	113.70
56	SB	65	ARG	NE-CZ-NH1	5.06	122.83	120.30
32	5	1522	G	C4'-C3'-C2'	-5.06	97.54	102.60
32	5	4094	G	C2'-C3'-O3'	5.06	121.79	113.70
54	S2	968	U	C2'-C3'-O3'	5.06	121.79	113.70
54	S2	1404	U	O4'-C1'-N1	-5.06	104.15	108.20
58	SE	235	TRP	CA-CB-CG	5.06	123.31	113.70
32	5	292	G	C4'-C3'-O3'	-5.05	98.78	109.40
32	5	1980	U	O4'-C1'-N1	5.05	112.24	108.20
38	F	228	HIS	N-CA-CB	5.05	119.70	110.60
32	5	1636	U	N1-C1'-C2'	5.05	120.57	114.00
54	S2	1109	C	C1'-O4'-C4'	-5.05	105.86	109.90
78	SQ	99	TYR	CB-CG-CD1	5.05	124.03	121.00
78	SQ	138	ARG	CG-CD-NE	5.05	122.40	111.80
88	S1	44	ASP	CB-CG-OD1	-5.05	113.76	118.30
5	J	35	ARG	NE-CZ-NH2	-5.05	117.78	120.30
6	L	99	ASP	N-CA-C	-5.05	97.38	111.00
32	5	4975	G	C3'-C2'-C1'	5.05	105.54	101.50
32	5	5044	A	C1'-C2'-O2'	-5.05	95.46	110.60
27	i	85	ARG	CD-NE-CZ	5.04	130.66	123.60
32	5	383	A	C1'-C2'-O2'	-5.04	95.46	110.60
32	5	3881	G	O4'-C1'-N9	-5.04	104.16	108.20
39	I	147	HIS	CB-CA-C	5.04	120.49	110.40
54	S2	1561	A	N9-C1'-C2'	-5.04	106.45	112.00
33	7	59	G	C2'-C3'-O3'	5.04	121.77	113.70
34	8	113	C	C2'-C3'-O3'	5.04	121.77	113.70
54	S2	992	A	N9-C1'-C2'	-5.04	106.45	112.00
11	R	108	ARG	CD-NE-CZ	5.04	130.66	123.60
54	S2	504	G	N9-C1'-C2'	5.04	120.56	114.00
10	Q	52	PHE	N-CA-CB	-5.04	101.53	110.60
32	5	20	U	N1-C1'-C2'	-5.04	106.46	112.00
54	S2	1416	C	C2'-C3'-O3'	5.04	121.76	113.70
54	S2	1830	U	N1-C1'-C2'	-5.04	106.46	112.00
12	S	111	ARG	NE-CZ-NH2	5.04	122.82	120.30
36	C	350	ARG	NE-CZ-NH2	-5.04	117.78	120.30
32	5	2545	U	C2'-C3'-O3'	5.03	121.75	113.70
54	S2	376	A	N9-C1'-C2'	-5.03	106.46	112.00
32	5	2666	U	C5'-C4'-O4'	5.03	115.14	109.10
32	5	1281	G	C5'-C4'-O4'	5.03	115.14	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	4606	G	N9-C1'-C2'	5.03	120.54	114.00
67	SW	28	ARG	NE-CZ-NH1	5.03	122.81	120.30
32	5	4976	U	N1-C1'-C2'	5.03	120.54	114.00
32	5	2511	A	C5'-C4'-O4'	5.03	115.13	109.10
30	m	111	ARG	NE-CZ-NH2	5.03	122.81	120.30
32	5	4436	U	N1-C1'-C2'	-5.03	106.47	112.00
54	S2	1339	U	C3'-C2'-C1'	5.03	105.52	101.50
60	SH	135	PHE	CB-CG-CD1	5.03	124.32	120.80
34	8	70	G	C3'-C2'-C1'	5.02	105.52	101.50
54	S2	127	C	C4'-C3'-O3'	5.02	123.05	113.00
54	S2	578	C	N1-C1'-C2'	-5.02	106.47	112.00
54	S2	821	G	C5'-C4'-O4'	5.02	115.13	109.10
73	SD	106	ARG	NE-CZ-NH1	5.02	122.81	120.30
4	H	124	ARG	NE-CZ-NH1	5.02	122.81	120.30
10	Q	32	TYR	CA-CB-CG	5.02	122.94	113.40
1	A	189	TYR	CB-CG-CD1	5.02	124.01	121.00
22	d	63	ARG	NE-CZ-NH1	5.02	122.81	120.30
32	5	286	U	C2-N1-C1'	5.02	123.72	117.70
34	8	34	U	C3'-C2'-C1'	5.02	105.52	101.50
40	P	42	ARG	NE-CZ-NH2	-5.02	117.79	120.30
54	S2	943	U	C2-N1-C1'	5.02	123.72	117.70
32	5	4939	C	O4'-C1'-C2'	-5.02	100.78	105.80
34	8	67	U	N1-C1'-C2'	5.02	120.52	114.00
86	Sf	146	LEU	N-CA-CB	5.02	120.43	110.40
2	D	35	ARG	NE-CZ-NH2	-5.02	117.79	120.30
54	S2	164	A	C3'-C2'-C1'	5.02	105.51	101.50
32	5	2055	G	N9-C1'-C2'	-5.01	106.48	112.00
32	5	2268	A	P-O3'-C3'	5.01	125.72	119.70
54	S2	1432	U	N1-C1'-C2'	5.01	120.52	114.00
54	S2	606	G	O4'-C1'-N9	5.01	112.21	108.20
32	5	4539	U	N1-C1'-C2'	5.01	120.51	114.00
32	5	1364	U	C4'-C3'-C2'	-5.01	97.59	102.60
32	5	1397	A	C2'-C3'-O3'	5.01	121.71	113.70
38	F	197	TYR	CB-CA-C	-5.01	100.39	110.40
80	SS	124	ARG	CG-CD-NE	5.01	122.31	111.80
54	S2	349	A	C4'-C3'-O3'	-5.00	98.89	109.40
14	U	97	ARG	NE-CZ-NH2	-5.00	117.80	120.30
48	z	237	LYS	CD-CE-NZ	5.00	123.20	111.70

There are no chirality outliers.

All (529) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
49	2	110	LYS	Peptide
32	5	100	C	Sidechain
32	5	120	A	Sidechain
32	5	1214	C	Sidechain
32	5	1319	U	Sidechain
32	5	1324	A	Sidechain
32	5	1365	C	Sidechain
32	5	1395	U	Sidechain
32	5	1398	A	Sidechain
32	5	147	A	Sidechain
32	5	1479	G	Sidechain
32	5	150	U	Sidechain
32	5	1501	C	Sidechain
32	5	151	G	Sidechain
32	5	1516	G	Sidechain
32	5	1521	C	Sidechain
32	5	1522	G	Sidechain
32	5	1534	A	Sidechain
32	5	1552	G	Sidechain
32	5	157	U	Sidechain
32	5	1613	A	Sidechain
32	5	1627	G	Sidechain
32	5	1631	A	Sidechain
32	5	1632	A	Sidechain
32	5	1650	A	Sidechain
32	5	1668	A	Sidechain
32	5	1671	U	Sidechain
32	5	1676	C	Sidechain
32	5	1682	A	Sidechain
32	5	1697	G	Sidechain
32	5	172	C	Sidechain
32	5	1740	C	Sidechain
32	5	1853	G	Sidechain
32	5	1887	G	Sidechain
32	5	1894	C	Sidechain
32	5	1930	U	Sidechain
32	5	1938	C	Sidechain
32	5	1946	G	Sidechain
32	5	2035	C	Sidechain
32	5	2037	C	Sidechain
32	5	2046	G	Sidechain
32	5	2056	G	Sidechain
32	5	2077	C	Sidechain

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Mol	Chain	Res	Type	Group
32	5	2081	C	Sidechain
32	5	2082	G	Sidechain
32	5	2087	C	Sidechain
32	5	22	G	Sidechain
32	5	2263	A	Sidechain
32	5	2268	A	Sidechain
32	5	2282	A	Sidechain
32	5	2305	U	Sidechain
32	5	2307	A	Sidechain
32	5	2325	C	Sidechain
32	5	2348	G	Sidechain
32	5	235	A	Sidechain
32	5	2361	G	Sidechain
32	5	2362	U	Sidechain
32	5	2394	G	Sidechain
32	5	2396	A	Sidechain
32	5	2406	G	Sidechain
32	5	2436	U	Sidechain
32	5	2438	A	Sidechain
32	5	2446	C	Sidechain
32	5	2450	G	Sidechain
32	5	2460	A	Sidechain
32	5	2465	C	Sidechain
32	5	2510	G	Sidechain
32	5	2511	A	Sidechain
32	5	2513	A	Sidechain
32	5	2515	G	Sidechain
32	5	2597	G	Sidechain
32	5	2649	G	Sidechain
32	5	2666	U	Sidechain
32	5	2675	G	Sidechain
32	5	2769	U	Sidechain
32	5	2796	G	Sidechain
32	5	280	G	Sidechain
32	5	2806	A	Sidechain
32	5	2827	G	Sidechain
32	5	2848	G	Sidechain
32	5	2851	G	Sidechain
32	5	2858	A	Sidechain
32	5	292	G	Sidechain
32	5	30	C	Sidechain
32	5	31	U	Sidechain

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Mol	Chain	Res	Type	Group
32	5	33	A	Sidechain
32	5	336	A	Sidechain
32	5	352	G	Sidechain
32	5	3621	A	Sidechain
32	5	3635	A	Sidechain
32	5	3648	A	Sidechain
32	5	3653	A	Sidechain
32	5	3663	A	Sidechain
32	5	3692	A	Sidechain
32	5	3726	A	Sidechain
32	5	3790	U	Sidechain
32	5	384	A	Sidechain
32	5	3843	C	Sidechain
32	5	3844	U	Sidechain
32	5	3860	A	Sidechain
32	5	3871	A	Sidechain
32	5	3875	G	Sidechain
32	5	3879	G	Sidechain
32	5	3880	G	Sidechain
32	5	3905	A	Sidechain
32	5	3906	A	Sidechain
32	5	3907	G	Sidechain
32	5	3938	G	Sidechain
32	5	394	G	Sidechain
32	5	405	U	Sidechain
32	5	4162	C	Sidechain
32	5	417	G	Sidechain
32	5	421	C	Sidechain
32	5	4228	G	Sidechain
32	5	4229	U	Sidechain
32	5	4234	A	Sidechain
32	5	4239	A	Sidechain
32	5	4270	C	Sidechain
32	5	4275	G	Sidechain
32	5	4280	A	Sidechain
32	5	4282	A	Sidechain
32	5	4283	G	Sidechain
32	5	43	U	Sidechain
32	5	4330	G	Sidechain
32	5	4331	G	Sidechain
32	5	4336	A	Sidechain
32	5	4341	C	Sidechain

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Mol	Chain	Res	Type	Group
32	5	4378	A	Sidechain
32	5	4404	U	Sidechain
32	5	4405	G	Sidechain
32	5	4449	A	Sidechain
32	5	4463	U	Sidechain
32	5	4464	A	Sidechain
32	5	4497	U	Sidechain
32	5	4498	U	Sidechain
32	5	4510	A	Sidechain
32	5	4519	C	Sidechain
32	5	4527	G	Sidechain
32	5	4528	G	Sidechain
32	5	4535	A	Sidechain
32	5	4589	A	Sidechain
32	5	4600	G	Sidechain
32	5	4670	C	Sidechain
32	5	4677	U	Sidechain
32	5	4693	C	Sidechain
32	5	4763	U	Sidechain
32	5	4871	C	Sidechain
32	5	4880	C	Sidechain
32	5	4911	A	Sidechain
32	5	4966	A	Sidechain
32	5	4976	U	Sidechain
32	5	4981	G	Sidechain
32	5	5001	U	Sidechain
32	5	5006	U	Sidechain
32	5	5040	U	Sidechain
32	5	5043	A	Sidechain
32	5	5044	A	Sidechain
32	5	5050	C	Sidechain
32	5	5066	U	Sidechain
32	5	53	C	Sidechain
32	5	54	G	Sidechain
32	5	55	G	Sidechain
32	5	62	A	Sidechain
32	5	664	G	Sidechain
32	5	72	C	Sidechain
32	5	77	U	Sidechain
32	5	84	A	Sidechain
32	5	85	G	Sidechain
32	5	89	C	Sidechain

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Mol	Chain	Res	Type	Group
32	5	91	G	Sidechain
32	5	92	C	Sidechain
32	5	93	G	Sidechain
32	5	94	A	Sidechain
32	5	964	A	Sidechain
32	5	97	G	Sidechain
32	5	99	A	Sidechain
33	7	42	A	Sidechain
33	7	56	G	Sidechain
34	8	10	G	Sidechain
34	8	104	A	Sidechain
34	8	14	U	Sidechain
34	8	34	U	Sidechain
34	8	35	C	Sidechain
34	8	38	U	Sidechain
34	8	39	G	Sidechain
34	8	70	G	Sidechain
34	8	73	U	Sidechain
34	8	9	A	Sidechain
34	8	94	G	Sidechain
1	A	18	ALA	Peptide
1	A	194	ASN	Peptide
1	A	196	TRP	Peptide
1	A	209	HIS	Sidechain
1	A	211	PHE	Sidechain
1	A	215	ASN	Peptide
1	A	66	PRO	Peptide
1	A	67	TYR	Sidechain
35	B	102	PHE	Peptide
35	B	108	GLU	Peptide
35	B	16	PHE	Peptide
35	B	179	HIS	Sidechain
35	B	257	TRP	Peptide
35	B	264	PHE	Peptide
35	B	322	HIS	Peptide
35	B	367	PHE	Sidechain
35	B	379	PHE	Peptide
35	B	387	ALA	Peptide
35	B	46	PHE	Peptide
35	B	55	HIS	Sidechain
36	C	113	ARG	Peptide
36	C	177	TRP	Peptide

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Mol	Chain	Res	Type	Group
36	C	265	GLY	Peptide
36	C	41	HIS	Sidechain
2	D	129	GLU	Peptide
2	D	190	PHE	Peptide
2	D	20	PHE	Peptide
2	D	218	ALA	Peptide
2	D	260	GLU	Peptide
2	D	266	TRP	Peptide
2	D	30	TYR	Peptide
2	D	41	LYS	Peptide
2	D	44	TYR	Sidechain
37	E	102	VAL	Peptide
37	E	103	VAL	Peptide
37	E	111	TYR	Peptide
37	E	123	SER	Peptide
37	E	152	ARG	Peptide
37	E	177	LEU	Peptide
37	E	216	LYS	Peptide
37	E	224	GLN	Peptide
37	E	230	ASP	Peptide
37	E	233	LYS	Peptide
37	E	235	LYS	Peptide
37	E	274	THR	Peptide
37	E	278	TYR	Sidechain
37	E	279	PRO	Peptide
37	E	280	HIS	Sidechain
37	E	281	LYS	Peptide
38	F	127	LEU	Peptide
38	F	197	TYR	Peptide
38	F	208	ASN	Peptide
38	F	228	HIS	Sidechain
38	F	237	ASN	Peptide
38	F	81	GLY	Peptide
38	F	82	ASN	Peptide
38	F	84	TYR	Peptide
3	G	101	LYS	Peptide
3	G	229	ARG	Peptide
3	G	54	PHE	Sidechain
3	G	66	GLN	Peptide
4	H	50	LYS	Peptide
4	H	59	LYS	Peptide
39	I	158	LYS	Peptide

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Mol	Chain	Res	Type	Group
39	I	77	VAL	Peptide
39	I	93	PRO	Peptide
5	J	87	LEU	Peptide
5	J	99	PHE	Sidechain
46	K	122	ALA	Peptide
46	K	123	ARG	Peptide
46	K	148	PRO	Peptide
46	K	54	LYS	Peptide
46	K	87	GLU	Peptide
46	K	88	PRO	Peptide
46	K	89	PRO	Peptide
46	K	9	GLU	Peptide
46	K	94	LYS	Peptide
46	K	97	ASN	Peptide
6	L	146	LEU	Peptide
6	L	46	ILE	Peptide
6	L	62	PRO	Peptide
6	L	66	TYR	Peptide
7	M	6	PHE	Sidechain
7	M	65	PRO	Peptide
7	M	94	LYS	Peptide
8	N	119	TYR	Sidechain
8	N	138	PHE	Peptide
8	N	139	HIS	Sidechain
8	N	180	PHE	Sidechain
8	N	181	HIS	Peptide
8	N	202	ARG	Peptide
8	N	29	GLN	Peptide
8	N	86	HIS	Peptide
8	N	90	ASN	Peptide
9	O	110	PRO	Peptide
9	O	117	ARG	Peptide
9	O	135	PHE	Sidechain
9	O	64	THR	Peptide
40	P	116	HIS	Sidechain
40	P	139	TYR	Sidechain
40	P	145	HIS	Sidechain
40	P	7	ASP	Peptide
10	Q	161	SER	Peptide
10	Q	3	VAL	Peptide
10	Q	32	TYR	Peptide
10	Q	34	PHE	Sidechain

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Mol	Chain	Res	Type	Group
10	Q	51	LEU	Peptide
11	R	132	PHE	Peptide,Sidechain
11	R	174	GLU	Peptide
11	R	19	LYS	Peptide
11	R	23	TRP	Peptide
11	R	31	GLU	Peptide
11	R	94	THR	Peptide
12	S	10	TYR	Sidechain
12	S	145	PHE	Peptide
12	S	152	PHE	Peptide
12	S	154	LEU	Peptide
12	S	159	LEU	Peptide
12	S	164	LYS	Peptide
12	S	32	ILE	Peptide
12	S	68	PHE	Peptide
88	S1	46	LEU	Peptide
88	S1	5	GLN	Mainchain,Peptide
88	S1	52	LYS	Peptide
54	S2	1036	A	Sidechain
54	S2	1063	C	Sidechain
54	S2	1085	C	Sidechain
54	S2	1088	U	Sidechain
54	S2	1142	G	Sidechain
54	S2	1167	G	Sidechain
54	S2	1168	G	Sidechain
54	S2	1221	G	Sidechain
54	S2	1247	C	Sidechain
54	S2	1249	C	Sidechain
54	S2	1378	A	Sidechain
54	S2	1408	U	Sidechain
54	S2	1452	A	Sidechain
54	S2	1453	C	Sidechain
54	S2	1537	A	Sidechain
54	S2	1552	G	Sidechain
54	S2	1578	U	Sidechain
54	S2	1603	G	Sidechain
54	S2	1606	G	Sidechain
54	S2	1623	A	Sidechain
54	S2	1659	U	Sidechain
54	S2	1835	A	Sidechain
54	S2	1838	U	Sidechain
54	S2	26	U	Sidechain

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Mol	Chain	Res	Type	Group
54	S2	27	A	Sidechain
54	S2	294	U	Sidechain
54	S2	3	C	Sidechain
54	S2	31	U	Sidechain
54	S2	313	A	Sidechain
54	S2	367	U	Sidechain
54	S2	381	C	Sidechain
54	S2	382	C	Sidechain
54	S2	399	C	Sidechain
54	S2	409	C	Sidechain
54	S2	421	G	Sidechain
54	S2	423	U	Sidechain
54	S2	426	A	Sidechain
54	S2	427	U	Sidechain
54	S2	428	U	Sidechain
54	S2	437	G	Sidechain
54	S2	447	A	Sidechain
54	S2	448	A	Sidechain
54	S2	482	G	Sidechain
54	S2	596	U	Sidechain
54	S2	617	G	Sidechain
54	S2	631	U	Sidechain
54	S2	642	U	Sidechain
54	S2	645	C	Sidechain
54	S2	648	A	Sidechain
54	S2	662	G	Sidechain
54	S2	821	G	Sidechain
54	S2	825	A	Sidechain
54	S2	841	G	Sidechain
54	S2	875	A	Sidechain
54	S2	876	C	Sidechain
54	S2	91	A	Sidechain
54	S2	92	A	Sidechain
54	S2	945	U	Sidechain
54	S2	999	G	Sidechain
55	SA	103	PHE	Sidechain
55	SA	115	ALA	Peptide
55	SA	163	CYS	Peptide
55	SA	2	SER	Peptide
55	SA	40	LYS	Peptide
56	SB	100	PHE	Sidechain
56	SB	205	TYR	Sidechain

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Mol	Chain	Res	Type	Group
56	SB	211	PHE	Peptide
56	SB	40	ASN	Peptide
56	SB	66	VAL	Peptide
56	SB	81	PHE	Peptide,Sidechain
57	SC	168	GLY	Peptide
57	SC	235	ASN	Peptide
57	SC	236	PHE	Sidechain
57	SC	240	THR	Peptide
57	SC	241	PHE	Sidechain
57	SC	60	TRP	Peptide
57	SC	96	PHE	Peptide
73	SD	159	HIS	Sidechain
73	SD	196	GLY	Peptide
73	SD	203	PRO	Peptide
58	SE	100	ARG	Peptide
58	SE	121	TYR	Sidechain
58	SE	17	HIS	Peptide
58	SE	205	PHE	Peptide
58	SE	41	CYS	Peptide
58	SE	86	PHE	Sidechain
74	SF	164	ARG	Peptide
74	SF	22	LYS	Peptide
74	SF	43	GLU	Peptide
74	SF	51	HIS	Sidechain
59	SG	57	ASP	Peptide
60	SH	108	SER	Peptide
60	SH	189	PHE	Peptide
61	SI	111	GLN	Peptide
61	SI	149	TYR	Peptide
61	SI	153	LYS	Peptide
61	SI	155	ASN	Peptide
61	SI	197	PHE	Peptide
61	SI	26	LYS	Peptide
61	SI	50	GLY	Peptide
61	SI	64	ASN	Peptide
61	SI	65	PHE	Peptide
62	SJ	18	ARG	Peptide
62	SJ	38	ARG	Peptide
62	SJ	93	LYS	Peptide
75	SK	60	GLU	Peptide
63	SL	15	THR	Peptide
63	SL	151	THR	Peptide

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Mol	Chain	Res	Type	Group
63	SL	62	PHE	Sidechain
76	SM	32	ALA	Peptide
76	SM	75	ASN	Peptide
64	SN	112	LYS	Peptide
64	SN	113	PHE	Peptide
64	SN	127	ARG	Peptide
64	SN	18	TYR	Sidechain
64	SN	57	SER	Peptide
65	SO	147	ARG	Sidechain
77	SP	11	THR	Peptide
77	SP	21	ASP	Sidechain
77	SP	36	LEU	Peptide
78	SQ	43	GLU	Peptide
80	SS	81	ASP	Peptide
81	ST	10	ASN	Peptide
81	ST	52	TRP	Peptide
82	SU	71	GLY	Peptide
66	SV	32	ILE	Peptide
66	SV	49	GLN	Peptide
66	SV	52	THR	Peptide
67	SW	44	HIS	Sidechain
67	SW	67	GLY	Peptide
67	SW	76	SER	Peptide
68	SX	16	HIS	Sidechain
68	SX	20	HIS	Sidechain
69	SY	34	THR	Peptide
83	SZ	108	ILE	Peptide
70	Sa	17	HIS	Sidechain
70	Sa	71	LEU	Peptide
70	Sa	9	GLY	Peptide
71	Sb	81	ARG	Peptide
85	Sd	10	HIS	Peptide
85	Sd	26	ASN	Peptide
85	Sd	8	TRP	Peptide
86	Sf	132	MET	Peptide
86	Sf	135	HIS	Peptide
86	Sf	138	ARG	Peptide
86	Sf	139	HIS	Peptide
87	Sg	125	ARG	Peptide
87	Sg	155	ARG	Peptide
87	Sg	64	HIS	Peptide
13	T	140	PHE	Sidechain

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Mol	Chain	Res	Type	Group
13	T	142	ARG	Peptide
15	V	108	ASN	Peptide
15	V	13	LYS	Peptide
15	V	98	PHE	Sidechain
41	W	16	GLY	Peptide
16	X	143	ASP	Peptide
16	X	73	HIS	Sidechain
17	Y	11	ARG	Sidechain
17	Y	61	HIS	Sidechain
17	Y	62	TYR	Peptide
18	Z	37	PRO	Peptide
19	a	142	GLY	Peptide
19	a	39	HIS	Peptide
19	a	60	HIS	Peptide
19	a	61	TYR	Peptide
19	a	62	HIS	Sidechain
19	a	91	ALA	Peptide
20	b	20	GLY	Peptide
20	b	7	HIS	Peptide
21	c	77	ASN	Peptide
22	d	103	TYR	Peptide
22	d	108	TYR	Peptide
22	d	25	TYR	Sidechain
22	d	37	GLY	Peptide
22	d	72	VAL	Peptide
23	e	74	PHE	Sidechain
24	f	100	ARG	Peptide
24	f	70	ILE	Peptide
25	g	6	THR	Peptide
25	g	95	PHE	Peptide
26	h	97	LYS	Peptide
27	i	26	HIS	Sidechain
27	i	39	PHE	Sidechain
27	i	49	GLY	Peptide
42	j	46	LYS	Peptide
42	j	48	ASN	Peptide
42	j	66	HIS	Sidechain
42	j	8	PHE	Sidechain
28	k	28	ASN	Peptide
30	m	117	HIS	Peptide
31	o	31	ASP	Peptide
31	o	43	ARG	Peptide

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Mol	Chain	Res	Type	Group
31	o	47	GLY	Peptide
44	p	17	ARG	Peptide
44	p	34	HIS	Sidechain
47	q	116	ILE	Peptide
47	q	117	ALA	Peptide
47	q	132	PRO	Peptide
47	q	202	GLU	Peptide
47	q	204	LEU	Peptide
47	q	5	ASP	Peptide
47	q	6	ARG	Peptide
47	q	94	ASP	Peptide
45	r	30	ASN	Peptide
45	r	70	GLN	Peptide
45	r	76	SER	Peptide
48	z	100	LYS	Peptide
48	z	196	LYS	Peptide
48	z	344	PRO	Mainchain,Peptide
48	z	482	UNK	Mainchain
48	z	69	LEU	Peptide
48	z	70	ASN	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/244 (99%)	194 (80%)	38 (16%)	10 (4%)	2	21
2	D	290/292 (99%)	228 (79%)	41 (14%)	21 (7%)	1	13
3	G	236/238 (99%)	188 (80%)	41 (17%)	7 (3%)	3	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	188/190 (99%)	162 (86%)	20 (11%)	6 (3%)	3	26
5	J	168/170 (99%)	126 (75%)	33 (20%)	9 (5%)	1	17
6	L	208/210 (99%)	166 (80%)	29 (14%)	13 (6%)	1	15
7	M	136/138 (99%)	111 (82%)	21 (15%)	4 (3%)	3	27
8	N	201/203 (99%)	159 (79%)	31 (15%)	11 (6%)	1	17
9	O	199/201 (99%)	177 (89%)	19 (10%)	3 (2%)	8	38
10	Q	185/187 (99%)	154 (83%)	24 (13%)	7 (4%)	2	23
11	R	178/180 (99%)	148 (83%)	23 (13%)	7 (4%)	2	22
12	S	173/175 (99%)	139 (80%)	27 (16%)	7 (4%)	2	22
13	T	157/159 (99%)	132 (84%)	20 (13%)	5 (3%)	3	26
14	U	97/99 (98%)	80 (82%)	14 (14%)	3 (3%)	3	27
15	V	129/131 (98%)	110 (85%)	14 (11%)	5 (4%)	2	22
16	X	117/119 (98%)	102 (87%)	12 (10%)	3 (3%)	4	29
17	Y	132/134 (98%)	105 (80%)	21 (16%)	6 (4%)	2	20
18	Z	133/135 (98%)	111 (84%)	15 (11%)	7 (5%)	1	18
19	a	145/147 (99%)	114 (79%)	24 (17%)	7 (5%)	2	19
20	b	73/75 (97%)	60 (82%)	10 (14%)	3 (4%)	2	21
21	c	92/94 (98%)	78 (85%)	10 (11%)	4 (4%)	2	20
22	d	105/107 (98%)	85 (81%)	16 (15%)	4 (4%)	2	23
23	e	126/128 (98%)	110 (87%)	14 (11%)	2 (2%)	8	37
24	f	107/109 (98%)	89 (83%)	11 (10%)	7 (6%)	1	15
25	g	112/114 (98%)	100 (89%)	10 (9%)	2 (2%)	7	35
26	h	120/122 (98%)	97 (81%)	21 (18%)	2 (2%)	7	36
27	i	100/102 (98%)	85 (85%)	13 (13%)	2 (2%)	6	34
28	k	67/69 (97%)	53 (79%)	11 (16%)	3 (4%)	2	20
29	l	48/50 (96%)	42 (88%)	5 (10%)	1 (2%)	5	33
30	m	50/52 (96%)	44 (88%)	6 (12%)	0	100	100
31	o	102/104 (98%)	79 (78%)	17 (17%)	6 (6%)	1	16
35	B	392/394 (100%)	309 (79%)	54 (14%)	29 (7%)	1	12
36	C	365/367 (100%)	292 (80%)	55 (15%)	18 (5%)	2	18
37	E	232/236 (98%)	144 (62%)	55 (24%)	33 (14%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	F	223/225 (99%)	180 (81%)	35 (16%)	8 (4%)	3	24
39	I	211/213 (99%)	170 (81%)	28 (13%)	13 (6%)	1	15
40	P	151/153 (99%)	134 (89%)	15 (10%)	2 (1%)	10	41
41	W	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
42	j	84/86 (98%)	64 (76%)	18 (21%)	2 (2%)	5	30
43	n	21/23 (91%)	20 (95%)	1 (5%)	0	100	100
44	p	89/91 (98%)	75 (84%)	14 (16%)	0	100	100
45	r	123/125 (98%)	96 (78%)	20 (16%)	7 (6%)	1	16
46	K	159/163 (98%)	91 (57%)	34 (21%)	34 (21%)	0	1
47	q	200/202 (99%)	141 (70%)	31 (16%)	28 (14%)	0	3
48	z	399/426 (94%)	350 (88%)	31 (8%)	18 (4%)	2	20
49	2	27/31 (87%)	15 (56%)	9 (33%)	3 (11%)	0	5
52	9	103/105 (98%)	96 (93%)	7 (7%)	0	100	100
53	6	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
55	SA	206/208 (99%)	163 (79%)	30 (15%)	13 (6%)	1	15
56	SB	211/213 (99%)	154 (73%)	36 (17%)	21 (10%)	0	7
57	SC	216/218 (99%)	182 (84%)	27 (12%)	7 (3%)	3	26
58	SE	260/262 (99%)	198 (76%)	44 (17%)	18 (7%)	1	13
59	SG	235/237 (99%)	195 (83%)	32 (14%)	8 (3%)	3	25
60	SH	187/189 (99%)	141 (75%)	29 (16%)	17 (9%)	0	8
61	SI	204/206 (99%)	165 (81%)	30 (15%)	9 (4%)	2	20
62	SJ	183/185 (99%)	133 (73%)	35 (19%)	15 (8%)	1	10
63	SL	150/152 (99%)	122 (81%)	22 (15%)	6 (4%)	2	22
64	SN	147/149 (99%)	115 (78%)	28 (19%)	4 (3%)	4	29
65	SO	134/136 (98%)	99 (74%)	21 (16%)	14 (10%)	0	6
66	SV	80/82 (98%)	58 (72%)	15 (19%)	7 (9%)	0	9
67	SW	127/129 (98%)	108 (85%)	16 (13%)	3 (2%)	5	30
68	SX	139/141 (99%)	109 (78%)	26 (19%)	4 (3%)	3	27
69	SY	124/126 (98%)	101 (82%)	16 (13%)	7 (6%)	1	17
70	Sa	96/98 (98%)	69 (72%)	18 (19%)	9 (9%)	0	8
71	Sb	81/83 (98%)	61 (75%)	16 (20%)	4 (5%)	2	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	Se	55/57 (96%)	41 (74%)	12 (22%)	2 (4%)	3	24
73	SD	225/227 (99%)	174 (77%)	41 (18%)	10 (4%)	2	20
74	SF	189/191 (99%)	145 (77%)	34 (18%)	10 (5%)	1	18
75	SK	96/98 (98%)	58 (60%)	26 (27%)	12 (12%)	0	4
76	SM	122/124 (98%)	78 (64%)	24 (20%)	20 (16%)	0	2
77	SP	94/96 (98%)	67 (71%)	17 (18%)	10 (11%)	0	6
78	SQ	139/141 (99%)	111 (80%)	20 (14%)	8 (6%)	1	16
79	SR	127/129 (98%)	111 (87%)	11 (9%)	5 (4%)	2	22
80	SS	135/137 (98%)	114 (84%)	12 (9%)	9 (7%)	1	14
81	ST	139/141 (99%)	115 (83%)	18 (13%)	6 (4%)	2	20
82	SU	102/104 (98%)	83 (81%)	13 (13%)	6 (6%)	1	16
83	SZ	73/75 (97%)	59 (81%)	9 (12%)	5 (7%)	1	14
84	Sc	60/64 (94%)	47 (78%)	12 (20%)	1 (2%)	7	36
85	Sd	50/52 (96%)	36 (72%)	11 (22%)	3 (6%)	1	15
86	Sf	69/71 (97%)	42 (61%)	15 (22%)	12 (17%)	0	2
87	Sg	311/313 (99%)	240 (77%)	56 (18%)	15 (5%)	2	19
88	S1	72/74 (97%)	61 (85%)	6 (8%)	5 (7%)	1	13
89	S4	72/76 (95%)	68 (94%)	4 (6%)	0	100	100
All	All	12341/12544 (98%)	9853 (80%)	1811 (15%)	677 (6%)	2	17

All (677) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	196	TRP
1	A	197	PRO
2	D	9	ASN
2	D	19	LYS
2	D	57	ASN
2	D	212	ILE
2	D	262	LYS
4	H	60	TRP
5	J	88	LYS
5	J	91	GLU
6	L	64	VAL
6	L	67	HIS

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Mol	Chain	Res	Type
6	L	83	VAL
6	L	100	PRO
7	M	7	VAL
8	N	30	TYR
8	N	79	ALA
8	N	89	VAL
9	O	5	GLN
9	O	111	PRO
10	Q	52	PHE
10	Q	55	ARG
10	Q	178	ARG
11	R	36	ASN
12	S	146	HIS
12	S	165	PRO
13	T	44	GLY
13	T	106	LEU
15	V	14	PHE
15	V	99	GLU
16	X	86	ALA
16	X	118	ASP
16	X	131	ASP
17	Y	63	LYS
19	a	62	HIS
19	a	76	ASP
19	a	92	LYS
19	a	110	LYS
20	b	7	HIS
20	b	12	GLN
24	f	4	ARG
25	g	7	TYR
27	i	64	SER
28	k	23	VAL
29	l	22	PRO
31	o	90	HIS
35	B	16	PHE
35	B	47	LEU
35	B	108	GLU
35	B	109	HIS
35	B	111	SER
35	B	138	GLN
35	B	143	ALA
35	B	147	ALA

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Mol	Chain	Res	Type
35	B	191	ALA
35	B	196	TRP
35	B	388	PHE
35	B	389	MET
36	C	49	ARG
36	C	69	THR
36	C	273	LEU
36	C	309	ILE
36	C	318	PRO
36	C	319	LEU
37	E	43	ASN
37	E	55	ARG
37	E	59	TYR
37	E	96	LYS
37	E	104	LYS
37	E	131	LYS
37	E	153	HIS
37	E	175	LEU
37	E	183	ARG
37	E	221	PRO
37	E	230	ASP
37	E	232	GLU
37	E	280	HIS
38	F	72	ARG
38	F	128	ASN
39	I	79	SER
39	I	187	LYS
40	P	41	ILE
45	r	34	ALA
45	r	44	ILE
45	r	45	HIS
45	r	107	ARG
46	K	2	PRO
46	K	7	PRO
46	K	8	ASN
46	K	9	GLU
46	K	30	PRO
46	K	31	LYS
46	K	38	SER
46	K	39	PRO
46	K	54	LYS
46	K	58	ILE

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Mol	Chain	Res	Type
46	K	67	ARG
46	K	87	GLU
46	K	95	GLN
46	K	96	LYS
46	K	120	SER
46	K	139	VAL
46	K	141	CYS
46	K	144	ASP
46	K	149	HIS
46	K	159	ALA
47	q	6	ARG
47	q	69	LEU
47	q	73	PRO
47	q	85	ASN
47	q	95	LEU
47	q	96	THR
47	q	107	VAL
47	q	117	ALA
47	q	125	ALA
47	q	133	GLU
47	q	134	LYS
47	q	182	PRO
47	q	185	PHE
47	q	187	LEU
47	q	188	VAL
48	z	44	VAL
48	z	70	ASN
48	z	71	LYS
48	z	101	GLN
48	z	344	PRO
48	z	345	PHE
49	2	113	PRO
49	2	120	SER
55	SA	44	ASP
55	SA	200	ASP
56	SB	53	GLN
56	SB	56	LYS
56	SB	59	SER
56	SB	147	ASN
56	SB	152	LYS
56	SB	179	ASN
56	SB	191	ASP

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Mol	Chain	Res	Type
56	SB	223	PHE
57	SC	264	SER
58	SE	95	THR
58	SE	98	ASN
58	SE	101	LEU
58	SE	109	PHE
58	SE	196	THR
59	SG	99	GLY
59	SG	105	ASN
59	SG	146	ASN
60	SH	16	PRO
60	SH	17	ASP
60	SH	18	GLU
60	SH	66	VAL
60	SH	115	LYS
60	SH	116	ARG
60	SH	170	VAL
61	SI	52	ASN
61	SI	138	ASN
61	SI	155	ASN
62	SJ	3	VAL
62	SJ	22	LYS
62	SJ	119	LEU
62	SJ	121	LYS
63	SL	100	ASN
63	SL	147	LYS
64	SN	108	ASP
64	SN	143	SER
65	SO	56	VAL
65	SO	65	ASP
65	SO	105	THR
65	SO	140	THR
66	SV	41	LYS
66	SV	65	SER
67	SW	107	SER
68	SX	34	THR
69	SY	60	PHE
69	SY	95	GLY
70	Sa	72	HIS
71	Sb	4	ALA
73	SD	5	ILE
73	SD	202	LYS

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Mol	Chain	Res	Type
73	SD	223	ILE
74	SF	34	SER
74	SF	68	ILE
75	SK	30	PRO
76	SM	15	ASN
76	SM	77	ILE
76	SM	91	LEU
76	SM	102	LYS
76	SM	103	VAL
76	SM	114	TYR
77	SP	27	ASP
77	SP	38	SER
77	SP	73	PRO
78	SQ	35	ASN
78	SQ	48	GLN
78	SQ	116	ASP
80	SS	12	ILE
80	SS	90	VAL
80	SS	118	ARG
80	SS	133	GLY
81	ST	29	LYS
81	ST	31	PRO
81	ST	34	VAL
82	SU	50	VAL
82	SU	107	GLU
83	SZ	42	ASP
83	SZ	113	THR
86	Sf	98	VAL
87	Sg	37	ASP
87	Sg	61	GLY
87	Sg	96	THR
87	Sg	161	SER
87	Sg	182	CYS
87	Sg	282	GLU
88	S1	6	THR
88	S1	47	VAL
88	S1	53	THR
88	S1	56	ALA
1	A	35	ALA
1	A	67	TYR
1	A	180	LEU
1	A	210	PRO

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Mol	Chain	Res	Type
2	D	129	GLU
2	D	159	VAL
2	D	188	LYS
2	D	260	GLU
2	D	281	ALA
2	D	285	ALA
2	D	293	ARG
3	G	42	GLY
3	G	108	GLN
3	G	128	VAL
4	H	51	LYS
5	J	26	VAL
5	J	124	GLY
5	J	169	LYS
6	L	62	PRO
6	L	134	PRO
6	L	143	GLU
6	L	172	GLU
7	M	87	ALA
8	N	96	ARG
8	N	158	HIS
10	Q	155	ALA
11	R	96	MET
11	R	116	ASP
11	R	131	VAL
12	S	10	TYR
12	S	101	THR
12	S	153	PRO
13	T	18	PRO
13	T	55	LYS
14	U	38	ASN
17	Y	6	PHE
17	Y	11	ARG
18	Z	33	THR
18	Z	91	LEU
18	Z	124	THR
21	c	32	LYS
21	c	80	GLU
21	c	81	LEU
22	d	38	PHE
23	e	4	LEU
24	f	80	ASN

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Mol	Chain	Res	Type
24	f	107	PRO
28	k	59	SER
31	o	94	GLY
35	B	120	LYS
35	B	264	PHE
35	B	295	ASP
35	B	314	ILE
35	B	394	LYS
36	C	66	SER
36	C	99	GLY
36	C	320	LYS
36	C	322	LEU
37	E	42	ARG
37	E	91	PRO
37	E	118	PRO
37	E	181	PRO
37	E	255	ARG
38	F	236	GLY
39	I	78	LYS
39	I	94	PHE
39	I	178	ALA
39	I	210	ARG
42	j	9	GLY
45	r	33	LYS
45	r	101	LYS
46	K	5	PHE
46	K	88	PRO
46	K	98	ILE
46	K	105	THR
46	K	127	GLY
47	q	118	PRO
48	z	43	ASP
48	z	267	LYS
48	z	346	SER
55	SA	3	GLY
55	SA	187	GLY
56	SB	54	GLY
56	SB	57	ILE
56	SB	83	LYS
56	SB	93	GLY
56	SB	151	ARG
57	SC	189	GLY

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Mol	Chain	Res	Type
57	SC	255	LEU
58	SE	12	VAL
58	SE	76	VAL
58	SE	163	ASP
58	SE	164	LEU
58	SE	171	ASP
58	SE	195	ILE
59	SG	124	LEU
60	SH	160	LYS
61	SI	27	TYR
61	SI	126	GLY
61	SI	137	LEU
62	SJ	39	ASN
62	SJ	89	GLU
62	SJ	92	MET
62	SJ	118	GLY
65	SO	32	HIS
67	SW	77	PRO
68	SX	113	GLY
68	SX	129	SER
70	Sa	8	ASN
70	Sa	97	PRO
71	Sb	58	GLY
73	SD	178	ARG
73	SD	196	GLY
73	SD	219	PRO
74	SF	43	GLU
74	SF	121	PRO
74	SF	132	GLY
74	SF	166	ILE
75	SK	3	MET
75	SK	58	VAL
75	SK	63	ALA
75	SK	65	ARG
75	SK	92	ALA
76	SM	30	GLY
76	SM	35	ILE
76	SM	79	VAL
77	SP	12	PHE
77	SP	14	LYS
78	SQ	32	ILE
78	SQ	77	HIS

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Mol	Chain	Res	Type
79	SR	95	ILE
79	SR	115	SER
81	ST	28	LEU
81	ST	39	LEU
82	SU	52	GLY
83	SZ	104	ARG
83	SZ	112	ASN
85	Sd	10	HIS
86	Sf	89	LYS
86	Sf	100	LEU
86	Sf	137	ASP
86	Sf	148	TYR
87	Sg	65	PHE
87	Sg	142	VAL
87	Sg	144	ASP
2	D	44	TYR
2	D	114	GLY
2	D	125	VAL
3	G	43	GLN
4	H	52	LYS
5	J	11	PRO
8	N	28	TRP
9	O	110	PRO
10	Q	177	ALA
11	R	39	GLN
11	R	130	ASN
15	V	50	ASN
15	V	110	GLY
18	Z	17	ARG
22	d	93	ASN
23	e	34	ASN
24	f	5	LEU
24	f	6	TRP
25	g	84	ALA
28	k	61	PRO
31	o	33	LEU
35	B	257	TRP
35	B	308	ASP
36	C	23	THR
36	C	310	HIS
37	E	40	CYS
37	E	92	VAL

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Mol	Chain	Res	Type
37	E	95	ASP
37	E	115	GLU
37	E	206	LYS
37	E	220	LYS
37	E	245	ASP
37	E	254	LEU
38	F	31	LYS
39	I	143	GLN
40	P	21	ASN
46	K	28	LEU
46	K	86	LYS
46	K	126	SER
47	q	70	GLU
47	q	74	ALA
47	q	94	ASP
47	q	110	ALA
47	q	149	ARG
47	q	183	PHE
48	z	72	ARG
48	z	92	LYS
48	z	152	ALA
55	SA	105	PRO
55	SA	191	ARG
56	SB	24	PRO
56	SB	67	PHE
58	SE	38	LEU
58	SE	68	ARG
59	SG	20	ASP
59	SG	122	PRO
60	SH	112	ASN
60	SH	113	LYS
60	SH	190	PRO
61	SI	143	LYS
62	SJ	4	ALA
63	SL	8	ARG
63	SL	19	ASN
63	SL	28	THR
65	SO	117	ARG
65	SO	128	ARG
65	SO	129	ILE
65	SO	147	ARG
66	SV	3	ASN

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Mol	Chain	Res	Type
68	SX	99	GLU
69	SY	30	PRO
69	SY	84	LYS
69	SY	118	ARG
70	Sa	10	ARG
70	Sa	62	TYR
71	Sb	59	CYS
74	SF	21	GLY
74	SF	143	PRO
75	SK	84	HIS
76	SM	85	LEU
76	SM	96	ARG
76	SM	116	LYS
77	SP	18	ARG
80	SS	7	GLU
82	SU	51	LYS
82	SU	118	ASP
85	Sd	7	TYR
85	Sd	8	TRP
86	Sf	150	PHE
1	A	31	ALA
1	A	217	GLN
2	D	21	ARG
2	D	32	ALA
2	D	187	SER
2	D	234	ASP
2	D	267	ASN
4	H	110	SER
6	L	82	ARG
8	N	3	ALA
8	N	40	PRO
10	Q	34	PHE
10	Q	146	ARG
12	S	80	ILE
14	U	98	ASP
17	Y	18	HIS
18	Z	30	ASP
19	a	17	HIS
19	a	98	ALA
21	c	77	ASN
22	d	102	LEU
24	f	106	TYR

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Mol	Chain	Res	Type
26	h	119	PHE
26	h	122	LYS
27	i	25	ARG
31	o	58	LYS
31	o	98	LYS
35	B	189	THR
35	B	258	HIS
36	C	73	VAL
36	C	104	PRO
37	E	61	ARG
37	E	208	LEU
37	E	218	LEU
37	E	229	PHE
39	I	47	PRO
39	I	77	VAL
39	I	172	GLY
45	r	123	PRO
46	K	10	ILE
46	K	34	PRO
46	K	138	SER
47	q	61	MET
47	q	186	GLY
48	z	19	ASN
48	z	23	ILE
49	2	127	MET
55	SA	43	SER
55	SA	110	ASN
55	SA	186	ARG
55	SA	207	PRO
56	SB	190	PRO
56	SB	204	ILE
57	SC	171	GLY
57	SC	190	SER
59	SG	152	ASP
60	SH	107	LYS
60	SH	159	ASP
61	SI	20	PRO
62	SJ	18	ARG
62	SJ	96	TYR
62	SJ	120	ALA
63	SL	69	ARG
65	SO	146	ARG

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Mol	Chain	Res	Type
69	SY	103	SER
70	Sa	15	ARG
70	Sa	61	ALA
73	SD	48	ILE
73	SD	218	LEU
74	SF	163	PHE
75	SK	31	LYS
76	SM	117	GLU
76	SM	119	GLN
77	SP	75	VAL
78	SQ	80	GLN
79	SR	127	ASN
80	SS	88	LYS
82	SU	106	ILE
86	Sf	83	LYS
86	Sf	87	THR
86	Sf	110	GLU
87	Sg	49	GLU
87	Sg	97	THR
87	Sg	163	PRO
87	Sg	172	LYS
87	Sg	283	PRO
1	A	234	LYS
3	G	28	VAL
3	G	125	LYS
3	G	165	GLU
6	L	28	GLN
6	L	47	ALA
7	M	44	GLN
7	M	60	PHE
8	N	55	ALA
8	N	77	LYS
15	V	96	LEU
17	Y	79	VAL
19	a	93	ASN
24	f	33	VAL
31	o	77	CYS
35	B	38	SER
35	B	110	ILE
35	B	112	ASP
35	B	310	SER
35	B	329	ASP

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Mol	Chain	Res	Type
36	C	58	ALA
36	C	305	PRO
36	C	342	ARG
37	E	85	LEU
37	E	174	PRO
37	E	251	SER
38	F	56	ALA
38	F	101	ASN
39	I	7	ARG
39	I	109	ASP
42	j	59	THR
46	K	94	LYS
46	K	104	ILE
46	K	119	ARG
47	q	60	MET
48	z	197	GLN
56	SB	86	LEU
56	SB	108	ASP
56	SB	207	LEU
57	SC	134	ASN
57	SC	256	TRP
58	SE	15	PRO
58	SE	30	ARG
60	SH	6	ALA
60	SH	100	ILE
61	SI	21	TYR
62	SJ	103	GLU
64	SN	28	LEU
65	SO	24	GLY
65	SO	33	ILE
66	SV	10	ASP
66	SV	42	VAL
66	SV	45	ARG
66	SV	53	TYR
67	SW	29	PRO
70	Sa	46	GLU
71	Sb	48	SER
73	SD	130	GLY
75	SK	34	GLU
76	SM	94	ILE
77	SP	87	PRO
78	SQ	47	LEU

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Mol	Chain	Res	Type
80	SS	92	ASP
81	ST	128	GLN
83	SZ	108	ILE
88	S1	45	ASP
2	D	263	LYS
4	H	40	HIS
6	L	10	LEU
6	L	169	ILE
11	R	19	LYS
13	T	53	PRO
17	Y	85	VAL
18	Z	4	PHE
20	b	21	ILE
22	d	58	GLY
35	B	301	ASN
36	C	72	ALA
38	F	168	ARG
47	q	111	ALA
60	SH	10	LYS
62	SJ	169	ARG
65	SO	54	CYS
65	SO	64	ALA
69	SY	6	THR
72	Se	26	LYS
75	SK	43	LEU
76	SM	78	LYS
76	SM	81	ASP
77	SP	37	TYR
77	SP	54	HIS
79	SR	52	GLY
86	Sf	99	LYS
86	Sf	122	PRO
86	Sf	145	CYS
87	Sg	190	GLY
5	J	27	GLY
18	Z	95	VAL
48	z	158	PRO
48	z	213	GLN
55	SA	45	GLY
56	SB	22	VAL
58	SE	90	ILE
58	SE	131	VAL

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Mol	Chain	Res	Type
60	SH	176	VAL
75	SK	41	PRO
75	SK	90	VAL
78	SQ	43	GLU
79	SR	121	GLN
80	SS	117	ILE
12	S	5	GLY
35	B	259	PRO
59	SG	182	PRO
64	SN	52	VAL
73	SD	222	PRO
76	SM	65	VAL
76	SM	89	VAL
4	H	104	VAL
5	J	127	GLY
14	U	27	HIS
35	B	17	LEU
38	F	105	PRO
39	I	149	ILE
47	q	142	GLY
48	z	161	GLY
70	Sa	98	PRO
72	Se	54	GLY
76	SM	104	VAL
84	Sc	7	GLN
5	J	174	ILE
8	N	52	GLY
47	q	84	GLY
55	SA	106	GLY
55	SA	199	PRO
58	SE	64	ILE
62	SJ	36	GLY
74	SF	92	ILE
80	SS	36	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/187 (100%)	137 (73%)	50 (27%)	0	3
2	D	246/247 (100%)	183 (74%)	63 (26%)	0	3
3	G	204/206 (99%)	150 (74%)	54 (26%)	0	3
4	H	169/169 (100%)	131 (78%)	38 (22%)	1	5
5	J	143/143 (100%)	108 (76%)	35 (24%)	0	4
6	L	176/176 (100%)	133 (76%)	43 (24%)	0	4
7	M	116/116 (100%)	87 (75%)	29 (25%)	0	3
8	N	171/171 (100%)	126 (74%)	45 (26%)	0	3
9	O	172/172 (100%)	138 (80%)	34 (20%)	1	7
10	Q	163/163 (100%)	126 (77%)	37 (23%)	0	5
11	R	159/159 (100%)	120 (76%)	39 (24%)	0	4
12	S	156/156 (100%)	124 (80%)	32 (20%)	1	6
13	T	139/139 (100%)	105 (76%)	34 (24%)	0	4
14	U	89/89 (100%)	65 (73%)	24 (27%)	0	2
15	V	101/101 (100%)	78 (77%)	23 (23%)	0	5
16	X	107/107 (100%)	88 (82%)	19 (18%)	1	9
17	Y	124/124 (100%)	94 (76%)	30 (24%)	0	4
18	Z	117/117 (100%)	93 (80%)	24 (20%)	1	6
19	a	119/119 (100%)	99 (83%)	20 (17%)	1	11
20	b	63/63 (100%)	48 (76%)	15 (24%)	0	4
21	c	79/79 (100%)	59 (75%)	20 (25%)	0	3
22	d	98/98 (100%)	65 (66%)	33 (34%)	0	1
23	e	114/114 (100%)	91 (80%)	23 (20%)	1	6
24	f	88/88 (100%)	73 (83%)	15 (17%)	1	11
25	g	98/98 (100%)	78 (80%)	20 (20%)	1	6
26	h	109/109 (100%)	91 (84%)	18 (16%)	2	12
27	i	86/86 (100%)	68 (79%)	18 (21%)	1	6
28	k	64/64 (100%)	51 (80%)	13 (20%)	1	6
29	l	47/47 (100%)	37 (79%)	10 (21%)	1	6
30	m	48/48 (100%)	33 (69%)	15 (31%)	0	1
31	o	92/92 (100%)	70 (76%)	22 (24%)	0	4
35	B	335/335 (100%)	260 (78%)	75 (22%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	C	305/305 (100%)	233 (76%)	72 (24%)	0	4
37	E	209/209 (100%)	163 (78%)	46 (22%)	1	5
38	F	194/194 (100%)	141 (73%)	53 (27%)	0	2
39	I	180/180 (100%)	126 (70%)	54 (30%)	0	2
40	P	134/134 (100%)	108 (81%)	26 (19%)	1	7
41	W	55/55 (100%)	38 (69%)	17 (31%)	0	1
42	j	73/73 (100%)	60 (82%)	13 (18%)	1	9
43	n	22/22 (100%)	16 (73%)	6 (27%)	0	2
44	p	74/74 (100%)	62 (84%)	12 (16%)	2	12
45	r	109/109 (100%)	83 (76%)	26 (24%)	0	4
46	K	136/136 (100%)	118 (87%)	18 (13%)	3	18
47	q	170/170 (100%)	134 (79%)	36 (21%)	1	6
48	z	340/340 (100%)	321 (94%)	19 (6%)	17	45
49	2	29/29 (100%)	26 (90%)	3 (10%)	6	25
52	9	92/94 (98%)	88 (96%)	4 (4%)	25	50
53	6	157/157 (100%)	151 (96%)	6 (4%)	28	53
55	SA	174/174 (100%)	132 (76%)	42 (24%)	0	4
56	SB	194/194 (100%)	155 (80%)	39 (20%)	1	7
57	SC	184/184 (100%)	141 (77%)	43 (23%)	0	4
58	SE	224/224 (100%)	172 (77%)	52 (23%)	0	5
59	SG	207/207 (100%)	166 (80%)	41 (20%)	1	7
60	SH	169/169 (100%)	145 (86%)	24 (14%)	2	17
61	SI	178/178 (100%)	144 (81%)	34 (19%)	1	7
62	SJ	161/161 (100%)	116 (72%)	45 (28%)	0	2
63	SL	136/136 (100%)	104 (76%)	32 (24%)	0	4
64	SN	130/130 (100%)	103 (79%)	27 (21%)	1	6
65	SO	106/106 (100%)	74 (70%)	32 (30%)	0	2
66	SV	66/66 (100%)	50 (76%)	16 (24%)	0	4
67	SW	112/112 (100%)	90 (80%)	22 (20%)	1	7
68	SX	113/113 (100%)	95 (84%)	18 (16%)	2	13
69	SY	108/108 (100%)	85 (79%)	23 (21%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	Sa	85/85 (100%)	71 (84%)	14 (16%)	2	12
71	Sb	75/75 (100%)	58 (77%)	17 (23%)	0	5
72	Se	46/46 (100%)	35 (76%)	11 (24%)	0	4
73	SD	190/190 (100%)	149 (78%)	41 (22%)	1	5
74	SF	161/161 (100%)	123 (76%)	38 (24%)	0	4
75	SK	89/89 (100%)	68 (76%)	21 (24%)	0	4
76	SM	104/104 (100%)	74 (71%)	30 (29%)	0	2
77	SP	88/88 (100%)	70 (80%)	18 (20%)	1	6
78	SQ	117/117 (100%)	91 (78%)	26 (22%)	1	5
79	SR	117/117 (100%)	102 (87%)	15 (13%)	3	19
80	SS	119/119 (100%)	96 (81%)	23 (19%)	1	7
81	ST	112/112 (100%)	88 (79%)	24 (21%)	1	6
82	SU	94/94 (100%)	82 (87%)	12 (13%)	3	19
83	SZ	66/66 (100%)	57 (86%)	9 (14%)	3	17
84	Sc	57/57 (100%)	47 (82%)	10 (18%)	1	10
85	Sd	45/45 (100%)	36 (80%)	9 (20%)	1	7
86	Sf	64/64 (100%)	45 (70%)	19 (30%)	0	2
87	Sg	272/272 (100%)	235 (86%)	37 (14%)	3	17
88	S1	67/67 (100%)	59 (88%)	8 (12%)	4	20
89	S4	69/69 (100%)	60 (87%)	9 (13%)	3	18
All	All	10757/10762 (100%)	8495 (79%)	2262 (21%)	2	6

All (2262) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	5	ILE
1	A	16	PHE
1	A	19	HIS
1	A	22	HIS
1	A	30	ARG
1	A	37	ARG
1	A	40	TYR
1	A	41	ILE
1	A	54	ARG

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Mol	Chain	Res	Type
1	A	63	PHE
1	A	74	GLU
1	A	83	HIS
1	A	84	THR
1	A	87	PHE
1	A	95	GLN
1	A	97	ASN
1	A	100	ASN
1	A	109	GLU
1	A	122	ASP
1	A	125	LYS
1	A	128	ARG
1	A	130	SER
1	A	139	HIS
1	A	142	GLU
1	A	144	LYS
1	A	147	ARG
1	A	162	ASN
1	A	163	ARG
1	A	174	ARG
1	A	181	LYS
1	A	186	TYR
1	A	187	HIS
1	A	189	TYR
1	A	190	LYS
1	A	193	ARG
1	A	194	ASN
1	A	196	TRP
1	A	200	ARG
1	A	205	ASN
1	A	215	ASN
1	A	216	HIS
1	A	218	HIS
1	A	221	LYS
1	A	226	ARG
1	A	227	ARG
1	A	233	ARG
1	A	242	ARG
1	A	243	THR
1	A	245	ARG
2	D	9	ASN
2	D	21	ARG

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Mol	Chain	Res	Type
2	D	23	ARG
2	D	30	TYR
2	D	35	ARG
2	D	39	GLN
2	D	42	ASN
2	D	44	TYR
2	D	45	ASN
2	D	50	ARG
2	D	59	ASP
2	D	63	GLN
2	D	66	TYR
2	D	79	TYR
2	D	81	HIS
2	D	92	LEU
2	D	94	ASN
2	D	95	TYR
2	D	99	TYR
2	D	104	LEU
2	D	107	ARG
2	D	111	ASN
2	D	113	PHE
2	D	116	ASP
2	D	118	ILE
2	D	119	TYR
2	D	124	GLU
2	D	129	GLU
2	D	131	ASN
2	D	136	ASP
2	D	138	GLN
2	D	157	ASN
2	D	168	ASP
2	D	177	THR
2	D	179	ARG
2	D	189	GLU
2	D	191	ASN
2	D	193	GLU
2	D	196	ARG
2	D	202	GLN
2	D	203	ASN
2	D	207	TYR
2	D	219	TYR
2	D	223	PHE

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Mol	Chain	Res	Type
2	D	225	GLN
2	D	229	ASN
2	D	232	THR
2	D	234	ASP
2	D	244	HIS
2	D	249	GLU
2	D	254	GLU
2	D	255	LYS
2	D	256	LYS
2	D	259	LYS
2	D	260	GLU
2	D	262	LYS
2	D	264	LYS
2	D	265	ARG
2	D	266	TRP
2	D	279	ARG
2	D	287	PHE
2	D	291	GLN
2	D	293	ARG
3	G	28	VAL
3	G	31	LEU
3	G	32	PHE
3	G	38	ASN
3	G	39	PHE
3	G	44	ASP
3	G	46	GLN
3	G	49	ARG
3	G	50	ASP
3	G	53	ARG
3	G	56	LYS
3	G	59	ARG
3	G	60	TYR
3	G	62	ARG
3	G	67	ARG
3	G	71	TYR
3	G	73	ARG
3	G	85	GLN
3	G	88	ASP
3	G	89	ARG
3	G	90	GLN
3	G	97	LYS
3	G	100	HIS

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Mol	Chain	Res	Type
3	G	101	LYS
3	G	102	TYR
3	G	103	ARG
3	G	106	THR
3	G	108	GLN
3	G	112	GLN
3	G	125	LYS
3	G	131	LYS
3	G	141	ASN
3	G	150	LYS
3	G	154	LEU
3	G	162	ASP
3	G	167	VAL
3	G	169	PHE
3	G	170	LEU
3	G	175	ARG
3	G	177	MET
3	G	189	ARG
3	G	202	VAL
3	G	210	GLU
3	G	217	LYS
3	G	220	GLU
3	G	223	ARG
3	G	227	ASN
3	G	230	TYR
3	G	231	ASN
3	G	234	ARG
3	G	235	ARG
3	G	240	ASN
3	G	249	ARG
3	G	254	GLU
4	H	11	ASP
4	H	15	ASN
4	H	18	ILE
4	H	26	ILE
4	H	36	ARG
4	H	40	HIS
4	H	51	LYS
4	H	52	LYS
4	H	54	ARG
4	H	58	ASP
4	H	59	LYS

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Mol	Chain	Res	Type
4	H	60	TRP
4	H	63	ASN
4	H	66	GLU
4	H	71	ARG
4	H	84	VAL
4	H	88	PHE
4	H	92	MET
4	H	94	SER
4	H	96	TYR
4	H	105	ILE
4	H	108	ASN
4	H	113	GLU
4	H	117	PHE
4	H	118	LEU
4	H	122	TYR
4	H	123	ILE
4	H	124	ARG
4	H	125	ARG
4	H	128	MET
4	H	140	GLN
4	H	141	LYS
4	H	161	ILE
4	H	168	LYS
4	H	171	ASP
4	H	173	ARG
4	H	177	ASP
4	H	180	TYR
5	J	18	ARG
5	J	21	CYS
5	J	23	ASN
5	J	26	VAL
5	J	35	ARG
5	J	46	GLN
5	J	54	ARG
5	J	55	TYR
5	J	63	ARG
5	J	71	HIS
5	J	72	CYS
5	J	73	THR
5	J	81	GLU
5	J	83	LEU
5	J	85	LYS

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Mol	Chain	Res	Type
5	J	87	LEU
5	J	90	ARG
5	J	96	LYS
5	J	97	ASN
5	J	98	ASN
5	J	101	ASP
5	J	105	PHE
5	J	113	ILE
5	J	119	TYR
5	J	126	TYR
5	J	128	LEU
5	J	139	PHE
5	J	143	ASP
5	J	146	ARG
5	J	154	LYS
5	J	155	HIS
5	J	164	ARG
5	J	165	TRP
5	J	168	GLN
5	J	171	ASP
6	L	5	ARG
6	L	10	LEU
6	L	13	HIS
6	L	19	GLN
6	L	31	ARG
6	L	34	ARG
6	L	36	ARG
6	L	39	ARG
6	L	45	ARG
6	L	49	ARG
6	L	56	ARG
6	L	65	ARG
6	L	66	TYR
6	L	67	HIS
6	L	74	ARG
6	L	80	GLU
6	L	82	ARG
6	L	92	ARG
6	L	99	ASP
6	L	101	ARG
6	L	103	ARG
6	L	111	GLN

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Mol	Chain	Res	Type
6	L	113	ASN
6	L	115	GLN
6	L	121	ARG
6	L	123	LYS
6	L	127	PHE
6	L	129	ARG
6	L	130	LYS
6	L	146	LEU
6	L	151	THR
6	L	159	ASN
6	L	162	LYS
6	L	163	ARG
6	L	165	LYS
6	L	172	GLU
6	L	175	ASN
6	L	176	PHE
6	L	181	SER
6	L	186	ARG
6	L	195	ARG
6	L	201	GLU
6	L	205	GLN
7	M	11	ARG
7	M	17	PHE
7	M	29	ASP
7	M	32	ASP
7	M	33	GLN
7	M	34	ASN
7	M	37	LEU
7	M	38	VAL
7	M	46	ARG
7	M	47	ARG
7	M	56	GLN
7	M	59	ASP
7	M	61	ILE
7	M	62	LEU
7	M	66	HIS
7	M	67	SER
7	M	71	LYS
7	M	74	ARG
7	M	78	GLU
7	M	79	LYS
7	M	81	ASP

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Mol	Chain	Res	Type
7	M	83	ASN
7	M	89	THR
7	M	90	ARG
7	M	91	TRP
7	M	98	ARG
7	M	99	GLU
7	M	109	ARG
7	M	119	ARG
8	N	4	TYR
8	N	9	GLU
8	N	11	TRP
8	N	24	ARG
8	N	26	ARG
8	N	29	GLN
8	N	30	TYR
8	N	43	THR
8	N	53	TYR
8	N	54	LYS
8	N	59	TYR
8	N	63	ARG
8	N	64	ILE
8	N	67	ARG
8	N	71	ARG
8	N	72	LYS
8	N	86	HIS
8	N	89	VAL
8	N	91	GLN
8	N	104	GLU
8	N	108	ARG
8	N	110	CYS
8	N	114	ARG
8	N	119	TYR
8	N	123	GLU
8	N	127	TYR
8	N	131	GLU
8	N	136	ASP
8	N	138	PHE
8	N	139	HIS
8	N	147	ASP
8	N	150	TRP
8	N	151	ILE
8	N	158	HIS

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Mol	Chain	Res	Type
8	N	162	ARG
8	N	166	SER
8	N	169	ARG
8	N	174	LEU
8	N	178	HIS
8	N	182	HIS
8	N	189	ARG
8	N	192	TRP
8	N	193	ARG
8	N	196	ASN
8	N	203	TYR
9	O	5	GLN
9	O	16	LEU
9	O	31	ARG
9	O	37	ARG
9	O	38	CYS
9	O	41	ILE
9	O	42	ASN
9	O	46	ASN
9	O	49	ARG
9	O	50	ASN
9	O	57	PHE
9	O	60	LYS
9	O	61	ARG
9	O	62	MET
9	O	72	HIS
9	O	74	ARG
9	O	78	ARG
9	O	82	ARG
9	O	85	ARG
9	O	110	PRO
9	O	113	ASP
9	O	125	LYS
9	O	140	ARG
9	O	147	TRP
9	O	160	ARG
9	O	167	HIS
9	O	173	GLN
9	O	178	ARG
9	O	187	LYS
9	O	188	LYS
9	O	192	PHE

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Mol	Chain	Res	Type
9	O	198	THR
9	O	199	HIS
9	O	202	LEU
10	Q	3	VAL
10	Q	4	ASP
10	Q	5	ILE
10	Q	9	LYS
10	Q	14	ARG
10	Q	15	ARG
10	Q	16	LYS
10	Q	26	ARG
10	Q	32	TYR
10	Q	37	ARG
10	Q	40	ASN
10	Q	44	ASN
10	Q	52	PHE
10	Q	58	ARG
10	Q	63	LEU
10	Q	65	ARG
10	Q	68	ARG
10	Q	72	LEU
10	Q	75	ARG
10	Q	79	THR
10	Q	85	THR
10	Q	89	ASP
10	Q	91	ARG
10	Q	92	VAL
10	Q	93	GLN
10	Q	97	LYS
10	Q	108	ARG
10	Q	110	ARG
10	Q	112	ARG
10	Q	119	LYS
10	Q	146	ARG
10	Q	159	PRO
10	Q	166	TYR
10	Q	168	ARG
10	Q	173	LYS
10	Q	178	ARG
10	Q	181	ARG
11	R	2	SER
11	R	6	LEU

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Mol	Chain	Res	Type
11	R	17	CYS
11	R	23	TRP
11	R	30	ASN
11	R	39	GLN
11	R	40	GLN
11	R	42	ARG
11	R	50	ILE
11	R	58	HIS
11	R	66	ASN
11	R	71	ARG
11	R	74	ARG
11	R	81	ARG
11	R	89	MET
11	R	94	THR
11	R	99	MET
11	R	104	ARG
11	R	105	LEU
11	R	107	ARG
11	R	108	ARG
11	R	113	LYS
11	R	117	ARG
11	R	118	HIS
11	R	120	TYR
11	R	124	TYR
11	R	131	VAL
11	R	133	LYS
11	R	136	ARG
11	R	138	LEU
11	R	141	HIS
11	R	168	GLU
11	R	170	ARG
11	R	172	ARG
11	R	175	GLU
11	R	176	ARG
11	R	177	LEU
11	R	178	GLN
11	R	180	LYS
12	S	2	LYS
12	S	17	LEU
12	S	28	TYR
12	S	29	ARG
12	S	44	PHE

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Mol	Chain	Res	Type
12	S	47	PHE
12	S	48	VAL
12	S	53	LYS
12	S	64	CYS
12	S	68	PHE
12	S	70	LYS
12	S	82	LEU
12	S	83	ARG
12	S	84	TYR
12	S	95	ARG
12	S	98	ARG
12	S	99	ASP
12	S	100	LEU
12	S	101	THR
12	S	111	ARG
12	S	116	ARG
12	S	128	LYS
12	S	138	ARG
12	S	146	HIS
12	S	149	LYS
12	S	150	ILE
12	S	156	HIS
12	S	159	LEU
12	S	162	GLN
12	S	167	PHE
12	S	168	THR
12	S	171	ARG
13	T	5	LYS
13	T	9	ARG
13	T	17	ARG
13	T	19	PHE
13	T	30	TYR
13	T	32	ARG
13	T	33	ILE
13	T	35	LYS
13	T	36	LYS
13	T	41	ASP
13	T	54	HIS
13	T	57	TYR
13	T	60	LYS
13	T	61	THR
13	T	67	VAL

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Mol	Chain	Res	Type
13	T	70	HIS
13	T	76	VAL
13	T	88	ARG
13	T	102	ARG
13	T	103	ASP
13	T	105	PHE
13	T	107	LYS
13	T	113	ASP
13	T	117	LYS
13	T	118	GLU
13	T	121	GLU
13	T	127	GLN
13	T	136	ARG
13	T	137	GLU
13	T	139	HIS
13	T	142	ARG
13	T	144	ASN
13	T	158	PHE
13	T	159	MET
14	U	23	LEU
14	U	27	HIS
14	U	33	ILE
14	U	39	PHE
14	U	40	GLU
14	U	42	PHE
14	U	46	ARG
14	U	52	LYS
14	U	62	THR
14	U	64	GLU
14	U	65	ARG
14	U	67	LYS
14	U	69	LYS
14	U	79	SER
14	U	81	ARG
14	U	82	TYR
14	U	89	LYS
14	U	90	TYR
14	U	97	ARG
14	U	98	ASP
14	U	100	LEU
14	U	101	ARG
14	U	110	TYR

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Mol	Chain	Res	Type
14	U	113	ARG
15	V	13	LYS
15	V	14	PHE
15	V	15	ARG
15	V	18	LEU
15	V	30	ASP
15	V	36	ASN
15	V	46	LYS
15	V	48	ARG
15	V	50	ASN
15	V	51	ARG
15	V	59	ASP
15	V	60	MET
15	V	73	ARG
15	V	77	HIS
15	V	84	GLN
15	V	91	LYS
15	V	92	ASP
15	V	98	PHE
15	V	100	ASP
15	V	107	ASN
15	V	109	LYS
15	V	111	GLU
15	V	123	LYS
16	X	39	LYS
16	X	41	ARG
16	X	45	THR
16	X	48	ARG
16	X	53	ARG
16	X	60	TYR
16	X	62	ARG
16	X	68	ARG
16	X	72	ASP
16	X	79	PHE
16	X	84	GLU
16	X	94	ASN
16	X	120	ASP
16	X	129	ARG
16	X	137	TYR
16	X	139	ARG
16	X	144	TYR
16	X	148	ASP

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Mol	Chain	Res	Type
16	X	151	ASN
17	Y	2	LYS
17	Y	4	ASN
17	Y	17	ARG
17	Y	18	HIS
17	Y	19	PHE
17	Y	27	ARG
17	Y	36	LYS
17	Y	42	TYR
17	Y	45	ARG
17	Y	49	ILE
17	Y	50	ARG
17	Y	53	ASP
17	Y	55	VAL
17	Y	56	GLN
17	Y	59	ARG
17	Y	62	TYR
17	Y	65	GLN
17	Y	72	GLN
17	Y	81	TYR
17	Y	82	ILE
17	Y	87	ARG
17	Y	91	ASN
17	Y	96	HIS
17	Y	108	ARG
17	Y	112	ASP
17	Y	114	ASP
17	Y	115	ARG
17	Y	121	ARG
17	Y	126	ARG
17	Y	127	GLN
18	Z	4	PHE
18	Z	5	MET
18	Z	17	ARG
18	Z	19	SER
18	Z	21	ARG
18	Z	36	ARG
18	Z	38	TYR
18	Z	57	MET
18	Z	60	LYS
18	Z	64	LYS
18	Z	75	TYR

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Mol	Chain	Res	Type
18	Z	78	ASN
18	Z	88	ASP
18	Z	91	LEU
18	Z	92	ASP
18	Z	93	LYS
18	Z	98	LYS
18	Z	108	ARG
18	Z	109	LYS
18	Z	112	ARG
18	Z	121	ARG
18	Z	122	TYR
18	Z	127	ASN
18	Z	136	PHE
19	a	7	LYS
19	a	14	HIS
19	a	19	HIS
19	a	21	ARG
19	a	40	HIS
19	a	41	HIS
19	a	46	ASP
19	a	47	LYS
19	a	49	HIS
19	a	52	TYR
19	a	59	ARG
19	a	61	TYR
19	a	65	ARG
19	a	67	GLN
19	a	77	LYS
19	a	83	SER
19	a	84	GLU
19	a	85	GLN
19	a	95	THR
19	a	105	ARG
20	b	12	GLN
20	b	16	TRP
20	b	22	LYS
20	b	25	ARG
20	b	27	GLN
20	b	28	ARG
20	b	30	GLU
20	b	36	ASP
20	b	39	PHE

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Mol	Chain	Res	Type
20	b	41	ARG
20	b	43	MET
20	b	44	ARG
20	b	51	LYS
20	b	55	LYS
20	b	65	MET
21	c	18	LEU
21	c	19	GLN
21	c	27	TYR
21	c	31	TYR
21	c	37	MET
21	c	42	LYS
21	c	44	LYS
21	c	55	LEU
21	c	56	ARG
21	c	59	GLU
21	c	65	MET
21	c	66	LEU
21	c	72	HIS
21	c	73	HIS
21	c	74	TYR
21	c	77	ASN
21	c	78	ASN
21	c	81	LEU
21	c	88	TYR
21	c	92	CYS
22	d	18	ASN
22	d	19	GLU
22	d	23	ARG
22	d	26	THR
22	d	28	ASN
22	d	31	LYS
22	d	32	ARG
22	d	34	HIS
22	d	38	PHE
22	d	39	LYS
22	d	44	ARG
22	d	67	ARG
22	d	73	TRP
22	d	78	ARG
22	d	79	ASN
22	d	83	ARG

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Mol	Chain	Res	Type
22	d	85	ARG
22	d	86	VAL
22	d	87	ARG
22	d	91	LYS
22	d	93	ASN
22	d	94	GLU
22	d	95	ASP
22	d	101	LYS
22	d	103	TYR
22	d	107	THR
22	d	109	VAL
22	d	116	ASN
22	d	117	LEU
22	d	118	GLN
22	d	119	THR
22	d	121	ASN
22	d	123	ASP
23	e	11	LYS
23	e	16	ARG
23	e	21	ILE
23	e	26	ASP
23	e	39	ARG
23	e	42	ASP
23	e	43	ASN
23	e	46	ARG
23	e	49	PHE
23	e	57	ASN
23	e	64	LYS
23	e	68	HIS
23	e	77	PHE
23	e	78	LEU
23	e	85	LEU
23	e	92	ASN
23	e	95	TYR
23	e	106	LYS
23	e	107	ASN
23	e	113	GLU
23	e	118	LEU
23	e	126	ASN
23	e	128	ARG
24	f	14	TYR
24	f	16	ARG

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Mol	Chain	Res	Type
24	f	19	ARG
24	f	24	HIS
24	f	25	THR
24	f	28	LEU
24	f	34	TYR
24	f	36	ARG
24	f	37	ASP
24	f	38	GLU
24	f	49	TYR
24	f	51	TYR
24	f	52	LYS
24	f	101	ILE
24	f	109	ARG
25	g	3	GLN
25	g	4	ARG
25	g	7	TYR
25	g	11	LEU
25	g	12	SER
25	g	14	ASN
25	g	29	ARG
25	g	32	TYR
25	g	52	ARG
25	g	54	ARG
25	g	60	ARG
25	g	64	LEU
25	g	66	ARG
25	g	75	SER
25	g	81	SER
25	g	88	ARG
25	g	93	ARG
25	g	95	PHE
25	g	114	GLN
25	g	115	LYS
26	h	10	ARG
26	h	15	GLU
26	h	23	ASP
26	h	28	LEU
26	h	48	ARG
26	h	51	ARG
26	h	67	GLU
26	h	68	ASN
26	h	69	LEU

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Mol	Chain	Res	Type
26	h	72	PHE
26	h	73	TYR
26	h	89	ARG
26	h	93	ARG
26	h	97	LYS
26	h	100	GLU
26	h	117	ARG
26	h	119	PHE
26	h	122	LYS
27	i	3	LEU
27	i	4	ARG
27	i	12	ASN
27	i	20	ASN
27	i	27	SER
27	i	30	ARG
27	i	32	ARG
27	i	33	LEU
27	i	42	ASP
27	i	45	ARG
27	i	46	GLU
27	i	50	PHE
27	i	54	GLU
27	i	68	ARG
27	i	85	ARG
27	i	87	ARG
27	i	89	GLU
27	i	103	LYS
28	k	14	THR
28	k	19	ASP
28	k	27	LYS
28	k	30	ASP
28	k	35	LYS
28	k	37	ARG
28	k	40	ARG
28	k	43	TYR
28	k	51	GLU
28	k	54	GLU
28	k	56	LEU
28	k	60	LEU
28	k	70	LYS
29	l	12	PHE
29	l	16	LYS

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Mol	Chain	Res	Type
29	l	17	GLN
29	l	21	ARG
29	l	36	ARG
29	l	39	SER
29	l	44	TRP
29	l	45	ARG
29	l	46	ARG
29	l	49	LEU
30	m	79	GLU
30	m	84	GLN
30	m	87	GLN
30	m	89	TYR
30	m	90	ASN
30	m	97	ARG
30	m	102	ARG
30	m	104	HIS
30	m	106	ARG
30	m	109	ASN
30	m	111	ARG
30	m	117	HIS
30	m	118	THR
30	m	119	ASN
30	m	122	ARG
31	o	8	ARG
31	o	11	PHE
31	o	26	TYR
31	o	31	ASP
31	o	33	LEU
31	o	36	GLN
31	o	40	ARG
31	o	45	GLN
31	o	48	TYR
31	o	57	ARG
31	o	59	LYS
31	o	61	LYS
31	o	64	LYS
31	o	69	ARG
31	o	76	ASN
31	o	77	CYS
31	o	78	ARG
31	o	79	SER
31	o	82	MET

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Mol	Chain	Res	Type
31	o	99	ARG
31	o	102	GLN
31	o	104	ILE
35	B	4	ARG
35	B	5	LYS
35	B	10	ARG
35	B	16	PHE
35	B	17	LEU
35	B	25	HIS
35	B	26	ARG
35	B	36	ASP
35	B	39	LYS
35	B	46	PHE
35	B	49	TYR
35	B	54	THR
35	B	56	ILE
35	B	58	ARG
35	B	59	GLU
35	B	61	ASP
35	B	62	ARG
35	B	66	LYS
35	B	74	GLU
35	B	78	ILE
35	B	95	THR
35	B	100	ARG
35	B	101	THR
35	B	103	LYS
35	B	104	THR
35	B	106	PHE
35	B	116	ARG
35	B	117	ARG
35	B	119	TYR
35	B	122	TRP
35	B	123	HIS
35	B	146	LEU
35	B	149	ASP
35	B	151	SER
35	B	152	SER
35	B	154	LYS
35	B	165	HIS
35	B	167	GLN
35	B	169	ARG

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Mol	Chain	Res	Type
35	B	174	ARG
35	B	189	THR
35	B	198	ARG
35	B	203	GLN
35	B	207	VAL
35	B	208	ASN
35	B	218	ASP
35	B	228	TYR
35	B	235	TRP
35	B	236	HIS
35	B	245	HIS
35	B	249	ARG
35	B	257	TRP
35	B	258	HIS
35	B	261	ARG
35	B	291	TYR
35	B	307	TYR
35	B	308	ASP
35	B	309	LEU
35	B	311	ASP
35	B	314	ILE
35	B	323	TYR
35	B	326	VAL
35	B	328	ASN
35	B	336	CYS
35	B	347	LEU
35	B	348	ARG
35	B	355	THR
35	B	356	LYS
35	B	357	ARG
35	B	364	ASP
35	B	369	ASP
35	B	374	PHE
35	B	378	ARG
35	B	381	THR
35	B	384	GLU
36	C	14	LYS
36	C	35	ASP
36	C	36	ILE
36	C	41	HIS
36	C	47	ASN
36	C	49	ARG

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Mol	Chain	Res	Type
36	C	65	GLU
36	C	69	THR
36	C	71	ARG
36	C	78	ARG
36	C	80	ARG
36	C	85	HIS
36	C	86	ARG
36	C	87	SER
36	C	92	PHE
36	C	94	ASN
36	C	95	MET
36	C	96	CYS
36	C	97	ARG
36	C	100	ARG
36	C	102	PHE
36	C	107	THR
36	C	112	HIS
36	C	113	ARG
36	C	114	ARG
36	C	122	TYR
36	C	126	SER
36	C	142	HIS
36	C	146	GLU
36	C	149	GLU
36	C	150	LEU
36	C	155	GLU
36	C	156	ASP
36	C	165	LYS
36	C	173	LYS
36	C	175	LYS
36	C	177	TRP
36	C	178	ASN
36	C	182	LYS
36	C	184	TYR
36	C	188	ARG
36	C	193	LYS
36	C	196	MET
36	C	198	ASN
36	C	201	ARG
36	C	203	GLN
36	C	208	CYS
36	C	212	ASN

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Mol	Chain	Res	Type
36	C	215	ASN
36	C	222	ARG
36	C	225	PRO
36	C	232	VAL
36	C	262	GLU
36	C	267	TRP
36	C	276	ASN
36	C	281	MET
36	C	284	MET
36	C	288	ASP
36	C	300	ARG
36	C	303	ARG
36	C	307	LYS
36	C	309	ILE
36	C	310	HIS
36	C	311	ARG
36	C	312	ARG
36	C	322	LEU
36	C	333	LYS
36	C	337	ARG
36	C	342	ARG
36	C	343	GLN
36	C	345	ARG
36	C	350	ARG
37	E	39	HIS
37	E	43	ASN
37	E	46	LEU
37	E	52	ARG
37	E	61	ARG
37	E	64	MET
37	E	66	LYS
37	E	68	LYS
37	E	101	ARG
37	E	104	LYS
37	E	111	TYR
37	E	112	TYR
37	E	114	THR
37	E	126	LYS
37	E	129	PHE
37	E	134	ARG
37	E	153	HIS
37	E	157	ARG

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Mol	Chain	Res	Type
37	E	166	SER
37	E	171	VAL
37	E	175	LEU
37	E	178	ASN
37	E	186	HIS
37	E	187	GLN
37	E	203	LYS
37	E	206	LYS
37	E	212	TYR
37	E	217	LYS
37	E	219	ARG
37	E	222	ARG
37	E	230	ASP
37	E	233	LYS
37	E	237	GLU
37	E	241	GLN
37	E	242	ARG
37	E	245	ASP
37	E	246	GLN
37	E	250	ASP
37	E	252	GLN
37	E	256	ARG
37	E	266	TYR
37	E	268	ARG
37	E	275	ASN
37	E	277	ILE
37	E	280	HIS
37	E	284	PHE
38	F	27	PHE
38	F	32	ILE
38	F	33	LYS
38	F	34	ARG
38	F	41	GLN
38	F	43	MET
38	F	44	LEU
38	F	49	ARG
38	F	50	LYS
38	F	57	LYS
38	F	68	ARG
38	F	69	THR
38	F	72	ARG
38	F	75	ARG

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Mol	Chain	Res	Type
38	F	82	ASN
38	F	83	PHE
38	F	84	TYR
38	F	85	VAL
38	F	90	LYS
38	F	93	PHE
38	F	100	ILE
38	F	101	ASN
38	F	104	SER
38	F	118	GLN
38	F	119	ILE
38	F	120	PHE
38	F	121	ASN
38	F	137	ILE
38	F	146	TYR
38	F	149	LEU
38	F	151	SER
38	F	154	GLU
38	F	190	GLU
38	F	192	LEU
38	F	195	GLU
38	F	201	LYS
38	F	202	ARG
38	F	204	LYS
38	F	207	ASN
38	F	209	PHE
38	F	213	PHE
38	F	214	LYS
38	F	216	SER
38	F	219	ARG
38	F	226	THR
38	F	227	THR
38	F	228	HIS
38	F	229	PHE
38	F	234	ASP
38	F	245	LEU
38	F	247	ARG
38	F	248	ARG
38	F	250	ASN
39	I	3	ARG
39	I	4	ARG
39	I	8	CYS

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Mol	Chain	Res	Type
39	I	9	TYR
39	I	13	LYS
39	I	14	ASN
39	I	17	TYR
39	I	21	ARG
39	I	24	ARG
39	I	28	ASP
39	I	32	ARG
39	I	34	PHE
39	I	36	LEU
39	I	39	LYS
39	I	40	LYS
39	I	43	VAL
39	I	44	ASP
39	I	45	GLU
39	I	46	PHE
39	I	48	LEU
39	I	55	ASP
39	I	58	GLU
39	I	71	CYS
39	I	74	LYS
39	I	78	LYS
39	I	80	CYS
39	I	85	PHE
39	I	86	HIS
39	I	92	HIS
39	I	95	HIS
39	I	99	ILE
39	I	100	ASN
39	I	101	LYS
39	I	102	MET
39	I	111	LEU
39	I	119	PHE
39	I	125	THR
39	I	139	ARG
39	I	142	LEU
39	I	143	GLN
39	I	146	GLU
39	I	150	GLU
39	I	153	ARG
39	I	159	PHE
39	I	164	LYS

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Mol	Chain	Res	Type
39	I	171	TRP
39	I	177	ASN
39	I	179	ASP
39	I	181	PHE
39	I	182	GLU
39	I	187	LYS
39	I	189	CYS
39	I	207	ASP
39	I	208	LYS
40	P	3	ARG
40	P	5	SER
40	P	9	GLU
40	P	10	ASN
40	P	13	LYS
40	P	18	ARG
40	P	22	LEU
40	P	23	ARG
40	P	24	VAL
40	P	26	PHE
40	P	28	ASN
40	P	30	ARG
40	P	40	HIS
40	P	42	ARG
40	P	54	GLN
40	P	57	CYS
40	P	69	ARG
40	P	78	TRP
40	P	90	PHE
40	P	91	LEU
40	P	110	ASP
40	P	115	GLU
40	P	128	ARG
40	P	133	HIS
40	P	135	ARG
40	P	154	GLU
41	W	1	MET
41	W	3	VAL
41	W	8	PHE
41	W	11	TYR
41	W	12	LYS
41	W	14	TYR
41	W	17	HIS

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Mol	Chain	Res	Type
41	W	31	PHE
41	W	33	ASN
41	W	41	LEU
41	W	44	ARG
41	W	50	ASN
41	W	51	TRP
41	W	55	TYR
41	W	56	ARG
41	W	57	ARG
41	W	59	HIS
42	j	10	LYS
42	j	25	LYS
42	j	27	TYR
42	j	28	HIS
42	j	39	TYR
42	j	47	TYR
42	j	48	ASN
42	j	55	ARG
42	j	56	ARG
42	j	57	ASN
42	j	71	TYR
42	j	79	ARG
42	j	80	GLU
43	n	2	ARG
43	n	8	LYS
43	n	9	ARG
43	n	18	ARG
43	n	20	MET
43	n	21	ARG
44	p	3	LYS
44	p	4	ARG
44	p	16	THR
44	p	18	TYR
44	p	34	HIS
44	p	49	ARG
44	p	69	TRP
44	p	71	TYR
44	p	84	ARG
44	p	85	ARG
44	p	87	LYS
44	p	92	GLN
45	r	7	TRP

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Mol	Chain	Res	Type
45	r	11	ARG
45	r	13	CYS
45	r	16	PHE
45	r	18	ILE
45	r	19	LYS
45	r	26	SER
45	r	28	GLU
45	r	31	ASN
45	r	35	ARG
45	r	36	ASN
45	r	39	ARG
45	r	45	HIS
45	r	46	HIS
45	r	64	ILE
45	r	66	ARG
45	r	67	ARG
45	r	71	ARG
45	r	83	ASN
45	r	101	LYS
45	r	105	ASP
45	r	106	LEU
45	r	107	ARG
45	r	112	ARG
45	r	113	ARG
45	r	115	SER
46	K	1	MET
46	K	5	PHE
46	K	14	TYR
46	K	16	ARG
46	K	22	VAL
46	K	40	LYS
46	K	45	ASP
46	K	61	LYS
46	K	90	ARG
46	K	96	LYS
46	K	104	ILE
46	K	107	ASP
46	K	108	GLU
46	K	111	ASN
46	K	117	ARG
46	K	125	LEU
46	K	130	LYS

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Mol	Chain	Res	Type
46	K	147	HIS
47	q	5	ASP
47	q	14	PHE
47	q	16	LYS
47	q	26	LYS
47	q	33	ASP
47	q	45	MET
47	q	48	ARG
47	q	50	LYS
47	q	57	LYS
47	q	58	ASN
47	q	59	THR
47	q	61	MET
47	q	62	ARG
47	q	69	LEU
47	q	70	GLU
47	q	77	LYS
47	q	81	HIS
47	q	83	ARG
47	q	91	THR
47	q	94	ASP
47	q	95	LEU
47	q	99	ARG
47	q	105	ASN
47	q	127	ASN
47	q	143	ILE
47	q	148	SER
47	q	149	ARG
47	q	155	LEU
47	q	158	VAL
47	q	176	ASN
47	q	183	PHE
47	q	187	LEU
47	q	191	GLN
47	q	194	ASP
47	q	202	GLU
47	q	203	VAL
48	z	8	ARG
48	z	15	ARG
48	z	24	ASN
48	z	28	LEU
48	z	29	ASN

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Mol	Chain	Res	Type
48	z	33	LYS
48	z	43	ASP
48	z	61	ASP
48	z	81	LYS
48	z	147	GLN
48	z	162	SER
48	z	200	SER
48	z	241	ASP
48	z	273	ILE
48	z	280	ASP
48	z	283	GLU
48	z	349	LEU
48	z	383	ASN
48	z	427	PHE
49	2	109	LEU
49	2	123	PHE
49	2	127	MET
52	9	72	TRP
52	9	77	GLN
52	9	79	ARG
52	9	89	GLU
53	6	84	ARG
53	6	91	ASN
53	6	108	ASP
53	6	122	ASP
53	6	129	TYR
53	6	142	ARG
55	SA	6	ASP
55	SA	8	LEU
55	SA	9	GLN
55	SA	32	PHE
55	SA	36	GLN
55	SA	39	TYR
55	SA	44	ASP
55	SA	53	ARG
55	SA	56	GLU
55	SA	58	LEU
55	SA	60	LEU
55	SA	70	ASN
55	SA	73	ASP
55	SA	75	SER
55	SA	81	ASN

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Mol	Chain	Res	Type
55	SA	84	GLN
55	SA	89	LYS
55	SA	90	PHE
55	SA	97	THR
55	SA	99	ILE
55	SA	102	ARG
55	SA	105	PRO
55	SA	111	GLN
55	SA	116	PHE
55	SA	117	ARG
55	SA	130	ASP
55	SA	131	HIS
55	SA	135	THR
55	SA	140	VAL
55	SA	141	ASN
55	SA	151	ASP
55	SA	158	ASP
55	SA	169	HIS
55	SA	181	GLU
55	SA	185	MET
55	SA	186	ARG
55	SA	195	TRP
55	SA	196	GLU
55	SA	203	PHE
55	SA	204	TYR
55	SA	206	ASP
55	SA	208	GLU
56	SB	27	LYS
56	SB	28	ARG
56	SB	30	TRP
56	SB	31	TYR
56	SB	32	ASP
56	SB	34	LYS
56	SB	43	ASN
56	SB	51	ARG
56	SB	52	THR
56	SB	53	GLN
56	SB	56	LYS
56	SB	65	ARG
56	SB	67	PHE
56	SB	68	GLU
56	SB	81	PHE

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Mol	Chain	Res	Type
56	SB	88	THR
56	SB	100	PHE
56	SB	104	ASP
56	SB	105	LEU
56	SB	107	ARG
56	SB	111	CYS
56	SB	119	THR
56	SB	133	TYR
56	SB	136	ARG
56	SB	138	PHE
56	SB	146	ARG
56	SB	148	ASN
56	SB	150	ILE
56	SB	151	ARG
56	SB	155	TYR
56	SB	158	HIS
56	SB	165	ARG
56	SB	181	LEU
56	SB	191	ASP
56	SB	196	ASP
56	SB	202	GLN
56	SB	205	TYR
56	SB	208	HIS
56	SB	223	PHE
57	SC	59	GLU
57	SC	60	TRP
57	SC	61	MET
57	SC	65	LYS
57	SC	68	ARG
57	SC	71	LYS
57	SC	72	ASP
57	SC	78	LEU
57	SC	79	GLU
57	SC	96	PHE
57	SC	97	PHE
57	SC	101	SER
57	SC	104	ASP
57	SC	110	MET
57	SC	114	LYS
57	SC	115	GLN
57	SC	120	GLN
57	SC	121	ARG

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Mol	Chain	Res	Type
57	SC	123	ARG
57	SC	134	ASN
57	SC	137	VAL
57	SC	142	LYS
57	SC	143	CYS
57	SC	152	ARG
57	SC	167	ARG
57	SC	169	TYR
57	SC	183	LYS
57	SC	192	LEU
57	SC	200	ARG
57	SC	206	SER
57	SC	215	MET
57	SC	220	ASP
57	SC	221	ASP
57	SC	223	TYR
57	SC	227	ARG
57	SC	242	ASP
57	SC	248	TYR
57	SC	250	TYR
57	SC	255	LEU
57	SC	261	PHE
57	SC	262	THR
57	SC	272	HIS
57	SC	275	LYS
58	SE	3	ARG
58	SE	8	HIS
58	SE	9	LEU
58	SE	11	ARG
58	SE	18	TRP
58	SE	21	ASP
58	SE	30	ARG
58	SE	39	ARG
58	SE	42	LEU
58	SE	49	ARG
58	SE	51	ARG
58	SE	54	TYR
58	SE	67	GLN
58	SE	73	ASP
58	SE	87	MET
58	SE	93	ASP
58	SE	95	THR

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Mol	Chain	Res	Type
58	SE	98	ASN
58	SE	99	PHE
58	SE	100	ARG
58	SE	103	TYR
58	SE	106	LYS
58	SE	108	ARG
58	SE	112	HIS
58	SE	115	THR
58	SE	117	GLU
58	SE	118	GLU
58	SE	121	TYR
58	SE	122	LYS
58	SE	130	PHE
58	SE	148	ARG
58	SE	155	LYS
58	SE	158	ASP
58	SE	164	LEU
58	SE	165	GLU
58	SE	179	ASN
58	SE	180	LEU
58	SE	188	ASN
58	SE	191	ARG
58	SE	198	ARG
58	SE	205	PHE
58	SE	220	THR
58	SE	221	ARG
58	SE	224	ASN
58	SE	226	PHE
58	SE	235	TRP
58	SE	240	ARG
58	SE	242	LYS
58	SE	245	ARG
58	SE	253	ASP
58	SE	259	LYS
58	SE	260	GLN
59	SG	20	ASP
59	SG	27	PHE
59	SG	29	GLU
59	SG	30	LYS
59	SG	31	ARG
59	SG	32	MET
59	SG	56	ASN

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Mol	Chain	Res	Type
59	SG	58	LYS
59	SG	59	GLN
59	SG	64	LYS
59	SG	65	GLN
59	SG	70	HIS
59	SG	74	ARG
59	SG	76	LEU
59	SG	87	ARG
59	SG	88	ARG
59	SG	98	ARG
59	SG	109	LEU
59	SG	110	ASN
59	SG	120	ASP
59	SG	126	ASP
59	SG	132	ARG
59	SG	133	LEU
59	SG	140	ARG
59	SG	143	LYS
59	SG	145	PHE
59	SG	152	ASP
59	SG	155	GLN
59	SG	159	ARG
59	SG	162	LEU
59	SG	164	LYS
59	SG	165	GLU
59	SG	170	ARG
59	SG	190	ARG
59	SG	191	ARG
59	SG	196	LYS
59	SG	198	ARG
59	SG	213	LEU
59	SG	224	ARG
59	SG	227	GLN
59	SG	236	SER
60	SH	12	ASN
60	SH	16	PRO
60	SH	23	ILE
60	SH	35	ASP
60	SH	36	LEU
60	SH	40	LEU
60	SH	46	THR
60	SH	57	ARG

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Mol	Chain	Res	Type
60	SH	81	ARG
60	SH	83	LEU
60	SH	109	ARG
60	SH	126	HIS
60	SH	135	PHE
60	SH	137	SER
60	SH	138	GLU
60	SH	148	LEU
60	SH	159	ASP
60	SH	160	LYS
60	SH	162	GLN
60	SH	166	VAL
60	SH	177	TYR
60	SH	184	ASP
60	SH	186	ASN
60	SH	190	PRO
61	SI	5	ARG
61	SI	6	ASP
61	SI	8	TRP
61	SI	12	ARG
61	SI	21	TYR
61	SI	22	HIS
61	SI	25	ARG
61	SI	27	TYR
61	SI	47	ARG
61	SI	52	ASN
61	SI	58	LEU
61	SI	65	PHE
61	SI	67	TRP
61	SI	72	CYS
61	SI	73	THR
61	SI	74	ARG
61	SI	83	TYR
61	SI	86	SER
61	SI	110	ARG
61	SI	111	GLN
61	SI	112	TRP
61	SI	113	TYR
61	SI	116	HIS
61	SI	123	ARG
61	SI	140	LYS
61	SI	149	TYR

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Mol	Chain	Res	Type
61	SI	155	ASN
61	SI	174	CYS
61	SI	178	ARG
61	SI	188	TYR
61	SI	191	GLU
61	SI	196	GLU
61	SI	203	LYS
61	SI	206	LYS
62	SJ	5	ARG
62	SJ	9	CYS
62	SJ	10	ARG
62	SJ	13	TYR
62	SJ	18	ARG
62	SJ	20	PHE
62	SJ	26	ASP
62	SJ	29	LEU
62	SJ	35	TYR
62	SJ	37	LEU
62	SJ	39	ASN
62	SJ	42	GLU
62	SJ	44	TRP
62	SJ	64	ASP
62	SJ	67	ASP
62	SJ	69	ARG
62	SJ	70	ARG
62	SJ	83	ARG
62	SJ	88	ASP
62	SJ	91	LYS
62	SJ	93	LYS
62	SJ	95	ASP
62	SJ	96	TYR
62	SJ	101	LYS
62	SJ	108	ARG
62	SJ	109	ARG
62	SJ	110	LEU
62	SJ	115	PHE
62	SJ	116	LYS
62	SJ	123	ILE
62	SJ	124	HIS
62	SJ	125	HIS
62	SJ	127	ARG
62	SJ	131	ARG

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Mol	Chain	Res	Type
62	SJ	136	ARG
62	SJ	138	ARG
62	SJ	139	LYS
62	SJ	147	PHE
62	SJ	150	ARG
62	SJ	158	ASP
62	SJ	162	ARG
62	SJ	165	TYR
62	SJ	169	ARG
62	SJ	172	ARG
62	SJ	174	LYS
63	SL	8	ARG
63	SL	13	GLN
63	SL	16	ILE
63	SL	20	LYS
63	SL	22	ARG
63	SL	25	LEU
63	SL	27	GLU
63	SL	35	ARG
63	SL	39	ASN
63	SL	40	ILE
63	SL	44	PHE
63	SL	57	ASP
63	SL	61	PRO
63	SL	65	ASN
63	SL	66	VAL
63	SL	69	ARG
63	SL	74	SER
63	SL	85	THR
63	SL	89	ARG
63	SL	90	ARG
63	SL	92	TYR
63	SL	97	ARG
63	SL	103	GLU
63	SL	108	ASN
63	SL	113	LEU
63	SL	117	PHE
63	SL	121	GLN
63	SL	124	ASP
63	SL	131	CYS
63	SL	132	ARG
63	SL	139	ARG

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Mol	Chain	Res	Type
63	SL	147	LYS
64	SN	3	ARG
64	SN	13	GLN
64	SN	14	SER
64	SN	20	ARG
64	SN	27	LYS
64	SN	31	ASP
64	SN	38	TYR
64	SN	55	ARG
64	SN	56	ASP
64	SN	58	HIS
64	SN	62	GLN
64	SN	64	ARG
64	SN	69	ASN
64	SN	76	LYS
64	SN	84	LEU
64	SN	86	GLU
64	SN	87	ASP
64	SN	89	TYR
64	SN	99	ARG
64	SN	101	HIS
64	SN	105	ASN
64	SN	113	PHE
64	SN	127	ARG
64	SN	128	TYR
64	SN	132	LYS
64	SN	139	TRP
64	SN	141	TYR
65	SO	17	LEU
65	SO	20	GLN
65	SO	26	ASN
65	SO	32	HIS
65	SO	34	PHE
65	SO	37	PHE
65	SO	39	ASP
65	SO	41	PHE
65	SO	43	HIS
65	SO	46	ASP
65	SO	50	LYS
65	SO	51	GLU
65	SO	60	MET
65	SO	63	LYS

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Mol	Chain	Res	Type
65	SO	65	ASP
65	SO	66	ARG
65	SO	80	ASP
65	SO	84	ARG
65	SO	86	LYS
65	SO	94	HIS
65	SO	103	ASN
65	SO	106	LYS
65	SO	116	LEU
65	SO	121	ARG
65	SO	128	ARG
65	SO	130	GLU
65	SO	131	ASP
65	SO	141	ARG
65	SO	146	ARG
65	SO	147	ARG
65	SO	149	ARG
65	SO	150	ARG
66	SV	1	MET
66	SV	2	GLN
66	SV	4	ASP
66	SV	11	LEU
66	SV	18	SER
66	SV	21	ASN
66	SV	39	VAL
66	SV	46	PHE
66	SV	47	ASN
66	SV	49	GLN
66	SV	50	PHE
66	SV	53	TYR
66	SV	66	ASP
66	SV	67	ASP
66	SV	81	LYS
66	SV	82	ASN
67	SW	12	LYS
67	SW	15	ASN
67	SW	18	GLU
67	SW	24	GLN
67	SW	28	ARG
67	SW	36	ARG
67	SW	37	PHE
67	SW	52	ILE

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Mol	Chain	Res	Type
67	SW	55	ASP
67	SW	57	ARG
67	SW	70	ASN
67	SW	80	ASP
67	SW	83	LEU
67	SW	85	ASP
67	SW	98	GLN
67	SW	105	THR
67	SW	111	MET
67	SW	113	HIS
67	SW	114	GLU
67	SW	117	ARG
67	SW	118	ARG
67	SW	120	HIS
68	SX	5	ARG
68	SX	9	THR
68	SX	17	ARG
68	SX	19	ASP
68	SX	32	LEU
68	SX	46	HIS
68	SX	61	GLN
68	SX	67	ARG
68	SX	84	PHE
68	SX	88	ASP
68	SX	105	PHE
68	SX	110	HIS
68	SX	114	ASP
68	SX	115	ILE
68	SX	131	LEU
68	SX	134	TYR
68	SX	135	LYS
68	SX	142	ARG
69	SY	16	ARG
69	SY	17	LEU
69	SY	19	GLN
69	SY	20	ARG
69	SY	22	GLN
69	SY	23	MET
69	SY	34	THR
69	SY	47	MET
69	SY	54	VAL
69	SY	61	ARG

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Mol	Chain	Res	Type
69	SY	63	HIS
69	SY	69	THR
69	SY	72	PHE
69	SY	77	ASP
69	SY	81	TYR
69	SY	96	LEU
69	SY	97	TYR
69	SY	98	GLU
69	SY	99	LYS
69	SY	107	ARG
69	SY	111	LYS
69	SY	118	ARG
69	SY	124	ASN
70	Sa	6	ARG
70	Sa	8	ASN
70	Sa	22	ARG
70	Sa	23	CYS
70	Sa	26	CYS
70	Sa	28	ARG
70	Sa	41	ILE
70	Sa	51	ARG
70	Sa	52	ASP
70	Sa	62	TYR
70	Sa	86	ASN
70	Sa	87	ARG
70	Sa	94	ASP
70	Sa	95	ARG
71	Sb	14	GLU
71	Sb	17	ARG
71	Sb	20	LYS
71	Sb	23	ARG
71	Sb	31	TYR
71	Sb	32	PHE
71	Sb	33	MET
71	Sb	34	ASP
71	Sb	37	CYS
71	Sb	47	PHE
71	Sb	51	GLN
71	Sb	72	ARG
71	Sb	75	GLU
71	Sb	78	SER
71	Sb	80	ARG

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Mol	Chain	Res	Type
71	Sb	83	GLN
71	Sb	84	HIS
72	Se	13	ARG
72	Se	15	GLN
72	Se	18	LYS
72	Se	26	LYS
72	Se	28	LYS
72	Se	31	ARG
72	Se	34	ARG
72	Se	37	GLN
72	Se	40	ARG
72	Se	41	ARG
72	Se	52	LYS
73	SD	4	GLN
73	SD	5	ILE
73	SD	6	SER
73	SD	9	ARG
73	SD	17	PHE
73	SD	22	ASN
73	SD	24	PHE
73	SD	28	GLU
73	SD	32	ASP
73	SD	40	ARG
73	SD	42	THR
73	SD	53	THR
73	SD	56	GLN
73	SD	67	ARG
73	SD	76	ARG
73	SD	87	TYR
73	SD	94	ARG
73	SD	103	GLU
73	SD	106	ARG
73	SD	107	TYR
73	SD	113	LEU
73	SD	135	GLU
73	SD	141	LYS
73	SD	152	PHE
73	SD	156	LEU
73	SD	158	ILE
73	SD	159	HIS
73	SD	162	ASP
73	SD	163	PRO

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Mol	Chain	Res	Type
73	SD	167	TYR
73	SD	169	ASP
73	SD	177	LEU
73	SD	178	ARG
73	SD	192	TRP
73	SD	206	ASP
73	SD	207	HIS
73	SD	212	GLU
73	SD	216	GLU
73	SD	218	LEU
73	SD	225	GLU
73	SD	226	GLN
74	SF	23	TRP
74	SF	27	ASP
74	SF	29	GLN
74	SF	35	LEU
74	SF	37	ASP
74	SF	42	LYS
74	SF	43	GLU
74	SF	49	LEU
74	SF	55	ARG
74	SF	63	LYS
74	SF	79	HIS
74	SF	82	ASN
74	SF	83	ASN
74	SF	88	MET
74	SF	94	LYS
74	SF	101	HIS
74	SF	106	GLU
74	SF	110	GLN
74	SF	114	ASN
74	SF	118	ASN
74	SF	122	ARG
74	SF	123	GLU
74	SF	130	ARG
74	SF	136	ARG
74	SF	137	GLN
74	SF	140	ASP
74	SF	145	ARG
74	SF	152	TRP
74	SF	164	ARG
74	SF	168	THR

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Mol	Chain	Res	Type
74	SF	171	GLU
74	SF	172	CYS
74	SF	184	SER
74	SF	186	ASN
74	SF	187	SER
74	SF	190	ILE
74	SF	194	ASP
74	SF	198	ARG
75	SK	1	MET
75	SK	2	LEU
75	SK	5	LYS
75	SK	8	ARG
75	SK	16	PHE
75	SK	32	HIS
75	SK	37	ASP
75	SK	39	ASN
75	SK	43	LEU
75	SK	46	MET
75	SK	54	SER
75	SK	61	GLN
75	SK	65	ARG
75	SK	66	HIS
75	SK	70	TYR
75	SK	74	GLU
75	SK	80	ARG
75	SK	81	ASP
75	SK	89	ILE
75	SK	95	ARG
75	SK	96	ARG
76	SM	12	MET
76	SM	18	LEU
76	SM	20	GLU
76	SM	26	LEU
76	SM	29	ASP
76	SM	31	LEU
76	SM	33	ARG
76	SM	43	ASP
76	SM	45	ARG
76	SM	48	HIS
76	SM	49	LEU
76	SM	52	GLN
76	SM	57	ASP

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Mol	Chain	Res	Type
76	SM	61	TYR
76	SM	72	HIS
76	SM	73	GLN
76	SM	77	ILE
76	SM	81	ASP
76	SM	83	LYS
76	SM	88	TRP
76	SM	91	LEU
76	SM	92	CYS
76	SM	95	ASP
76	SM	96	ARG
76	SM	99	ASN
76	SM	101	ARG
76	SM	102	LYS
76	SM	113	ASP
76	SM	114	TYR
76	SM	127	TYR
77	SP	5	GLU
77	SP	7	LYS
77	SP	10	ARG
77	SP	15	PHE
77	SP	18	ARG
77	SP	27	ASP
77	SP	30	TYR
77	SP	40	ARG
77	SP	41	GLN
77	SP	42	ARG
77	SP	43	ARG
77	SP	44	ARG
77	SP	50	ARG
77	SP	51	ARG
77	SP	52	LYS
77	SP	81	ARG
77	SP	82	ASP
77	SP	86	LEU
78	SQ	15	ARG
78	SQ	26	LYS
78	SQ	27	ARG
78	SQ	33	LYS
78	SQ	35	ASN
78	SQ	41	MET
78	SQ	45	ARG

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Mol	Chain	Res	Type
78	SQ	50	LYS
78	SQ	63	PHE
78	SQ	69	ARG
78	SQ	71	ARG
78	SQ	73	LYS
78	SQ	77	HIS
78	SQ	90	LYS
78	SQ	99	TYR
78	SQ	107	GLU
78	SQ	114	GLN
78	SQ	115	TYR
78	SQ	116	ASP
78	SQ	117	ARG
78	SQ	119	LEU
78	SQ	123	ASP
78	SQ	128	GLU
78	SQ	138	ARG
78	SQ	140	ARG
78	SQ	145	TYR
79	SR	1	MET
79	SR	3	ARG
79	SR	6	THR
79	SR	28	PHE
79	SR	31	ASN
79	SR	33	ARG
79	SR	37	GLU
79	SR	49	LYS
79	SR	56	HIS
79	SR	58	MET
79	SR	99	ASP
79	SR	102	THR
79	SR	105	MET
79	SR	116	ASN
79	SR	127	ASN
80	SS	8	LYS
80	SS	10	GLN
80	SS	14	ARG
80	SS	34	LYS
80	SS	39	ARG
80	SS	42	HIS
80	SS	55	ARG
80	SS	63	GLU

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Mol	Chain	Res	Type
80	SS	72	GLN
80	SS	78	LYS
80	SS	81	ASP
80	SS	82	TRP
80	SS	85	ASN
80	SS	86	ARG
80	SS	87	GLN
80	SS	92	ASP
80	SS	95	TYR
80	SS	108	ARG
80	SS	113	ARG
80	SS	118	ARG
80	SS	124	ARG
80	SS	134	GLN
80	SS	135	HIS
81	ST	8	ASP
81	ST	11	GLN
81	ST	16	ARG
81	ST	21	PHE
81	ST	28	LEU
81	ST	35	ASP
81	ST	42	HIS
81	ST	52	TRP
81	ST	53	PHE
81	ST	62	ARG
81	ST	63	HIS
81	ST	74	SER
81	ST	79	TYR
81	ST	82	ARG
81	ST	84	ARG
81	ST	90	SER
81	ST	92	PHE
81	ST	94	ARG
81	ST	97	LYS
81	ST	102	ARG
81	ST	118	ASP
81	ST	121	ARG
81	ST	123	LEU
81	ST	128	GLN
82	SU	19	ARG
82	SU	47	ASN
82	SU	48	LEU

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Mol	Chain	Res	Type
82	SU	55	ARG
82	SU	56	MET
82	SU	62	ARG
82	SU	64	THR
82	SU	79	ARG
82	SU	84	ILE
82	SU	87	ARG
82	SU	93	SER
82	SU	111	GLU
83	SZ	44	LEU
83	SZ	45	ASN
83	SZ	51	ASP
83	SZ	64	ASN
83	SZ	94	LYS
83	SZ	97	ILE
83	SZ	109	TYR
83	SZ	110	THR
83	SZ	114	LYS
84	Sc	5	ARG
84	Sc	7	GLN
84	Sc	13	ARG
84	Sc	21	THR
84	Sc	26	GLN
84	Sc	51	ARG
84	Sc	54	ASP
84	Sc	60	GLU
84	Sc	62	GLU
84	Sc	67	ARG
85	Sd	6	PHE
85	Sd	8	TRP
85	Sd	9	SER
85	Sd	12	ARG
85	Sd	26	ASN
85	Sd	30	LEU
85	Sd	34	TYR
85	Sd	43	PHE
85	Sd	56	ASP
86	Sf	87	THR
86	Sf	89	LYS
86	Sf	95	ARG
86	Sf	104	LYS
86	Sf	106	TYR

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Mol	Chain	Res	Type
86	Sf	116	ARG
86	Sf	119	ARG
86	Sf	121	CYS
86	Sf	126	CYS
86	Sf	131	PHE
86	Sf	138	ARG
86	Sf	139	HIS
86	Sf	140	TYR
86	Sf	141	CYS
86	Sf	146	LEU
86	Sf	147	THR
86	Sf	148	TYR
86	Sf	149	CYS
86	Sf	150	PHE
87	Sg	8	ARG
87	Sg	15	ASN
87	Sg	17	TRP
87	Sg	20	GLN
87	Sg	24	THR
87	Sg	36	ARG
87	Sg	44	LYS
87	Sg	47	ARG
87	Sg	48	ASP
87	Sg	49	GLU
87	Sg	59	LEU
87	Sg	65	PHE
87	Sg	84	ASP
87	Sg	100	ARG
87	Sg	107	ASP
87	Sg	118	ARG
87	Sg	143	GLN
87	Sg	172	LYS
87	Sg	186	THR
87	Sg	187	ASN
87	Sg	194	TYR
87	Sg	213	ASP
87	Sg	215	GLN
87	Sg	226	HIS
87	Sg	229	THR
87	Sg	234	ASP
87	Sg	240	CYS
87	Sg	247	TRP

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Mol	Chain	Res	Type
87	Sg	268	ASP
87	Sg	269	GLU
87	Sg	273	GLU
87	Sg	289	LEU
87	Sg	294	ASP
87	Sg	299	PHE
87	Sg	302	TYR
87	Sg	306	LEU
87	Sg	310	TRP
88	S1	9	GLU
88	S1	18	TYR
88	S1	32	ARG
88	S1	35	ASP
88	S1	43	THR
88	S1	46	LEU
88	S1	54	ASP
88	S1	63	GLU
89	S4	21	ARG
89	S4	32	LYS
89	S4	34	ASP
89	S4	56	CYS
89	S4	77	ASN
89	S4	85	ASN
89	S4	92	ASP
89	S4	94	LEU
89	S4	95	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (269) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	50	HIS
1	A	100	ASN
1	A	194	ASN
1	A	209	HIS
1	A	215	ASN
2	D	45	ASN
2	D	94	ASN
2	D	122	GLN
2	D	195	HIS
2	D	202	GLN
2	D	244	HIS

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Mol	Chain	Res	Type
2	D	250	ASN
3	G	43	GLN
3	G	81	ASN
3	G	108	GLN
3	G	112	GLN
3	G	231	ASN
4	H	40	HIS
4	H	42	ASN
4	H	63	ASN
4	H	78	GLN
4	H	106	GLN
5	J	46	GLN
5	J	155	HIS
6	L	15	HIS
6	L	28	GLN
6	L	87	HIS
6	L	113	ASN
6	L	159	ASN
7	M	33	GLN
7	M	34	ASN
8	N	8	GLN
8	N	90	ASN
8	N	145	ASN
8	N	158	HIS
8	N	178	HIS
8	N	181	HIS
8	N	182	HIS
8	N	196	ASN
9	O	65	ASN
9	O	72	HIS
9	O	173	GLN
9	O	184	ASN
9	O	199	HIS
10	Q	7	HIS
10	Q	40	ASN
11	R	66	ASN
11	R	75	HIS
11	R	118	HIS
11	R	143	HIS
12	S	91	HIS
12	S	92	ASN
12	S	122	HIS

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Mol	Chain	Res	Type
12	S	163	HIS
13	T	70	HIS
13	T	98	HIS
13	T	139	HIS
14	U	55	ASN
16	X	93	ASN
17	Y	24	HIS
17	Y	72	GLN
17	Y	100	HIS
18	Z	28	ASN
18	Z	79	HIS
18	Z	127	ASN
19	a	19	HIS
19	a	40	HIS
19	a	66	ASN
20	b	6	ASN
20	b	12	GLN
20	b	19	ASN
20	b	27	GLN
20	b	42	ASN
21	c	19	GLN
21	c	77	ASN
22	d	93	ASN
23	e	24	GLN
23	e	43	ASN
23	e	57	ASN
23	e	92	ASN
23	e	126	ASN
24	f	21	GLN
24	f	55	ASN
24	f	80	ASN
24	f	99	HIS
25	g	18	ASN
25	g	110	GLN
25	g	112	GLN
26	h	30	GLN
26	h	63	GLN
26	h	68	ASN
26	h	98	HIS
27	i	12	ASN
27	i	26	HIS
30	m	87	GLN

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Mol	Chain	Res	Type
31	o	21	HIS
31	o	45	GLN
31	o	76	ASN
35	B	167	GLN
35	B	179	HIS
35	B	203	GLN
35	B	204	GLN
35	B	213	GLN
35	B	258	HIS
35	B	302	ASN
35	B	376	HIS
36	C	50	GLN
36	C	60	HIS
36	C	85	HIS
36	C	94	ASN
36	C	112	HIS
36	C	142	HIS
36	C	178	ASN
36	C	198	ASN
36	C	203	GLN
36	C	215	ASN
36	C	223	ASN
36	C	286	ASN
36	C	338	ASN
36	C	343	GLN
37	E	178	ASN
37	E	186	HIS
37	E	246	GLN
38	F	41	GLN
38	F	82	ASN
38	F	128	ASN
38	F	153	ASN
38	F	174	ASN
38	F	194	HIS
38	F	250	ASN
39	I	51	HIS
39	I	86	HIS
39	I	100	ASN
39	I	213	HIS
40	P	28	ASN
40	P	64	ASN
40	P	72	GLN

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Mol	Chain	Res	Type
40	P	80	GLN
40	P	133	HIS
40	P	145	HIS
41	W	17	HIS
41	W	59	HIS
42	j	16	HIS
42	j	48	ASN
42	j	66	HIS
44	p	92	GLN
45	r	6	GLN
45	r	12	ASN
45	r	36	ASN
46	K	147	HIS
46	K	149	HIS
47	q	68	HIS
47	q	85	ASN
47	q	200	ASN
48	z	76	GLN
48	z	102	ASN
48	z	126	GLN
48	z	151	ASN
48	z	197	GLN
48	z	227	GLN
48	z	347	GLN
48	z	364	ASN
48	z	383	ASN
48	z	404	GLN
48	z	429	GLN
55	SA	33	GLN
55	SA	36	GLN
55	SA	70	ASN
55	SA	84	GLN
55	SA	132	GLN
55	SA	169	HIS
56	SB	40	ASN
56	SB	53	GLN
56	SB	75	GLN
56	SB	99	ASN
56	SB	124	HIS
56	SB	148	ASN
56	SB	158	HIS
56	SB	232	HIS

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Mol	Chain	Res	Type
57	SC	113	GLN
57	SC	115	GLN
57	SC	120	GLN
57	SC	134	ASN
58	SE	36	HIS
58	SE	138	HIS
58	SE	142	HIS
58	SE	188	ASN
59	SG	59	GLN
59	SG	65	GLN
59	SG	81	HIS
59	SG	110	ASN
60	SH	112	ASN
60	SH	114	GLN
61	SI	44	HIS
61	SI	64	ASN
61	SI	155	ASN
61	SI	165	GLN
61	SI	168	GLN
62	SJ	111	GLN
63	SL	19	ASN
63	SL	65	ASN
63	SL	106	HIS
64	SN	5	HIS
64	SN	69	ASN
65	SO	26	ASN
65	SO	43	HIS
66	SV	47	ASN
67	SW	64	ASN
67	SW	82	GLN
67	SW	91	ASN
67	SW	98	GLN
67	SW	113	HIS
68	SX	20	HIS
68	SX	23	HIS
69	SY	112	ASN
71	Sb	9	HIS
71	Sb	26	GLN
72	Se	37	GLN
73	SD	4	GLN
73	SD	22	ASN
73	SD	56	GLN

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Mol	Chain	Res	Type
74	SF	29	GLN
74	SF	65	GLN
74	SF	83	ASN
74	SF	101	HIS
74	SF	107	ASN
74	SF	137	GLN
74	SF	186	ASN
74	SF	203	ASN
75	SK	28	HIS
75	SK	32	HIS
75	SK	39	ASN
75	SK	66	HIS
76	SM	19	GLN
76	SM	48	HIS
76	SM	99	ASN
78	SQ	24	HIS
78	SQ	80	GLN
78	SQ	142	GLN
79	SR	48	ASN
79	SR	74	GLN
79	SR	83	ASN
79	SR	118	GLN
79	SR	121	GLN
80	SS	10	GLN
80	SS	17	ASN
80	SS	19	ASN
80	SS	120	HIS
80	SS	125	HIS
80	SS	135	HIS
81	ST	11	GLN
81	ST	63	HIS
82	SU	47	ASN
83	SZ	46	ASN
83	SZ	89	GLN
83	SZ	103	HIS
84	Sc	7	GLN
84	Sc	45	ASN
85	Sd	26	ASN
87	Sg	64	HIS
87	Sg	187	ASN
87	Sg	191	HIS
87	Sg	215	GLN

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Mol	Chain	Res	Type
87	Sg	237	ASN
88	S1	3	GLN
88	S1	5	GLN
89	S4	80	GLN
89	S4	85	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	5	3642/3658 (99%)	1678 (46%)	666 (18%)
33	7	119/120 (99%)	38 (31%)	15 (12%)
34	8	155/156 (99%)	63 (40%)	30 (19%)
50	3	73/76 (96%)	27 (36%)	5 (6%)
51	4	197/206 (95%)	43 (21%)	10 (5%)
54	S2	1714/1742 (98%)	829 (48%)	303 (17%)
All	All	5900/5958 (99%)	2678 (45%)	1029 (17%)

All (2678) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
32	5	2	G
32	5	8	U
32	5	12	A
32	5	13	U
32	5	20	U
32	5	21	G
32	5	25	A
32	5	33	A
32	5	39	A
32	5	42	A
32	5	43	U
32	5	44	A
32	5	47	A
32	5	48	G
32	5	49	U
32	5	50	C
32	5	53	C
32	5	54	G
32	5	55	G
32	5	56	A
32	5	58	G

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Mol	Chain	Res	Type
32	5	59	A
32	5	62	A
32	5	63	G
32	5	65	A
32	5	67	C
32	5	69	A
32	5	70	A
32	5	71	C
32	5	72	C
32	5	74	G
32	5	81	C
32	5	83	C
32	5	84	A
32	5	85	G
32	5	88	A
32	5	89	C
32	5	91	G
32	5	92	C
32	5	93	G
32	5	94	A
32	5	95	G
32	5	96	U
32	5	98	A
32	5	99	A
32	5	100	C
32	5	101	A
32	5	107	G
32	5	108	A
32	5	109	G
32	5	110	C
32	5	111	C
32	5	112	C
32	5	115	C
32	5	116	G
32	5	118	C
32	5	119	G
32	5	120	A
32	5	121	A
32	5	126	C
32	5	128	C
32	5	129	C
32	5	134	G

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Mol	Chain	Res	Type
32	5	135	G
32	5	136	C
32	5	138	G
32	5	139	G
32	5	143	C
32	5	144	G
32	5	145	G
32	5	150	U
32	5	151	G
32	5	152	U
32	5	157	U
32	5	158	A
32	5	159	C
32	5	164	G
32	5	166	C
32	5	167	C
32	5	170	C
32	5	171	U
32	5	172	C
32	5	173	C
32	5	178	C
32	5	182	G
32	5	183	C
32	5	184	U
32	5	185	C
32	5	186	G
32	5	187	U
32	5	188	G
32	5	189	G
32	5	194	C
32	5	195	C
32	5	196	C
32	5	197	A
32	5	198	A
32	5	200	U
32	5	201	C
32	5	202	C
32	5	203	U
32	5	205	C
32	5	206	U
32	5	208	A
32	5	209	U

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Mol	Chain	Res	Type
32	5	211	G
32	5	216	C
32	5	217	C
32	5	218	A
32	5	219	G
32	5	220	C
32	5	221	C
32	5	224	U
32	5	225	G
32	5	226	G
32	5	227	A
32	5	231	U
32	5	232	G
32	5	233	U
32	5	234	G
32	5	235	A
32	5	237	G
32	5	238	C
32	5	239	C
32	5	245	C
32	5	246	G
32	5	255	C
32	5	257	C
32	5	262	G
32	5	264	C
32	5	265	C
32	5	266	C
32	5	267	G
32	5	269	G
32	5	270	U
32	5	272	U
32	5	273	U
32	5	274	C
32	5	275	C
32	5	276	C
32	5	277	G
32	5	278	G
32	5	279	A
32	5	280	G
32	5	281	U
32	5	287	U
32	5	291	U

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Mol	Chain	Res	Type
32	5	292	G
32	5	293	G
32	5	294	G
32	5	295	A
32	5	296	A
32	5	297	U
32	5	300	A
32	5	305	A
32	5	306	A
32	5	309	C
32	5	310	G
32	5	315	G
32	5	322	C
32	5	323	C
32	5	324	A
32	5	325	U
32	5	328	A
32	5	329	A
32	5	330	G
32	5	334	A
32	5	336	A
32	5	339	C
32	5	340	C
32	5	342	G
32	5	345	C
32	5	347	A
32	5	349	A
32	5	352	G
32	5	353	A
32	5	354	U
32	5	355	A
32	5	357	U
32	5	358	C
32	5	360	A
32	5	361	C
32	5	362	A
32	5	363	A
32	5	370	U
32	5	381	U
32	5	383	A
32	5	384	A
32	5	385	A

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Mol	Chain	Res	Type
32	5	386	A
32	5	387	G
32	5	388	A
32	5	394	G
32	5	395	A
32	5	396	A
32	5	399	G
32	5	406	C
32	5	407	A
32	5	408	A
32	5	409	G
32	5	410	A
32	5	411	G
32	5	412	G
32	5	413	G
32	5	414	C
32	5	415	G
32	5	417	G
32	5	418	A
32	5	424	U
32	5	431	G
32	5	432	U
32	5	433	A
32	5	436	C
32	5	440	U
32	5	446	C
32	5	449	C
32	5	450	G
32	5	451	C
32	5	452	A
32	5	453	G
32	5	454	U
32	5	455	C
32	5	456	C
32	5	458	C
32	5	467	U
32	5	468	U
32	5	469	C
32	5	470	A
32	5	473	C
32	5	485	C
32	5	486	C

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Mol	Chain	Res	Type
32	5	487	G
32	5	491	G
32	5	498	C
32	5	500	G
32	5	502	C
32	5	503	C
32	5	504	G
32	5	506	C
32	5	509	A
32	5	510	U
32	5	511	C
32	5	514	U
32	5	515	C
32	5	519	C
32	5	647	G
32	5	648	G
32	5	649	A
32	5	650	C
32	5	653	U
32	5	654	C
32	5	656	C
32	5	658	C
32	5	659	G
32	5	663	G
32	5	664	G
32	5	665	C
32	5	666	G
32	5	667	A
32	5	668	C
32	5	669	C
32	5	671	G
32	5	673	C
32	5	682	G
32	5	683	C
32	5	684	G
32	5	685	C
32	5	686	A
32	5	687	U
32	5	689	U
32	5	690	C
32	5	694	C
32	5	695	G

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Mol	Chain	Res	Type
32	5	696	C
32	5	697	G
32	5	700	G
32	5	702	U
32	5	703	G
32	5	704	C
32	5	707	C
32	5	716	C
32	5	721	G
32	5	724	C
32	5	727	C
32	5	728	U
32	5	729	G
32	5	730	G
32	5	731	G
32	5	732	A
32	5	737	C
32	5	742	G
32	5	743	G
32	5	745	G
32	5	746	A
32	5	747	A
32	5	748	G
32	5	749	G
32	5	756	G
32	5	912	G
32	5	913	U
32	5	915	A
32	5	917	A
32	5	918	G
32	5	920	C
32	5	921	C
32	5	925	C
32	5	926	G
32	5	927	G
32	5	928	C
32	5	929	A
32	5	930	G
32	5	931	C
32	5	932	A
32	5	933	G
32	5	934	C

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Mol	Chain	Res	Type
32	5	935	A
32	5	936	C
32	5	937	U
32	5	938	C
32	5	939	G
32	5	940	C
32	5	943	A
32	5	944	A
32	5	945	U
32	5	946	C
32	5	950	G
32	5	952	G
32	5	956	A
32	5	957	G
32	5	958	G
32	5	959	G
32	5	960	A
32	5	961	G
32	5	962	C
32	5	963	G
32	5	964	A
32	5	965	G
32	5	966	A
32	5	967	C
32	5	968	C
32	5	969	C
32	5	970	G
32	5	971	U
32	5	972	C
32	5	974	C
32	5	975	C
32	5	976	G
32	5	977	C
32	5	978	G
32	5	979	C
32	5	980	U
32	5	982	U
32	5	983	C
32	5	990	C
32	5	1051	G
32	5	1068	G
32	5	1070	G

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Mol	Chain	Res	Type
32	5	1072	C
32	5	1075	G
32	5	1076	C
32	5	1078	A
32	5	1081	C
32	5	1083	U
32	5	1084	C
32	5	1086	C
32	5	1168	G
32	5	1177	U
32	5	1181	C
32	5	1193	C
32	5	1210	C
32	5	1211	G
32	5	1212	G
32	5	1214	C
32	5	1215	C
32	5	1217	G
32	5	1219	G
32	5	1220	G
32	5	1221	G
32	5	1222	A
32	5	1233	G
32	5	1235	G
32	5	1236	C
32	5	1237	C
32	5	1238	A
32	5	1239	C
32	5	1240	G
32	5	1242	G
32	5	1243	C
32	5	1244	G
32	5	1245	C
32	5	1255	A
32	5	1265	G
32	5	1266	G
32	5	1267	C
32	5	1268	G
32	5	1269	G
32	5	1270	A
32	5	1271	G
32	5	1272	C

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Mol	Chain	Res	Type
32	5	1273	G
32	5	1274	A
32	5	1275	G
32	5	1277	G
32	5	1279	A
32	5	1280	C
32	5	1283	G
32	5	1284	G
32	5	1285	U
32	5	1288	G
32	5	1289	C
32	5	1290	G
32	5	1291	G
32	5	1293	G
32	5	1294	A
32	5	1295	C
32	5	1296	G
32	5	1297	U
32	5	1298	C
32	5	1299	G
32	5	1300	G
32	5	1301	C
32	5	1302	U
32	5	1303	A
32	5	1304	C
32	5	1313	C
32	5	1314	C
32	5	1318	C
32	5	1319	U
32	5	1320	U
32	5	1325	C
32	5	1326	A
32	5	1328	G
32	5	1329	G
32	5	1330	A
32	5	1333	A
32	5	1338	G
32	5	1344	C
32	5	1354	A
32	5	1355	G
32	5	1357	C
32	5	1358	G

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Mol	Chain	Res	Type
32	5	1359	G
32	5	1360	G
32	5	1362	G
32	5	1364	U
32	5	1365	C
32	5	1366	G
32	5	1367	C
32	5	1368	A
32	5	1369	C
32	5	1370	G
32	5	1371	A
32	5	1372	A
32	5	1377	G
32	5	1378	C
32	5	1379	C
32	5	1380	G
32	5	1381	U
32	5	1386	C
32	5	1387	A
32	5	1388	A
32	5	1389	U
32	5	1390	G
32	5	1394	G
32	5	1397	A
32	5	1398	A
32	5	1399	G
32	5	1402	C
32	5	1405	C
32	5	1406	G
32	5	1407	C
32	5	1408	G
32	5	1409	C
32	5	1410	U
32	5	1411	C
32	5	1415	G
32	5	1420	A
32	5	1421	G
32	5	1426	G
32	5	1427	A
32	5	1428	U
32	5	1429	C
32	5	1431	C

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Mol	Chain	Res	Type
32	5	1432	G
32	5	1435	G
32	5	1436	C
32	5	1439	C
32	5	1440	U
32	5	1441	C
32	5	1445	U
32	5	1446	C
32	5	1448	G
32	5	1454	G
32	5	1455	G
32	5	1456	C
32	5	1457	G
32	5	1463	C
32	5	1465	G
32	5	1466	G
32	5	1474	C
32	5	1475	G
32	5	1478	C
32	5	1479	G
32	5	1480	C
32	5	1481	C
32	5	1482	G
32	5	1483	C
32	5	1484	G
32	5	1485	C
32	5	1486	C
32	5	1488	G
32	5	1489	G
32	5	1490	G
32	5	1493	G
32	5	1497	A
32	5	1498	G
32	5	1501	C
32	5	1503	A
32	5	1504	G
32	5	1508	A
32	5	1514	U
32	5	1516	G
32	5	1518	A
32	5	1519	C
32	5	1520	C

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Mol	Chain	Res	Type
32	5	1521	C
32	5	1522	G
32	5	1523	A
32	5	1525	A
32	5	1530	G
32	5	1534	A
32	5	1535	C
32	5	1538	U
32	5	1543	G
32	5	1547	A
32	5	1562	G
32	5	1563	A
32	5	1564	A
32	5	1566	C
32	5	1571	G
32	5	1572	U
32	5	1577	G
32	5	1578	U
32	5	1583	A
32	5	1590	C
32	5	1591	U
32	5	1596	U
32	5	1597	G
32	5	1604	G
32	5	1611	C
32	5	1612	G
32	5	1613	A
32	5	1614	C
32	5	1615	C
32	5	1624	G
32	5	1625	G
32	5	1626	G
32	5	1631	A
32	5	1632	A
32	5	1633	G
32	5	1634	A
32	5	1636	U
32	5	1637	A
32	5	1638	A
32	5	1640	C
32	5	1641	G
32	5	1642	A

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Mol	Chain	Res	Type
32	5	1643	A
32	5	1649	U
32	5	1650	A
32	5	1654	G
32	5	1656	U
32	5	1661	C
32	5	1662	C
32	5	1670	G
32	5	1671	U
32	5	1673	U
32	5	1676	C
32	5	1678	C
32	5	1679	A
32	5	1680	G
32	5	1681	G
32	5	1684	A
32	5	1685	G
32	5	1686	C
32	5	1687	U
32	5	1691	G
32	5	1692	C
32	5	1694	C
32	5	1696	C
32	5	1697	G
32	5	1698	C
32	5	1699	A
32	5	1719	A
32	5	1720	C
32	5	1721	G
32	5	1722	C
32	5	1723	A
32	5	1724	G
32	5	1725	U
32	5	1731	C
32	5	1734	G
32	5	1735	U
32	5	1736	A
32	5	1741	G
32	5	1742	A
32	5	1746	A
32	5	1750	G
32	5	1751	A

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Mol	Chain	Res	Type
32	5	1753	G
32	5	1754	U
32	5	1755	C
32	5	1756	U
32	5	1757	U
32	5	1758	G
32	5	1759	G
32	5	1760	G
32	5	1761	G
32	5	1762	C
32	5	1764	G
32	5	1766	A
32	5	1767	A
32	5	1768	C
32	5	1769	G
32	5	1770	A
32	5	1772	C
32	5	1776	A
32	5	1777	C
32	5	1778	C
32	5	1779	U
32	5	1781	U
32	5	1787	A
32	5	1788	A
32	5	1790	U
32	5	1791	U
32	5	1797	G
32	5	1799	G
32	5	1800	U
32	5	1803	G
32	5	1804	A
32	5	1805	A
32	5	1815	G
32	5	1816	C
32	5	1817	U
32	5	1818	G
32	5	1819	G
32	5	1820	C
32	5	1821	G
32	5	1822	U
32	5	1827	C
32	5	1828	C

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Mol	Chain	Res	Type
32	5	1830	G
32	5	1832	C
32	5	1833	G
32	5	1834	U
32	5	1835	G
32	5	1836	G
32	5	1843	A
32	5	1847	C
32	5	1848	C
32	5	1849	U
32	5	1850	A
32	5	1851	G
32	5	1855	G
32	5	1864	G
32	5	1866	U
32	5	1867	A
32	5	1869	G
32	5	1876	U
32	5	1878	G
32	5	1881	C
32	5	1882	U
32	5	1889	U
32	5	1890	G
32	5	1891	A
32	5	1897	A
32	5	1899	G
32	5	1900	C
32	5	1903	G
32	5	1907	A
32	5	1910	G
32	5	1912	G
32	5	1913	C
32	5	1916	G
32	5	1917	A
32	5	1918	U
32	5	1920	C
32	5	1921	C
32	5	1922	G
32	5	1923	A
32	5	1925	G
32	5	1929	A
32	5	1930	U

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Mol	Chain	Res	Type
32	5	1931	C
32	5	1932	A
32	5	1935	C
32	5	1936	C
32	5	1938	C
32	5	1939	A
32	5	1941	A
32	5	1945	G
32	5	1947	U
32	5	1948	G
32	5	1949	U
32	5	1951	G
32	5	1952	G
32	5	1956	A
32	5	1959	U
32	5	1961	G
32	5	1962	A
32	5	1967	A
32	5	1971	C
32	5	1974	U
32	5	1975	G
32	5	1976	G
32	5	1977	C
32	5	1979	A
32	5	1980	U
32	5	1981	G
32	5	1983	A
32	5	1984	A
32	5	1985	G
32	5	1986	U
32	5	1987	C
32	5	1988	G
32	5	1991	A
32	5	1992	U
32	5	1993	C
32	5	1995	G
32	5	1997	U
32	5	1998	A
32	5	1999	A
32	5	2001	G
32	5	2002	A
32	5	2003	G

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Mol	Chain	Res	Type
32	5	2004	U
32	5	2005	G
32	5	2007	G
32	5	2008	U
32	5	2009	A
32	5	2010	A
32	5	2011	C
32	5	2015	U
32	5	2018	C
32	5	2024	G
32	5	2025	A
32	5	2026	A
32	5	2027	U
32	5	2033	A
32	5	2034	G
32	5	2036	C
32	5	2040	A
32	5	2044	U
32	5	2045	G
32	5	2046	G
32	5	2047	A
32	5	2048	U
32	5	2052	G
32	5	2054	U
32	5	2055	G
32	5	2056	G
32	5	2057	A
32	5	2058	G
32	5	2059	C
32	5	2062	C
32	5	2063	G
32	5	2064	G
32	5	2069	A
32	5	2070	U
32	5	2075	G
32	5	2077	C
32	5	2078	C
32	5	2082	G
32	5	2084	C
32	5	2085	G
32	5	2088	A
32	5	2089	G

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Mol	Chain	Res	Type
32	5	2090	U
32	5	2091	C
32	5	2092	G
32	5	2093	A
32	5	2094	G
32	5	2095	A
32	5	2096	G
32	5	2097	U
32	5	2100	A
32	5	2102	G
32	5	2105	A
32	5	2107	C
32	5	2108	G
32	5	2109	G
32	5	2110	C
32	5	2111	G
32	5	2112	G
32	5	2113	G
32	5	2114	G
32	5	2115	G
32	5	2116	C
32	5	2117	G
32	5	2118	G
32	5	2119	C
32	5	2120	G
32	5	2122	G
32	5	2123	C
32	5	2124	G
32	5	2125	C
32	5	2126	G
32	5	2127	C
32	5	2247	C
32	5	2248	C
32	5	2250	C
32	5	2251	G
32	5	2252	G
32	5	2253	A
32	5	2254	G
32	5	2255	C
32	5	2256	C
32	5	2257	C
32	5	2258	C

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Mol	Chain	Res	Type
32	5	2259	G
32	5	2260	C
32	5	2261	G
32	5	2262	G
32	5	2263	A
32	5	2264	C
32	5	2265	G
32	5	2266	C
32	5	2267	U
32	5	2268	A
32	5	2269	C
32	5	2270	G
32	5	2273	G
32	5	2275	G
32	5	2277	C
32	5	2279	A
32	5	2280	G
32	5	2283	G
32	5	2288	G
32	5	2289	C
32	5	2299	G
32	5	2300	A
32	5	2301	G
32	5	2305	U
32	5	2309	G
32	5	2311	C
32	5	2312	U
32	5	2313	A
32	5	2314	G
32	5	2315	G
32	5	2316	G
32	5	2319	C
32	5	2321	G
32	5	2322	G
32	5	2324	C
32	5	2325	C
32	5	2328	G
32	5	2329	U
32	5	2330	G
32	5	2331	G
32	5	2332	A
32	5	2333	G

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Mol	Chain	Res	Type
32	5	2334	C
32	5	2335	C
32	5	2337	C
32	5	2339	G
32	5	2342	G
32	5	2343	G
32	5	2347	A
32	5	2348	G
32	5	2349	A
32	5	2350	U
32	5	2351	C
32	5	2357	G
32	5	2360	A
32	5	2361	G
32	5	2362	U
32	5	2364	G
32	5	2366	A
32	5	2367	A
32	5	2369	U
32	5	2370	A
32	5	2372	U
32	5	2378	G
32	5	2382	A
32	5	2383	C
32	5	2384	U
32	5	2389	A
32	5	2390	G
32	5	2391	G
32	5	2394	G
32	5	2395	A
32	5	2396	A
32	5	2397	G
32	5	2399	G
32	5	2407	G
32	5	2408	U
32	5	2417	A
32	5	2422	C
32	5	2425	U
32	5	2426	U
32	5	2428	A
32	5	2429	A
32	5	2432	U

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Mol	Chain	Res	Type
32	5	2433	G
32	5	2434	G
32	5	2437	C
32	5	2438	A
32	5	2439	G
32	5	2440	U
32	5	2441	C
32	5	2443	G
32	5	2448	G
32	5	2449	A
32	5	2450	G
32	5	2454	U
32	5	2456	G
32	5	2460	A
32	5	2463	G
32	5	2465	C
32	5	2467	U
32	5	2468	U
32	5	2469	C
32	5	2470	C
32	5	2471	G
32	5	2472	A
32	5	2474	G
32	5	2475	G
32	5	2476	G
32	5	2488	C
32	5	2489	C
32	5	2490	U
32	5	2491	C
32	5	2499	C
32	5	2503	G
32	5	2504	C
32	5	2505	C
32	5	2507	A
32	5	2508	U
32	5	2510	G
32	5	2511	A
32	5	2512	A
32	5	2513	A
32	5	2514	G
32	5	2517	A
32	5	2518	G

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Mol	Chain	Res	Type
32	5	2526	C
32	5	2527	A
32	5	2529	A
32	5	2530	U
32	5	2531	C
32	5	2532	C
32	5	2533	C
32	5	2534	C
32	5	2537	A
32	5	2544	G
32	5	2545	U
32	5	2546	G
32	5	2547	G
32	5	2549	G
32	5	2551	A
32	5	2552	G
32	5	2553	A
32	5	2554	U
32	5	2555	G
32	5	2560	C
32	5	2563	C
32	5	2566	G
32	5	2571	C
32	5	2572	C
32	5	2577	C
32	5	2580	U
32	5	2581	A
32	5	2583	C
32	5	2586	G
32	5	2587	A
32	5	2588	C
32	5	2589	C
32	5	2600	A
32	5	2601	A
32	5	2602	G
32	5	2615	C
32	5	2620	G
32	5	2623	A
32	5	2627	C
32	5	2630	U
32	5	2631	U
32	5	2638	G

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Mol	Chain	Res	Type
32	5	2639	U
32	5	2640	G
32	5	2643	G
32	5	2648	G
32	5	2649	G
32	5	2658	G
32	5	2659	A
32	5	2660	A
32	5	2661	U
32	5	2662	G
32	5	2664	G
32	5	2666	U
32	5	2667	C
32	5	2670	C
32	5	2673	G
32	5	2674	A
32	5	2675	G
32	5	2676	A
32	5	2678	A
32	5	2684	C
32	5	2686	G
32	5	2687	U
32	5	2688	G
32	5	2689	C
32	5	2694	G
32	5	2696	A
32	5	2703	G
32	5	2704	C
32	5	2707	U
32	5	2710	C
32	5	2711	G
32	5	2712	G
32	5	2713	C
32	5	2716	C
32	5	2721	G
32	5	2722	G
32	5	2725	A
32	5	2726	G
32	5	2737	C
32	5	2739	C
32	5	2740	U
32	5	2743	A

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Mol	Chain	Res	Type
32	5	2744	A
32	5	2745	A
32	5	2747	U
32	5	2751	G
32	5	2752	G
32	5	2754	G
32	5	2756	G
32	5	2757	A
32	5	2758	G
32	5	2760	G
32	5	2761	U
32	5	2762	G
32	5	2764	A
32	5	2765	A
32	5	2766	A
32	5	2767	U
32	5	2768	C
32	5	2769	U
32	5	2770	C
32	5	2782	U
32	5	2783	A
32	5	2786	C
32	5	2787	A
32	5	2788	U
32	5	2789	A
32	5	2790	U
32	5	2794	C
32	5	2797	C
32	5	2798	A
32	5	2799	G
32	5	2806	A
32	5	2807	A
32	5	2812	A
32	5	2813	A
32	5	2814	C
32	5	2815	A
32	5	2818	C
32	5	2820	C
32	5	2823	G
32	5	2824	C
32	5	2826	U
32	5	2827	G

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Mol	Chain	Res	Type
32	5	2828	U
32	5	2829	U
32	5	2833	A
32	5	2834	C
32	5	2835	A
32	5	2838	G
32	5	2841	G
32	5	2842	G
32	5	2845	A
32	5	2848	G
32	5	2849	A
32	5	2850	A
32	5	2852	U
32	5	2854	G
32	5	2855	G
32	5	2858	A
32	5	2859	G
32	5	2860	C
32	5	2864	A
32	5	2867	C
32	5	2873	U
32	5	2874	U
32	5	2875	C
32	5	2879	A
32	5	2880	U
32	5	2897	G
32	5	2898	G
32	5	2900	U
32	5	2904	U
32	5	2905	C
32	5	2910	G
32	5	3591	C
32	5	3592	G
32	5	3594	C
32	5	3595	U
32	5	3596	A
32	5	3597	G
32	5	3598	C
32	5	3603	G
32	5	3605	C
32	5	3606	U
32	5	3615	G

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Mol	Chain	Res	Type
32	5	3616	U
32	5	3617	G
32	5	3620	G
32	5	3621	A
32	5	3623	C
32	5	3625	G
32	5	3626	G
32	5	3627	G
32	5	3630	A
32	5	3635	A
32	5	3636	C
32	5	3638	G
32	5	3644	U
32	5	3645	U
32	5	3648	A
32	5	3649	A
32	5	3650	C
32	5	3657	U
32	5	3658	C
32	5	3661	G
32	5	3662	A
32	5	3663	A
32	5	3667	C
32	5	3668	C
32	5	3671	G
32	5	3673	C
32	5	3674	G
32	5	3675	G
32	5	3676	G
32	5	3677	U
32	5	3678	G
32	5	3679	U
32	5	3680	U
32	5	3681	G
32	5	3682	A
32	5	3688	U
32	5	3696	C
32	5	3698	G
32	5	3699	C
32	5	3701	C
32	5	3709	U
32	5	3710	G

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Mol	Chain	Res	Type
32	5	3711	A
32	5	3712	A
32	5	3713	U
32	5	3714	G
32	5	3715	U
32	5	3716	C
32	5	3717	A
32	5	3718	A
32	5	3719	A
32	5	3727	A
32	5	3728	A
32	5	3729	U
32	5	3735	G
32	5	3736	A
32	5	3737	A
32	5	3738	G
32	5	3739	C
32	5	3743	G
32	5	3744	G
32	5	3747	A
32	5	3748	A
32	5	3750	G
32	5	3754	G
32	5	3755	G
32	5	3756	A
32	5	3759	A
32	5	3760	A
32	5	3763	A
32	5	3765	G
32	5	3766	A
32	5	3770	U
32	5	3771	C
32	5	3773	U
32	5	3774	A
32	5	3775	A
32	5	3776	G
32	5	3777	G
32	5	3784	A
32	5	3785	A
32	5	3786	U
32	5	3791	C
32	5	3799	A

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Mol	Chain	Res	Type
32	5	3802	U
32	5	3803	A
32	5	3807	A
32	5	3809	G
32	5	3810	C
32	5	3811	G
32	5	3812	C
32	5	3813	A
32	5	3814	U
32	5	3817	A
32	5	3819	G
32	5	3822	U
32	5	3827	G
32	5	3828	A
32	5	3831	U
32	5	3838	U
32	5	3839	G
32	5	3840	U
32	5	3841	C
32	5	3843	C
32	5	3851	U
32	5	3859	G
32	5	3860	A
32	5	3861	A
32	5	3865	A
32	5	3867	A
32	5	3876	A
32	5	3877	A
32	5	3878	C
32	5	3879	G
32	5	3880	G
32	5	3881	G
32	5	3882	C
32	5	3887	C
32	5	3889	G
32	5	3892	U
32	5	3895	G
32	5	3897	G
32	5	3898	G
32	5	3899	G
32	5	3900	G
32	5	3901	A

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Mol	Chain	Res	Type
32	5	3902	A
32	5	3905	A
32	5	3906	A
32	5	3907	G
32	5	3908	A
32	5	3909	C
32	5	3912	U
32	5	3913	G
32	5	3914	U
32	5	3915	U
32	5	3916	G
32	5	3917	A
32	5	3923	A
32	5	3926	C
32	5	3936	A
32	5	3937	C
32	5	3938	G
32	5	3939	G
32	5	3943	A
32	5	4069	U
32	5	4070	U
32	5	4073	A
32	5	4074	C
32	5	4075	U
32	5	4076	G
32	5	4079	C
32	5	4083	U
32	5	4084	G
32	5	4085	A
32	5	4086	G
32	5	4088	C
32	5	4089	G
32	5	4091	G
32	5	4092	G
32	5	4093	G
32	5	4094	G
32	5	4095	G
32	5	4097	G
32	5	4104	G
32	5	4105	A
32	5	4107	G
32	5	4114	C

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Mol	Chain	Res	Type
32	5	4115	G
32	5	4116	C
32	5	4117	U
32	5	4118	U
32	5	4119	C
32	5	4120	U
32	5	4121	G
32	5	4122	G
32	5	4123	C
32	5	4125	C
32	5	4126	C
32	5	4127	A
32	5	4128	A
32	5	4132	C
32	5	4140	C
32	5	4143	G
32	5	4144	C
32	5	4145	C
32	5	4158	C
32	5	4162	C
32	5	4164	C
32	5	4165	C
32	5	4166	G
32	5	4169	G
32	5	4171	C
32	5	4172	A
32	5	4173	G
32	5	4180	G
32	5	4183	G
32	5	4184	G
32	5	4191	G
32	5	4195	G
32	5	4196	G
32	5	4197	G
32	5	4199	C
32	5	4203	A
32	5	4205	A
32	5	4206	C
32	5	4212	A
32	5	4213	A
32	5	4214	A
32	5	4215	C

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Mol	Chain	Res	Type
32	5	4216	G
32	5	4217	G
32	5	4218	U
32	5	4219	A
32	5	4220	A
32	5	4221	C
32	5	4222	G
32	5	4223	C
32	5	4225	G
32	5	4226	G
32	5	4228	G
32	5	4229	U
32	5	4230	C
32	5	4232	U
32	5	4233	A
32	5	4234	A
32	5	4235	G
32	5	4236	G
32	5	4239	A
32	5	4241	C
32	5	4243	C
32	5	4249	G
32	5	4251	A
32	5	4252	C
32	5	4254	G
32	5	4255	A
32	5	4257	A
32	5	4265	U
32	5	4268	A
32	5	4270	C
32	5	4271	A
32	5	4273	A
32	5	4274	A
32	5	4279	A
32	5	4280	A
32	5	4281	A
32	5	4282	A
32	5	4283	G
32	5	4286	C
32	5	4288	C
32	5	4290	U
32	5	4291	G

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Mol	Chain	Res	Type
32	5	4296	U
32	5	4297	G
32	5	4305	G
32	5	4306	U
32	5	4311	A
32	5	4314	C
32	5	4316	G
32	5	4317	A
32	5	4318	C
32	5	4322	G
32	5	4323	A
32	5	4329	G
32	5	4330	G
32	5	4331	G
32	5	4332	C
32	5	4334	U
32	5	4335	C
32	5	4336	A
32	5	4337	C
32	5	4339	A
32	5	4344	U
32	5	4348	A
32	5	4349	C
32	5	4350	C
32	5	4354	U
32	5	4356	G
32	5	4364	G
32	5	4368	G
32	5	4369	A
32	5	4373	G
32	5	4374	U
32	5	4375	C
32	5	4376	A
32	5	4377	G
32	5	4378	A
32	5	4380	A
32	5	4385	A
32	5	4387	C
32	5	4391	G
32	5	4393	G
32	5	4394	A
32	5	4395	U

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Mol	Chain	Res	Type
32	5	4396	A
32	5	4401	G
32	5	4414	A
32	5	4419	U
32	5	4420	U
32	5	4422	A
32	5	4425	G
32	5	4426	C
32	5	4434	C
32	5	4436	U
32	5	4437	U
32	5	4438	U
32	5	4440	G
32	5	4441	A
32	5	4444	C
32	5	4448	G
32	5	4449	A
32	5	4450	U
32	5	4451	G
32	5	4452	U
32	5	4454	G
32	5	4459	U
32	5	4463	U
32	5	4464	A
32	5	4465	U
32	5	4466	C
32	5	4473	A
32	5	4475	G
32	5	4476	C
32	5	4477	A
32	5	4482	U
32	5	4483	C
32	5	4484	A
32	5	4488	A
32	5	4489	G
32	5	4491	G
32	5	4495	G
32	5	4497	U
32	5	4498	U
32	5	4500	U
32	5	4503	A
32	5	4510	A

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Mol	Chain	Res	Type
32	5	4511	A
32	5	4512	U
32	5	4513	A
32	5	4518	A
32	5	4519	C
32	5	4520	G
32	5	4522	G
32	5	4523	A
32	5	4524	G
32	5	4527	G
32	5	4528	G
32	5	4529	G
32	5	4530	U
32	5	4531	U
32	5	4532	U
32	5	4534	G
32	5	4537	C
32	5	4543	G
32	5	4544	A
32	5	4548	A
32	5	4549	G
32	5	4550	G
32	5	4552	U
32	5	4556	U
32	5	4557	U
32	5	4558	U
32	5	4560	C
32	5	4561	C
32	5	4564	A
32	5	4569	U
32	5	4570	G
32	5	4574	U
32	5	4575	G
32	5	4581	G
32	5	4582	C
32	5	4583	C
32	5	4584	A
32	5	4586	G
32	5	4589	A
32	5	4590	A
32	5	4592	C
32	5	4599	A

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Mol	Chain	Res	Type
32	5	4600	G
32	5	4601	U
32	5	4605	A
32	5	4606	G
32	5	4608	G
32	5	4616	A
32	5	4617	G
32	5	4623	G
32	5	4624	A
32	5	4627	U
32	5	4636	U
32	5	4637	G
32	5	4641	U
32	5	4646	U
32	5	4647	G
32	5	4648	A
32	5	4652	G
32	5	4656	A
32	5	4657	U
32	5	4661	G
32	5	4664	A
32	5	4669	A
32	5	4670	C
32	5	4671	C
32	5	4672	A
32	5	4676	G
32	5	4677	U
32	5	4687	A
32	5	4693	C
32	5	4694	G
32	5	4695	C
32	5	4698	C
32	5	4699	U
32	5	4700	A
32	5	4701	A
32	5	4703	U
32	5	4709	U
32	5	4714	C
32	5	4715	C
32	5	4717	A
32	5	4718	G
32	5	4719	G

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Mol	Chain	Res	Type
32	5	4720	C
32	5	4722	G
32	5	4728	U
32	5	4729	A
32	5	4730	C
32	5	4731	G
32	5	4732	G
32	5	4733	C
32	5	4734	A
32	5	4736	C
32	5	4737	G
32	5	4738	C
32	5	4739	C
32	5	4740	G
32	5	4741	C
32	5	4743	G
32	5	4745	G
32	5	4746	C
32	5	4748	U
32	5	4749	C
32	5	4750	G
32	5	4751	G
32	5	4752	U
32	5	4753	U
32	5	4756	C
32	5	4757	C
32	5	4758	U
32	5	4759	C
32	5	4760	G
32	5	4763	U
32	5	4764	A
32	5	4770	U
32	5	4771	C
32	5	4860	G
32	5	4865	C
32	5	4869	U
32	5	4870	G
32	5	4871	C
32	5	4872	G
32	5	4873	G
32	5	4874	A
32	5	4875	G

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Mol	Chain	Res	Type
32	5	4876	U
32	5	4877	G
32	5	4878	C
32	5	4879	C
32	5	4881	U
32	5	4882	U
32	5	4883	C
32	5	4884	G
32	5	4885	U
32	5	4886	C
32	5	4888	U
32	5	4889	G
32	5	4890	G
32	5	4891	G
32	5	4893	A
32	5	4895	C
32	5	4896	G
32	5	4898	G
32	5	4900	C
32	5	4901	G
32	5	4903	G
32	5	4906	C
32	5	4910	G
32	5	4911	A
32	5	4912	G
32	5	4913	G
32	5	4926	C
32	5	4927	G
32	5	4930	C
32	5	4932	U
32	5	4934	A
32	5	4935	C
32	5	4936	G
32	5	4937	C
32	5	4938	A
32	5	4939	C
32	5	4945	G
32	5	4946	U
32	5	4947	U
32	5	4948	C
32	5	4949	G
32	5	4950	U

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Mol	Chain	Res	Type
32	5	4951	G
32	5	4952	G
32	5	4956	A
32	5	4957	C
32	5	4959	U
32	5	4960	G
32	5	4961	G
32	5	4962	C
32	5	4964	C
32	5	4965	U
32	5	4966	A
32	5	4967	A
32	5	4975	G
32	5	4976	U
32	5	4977	A
32	5	4979	A
32	5	4980	C
32	5	4981	G
32	5	4982	A
32	5	4985	U
32	5	4988	U
32	5	4989	U
32	5	4990	C
32	5	4991	U
32	5	4992	G
32	5	4993	G
32	5	4999	G
32	5	5002	U
32	5	5003	U
32	5	5005	G
32	5	5006	U
32	5	5013	C
32	5	5014	A
32	5	5016	A
32	5	5017	G
32	5	5018	C
32	5	5019	A
32	5	5023	C
32	5	5035	U
32	5	5039	U
32	5	5040	U
32	5	5041	G

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Mol	Chain	Res	Type
32	5	5042	A
32	5	5043	A
32	5	5044	A
32	5	5045	G
32	5	5046	U
32	5	5047	C
32	5	5048	A
32	5	5049	G
32	5	5050	C
32	5	5052	C
32	5	5053	U
32	5	5054	C
32	5	5056	A
32	5	5057	C
32	5	5058	A
32	5	5061	A
32	5	5062	G
32	5	5063	G
32	5	5066	U
33	7	7	G
33	7	11	A
33	7	17	C
33	7	21	G
33	7	22	A
33	7	23	A
33	7	24	C
33	7	25	G
33	7	30	C
33	7	31	G
33	7	38	U
33	7	39	C
33	7	41	G
33	7	42	A
33	7	49	A
33	7	50	A
33	7	53	U
33	7	54	A
33	7	57	C
33	7	60	G
33	7	63	C
33	7	64	G
33	7	65	G

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Mol	Chain	Res	Type
33	7	70	G
33	7	73	U
33	7	74	A
33	7	80	U
33	7	84	U
33	7	90	A
33	7	91	C
33	7	100	A
33	7	102	U
33	7	105	C
33	7	106	G
33	7	110	G
33	7	112	U
33	7	115	A
33	7	120	U
34	8	2	G
34	8	3	A
34	8	9	A
34	8	11	C
34	8	14	U
34	8	16	G
34	8	23	C
34	8	32	C
34	8	33	G
34	8	34	U
34	8	35	C
34	8	36	G
34	8	37	A
34	8	38	U
34	8	39	G
34	8	40	A
34	8	43	A
34	8	46	G
34	8	48	A
34	8	50	C
34	8	51	U
34	8	59	A
34	8	60	G
34	8	61	A
34	8	62	A
34	8	63	U
34	8	70	G

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Mol	Chain	Res	Type
34	8	71	A
34	8	74	U
34	8	75	G
34	8	80	A
34	8	81	C
34	8	82	A
34	8	83	C
34	8	84	A
34	8	85	U
34	8	86	U
34	8	87	G
34	8	90	C
34	8	94	G
34	8	95	A
34	8	99	U
34	8	103	A
34	8	104	A
34	8	105	C
34	8	107	C
34	8	109	C
34	8	110	U
34	8	111	U
34	8	112	G
34	8	114	G
34	8	117	C
34	8	118	C
34	8	122	G
34	8	125	C
34	8	126	C
34	8	127	U
34	8	131	G
34	8	132	G
34	8	147	G
34	8	151	G
34	8	153	C
34	8	156	U
50	3	2	U
50	3	6	C
50	3	8	U
50	3	9	A
50	3	17	G
50	3	18	G

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Mol	Chain	Res	Type
50	3	19	U
50	3	20	U
50	3	21	A
50	3	22	U
50	3	33	U
50	3	37	A
50	3	39	G
50	3	40	C
50	3	42	A
50	3	46	G
50	3	48	C
50	3	51	C
50	3	52	G
50	3	59	A
50	3	60	A
50	3	61	C
50	3	69	A
50	3	73	A
50	3	74	C
50	3	75	C
50	3	76	A
51	4	4	G
51	4	12	U
51	4	24	G
51	4	28	U
51	4	29	C
51	4	32	A
51	4	33	G
51	4	35	U
51	4	36	A
51	4	38	U
51	4	39	C
51	4	40	G
51	4	47	U
51	4	48	G
51	4	53	U
51	4	54	G
51	4	65	U
51	4	287	A
51	4	115	A
51	4	116	C
51	4	120	G

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Mol	Chain	Res	Type
51	4	139	A
51	4	144	C
51	4	151	C
51	4	170	C
51	4	172	A
51	4	173	A
51	4	174	G
51	4	175	G
51	4	176	A
51	4	177	G
51	4	178	G
51	4	183	A
51	4	186	C
51	4	190	C
51	4	191	C
51	4	206	G
51	4	212	C
51	4	215	A
51	4	227	G
51	4	234	A
51	4	235	G
51	4	236	U
54	S2	3	C
54	S2	4	C
54	S2	5	U
54	S2	9	U
54	S2	10	G
54	S2	17	C
54	S2	18	C
54	S2	20	G
54	S2	21	U
54	S2	26	U
54	S2	28	U
54	S2	33	G
54	S2	37	C
54	S2	42	A
54	S2	44	U
54	S2	46	A
54	S2	49	C
54	S2	51	U
54	S2	53	C
54	S2	54	A

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Mol	Chain	Res	Type
54	S2	56	G
54	S2	57	U
54	S2	58	C
54	S2	59	U
54	S2	60	A
54	S2	61	A
54	S2	62	G
54	S2	63	U
54	S2	64	A
54	S2	65	C
54	S2	66	G
54	S2	67	C
54	S2	68	A
54	S2	72	C
54	S2	73	C
54	S2	74	G
54	S2	75	G
54	S2	77	A
54	S2	78	C
54	S2	79	A
54	S2	80	G
54	S2	81	U
54	S2	84	A
54	S2	89	C
54	S2	92	A
54	S2	93	U
54	S2	98	C
54	S2	99	A
54	S2	101	U
54	S2	103	A
54	S2	104	A
54	S2	105	U
54	S2	111	A
54	S2	113	G
54	S2	114	G
54	S2	115	U
54	S2	116	U
54	S2	123	G
54	S2	124	U
54	S2	125	C
54	S2	126	G
54	S2	127	C

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Mol	Chain	Res	Type
54	S2	139	C
54	S2	140	C
54	S2	141	A
54	S2	142	C
54	S2	144	U
54	S2	146	G
54	S2	147	A
54	S2	148	U
54	S2	153	G
54	S2	154	U
54	S2	155	G
54	S2	159	A
54	S2	160	U
54	S2	161	U
54	S2	162	C
54	S2	163	U
54	S2	164	A
54	S2	165	G
54	S2	167	G
54	S2	168	C
54	S2	169	U
54	S2	170	A
54	S2	171	A
54	S2	172	U
54	S2	173	A
54	S2	180	G
54	S2	181	A
54	S2	182	C
54	S2	183	G
54	S2	184	G
54	S2	188	C
54	S2	189	U
54	S2	191	A
54	S2	192	C
54	S2	200	G
54	S2	202	G
54	S2	206	G
54	S2	208	G
54	S2	209	A
54	S2	213	G
54	S2	214	U
54	S2	215	G

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Mol	Chain	Res	Type
54	S2	216	C
54	S2	217	A
54	S2	290	U
54	S2	291	G
54	S2	292	A
54	S2	293	C
54	S2	294	U
54	S2	295	C
54	S2	297	A
54	S2	302	A
54	S2	305	U
54	S2	306	C
54	S2	307	G
54	S2	308	G
54	S2	309	G
54	S2	310	C
54	S2	311	C
54	S2	312	G
54	S2	313	A
54	S2	314	U
54	S2	315	C
54	S2	317	C
54	S2	319	C
54	S2	321	C
54	S2	323	C
54	S2	324	C
54	S2	325	C
54	S2	326	C
54	S2	327	G
54	S2	328	U
54	S2	334	C
54	S2	335	G
54	S2	338	G
54	S2	340	C
54	S2	341	C
54	S2	342	C
54	S2	343	A
54	S2	346	C
54	S2	347	G
54	S2	350	C
54	S2	355	G
54	S2	356	C

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Mol	Chain	Res	Type
54	S2	357	C
54	S2	360	A
54	S2	361	U
54	S2	362	C
54	S2	364	A
54	S2	365	C
54	S2	366	U
54	S2	367	U
54	S2	368	U
54	S2	369	C
54	S2	370	G
54	S2	372	U
54	S2	373	G
54	S2	380	G
54	S2	381	C
54	S2	382	C
54	S2	383	G
54	S2	384	U
54	S2	385	G
54	S2	386	C
54	S2	387	C
54	S2	394	G
54	S2	395	G
54	S2	398	A
54	S2	399	C
54	S2	400	C
54	S2	401	A
54	S2	407	G
54	S2	408	A
54	S2	409	C
54	S2	411	G
54	S2	416	U
54	S2	417	C
54	S2	418	A
54	S2	419	G
54	S2	421	G
54	S2	422	U
54	S2	425	G
54	S2	426	A
54	S2	427	U
54	S2	428	U
54	S2	429	C

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Mol	Chain	Res	Type
54	S2	435	A
54	S2	436	G
54	S2	437	G
54	S2	438	G
54	S2	441	C
54	S2	442	C
54	S2	444	G
54	S2	445	A
54	S2	446	G
54	S2	447	A
54	S2	448	A
54	S2	449	A
54	S2	450	C
54	S2	453	C
54	S2	454	U
54	S2	455	A
54	S2	458	A
54	S2	459	C
54	S2	460	A
54	S2	464	A
54	S2	465	A
54	S2	466	G
54	S2	467	G
54	S2	469	A
54	S2	471	G
54	S2	472	C
54	S2	473	A
54	S2	474	G
54	S2	476	A
54	S2	482	G
54	S2	485	A
54	S2	487	U
54	S2	489	A
54	S2	492	C
54	S2	493	A
54	S2	496	C
54	S2	504	G
54	S2	507	G
54	S2	508	A
54	S2	516	A
54	S2	518	G
54	S2	523	A

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Mol	Chain	Res	Type
54	S2	525	A
54	S2	528	A
54	S2	530	U
54	S2	532	C
54	S2	533	A
54	S2	534	G
54	S2	540	U
54	S2	542	U
54	S2	544	G
54	S2	548	C
54	S2	549	C
54	S2	550	C
54	S2	551	U
54	S2	552	G
54	S2	554	A
54	S2	556	U
54	S2	557	U
54	S2	559	G
54	S2	560	A
54	S2	563	G
54	S2	564	A
54	S2	568	C
54	S2	569	A
54	S2	575	A
54	S2	576	A
54	S2	579	C
54	S2	580	U
54	S2	583	C
54	S2	588	G
54	S2	589	G
54	S2	590	A
54	S2	591	U
54	S2	592	C
54	S2	593	C
54	S2	595	U
54	S2	596	U
54	S2	597	G
54	S2	598	G
54	S2	600	G
54	S2	601	G
54	S2	602	G
54	S2	604	A

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Mol	Chain	Res	Type
54	S2	605	A
54	S2	607	U
54	S2	608	C
54	S2	612	U
54	S2	613	G
54	S2	614	C
54	S2	616	A
54	S2	617	G
54	S2	620	G
54	S2	621	C
54	S2	623	G
54	S2	624	C
54	S2	626	G
54	S2	627	U
54	S2	628	A
54	S2	629	A
54	S2	630	U
54	S2	631	U
54	S2	634	A
54	S2	639	C
54	S2	640	A
54	S2	642	U
54	S2	643	A
54	S2	644	G
54	S2	646	G
54	S2	647	U
54	S2	649	U
54	S2	651	U
54	S2	655	A
54	S2	656	G
54	S2	657	U
54	S2	660	C
54	S2	664	A
54	S2	666	U
54	S2	668	A
54	S2	669	A
54	S2	671	A
54	S2	672	A
54	S2	673	G
54	S2	679	A
54	S2	682	U
54	S2	683	G

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Mol	Chain	Res	Type
54	S2	684	G
54	S2	687	C
54	S2	688	U
54	S2	689	U
54	S2	690	G
54	S2	693	A
54	S2	694	G
54	S2	698	G
54	S2	731	G
54	S2	733	C
54	S2	735	C
54	S2	738	C
54	S2	739	C
54	S2	747	U
54	S2	748	C
54	S2	749	U
54	S2	751	G
54	S2	752	G
54	S2	753	C
54	S2	788	G
54	S2	791	C
54	S2	793	G
54	S2	794	A
54	S2	797	C
54	S2	798	A
54	S2	799	U
54	S2	800	U
54	S2	807	G
54	S2	810	A
54	S2	811	A
54	S2	812	A
54	S2	820	U
54	S2	821	G
54	S2	822	U
54	S2	825	A
54	S2	827	A
54	S2	830	A
54	S2	833	C
54	S2	834	C
54	S2	835	C
54	S2	836	G
54	S2	837	A

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Mol	Chain	Res	Type
54	S2	838	G
54	S2	839	C
54	S2	840	C
54	S2	841	G
54	S2	842	C
54	S2	843	C
54	S2	845	G
54	S2	846	G
54	S2	847	A
54	S2	848	U
54	S2	853	C
54	S2	859	G
54	S2	862	A
54	S2	864	A
54	S2	867	G
54	S2	868	G
54	S2	869	A
54	S2	870	A
54	S2	871	U
54	S2	872	A
54	S2	873	G
54	S2	875	A
54	S2	876	C
54	S2	877	C
54	S2	878	G
54	S2	879	C
54	S2	880	G
54	S2	881	G
54	S2	887	U
54	S2	888	U
54	S2	890	U
54	S2	891	G
54	S2	892	U
54	S2	893	U
54	S2	897	U
54	S2	898	U
54	S2	903	A
54	S2	913	A
54	S2	914	U
54	S2	918	U
54	S2	919	A
54	S2	920	A

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Mol	Chain	Res	Type
54	S2	921	G
54	S2	930	C
54	S2	933	G
54	S2	934	G
54	S2	938	A
54	S2	943	U
54	S2	946	U
54	S2	955	A
54	S2	956	G
54	S2	957	A
54	S2	958	G
54	S2	959	G
54	S2	960	U
54	S2	961	G
54	S2	962	A
54	S2	964	A
54	S2	965	U
54	S2	968	U
54	S2	969	U
54	S2	971	G
54	S2	974	C
54	S2	975	G
54	S2	979	C
54	S2	980	A
54	S2	981	A
54	S2	989	C
54	S2	990	A
54	S2	991	G
54	S2	992	A
54	S2	994	C
54	S2	996	A
54	S2	997	A
54	S2	999	G
54	S2	1001	A
54	S2	1002	U
54	S2	1008	A
54	S2	1016	U
54	S2	1017	U
54	S2	1023	A
54	S2	1024	A
54	S2	1030	A
54	S2	1033	G

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Mol	Chain	Res	Type
54	S2	1034	A
54	S2	1035	A
54	S2	1039	C
54	S2	1040	G
54	S2	1041	G
54	S2	1042	A
54	S2	1044	G
54	S2	1045	U
54	S2	1049	A
54	S2	1050	A
54	S2	1060	A
54	S2	1062	A
54	S2	1070	A
54	S2	1072	U
54	S2	1073	U
54	S2	1077	A
54	S2	1078	C
54	S2	1083	A
54	S2	1084	A
54	S2	1085	C
54	S2	1087	A
54	S2	1088	U
54	S2	1089	G
54	S2	1093	A
54	S2	1096	G
54	S2	1099	G
54	S2	1100	A
54	S2	1108	G
54	S2	1109	C
54	S2	1110	G
54	S2	1111	U
54	S2	1113	A
54	S2	1114	U
54	S2	1115	U
54	S2	1116	C
54	S2	1118	C
54	S2	1120	U
54	S2	1121	G
54	S2	1123	C
54	S2	1124	C
54	S2	1130	G
54	S2	1131	G

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Mol	Chain	Res	Type
54	S2	1133	A
54	S2	1138	C
54	S2	1139	C
54	S2	1143	A
54	S2	1144	A
54	S2	1146	C
54	S2	1148	A
54	S2	1149	A
54	S2	1150	A
54	S2	1151	G
54	S2	1153	C
54	S2	1154	U
54	S2	1157	G
54	S2	1165	G
54	S2	1166	G
54	S2	1180	C
54	S2	1182	A
54	S2	1191	C
54	S2	1194	A
54	S2	1195	A
54	S2	1199	A
54	S2	1200	A
54	S2	1201	U
54	S2	1203	G
54	S2	1204	A
54	S2	1205	C
54	S2	1206	G
54	S2	1207	G
54	S2	1208	A
54	S2	1210	G
54	S2	1211	G
54	S2	1214	A
54	S2	1215	C
54	S2	1216	C
54	S2	1217	A
54	S2	1221	G
54	S2	1222	G
54	S2	1224	G
54	S2	1234	C
54	S2	1240	A
54	S2	1242	U
54	S2	1243	U

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Mol	Chain	Res	Type
54	S2	1245	G
54	S2	1247	C
54	S2	1248	U
54	S2	1249	C
54	S2	1250	A
54	S2	1251	A
54	S2	1252	C
54	S2	1253	A
54	S2	1254	C
54	S2	1256	G
54	S2	1257	G
54	S2	1258	A
54	S2	1259	A
54	S2	1264	C
54	S2	1265	A
54	S2	1266	C
54	S2	1267	C
54	S2	1268	C
54	S2	1269	G
54	S2	1271	C
54	S2	1273	C
54	S2	1274	G
54	S2	1275	G
54	S2	1276	A
54	S2	1280	G
54	S2	1282	A
54	S2	1283	C
54	S2	1284	A
54	S2	1285	G
54	S2	1286	G
54	S2	1288	U
54	S2	1289	U
54	S2	1292	C
54	S2	1293	A
54	S2	1296	U
54	S2	1298	G
54	S2	1299	A
54	S2	1301	A
54	S2	1302	G
54	S2	1303	C
54	S2	1304	U
54	S2	1305	C

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Mol	Chain	Res	Type
54	S2	1306	U
54	S2	1308	U
54	S2	1309	C
54	S2	1312	G
54	S2	1313	A
54	S2	1314	U
54	S2	1315	U
54	S2	1316	C
54	S2	1322	G
54	S2	1324	G
54	S2	1326	U
54	S2	1331	C
54	S2	1332	A
54	S2	1337	C
54	S2	1339	U
54	S2	1340	U
54	S2	1341	C
54	S2	1342	U
54	S2	1343	U
54	S2	1344	A
54	S2	1345	G
54	S2	1347	U
54	S2	1348	G
54	S2	1349	G
54	S2	1351	G
54	S2	1352	G
54	S2	1353	A
54	S2	1354	G
54	S2	1355	C
54	S2	1356	G
54	S2	1357	A
54	S2	1358	U
54	S2	1364	U
54	S2	1367	U
54	S2	1368	U
54	S2	1370	A
54	S2	1371	U
54	S2	1372	U
54	S2	1373	C
54	S2	1374	C
54	S2	1378	A
54	S2	1379	A

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Mol	Chain	Res	Type
54	S2	1380	C
54	S2	1385	G
54	S2	1394	G
54	S2	1395	C
54	S2	1396	A
54	S2	1397	U
54	S2	1398	G
54	S2	1401	A
54	S2	1402	A
54	S2	1403	C
54	S2	1404	U
54	S2	1405	A
54	S2	1407	U
54	S2	1408	U
54	S2	1410	C
54	S2	1411	G
54	S2	1412	C
54	S2	1413	G
54	S2	1414	A
54	S2	1417	C
54	S2	1418	C
54	S2	1419	C
54	S2	1420	G
54	S2	1423	C
54	S2	1424	G
54	S2	1425	G
54	S2	1426	U
54	S2	1430	C
54	S2	1432	U
54	S2	1433	C
54	S2	1434	C
54	S2	1435	C
54	S2	1437	C
54	S2	1438	A
54	S2	1439	A
54	S2	1441	U
54	S2	1442	U
54	S2	1444	U
54	S2	1449	G
54	S2	1452	A
54	S2	1453	C
54	S2	1454	A

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Mol	Chain	Res	Type
54	S2	1455	A
54	S2	1462	U
54	S2	1463	U
54	S2	1464	C
54	S2	1465	A
54	S2	1466	G
54	S2	1473	G
54	S2	1475	G
54	S2	1476	A
54	S2	1477	U
54	S2	1478	U
54	S2	1488	C
54	S2	1489	A
54	S2	1490	G
54	S2	1493	C
54	S2	1494	U
54	S2	1495	G
54	S2	1496	U
54	S2	1497	G
54	S2	1501	C
54	S2	1507	G
54	S2	1508	A
54	S2	1509	U
54	S2	1510	G
54	S2	1511	U
54	S2	1512	C
54	S2	1513	C
54	S2	1514	G
54	S2	1515	G
54	S2	1520	G
54	S2	1521	C
54	S2	1522	A
54	S2	1523	C
54	S2	1525	C
54	S2	1527	C
54	S2	1531	A
54	S2	1533	A
54	S2	1534	C
54	S2	1535	U
54	S2	1537	A
54	S2	1540	G
54	S2	1541	G

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Mol	Chain	Res	Type
54	S2	1543	U
54	S2	1544	C
54	S2	1545	A
54	S2	1546	G
54	S2	1547	C
54	S2	1548	G
54	S2	1550	G
54	S2	1551	U
54	S2	1552	G
54	S2	1553	C
54	S2	1555	U
54	S2	1556	A
54	S2	1557	C
54	S2	1558	C
54	S2	1560	U
54	S2	1563	G
54	S2	1567	G
54	S2	1568	C
54	S2	1570	G
54	S2	1574	C
54	S2	1578	U
54	S2	1579	A
54	S2	1580	A
54	S2	1581	C
54	S2	1582	C
54	S2	1585	U
54	S2	1586	U
54	S2	1587	G
54	S2	1588	A
54	S2	1589	A
54	S2	1590	C
54	S2	1593	C
54	S2	1594	A
54	S2	1595	U
54	S2	1598	G
54	S2	1599	U
54	S2	1600	G
54	S2	1601	A
54	S2	1602	U
54	S2	1604	G
54	S2	1606	G
54	S2	1607	A

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Mol	Chain	Res	Type
54	S2	1609	C
54	S2	1610	G
54	S2	1621	U
54	S2	1622	U
54	S2	1623	A
54	S2	1625	U
54	S2	1632	G
54	S2	1633	A
54	S2	1634	A
54	S2	1637	A
54	S2	1638	G
54	S2	1641	A
54	S2	1644	C
54	S2	1645	C
54	S2	1646	C
54	S2	1647	A
54	S2	1648	G
54	S2	1649	U
54	S2	1654	G
54	S2	1659	U
54	S2	1660	C
54	S2	1663	A
54	S2	1664	A
54	S2	1665	G
54	S2	1666	C
54	S2	1667	U
54	S2	1668	U
54	S2	1669	G
54	S2	1674	G
54	S2	1679	A
54	S2	1680	G
54	S2	1682	C
54	S2	1683	C
54	S2	1684	C
54	S2	1688	C
54	S2	1689	C
54	S2	1695	A
54	S2	1698	C
54	S2	1700	C
54	S2	1701	C
54	S2	1702	G
54	S2	1714	U

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Mol	Chain	Res	Type
54	S2	1720	U
54	S2	1721	U
54	S2	1722	G
54	S2	1724	A
54	S2	1725	U
54	S2	1729	U
54	S2	1730	U
54	S2	1734	G
54	S2	1737	G
54	S2	1745	A
54	S2	1746	U
54	S2	1751	C
54	S2	1753	C
54	S2	1757	G
54	S2	1760	G
54	S2	1761	U
54	S2	1779	G
54	S2	1783	C
54	S2	1784	G
54	S2	1785	C
54	S2	1786	U
54	S2	1792	G
54	S2	1795	G
54	S2	1797	U
54	S2	1798	C
54	S2	1805	G
54	S2	1810	U
54	S2	1817	G
54	S2	1819	A
54	S2	1823	A
54	S2	1824	A
54	S2	1825	A
54	S2	1826	G
54	S2	1827	U
54	S2	1831	A
54	S2	1835	A
54	S2	1836	G
54	S2	1838	U
54	S2	1839	U
54	S2	1840	U
54	S2	1841	C
54	S2	1844	U

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Mol	Chain	Res	Type
54	S2	1847	G
54	S2	1850	A
54	S2	1852	C
54	S2	1860	A
54	S2	1861	G
54	S2	1862	G
54	S2	1863	A
54	S2	1864	U
54	S2	1865	C
54	S2	1868	U
54	S2	1869	A

All (1029) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
32	5	1	C
32	5	20	U
32	5	33	A
32	5	36	U
32	5	37	U
32	5	42	A
32	5	43	U
32	5	47	A
32	5	48	G
32	5	52	G
32	5	53	C
32	5	54	G
32	5	55	G
32	5	62	A
32	5	64	A
32	5	65	A
32	5	68	U
32	5	82	U
32	5	84	A
32	5	88	A
32	5	92	C
32	5	93	G
32	5	94	A
32	5	96	U
32	5	97	G
32	5	98	A
32	5	99	A

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Mol	Chain	Res	Type
32	5	100	C
32	5	107	G
32	5	111	C
32	5	112	C
32	5	117	C
32	5	119	G
32	5	120	A
32	5	123	C
32	5	124	C
32	5	125	C
32	5	134	G
32	5	143	C
32	5	150	U
32	5	151	G
32	5	163	A
32	5	165	A
32	5	170	C
32	5	172	C
32	5	183	C
32	5	187	U
32	5	194	C
32	5	197	A
32	5	207	G
32	5	209	U
32	5	212	A
32	5	216	C
32	5	218	A
32	5	219	G
32	5	226	G
32	5	237	G
32	5	245	C
32	5	252	C
32	5	253	G
32	5	265	C
32	5	266	C
32	5	268	G
32	5	274	C
32	5	275	C
32	5	276	C
32	5	278	G
32	5	280	G
32	5	292	G

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Mol	Chain	Res	Type
32	5	293	G
32	5	296	A
32	5	297	U
32	5	308	G
32	5	315	G
32	5	333	U
32	5	340	C
32	5	349	A
32	5	353	A
32	5	360	A
32	5	361	C
32	5	362	A
32	5	364	G
32	5	371	A
32	5	385	A
32	5	394	G
32	5	406	C
32	5	407	A
32	5	411	G
32	5	414	C
32	5	417	G
32	5	421	C
32	5	432	U
32	5	435	A
32	5	450	G
32	5	451	C
32	5	454	U
32	5	465	G
32	5	480	C
32	5	485	C
32	5	486	C
32	5	493	G
32	5	495	C
32	5	497	G
32	5	502	C
32	5	505	G
32	5	514	U
32	5	647	G
32	5	648	G
32	5	658	C
32	5	659	G
32	5	664	G

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Mol	Chain	Res	Type
32	5	666	G
32	5	668	C
32	5	673	C
32	5	684	G
32	5	686	A
32	5	693	C
32	5	700	G
32	5	727	C
32	5	728	U
32	5	732	A
32	5	733	A
32	5	738	C
32	5	746	A
32	5	747	A
32	5	911	U
32	5	917	A
32	5	920	C
32	5	922	C
32	5	927	G
32	5	930	G
32	5	931	C
32	5	932	A
32	5	936	C
32	5	943	A
32	5	956	A
32	5	957	G
32	5	958	G
32	5	961	G
32	5	965	G
32	5	968	C
32	5	970	G
32	5	974	C
32	5	977	C
32	5	978	G
32	5	979	C
32	5	981	C
32	5	989	U
32	5	1067	G
32	5	1068	G
32	5	1069	G
32	5	1074	G
32	5	1076	C

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Mol	Chain	Res	Type
32	5	1172	C
32	5	1179	U
32	5	1186	U
32	5	1188	C
32	5	1210	C
32	5	1211	G
32	5	1214	C
32	5	1216	C
32	5	1217	G
32	5	1221	G
32	5	1232	G
32	5	1235	G
32	5	1236	C
32	5	1237	C
32	5	1238	A
32	5	1239	C
32	5	1241	C
32	5	1243	C
32	5	1254	A
32	5	1264	C
32	5	1266	G
32	5	1268	G
32	5	1274	A
32	5	1279	A
32	5	1280	C
32	5	1281	G
32	5	1292	C
32	5	1293	G
32	5	1296	G
32	5	1301	C
32	5	1319	U
32	5	1322	A
32	5	1324	A
32	5	1325	C
32	5	1329	G
32	5	1338	G
32	5	1355	G
32	5	1356	U
32	5	1357	C
32	5	1359	G
32	5	1364	U
32	5	1365	C

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Mol	Chain	Res	Type
32	5	1368	A
32	5	1370	G
32	5	1371	A
32	5	1377	G
32	5	1378	C
32	5	1379	C
32	5	1380	G
32	5	1385	G
32	5	1386	C
32	5	1397	A
32	5	1405	C
32	5	1406	G
32	5	1407	C
32	5	1409	C
32	5	1410	U
32	5	1419	G
32	5	1420	A
32	5	1435	G
32	5	1438	U
32	5	1439	C
32	5	1440	U
32	5	1445	U
32	5	1455	G
32	5	1464	C
32	5	1474	C
32	5	1478	C
32	5	1479	G
32	5	1480	C
32	5	1481	C
32	5	1483	C
32	5	1484	G
32	5	1488	G
32	5	1489	G
32	5	1497	A
32	5	1500	A
32	5	1501	C
32	5	1509	C
32	5	1518	A
32	5	1520	C
32	5	1521	C
32	5	1522	G
32	5	1533	A

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Mol	Chain	Res	Type
32	5	1534	A
32	5	1539	G
32	5	1554	A
32	5	1555	G
32	5	1596	U
32	5	1609	U
32	5	1611	C
32	5	1614	C
32	5	1615	C
32	5	1617	G
32	5	1627	G
32	5	1632	A
32	5	1633	G
32	5	1636	U
32	5	1637	A
32	5	1639	U
32	5	1654	G
32	5	1671	U
32	5	1681	G
32	5	1682	A
32	5	1691	G
32	5	1696	C
32	5	1697	G
32	5	1724	G
32	5	1725	U
32	5	1733	G
32	5	1734	G
32	5	1742	A
32	5	1745	G
32	5	1763	C
32	5	1764	G
32	5	1788	A
32	5	1790	U
32	5	1793	A
32	5	1804	A
32	5	1808	C
32	5	1819	G
32	5	1820	C
32	5	1822	U
32	5	1835	G
32	5	1847	C
32	5	1864	G

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Mol	Chain	Res	Type
32	5	1876	U
32	5	1881	C
32	5	1884	C
32	5	1886	G
32	5	1887	G
32	5	1890	G
32	5	1891	A
32	5	1919	G
32	5	1920	C
32	5	1921	C
32	5	1925	G
32	5	1928	C
32	5	1930	U
32	5	1934	A
32	5	1935	C
32	5	1938	C
32	5	1941	A
32	5	1945	G
32	5	1946	G
32	5	1947	U
32	5	1959	U
32	5	1964	A
32	5	1975	G
32	5	1980	U
32	5	1986	U
32	5	1992	U
32	5	2007	G
32	5	2008	U
32	5	2009	A
32	5	2014	C
32	5	2034	G
32	5	2035	C
32	5	2046	G
32	5	2054	U
32	5	2057	A
32	5	2068	C
32	5	2075	G
32	5	2076	G
32	5	2077	C
32	5	2079	G
32	5	2083	C
32	5	2087	C

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Mol	Chain	Res	Type
32	5	2088	A
32	5	2089	G
32	5	2093	A
32	5	2096	G
32	5	2107	C
32	5	2111	G
32	5	2114	G
32	5	2116	C
32	5	2118	G
32	5	2119	C
32	5	2122	G
32	5	2123	C
32	5	2124	G
32	5	2126	G
32	5	2246	C
32	5	2249	C
32	5	2251	G
32	5	2256	C
32	5	2257	C
32	5	2260	C
32	5	2261	G
32	5	2262	G
32	5	2264	C
32	5	2265	G
32	5	2266	C
32	5	2268	A
32	5	2272	C
32	5	2276	A
32	5	2278	G
32	5	2311	C
32	5	2313	A
32	5	2315	G
32	5	2321	G
32	5	2323	C
32	5	2324	C
32	5	2328	G
32	5	2331	G
32	5	2332	A
32	5	2333	G
32	5	2347	A
32	5	2351	C
32	5	2361	G

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Mol	Chain	Res	Type
32	5	2362	U
32	5	2369	U
32	5	2378	G
32	5	2389	A
32	5	2394	G
32	5	2396	A
32	5	2398	U
32	5	2436	U
32	5	2438	A
32	5	2442	G
32	5	2446	C
32	5	2448	G
32	5	2451	A
32	5	2459	G
32	5	2464	C
32	5	2468	U
32	5	2470	C
32	5	2474	G
32	5	2479	G
32	5	2487	G
32	5	2490	U
32	5	2502	G
32	5	2507	A
32	5	2509	C
32	5	2512	A
32	5	2515	G
32	5	2517	A
32	5	2523	G
32	5	2533	C
32	5	2544	G
32	5	2545	U
32	5	2546	G
32	5	2553	A
32	5	2554	U
32	5	2576	G
32	5	2587	A
32	5	2588	C
32	5	2589	C
32	5	2600	A
32	5	2613	C
32	5	2614	C
32	5	2618	G

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Mol	Chain	Res	Type
32	5	2631	U
32	5	2658	G
32	5	2661	U
32	5	2665	U
32	5	2666	U
32	5	2673	G
32	5	2674	A
32	5	2675	G
32	5	2686	G
32	5	2688	G
32	5	2695	A
32	5	2708	U
32	5	2711	G
32	5	2732	G
32	5	2733	C
32	5	2735	G
32	5	2739	C
32	5	2744	A
32	5	2745	A
32	5	2757	A
32	5	2761	U
32	5	2768	C
32	5	2769	U
32	5	2782	U
32	5	2787	A
32	5	2796	G
32	5	2806	A
32	5	2811	G
32	5	2812	A
32	5	2817	C
32	5	2825	A
32	5	2827	G
32	5	2828	U
32	5	2837	U
32	5	2840	A
32	5	2841	G
32	5	2848	G
32	5	2851	G
32	5	2854	G
32	5	2857	A
32	5	2867	C
32	5	2879	A

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Mol	Chain	Res	Type
32	5	2896	G
32	5	2902	G
32	5	3590	G
32	5	3593	C
32	5	3615	G
32	5	3620	G
32	5	3622	C
32	5	3625	G
32	5	3626	G
32	5	3636	C
32	5	3644	U
32	5	3648	A
32	5	3652	A
32	5	3653	A
32	5	3654	G
32	5	3663	A
32	5	3666	C
32	5	3667	C
32	5	3671	G
32	5	3676	G
32	5	3679	U
32	5	3692	A
32	5	3697	U
32	5	3712	A
32	5	3719	A
32	5	3727	A
32	5	3729	U
32	5	3730	U
32	5	3734	U
32	5	3735	G
32	5	3754	G
32	5	3773	U
32	5	3774	A
32	5	3776	G
32	5	3784	A
32	5	3791	C
32	5	3802	U
32	5	3803	A
32	5	3809	G
32	5	3812	C
32	5	3817	A
32	5	3827	G

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Mol	Chain	Res	Type
32	5	3829	G
32	5	3839	G
32	5	3854	C
32	5	3860	A
32	5	3875	G
32	5	3876	A
32	5	3877	A
32	5	3879	G
32	5	3888	G
32	5	3904	G
32	5	3905	A
32	5	3906	A
32	5	3908	A
32	5	3909	C
32	5	3911	C
32	5	3912	U
32	5	3914	U
32	5	3922	G
32	5	3941	G
32	5	3944	G
32	5	4069	U
32	5	4074	C
32	5	4075	U
32	5	4078	C
32	5	4084	G
32	5	4091	G
32	5	4092	G
32	5	4095	G
32	5	4103	C
32	5	4104	G
32	5	4115	G
32	5	4117	U
32	5	4118	U
32	5	4119	C
32	5	4121	G
32	5	4122	G
32	5	4124	G
32	5	4127	A
32	5	4143	G
32	5	4144	C
32	5	4163	U
32	5	4165	C

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Mol	Chain	Res	Type
32	5	4170	A
32	5	4173	G
32	5	4195	G
32	5	4217	G
32	5	4219	A
32	5	4221	C
32	5	4227	U
32	5	4228	G
32	5	4229	U
32	5	4232	U
32	5	4233	A
32	5	4238	G
32	5	4239	A
32	5	4251	A
32	5	4254	G
32	5	4257	A
32	5	4270	C
32	5	4275	G
32	5	4276	G
32	5	4279	A
32	5	4280	A
32	5	4282	A
32	5	4283	G
32	5	4295	U
32	5	4297	G
32	5	4322	G
32	5	4336	A
32	5	4342	C
32	5	4348	A
32	5	4349	C
32	5	4368	G
32	5	4374	U
32	5	4375	C
32	5	4378	A
32	5	4379	A
32	5	4385	A
32	5	4395	U
32	5	4399	U
32	5	4419	U
32	5	4436	U
32	5	4440	G
32	5	4448	G

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Mol	Chain	Res	Type
32	5	4449	A
32	5	4450	U
32	5	4451	G
32	5	4452	U
32	5	4454	G
32	5	4463	U
32	5	4464	A
32	5	4474	A
32	5	4475	G
32	5	4479	A
32	5	4488	A
32	5	4489	G
32	5	4497	U
32	5	4501	U
32	5	4507	A
32	5	4519	C
32	5	4522	G
32	5	4527	G
32	5	4528	G
32	5	4532	U
32	5	4533	A
32	5	4535	A
32	5	4536	C
32	5	4543	G
32	5	4548	A
32	5	4574	U
32	5	4583	C
32	5	4600	G
32	5	4605	A
32	5	4610	A
32	5	4626	A
32	5	4634	U
32	5	4656	A
32	5	4670	C
32	5	4691	A
32	5	4693	C
32	5	4699	U
32	5	4700	A
32	5	4709	U
32	5	4718	G
32	5	4719	G
32	5	4730	C

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Mol	Chain	Res	Type
32	5	4731	G
32	5	4733	C
32	5	4735	G
32	5	4736	C
32	5	4737	G
32	5	4739	C
32	5	4740	G
32	5	4741	C
32	5	4756	C
32	5	4757	C
32	5	4763	U
32	5	4770	U
32	5	4871	C
32	5	4872	G
32	5	4873	G
32	5	4874	A
32	5	4884	G
32	5	4885	U
32	5	4887	C
32	5	4888	U
32	5	4889	G
32	5	4900	C
32	5	4911	A
32	5	4912	G
32	5	4926	C
32	5	4935	C
32	5	4938	A
32	5	4945	G
32	5	4948	C
32	5	4949	G
32	5	4950	U
32	5	4951	G
32	5	4981	G
32	5	4990	C
32	5	4991	U
32	5	4996	C
32	5	4997	G
32	5	5001	U
32	5	5002	U
32	5	5006	U
32	5	5022	U
32	5	5041	G

*Continued on next page...*



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Mol	Chain	Res	Type
32	5	5043	A
32	5	5045	G
32	5	5046	U
32	5	5049	G
32	5	5050	C
32	5	5056	A
32	5	5060	A
32	5	5061	A
32	5	5062	G
33	7	7	G
33	7	21	G
33	7	26	C
33	7	39	C
33	7	41	G
33	7	42	A
33	7	49	A
33	7	56	G
33	7	57	C
33	7	58	A
33	7	59	G
33	7	60	G
33	7	72	U
33	7	75	G
33	7	82	G
34	8	2	G
34	8	9	A
34	8	10	G
34	8	11	C
34	8	22	U
34	8	34	U
34	8	35	C
34	8	37	A
34	8	51	U
34	8	60	G
34	8	64	U
34	8	70	G
34	8	73	U
34	8	81	C
34	8	82	A
34	8	83	C
34	8	85	U
34	8	94	G

*Continued on next page...*

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Mol	Chain	Res	Type
34	8	95	A
34	8	109	C
34	8	110	U
34	8	111	U
34	8	113	C
34	8	115	G
34	8	116	C
34	8	124	U
34	8	125	C
34	8	126	C
34	8	130	C
34	8	131	G
50	3	9	A
50	3	17	G
50	3	19	U
50	3	60	A
50	3	75	C
51	4	10	G
51	4	35	U
51	4	37	C
51	4	38	U
51	4	39	C
51	4	45	G
51	4	47	U
51	4	176	A
51	4	234	A
51	4	235	G
54	S2	2	A
54	S2	3	C
54	S2	9	U
54	S2	19	A
54	S2	25	A
54	S2	27	A
54	S2	37	C
54	S2	55	U
54	S2	61	A
54	S2	65	C
54	S2	67	C
54	S2	72	C
54	S2	73	C
54	S2	74	G
54	S2	91	A

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Mol	Chain	Res	Type
54	S2	98	C
54	S2	102	A
54	S2	104	A
54	S2	105	U
54	S2	110	U
54	S2	113	G
54	S2	126	G
54	S2	127	C
54	S2	139	C
54	S2	140	C
54	S2	141	A
54	S2	158	A
54	S2	160	U
54	S2	163	U
54	S2	171	A
54	S2	180	G
54	S2	181	A
54	S2	182	C
54	S2	183	G
54	S2	190	G
54	S2	215	G
54	S2	291	G
54	S2	294	U
54	S2	297	A
54	S2	305	U
54	S2	312	G
54	S2	313	A
54	S2	325	C
54	S2	327	G
54	S2	334	C
54	S2	340	C
54	S2	357	C
54	S2	360	A
54	S2	366	U
54	S2	367	U
54	S2	368	U
54	S2	369	C
54	S2	376	A
54	S2	377	G
54	S2	384	U
54	S2	393	U
54	S2	394	G

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Mol	Chain	Res	Type
54	S2	398	A
54	S2	399	C
54	S2	402	C
54	S2	409	C
54	S2	413	G
54	S2	421	G
54	S2	426	A
54	S2	428	U
54	S2	437	G
54	S2	442	C
54	S2	443	U
54	S2	444	G
54	S2	446	G
54	S2	447	A
54	S2	448	A
54	S2	452	G
54	S2	453	C
54	S2	457	C
54	S2	465	A
54	S2	468	A
54	S2	470	G
54	S2	473	A
54	S2	474	G
54	S2	499	G
54	S2	505	G
54	S2	515	G
54	S2	532	C
54	S2	550	C
54	S2	559	G
54	S2	577	U
54	S2	578	C
54	S2	579	C
54	S2	596	U
54	S2	604	A
54	S2	607	U
54	S2	608	C
54	S2	613	G
54	S2	617	G
54	S2	639	C
54	S2	641	A
54	S2	642	U
54	S2	643	A

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Mol	Chain	Res	Type
54	S2	645	C
54	S2	649	U
54	S2	650	A
54	S2	656	G
54	S2	687	C
54	S2	688	U
54	S2	732	U
54	S2	734	C
54	S2	746	C
54	S2	747	U
54	S2	752	G
54	S2	797	C
54	S2	798	A
54	S2	799	U
54	S2	800	U
54	S2	802	A
54	S2	807	G
54	S2	810	A
54	S2	811	A
54	S2	815	U
54	S2	818	A
54	S2	821	G
54	S2	822	U
54	S2	829	C
54	S2	833	C
54	S2	841	G
54	S2	842	C
54	S2	868	G
54	S2	870	A
54	S2	871	U
54	S2	875	A
54	S2	913	A
54	S2	914	U
54	S2	918	U
54	S2	919	A
54	S2	920	A
54	S2	924	G
54	S2	955	A
54	S2	959	G
54	S2	960	U
54	S2	962	A
54	S2	964	A

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Mol	Chain	Res	Type
54	S2	967	C
54	S2	968	U
54	S2	975	G
54	S2	980	A
54	S2	991	G
54	S2	993	G
54	S2	999	G
54	S2	1001	A
54	S2	1016	U
54	S2	1036	A
54	S2	1037	G
54	S2	1050	A
54	S2	1063	C
54	S2	1087	A
54	S2	1088	U
54	S2	1092	G
54	S2	1093	A
54	S2	1096	G
54	S2	1098	C
54	S2	1099	G
54	S2	1107	G
54	S2	1109	C
54	S2	1110	G
54	S2	1113	A
54	S2	1114	U
54	S2	1115	U
54	S2	1121	G
54	S2	1132	C
54	S2	1137	U
54	S2	1141	G
54	S2	1142	G
54	S2	1153	C
54	S2	1165	G
54	S2	1194	A
54	S2	1199	A
54	S2	1204	A
54	S2	1207	G
54	S2	1221	G
54	S2	1223	A
54	S2	1224	G
54	S2	1225	U
54	S2	1226	G

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Mol	Chain	Res	Type
54	S2	1244	U
54	S2	1247	C
54	S2	1249	C
54	S2	1250	A
54	S2	1253	A
54	S2	1265	A
54	S2	1273	C
54	S2	1274	G
54	S2	1283	C
54	S2	1288	U
54	S2	1289	U
54	S2	1292	C
54	S2	1298	G
54	S2	1302	G
54	S2	1312	G
54	S2	1313	A
54	S2	1315	U
54	S2	1341	C
54	S2	1342	U
54	S2	1350	U
54	S2	1352	G
54	S2	1355	C
54	S2	1362	U
54	S2	1363	C
54	S2	1367	U
54	S2	1368	U
54	S2	1370	A
54	S2	1372	U
54	S2	1373	C
54	S2	1378	A
54	S2	1379	A
54	S2	1386	A
54	S2	1391	C
54	S2	1395	C
54	S2	1396	A
54	S2	1401	A
54	S2	1418	C
54	S2	1419	C
54	S2	1421	A
54	S2	1423	C
54	S2	1429	G
54	S2	1430	C

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Mol	Chain	Res	Type
54	S2	1433	C
54	S2	1438	A
54	S2	1440	C
54	S2	1441	U
54	S2	1442	U
54	S2	1446	A
54	S2	1452	A
54	S2	1454	A
54	S2	1462	U
54	S2	1463	U
54	S2	1474	A
54	S2	1475	G
54	S2	1477	U
54	S2	1480	A
54	S2	1488	C
54	S2	1489	A
54	S2	1495	G
54	S2	1512	C
54	S2	1515	G
54	S2	1521	C
54	S2	1522	A
54	S2	1524	G
54	S2	1533	A
54	S2	1534	C
54	S2	1537	A
54	S2	1540	G
54	S2	1543	U
54	S2	1546	G
54	S2	1551	U
54	S2	1552	G
54	S2	1556	A
54	S2	1568	C
54	S2	1571	G
54	S2	1578	U
54	S2	1579	A
54	S2	1581	C
54	S2	1591	C
54	S2	1597	C
54	S2	1598	G
54	S2	1599	U
54	S2	1601	A
54	S2	1603	G

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Mol	Chain	Res	Type
54	S2	1605	G
54	S2	1617	G
54	S2	1621	U
54	S2	1623	A
54	S2	1629	C
54	S2	1637	A
54	S2	1639	G
54	S2	1641	A
54	S2	1644	C
54	S2	1645	C
54	S2	1657	G
54	S2	1659	U
54	S2	1664	A
54	S2	1668	U
54	S2	1678	A
54	S2	1679	A
54	S2	1682	C
54	S2	1695	A
54	S2	1697	A
54	S2	1700	C
54	S2	1726	G
54	S2	1804	U
54	S2	1821	U
54	S2	1823	A
54	S2	1824	A
54	S2	1825	A
54	S2	1826	G
54	S2	1830	U
54	S2	1837	G
54	S2	1838	U
54	S2	1843	G
54	S2	1849	G
54	S2	1857	G
54	S2	1858	G
54	S2	1863	A
54	S2	1868	U

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

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 170 ligands modelled in this entry, 170 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
32	5	16
54	S2	6
48	z	5
51	4	3
50	3	3
46	K	2
49	2	1
37	E	1
89	S4	1
53	6	1
84	Sc	1
11	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	298:C	O3'	114:G	P	140.85

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	85:LEU	C	109:LEU	N	48.29
1	z	297:MET	C	326:GLN	N	33.03
1	E	72:ALA	C	84:VAL	N	24.28
1	S2	753:C	O3'	785:C	P	22.70
1	z	434:MET	C	455:UNK	N	20.61
1	S2	698:G	O3'	730:C	P	20.30
1	5	4776:G	O3'	4859:C	P	17.65
1	5	757:G	O3'	906:C	P	17.08
1	5	519:C	O3'	642:G	P	16.81
1	5	2910:G	O3'	3583:U	P	16.80
1	4	65:U	O3'	282:U	P	15.74
1	5	2131:C	O3'	2243:C	P	14.84
1	z	465:UNK	C	477:UNK	N	14.59
1	5	3950:U	O3'	4065:G	P	13.89
1	S4	35:GLY	C	54:ASN	N	13.11
1	5	997:C	O3'	1047:C	P	13.04
1	6	91:ASN	C	108:ASP	N	12.86
1	5	5023:C	O3'	5028:G	P	12.61
1	5	1051:G	O3'	1064:G	P	9.59
1	S2	739:C	O3'	744:G	P	7.80
1	S2	225:G	O3'	287:U	P	7.53
1	5	1699:A	O3'	1718:C	P	4.22
1	5	1222:A	O3'	1232:G	P	4.18
1	3	46:G	O3'	47:U	P	3.74
1	5	4939:C	O3'	4941:G	P	3.43
1	5	1100:U	O3'	1167:C	P	3.38
1	5	4942:C	O3'	4944:C	P	3.33
1	K	154:ASP	C	155:ILE	N	2.99
1	S2	1690:U	O3'	1691:U	P	2.73
1	5	1840:G	O3'	1842:G	P	2.69
1	3	56:C	O3'	57:G	P	2.58
1	S2	1686:G	O3'	1687:C	P	2.41
1	Sc	54:ASP	C	55:VAL	N	2.23
1	5	1823:G	O3'	1825:A	P	2.03
1	z	340:MET	C	341:LYS	N	1.86
1	R	149:LYS	C	150:ALA	N	1.67
1	K	9:GLU	C	10:ILE	N	1.11
1	4	183:A	O3'	184:A	P	1.08
1	z	345:PHE	C	346:SER	N	0.91
1	3	31:C	O3'	32:C	P	0.86

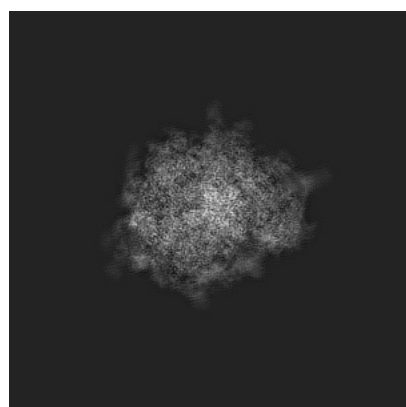
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3037. These allow visual inspection of the internal detail of the map and identification of artifacts.

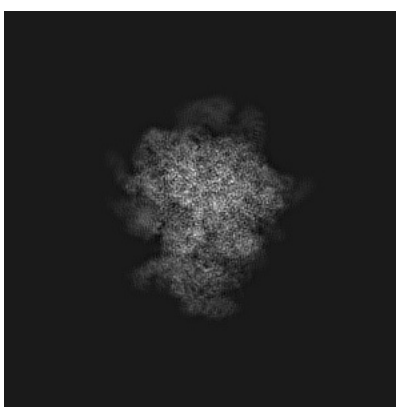
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

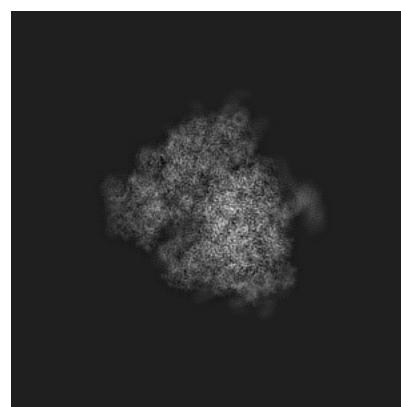
#### 6.1.1 Primary map



X



Y

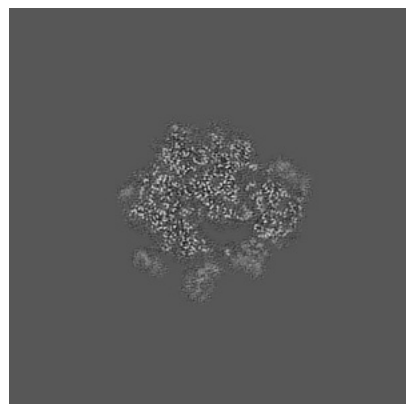


Z

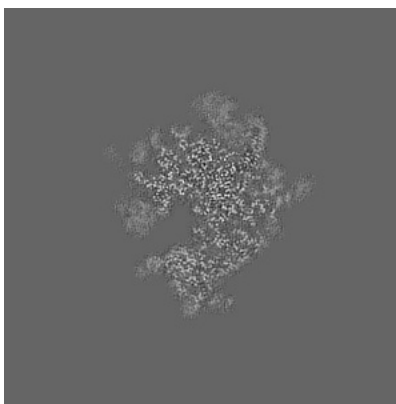
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

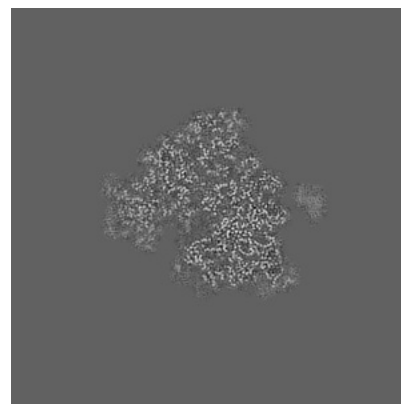
#### 6.2.1 Primary map



X Index: 210



Y Index: 210

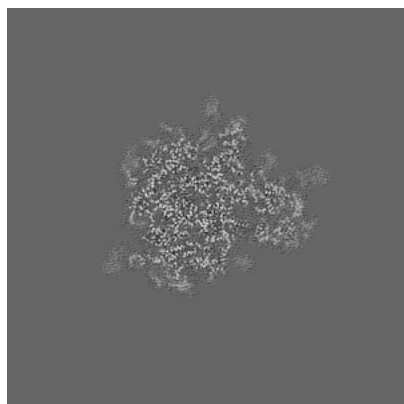


Z Index: 210

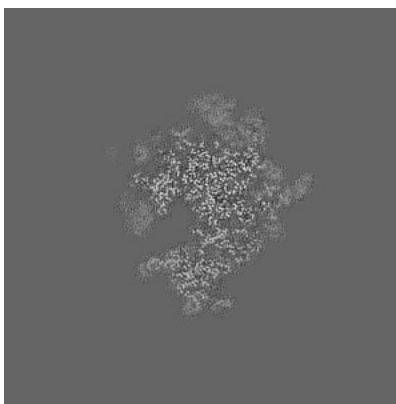
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

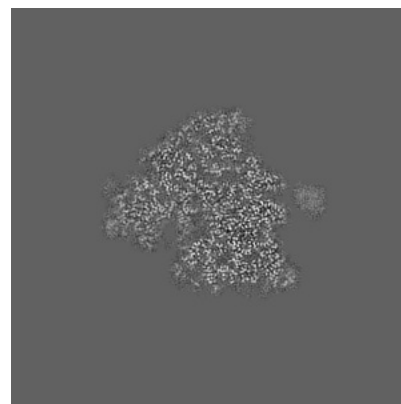
### 6.3.1 Primary map



X Index: 234



Y Index: 212

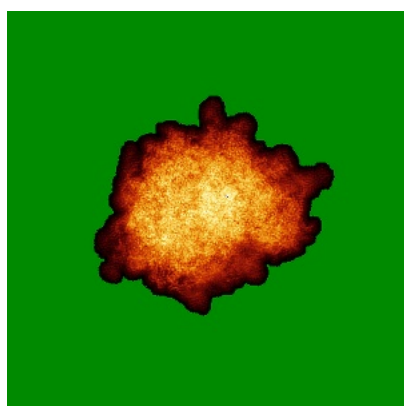


Z Index: 208

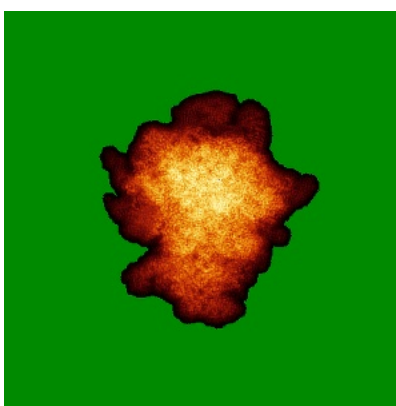
The images above show the largest variance slices of the map in three orthogonal directions.

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

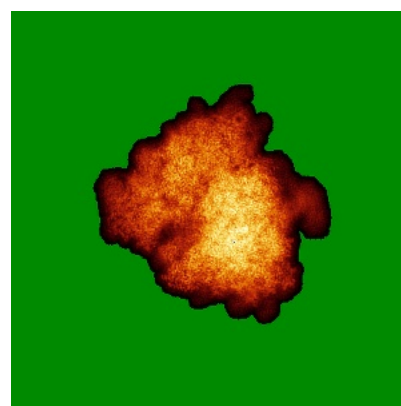
### 6.4.1 Primary map



X



Y

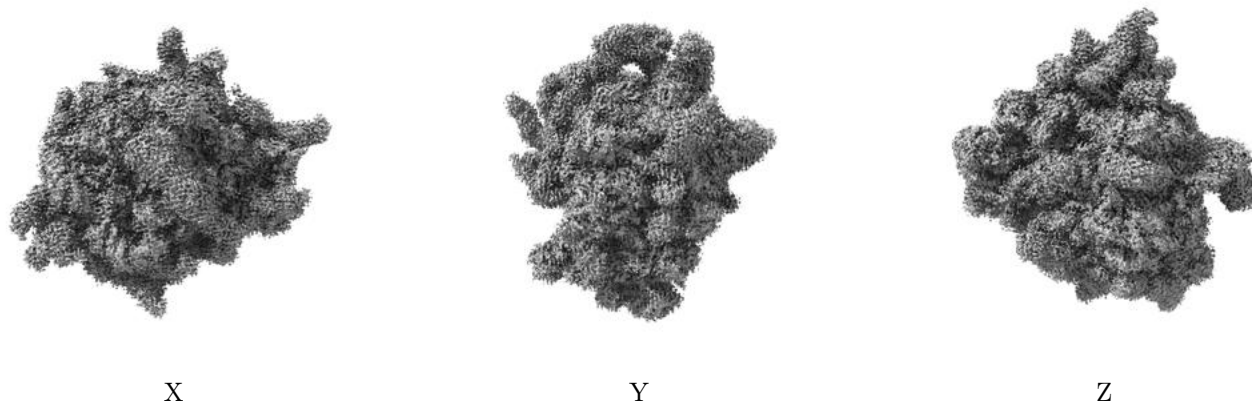


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

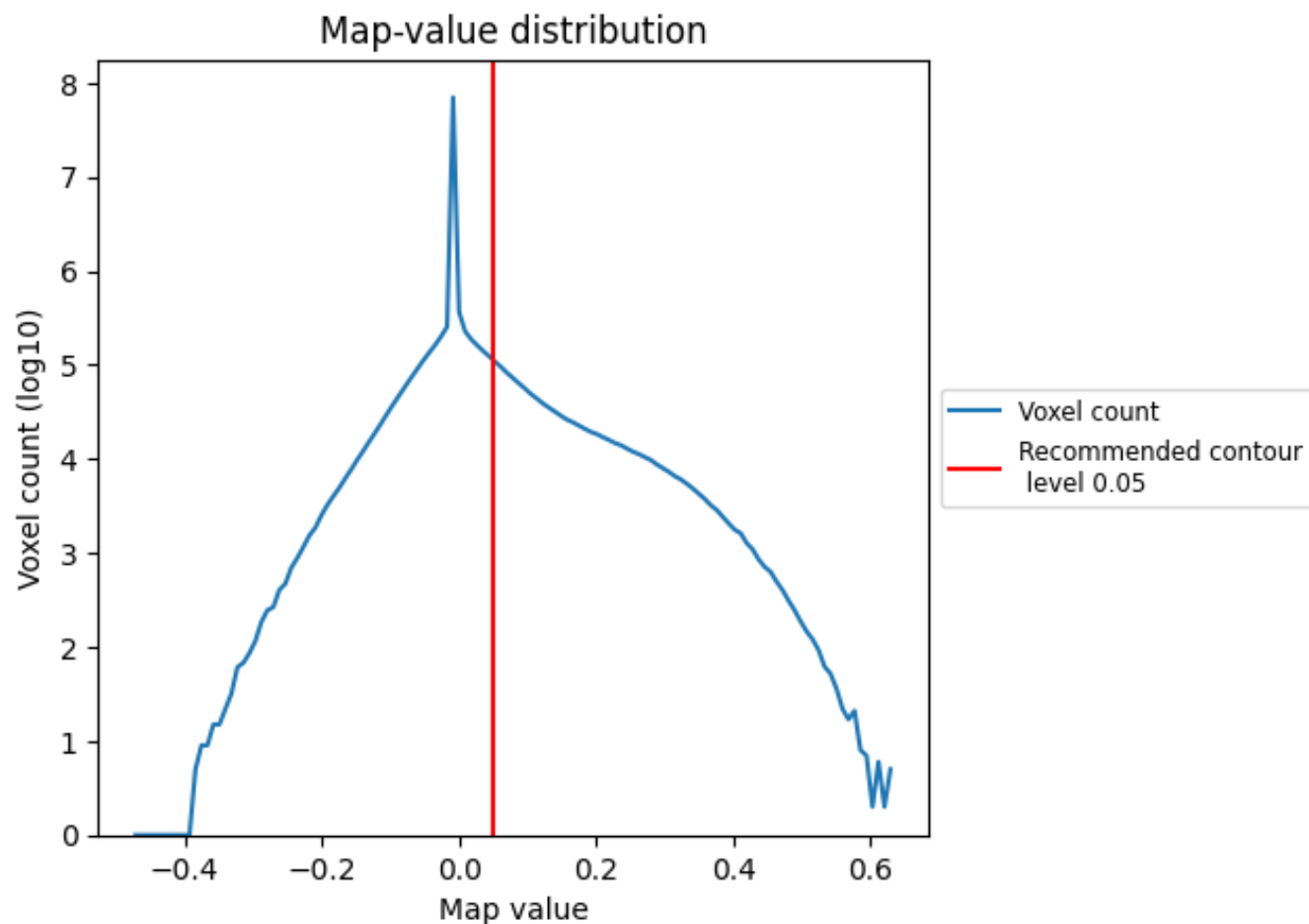
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

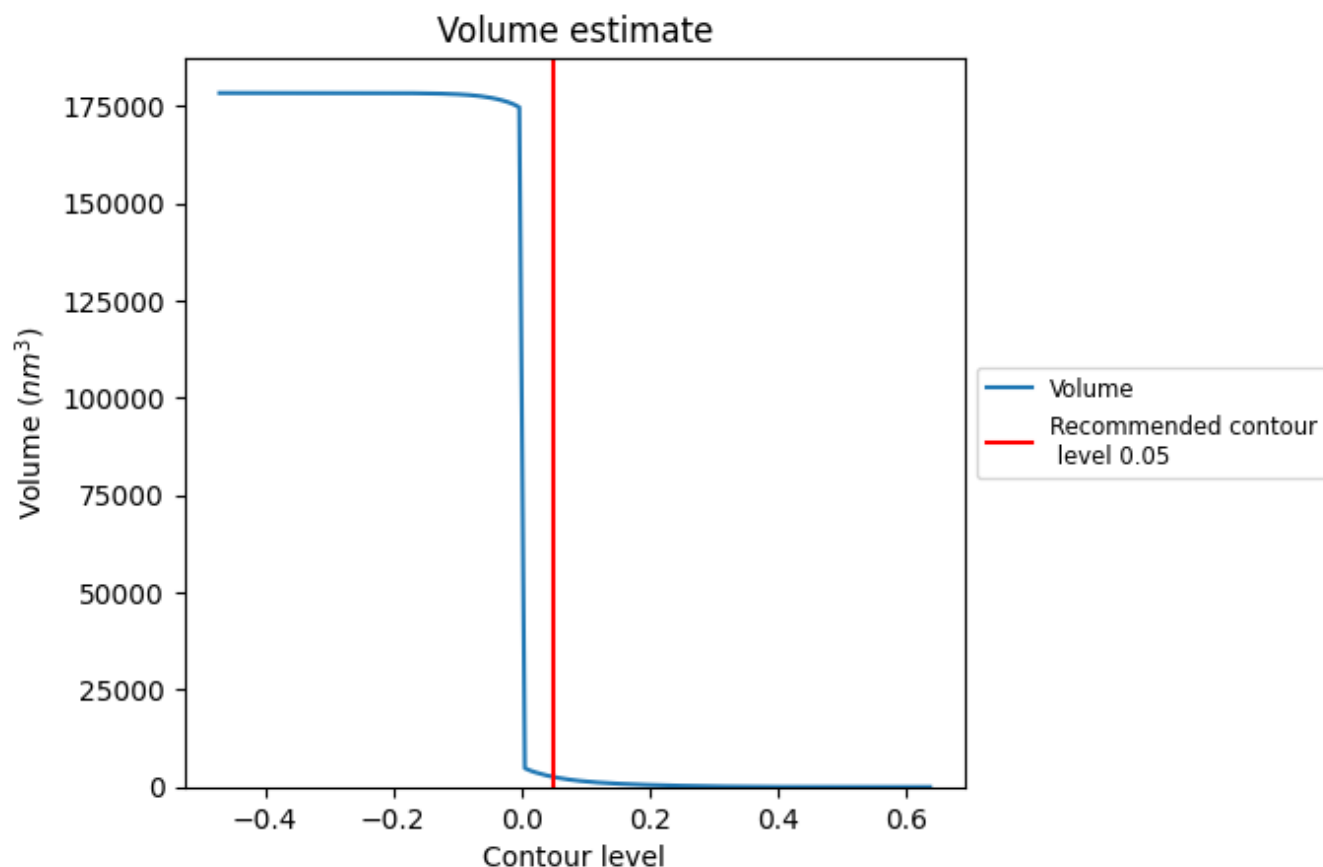
This section contains the results of statistical analysis of the map.

### 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](#)

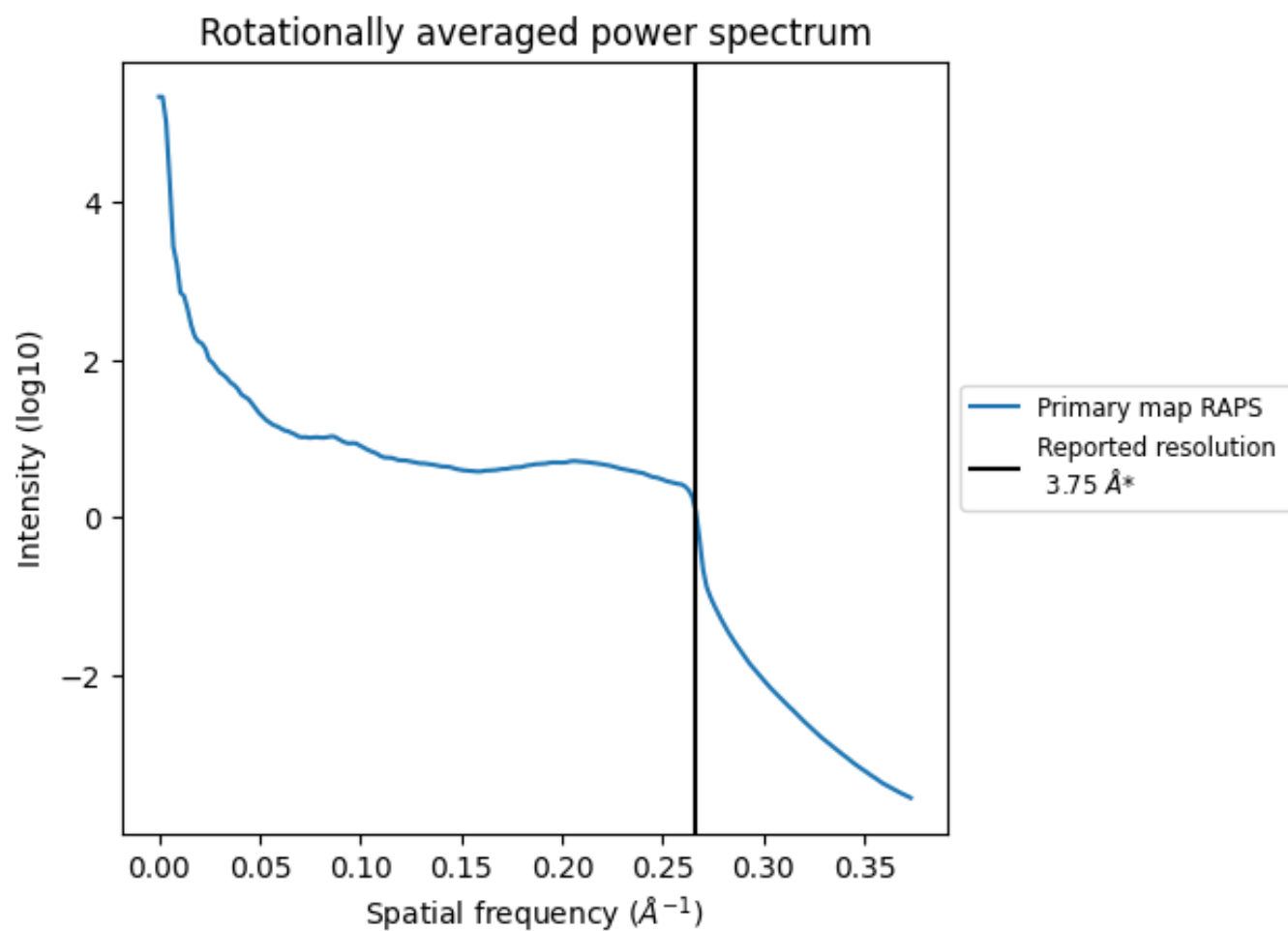


The volume at the recommended contour level is 2578  $\text{nm}^3$ ; this corresponds to an approximate mass of 2329 kDa.

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 0.267 Å<sup>-1</sup>

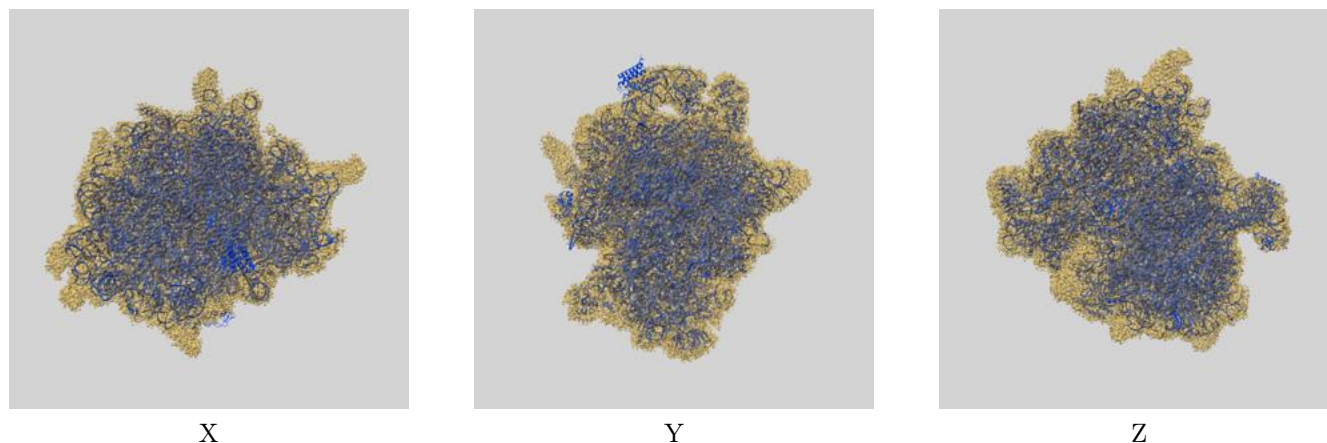
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

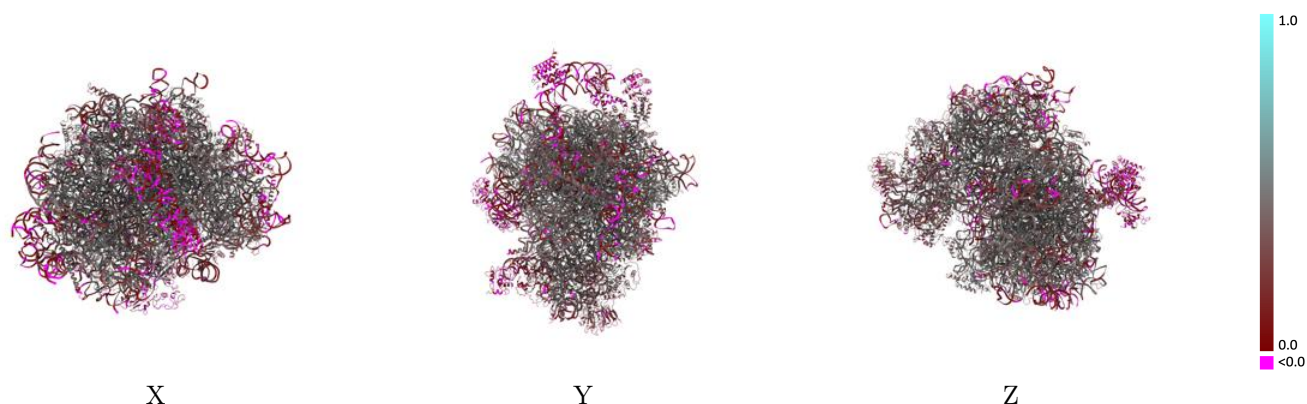
This section contains information regarding the fit between EMDB map EMD-3037 and PDB model 3JAJ. Per-residue inclusion information can be found in section [3](#) on page [21](#).

### 9.1 Map-model overlay [i](#)



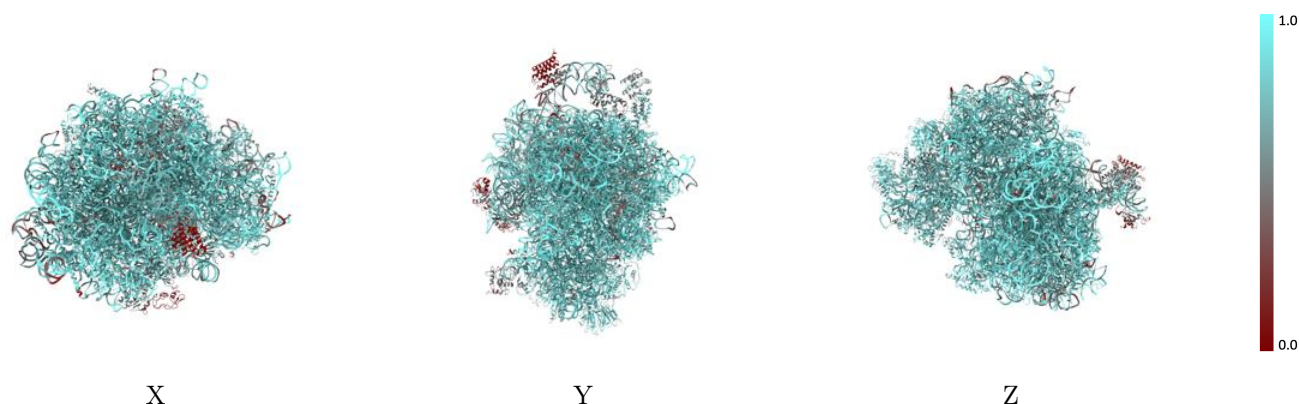
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



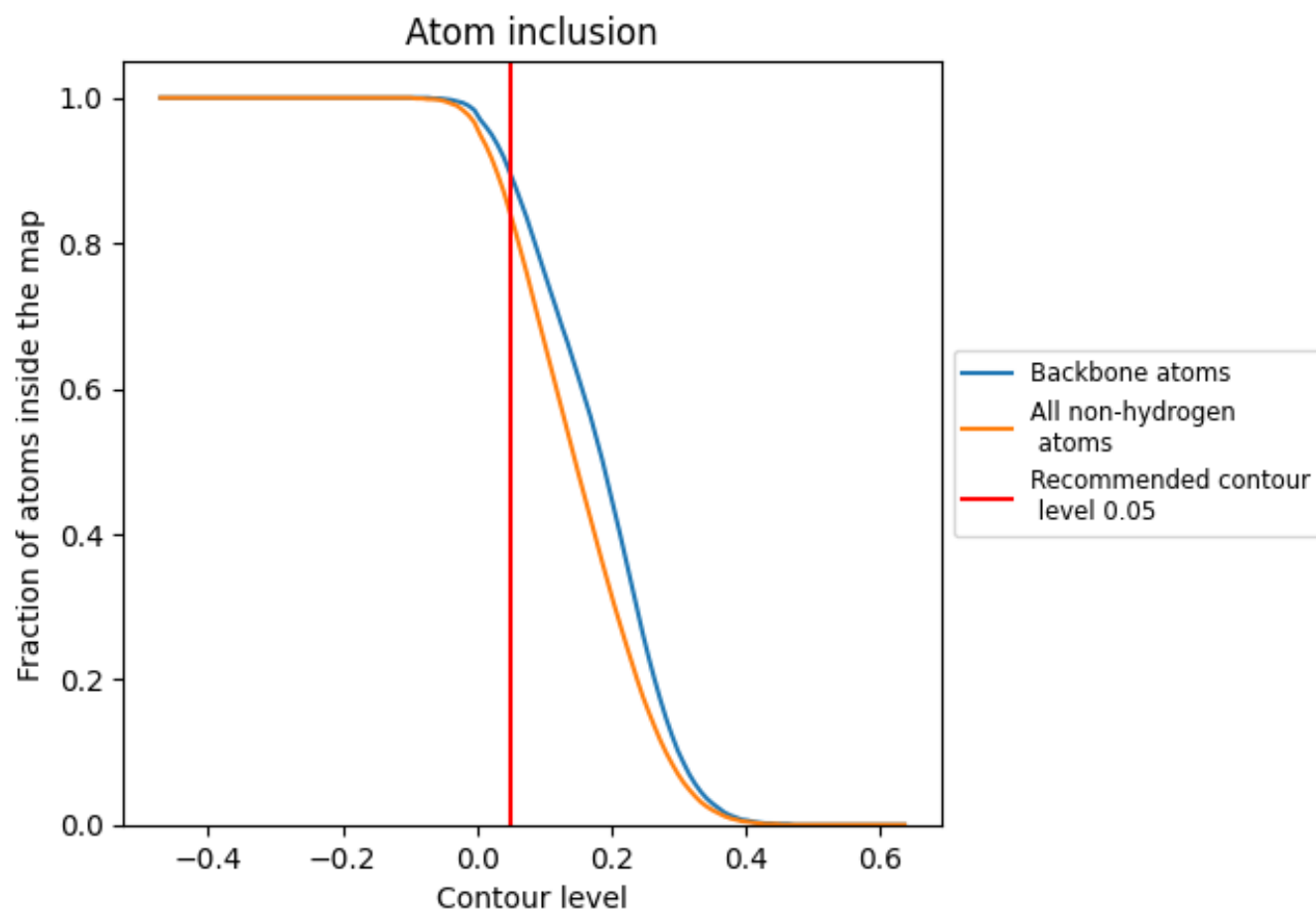
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8410	 0.3550
2	 0.6090	 0.2570
3	 0.8600	 0.3180
4	 0.6920	 0.0860
5	 0.8750	 0.3540
6	 0.1830	 0.0010
7	 0.9440	 0.4200
8	 0.9040	 0.3840
9	 0.4040	 0.0380
A	 0.8800	 0.4640
B	 0.8870	 0.4580
C	 0.8760	 0.4500
D	 0.8740	 0.4050
E	 0.8240	 0.3760
F	 0.8690	 0.4420
G	 0.8220	 0.3960
H	 0.8690	 0.4440
I	 0.8600	 0.4360
J	 0.8550	 0.4050
K	 0.3210	 0.0010
L	 0.8460	 0.4130
M	 0.8830	 0.4320
N	 0.8940	 0.4690
O	 0.8680	 0.4490
P	 0.8730	 0.4670
Q	 0.8840	 0.4620
R	 0.8490	 0.4020
S	 0.8950	 0.4590
S1	 0.7230	 0.2760
S2	 0.8780	 0.3390
S4	 0.7450	 0.3270
SA	 0.8470	 0.4070
SB	 0.8510	 0.4230
SC	 0.8660	 0.4430
SD	 0.7820	 0.3440





























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Chain	Atom inclusion	Q-score
SE	 0.8720	 0.4350
SF	 0.7430	 0.2860
SG	 0.7920	 0.3240
SH	 0.7760	 0.3330
SI	 0.8370	 0.3970
SJ	 0.8700	 0.4090
SK	 0.7370	 0.2330
SL	 0.8270	 0.4230
SM	 0.3940	 0.0260
SN	 0.8650	 0.4240
SO	 0.8460	 0.4190
SP	 0.6990	 0.2310
SQ	 0.8310	 0.3800
SR	 0.7500	 0.3240
SS	 0.8240	 0.3380
ST	 0.8200	 0.3430
SU	 0.8050	 0.3520
SV	 0.8400	 0.4170
SW	 0.8920	 0.4550
SX	 0.8770	 0.4640
SY	 0.8290	 0.3870
SZ	 0.7530	 0.2770
Sa	 0.8800	 0.4460
Sb	 0.8360	 0.3870
Sc	 0.7570	 0.3270
Sd	 0.8390	 0.3930
Se	 0.7730	 0.3460
Sf	 0.4470	 0.0610
Sg	 0.7590	 0.2530
T	 0.8730	 0.4480
U	 0.8460	 0.3830
V	 0.8760	 0.4710
W	 0.8550	 0.4330
X	 0.8500	 0.4440
Y	 0.8580	 0.4280
Z	 0.8970	 0.4320
a	 0.9040	 0.4650
b	 0.8010	 0.3750
c	 0.8890	 0.4450
d	 0.8600	 0.4310
e	 0.8720	 0.4570
f	 0.9180	 0.4670

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Chain	Atom inclusion	Q-score
g	 0.8580	 0.4430
h	 0.8480	 0.4100
i	 0.8660	 0.4250
j	 0.9040	 0.4570
k	 0.7920	 0.3760
l	 0.8720	 0.4600
m	 0.8990	 0.4470
n	 0.8160	 0.3670
o	 0.8760	 0.4500
p	 0.8460	 0.4490
q	 0.3190	 0.0460
r	 0.9030	 0.4530
z	 0.6100	 0.1370