Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 04:40 PM EST

PDB ID	:	3JAN
EMDB ID	:	EMD-3045
Title	:	Structure of the scanning state of the mammalian SRP-ribosome complex
Authors	:	Voorhees, R.M.; Hegde, R.S.
Deposited on	:	2015-06-17
Resolution	:	3.75 Å(reported)
Based on initial model	:	3JAJ

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

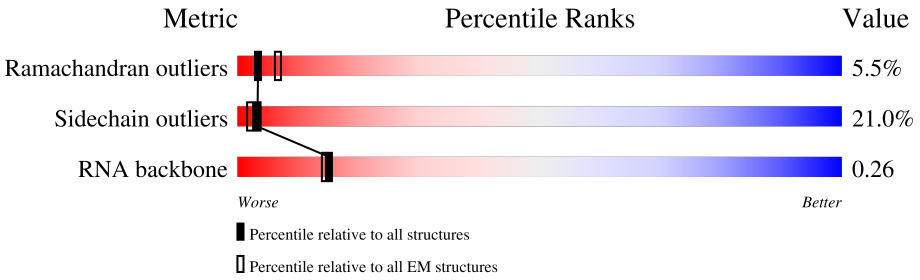
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.75 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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	74% 20% 5%
2	D	292	70% 24%
3	G	238	74% 22% 5%
4	H	190	78% 15% 6%
5	J	170	72% 24%
6	L	210	74% 20% 6%
7	M	138	75% 23%
8	N	203	70% 23% 6%

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Mol	Chain	Length	Quality of chain
9	O	201	80% 15%
10	Q	187	74% 17% 7%
11	R	180	70% 25% 5%
12	S	175	71% 20% 7%
13	T	159	74% 23%
14	U	99	74% 23%
15	V	131	79% 17%
16	X	119	81% 18%
17	Y	134	71% 22% 7%
18	Z	135	79% 16% 5%
19	a	147	78% 20%
20	b	75	8% 75% 19% 5%
21	c	94	74% 22%
22	d	107	64% 28% 8%
23	e	128	77% 22%
24	f	109	76% 19% 5%
25	g	114	79% 17%
26	h	122	84% 11%
27	i	102	76% 20%
28	k	69	6% 75% 25%
29	l	50	78% 20%
30	m	52	71% 25%
31	o	104	72% 21% 6%
32	5	3658	5% 46% 40% 10%
33	7	120	59% 30% 9%

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Mol	Chain	Length	Quality of chain
34	8	156	48% 40% 6% 6%
35	B	394	73% 22% 5%
36	C	367	76% 19% 5%
37	E	236	8% 64% 27% 7%
38	F	225	70% 25%
39	I	213	68% 28%
40	P	153	78% 18%
41	W	63	71% 24% 5%
42	j	86	76% 17% 7%
43	n	23	74% 26%
44	p	91	86% 11%
45	r	125	74% 24%
46	K	163	64% 66% 28% 6%
47	q	202	78% 70% 23% 6%
48	z	426	48% 87% 12%
49	3	76	14% 62% 34%
50	4	206	39% 76% 21%
51	9	105	72% 96%
52	6	179	88% 97%
53	S2	1742	44% 44% 9%
54	SA	208	72% 23% 5%
55	SB	213	71% 23%
56	SC	218	75% 20% 5%
57	SE	262	74% 21% 5%
58	SG	237	10% 78% 20%

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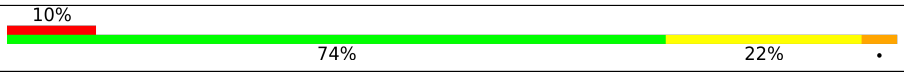
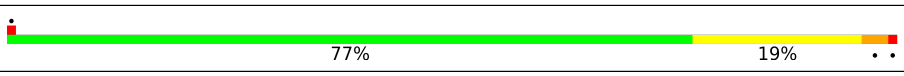
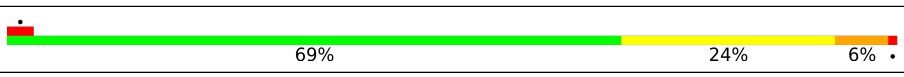
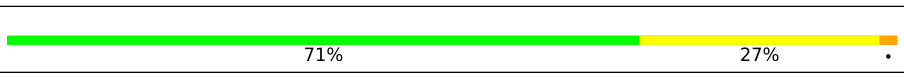
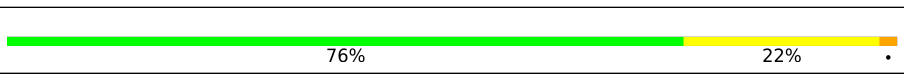
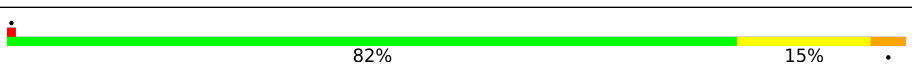
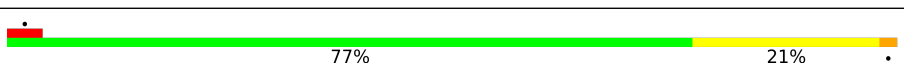
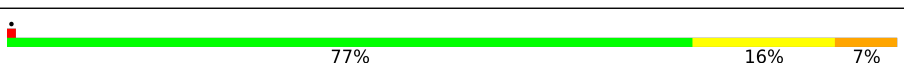
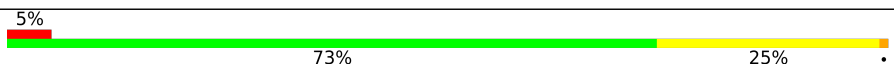
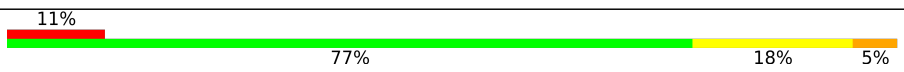
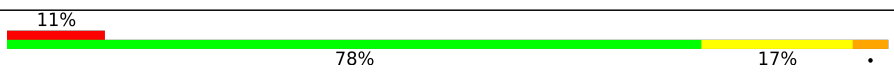
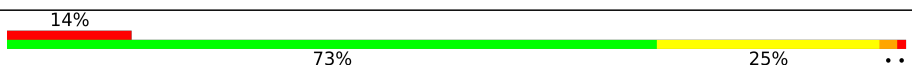
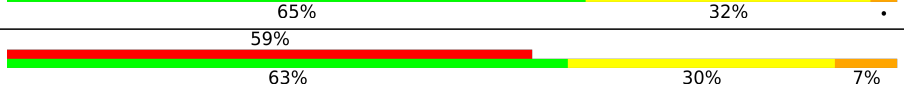
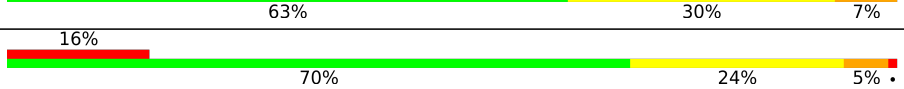
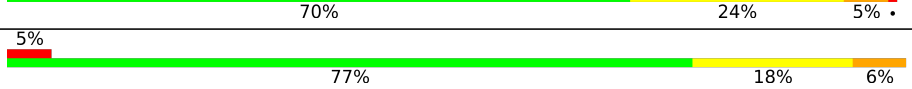
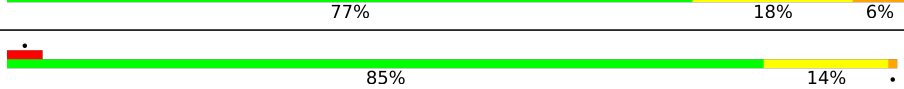
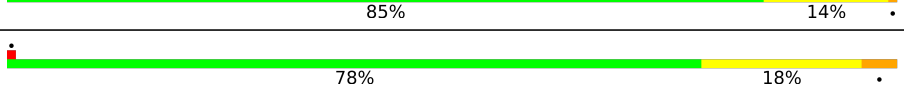
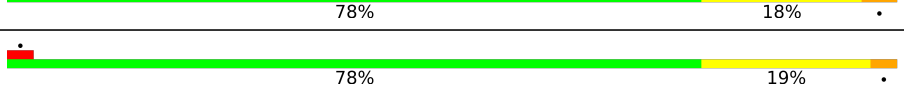
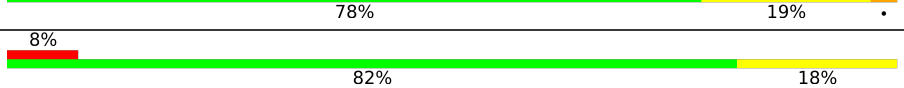
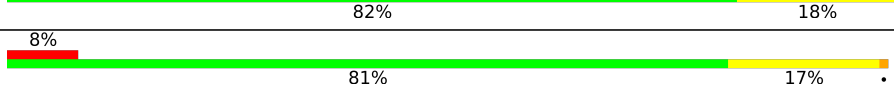
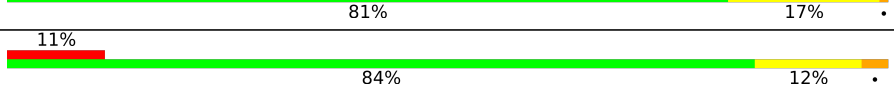
Mol	Chain	Length	Quality of chain
59	SH	189	
60	SI	206	
61	SJ	185	
62	SL	152	
63	SN	149	
64	SO	136	
65	SV	82	
66	SW	129	
67	SX	141	
68	SY	126	
69	Sa	98	
70	Sb	83	
71	Se	57	
72	SD	227	
73	SF	191	
74	SK	98	
75	SM	124	
76	SP	96	
77	SQ	141	
78	SR	129	
79	SS	137	
80	ST	141	
81	SU	104	
82	SZ	75	
83	Sc	64	

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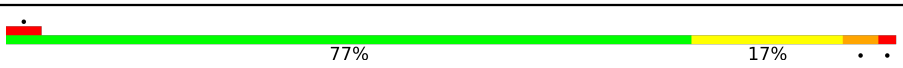
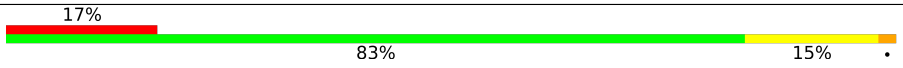
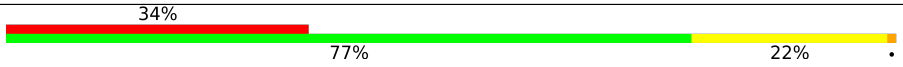
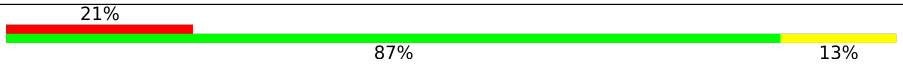
Mol	Chain	Length	Quality of chain
84	Sd	52	
85	Sf	71	
86	Sg	313	
87	S1	74	
88	S4	76	

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 227964 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribosomal protein uL2.

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

- Molecule 2 is a protein called Ribosomal protein uL18.

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

- Molecule 3 is a protein called Ribosomal protein eL8.

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

- Molecule 4 is a protein called Ribosomal protein uL6.

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

- Molecule 5 is a protein called Ribosomal protein uL5.

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

- Molecule 6 is a protein called Ribosomal protein eL13.

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

- 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 RNA chain called Val tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	3	76	Total	C	N	O	P	0	0
			1616	723	290	528	75		

- Molecule 50 is a RNA chain called SRP 7S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	4	206	Total	C	N	O	P	6	0
			4551	2026	836	1477	212		

- Molecule 51 is a protein called SRP19.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	9	105	Total	C	N	O	S	0	0
			844	534	152	152	6		

- Molecule 52 is a protein called SRP68.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	6	179	Total	C	N	O	S	0	0
			1497	939	280	271	7		

- Molecule 53 is a RNA chain called 18S ribosomal RNA.

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

- Molecule 54 is a protein called Ribosomal protein uS2.

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

- Molecule 55 is a protein called Ribosomal protein eS1.

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

- Molecule 56 is a protein called Ribosomal protein uS5.

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

- Molecule 57 is a protein called Ribosomal protein eS4.

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

- Molecule 58 is a protein called Ribosomal protein eS6.

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

- Molecule 59 is a protein called Ribosomal protein eS7.

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

- Molecule 60 is a protein called Ribosomal protein eS8.

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

- Molecule 61 is a protein called Ribosomal protein uS4.

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

- Molecule 62 is a protein called Ribosomal protein uS17.

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

- Molecule 63 is a protein called Ribosomal protein uS15.

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

- Molecule 64 is a protein called Ribosomal protein uS11.

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

- Molecule 65 is a protein called Ribosomal protein eS21.

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

- Molecule 66 is a protein called Ribosomal protein uS8.

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

- Molecule 67 is a protein called Ribosomal protein uS12.

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

- Molecule 68 is a protein called Ribosomal protein eS24.

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

- Molecule 69 is a protein called Ribosomal protein eS26.

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

- Molecule 70 is a protein called Ribosomal protein eS27.

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

- Molecule 71 is a protein called Ribosomal protein eS30.

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

- Molecule 72 is a protein called Ribosomal protein uS3.

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

- Molecule 73 is a protein called Ribosomal protein uS7.

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

- Molecule 74 is a protein called Ribosomal protein eS10.

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

- Molecule 75 is a protein called Ribosomal protein eS12.

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

- Molecule 76 is a protein called Ribosomal protein uS19.

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

- Molecule 77 is a protein called Ribosomal protein uS9.

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

- Molecule 78 is a protein called Ribosomal protein eS17.

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

- Molecule 79 is a protein called Ribosomal protein uS13.

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

- Molecule 80 is a protein called Ribosomal protein eS19.

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

- Molecule 81 is a protein called Ribosomal protein uS10.

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

- Molecule 82 is a protein called Ribosomal protein es25.

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

- Molecule 83 is a protein called Ribosomal protein eS28.

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

- Molecule 84 is a protein called Ribosomal protein uS14.

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

- Molecule 85 is a protein called Ribosomal protein eS31.

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

- Molecule 86 is a protein called Ribosomal protein RACK1.

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

- Molecule 87 is a protein called SRP9.

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

- Molecule 88 is a protein called SRP14.

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

- Molecule 89 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
89	D	1	Total	Mg	0
			1	1	
89	V	1	Total	Mg	0
			1	1	
89	g	1	Total	Mg	0
			1	1	
89	5	116	Total	Mg	0
			116	116	
89	7	5	Total	Mg	0
			5	5	
89	8	6	Total	Mg	0
			6	6	

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Mol	Chain	Residues	Atoms	AltConf
89	S2	36	Total Mg 36 36	0

- Molecule 90 is ZINC ION (three-letter code: ZN) (formula: Zn).

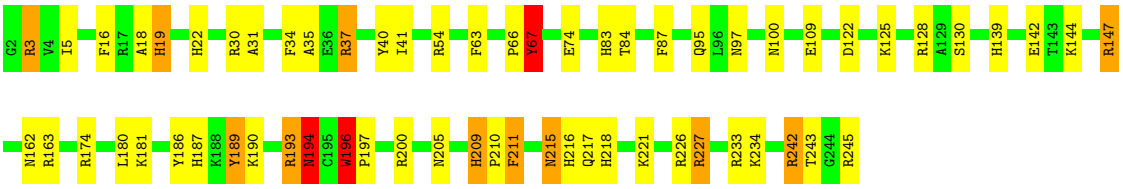
Mol	Chain	Residues	Atoms	AltConf
90	m	1	Total Zn 1 1	0
90	o	1	Total Zn 1 1	0
90	j	1	Total Zn 1 1	0
90	Sa	1	Total Zn 1 1	0

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.

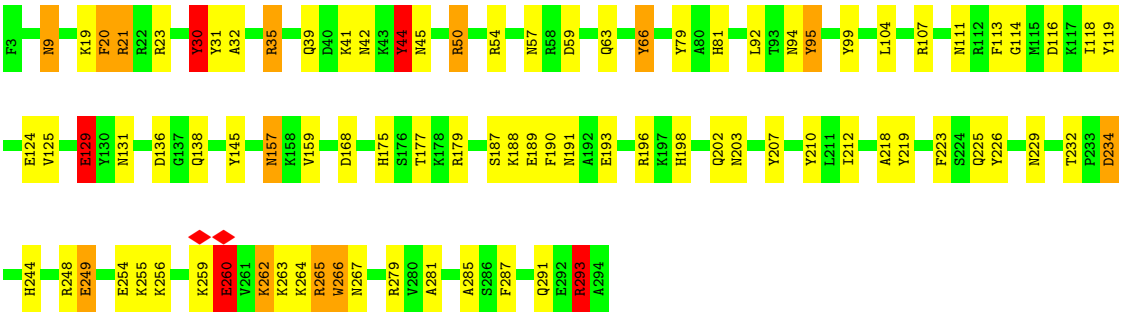
• Molecule 1: Ribosomal protein uL2

Chain A:



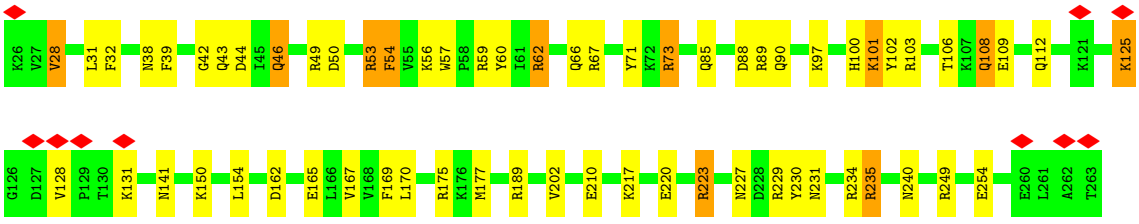
• Molecule 2: Ribosomal protein uL18

Chain D:



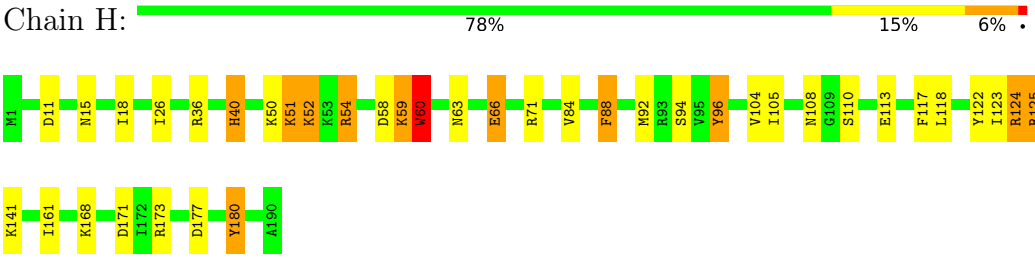
• Molecule 3: Ribosomal protein eL8

Chain G:



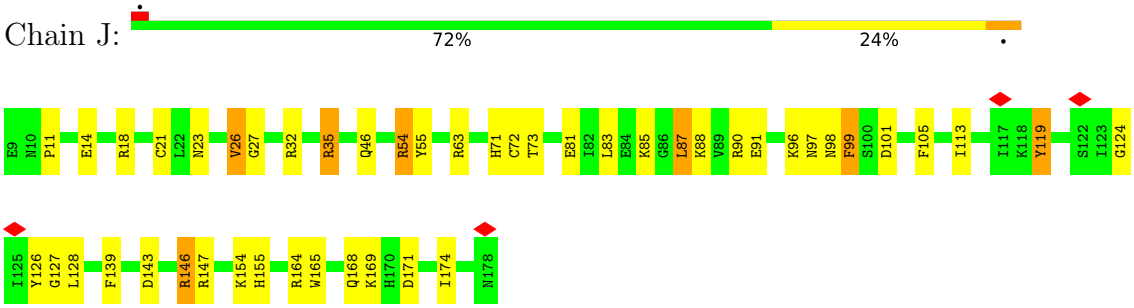
• Molecule 4: Ribosomal protein uL6

Chain H:



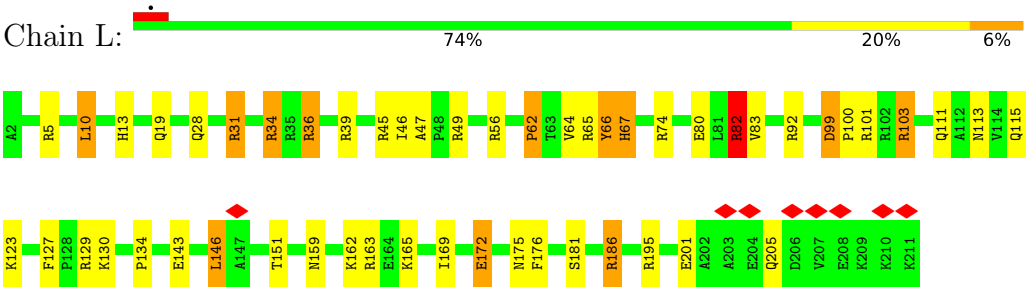
• Molecule 5: Ribosomal protein uL5

Chain J:



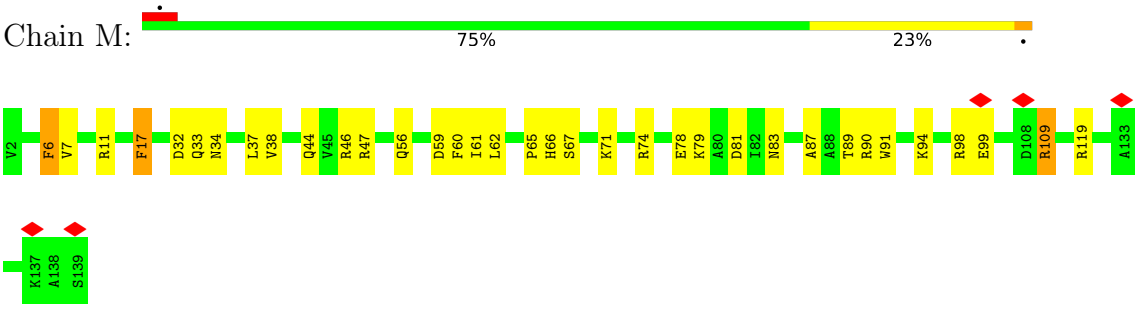
• Molecule 6: Ribosomal protein eL13

Chain L:



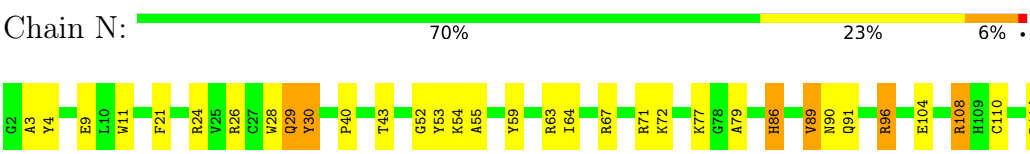
• Molecule 7: Ribosomal protein eL14

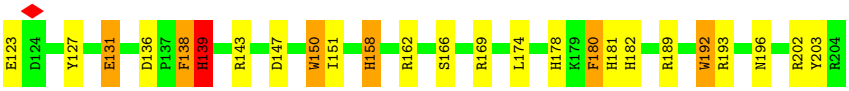
Chain M:



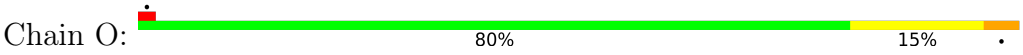
• Molecule 8: Ribosomal protein eL15

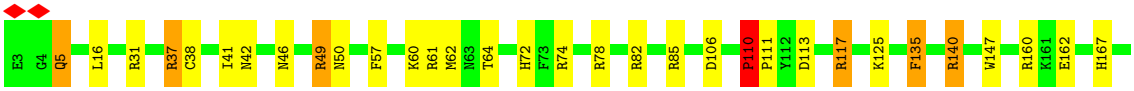
Chain N:

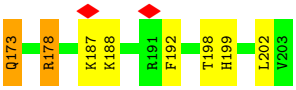




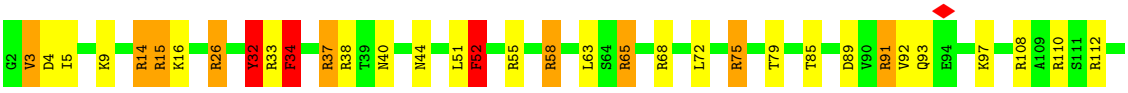
• Molecule 9: Ribosomal protein uL13

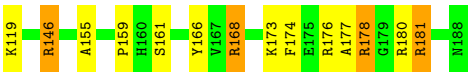




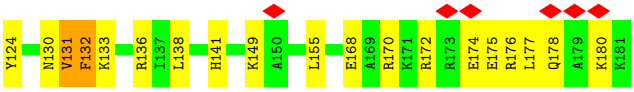


• Molecule 10: Ribosomal protein eL18

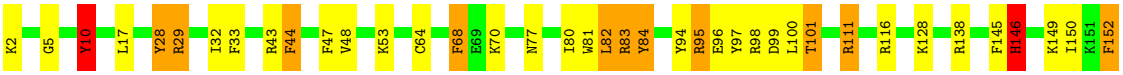


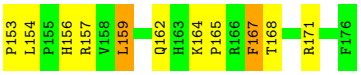


• Molecule 11: Ribosomal protein eL19

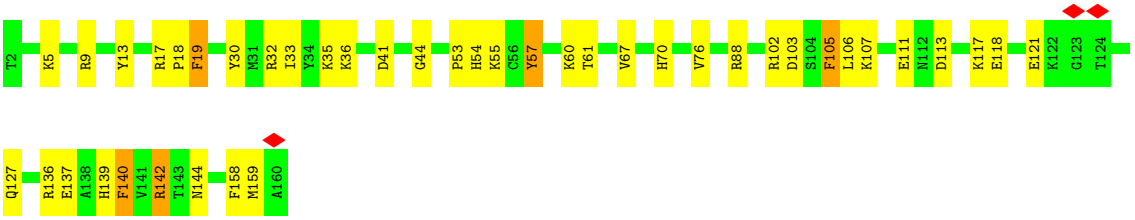


• Molecule 12: Ribosomal protein eL20



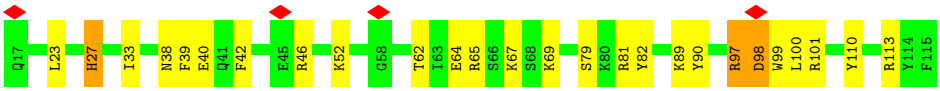


• Molecule 13: Ribosomal protein eL21



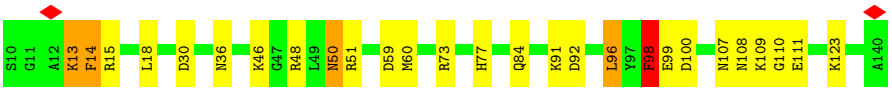
• Molecule 14: Ribosomal protein eL22

Chain U:



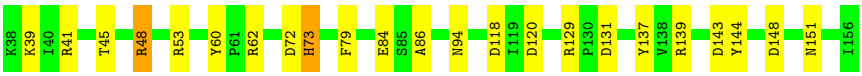
• Molecule 15: Ribosomal protein uL14

Chain V:



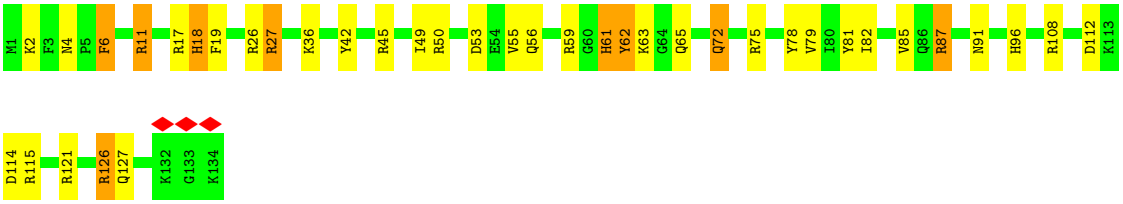
• Molecule 16: Ribosomal protein uL23

Chain X:



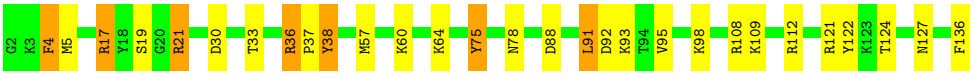
• Molecule 17: Ribosomal protein uL24

Chain Y:



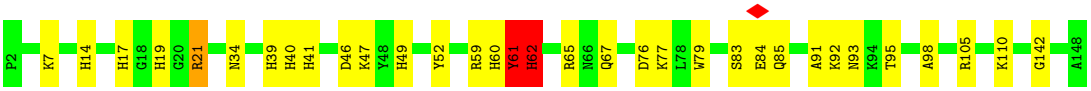
• Molecule 18: Ribosomal protein eL27

Chain Z:



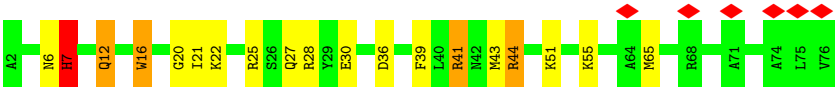
• Molecule 19: Ribosomal protein uL15

Chain a:



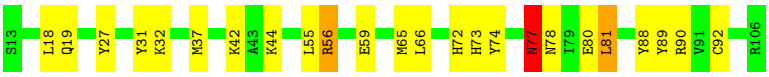
• Molecule 20: Ribosomal protein eL29

Chain b:



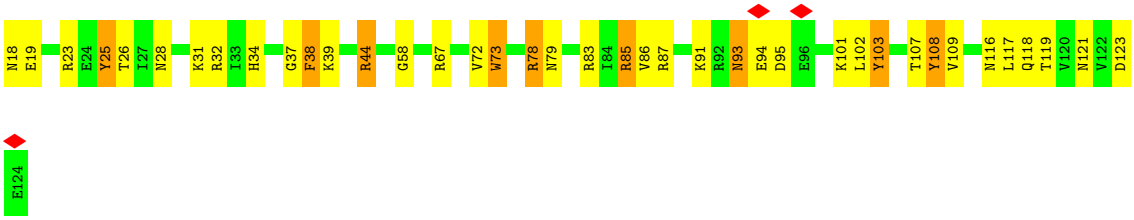
• Molecule 21: Ribosomal protein eL30

Chain c:



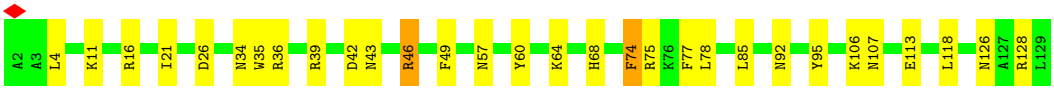
• Molecule 22: Ribosomal protein eL31

Chain d:



• Molecule 23: Ribosomal protein eL32

Chain e:

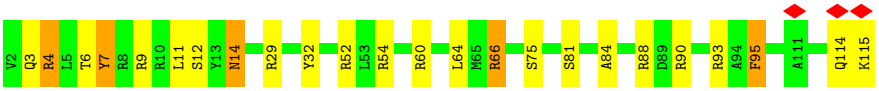


• Molecule 24: Ribosomal protein eL33

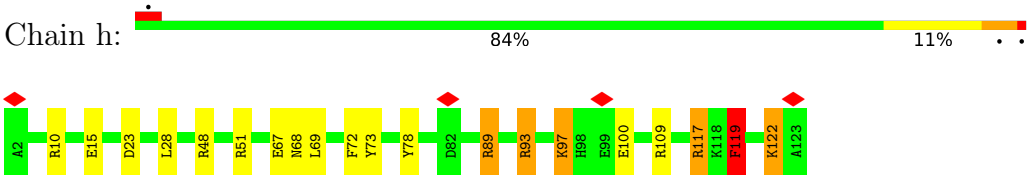
Chain f:

• Molecule 25: Ribosomal protein eL34

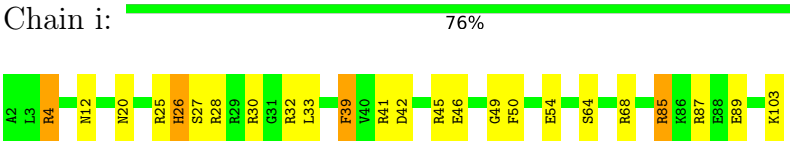
Chain g:



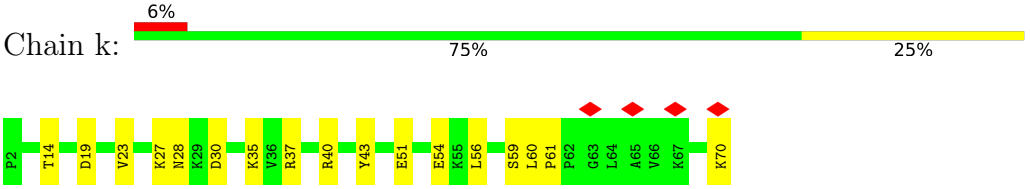
• Molecule 26: Ribosomal protein uL29



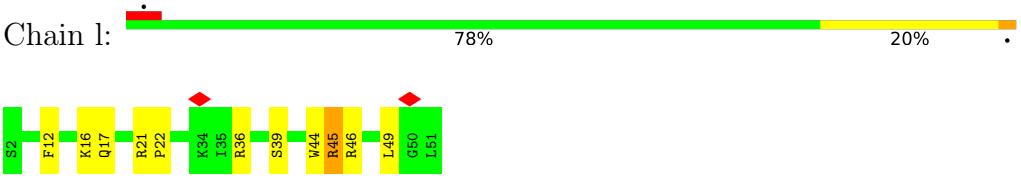
• Molecule 27: Ribosomal protein eL36



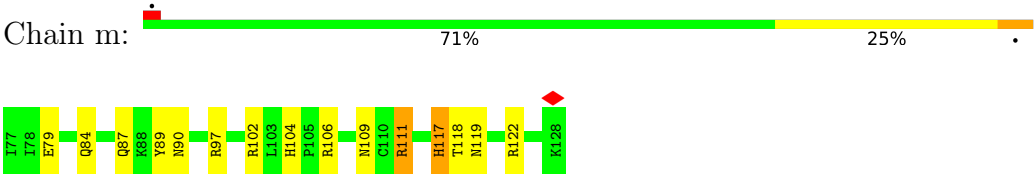
• Molecule 28: Ribosomal protein eL38



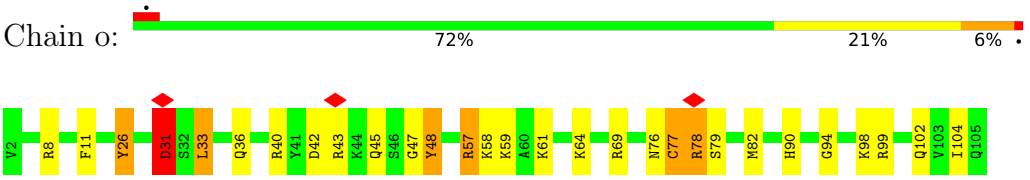
• Molecule 29: Ribosomal protein eL39



• Molecule 30: Ribosomal protein eL40

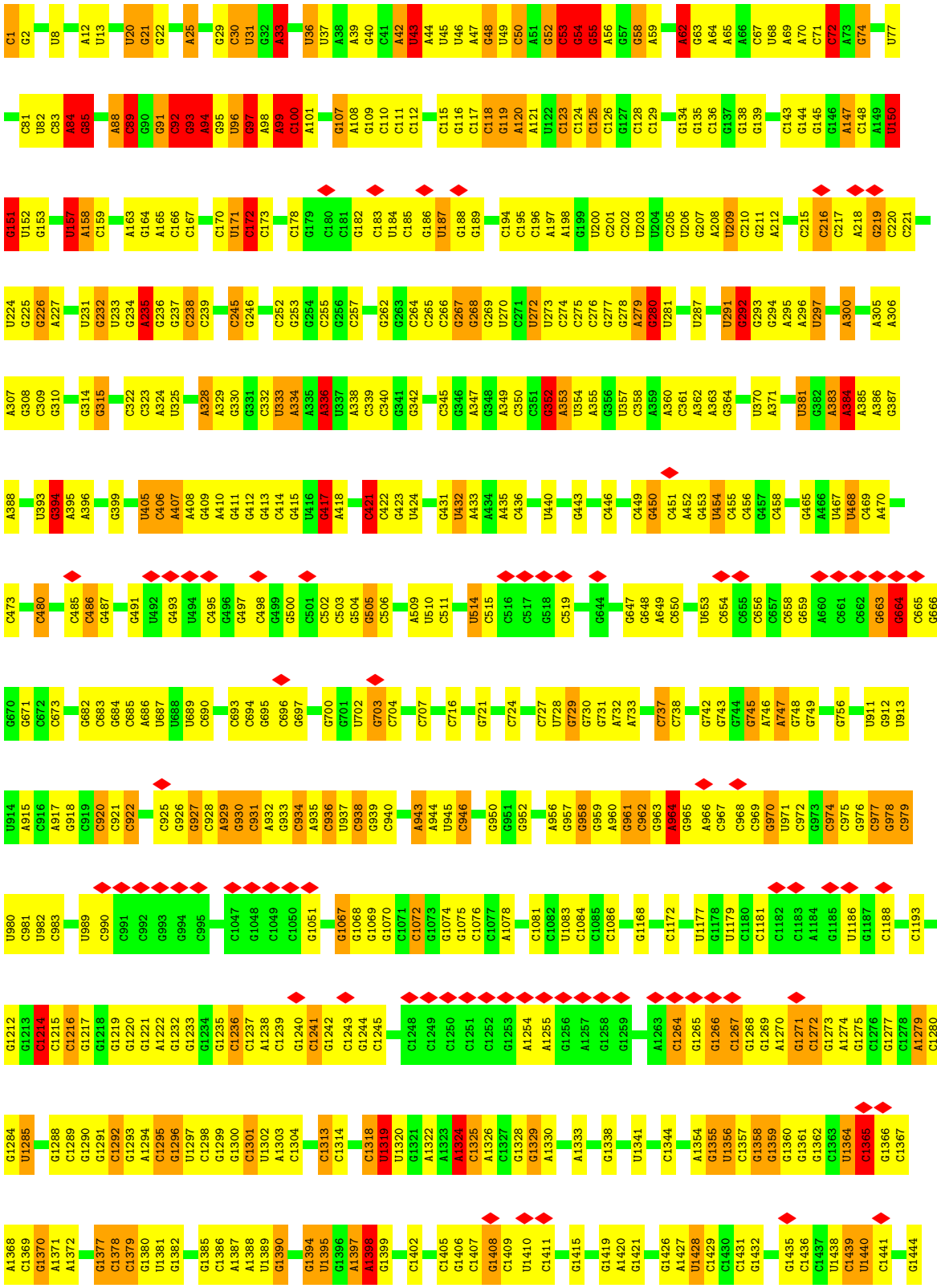


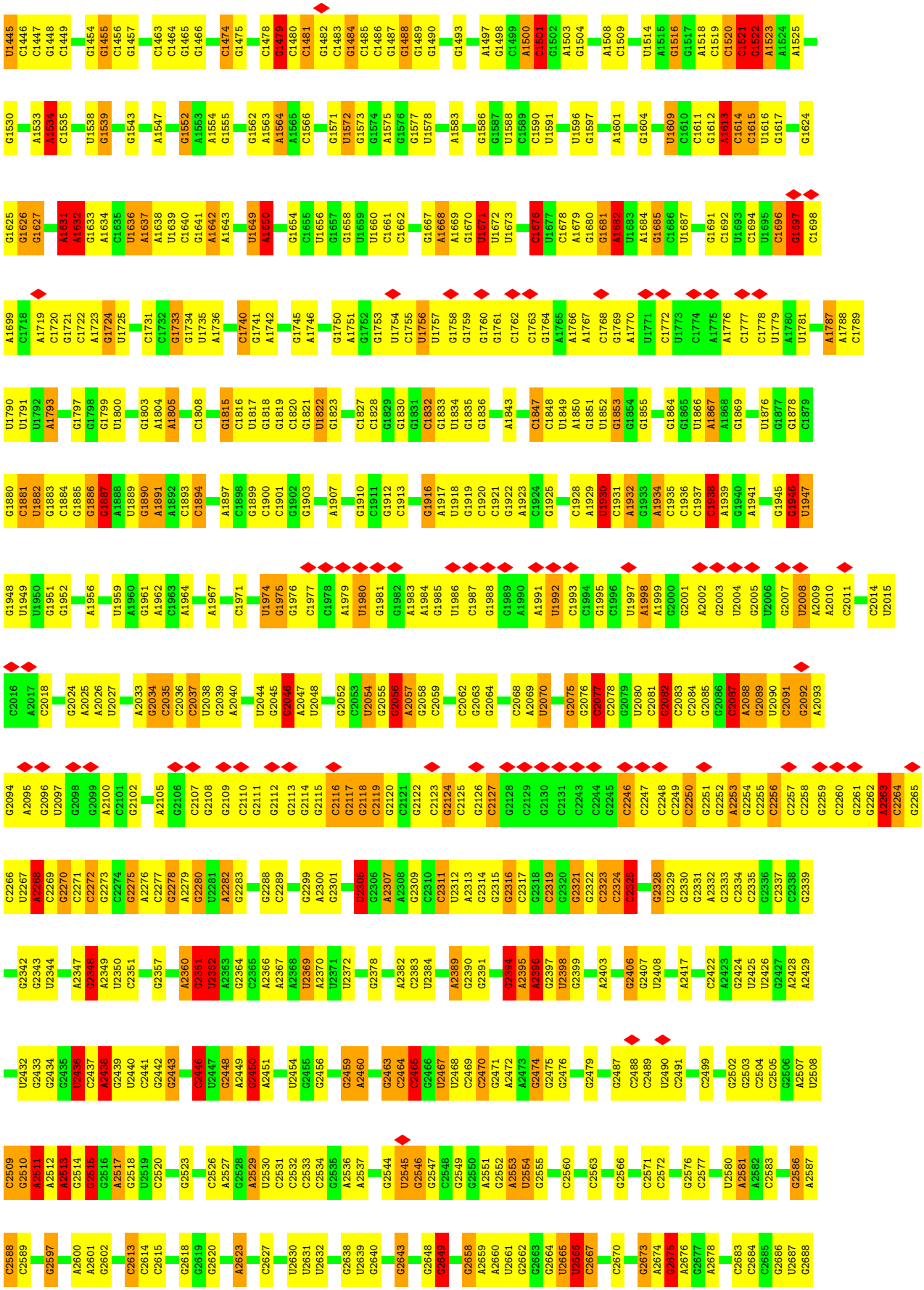
• Molecule 31: Ribosomal protein eL42

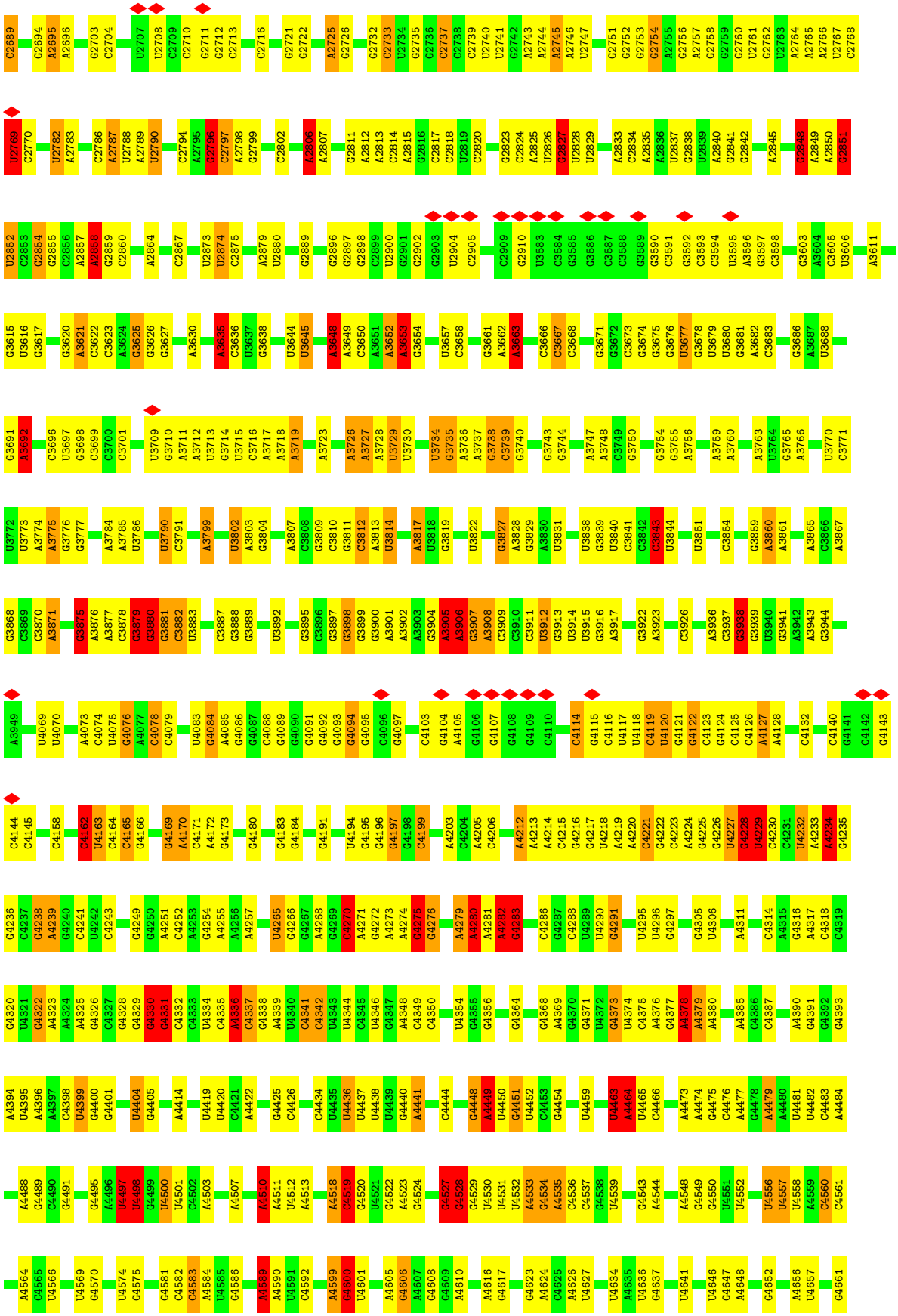


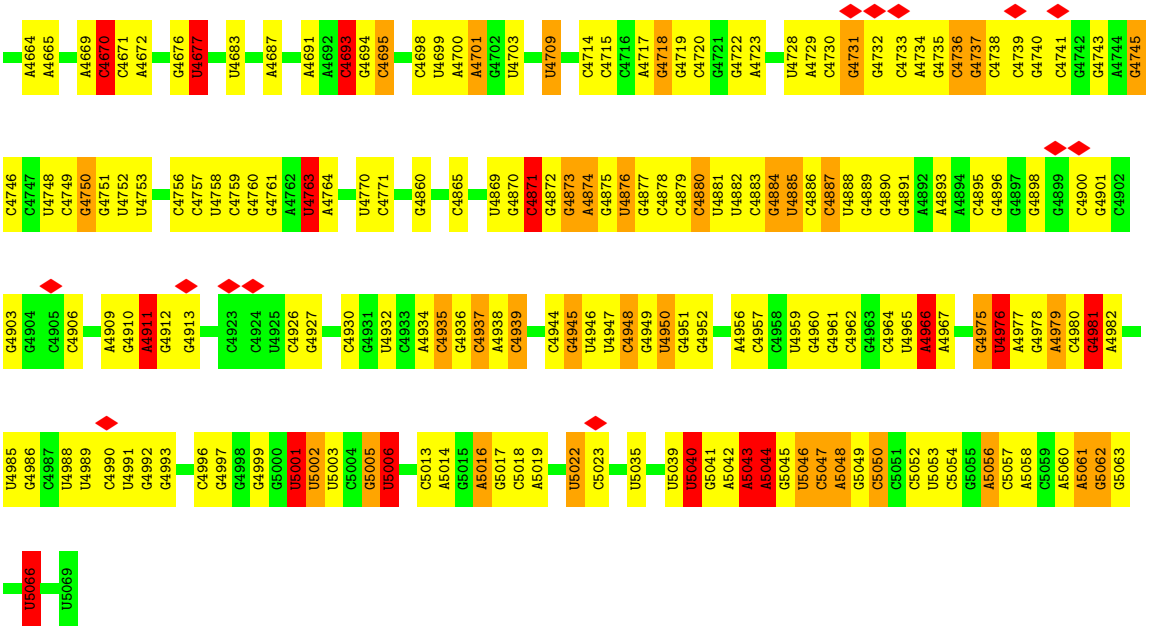
• Molecule 32: 28S ribosomal RNA

Chain 5:



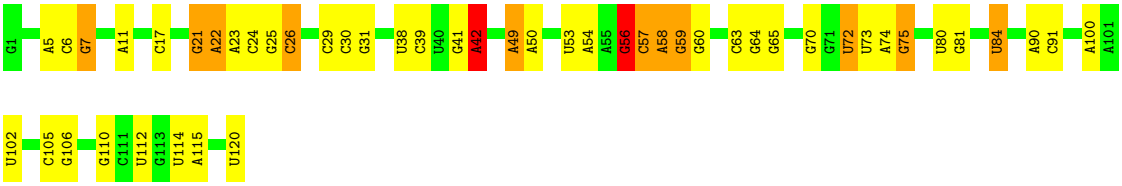






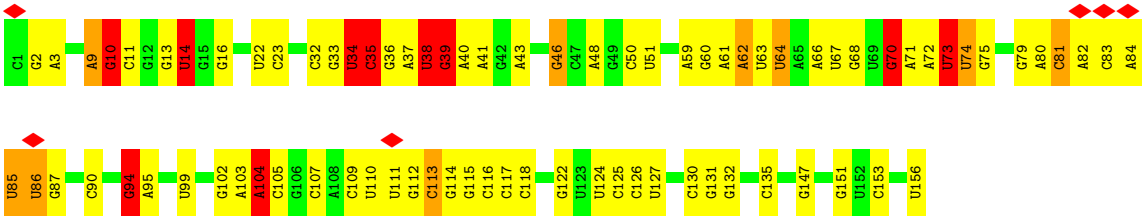
• Molecule 33: 5S ribosomal RNA

Chain 7:



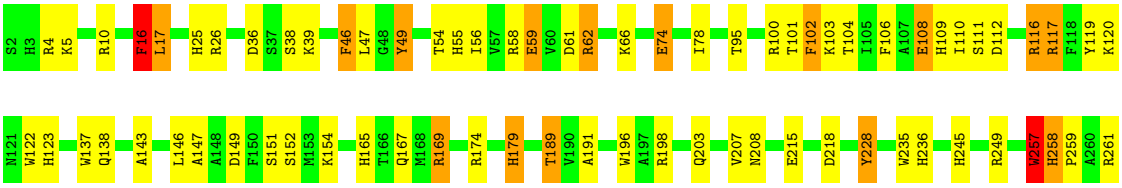
• Molecule 34: 5.8S ribosomal RNA

Chain 8:



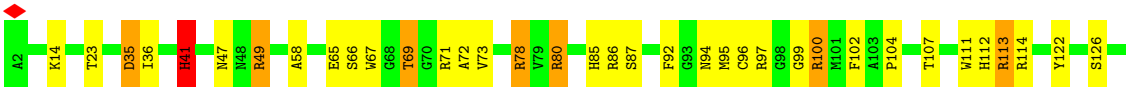
• Molecule 35: Ribosomal protein uL3

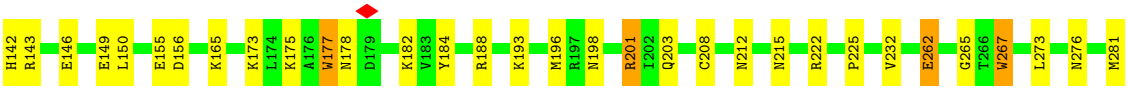
Chain B:

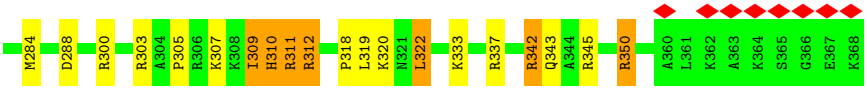


• Molecule 36: Ribosomal protein uL4

Chain C:

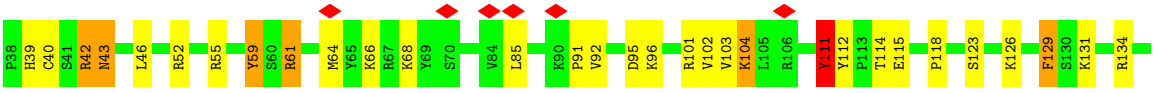


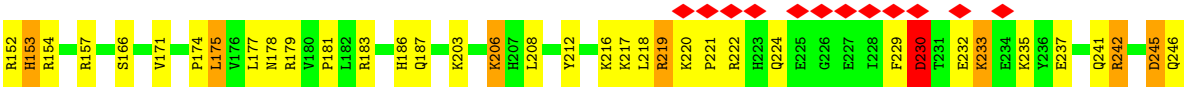


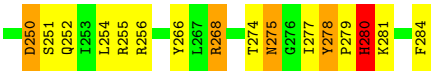


• Molecule 37: Ribosomal protein eL6

Chain E:

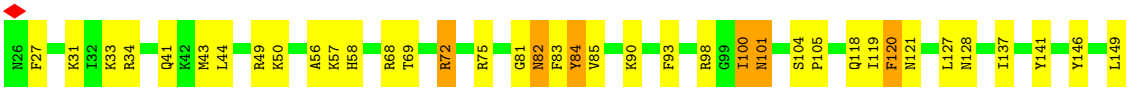


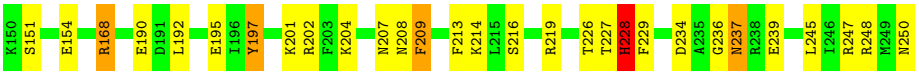




• Molecule 38: Ribosomal protein uL30

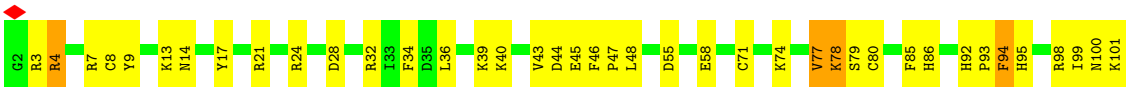
Chain F:

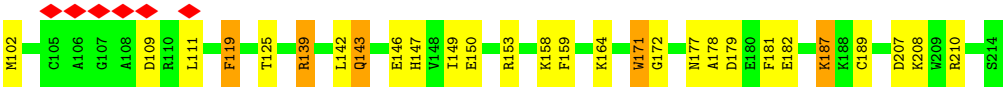




• Molecule 39: Ribosomal protein uL16

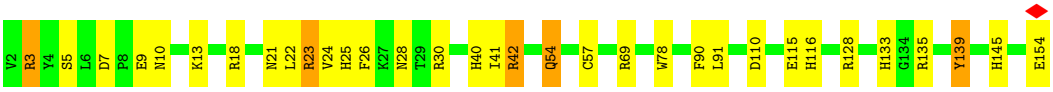
Chain I:





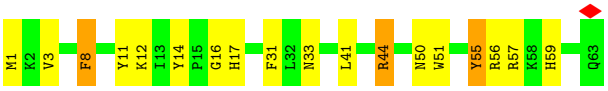
• Molecule 40: Ribosomal protein uL22

Chain P:



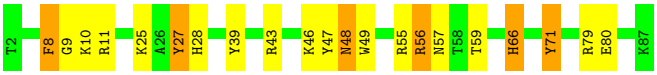
• Molecule 41: Ribosomal protein eL24

Chain W:



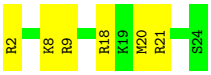
• Molecule 42: Ribosomal protein eL37

Chain j:



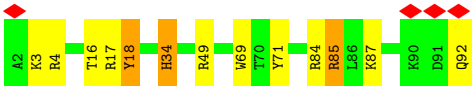
• Molecule 43: Ribosomal protein eL41

Chain n:



• Molecule 44: Ribosomal protein eL43

Chain p:

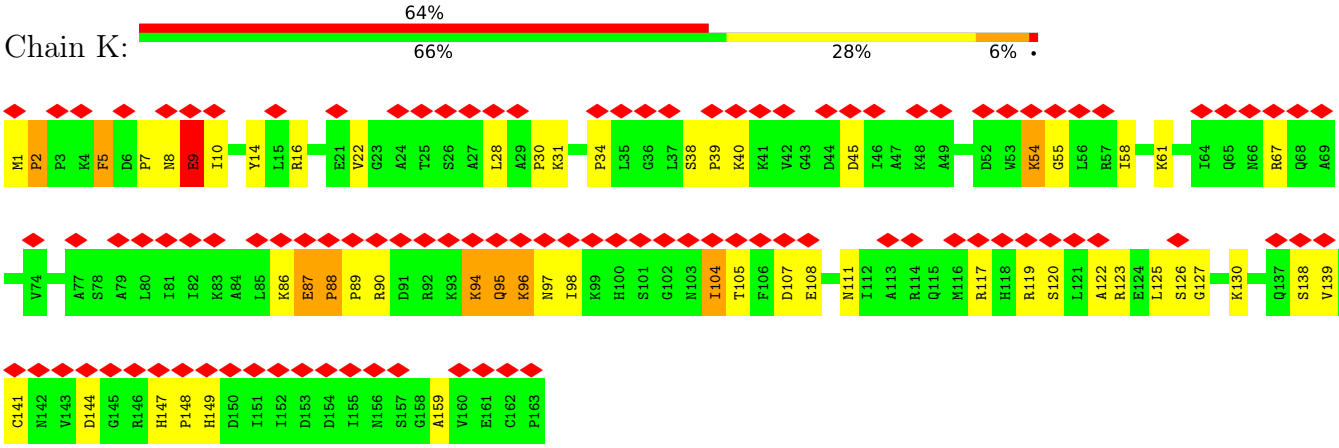


• Molecule 45: Ribosomal protein eL28

Chain r:

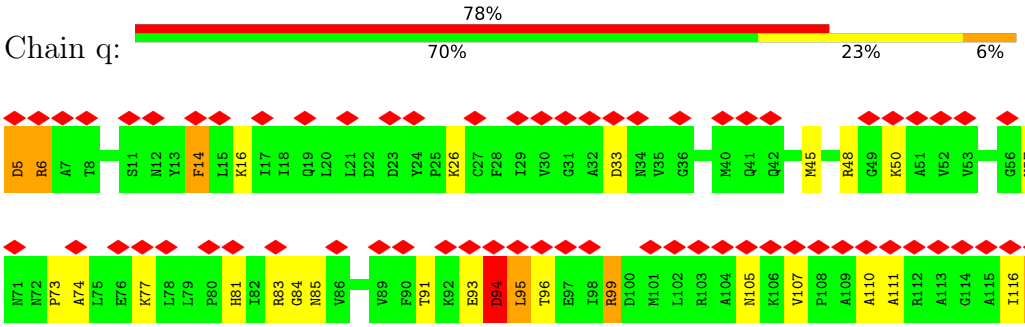
• Molecule 46: Ribosomal protein uL11

Chain K:



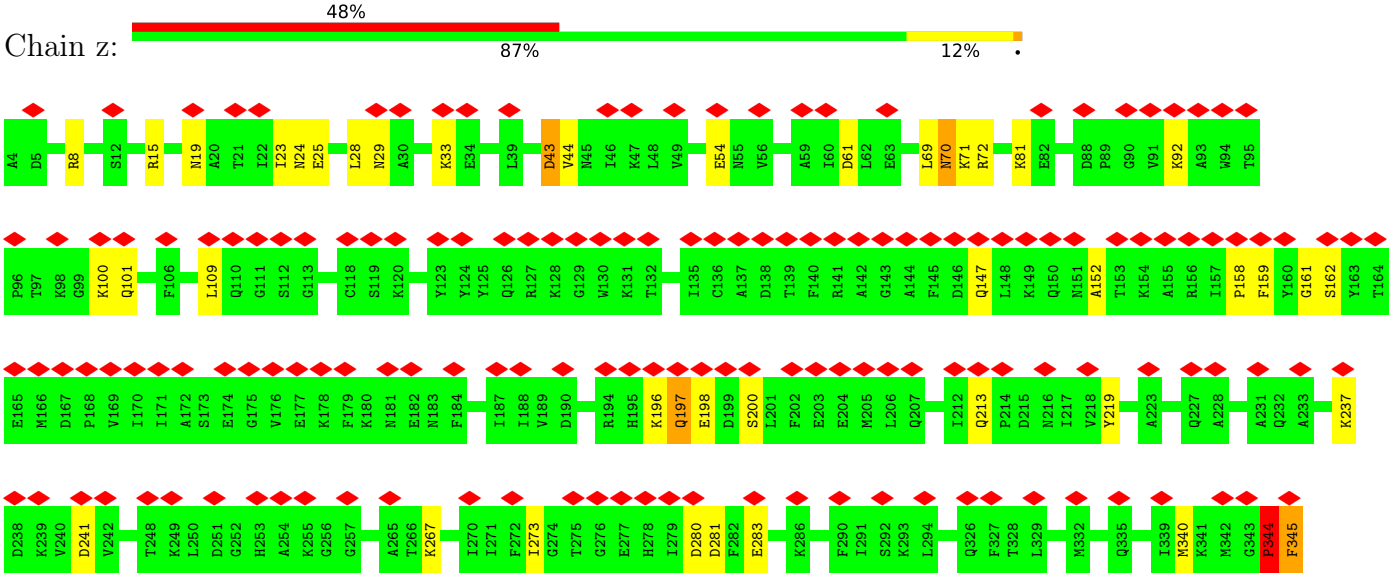
• Molecule 47: Ribosomal protein uL10

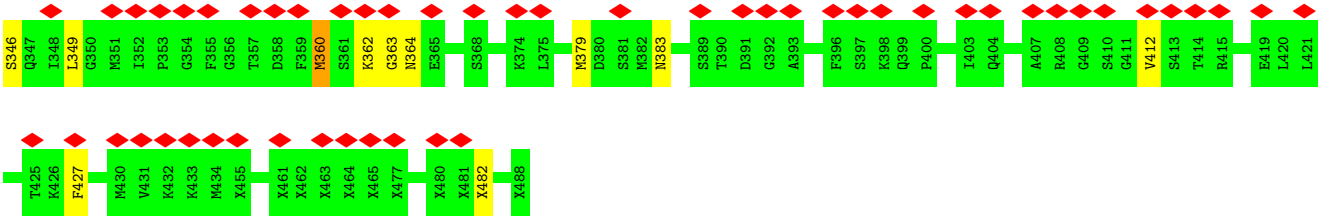
Chain q:



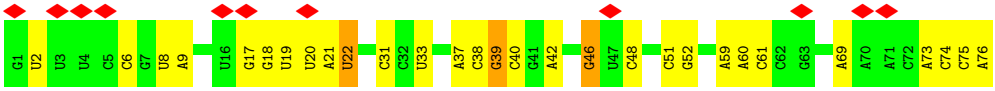
• Molecule 48: SRP54

Chain z:

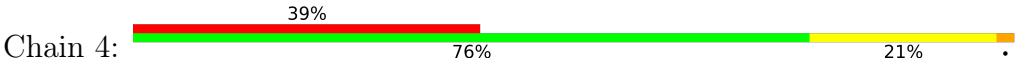


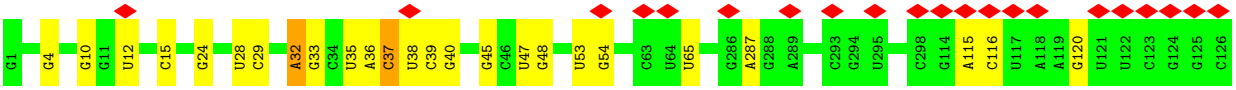


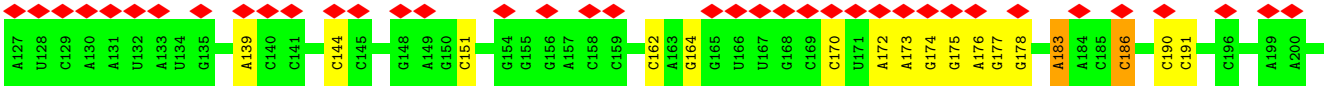
• Molecule 49: Val tRNA

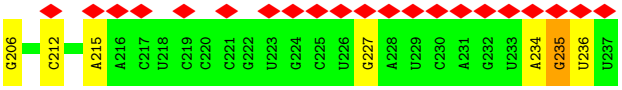


• Molecule 50: SRP 7S RNA

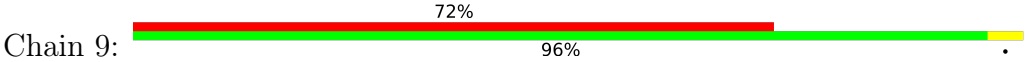


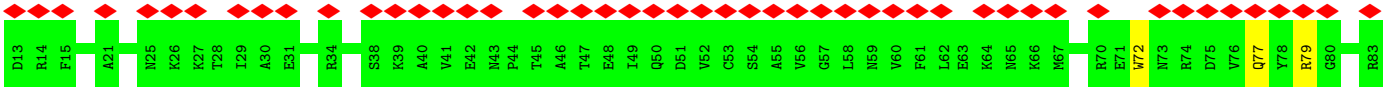


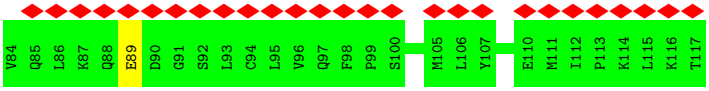




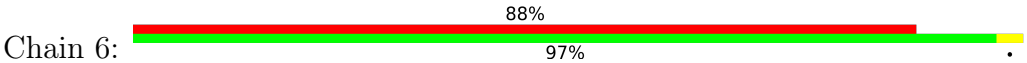
• Molecule 51: SRP19

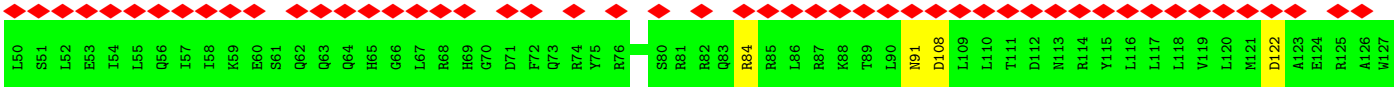






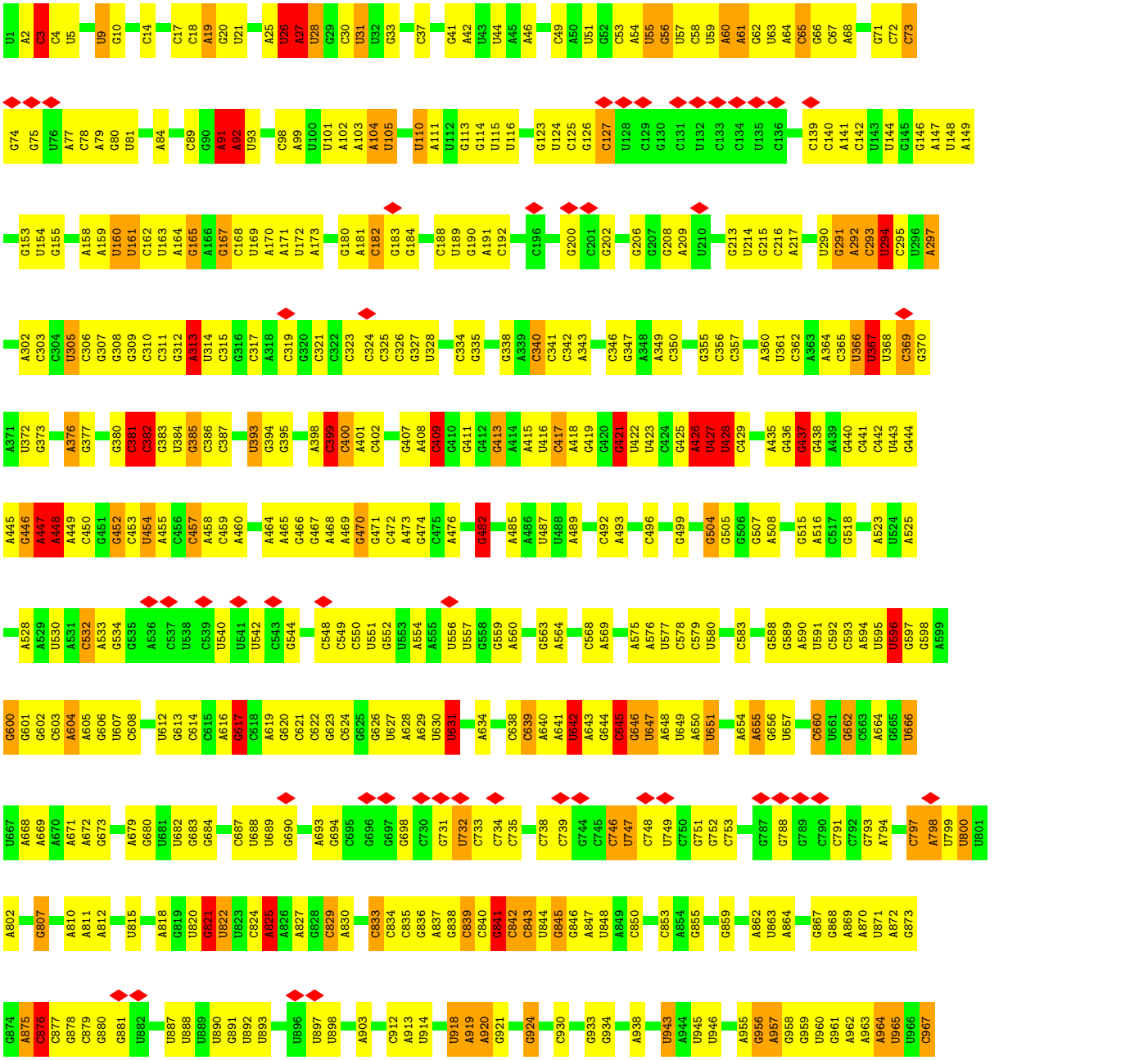
• Molecule 52: SRP68

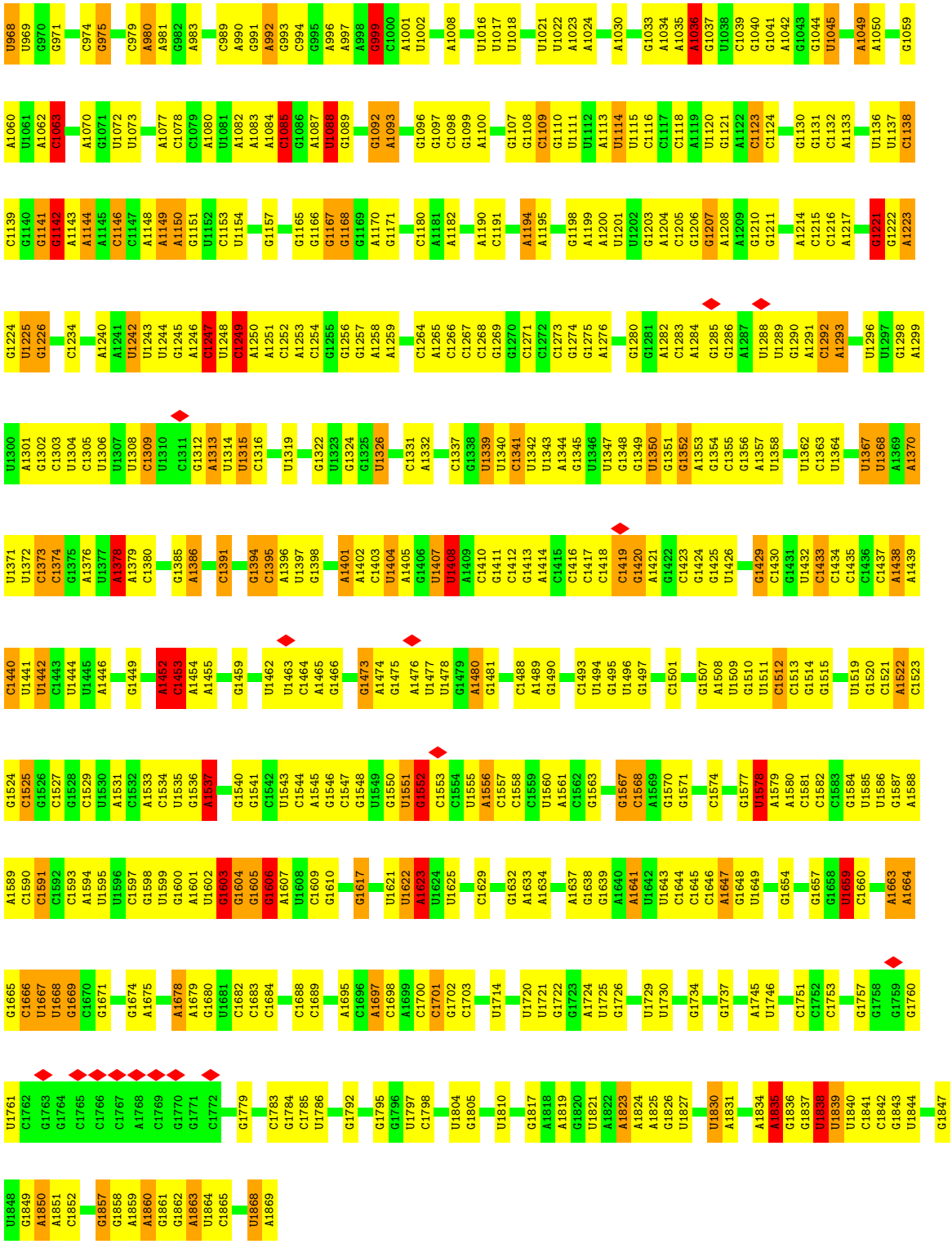




• Molecule 53: 18S ribosomal RNA

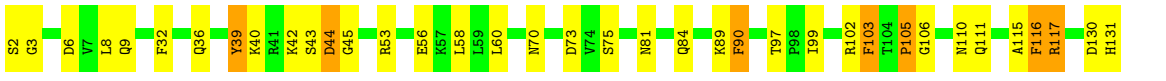
Chain S2:

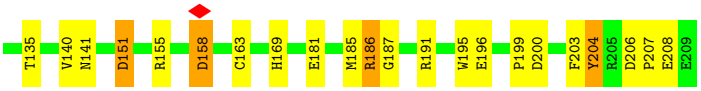




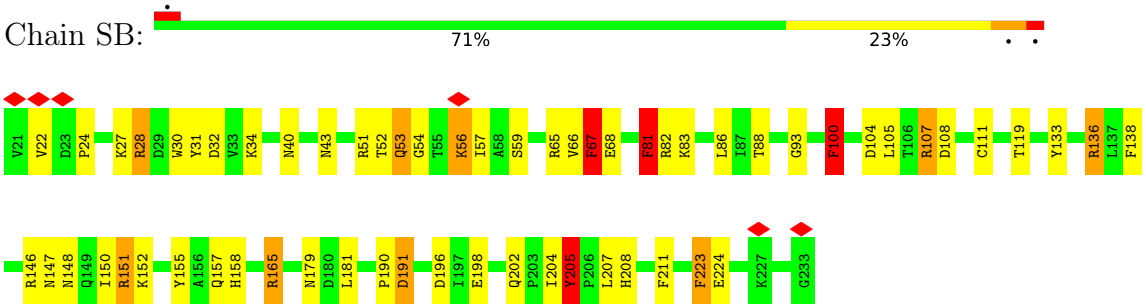
• Molecule 54: Ribosomal protein uS2

Chain SA:

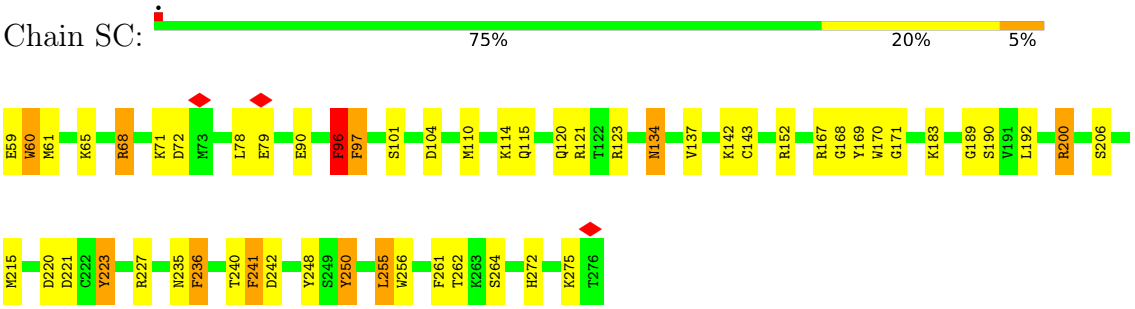




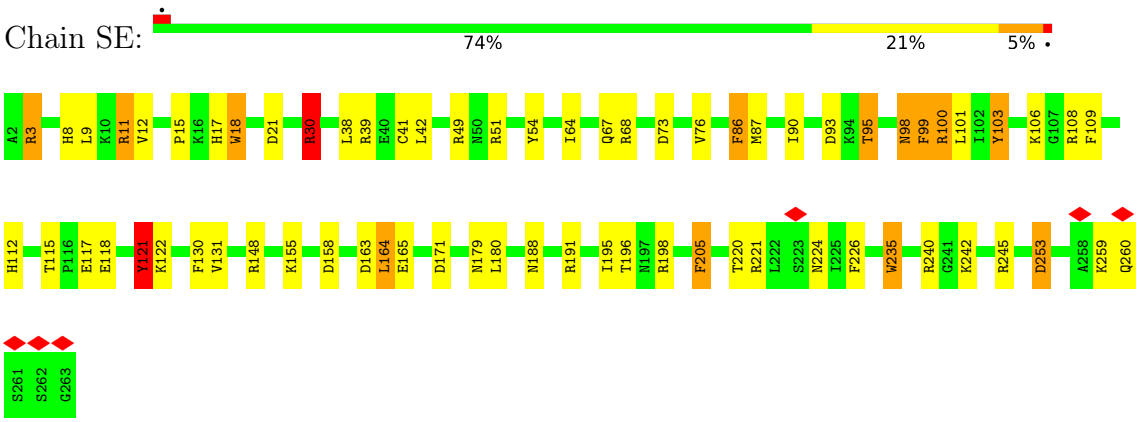
• Molecule 55: Ribosomal protein eS1



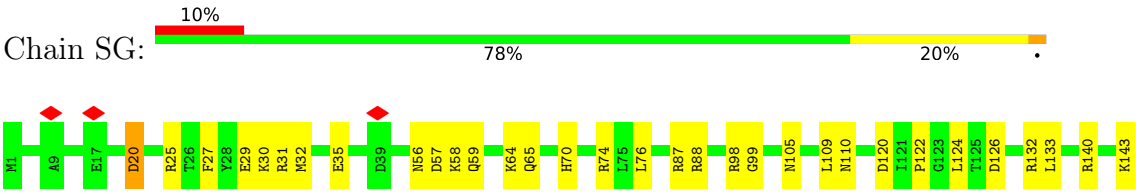
• Molecule 56: Ribosomal protein uS5

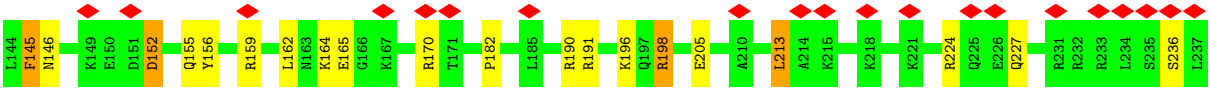


• Molecule 57: Ribosomal protein eS4

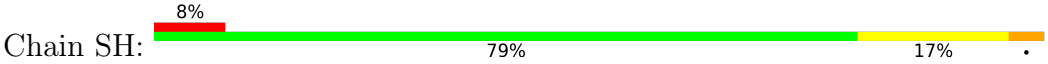


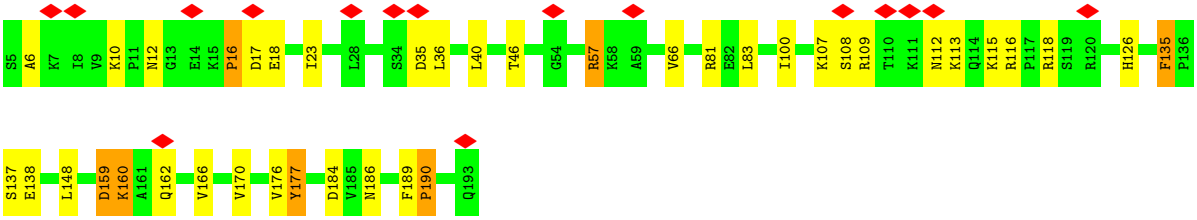
• Molecule 58: Ribosomal protein eS6



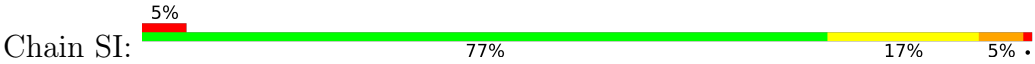


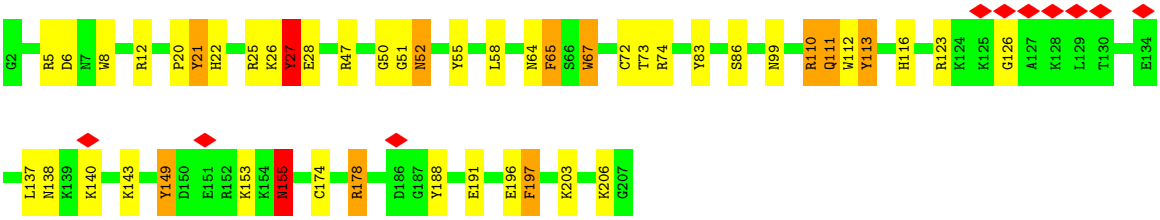
• Molecule 59: Ribosomal protein eS7



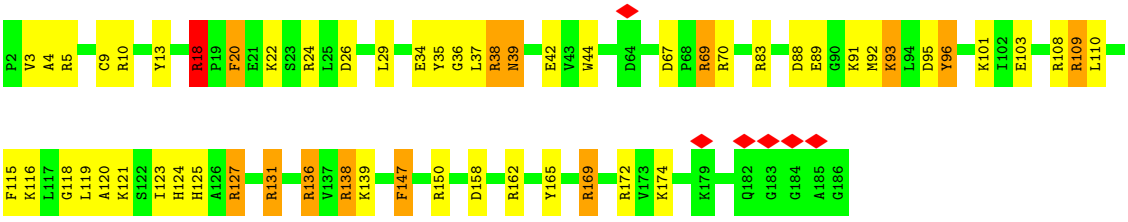


• Molecule 60: Ribosomal protein eS8

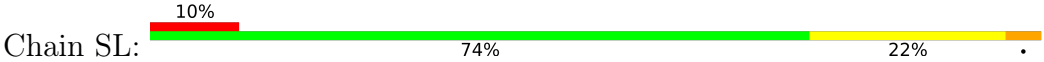


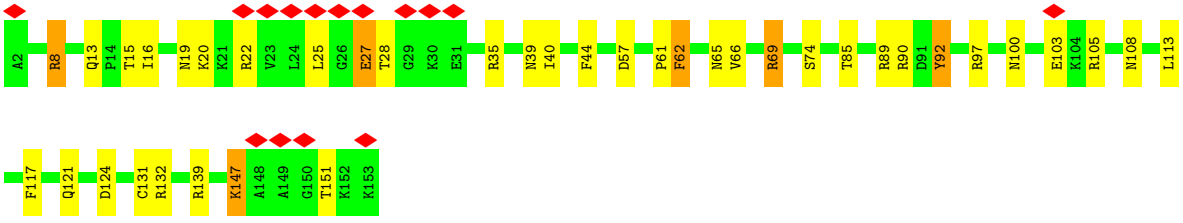


• Molecule 61: Ribosomal protein uS4



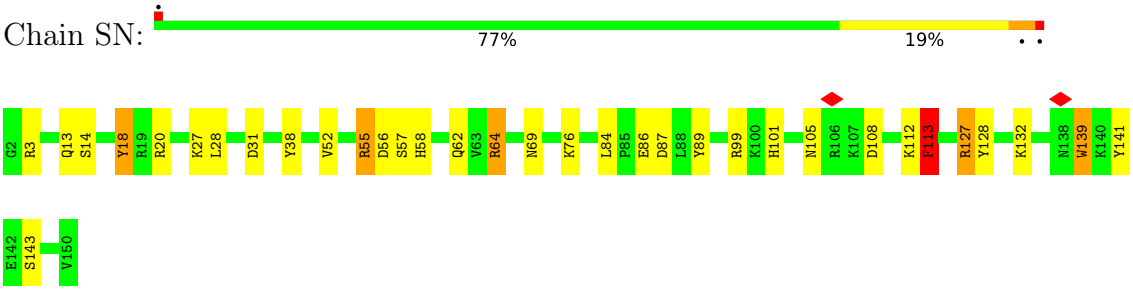
• Molecule 62: Ribosomal protein uS17





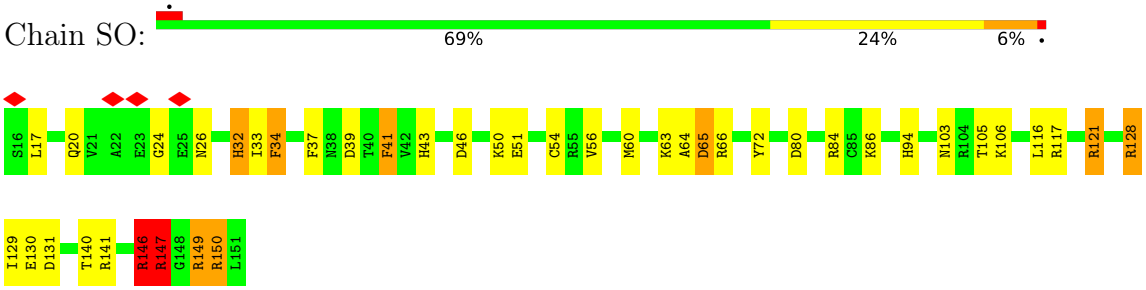
• Molecule 63: Ribosomal protein uS15

Chain SN:



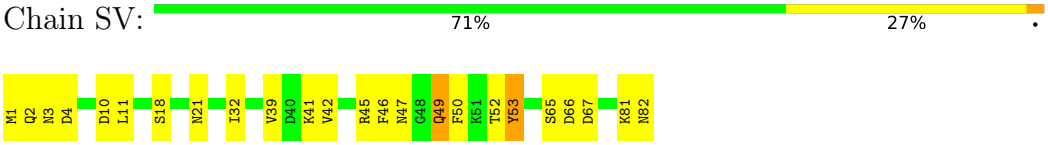
• Molecule 64: Ribosomal protein uS11

Chain SO:



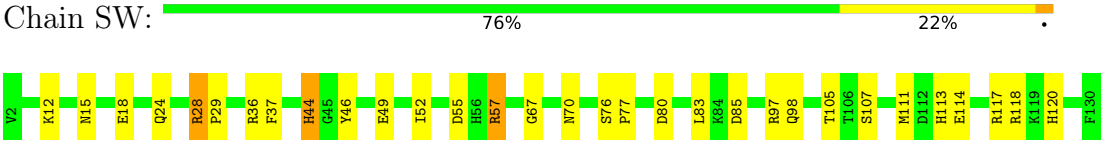
• Molecule 65: Ribosomal protein eS21

Chain SV:



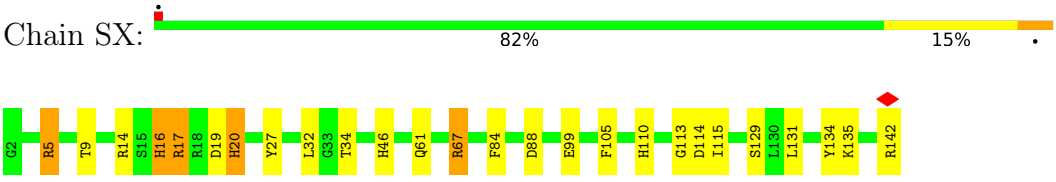
• Molecule 66: Ribosomal protein uS8

Chain SW:



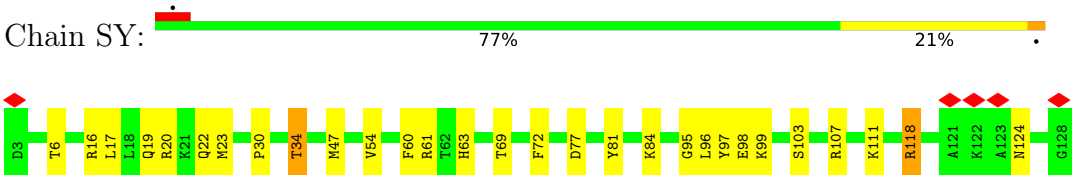
• Molecule 67: Ribosomal protein uS12

Chain SX:



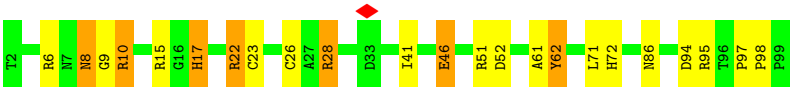
• Molecule 68: Ribosomal protein eS24

Chain SY:



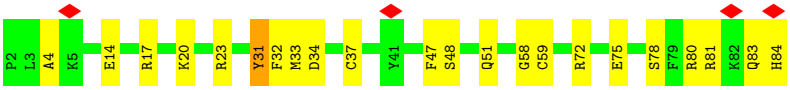
• Molecule 69: Ribosomal protein eS26

Chain Sa:



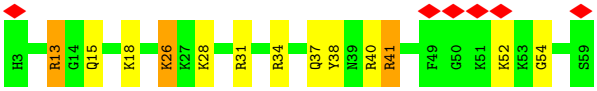
• Molecule 70: Ribosomal protein eS27

Chain Sb:



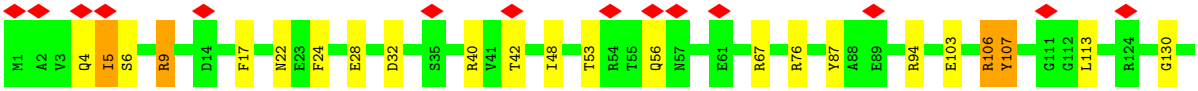
• Molecule 71: Ribosomal protein eS30

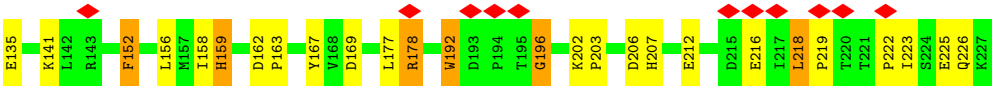
Chain Se:



• Molecule 72: Ribosomal protein uS3

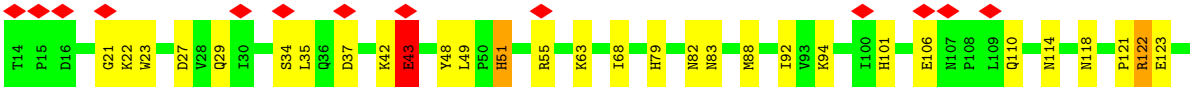
Chain SD:

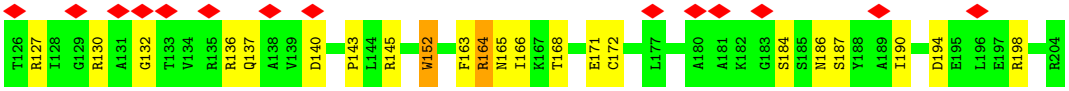




• Molecule 73: Ribosomal protein uS7

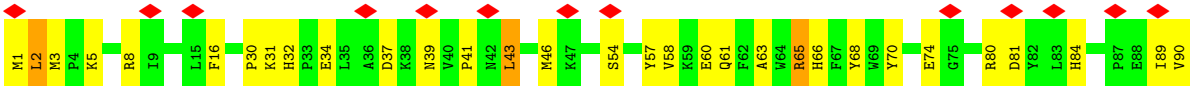
Chain SF:

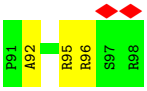




• Molecule 74: Ribosomal protein eS10

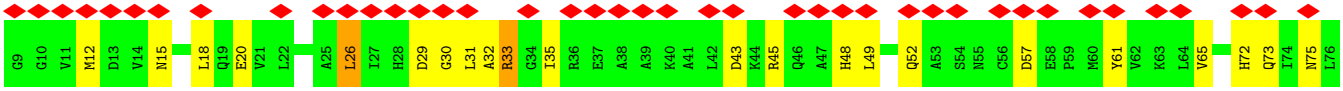
Chain SK:

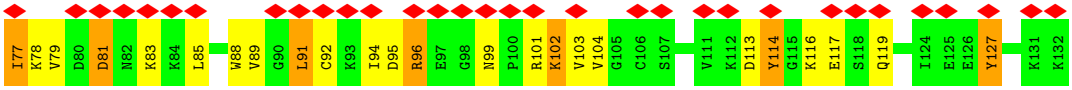




• Molecule 75: Ribosomal protein eS12

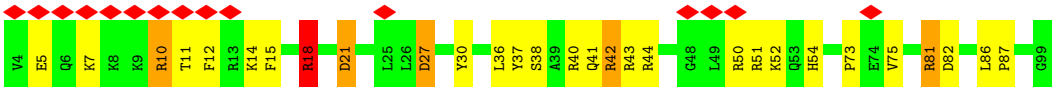
Chain SM:





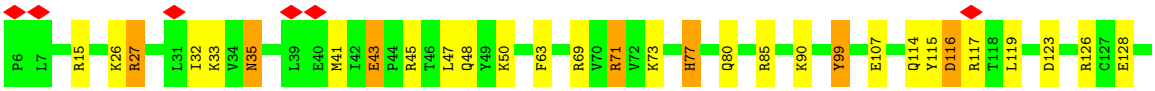
• Molecule 76: Ribosomal protein uS19

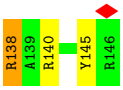
Chain SP:



• Molecule 77: Ribosomal protein uS9

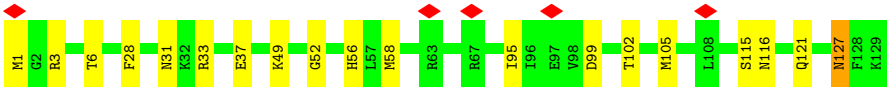
Chain SQ:





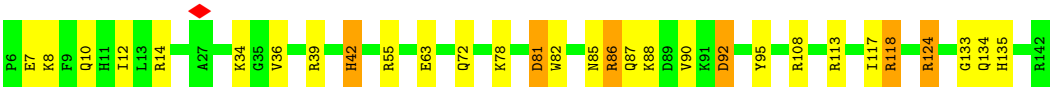
• Molecule 78: Ribosomal protein eS17

Chain SR:



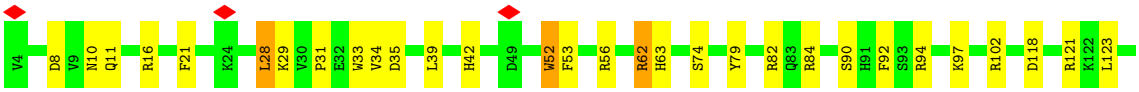
• Molecule 79: Ribosomal protein uS13

Chain SS:



• Molecule 80: Ribosomal protein eS19

Chain ST:

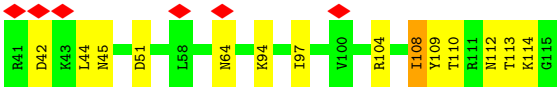


• Molecule 81: Ribosomal protein uS10

Chain SU:

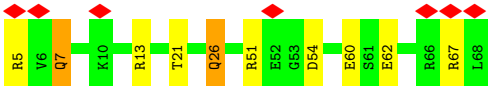
• Molecule 82: Ribosomal protein es25

Chain SZ:



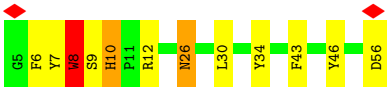
• Molecule 83: Ribosomal protein eS28

Chain Sc:



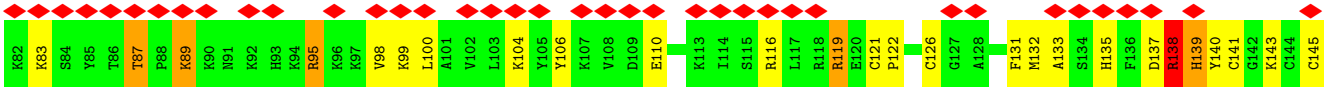
• Molecule 84: Ribosomal protein uS14

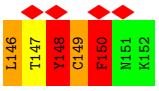
Chain Sd:



• Molecule 85: Ribosomal protein eS31

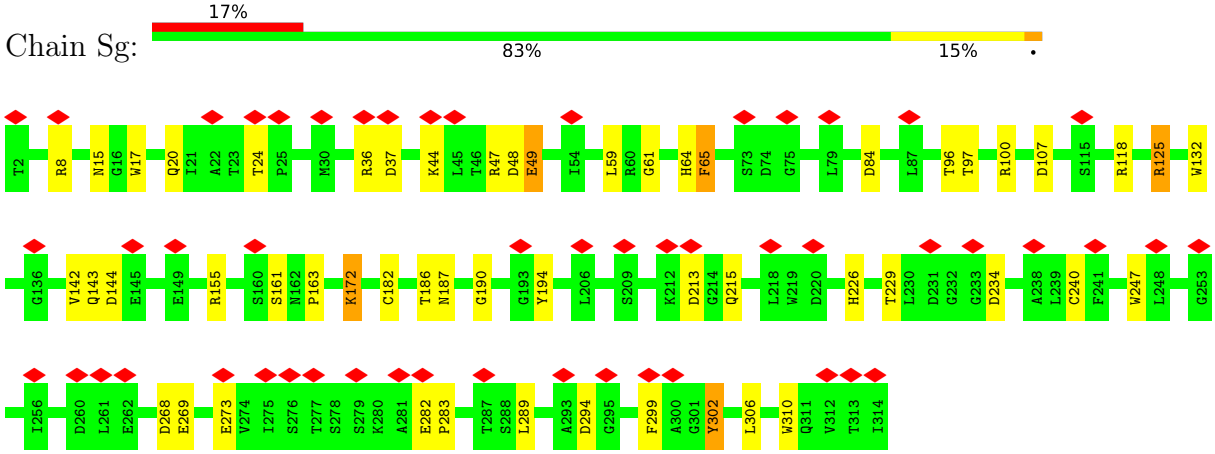
Chain Sf:





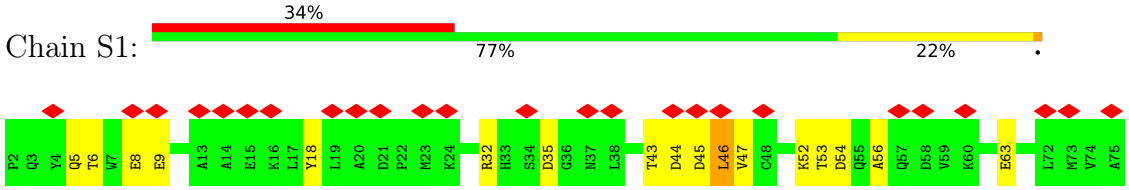
• Molecule 86: Ribosomal protein RACK1

Chain Sg:



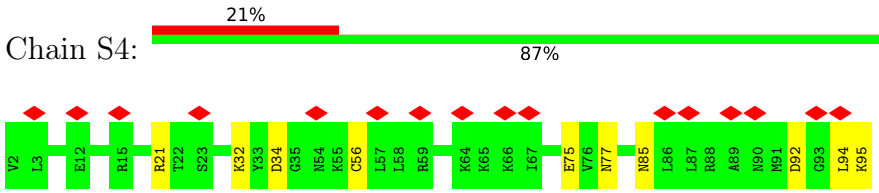
• Molecule 87: SRP9

Chain S1:



• Molecule 88: SRP14

Chain S4:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27627	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 ($e^-/Å^2$)	27	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.577	Depositor
Minimum map value	-0.384	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	562.8, 562.8, 562.8	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: ZN, MG

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	18/2556 (0.7%)
2	D	0.67	2/2426 (0.1%)	1.17	24/3252 (0.7%)
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	0.62	1/1152 (0.1%)	1.10	6/1539 (0.4%)
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	5/1770 (0.3%)
14	U	0.61	1/822 (0.1%)	0.99	1/1103 (0.1%)
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	1/903 (0.1%)	1.28	10/1216 (0.8%)
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	802/136805 (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	39/5766 (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	1.18	3/720 (0.4%)
42	j	0.83	1/721 (0.1%)	1.30	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	8/3171 (0.3%)	0.95	11/4257 (0.3%)
49	3	1.56	2/1804 (0.1%)	1.07	7/2805 (0.2%)
50	4	0.77	1/5090 (0.0%)	1.05	13/7936 (0.2%)
51	9	0.35	0/858	0.58	0/1156
52	6	0.30	0/1521	0.49	0/2039
53	S2	0.60	27/41241 (0.1%)	1.15	363/64249 (0.6%)
54	SA	0.63	1/1679 (0.1%)	1.05	10/2283 (0.4%)
55	SB	0.74	6/1753 (0.3%)	1.12	14/2350 (0.6%)
56	SC	0.69	1/1726 (0.1%)	1.05	14/2332 (0.6%)
57	SE	0.64	3/2118 (0.1%)	1.09	15/2849 (0.5%)
58	SG	0.69	4/1946 (0.2%)	1.05	8/2590 (0.3%)
59	SH	0.51	0/1544	0.94	5/2068 (0.2%)
60	SI	0.76	3/1715 (0.2%)	1.11	12/2287 (0.5%)
61	SJ	0.59	1/1550 (0.1%)	1.20	12/2069 (0.6%)
62	SL	0.66	1/1259 (0.1%)	1.05	4/1684 (0.2%)
63	SN	0.60	0/1226	1.05	7/1649 (0.4%)
64	SO	0.61	0/1029	1.23	13/1380 (0.9%)
65	SV	0.54	0/631	0.93	0/844
66	SW	0.64	1/1051 (0.1%)	1.03	6/1406 (0.4%)
67	SX	0.60	0/1118	1.06	10/1493 (0.7%)
68	SY	0.55	0/1040	0.94	0/1382
69	Sa	0.71	1/794 (0.1%)	1.16	6/1065 (0.6%)
70	Sb	0.48	0/665	0.90	1/891 (0.1%)
71	Se	0.50	0/458	0.97	3/602 (0.5%)
72	SD	0.60	1/1793 (0.1%)	1.01	5/2414 (0.2%)
73	SF	0.62	2/1531 (0.1%)	1.00	6/2059 (0.3%)
74	SK	0.58	0/851	1.01	5/1147 (0.4%)
75	SM	0.69	0/970	1.05	6/1300 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	SP	0.88	2/816 (0.2%)	1.19	10/1084 (0.9%)
77	SQ	0.51	0/1142	1.08	12/1528 (0.8%)
78	SR	0.50	0/1060	0.73	0/1421
79	SS	0.46	0/1157	1.00	5/1548 (0.3%)
80	ST	0.61	1/1119 (0.1%)	1.05	3/1499 (0.2%)
81	SU	0.52	0/828	0.91	0/1112
82	SZ	0.47	0/604	0.84	0/810
83	Sc	0.57	2/507 (0.4%)	0.75	0/677
84	Sd	0.66	0/445	1.12	2/589 (0.3%)
85	Sf	0.96	3/593 (0.5%)	1.61	15/786 (1.9%)
86	Sg	0.56	0/2493	0.85	3/3394 (0.1%)
87	S1	1.04	4/619 (0.6%)	0.90	1/832 (0.1%)
88	S4	0.88	2/608 (0.3%)	0.77	0/809
All	All	0.65	184/244482 (0.1%)	1.12	1884/358687 (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
22	d	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
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	173
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	1
45	r	0	3
46	K	0	10
47	q	0	8
48	z	0	7
53	S2	0	59
54	SA	0	5
55	SB	0	7
56	SC	0	7
57	SE	0	6
58	SG	0	1
59	SH	0	2
60	SI	0	9
61	SJ	0	3
62	SL	0	3
63	SN	0	5
64	SO	0	1
65	SV	0	3
66	SW	0	3
67	SX	0	2
68	SY	0	1
69	Sa	0	3
70	Sb	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
72	SD	0	3
73	SF	0	4
74	SK	0	1
75	SM	0	2
76	SP	0	3
77	SQ	0	1
79	SS	0	1
80	ST	0	2
81	SU	0	1
82	SZ	0	1
84	Sd	0	3
85	Sf	0	4
86	Sg	0	3
87	S1	0	4
All	All	0	525

All (184) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	3	31	C	O3'-P	-62.25	0.86	1.61
50	4	183	A	O3'-P	-44.21	1.08	1.61
32	5	1823	G	O3'-P	35.64	2.04	1.61
48	z	340	MET	C-N	22.91	1.86	1.34
48	z	345	PHE	C-N	-18.41	0.91	1.34
4	H	66	GLU	CD-OE1	18.34	1.45	1.25
12	S	96	GLU	CD-OE1	17.61	1.45	1.25
48	z	25	GLU	CD-OE2	16.69	1.44	1.25
88	S4	75	GLU	CD-OE1	15.11	1.42	1.25
49	3	39	G	O3'-P	-15.00	1.43	1.61
48	z	25	GLU	CD-OE1	14.67	1.41	1.25
11	R	149	LYS	C-N	14.58	1.67	1.34
76	SP	21	ASP	CG-OD1	13.73	1.56	1.25
58	SG	35	GLU	CD-OE1	13.71	1.40	1.25
12	S	96	GLU	CD-OE2	13.65	1.40	1.25
35	B	59	GLU	CD-OE2	13.58	1.40	1.25
87	S1	8	GLU	CD-OE1	13.57	1.40	1.25
3	G	54	PHE	CB-CG	-12.53	1.30	1.51
47	q	93	GLU	CD-OE1	12.50	1.39	1.25
5	J	14	GLU	CD-OE1	11.98	1.38	1.25
6	L	119	GLU	CD-OE1	11.74	1.38	1.25
12	S	81	TRP	CB-CG	-11.61	1.29	1.50
87	S1	44	ASP	CG-OD2	11.45	1.51	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	SC	90	GLU	CD-OE1	10.82	1.37	1.25
4	H	66	GLU	CD-OE2	10.73	1.37	1.25
60	SI	99	ASN	CG-OD1	10.67	1.47	1.24
88	S4	75	GLU	CD-OE2	10.62	1.37	1.25
48	z	198	GLU	CD-OE2	10.48	1.37	1.25
53	S2	1292	C	O3'-P	10.02	1.73	1.61
46	K	9	GLU	C-N	-9.96	1.11	1.34
11	R	95	TRP	CB-CG	-9.95	1.32	1.50
87	S1	8	GLU	CD-OE2	9.88	1.36	1.25
24	f	6	TRP	CB-CG	-9.74	1.32	1.50
48	z	198	GLU	CD-OE1	9.69	1.36	1.25
35	B	215	GLU	CD-OE1	9.29	1.35	1.25
60	SI	99	ASN	CG-ND2	9.21	1.55	1.32
12	S	81	TRP	CA-CB	9.19	1.74	1.53
55	SB	224	GLU	CD-OE2	9.06	1.35	1.25
53	S2	1309	C	O3'-P	9.05	1.72	1.61
36	C	35	ASP	CG-OD1	9.04	1.46	1.25
53	S2	1290	G	O3'-P	8.99	1.72	1.61
76	SP	21	ASP	CG-OD2	8.76	1.45	1.25
3	G	109	GLU	CD-OE2	8.62	1.35	1.25
73	SF	127	ARG	CZ-NH1	8.53	1.44	1.33
62	SL	27	GLU	CD-OE2	8.46	1.34	1.25
20	b	16	TRP	CB-CG	-8.43	1.35	1.50
36	C	35	ASP	CB-CG	8.42	1.69	1.51
40	P	139	TYR	CB-CG	-8.36	1.39	1.51
53	S2	1291	A	O3'-P	7.94	1.70	1.61
87	S1	44	ASP	CG-OD1	7.76	1.43	1.25
58	SG	205	GLU	CD-OE2	7.66	1.34	1.25
37	E	278	TYR	CB-CG	-7.55	1.40	1.51
35	B	74	GLU	CD-OE1	7.51	1.33	1.25
32	5	964	A	O3'-P	7.28	1.69	1.61
32	5	4390	A	O3'-P	-7.28	1.52	1.61
32	5	4497	U	O3'-P	7.26	1.69	1.61
37	E	278	TYR	CA-CB	7.24	1.69	1.53
40	P	139	TYR	CA-CB	7.21	1.69	1.53
58	SG	35	GLU	CD-OE2	7.15	1.33	1.25
3	G	109	GLU	CG-CD	7.13	1.62	1.51
5	J	14	GLU	CD-OE2	7.10	1.33	1.25
32	5	1887	G	O3'-P	7.04	1.69	1.61
32	5	514	U	O3'-P	6.97	1.69	1.61
3	G	54	PHE	N-CA	6.96	1.60	1.46
3	G	57	TRP	CB-CG	-6.95	1.37	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	46	GLN	CD-NE2	6.93	1.50	1.32
69	Sa	46	GLU	CD-OE1	6.79	1.33	1.25
32	5	3729	U	C4-O4	-6.72	1.18	1.23
53	S2	409	C	O3'-P	6.70	1.69	1.61
53	S2	1838	U	O3'-P	6.69	1.69	1.61
83	Sc	26	GLN	CD-OE1	6.67	1.38	1.24
57	SE	121	TYR	CB-CG	-6.67	1.41	1.51
8	N	119	TYR	CB-CG	-6.67	1.41	1.51
53	S2	662	G	O3'-P	6.64	1.69	1.61
32	5	2362	U	O3'-P	6.58	1.69	1.61
32	5	1669	A	O3'-P	-6.51	1.53	1.61
6	L	119	GLU	CD-OE2	6.49	1.32	1.25
32	5	1365	C	O3'-P	6.49	1.69	1.61
12	S	10	TYR	CB-CG	-6.48	1.42	1.51
3	G	54	PHE	CA-CB	6.47	1.68	1.53
46	K	2	PRO	CA-C	6.46	1.65	1.52
11	R	132	PHE	CB-CG	-6.42	1.40	1.51
10	Q	34	PHE	CA-CB	6.41	1.68	1.53
42	j	49	TRP	CB-CG	-6.40	1.38	1.50
58	SG	205	GLU	CD-OE1	6.36	1.32	1.25
32	5	1364	U	O3'-P	6.35	1.68	1.61
32	5	171	U	O3'-P	-6.33	1.53	1.61
32	5	2037	C	C2-O2	-6.30	1.18	1.24
13	T	111	GLU	CD-OE1	6.29	1.32	1.25
54	SA	151	ASP	CB-CG	6.28	1.65	1.51
12	S	10	TYR	CA-CB	6.24	1.67	1.53
32	5	2278	G	O3'-P	6.24	1.68	1.61
48	z	54	GLU	CD-OE2	6.21	1.32	1.25
32	5	1632	A	O3'-P	6.18	1.68	1.61
73	SF	152	TRP	CB-CG	-6.17	1.39	1.50
53	S2	1378	A	O3'-P	6.15	1.68	1.61
32	5	1522	G	O3'-P	6.14	1.68	1.61
32	5	3652	A	O3'-P	6.13	1.68	1.61
32	5	3905	A	O3'-P	6.13	1.68	1.61
35	B	257	TRP	CA-CB	6.11	1.67	1.53
53	S2	1623	A	O3'-P	6.08	1.68	1.61
39	I	171	TRP	CB-CG	-6.05	1.39	1.50
32	5	45	U	O3'-P	-6.02	1.53	1.61
32	5	3635	A	O3'-P	6.01	1.68	1.61
55	SB	198	GLU	CG-CD	6.00	1.60	1.51
85	Sf	146	LEU	CA-CB	5.96	1.67	1.53
32	5	4464	A	O3'-P	5.93	1.68	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	262	GLU	CD-OE2	5.92	1.32	1.25
32	5	1883	G	O3'-P	-5.92	1.54	1.61
2	D	44	TYR	CA-CB	5.91	1.67	1.53
53	S2	1207	G	O3'-P	-5.91	1.54	1.61
66	SW	49	GLU	CD-OE1	5.91	1.32	1.25
32	5	2268	A	O3'-P	5.90	1.68	1.61
60	SI	27	TYR	CB-CG	-5.87	1.42	1.51
53	S2	999	G	O3'-P	5.84	1.68	1.61
32	5	2459	G	O3'-P	5.81	1.68	1.61
53	S2	294	U	O3'-P	5.79	1.68	1.61
72	SD	192	TRP	CB-CG	5.79	1.60	1.50
80	ST	33	TRP	CA-CB	5.76	1.66	1.53
57	SE	18	TRP	CA-CB	5.74	1.66	1.53
55	SB	157	GLN	CD-OE1	5.73	1.36	1.24
83	Sc	26	GLN	CD-NE2	5.72	1.47	1.32
36	C	111	TRP	CB-CG	-5.72	1.40	1.50
53	S2	639	C	O3'-P	-5.70	1.54	1.61
55	SB	205	TYR	CB-CG	-5.70	1.43	1.51
32	5	1946	G	O3'-P	5.63	1.68	1.61
53	S2	876	C	O3'-P	5.63	1.68	1.61
47	q	93	GLU	CD-OE2	5.60	1.31	1.25
12	S	152	PHE	CB-CG	-5.60	1.41	1.51
7	M	6	PHE	CB-CG	-5.59	1.41	1.51
12	S	94	TYR	CE1-CZ	-5.56	1.31	1.38
53	S2	1473	G	O3'-P	5.54	1.67	1.61
32	5	1756	U	C4-O4	-5.50	1.19	1.23
12	S	33	PHE	CB-CG	-5.49	1.42	1.51
23	e	35	TRP	CB-CG	-5.49	1.40	1.50
55	SB	81	PHE	CB-CG	-5.49	1.42	1.51
53	S2	9	U	O3'-P	5.48	1.67	1.61
32	5	2520	C	O3'-P	-5.45	1.54	1.61
8	N	119	TYR	CA-CB	5.44	1.66	1.53
32	5	1681	G	O3'-P	5.44	1.67	1.61
55	SB	198	GLU	CD-OE2	5.43	1.31	1.25
20	b	16	TRP	CA-CB	5.42	1.65	1.53
32	5	4566	U	O3'-P	-5.41	1.54	1.61
14	U	99	TRP	CB-CG	-5.40	1.40	1.50
32	5	1301	C	O3'-P	5.39	1.67	1.61
53	S2	427	U	O5'-C5'	5.39	1.53	1.44
48	z	379	MET	C-N	5.39	1.46	1.34
32	5	3875	G	O3'-P	5.37	1.67	1.61
32	5	85	G	O3'-P	5.36	1.67	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	p	18	TYR	CB-CG	-5.35	1.43	1.51
3	G	53	ARG	CA-C	5.29	1.66	1.52
53	S2	1341	C	O3'-P	5.28	1.67	1.61
53	S2	92	A	O3'-P	5.28	1.67	1.61
22	d	108	TYR	CB-CG	-5.27	1.43	1.51
9	O	173	GLN	CD-OE1	5.26	1.35	1.24
6	L	31	ARG	CZ-NH2	5.24	1.39	1.33
8	N	120	TRP	CE3-CZ3	-5.22	1.29	1.38
32	5	2667	C	O3'-P	-5.22	1.54	1.61
32	5	2034	G	O3'-P	5.22	1.67	1.61
85	Sf	149	CYS	N-CA	5.22	1.56	1.46
53	S2	1170	A	O3'-P	-5.20	1.54	1.61
32	5	2253	A	O3'-P	5.19	1.67	1.61
53	S2	1839	U	O3'-P	5.19	1.67	1.61
32	5	3653	A	O3'-P	5.16	1.67	1.61
53	S2	1659	U	O3'-P	5.16	1.67	1.61
53	S2	1293	A	O3'-P	5.16	1.67	1.61
1	A	211	PHE	CB-CG	-5.15	1.42	1.51
61	SJ	34	GLU	CG-CD	5.15	1.59	1.51
85	Sf	150	PHE	CB-CG	5.14	1.60	1.51
35	B	257	TRP	CE3-CZ3	-5.14	1.29	1.38
53	S2	440	G	O3'-P	-5.13	1.54	1.61
53	S2	426	A	O3'-P	5.13	1.67	1.61
10	Q	34	PHE	CB-CG	-5.12	1.42	1.51
9	O	162	GLU	CD-OE1	5.12	1.31	1.25
2	D	95	TYR	CA-CB	5.09	1.65	1.53
53	S2	1370	A	O3'-P	5.09	1.67	1.61
40	P	139	TYR	CD1-CE1	-5.09	1.31	1.39
53	S2	427	U	C5'-C4'	5.07	1.57	1.51
57	SE	86	PHE	CA-CB	5.06	1.65	1.53
34	8	73	U	O3'-P	5.06	1.67	1.61
12	S	29	ARG	CA-CB	5.04	1.65	1.53
35	B	367	PHE	CB-CG	-5.04	1.42	1.51
37	E	250	ASP	CG-OD2	5.00	1.36	1.25
32	5	1609	U	O3'-P	5.00	1.67	1.61

All (1884) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	3	38	C	P-O3'-C3'	-20.62	94.95	119.70
48	z	340	MET	O-C-N	19.47	153.86	122.70
49	3	31	C	O3'-P-O5'	-18.73	68.41	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	z	340	MET	C-N-CA	-18.61	75.16	121.70
85	Sf	146	LEU	CA-CB-CG	16.38	152.97	115.30
48	z	340	MET	CA-C-N	-16.02	81.95	117.20
53	S2	3	C	N1-C1'-C2'	15.70	134.41	114.00
53	S2	1838	U	N1-C1'-C2'	14.63	133.03	114.00
32	5	1501	C	N1-C1'-C2'	14.22	132.48	114.00
53	S2	92	A	N9-C1'-C2'	13.96	132.15	114.00
32	5	1501	C	O4'-C1'-N1	12.76	118.41	108.20
32	5	1697	G	N9-C1'-C2'	12.64	130.43	114.00
53	S2	367	U	N1-C1'-C2'	-12.63	97.58	114.00
53	S2	294	U	N1-C1'-C2'	12.62	130.41	114.00
32	5	2396	A	N9-C1'-C2'	12.09	129.72	114.00
1	A	67	TYR	CA-CB-CG	12.03	136.26	113.40
69	Sa	28	ARG	NE-CZ-NH1	11.86	126.23	120.30
53	S2	428	U	N1-C1'-C2'	11.82	129.36	114.00
32	5	336	A	O4'-C1'-N9	11.76	117.61	108.20
53	S2	1835	A	N9-C1'-C2'	11.75	129.27	114.00
53	S2	447	A	O4'-C1'-N9	11.66	117.53	108.20
32	5	1	C	N1-C1'-C2'	11.66	129.16	114.00
32	5	2513	A	N9-C1'-C2'	11.65	129.14	114.00
3	G	54	PHE	CB-CG-CD1	-11.60	112.68	120.80
48	z	345	PHE	C-N-CA	11.60	150.69	121.70
32	5	2361	G	N9-C1'-C2'	-11.50	99.05	114.00
53	S2	1063	C	N1-C1'-C2'	-11.45	99.12	114.00
32	5	664	G	O4'-C1'-N9	11.39	117.31	108.20
53	S2	1452	A	N9-C1'-C2'	11.36	128.77	114.00
32	5	5040	U	N1-C1'-C2'	11.24	128.61	114.00
50	4	186	C	O3'-P-O5'	-11.24	82.65	104.00
32	5	151	G	N9-C1'-C2'	-11.21	99.43	114.00
32	5	2046	G	O4'-C1'-N9	11.21	117.17	108.20
32	5	336	A	C8-N9-C1'	-11.11	107.71	127.70
32	5	4234	A	N9-C1'-C2'	11.05	128.36	114.00
32	5	1370	G	N9-C1'-C2'	11.05	128.36	114.00
53	S2	1247	C	N1-C1'-C2'	11.00	128.30	114.00
32	5	2268	A	N9-C1'-C2'	11.00	128.30	114.00
32	5	2438	A	N9-C1'-C2'	-10.97	99.73	114.00
53	S2	1823	A	N9-C1'-C2'	10.92	128.19	114.00
32	5	1938	C	N1-C1'-C2'	10.89	128.16	114.00
1	A	3	ARG	NE-CZ-NH1	10.81	125.71	120.30
32	5	2586	G	N9-C1'-C2'	10.79	128.03	114.00
32	5	4911	A	O4'-C1'-N9	10.76	116.81	108.20
32	5	4693	C	O4'-C1'-N1	-10.71	99.63	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	R	132	PHE	CB-CA-C	10.67	131.75	110.40
32	5	2436	U	N1-C1'-C2'	10.61	127.80	114.00
32	5	4373	G	N9-C1'-C2'	10.61	127.79	114.00
32	5	2806	A	N9-C1'-C2'	-10.59	100.23	114.00
37	E	278	TYR	CA-CB-CG	-10.55	93.36	113.40
32	5	4871	C	N1-C1'-C2'	10.49	127.64	114.00
32	5	2389	A	C2'-C3'-O3'	10.45	132.49	109.50
32	5	2394	G	N9-C1'-C2'	-10.43	100.44	114.00
32	5	4275	G	N9-C1'-C2'	-10.40	100.48	114.00
34	8	70	G	N9-C1'-C2'	-10.38	100.51	114.00
32	5	2553	A	N9-C1'-C2'	10.35	127.45	114.00
33	7	56	G	N9-C1'-C2'	10.30	127.40	114.00
26	h	93	ARG	NE-CZ-NH1	10.27	125.44	120.30
32	5	4162	C	N1-C1'-C2'	10.24	127.31	114.00
12	S	81	TRP	CA-CB-CG	-10.22	94.27	113.70
53	S2	1088	U	N1-C1'-C2'	10.20	127.26	114.00
32	5	2465	C	N1-C1'-C2'	10.20	127.26	114.00
85	Sf	119	ARG	NE-CZ-NH1	10.16	125.38	120.30
32	5	280	G	O4'-C1'-N9	10.15	116.32	108.20
53	S2	421	G	N9-C1'-C2'	10.13	127.17	114.00
32	5	30	C	N1-C1'-C2'	10.13	127.17	114.00
32	5	4163	U	C4'-C3'-O3'	10.12	133.24	113.00
32	5	3938	G	N9-C1'-C2'	10.11	127.14	114.00
76	SP	21	ASP	CB-CG-OD1	-10.08	109.23	118.30
53	S2	437	G	N9-C1'-C2'	10.07	127.09	114.00
3	G	54	PHE	CB-CG-CD2	-10.07	113.75	120.80
34	8	85	U	C2'-C3'-O3'	10.04	131.60	109.50
34	8	14	U	N1-C1'-C2'	9.99	126.99	114.00
53	S2	1552	G	C2'-C3'-O3'	9.98	131.46	109.50
10	Q	34	PHE	N-CA-CB	9.97	128.54	110.60
61	SJ	127	ARG	NE-CZ-NH1	9.88	125.24	120.30
53	S2	1408	U	N1-C1'-C2'	9.86	126.81	114.00
64	SO	146	ARG	NE-CZ-NH2	-9.86	115.37	120.30
11	R	108	ARG	NE-CZ-NH1	9.85	125.23	120.30
32	5	1398	A	N9-C1'-C2'	9.82	126.77	114.00
32	5	4528	G	C2'-C3'-O3'	9.82	131.10	109.50
22	d	85	ARG	NE-CZ-NH1	9.82	125.21	120.30
61	SJ	131	ARG	NE-CZ-NH2	-9.80	115.40	120.30
10	Q	37	ARG	NE-CZ-NH2	9.78	125.19	120.30
19	a	79	TRP	CA-CB-CG	-9.78	95.12	113.70
32	5	1474	C	C2'-C3'-O3'	9.76	130.98	109.50
12	S	81	TRP	CB-CA-C	9.75	129.91	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	Sf	143	LYS	CD-CE-NZ	9.75	134.12	111.70
32	5	4464	A	O4'-C1'-N9	-9.73	100.41	108.20
53	S2	833	C	C2'-C3'-O3'	9.72	130.89	109.50
42	j	66	HIS	N-CA-CB	9.71	128.08	110.60
32	5	4404	U	N1-C1'-C2'	-9.70	101.33	112.00
32	5	5043	A	N9-C1'-C2'	9.69	126.59	114.00
32	5	4693	C	N1-C1'-C2'	9.65	126.55	114.00
32	5	3938	G	O4'-C1'-N9	-9.64	100.49	108.20
42	j	11	ARG	NE-CZ-NH2	-9.63	115.49	120.30
20	b	44	ARG	NE-CZ-NH1	9.60	125.10	120.30
22	d	44	ARG	NE-CZ-NH1	9.60	125.10	120.30
46	K	9	GLU	O-C-N	-9.60	107.35	122.70
37	E	278	TYR	CB-CA-C	9.58	129.55	110.40
77	SQ	71	ARG	NE-CZ-NH1	9.54	125.07	120.30
32	5	93	G	N9-C1'-C2'	9.54	126.40	114.00
32	5	2666	U	N1-C1'-C2'	-9.54	101.51	112.00
32	5	1974	U	N1-C1'-C2'	9.52	126.37	114.00
22	d	25	TYR	CA-CB-CG	-9.50	95.34	113.40
32	5	2446	C	N1-C1'-C2'	9.49	126.34	114.00
32	5	31	U	N1-C1'-C2'	9.49	126.33	114.00
32	5	2087	C	N1-C1'-C2'	-9.47	101.58	112.00
31	o	78	ARG	NE-CZ-NH2	9.47	125.03	120.30
27	i	85	ARG	NE-CZ-NH1	9.40	125.00	120.30
8	N	131	GLU	CA-CB-CG	9.39	134.07	113.40
32	5	4221	C	N1-C1'-C2'	-9.38	101.68	112.00
60	SI	197	PHE	N-CA-CB	9.38	127.49	110.60
32	5	1815	G	N9-C1'-C2'	9.37	126.18	114.00
53	S2	666	U	N1-C1'-C2'	9.35	126.16	114.00
9	O	135	PHE	N-CA-C	9.34	136.21	111.00
54	SA	117	ARG	NE-CZ-NH1	9.32	124.96	120.30
32	5	2851	G	N9-C1'-C2'	-9.32	101.75	112.00
4	H	54	ARG	NE-CZ-NH1	9.31	124.96	120.30
32	5	1211	G	C2'-C3'-O3'	9.27	129.90	109.50
32	5	4265	U	N1-C1'-C2'	9.27	126.05	114.00
53	S2	1838	U	O4'-C1'-N1	-9.26	100.79	108.20
53	S2	1249	C	N1-C1'-C2'	-9.26	101.82	112.00
53	S2	313	A	O4'-C1'-N9	9.25	115.60	108.20
32	5	974	C	C2'-C3'-O3'	9.24	129.82	109.50
32	5	2511	A	C4'-C3'-O3'	-9.23	90.02	109.40
76	SP	81	ARG	NE-CZ-NH1	9.22	124.91	120.30
7	M	109	ARG	NE-CZ-NH2	9.20	124.90	120.30
53	S2	631	U	N1-C1'-C2'	9.18	125.94	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	R	132	PHE	N-CA-C	-9.18	86.22	111.00
32	5	3790	U	N1-C1'-C2'	9.18	125.93	114.00
5	J	54	ARG	NE-CZ-NH1	9.17	124.89	120.30
32	5	1853	G	N9-C1'-C2'	-9.16	101.92	112.00
3	G	235	ARG	NE-CZ-NH1	9.14	124.87	120.30
32	5	1379	C	O4'-C1'-N1	9.10	115.48	108.20
11	R	132	PHE	CB-CG-CD1	-9.09	114.44	120.80
32	5	4228	G	N9-C1'-C2'	-9.07	102.03	112.00
61	SJ	69	ARG	NE-CZ-NH2	9.06	124.83	120.30
7	M	6	PHE	CB-CG-CD2	-9.04	114.47	120.80
32	5	5046	U	C2'-C3'-O3'	9.04	129.39	109.50
53	S2	73	C	O4'-C1'-N1	9.04	115.43	108.20
3	G	57	TRP	CA-CB-CG	-9.04	96.53	113.70
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
25	g	66	ARG	NE-CZ-NH1	9.01	124.80	120.30
56	SC	200	ARG	NE-CZ-NH2	8.99	124.80	120.30
32	5	1324	A	N9-C1'-C2'	8.98	125.67	114.00
53	S2	1429	G	C2'-C3'-O3'	8.97	129.25	109.50
86	Sg	125	ARG	NE-CZ-NH2	-8.96	115.82	120.30
32	5	1214	C	N1-C1'-C2'	8.96	125.64	114.00
57	SE	103	TYR	CA-CB-CG	8.95	130.41	113.40
32	5	62	A	N9-C1'-C2'	8.93	125.60	114.00
53	S2	1292	C	C4'-C3'-O3'	8.93	130.85	113.00
79	SS	86	ARG	NE-CZ-NH1	-8.90	115.85	120.30
32	5	1296	G	O4'-C1'-N9	8.86	115.29	108.20
44	p	85	ARG	NE-CZ-NH1	8.85	124.72	120.30
64	SO	147	ARG	CA-CB-CG	8.82	132.81	113.40
53	S2	1313	A	N9-C1'-C2'	8.82	125.46	114.00
77	SQ	138	ARG	NE-CZ-NH1	8.81	124.71	120.30
32	5	1668	A	N9-C1'-C2'	8.80	125.44	114.00
24	f	36	ARG	NE-CZ-NH1	8.80	124.70	120.30
66	SW	57	ARG	NE-CZ-NH1	8.80	124.70	120.30
5	J	35	ARG	NE-CZ-NH1	8.77	124.69	120.30
32	5	315	G	O4'-C1'-N9	8.77	115.21	108.20
32	5	514	U	N1-C1'-C2'	-8.76	102.37	112.00
32	5	1887	G	N9-C1'-C2'	-8.75	102.38	112.00
53	S2	1419	C	C2'-C3'-O3'	8.75	128.74	109.50
19	a	62	HIS	N-CA-CB	8.74	126.33	110.60
32	5	336	A	C1'-O4'-C4'	-8.74	102.91	109.90
40	P	3	ARG	NE-CZ-NH1	8.73	124.67	120.30
79	SS	124	ARG	NE-CZ-NH1	8.73	124.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
67	SX	27	TYR	CA-CB-CG	8.72	129.97	113.40
32	5	150	U	O4'-C1'-N1	8.70	115.16	108.20
80	ST	62	ARG	NE-CZ-NH2	8.69	124.65	120.30
32	5	3683	C	N1-C1'-C2'	8.69	125.29	114.00
32	5	3906	A	N9-C1'-C2'	-8.68	102.45	112.00
32	5	3908	A	N9-C1'-C2'	8.67	125.27	114.00
32	5	2263	A	O4'-C1'-N9	-8.66	101.27	108.20
17	Y	75	ARG	CG-CD-NE	8.65	129.96	111.80
2	D	265	ARG	NE-CZ-NH1	8.63	124.62	120.30
63	SN	18	TYR	N-CA-CB	8.63	126.14	110.60
18	Z	36	ARG	NE-CZ-NH1	8.62	124.61	120.30
12	S	28	TYR	CB-CG-CD1	8.60	126.16	121.00
32	5	2406	G	N9-C1'-C2'	-8.60	102.54	112.00
53	S2	399	C	N1-C1'-C2'	-8.59	102.55	112.00
32	5	1916	G	N9-C1'-C2'	8.58	125.16	114.00
32	5	72	C	O4'-C1'-N1	8.57	115.06	108.20
53	S2	747	U	C2'-C3'-O3'	8.56	128.34	109.50
39	I	171	TRP	CA-CB-CG	-8.56	97.44	113.70
32	5	4880	C	N1-C1'-C2'	8.55	125.11	114.00
32	5	336	A	C4-N9-C1'	8.53	141.65	126.30
32	5	962	C	N1-C1'-C2'	8.50	125.05	114.00
32	5	3868	G	N9-C1'-C2'	-8.50	102.64	112.00
53	S2	448	A	N9-C1'-C2'	-8.49	102.66	112.00
32	5	292	G	N9-C1'-C2'	8.49	125.03	114.00
34	8	81	C	O4'-C1'-N1	8.49	114.99	108.20
32	5	42	A	O4'-C1'-N9	8.48	114.99	108.20
53	S2	1623	A	C2'-C3'-O3'	8.48	128.15	109.50
32	5	1637	A	N9-C1'-C2'	-8.47	102.68	112.00
32	5	92	C	N1-C1'-C2'	-8.47	102.68	112.00
32	5	118	C	C2'-C3'-O3'	8.46	128.12	109.50
32	5	1534	A	O4'-C1'-N9	-8.44	101.44	108.20
32	5	4234	A	O4'-C1'-N9	-8.44	101.45	108.20
32	5	2796	G	N9-C1'-C2'	8.44	124.97	114.00
32	5	5001	U	N1-C1'-C2'	8.43	124.96	114.00
8	N	180	PHE	CB-CA-C	8.42	127.25	110.40
32	5	4464	A	C2'-C3'-O3'	8.42	128.03	109.50
32	5	1631	A	O4'-C1'-N9	-8.41	101.47	108.20
32	5	2398	U	C2'-C3'-O3'	8.41	127.99	109.50
53	S2	1578	U	N1-C1'-C2'	8.40	124.92	114.00
32	5	1325	C	N1-C1'-C2'	8.40	124.92	114.00
32	5	3879	G	N9-C1'-C2'	-8.39	102.77	112.00
64	SO	146	ARG	NE-CZ-NH1	8.39	124.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	S2	596	U	N1-C1'-C2'	8.38	124.90	114.00
32	5	4194	U	N1-C1'-C2'	-8.38	102.78	112.00
53	S2	91	A	N9-C1'-C2'	-8.37	102.79	112.00
32	5	4280	A	C2'-C3'-O3'	8.35	127.87	109.50
32	5	292	G	O4'-C1'-N9	-8.35	101.52	108.20
17	Y	126	ARG	NE-CZ-NH1	8.35	124.47	120.30
53	S2	1114	U	N1-C1'-C2'	8.35	124.85	114.00
32	5	4280	A	N9-C1'-C2'	-8.33	102.84	112.00
21	c	56	ARG	NE-CZ-NH1	8.33	124.46	120.30
32	5	1329	G	C2'-C3'-O3'	8.32	127.81	109.50
32	5	1356	U	C2'-C3'-O3'	8.32	127.80	109.50
32	5	1946	G	N9-C1'-C2'	-8.31	102.86	112.00
32	5	4119	C	C2'-C3'-O3'	8.31	127.78	109.50
32	5	4464	A	C5'-C4'-O4'	8.31	119.07	109.10
32	5	2280	G	N9-C1'-C2'	8.30	124.79	114.00
53	S2	956	G	N9-C1'-C2'	8.30	124.79	114.00
32	5	668	C	C2'-C3'-O3'	8.29	127.74	109.50
55	SB	107	ARG	NE-CZ-NH1	8.29	124.44	120.30
53	S2	604	A	C2'-C3'-O3'	8.29	127.73	109.50
32	5	3790	U	O4'-C1'-N1	-8.28	101.57	108.20
53	S2	645	C	N1-C1'-C2'	-8.28	102.89	112.00
9	O	140	ARG	NE-CZ-NH2	8.24	124.42	120.30
32	5	977	C	C2'-C3'-O3'	8.24	127.62	109.50
32	5	1481	C	C2'-C3'-O3'	8.22	127.59	109.50
32	5	1890	G	N9-C1'-C2'	-8.22	102.96	112.00
32	5	964	A	C4'-C3'-O3'	8.20	129.39	113.00
32	5	2124	G	C2'-C3'-O3'	8.20	127.53	109.50
16	X	73	HIS	CB-CA-C	8.19	126.78	110.40
32	5	1522	G	N9-C1'-C2'	-8.19	102.99	112.00
32	5	4885	U	C2'-C3'-O3'	8.19	127.52	109.50
32	5	2046	G	C1'-O4'-C4'	-8.18	103.36	109.90
32	5	157	U	O4'-C1'-N1	8.17	114.74	108.20
41	W	44	ARG	NE-CZ-NH1	8.17	124.39	120.30
53	S2	1167	G	N9-C1'-C2'	8.17	124.62	114.00
32	5	1881	C	N1-C1'-C2'	8.16	124.60	114.00
32	5	2848	G	N9-C1'-C2'	-8.15	103.03	112.00
19	a	79	TRP	CB-CA-C	8.15	126.70	110.40
32	5	5040	U	C4'-C3'-O3'	-8.15	92.29	109.40
22	d	25	TYR	CB-CA-C	8.14	126.69	110.40
32	5	157	U	N1-C1'-C2'	-8.14	103.04	112.00
55	SB	205	TYR	CA-CB-CG	-8.14	97.93	113.40
32	5	1685	G	N9-C1'-C2'	8.14	124.58	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	5	1650	A	C4-N9-C1'	-8.14	111.65	126.30
67	SX	5	ARG	NE-CZ-NH2	8.14	124.37	120.30
37	E	268	ARG	NE-CZ-NH1	8.12	124.36	120.30
53	S2	1352	G	C2'-C3'-O3'	8.12	127.37	109.50
32	5	1805	A	N9-C1'-C2'	8.12	124.55	114.00
32	5	2271	C	N1-C1'-C2'	8.12	124.55	114.00
32	5	4163	U	N1-C1'-C2'	-8.12	103.07	112.00
32	5	72	C	C1'-O4'-C4'	-8.11	103.41	109.90
34	8	34	U	C4'-C3'-O3'	-8.11	92.37	109.40
49	3	31	C	OP2-P-O3'	8.11	123.04	105.20
73	SF	127	ARG	NE-CZ-NH2	-8.08	116.26	120.30
57	SE	30	ARG	NE-CZ-NH1	8.07	124.33	120.30
32	5	1272	C	O4'-C1'-N1	8.06	114.65	108.20
32	5	1365	C	N1-C1'-C2'	8.05	124.47	114.00
53	S2	1519	U	N1-C1'-C2'	8.06	124.47	114.00
32	5	172	C	O4'-C1'-N1	8.05	114.64	108.20
36	C	78	ARG	NE-CZ-NH1	8.05	124.33	120.30
53	S2	1225	U	N1-C1'-C2'	-8.04	103.15	112.00
63	SN	18	TYR	CA-CB-CG	-8.04	98.12	113.40
32	5	3905	A	C2'-C3'-O3'	8.04	127.19	109.50
55	SB	165	ARG	NE-CZ-NH2	8.03	124.32	120.30
76	SP	10	ARG	NE-CZ-NH1	8.03	124.32	120.30
32	5	187	U	C2'-C3'-O3'	8.03	127.16	109.50
53	S2	73	C	N1-C1'-C2'	8.03	124.44	114.00
32	5	4464	A	N9-C1'-C2'	8.03	124.43	114.00
32	5	3635	A	N9-C1'-C2'	-8.02	103.18	112.00
39	I	4	ARG	CG-CD-NE	-8.01	94.98	111.80
53	S2	798	A	C2'-C3'-O3'	8.00	127.10	109.50
32	5	88	A	N9-C1'-C2'	7.99	124.39	114.00
25	g	9	ARG	CG-CD-NE	-7.97	95.06	111.80
32	5	1279	A	C2'-C3'-O3'	7.97	127.04	109.50
32	5	2394	G	O4'-C1'-N9	7.97	114.58	108.20
32	5	2790	U	N1-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	-7.95	98.29	113.40
32	5	219	G	O5'-P-OP2	-7.95	98.55	105.70
53	S2	662	G	N9-C1'-C2'	7.95	124.33	114.00
32	5	3880	G	N9-C1'-C2'	7.94	124.32	114.00
57	SE	86	PHE	N-CA-CB	7.93	124.88	110.60
32	5	5066	U	N1-C1'-C2'	7.93	124.31	114.00
32	5	4693	C	C2'-C3'-O3'	7.93	126.94	109.50
32	5	4379	A	N9-C1'-C2'	-7.91	103.30	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	5	53	C	C2'-C3'-O3'	7.91	126.91	109.50
32	5	1552	G	N9-C1'-C2'	-7.91	103.30	112.00
32	5	4169	G	N9-C1'-C2'	7.90	124.27	114.00
53	S2	1394	G	C2'-C3'-O3'	7.89	126.86	109.50
32	5	1379	C	N1-C1'-C2'	7.89	124.25	114.00
32	5	2282	A	N9-C1'-C2'	7.88	124.24	114.00
85	Sf	138	ARG	NE-CZ-NH1	7.87	124.24	120.30
32	5	1359	G	C2'-C3'-O3'	7.86	126.79	109.50
4	H	125	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	A	242	ARG	NE-CZ-NH1	7.85	124.22	120.30
32	5	1521	C	N1-C1'-C2'	-7.84	103.38	112.00
32	5	5006	U	N1-C1'-C2'	-7.84	103.37	112.00
32	5	4911	A	C1'-O4'-C4'	-7.84	103.63	109.90
34	8	35	C	N1-C1'-C2'	7.84	124.19	114.00
32	5	2369	U	N1-C1'-C2'	-7.83	103.38	112.00
76	SP	18	ARG	NE-CZ-NH1	7.83	124.22	120.30
34	8	38	U	O4'-C1'-N1	7.82	114.46	108.20
32	5	29	G	N9-C1'-C2'	7.82	124.16	114.00
32	5	2658	G	N9-C1'-C2'	-7.81	103.41	112.00
53	S2	92	A	O4'-C1'-N9	-7.81	101.95	108.20
1	A	193	ARG	CG-CD-NE	-7.80	95.41	111.80
67	SX	20	HIS	CB-CA-C	7.80	126.01	110.40
32	5	1930	U	N1-C1'-C2'	7.80	124.14	114.00
32	5	4463	U	N1-C1'-C2'	-7.80	103.42	112.00
3	G	53	ARG	NE-CZ-NH2	-7.79	116.41	120.30
32	5	978	G	C2'-C3'-O3'	7.79	126.63	109.50
32	5	4693	C	C5'-C4'-O4'	7.78	118.44	109.10
32	5	1379	C	C1'-O4'-C4'	-7.78	103.68	109.90
32	5	4718	G	N9-C1'-C2'	-7.76	103.46	112.00
40	P	23	ARG	NE-CZ-NH1	7.76	124.18	120.30
53	S2	41	G	N9-C1'-C2'	-7.76	103.47	112.00
32	5	54	G	N9-C1'-C2'	-7.75	103.48	112.00
32	5	2046	G	C2'-C3'-O3'	7.75	126.55	109.50
27	i	39	PHE	N-CA-CB	7.75	124.54	110.60
32	5	3625	G	C2'-C3'-O3'	7.75	126.54	109.50
32	5	1455	G	C2'-C3'-O3'	7.75	126.54	109.50
57	SE	86	PHE	CB-CG-CD1	-7.75	115.38	120.80
61	SJ	131	ARG	NE-CZ-NH1	7.74	124.17	120.30
32	5	4498	U	N1-C1'-C2'	-7.74	103.49	112.00
53	S2	1407	U	N1-C1'-C2'	7.73	124.05	114.00
47	q	99	ARG	CG-CD-NE	7.72	128.02	111.80
32	5	350	C	N1-C1'-C2'	7.71	124.03	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	7	72	U	C2'-C3'-O3'	7.71	126.47	109.50
75	SM	127	TYR	CA-CB-CG	7.71	128.06	113.40
32	5	353	A	N9-C1'-C2'	-7.71	103.52	112.00
53	S2	1668	U	N1-C1'-C2'	7.71	124.02	114.00
32	5	2263	A	C5'-C4'-O4'	7.70	118.34	109.10
32	5	4976	U	O4'-C1'-N1	-7.70	102.04	108.20
75	SM	33	ARG	NE-CZ-NH1	7.70	124.15	120.30
53	S2	110	U	C2'-C3'-O3'	7.69	126.42	109.50
53	S2	1168	G	N9-C1'-C2'	7.68	123.98	114.00
32	5	5056	A	N9-C1'-C2'	7.67	123.98	114.00
7	M	17	PHE	CB-CG-CD2	7.67	126.17	120.80
17	Y	27	ARG	NE-CZ-NH2	7.67	124.14	120.30
11	R	149	LYS	C-N-CA	-7.67	102.53	121.70
46	K	9	GLU	C-N-CA	7.67	140.87	121.70
53	S2	1697	A	C4-N9-C1'	7.67	140.10	126.30
32	5	3663	A	O4'-C1'-N9	-7.66	102.07	108.20
32	5	1649	U	N1-C1'-C2'	7.65	123.94	114.00
53	S2	1194	A	N9-C1'-C2'	-7.65	103.59	112.00
2	D	54	ARG	CG-CD-NE	-7.64	95.75	111.80
53	S2	825	A	N9-C1'-C2'	7.64	123.93	114.00
10	Q	75	ARG	NE-CZ-NH1	7.63	124.12	120.30
32	5	352	G	N9-C1'-C2'	-7.63	103.61	112.00
55	SB	82	ARG	CG-CD-NE	-7.62	95.79	111.80
32	5	2082	G	N9-C1'-C2'	7.62	123.91	114.00
53	S2	1697	A	C8-N9-C1'	-7.62	113.98	127.70
10	Q	26	ARG	NE-CZ-NH2	-7.62	116.49	120.30
53	S2	642	U	N1-C1'-C2'	-7.62	103.62	112.00
53	S2	662	G	O4'-C1'-N9	-7.61	102.11	108.20
32	5	2119	C	O4'-C1'-N1	7.61	114.29	108.20
32	5	300	A	C4-N9-C1'	7.60	139.99	126.30
32	5	4737	G	N9-C1'-C2'	7.60	123.88	114.00
53	S2	1606	G	N9-C1'-C2'	-7.60	103.64	112.00
60	SI	197	PHE	CB-CA-C	-7.59	95.23	110.40
53	S2	1419	C	O5'-P-OP2	-7.58	98.87	105.70
32	5	2246	C	C2'-C3'-O3'	7.58	126.19	109.50
32	5	42	A	C1'-O4'-C4'	-7.58	103.83	109.90
32	5	315	G	C1'-O4'-C4'	-7.58	103.84	109.90
32	5	33	A	N9-C1'-C2'	7.57	123.85	114.00
32	5	664	G	C1'-O4'-C4'	-7.57	103.85	109.90
32	5	2827	G	O4'-C1'-N9	-7.57	102.15	108.20
64	SO	121	ARG	NE-CZ-NH1	7.56	124.08	120.30
19	a	34	ASN	CB-CA-C	7.56	125.51	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	h	117	ARG	CG-CD-NE	-7.56	95.93	111.80
53	S2	1842	C	N1-C1'-C2'	7.55	123.82	114.00
32	5	958	G	C2'-C3'-O3'	7.55	126.12	109.50
53	S2	1395	C	C2'-C3'-O3'	7.55	126.12	109.50
32	5	1	C	C5'-C4'-O4'	7.54	118.15	109.10
26	h	89	ARG	NE-CZ-NH1	7.54	124.07	120.30
53	S2	313	A	C1'-O4'-C4'	-7.54	103.87	109.90
32	5	4876	U	N1-C1'-C2'	7.53	123.79	114.00
34	8	81	C	C1'-O4'-C4'	-7.53	103.87	109.90
8	N	139	HIS	N-CA-CB	7.53	124.15	110.60
32	5	3843	C	N1-C1'-C2'	7.53	123.79	114.00
53	S2	3	C	O4'-C1'-N1	7.53	114.22	108.20
32	5	3817	A	N9-C1'-C2'	7.52	123.78	114.00
73	SF	51	HIS	N-CA-CB	7.52	124.13	110.60
32	5	1292	C	C2'-C3'-O3'	7.52	126.04	109.50
40	P	139	TYR	CB-CG-CD1	-7.51	116.49	121.00
32	5	946	C	O4'-C1'-N1	7.51	114.21	108.20
32	5	94	A	N9-C1'-C2'	7.50	123.76	114.00
32	5	58	G	N9-C1'-C2'	7.50	123.75	114.00
39	I	171	TRP	N-CA-CB	7.50	124.10	110.60
50	4	37	C	C2'-C3'-O3'	7.50	126.00	109.50
32	5	454	U	C2'-C3'-O3'	7.50	125.99	109.50
32	5	3735	G	C4'-C3'-O3'	-7.49	93.67	109.40
32	5	1534	A	N9-C1'-C2'	7.48	123.72	114.00
53	S2	427	U	C5'-C4'-O4'	7.48	118.07	109.10
36	C	35	ASP	CB-CG-OD1	7.48	125.03	118.30
32	5	300	A	C8-N9-C1'	-7.47	114.25	127.70
34	8	104	A	O4'-C1'-N9	-7.47	102.22	108.20
32	5	4723	A	C4-N9-C1'	7.47	139.74	126.30
32	5	147	A	N9-C1'-C2'	7.47	123.70	114.00
74	SK	68	TYR	CA-CB-CG	-7.47	99.21	113.40
32	5	2517	A	N9-C1'-C2'	7.45	123.69	114.00
2	D	44	TYR	CB-CA-C	7.45	125.29	110.40
34	8	94	G	O4'-C1'-N9	-7.45	102.24	108.20
32	5	4497	U	N1-C1'-C2'	-7.44	103.81	112.00
1	A	37	ARG	NE-CZ-NH2	-7.44	116.58	120.30
53	S2	1433	C	C4'-C3'-O3'	7.43	127.86	113.00
32	5	2797	C	N1-C1'-C2'	-7.42	103.83	112.00
32	5	4371	G	O4'-C1'-N9	7.42	114.14	108.20
53	S2	1603	G	N9-C1'-C2'	7.42	123.64	114.00
53	S2	1623	A	N9-C1'-C2'	-7.42	103.84	112.00
32	5	332	C	N1-C1'-C2'	7.42	123.64	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	53	ARG	CA-CB-CG	7.41	129.71	113.40
53	S2	829	C	N1-C1'-C2'	-7.41	103.85	112.00
69	Sa	22	ARG	NE-CZ-NH2	-7.41	116.59	120.30
32	5	3875	G	N9-C1'-C2'	-7.40	103.86	112.00
32	5	1676	C	C1'-C2'-O2'	-7.40	88.39	110.60
53	S2	822	U	N1-C1'-C2'	7.40	123.62	114.00
32	5	235	A	N9-C1'-C2'	-7.39	103.87	112.00
53	S2	1221	G	N9-C1'-C2'	7.39	123.61	114.00
32	5	209	U	C4'-C3'-O3'	7.39	127.78	113.00
53	S2	447	A	C1'-O4'-C4'	-7.38	104.00	109.90
53	S2	31	U	N1-C1'-C2'	7.37	123.58	114.00
53	S2	821	G	O4'-C1'-N9	-7.37	102.30	108.20
32	5	2553	A	O4'-C1'-N9	7.37	114.10	108.20
32	5	3882	C	N1-C1'-C2'	7.37	123.58	114.00
53	S2	30	C	N1-C1'-C2'	7.36	123.57	114.00
56	SC	170	TRP	CA-CB-CG	-7.36	99.72	113.70
57	SE	3	ARG	NE-CZ-NH1	7.36	123.98	120.30
53	S2	161	U	N1-C1'-C2'	7.36	123.56	114.00
57	SE	18	TRP	CB-CA-C	7.36	125.11	110.40
32	5	1319	U	N1-C1'-C2'	-7.35	103.91	112.00
32	5	1642	A	C4'-C3'-O3'	-7.35	93.97	109.40
73	SF	122	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	A	189	TYR	CA-CB-CG	7.33	127.33	113.40
53	S2	55	U	N1-C1'-C2'	7.33	123.53	114.00
53	S2	1109	C	O4'-C1'-N1	7.33	114.06	108.20
4	H	60	TRP	CB-CA-C	7.32	125.04	110.40
32	5	4282	A	N9-C1'-C2'	7.31	123.51	114.00
32	5	84	A	O4'-C1'-N9	-7.31	102.35	108.20
32	5	4272	G	N9-C1'-C2'	7.31	123.50	114.00
32	5	4120	U	N1-C1'-C2'	-7.30	103.97	112.00
53	S2	1085	C	N1-C1'-C2'	7.30	123.49	114.00
32	5	4723	A	C8-N9-C1'	-7.30	114.56	127.70
32	5	85	G	O4'-C1'-N9	7.30	114.04	108.20
53	S2	968	U	N1-C1'-C2'	-7.30	103.97	112.00
32	5	3677	U	N1-C1'-C2'	7.29	123.48	114.00
32	5	432	U	N1-C1'-C2'	-7.29	103.98	112.00
32	5	1364	U	C2'-C3'-O3'	7.28	125.52	109.50
32	5	1894	C	N1-C1'-C2'	7.28	123.46	114.00
32	5	54	G	C2'-C3'-O3'	7.28	125.50	109.50
32	5	1214	C	O4'-C1'-N1	-7.27	102.38	108.20
32	5	4336	A	N9-C1'-C2'	-7.26	104.01	112.00
53	S2	746	C	C2'-C3'-O3'	7.26	125.47	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	35	ARG	NE-CZ-NH1	7.25	123.93	120.30
34	8	73	U	N1-C1'-C2'	-7.25	104.02	112.00
85	Sf	146	LEU	CB-CG-CD1	7.24	123.31	111.00
32	5	1377	G	C2'-C3'-O3'	7.24	125.43	109.50
34	8	86	U	O4'-C1'-C2'	-7.24	98.56	105.80
53	S2	532	C	C2'-C3'-O3'	7.24	125.42	109.50
32	5	1500	A	C4'-C3'-O3'	7.21	127.43	113.00
32	5	2597	G	N9-C1'-C2'	7.21	123.38	114.00
38	F	120	PHE	CB-CA-C	7.21	124.81	110.40
53	S2	1452	A	C2'-C3'-O3'	7.21	125.36	109.50
5	J	119	TYR	CA-CB-CG	7.21	127.09	113.40
19	a	61	TYR	CB-CA-C	7.20	124.81	110.40
32	5	2511	A	O4'-C1'-N9	-7.20	102.44	108.20
53	S2	1059	G	N9-C1'-C2'	7.20	123.36	114.00
32	5	394	G	N9-C1'-C2'	-7.20	104.08	112.00
32	5	3905	A	N9-C1'-C2'	-7.20	104.08	112.00
53	S2	1701	C	N1-C1'-C2'	7.19	123.35	114.00
53	S2	1341	C	N1-C1'-C2'	7.19	123.35	114.00
53	S2	1567	G	O4'-C1'-N9	7.18	113.95	108.20
32	5	4600	G	N9-C1'-C2'	-7.17	104.11	112.00
32	5	125	C	C2'-C3'-O3'	7.17	125.28	109.50
60	SI	55	TYR	CA-CB-CG	-7.17	99.77	113.40
85	Sf	95	ARG	NE-CZ-NH1	7.17	123.89	120.30
42	j	11	ARG	NE-CZ-NH1	7.17	123.88	120.30
8	N	131	GLU	CB-CA-C	7.16	124.72	110.40
32	5	406	C	C2'-C3'-O3'	7.16	125.25	109.50
20	b	7	HIS	CB-CA-C	-7.16	96.09	110.40
12	S	29	ARG	CG-CD-NE	-7.14	96.80	111.80
32	5	2511	A	C2'-C3'-O3'	7.14	125.21	109.50
40	P	42	ARG	NE-CZ-NH1	7.14	123.87	120.30
53	S2	1664	A	C2'-C3'-O3'	7.14	125.20	109.50
64	SO	147	ARG	CG-CD-NE	-7.13	96.83	111.80
32	5	171	U	C4'-C3'-O3'	-7.13	94.43	109.40
32	5	929	A	N9-C1'-C2'	-7.13	104.16	112.00
17	Y	78	TYR	CB-CA-C	7.12	124.65	110.40
53	S2	594	A	N9-C1'-C2'	-7.12	104.17	112.00
26	h	78	TYR	CA-CB-CG	-7.12	99.88	113.40
32	5	52	G	C2'-C3'-O3'	7.12	125.16	109.50
32	5	514	U	C2'-C3'-O3'	7.12	125.15	109.50
62	SL	62	PHE	CB-CA-C	7.12	124.63	110.40
12	S	157	ARG	CG-CD-NE	7.11	126.73	111.80
53	S2	91	A	C2'-C3'-O3'	7.11	125.15	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	5	1650	A	O4'-C1'-N9	-7.11	102.52	108.20
32	5	1893	C	N1-C1'-C2'	7.11	123.24	114.00
32	5	226	G	N9-C1'-C2'	-7.10	104.19	112.00
38	F	58	HIS	CB-CA-C	-7.10	96.20	110.40
53	S2	165	G	O4'-C1'-N9	7.10	113.88	108.20
53	S2	427	U	N1-C1'-C2'	7.10	123.23	114.00
55	SB	28	ARG	NE-CZ-NH1	7.10	123.85	120.30
53	S2	841	G	O4'-C1'-C2'	-7.10	98.70	105.80
32	5	4518	A	O5'-P-OP2	-7.09	99.32	105.70
32	5	3653	A	N9-C1'-C2'	-7.09	104.20	112.00
32	5	2695	A	C2'-C3'-O3'	7.09	125.10	109.50
53	S2	1082	A	N9-C1'-C2'	7.09	123.22	114.00
32	5	4945	G	O5'-P-OP1	-7.09	99.32	105.70
32	5	4966	A	N9-C1'-C2'	7.09	123.21	114.00
32	5	4279	A	N9-C1'-C2'	-7.08	104.22	112.00
12	S	167	PHE	CB-CG-CD1	-7.07	115.85	120.80
27	i	39	PHE	CB-CG-CD1	-7.07	115.85	120.80
32	5	1534	A	C5'-C4'-O4'	7.07	117.58	109.10
53	S2	349	A	C2'-C3'-O3'	7.07	125.05	109.50
32	5	3883	U	N1-C1'-C2'	7.07	123.19	114.00
32	5	4979	A	N9-C1'-C2'	7.07	123.19	114.00
31	o	57	ARG	NE-CZ-NH1	7.07	123.83	120.30
53	S2	957	A	N9-C1'-C2'	7.07	123.19	114.00
53	S2	980	A	C2'-C3'-O3'	7.06	125.03	109.50
1	A	211	PHE	CB-CA-C	7.05	124.50	110.40
9	O	178	ARG	NE-CZ-NH1	7.05	123.82	120.30
36	C	41	HIS	N-CA-CB	7.05	123.28	110.60
53	S2	1556	A	N9-C1'-C2'	7.04	123.15	114.00
32	5	267	G	C2'-C3'-O3'	7.04	124.98	109.50
32	5	1067	G	C2'-C3'-O3'	7.04	124.98	109.50
32	5	5061	A	C2'-C3'-O3'	7.03	124.97	109.50
18	Z	38	TYR	N-CA-C	-7.03	92.03	111.00
53	S2	1293	A	C4'-C3'-O3'	7.02	127.05	113.00
32	5	2443	G	N9-C1'-C2'	7.02	123.13	114.00
36	C	311	ARG	NE-CZ-NH2	-7.02	116.79	120.30
32	5	3692	A	C2'-C3'-O3'	7.02	124.94	109.50
32	5	1398	A	O4'-C1'-N9	7.01	113.81	108.20
32	5	84	A	N9-C1'-C2'	7.01	123.11	114.00
32	5	3729	U	C2'-C3'-O3'	7.01	124.92	109.50
35	B	367	PHE	CB-CG-CD1	-7.01	115.89	120.80
32	5	157	U	C1'-O4'-C4'	-7.01	104.30	109.90
18	Z	75	TYR	CA-CB-CG	7.00	126.71	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	S	167	PHE	CB-CG-CD2	7.00	125.70	120.80
53	S2	845	G	N9-C1'-C2'	7.00	123.11	114.00
53	S2	1529	C	N1-C1'-C2'	7.00	123.10	114.00
32	5	2546	G	C4'-C3'-O3'	7.00	126.99	113.00
32	5	3691	G	N9-C1'-C2'	7.00	123.10	114.00
32	5	279	A	C4'-C3'-O3'	-7.00	94.71	109.40
32	5	3667	C	C2'-C3'-O3'	6.99	124.88	113.70
32	5	3692	A	N9-C1'-C2'	-6.99	104.31	112.00
53	S2	1453	C	O4'-C1'-N1	6.98	113.78	108.20
32	5	2581	A	N9-C1'-C2'	6.98	123.07	114.00
32	5	2632	U	N1-C1'-C2'	6.98	123.07	114.00
32	5	1992	U	N1-C1'-C2'	6.97	123.06	114.00
32	5	48	G	C2'-C3'-O3'	6.97	124.85	113.70
32	5	97	G	N9-C1'-C2'	-6.97	104.33	112.00
53	S2	1350	U	C2'-C3'-O3'	6.97	124.85	113.70
32	5	4599	A	N9-C1'-C2'	6.96	123.05	114.00
32	5	4497	U	C2'-C3'-O3'	6.96	124.84	113.70
53	S2	1114	U	O4'-C1'-N1	6.95	113.76	108.20
32	5	2054	U	C1'-O4'-C4'	-6.95	104.34	109.90
57	SE	103	TYR	CB-CG-CD1	-6.95	116.83	121.00
40	P	139	TYR	CA-CB-CG	-6.95	100.20	113.40
32	5	1998	A	N9-C1'-C2'	6.94	123.03	114.00
26	h	119	PHE	CB-CA-C	-6.94	96.52	110.40
32	5	1355	G	N9-C1'-C2'	6.94	123.02	114.00
32	5	3739	C	O4'-C1'-C2'	-6.94	98.86	105.80
53	S2	393	U	O4'-C1'-N1	6.93	113.74	108.20
53	S2	631	U	O4'-C1'-N1	-6.92	102.66	108.20
8	N	143	ARG	CG-CD-NE	-6.92	97.27	111.80
32	5	4986	G	N9-C1'-C2'	6.92	123.00	114.00
54	SA	103	PHE	N-CA-CB	6.92	123.06	110.60
32	5	2463	G	N9-C1'-C2'	6.92	122.99	114.00
32	5	4378	A	O4'-C1'-N9	6.91	113.72	108.20
32	5	4589	A	O4'-C1'-N9	-6.91	102.67	108.20
34	8	94	G	C2'-C3'-O3'	6.90	124.74	113.70
32	5	2319	C	N1-C1'-C2'	6.90	122.96	114.00
53	S2	1109	C	N1-C1'-C2'	6.89	122.96	114.00
75	SM	33	ARG	CG-CD-NE	6.89	126.26	111.80
10	Q	33	ARG	CA-CB-CG	6.88	128.55	113.40
32	5	1937	C	N1-C1'-C2'	6.88	122.94	114.00
32	5	4238	G	N9-C1'-C2'	-6.86	104.45	112.00
16	X	48	ARG	NE-CZ-NH2	-6.85	116.87	120.30
11	R	95	TRP	N-CA-CB	6.85	122.93	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	5	747	A	C2'-C3'-O3'	6.85	124.66	113.70
32	5	979	C	C2'-C3'-O3'	6.85	124.66	113.70
10	Q	91	ARG	NE-CZ-NH2	6.84	123.72	120.30
12	S	29	ARG	CA-CB-CG	6.84	128.46	113.40
32	5	2623	A	C4-N9-C1'	6.84	138.62	126.30
32	5	4510	A	O4'-C1'-N9	-6.84	102.73	108.20
53	S2	1114	U	C1'-O4'-C4'	-6.84	104.43	109.90
45	r	45	HIS	N-CA-CB	-6.83	98.30	110.60
32	5	53	C	N1-C1'-C2'	-6.83	104.49	112.00
32	5	235	A	O4'-C1'-N9	6.83	113.66	108.20
32	5	2081	C	N1-C1'-C2'	6.83	122.87	114.00
32	5	2467	U	N1-C1'-C2'	-6.83	104.49	112.00
33	7	84	U	N1-C1'-C2'	6.82	122.87	114.00
32	5	43	U	C5'-C4'-O4'	6.82	117.28	109.10
32	5	486	C	C2'-C3'-O3'	6.82	124.61	113.70
34	8	79	G	N9-C1'-C2'	6.81	122.86	114.00
32	5	2270	G	N9-C1'-C2'	6.81	122.85	114.00
32	5	4170	A	N9-C1'-C2'	6.81	122.85	114.00
24	f	4	ARG	CA-CB-CG	6.80	128.37	113.40
32	5	100	C	N1-C1'-C2'	-6.80	104.52	112.00
6	L	34	ARG	NE-CZ-NH1	6.80	123.70	120.30
53	S2	1144	A	C4-N9-C1'	6.80	138.54	126.30
9	O	49	ARG	CG-CD-NE	-6.80	97.52	111.80
34	8	66	A	N9-C1'-C2'	6.80	122.83	114.00
32	5	100	C	C2'-C3'-O3'	6.79	124.57	113.70
53	S2	1567	G	C1'-O4'-C4'	-6.79	104.47	109.90
32	5	450	G	N9-C1'-C2'	-6.79	104.53	112.00
64	SO	149	ARG	NE-CZ-NH1	6.79	123.69	120.30
53	S2	965	U	N1-C1'-C2'	6.78	122.82	114.00
12	S	83	ARG	CG-CD-NE	6.78	126.04	111.80
32	5	514	U	C5'-C4'-O4'	6.78	117.24	109.10
34	8	38	U	C1'-O4'-C4'	-6.77	104.48	109.90
32	5	2588	C	C4'-C3'-O3'	6.77	126.54	113.00
32	5	2307	A	N9-C1'-C2'	6.77	122.80	114.00
53	S2	1850	A	N9-C1'-C2'	6.77	122.80	114.00
59	SH	177	TYR	N-CA-CB	6.76	122.77	110.60
32	5	1501	C	C1'-O4'-C4'	-6.76	104.49	109.90
36	C	80	ARG	NE-CZ-NH1	6.76	123.68	120.30
32	5	4224	A	N9-C1'-C2'	-6.75	104.57	112.00
58	SG	156	TYR	CA-CB-CG	-6.75	100.58	113.40
32	5	1934	A	N9-C1'-C2'	-6.75	104.58	112.00
32	5	3648	A	C1'-O4'-C4'	-6.74	104.51	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	S2	924	G	N9-C1'-C2'	-6.73	104.59	112.00
3	G	62	ARG	NE-CZ-NH2	-6.73	116.94	120.30
53	S2	1293	A	N9-C1'-C2'	6.73	122.75	114.00
7	M	17	PHE	CB-CG-CD1	-6.72	116.09	120.80
32	5	4950	U	N1-C1'-C2'	6.72	122.73	114.00
32	5	3775	A	N9-C1'-C2'	6.72	122.73	114.00
32	5	1614	C	C2'-C3'-O3'	6.71	124.43	113.70
69	Sa	10	ARG	N-CA-C	-6.71	92.89	111.00
53	S2	1552	G	N9-C1'-C2'	-6.70	104.63	112.00
32	5	4238	G	C2'-C3'-O3'	6.70	124.42	113.70
53	S2	1401	A	C2'-C3'-O3'	6.70	124.42	113.70
54	SA	117	ARG	NE-CZ-NH2	-6.70	116.95	120.30
53	S2	1678	A	N9-C1'-C2'	-6.69	104.64	112.00
76	SP	42	ARG	NE-CZ-NH2	-6.69	116.95	120.30
53	S2	1144	A	C8-N9-C1'	-6.69	115.66	127.70
32	5	920	C	C5'-C4'-O4'	6.69	117.12	109.10
53	S2	1150	A	N9-C1'-C2'	6.69	122.69	114.00
50	4	186	C	OP2-P-O3'	6.68	119.91	105.20
32	5	4911	A	O5'-P-OP2	-6.68	99.69	105.70
25	g	4	ARG	NE-CZ-NH2	-6.67	116.96	120.30
32	5	1586	G	N9-C1'-C2'	6.67	122.67	114.00
32	5	43	U	N1-C1'-C2'	-6.67	104.66	112.00
32	5	2649	G	N9-C1'-C2'	6.67	122.67	114.00
10	Q	58	ARG	NE-CZ-NH1	6.67	123.63	120.30
34	8	13	G	N9-C1'-C2'	6.66	122.66	114.00
56	SC	241	PHE	N-CA-CB	6.66	122.59	110.60
32	5	1789	C	N1-C1'-C2'	6.66	122.66	114.00
53	S2	964	A	N9-C1'-C2'	6.66	122.66	114.00
32	5	1740	C	N1-C1'-C2'	-6.65	104.69	112.00
32	5	3912	U	C1'-C2'-O2'	-6.65	90.66	110.60
32	5	4449	A	N9-C1'-C2'	-6.64	104.69	112.00
32	5	1671	U	O4'-C1'-C2'	-6.64	99.16	105.80
32	5	3799	A	N9-C1'-C2'	6.64	122.63	114.00
32	5	1440	U	C2'-C3'-O3'	6.64	124.32	113.70
53	S2	65	C	O4'-C1'-N1	6.63	113.51	108.20
32	5	2623	A	C8-N9-C1'	-6.63	115.76	127.70
64	SO	150	ARG	NE-CZ-NH2	6.63	123.61	120.30
32	5	291	U	N1-C1'-C2'	6.63	122.61	114.00
32	5	1867	A	N9-C1'-C2'	6.63	122.62	114.00
25	g	14	ASN	N-CA-CB	6.62	122.51	110.60
32	5	89	C	N1-C1'-C2'	6.62	122.60	114.00
18	Z	21	ARG	NE-CZ-NH1	6.61	123.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	5	5044	A	N9-C1'-C2'	6.61	122.59	114.00
32	5	292	G	C4-N9-C1'	-6.61	117.91	126.50
53	S2	1591	C	C2'-C3'-O3'	6.61	124.28	113.70
33	7	58	A	C2'-C3'-O3'	6.61	124.28	113.70
61	SJ	24	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	A	37	ARG	NE-CZ-NH1	6.61	123.60	120.30
32	5	171	U	N1-C1'-C2'	6.60	122.58	114.00
53	S2	426	A	O4'-C1'-N9	6.60	113.48	108.20
32	5	4510	A	N9-C1'-C2'	6.60	122.58	114.00
60	SI	197	PHE	CB-CG-CD2	-6.60	116.18	120.80
85	Sf	148	TYR	CA-CB-CG	6.59	125.93	113.40
32	5	1564	A	N9-C1'-C2'	6.59	122.57	114.00
1	A	34	PHE	N-CA-CB	6.59	122.46	110.60
35	B	169	ARG	NE-CZ-NH1	6.58	123.59	120.30
26	h	78	TYR	CB-CA-C	6.58	123.56	110.40
32	5	1390	G	N9-C1'-C2'	-6.58	104.76	112.00
32	5	1479	G	N9-C1'-C2'	6.58	122.55	114.00
53	S2	385	G	N9-C1'-C2'	6.58	122.55	114.00
32	5	384	A	N9-C1'-C2'	6.57	122.54	114.00
64	SO	41	PHE	CB-CG-CD1	6.57	125.40	120.80
32	5	4589	A	N9-C1'-C2'	6.57	122.53	114.00
32	5	2317	C	N1-C1'-C2'	6.56	122.53	114.00
23	e	35	TRP	CA-CB-CG	-6.56	101.23	113.70
57	SE	121	TYR	CA-CB-CG	-6.56	100.94	113.40
32	5	417	G	O4'-C1'-N9	6.56	113.45	108.20
32	5	1523	A	O5'-P-OP1	-6.55	99.80	105.70
32	5	3611	A	N9-C1'-C2'	6.55	122.52	114.00
37	E	278	TYR	CB-CG-CD2	-6.54	117.07	121.00
32	5	1631	A	C4'-C3'-O3'	-6.54	95.66	109.40
3	G	57	TRP	CB-CA-C	6.54	123.48	110.40
48	z	344	PRO	O-C-N	-6.54	112.24	122.70
53	S2	1190	A	N9-C1'-C2'	6.54	122.50	114.00
32	5	4976	U	C5'-C4'-O4'	6.53	116.94	109.10
32	5	4341	C	N1-C1'-C2'	-6.53	104.82	112.00
34	8	68	G	N9-C1'-C2'	6.53	122.49	114.00
32	5	1573	G	N9-C1'-C2'	6.53	122.49	114.00
32	5	4871	C	O4'-C1'-N1	-6.53	102.98	108.20
32	5	421	C	N1-C1'-C2'	-6.53	104.82	112.00
32	5	4291	G	N9-C1'-C2'	6.51	122.47	114.00
40	P	54	GLN	CA-CB-CG	6.51	127.72	113.40
32	5	1886	G	N9-C1'-C2'	-6.51	104.84	112.00
63	SN	139	TRP	CA-CB-CG	6.51	126.07	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	I	98	ARG	NE-CZ-NH2	6.51	123.55	120.30
32	5	1484	G	O4'-C4'-C3'	-6.51	97.49	104.00
32	5	2675	G	N9-C1'-C2'	-6.51	104.84	112.00
32	5	3723	A	C4-N9-C1'	6.51	138.01	126.30
32	5	280	G	C1'-O4'-C4'	-6.50	104.70	109.90
25	g	66	ARG	NE-CZ-NH2	-6.50	117.05	120.30
32	5	1932	A	N9-C1'-C2'	6.50	122.45	114.00
53	S2	850	C	N1-C1'-C2'	6.50	122.45	114.00
32	5	4887	C	C2'-C3'-O3'	6.50	124.10	113.70
53	S2	919	A	C4'-C3'-O3'	6.50	126.00	113.00
61	SJ	138	ARG	NE-CZ-NH1	6.50	123.55	120.30
32	5	1658	G	N9-C1'-C2'	6.50	122.45	114.00
53	S2	1868	U	N1-C1'-C2'	6.50	122.44	114.00
2	D	210	TYR	N-CA-CB	6.49	122.28	110.60
32	5	1378	C	N1-C1'-C2'	6.49	122.44	114.00
53	S2	454	U	N1-C1'-C2'	6.49	122.44	114.00
27	i	4	ARG	NE-CZ-NH1	6.48	123.54	120.30
32	5	4326	G	N9-C1'-C2'	6.48	122.43	114.00
32	5	1521	C	C2'-C3'-O3'	6.48	124.06	113.70
50	4	186	C	C2-N1-C1'	6.48	125.92	118.80
53	S2	666	U	C6-N1-C1'	-6.48	112.13	121.20
53	S2	732	U	C2'-C3'-O3'	6.47	124.06	113.70
53	S2	1394	G	O4'-C1'-C2'	-6.46	99.33	105.80
32	5	4978	G	N9-C1'-C2'	6.46	122.40	114.00
53	S2	1374	C	N1-C1'-C2'	6.46	122.40	114.00
32	5	3827	G	N9-C1'-C2'	-6.46	104.89	112.00
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
8	N	150	TRP	CA-CB-CG	6.46	125.97	113.70
23	e	46	ARG	NE-CZ-NH1	6.46	123.53	120.30
74	SK	2	LEU	CA-CB-CG	6.46	130.15	115.30
32	5	216	C	C2'-C3'-O3'	6.45	124.02	113.70
53	S2	26	U	C2'-C3'-O3'	6.45	124.02	113.70
56	SC	236	PHE	N-CA-CB	6.45	122.21	110.60
32	5	1882	U	O5'-P-OP1	-6.45	99.90	105.70
67	SX	67	ARG	NE-CZ-NH2	6.44	123.52	120.30
53	S2	1292	C	P-O5'-C5'	6.44	131.20	120.90
12	S	77	ASN	CB-CA-C	6.43	123.27	110.40
32	5	50	C	N1-C1'-C2'	6.43	122.36	114.00
32	5	1696	C	C2'-C3'-O3'	6.43	123.99	113.70
46	K	95	GLN	N-CA-C	-6.43	93.64	111.00
32	5	4378	A	N9-C1'-C2'	6.43	122.36	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	S2	381	C	O4'-C1'-N1	-6.43	103.06	108.20
61	SJ	147	PHE	CB-CG-CD1	6.43	125.30	120.80
32	5	2116	C	C2'-C3'-O3'	6.42	123.97	113.70
53	S2	1309	C	C4'-C3'-O3'	6.42	125.84	113.00
76	SP	81	ARG	NE-CZ-NH2	-6.42	117.09	120.30
67	SX	16	HIS	N-CA-CB	6.41	122.14	110.60
53	S2	426	A	C4'-C3'-O3'	6.41	125.81	113.00
47	q	99	ARG	NE-CZ-NH1	6.40	123.50	120.30
32	5	4556	U	O4'-C1'-N1	6.40	113.32	108.20
22	d	85	ARG	NE-CZ-NH2	-6.40	117.10	120.30
53	S2	666	U	C2-N1-C1'	6.39	125.37	117.70
53	S2	968	U	C4'-C3'-O3'	6.39	125.78	113.00
32	5	964	A	N9-C1'-C2'	-6.39	104.97	112.00
32	5	4331	G	N9-C1'-C2'	-6.39	104.97	112.00
32	5	4981	G	N9-C1'-C2'	-6.39	104.97	112.00
53	S2	841	G	N9-C1'-C2'	-6.39	104.97	112.00
69	Sa	22	ARG	CG-CD-NE	-6.38	98.40	111.80
77	SQ	85	ARG	NE-CZ-NH1	6.38	123.49	120.30
79	SS	86	ARG	NE-CZ-NH2	6.38	123.49	120.30
32	5	2874	U	O4'-C1'-N1	-6.38	103.10	108.20
46	K	9	GLU	CA-C-N	6.38	131.23	117.20
32	5	245	C	C2'-C3'-O3'	6.38	123.90	113.70
53	S2	393	U	O4'-C1'-C2'	-6.38	99.42	105.80
53	S2	19	A	C2'-C3'-O3'	6.38	123.90	113.70
32	5	4378	A	C1'-O4'-C4'	-6.37	104.80	109.90
2	D	198	HIS	CB-CA-C	6.37	123.14	110.40
32	5	1211	G	N9-C1'-C2'	-6.37	105.00	112.00
32	5	4731	G	O4'-C1'-N9	6.37	113.29	108.20
16	X	48	ARG	NE-CZ-NH1	6.36	123.48	120.30
32	5	4338	G	N9-C1'-C2'	-6.36	105.00	112.00
39	I	139	ARG	CG-CD-NE	6.36	125.16	111.80
53	S2	1857	G	N9-C1'-C2'	-6.35	105.01	112.00
32	5	3723	A	C8-N9-C1'	-6.35	116.28	127.70
32	5	1379	C	C5'-C4'-O4'	6.34	116.71	109.10
38	F	141	TYR	CA-CB-CG	6.34	125.45	113.40
5	J	99	PHE	CB-CA-C	6.34	123.08	110.40
32	5	46	U	N1-C1'-C2'	6.34	122.24	114.00
37	E	59	TYR	N-CA-C	-6.33	93.92	111.00
73	SF	165	ASN	N-CA-CB	6.32	121.98	110.60
49	3	46	G	N9-C1'-C2'	6.32	122.22	114.00
32	5	2118	G	C4'-C3'-O3'	6.31	125.63	113.00
53	S2	1142	G	C2'-C3'-O3'	6.31	123.80	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Y	6	PHE	CB-CA-C	6.31	123.01	110.40
9	O	117	ARG	NE-CZ-NH1	6.31	123.45	120.30
55	SB	165	ARG	CG-CD-NE	6.31	125.04	111.80
58	SG	25	ARG	CG-CD-NE	-6.31	98.56	111.80
32	5	2632	U	C2-N1-C1'	6.30	125.27	117.70
32	5	4583	C	N1-C1'-C2'	-6.30	105.06	112.00
53	S2	1667	U	N1-C1'-C2'	6.30	122.19	114.00
5	J	119	TYR	CB-CG-CD1	6.30	124.78	121.00
32	5	4076	G	N9-C1'-C2'	-6.30	105.07	112.00
32	5	2769	U	N1-C1'-C2'	-6.30	105.07	112.00
32	5	4560	C	O4'-C1'-N1	-6.30	103.16	108.20
1	A	211	PHE	CB-CG-CD2	-6.30	116.39	120.80
50	4	235	G	P-O3'-C3'	6.29	127.25	119.70
58	SG	145	PHE	CB-CG-CD1	6.29	125.20	120.80
32	5	1887	G	C2'-C3'-O3'	6.29	123.77	113.70
53	S2	9	U	C2'-C3'-O3'	6.29	123.77	113.70
42	j	27	TYR	CA-CB-CG	-6.29	101.45	113.40
32	5	1211	G	C4'-C3'-O3'	6.28	125.55	113.00
32	5	2075	G	C2'-C3'-O3'	6.27	123.74	113.70
66	SW	44	HIS	CB-CA-C	6.27	122.94	110.40
22	d	108	TYR	CA-CB-CG	-6.27	101.49	113.40
53	S2	340	C	C2'-C3'-O3'	6.27	123.72	113.70
2	D	210	TYR	CA-CB-CG	-6.26	101.50	113.40
8	N	192	TRP	CA-CB-CG	6.26	125.60	113.70
18	Z	75	TYR	CB-CG-CD2	6.26	124.76	121.00
53	S2	427	U	O4'-C1'-N1	-6.26	103.19	108.20
9	O	106	ASP	CB-CG-OD1	-6.26	112.67	118.30
53	S2	9	U	N1-C1'-C2'	-6.26	105.11	112.00
11	R	88	ARG	NE-CZ-NH1	6.26	123.43	120.30
32	5	1216	C	C2'-C3'-O3'	6.26	123.71	113.70
53	S2	1063	C	C1'-C2'-O2'	6.26	129.37	110.60
32	5	4122	G	C2'-C3'-O3'	6.25	123.71	113.70
53	S2	104	A	C2'-C3'-O3'	6.25	123.70	113.70
32	5	1613	A	C8-N9-C1'	-6.25	116.45	127.70
32	5	2470	C	O4'-C1'-C2'	-6.25	99.55	105.80
32	5	5022	U	C2'-C3'-O3'	6.25	123.70	113.70
32	5	3938	G	C5'-C4'-O4'	6.25	116.59	109.10
23	e	60	TYR	CB-CA-C	6.25	122.89	110.40
32	5	2348	G	O4'-C1'-N9	-6.24	103.20	108.20
32	5	2827	G	N9-C1'-C2'	6.24	122.12	114.00
50	4	164	G	N3-C4-C5	6.24	131.72	128.60
34	8	94	G	C5'-C4'-O4'	6.23	116.58	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
71	Se	38	TYR	CA-CB-CG	6.23	125.24	113.40
84	Sd	46	TYR	CA-CB-CG	-6.23	101.56	113.40
32	5	1615	C	N1-C1'-C2'	-6.23	105.15	112.00
32	5	2038	U	N1-C1'-C2'	6.23	122.10	114.00
32	5	1370	G	C1'-O4'-C4'	-6.22	104.92	109.90
53	S2	1584	G	N9-C1'-C2'	6.22	122.09	114.00
53	S2	426	A	N9-C1'-C2'	-6.22	105.16	112.00
32	5	1650	A	C8-N9-C1'	6.22	138.90	127.70
32	5	2529	A	C1'-O4'-C4'	-6.22	104.92	109.90
60	SI	178	ARG	NE-CZ-NH1	6.22	123.41	120.30
32	5	2683	C	C2'-C3'-O3'	6.22	123.65	113.70
38	F	168	ARG	NE-CZ-NH1	6.21	123.41	120.30
32	5	3739	C	C2'-C3'-O3'	6.21	123.64	113.70
36	C	267	TRP	CA-CB-CG	6.21	125.50	113.70
32	5	407	A	N9-C1'-C2'	-6.21	105.17	112.00
32	5	1631	A	N9-C1'-C2'	6.21	122.07	114.00
53	S2	967	C	N1-C1'-C2'	-6.21	105.17	112.00
32	5	3727	A	N9-C1'-C2'	6.21	122.07	114.00
2	D	35	ARG	CG-CD-NE	6.20	124.83	111.80
12	S	28	TYR	CB-CG-CD2	-6.20	117.28	121.00
32	5	3879	G	O4'-C1'-N9	6.20	113.16	108.20
57	SE	11	ARG	NE-CZ-NH2	6.20	123.40	120.30
10	Q	52	PHE	N-CA-C	6.20	127.73	111.00
18	Z	75	TYR	CB-CG-CD1	-6.20	117.28	121.00
53	S2	26	U	O4'-C1'-C2'	-6.20	99.60	105.80
9	O	110	PRO	C-N-CD	-6.19	106.98	120.60
26	h	93	ARG	NE-CZ-NH2	-6.19	117.20	120.30
21	c	90	ARG	CA-CB-CG	6.19	127.02	113.40
32	5	1210	C	N1-C1'-C2'	6.19	122.05	114.00
2	D	293	ARG	NE-CZ-NH1	6.19	123.39	120.30
32	5	2395	A	C2'-C3'-O3'	6.18	123.59	113.70
32	5	1626	G	N9-C1'-C2'	-6.18	105.20	112.00
53	S2	1123	C	O4'-C1'-C2'	-6.18	99.62	105.80
32	5	505	G	C2'-C3'-O3'	6.18	123.59	113.70
50	4	186	C	C6-N1-C1'	-6.18	113.39	120.80
53	S2	1226	G	N9-C1'-C2'	-6.18	105.20	112.00
32	5	970	G	N9-C1'-C2'	6.17	122.02	114.00
22	d	78	ARG	NE-CZ-NH1	6.17	123.38	120.30
53	S2	1669	G	N9-C1'-C2'	6.17	122.02	114.00
32	5	2325	C	O4'-C1'-C2'	-6.17	99.63	105.80
32	5	2675	G	C5'-C4'-O4'	6.17	116.50	109.10
24	f	51	TYR	CA-CB-CG	6.16	125.10	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	R	74	ARG	NE-CZ-NH2	6.16	123.38	120.30
32	5	1613	A	C4-N9-C1'	6.16	137.38	126.30
32	5	2673	G	O4'-C1'-C2'	-6.16	99.64	105.80
32	5	4519	C	C2'-C3'-O3'	6.15	123.55	113.70
36	C	312	ARG	CG-CD-NE	-6.15	98.88	111.80
53	S2	983	A	C8-N9-C1'	-6.15	116.63	127.70
10	Q	33	ARG	NE-CZ-NH2	-6.15	117.23	120.30
25	g	14	ASN	N-CA-C	-6.15	94.40	111.00
32	5	514	U	C4'-C3'-C2'	-6.14	96.45	102.60
53	S2	1246	A	N9-C1'-C2'	-6.14	105.24	112.00
32	5	1575	A	N9-C1'-C2'	6.14	121.98	114.00
32	5	3843	C	O4'-C1'-N1	-6.14	103.29	108.20
32	5	1285	U	O4'-C1'-N1	6.14	113.11	108.20
32	5	123	C	C2'-C3'-O3'	6.14	123.52	113.70
32	5	2118	G	O4'-C4'-C3'	-6.14	97.86	104.00
32	5	3648	A	O4'-C1'-N9	6.14	113.11	108.20
32	5	1295	C	N1-C1'-C2'	6.13	121.97	114.00
32	5	4127	A	O4'-C1'-N9	6.13	113.10	108.20
53	S2	400	C	N1-C1'-C2'	-6.13	105.26	112.00
32	5	4276	G	N9-C1'-C2'	-6.12	105.27	112.00
53	S2	1223	A	N9-C1'-C2'	-6.12	105.27	112.00
53	S2	617	G	N9-C1'-C2'	-6.12	105.27	112.00
53	S2	1859	A	C8-N9-C1'	-6.12	116.69	127.70
12	S	28	TYR	CA-CB-CG	6.12	125.02	113.40
32	5	150	U	C1'-O4'-C4'	-6.12	105.01	109.90
53	S2	71	G	N9-C1'-C2'	6.12	121.95	114.00
32	5	40	G	N9-C1'-C2'	6.11	121.95	114.00
53	S2	1603	G	O4'-C1'-N9	-6.11	103.31	108.20
59	SH	57	ARG	NE-CZ-NH1	-6.11	117.24	120.30
32	5	2529	A	O4'-C1'-N9	6.11	113.09	108.20
32	5	1359	G	N9-C1'-C2'	6.10	121.94	114.00
32	5	2403	A	N9-C1'-C2'	6.10	121.94	114.00
32	5	2448	G	N9-C1'-C2'	6.10	121.93	114.00
32	5	4731	G	N9-C1'-C2'	6.10	121.93	114.00
53	S2	417	C	C2'-C3'-O3'	6.10	123.46	113.70
32	5	215	C	C2'-C3'-O3'	6.10	123.45	113.70
58	SG	156	TYR	CB-CA-C	6.10	122.59	110.40
53	S2	1577	G	N9-C1'-C2'	6.09	121.92	114.00
77	SQ	27	ARG	NE-CZ-NH1	6.09	123.35	120.30
79	SS	42	HIS	N-CA-CB	6.09	121.57	110.60
1	A	3	ARG	NE-CZ-NH2	-6.09	117.25	120.30
32	5	314	G	N9-C1'-C2'	-6.09	105.30	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	5	4400	G	N9-C1'-C2'	-6.09	105.30	112.00
32	5	1724	G	O4'-C4'-C3'	-6.09	97.91	104.00
32	5	4745	G	N9-C1'-C2'	6.09	121.92	114.00
37	E	219	ARG	NE-CZ-NH1	6.09	123.34	120.30
60	SI	51	GLY	N-CA-C	-6.09	97.87	113.10
66	SW	46	TYR	CA-CB-CG	-6.09	101.83	113.40
34	8	34	U	C5'-C4'-O4'	6.08	116.40	109.10
53	S2	1242	U	N1-C1'-C2'	6.08	121.91	114.00
32	5	938	C	N1-C1'-C2'	6.08	121.90	114.00
32	5	2851	G	C2'-C3'-O3'	6.07	123.42	113.70
32	5	1382	G	N9-C1'-C2'	6.07	121.89	114.00
32	5	1479	G	C1'-C2'-O2'	-6.07	92.39	110.60
32	5	158	A	N9-C1'-C2'	-6.07	105.33	112.00
32	5	4527	G	N9-C1'-C2'	-6.07	105.33	112.00
32	5	119	G	O4'-C4'-C3'	-6.07	97.94	104.00
53	S2	532	C	O5'-P-OP1	6.07	117.98	110.70
77	SQ	85	ARG	NE-CZ-NH2	-6.06	117.27	120.30
32	5	4342	C	C2'-C3'-O3'	6.06	123.40	113.70
53	S2	1663	A	N9-C1'-C2'	-6.06	105.34	112.00
32	5	4199	C	O4'-C1'-C2'	-6.05	99.75	105.80
53	S2	912	C	C2'-C3'-O3'	6.05	123.39	113.70
53	S2	1440	C	C5'-C4'-O4'	6.05	116.36	109.10
53	S2	1643	U	N1-C1'-C2'	6.05	121.87	114.00
77	SQ	99	TYR	CA-CB-CG	6.05	124.90	113.40
10	Q	15	ARG	NE-CZ-NH2	-6.05	117.27	120.30
63	SN	113	PHE	CB-CA-C	-6.05	98.30	110.40
72	SD	152	PHE	CB-CG-CD1	-6.05	116.56	120.80
32	5	55	G	N9-C1'-C2'	-6.05	105.35	112.00
42	j	56	ARG	CG-CD-NE	6.04	124.49	111.80
84	Sd	46	TYR	CB-CA-C	6.04	122.48	110.40
85	Sf	138	ARG	CG-CD-NE	6.04	124.48	111.80
53	S2	824	C	N1-C1'-C2'	6.03	121.84	114.00
53	S2	470	G	C5'-C4'-O4'	6.03	116.34	109.10
32	5	2858	A	O4'-C1'-N9	-6.03	103.38	108.20
53	S2	1339	U	N1-C1'-C2'	-6.03	105.37	112.00
53	S2	160	U	C2'-C3'-O3'	6.03	123.35	113.70
12	S	146	HIS	N-CA-C	6.03	127.27	111.00
32	5	927	G	O4'-C1'-N9	6.02	113.02	108.20
53	S2	382	C	N1-C1'-C2'	6.02	121.83	114.00
42	j	71	TYR	CA-CB-CG	6.02	124.83	113.40
53	S2	622	C	N1-C1'-C2'	-6.01	105.39	112.00
53	S2	1292	C	C4'-C3'-C2'	-6.01	96.59	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	S2	1622	U	O4'-C1'-N1	-6.01	103.39	108.20
35	B	62	ARG	NE-CZ-NH1	6.01	123.31	120.30
53	S2	680	G	N9-C1'-C2'	6.01	121.81	114.00
32	5	4448	G	N9-C1'-C2'	6.01	121.81	114.00
24	f	19	ARG	CA-CB-CG	6.00	126.61	113.40
35	B	117	ARG	NE-CZ-NH2	-6.00	117.30	120.30
35	B	169	ARG	CG-CD-NE	6.00	124.40	111.80
32	5	29	G	C8-N9-C1'	-6.00	119.21	127.00
53	S2	291	G	C4'-C3'-O3'	-6.00	96.81	109.40
32	5	4078	C	N1-C1'-C2'	-6.00	105.41	112.00
37	E	179	ARG	NE-CZ-NH1	5.99	123.30	120.30
56	SC	223	TYR	CB-CG-CD1	-5.99	117.40	121.00
27	i	28	ARG	CG-CD-NE	-5.99	99.22	111.80
53	S2	1835	A	O4'-C1'-N9	-5.99	103.41	108.20
2	D	50	ARG	NE-CZ-NH2	5.99	123.29	120.30
25	g	66	ARG	CG-CD-NE	5.99	124.37	111.80
32	5	1632	A	N9-C1'-C2'	-5.99	105.42	112.00
38	F	237	ASN	N-CA-CB	5.98	121.37	110.60
31	o	26	TYR	CB-CG-CD1	5.98	124.59	121.00
32	5	4481	U	N1-C1'-C2'	5.98	121.78	114.00
53	S2	1378	A	O4'-C1'-N9	-5.98	103.41	108.20
32	5	4736	C	N1-C1'-C2'	5.98	121.77	114.00
32	5	5062	G	P-O5'-C5'	5.98	130.46	120.90
53	S2	1367	U	C2'-C3'-O3'	5.98	123.27	113.70
20	b	6	ASN	CB-CA-C	5.98	122.35	110.40
32	5	85	G	O4'-C1'-C2'	-5.98	99.82	105.80
10	Q	26	ARG	NE-CZ-NH1	5.97	123.29	120.30
31	o	48	TYR	CB-CA-C	5.97	122.35	110.40
32	5	3726	A	N9-C1'-C2'	5.97	121.77	114.00
32	5	2305	U	O4'-C1'-N1	-5.97	103.42	108.20
41	W	55	TYR	CB-CG-CD1	5.97	124.58	121.00
19	a	21	ARG	NE-CZ-NH2	5.97	123.28	120.30
32	5	297	U	N1-C1'-C2'	-5.97	105.43	112.00
32	5	4197	G	N9-C1'-C2'	-5.97	105.43	112.00
53	S2	1378	A	O4'-C4'-C3'	-5.97	98.03	104.00
32	5	292	G	O4'-C4'-C3'	-5.97	98.03	104.00
53	S2	983	A	C4-N9-C1'	5.97	137.04	126.30
32	5	1601	A	N9-C1'-C2'	-5.96	105.44	112.00
32	5	1631	A	C5'-C4'-O4'	5.96	116.25	109.10
32	5	2321	G	N9-C1'-C2'	5.96	121.75	114.00
32	5	423	G	C5'-C4'-O4'	5.96	116.25	109.10
32	5	4527	G	O4'-C1'-N9	5.96	112.97	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	E	242	ARG	NE-CZ-NH1	5.96	123.28	120.30
53	S2	1480	A	N9-C1'-C2'	5.96	121.74	114.00
58	SG	213	LEU	CA-CB-CG	5.96	129.00	115.30
32	5	4519	C	O4'-C4'-C3'	-5.95	98.05	104.00
3	G	53	ARG	CG-CD-NE	-5.95	99.30	111.80
26	h	89	ARG	CG-CD-NE	5.95	124.29	111.80
32	5	2613	C	C2'-C3'-O3'	5.94	123.21	113.70
59	SH	57	ARG	NE-CZ-NH2	5.94	123.27	120.30
24	f	4	ARG	N-CA-CB	5.94	121.29	110.60
32	5	4600	G	O4'-C1'-N9	5.94	112.95	108.20
32	5	1292	C	N1-C1'-C2'	5.94	121.72	114.00
61	SJ	20	PHE	CB-CG-CD1	5.94	124.96	120.80
26	h	119	PHE	CB-CG-CD2	-5.94	116.64	120.80
32	5	964	A	C5'-C4'-O4'	-5.93	101.98	109.10
55	SB	67	PHE	N-CA-CB	-5.93	99.92	110.60
34	8	135	C	N1-C1'-C2'	5.93	121.71	114.00
32	5	1	C	C5'-C4'-C3'	5.93	125.48	116.00
32	5	4084	G	C2'-C3'-O3'	5.93	123.18	113.70
32	5	4948	C	C2'-C3'-O3'	5.93	123.18	113.70
53	S2	366	U	N1-C1'-C2'	-5.92	105.48	112.00
32	5	1484	G	O4'-C1'-N9	-5.92	103.46	108.20
32	5	3738	G	N9-C1'-C2'	-5.92	105.49	112.00
42	j	8	PHE	CB-CA-C	5.92	122.23	110.40
2	D	20	PHE	CB-CA-C	5.91	122.23	110.40
32	5	669	C	O4'-C1'-N1	5.91	112.93	108.20
1	A	209	HIS	N-CA-CB	5.90	121.22	110.60
32	5	2344	U	N1-C1'-C2'	5.90	121.67	114.00
32	5	2666	U	C4'-C3'-C2'	-5.90	96.70	102.60
53	S2	426	A	C4'-C3'-C2'	-5.90	96.70	102.60
53	S2	603	C	N1-C1'-C2'	-5.90	105.52	112.00
36	C	78	ARG	NE-CZ-NH2	-5.89	117.35	120.30
53	S2	798	A	N9-C1'-C2'	-5.89	105.52	112.00
53	S2	1022	U	O4'-C1'-N1	5.89	112.92	108.20
32	5	4266	G	N9-C1'-C2'	-5.89	105.52	112.00
37	E	111	TYR	N-CA-CB	5.89	121.21	110.60
53	S2	1863	A	N9-C1'-C2'	5.89	121.66	114.00
53	S2	863	U	N1-C1'-C2'	5.88	121.65	114.00
12	S	84	TYR	CB-CG-CD1	5.88	124.53	121.00
53	S2	399	C	C3'-C2'-C1'	5.88	106.20	101.50
32	5	2673	G	C1'-O4'-C4'	-5.88	105.20	109.90
38	F	98	ARG	NE-CZ-NH2	-5.88	117.36	120.30
34	8	10	G	N9-C1'-C2'	-5.88	105.54	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	K	2	PRO	C-N-CD	5.88	140.74	128.40
32	5	209	U	N1-C1'-C2'	-5.87	105.54	112.00
32	5	2450	G	N9-C1'-C2'	-5.87	105.55	112.00
34	8	74	U	O4'-C1'-C2'	-5.86	99.94	105.80
53	S2	1326	U	N1-C1'-C2'	5.86	121.62	114.00
64	SO	34	PHE	CB-CG-CD1	5.86	124.90	120.80
53	S2	842	C	N1-C1'-C2'	5.86	121.62	114.00
32	5	1672	U	C2-N1-C1'	5.86	124.73	117.70
32	5	2324	C	C2'-C3'-O3'	5.86	123.07	113.70
53	S2	426	A	O4'-C4'-C3'	-5.86	98.14	104.00
74	SK	57	TYR	CA-CB-CG	-5.86	102.28	113.40
29	l	45	ARG	CG-CD-NE	-5.85	99.51	111.80
32	5	2782	U	C4'-C3'-O3'	5.85	124.70	113.00
18	Z	36	ARG	CG-CD-NE	5.85	124.08	111.80
53	S2	1291	A	P-O3'-C3'	5.85	126.72	119.70
53	S2	1859	A	C4-N9-C1'	5.85	136.83	126.30
76	SP	42	ARG	NE-CZ-NH1	5.85	123.22	120.30
32	5	36	U	C2'-C3'-O3'	5.85	123.06	113.70
32	5	1359	G	C4'-C3'-O3'	-5.85	97.12	109.40
44	p	34	HIS	CB-CA-C	5.84	122.09	110.40
53	S2	1536	G	N9-C1'-C2'	-5.84	105.57	112.00
32	5	1361	G	C2'-C3'-O3'	5.84	123.05	113.70
56	SC	241	PHE	CB-CG-CD2	-5.84	116.71	120.80
32	5	1887	G	C4'-C3'-C2'	-5.84	96.76	102.60
53	S2	1522	A	C5'-C4'-O4'	5.84	116.11	109.10
32	5	934	C	O4'-C1'-N1	-5.83	103.53	108.20
32	5	4911	A	C4-N9-C1'	-5.83	115.80	126.30
32	5	4944	C	N1-C1'-C2'	5.83	121.58	114.00
32	5	3686	G	N9-C1'-C2'	-5.83	105.58	112.00
53	S2	647	U	O4'-C1'-C2'	-5.83	99.97	105.80
6	L	103	ARG	NE-CZ-NH2	-5.83	117.39	120.30
32	5	4528	G	O4'-C1'-C2'	-5.83	99.97	105.80
32	5	4873	G	N9-C1'-C2'	5.82	121.57	114.00
60	SI	67	TRP	N-CA-CB	5.82	121.08	110.60
56	SC	250	TYR	CA-CB-CG	-5.82	102.34	113.40
32	5	1236	C	C2'-C3'-O3'	5.82	123.01	113.70
2	D	248	ARG	NE-CZ-NH2	-5.82	117.39	120.30
12	S	81	TRP	N-CA-C	-5.82	95.29	111.00
32	5	2323	C	C2'-C3'-O3'	5.82	123.01	113.70
32	5	2515	G	N9-C1'-C2'	-5.82	105.60	112.00
32	5	25	A	N9-C1'-C2'	5.82	121.56	114.00
34	8	72	A	N9-C1'-C2'	-5.81	105.61	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	8	41	A	N9-C1'-C2'	-5.81	105.61	112.00
53	S2	797	C	O4'-C1'-N1	5.81	112.85	108.20
32	5	1487	G	C2'-C3'-O3'	5.81	122.99	113.70
34	8	104	A	N9-C1'-C2'	5.81	121.55	114.00
38	F	209	PHE	N-CA-CB	5.81	121.05	110.60
53	S2	1551	U	C2'-C3'-O3'	5.81	122.99	113.70
32	5	4212	A	N9-C1'-C2'	5.80	121.54	114.00
53	S2	3	C	C1'-O4'-C4'	-5.80	105.26	109.90
32	5	5048	A	C2'-C3'-O3'	5.80	122.97	113.70
60	SI	55	TYR	CB-CA-C	5.79	121.98	110.40
32	5	74	G	N9-C1'-C2'	5.79	121.53	114.00
85	Sf	146	LEU	CB-CA-C	5.79	121.20	110.20
32	5	4519	C	O4'-C1'-N1	5.79	112.83	108.20
3	G	235	ARG	NE-CZ-NH2	-5.78	117.41	120.30
10	Q	33	ARG	CB-CG-CD	5.78	126.64	111.60
33	7	75	G	O4'-C1'-N9	5.78	112.83	108.20
32	5	1428	U	C2'-C3'-O3'	5.78	122.95	113.70
32	5	2119	C	C1'-O4'-C4'	-5.78	105.28	109.90
63	SN	55	ARG	NE-CZ-NH1	5.77	123.19	120.30
9	O	117	ARG	NE-CZ-NH2	-5.77	117.42	120.30
72	SD	106	ARG	NE-CZ-NH2	-5.77	117.41	120.30
53	S2	1368	U	C4'-C3'-O3'	5.77	124.54	113.00
11	R	74	ARG	NE-CZ-NH1	-5.77	117.42	120.30
32	5	4232	U	N1-C1'-C2'	5.77	121.50	114.00
4	H	124	ARG	NE-CZ-NH2	-5.76	117.42	120.30
37	E	250	ASP	CB-CA-C	5.76	121.93	110.40
53	S2	660	C	N1-C1'-C2'	-5.76	105.66	112.00
12	S	83	ARG	NE-CZ-NH2	5.76	123.18	120.30
32	5	930	G	C4'-C3'-O3'	5.76	124.52	113.00
33	7	26	C	N1-C1'-C2'	-5.76	105.66	112.00
53	S2	1319	U	N1-C1'-C2'	5.76	121.49	114.00
10	Q	38	ARG	NE-CZ-NH2	-5.76	117.42	120.30
26	h	119	PHE	CB-CG-CD1	5.76	124.83	120.80
53	S2	1141	G	C2'-C3'-O3'	5.76	122.92	113.70
32	5	2077	C	C2'-C3'-O3'	5.75	122.91	113.70
53	S2	1851	A	N9-C1'-C2'	5.75	121.48	114.00
32	5	99	A	C2'-C3'-O3'	5.75	122.91	113.70
32	5	232	G	N9-C1'-C2'	-5.75	105.67	112.00
32	5	3938	G	C4'-C3'-O3'	-5.75	97.32	109.40
5	J	99	PHE	CB-CG-CD2	-5.75	116.77	120.80
10	Q	176	ARG	CG-CD-NE	-5.75	99.72	111.80
11	R	107	ARG	NE-CZ-NH1	5.75	123.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	5	1697	G	C3'-C2'-C1'	-5.75	96.90	101.50
33	7	59	G	N9-C1'-C2'	-5.75	105.67	112.00
53	S2	294	U	O4'-C1'-N1	-5.75	103.60	108.20
53	S2	855	G	N9-C1'-C2'	-5.75	105.68	112.00
53	S2	1291	A	C5'-C4'-O4'	5.75	116.00	109.10
12	S	111	ARG	CB-CG-CD	5.75	126.54	111.60
53	S2	381	C	C5'-C4'-O4'	5.75	116.00	109.10
32	5	4909	A	C1'-O4'-C4'	-5.74	105.31	109.90
64	SO	147	ARG	NE-CZ-NH2	-5.74	117.43	120.30
9	O	37	ARG	NE-CZ-NH1	5.74	123.17	120.30
14	U	97	ARG	NE-CZ-NH1	5.74	123.17	120.30
32	5	3870	C	N1-C1'-C2'	5.74	121.46	114.00
31	o	31	ASP	CB-CA-C	5.74	121.88	110.40
32	5	3663	A	N9-C1'-C2'	5.74	121.46	114.00
38	F	197	TYR	N-CA-CB	5.74	120.93	110.60
54	SA	155	ARG	CG-CD-NE	-5.74	99.75	111.80
67	SX	14	ARG	NE-CZ-NH1	5.74	123.17	120.30
32	5	1394	G	N9-C1'-C2'	5.74	121.46	114.00
35	B	49	TYR	CA-CB-CG	5.74	124.30	113.40
32	5	4165	C	O4'-C1'-C2'	-5.74	100.06	105.80
53	S2	1291	A	C3'-C2'-C1'	5.74	106.09	101.50
48	z	159	PHE	CB-CG-CD1	-5.73	116.79	120.80
6	L	34	ARG	NE-CZ-NH2	-5.73	117.43	120.30
10	Q	181	ARG	CA-CB-CG	5.73	126.01	113.40
32	5	1930	U	O4'-C1'-N1	-5.73	103.61	108.20
53	S2	14	C	N1-C1'-C2'	5.73	121.45	114.00
53	S2	1136	U	N1-C1'-C2'	5.73	121.45	114.00
34	8	64	U	C5'-C4'-O4'	5.73	115.97	109.10
32	5	1318	C	N1-C1'-C2'	-5.72	105.70	112.00
35	B	137	TRP	CA-CB-CG	-5.72	102.83	113.70
26	h	109	ARG	CG-CD-NE	5.72	123.81	111.80
45	r	107	ARG	NE-CZ-NH1	5.72	123.16	120.30
53	S2	1171	G	O4'-C1'-N9	5.72	112.78	108.20
53	S2	1315	U	C2'-C3'-O3'	5.72	122.86	113.70
15	V	98	PHE	CB-CG-CD1	-5.72	116.80	120.80
32	5	1822	U	N1-C1'-C2'	5.72	121.43	114.00
53	S2	1647	A	N9-C1'-C2'	5.72	121.43	114.00
53	S2	293	C	N1-C1'-C2'	5.72	121.43	114.00
53	S2	918	U	N1-C1'-C2'	5.72	121.43	114.00
37	E	275	ASN	N-CA-CB	5.71	120.88	110.60
85	Sf	119	ARG	NE-CZ-NH2	-5.71	117.44	120.30
9	O	37	ARG	NE-CZ-NH2	-5.71	117.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	5	4270	C	C2'-C3'-O3'	5.71	122.83	113.70
3	G	235	ARG	CG-CD-NE	5.70	123.78	111.80
17	Y	87	ARG	CG-CD-NE	5.70	123.78	111.80
32	5	1667	G	C2'-C3'-O3'	5.70	122.83	113.70
55	SB	67	PHE	CB-CG-CD2	-5.70	116.81	120.80
32	5	1241	C	C2'-C3'-O3'	5.70	122.82	113.70
32	5	3653	A	O5'-P-OP1	-5.70	100.57	105.70
32	5	4399	U	N1-C1'-C2'	-5.69	105.74	112.00
8	N	108	ARG	CG-CD-NE	-5.69	99.85	111.80
53	S2	60	A	C1'-C2'-O2'	-5.69	93.54	110.60
63	SN	113	PHE	N-CA-CB	5.69	120.84	110.60
53	S2	1659	U	C4'-C3'-C2'	-5.68	96.92	102.60
53	S2	1021	U	N1-C1'-C2'	5.68	121.38	114.00
53	S2	482	G	N9-C1'-C2'	-5.68	105.75	112.00
32	5	1632	A	O4'-C1'-N9	5.67	112.74	108.20
53	S2	920	A	N9-C1'-C2'	5.67	121.37	114.00
53	S2	1341	C	O4'-C1'-N1	-5.67	103.67	108.20
32	5	2070	U	N1-C1'-C2'	5.67	121.37	114.00
42	j	27	TYR	N-CA-CB	5.66	120.80	110.60
53	S2	305	U	C2'-C3'-O3'	5.66	122.76	113.70
53	S2	1198	G	C2'-C3'-O3'	5.66	122.76	113.70
33	7	7	G	C5'-C4'-O4'	5.66	115.89	109.10
20	b	41	ARG	CG-CD-NE	-5.66	99.91	111.80
32	5	2464	C	N1-C1'-C2'	5.66	121.36	114.00
34	8	39	G	N9-C1'-C2'	-5.66	105.77	112.00
32	5	4937	C	N1-C1'-C2'	5.66	121.36	114.00
32	5	4534	G	N9-C1'-C2'	-5.66	105.78	112.00
34	8	81	C	N1-C1'-C2'	5.65	121.35	114.00
40	P	139	TYR	CB-CA-C	5.65	121.71	110.40
75	SM	26	LEU	CA-CB-CG	5.65	128.30	115.30
72	SD	9	ARG	NE-CZ-NH1	5.65	123.12	120.30
35	B	116	ARG	CG-CD-NE	5.65	123.66	111.80
49	3	22	U	N1-C1'-C2'	5.65	121.34	114.00
53	S2	28	U	N1-C1'-C2'	5.65	121.34	114.00
53	S2	1085	C	O4'-C1'-N1	-5.65	103.68	108.20
53	S2	1438	A	N9-C1'-C2'	5.64	121.34	114.00
32	5	1676	C	N1-C1'-C2'	5.64	121.34	114.00
53	S2	1378	A	N9-C1'-C2'	5.64	121.33	114.00
38	F	239	GLU	CA-CB-CG	5.64	125.80	113.40
23	e	46	ARG	NE-CZ-NH2	-5.63	117.48	120.30
32	5	92	C	C3'-C2'-C1'	5.63	106.01	101.50
58	SG	213	LEU	CB-CG-CD1	5.63	120.58	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
72	SD	107	TYR	CA-CB-CG	5.63	124.11	113.40
12	S	95	ARG	NE-CZ-NH1	5.63	123.12	120.30
32	5	328	A	C1'-O4'-C4'	-5.63	105.39	109.90
32	5	1408	G	N9-C1'-C2'	-5.63	105.81	112.00
53	S2	182	C	C2'-C3'-O3'	5.63	122.71	113.70
24	f	42	TYR	CA-CB-CG	-5.63	102.71	113.40
32	5	4280	A	C4'-C3'-C2'	-5.63	96.97	102.60
49	3	38	C	O3'-P-O5'	-5.63	93.31	104.00
53	S2	1459	G	C2'-C3'-O3'	5.63	122.70	113.70
60	SI	110	ARG	NE-CZ-NH1	5.63	123.11	120.30
69	Sa	17	HIS	N-CA-CB	5.63	120.73	110.60
32	5	1	C	O4'-C1'-N1	5.62	112.70	108.20
32	5	2827	G	O4'-C4'-C3'	-5.62	98.38	104.00
53	S2	65	C	C1'-O4'-C4'	-5.62	105.40	109.90
4	H	54	ARG	NE-CZ-NH2	-5.62	117.49	120.30
32	5	2057	A	N9-C1'-C2'	5.62	121.30	114.00
53	S2	1373	C	N1-C1'-C2'	5.61	121.30	114.00
32	5	72	C	C5'-C4'-O4'	5.61	115.83	109.10
53	S2	452	G	N9-C1'-C2'	5.61	121.30	114.00
53	S2	1834	A	N9-C1'-C2'	5.61	121.30	114.00
57	SE	103	TYR	CB-CG-CD2	5.61	124.37	121.00
32	5	964	A	O4'-C1'-C2'	-5.61	100.19	105.80
53	S2	963	A	N9-C1'-C2'	5.61	121.29	114.00
53	S2	1838	U	O4'-C4'-C3'	-5.61	98.39	104.00
32	5	2311	C	N1-C1'-C2'	-5.61	105.83	112.00
32	5	3734	U	N1-C1'-C2'	5.61	121.29	114.00
53	S2	165	G	C1'-O4'-C4'	-5.61	105.41	109.90
8	N	21	PHE	N-CA-CB	5.61	120.69	110.60
11	R	52	ARG	NE-CZ-NH1	5.61	123.10	120.30
32	5	236	G	N9-C1'-C2'	5.61	121.29	114.00
32	5	443	G	N9-C1'-C2'	5.61	121.29	114.00
32	5	2745	A	N9-C1'-C2'	5.61	121.29	114.00
2	D	50	ARG	NE-CZ-NH1	-5.60	117.50	120.30
32	5	1072	C	N1-C1'-C2'	5.60	121.29	114.00
32	5	2632	U	C6-N1-C1'	-5.60	113.36	121.20
32	5	4874	A	O4'-C1'-C2'	-5.60	100.20	105.80
57	SE	99	PHE	CB-CG-CD1	5.60	124.72	120.80
27	i	26	HIS	N-CA-CB	5.60	120.68	110.60
32	5	2092	G	N9-C1'-C2'	5.60	121.28	114.00
32	5	4451	G	N9-C1'-C2'	5.60	121.28	114.00
47	q	14	PHE	CB-CG-CD1	5.60	124.72	120.80
53	S2	797	C	C1'-O4'-C4'	-5.60	105.42	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	S2	797	C	O4'-C1'-C2'	-5.60	100.20	105.80
32	5	2039	G	N9-C1'-C2'	5.60	121.28	114.00
32	5	4518	A	O5'-P-OP1	5.60	117.42	110.70
53	S2	413	G	N9-C1'-C2'	5.60	121.28	114.00
24	f	36	ARG	NE-CZ-NH2	-5.59	117.50	120.30
26	h	109	ARG	NE-CZ-NH1	5.59	123.10	120.30
32	5	2091	C	N1-C1'-C2'	5.59	121.27	114.00
53	S2	1622	U	N1-C1'-C2'	5.59	121.27	114.00
53	S2	617	G	C2'-C3'-O3'	5.59	122.65	113.70
2	D	248	ARG	NE-CZ-NH1	5.59	123.09	120.30
22	d	25	TYR	CB-CG-CD1	-5.58	117.65	121.00
53	S2	1567	G	N9-C1'-C2'	5.58	121.26	114.00
56	SC	170	TRP	N-CA-CB	5.58	120.65	110.60
32	5	3802	U	C1'-O4'-C4'	-5.58	105.44	109.90
40	P	3	ARG	CG-CD-NE	5.58	123.51	111.80
53	S2	844	U	C1'-O4'-C4'	-5.58	105.44	109.90
80	ST	62	ARG	NE-CZ-NH1	-5.58	117.51	120.30
21	c	89	TYR	CA-CB-CG	5.57	123.99	113.40
32	5	943	A	N9-C1'-C2'	-5.57	105.87	112.00
13	T	13	TYR	N-CA-CB	-5.57	100.57	110.60
39	I	94	PHE	CB-CG-CD2	-5.57	116.90	120.80
32	5	4464	A	C8-N9-C1'	-5.57	117.67	127.70
32	5	1650	A	O4'-C4'-C3'	-5.57	98.43	104.00
12	S	82	LEU	CA-CB-CG	5.56	128.10	115.30
34	8	62	A	C8-N9-C1'	5.56	137.71	127.70
50	4	186	C	O4'-C1'-N1	5.56	112.65	108.20
32	5	1682	A	C8-N9-C1'	-5.56	117.70	127.70
35	B	102	PHE	CB-CA-C	-5.56	99.29	110.40
17	Y	72	GLN	CA-CB-CG	5.55	125.62	113.40
32	5	172	C	O4'-C1'-C2'	-5.55	100.25	105.80
48	z	219	TYR	CA-CB-CG	5.55	123.95	113.40
25	g	90	ARG	CG-CD-NE	-5.55	100.15	111.80
32	5	1787	A	N9-C1'-C2'	5.55	121.22	114.00
32	5	4283	G	O4'-C1'-C2'	-5.55	100.25	105.80
32	5	422	C	C2'-C3'-O3'	5.55	122.57	113.70
64	SO	72	TYR	CA-CB-CG	5.54	123.93	113.40
32	5	1	C	C1'-O4'-C4'	-5.54	105.47	109.90
32	5	2509	C	C1'-C2'-O2'	-5.54	93.98	110.60
60	SI	113	TYR	CB-CG-CD2	-5.54	117.68	121.00
32	5	2474	G	C2'-C3'-O3'	5.54	122.56	113.70
53	S2	366	U	C2'-C3'-O3'	5.54	122.56	113.70
32	5	1449	C	C2'-C3'-O3'	5.53	122.55	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	5	4076	G	C1'-O4'-C4'	-5.53	105.47	109.90
32	5	5016	A	C1'-O4'-C4'	-5.53	105.47	109.90
32	5	1901	C	N1-C1'-C2'	5.53	121.19	114.00
32	5	4346	U	N1-C1'-C2'	5.53	121.19	114.00
32	5	4479	A	N9-C1'-C2'	-5.53	105.92	112.00
62	SL	92	TYR	CA-CB-CG	5.53	123.90	113.40
32	5	1447	C	C1'-O4'-C4'	-5.52	105.48	109.90
32	5	1539	G	N9-C1'-C2'	-5.52	105.92	112.00
32	5	153	G	C5'-C4'-O4'	5.52	115.73	109.10
48	z	197	GLN	N-CA-C	5.52	125.91	111.00
53	S2	1036	A	N9-C1'-C2'	-5.52	105.92	112.00
53	S2	1292	C	C5'-C4'-C3'	5.52	124.83	116.00
32	5	1325	C	O4'-C1'-N1	-5.51	103.79	108.20
50	4	164	G	N3-C4-N9	-5.51	122.69	126.00
77	SQ	126	ARG	NE-CZ-NH2	5.51	123.06	120.30
32	5	2643	G	C2'-C3'-O3'	5.51	122.52	113.70
61	SJ	136	ARG	NE-CZ-NH1	5.51	123.06	120.30
32	5	2858	A	C4'-C3'-O3'	-5.51	97.83	109.40
11	R	52	ARG	NE-CZ-NH2	-5.51	117.55	120.30
32	5	2754	G	N9-C1'-C2'	-5.51	105.94	112.00
32	5	55	G	C5'-C4'-O4'	5.50	115.71	109.10
32	5	334	A	N9-C1'-C2'	5.50	121.16	114.00
32	5	3814	U	N1-C1'-C2'	5.50	121.16	114.00
53	S2	303	C	N1-C1'-C2'	5.50	121.15	114.00
53	S2	1442	U	O4'-C1'-C2'	-5.50	100.30	105.80
53	S2	1860	A	C3'-C2'-C1'	5.50	105.90	101.50
32	5	4935	C	C2'-C3'-O3'	5.50	122.50	113.70
32	5	1572	U	N1-C1'-C2'	5.50	121.15	114.00
33	7	21	G	N9-C1'-C2'	5.50	121.14	114.00
53	S2	655	A	N9-C1'-C2'	5.50	121.14	114.00
13	T	57	TYR	CA-CB-CG	5.50	123.84	113.40
32	5	2554	U	C2'-C3'-O3'	5.50	122.49	113.70
38	F	58	HIS	N-CA-CB	5.50	120.49	110.60
32	5	2305	U	N1-C1'-C2'	5.49	121.14	114.00
53	S2	27	A	C5'-C4'-O4'	5.49	115.69	109.10
58	SG	145	PHE	CB-CG-CD2	-5.49	116.95	120.80
32	5	215	C	C4'-C3'-O3'	-5.49	97.87	109.40
32	5	977	C	C5'-C4'-O4'	5.49	115.69	109.10
32	5	328	A	O4'-C1'-N9	5.49	112.59	108.20
32	5	1615	C	C2'-C3'-O3'	5.49	122.48	113.70
86	Sg	132	TRP	CA-CB-CG	-5.49	103.27	113.70
24	f	51	TYR	CB-CG-CD2	-5.49	117.71	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	S2	1123	C	O5'-P-OP1	-5.49	100.76	105.70
32	5	1539	G	C2'-C3'-O3'	5.48	122.47	113.70
53	S2	1088	U	O4'-C1'-N1	-5.48	103.81	108.20
53	S2	415	A	C4-N9-C1'	-5.48	116.43	126.30
12	S	43	ARG	NE-CZ-NH2	5.48	123.04	120.30
32	5	2325	C	C2'-C3'-O3'	5.48	122.47	113.70
12	S	10	TYR	CB-CA-C	5.48	121.36	110.40
32	5	2852	U	C4'-C3'-O3'	5.48	123.96	113.00
26	h	119	PHE	N-CA-CB	5.48	120.46	110.60
32	5	3804	G	N9-C1'-C2'	-5.48	105.98	112.00
53	S2	1512	C	N1-C1'-C2'	5.48	121.12	114.00
32	5	85	G	N9-C1'-C2'	-5.48	105.98	112.00
32	5	1891	A	N9-C1'-C2'	5.48	121.12	114.00
32	5	307	A	N9-C1'-C2'	5.47	121.12	114.00
23	e	36	ARG	NE-CZ-NH1	-5.47	117.56	120.30
32	5	235	A	C1'-O4'-C4'	-5.47	105.52	109.90
32	5	1588	U	N1-C1'-C2'	5.47	121.11	114.00
32	5	3645	U	N1-C1'-C2'	5.47	121.11	114.00
12	S	96	GLU	OE1-CD-OE2	5.47	129.87	123.30
32	5	977	C	C4'-C3'-C2'	-5.47	97.13	102.60
32	5	1319	U	C2'-C3'-O3'	5.47	122.45	113.70
53	S2	1617	G	N9-C1'-C2'	-5.47	105.98	112.00
32	5	2666	U	C2'-C3'-O3'	5.47	122.45	113.70
32	5	4199	C	C4'-C3'-O3'	5.47	123.94	113.00
34	8	102	G	N9-C1'-C2'	5.47	121.11	114.00
3	G	223	ARG	NE-CZ-NH1	5.46	123.03	120.30
10	Q	26	ARG	CG-CD-NE	-5.46	100.32	111.80
10	Q	174	PHE	CB-CA-C	5.46	121.33	110.40
32	5	4665	A	N9-C1'-C2'	-5.46	105.99	112.00
7	M	6	PHE	CB-CA-C	5.46	121.32	110.40
53	S2	385	G	O4'-C1'-N9	-5.46	103.83	108.20
47	q	99	ARG	NE-CZ-NH2	-5.46	117.57	120.30
53	S2	292	A	C2'-C3'-O3'	5.46	122.43	113.70
32	5	4328	G	N9-C1'-C2'	-5.46	106.00	112.00
53	S2	1292	C	C5'-C4'-O4'	5.46	115.65	109.10
32	5	4701	A	C8-N9-C1'	-5.45	117.89	127.70
53	S2	807	G	N9-C1'-C2'	5.45	121.09	114.00
32	5	268	G	C2'-C3'-O3'	5.45	122.42	113.70
37	E	154	ARG	NE-CZ-NH1	5.45	123.03	120.30
57	SE	253	ASP	CB-CG-OD1	5.45	123.20	118.30
58	SG	198	ARG	NE-CZ-NH1	5.45	123.03	120.30
2	D	249	GLU	CA-CB-CG	5.45	125.38	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	5	3879	G	O4'-C1'-C2'	-5.44	100.36	105.80
53	S2	415	A	C8-N9-C1'	5.44	137.50	127.70
33	7	29	C	N1-C1'-C2'	5.44	121.07	114.00
56	SC	200	ARG	CG-CD-NE	5.44	123.22	111.80
32	5	100	C	C5'-C4'-O4'	5.44	115.62	109.10
10	Q	65	ARG	NE-CZ-NH1	5.43	123.02	120.30
32	5	4557	U	N1-C1'-C2'	5.43	121.06	114.00
3	G	53	ARG	NE-CZ-NH1	5.43	123.02	120.30
85	Sf	146	LEU	N-CA-C	-5.43	96.33	111.00
32	5	2536	A	C2'-C3'-O3'	5.43	122.39	113.70
56	SC	200	ARG	NE-CZ-NH1	-5.43	117.58	120.30
32	5	1279	A	N9-C1'-C2'	5.43	121.06	114.00
32	5	4944	C	O4'-C1'-N1	-5.43	103.86	108.20
4	H	180	TYR	CA-CB-CG	5.43	123.71	113.40
5	J	146	ARG	NE-CZ-NH1	-5.43	117.59	120.30
34	8	62	A	C4-N9-C1'	-5.43	116.53	126.30
32	5	2395	A	N9-C1'-C2'	-5.42	106.03	112.00
76	SP	42	ARG	CA-CB-CG	5.42	125.33	113.40
32	5	4451	G	C4'-C3'-O3'	5.42	123.84	113.00
11	R	9	ARG	NE-CZ-NH1	5.42	123.01	120.30
44	p	18	TYR	CB-CG-CD2	-5.42	117.75	121.00
53	S2	1045	U	O4'-C1'-C2'	-5.42	100.38	105.80
53	S2	1839	U	C2-N1-C1'	5.42	124.21	117.70
32	5	4677	U	N1-C1'-C2'	-5.42	106.04	112.00
2	D	30	TYR	CB-CA-C	5.42	121.23	110.40
32	5	3812	C	C2'-C3'-O3'	5.42	122.37	113.70
10	Q	15	ARG	NE-CZ-NH1	5.42	123.01	120.30
12	S	152	PHE	CB-CG-CD2	-5.42	117.01	120.80
32	5	238	C	N1-C1'-C2'	5.42	121.04	114.00
32	5	2275	G	C2'-C3'-O3'	5.42	122.37	113.70
53	S2	369	C	N1-C1'-C2'	5.42	121.04	114.00
53	S2	975	G	C5'-C4'-O4'	5.42	115.60	109.10
32	5	2054	U	N1-C1'-C2'	5.42	121.04	114.00
5	J	35	ARG	CG-CD-NE	5.41	123.17	111.80
53	S2	426	A	O5'-P-OP1	-5.41	100.83	105.70
10	Q	176	ARG	NE-CZ-NH2	-5.41	117.59	120.30
53	S2	457	C	C2'-C3'-O3'	5.41	122.36	113.70
32	5	1439	C	O4'-C1'-C2'	-5.41	100.39	105.80
32	5	1975	G	O4'-C1'-N9	-5.41	103.87	108.20
32	5	2854	G	N9-C1'-C2'	-5.41	106.05	112.00
53	S2	427	U	P-O5'-C5'	5.41	129.55	120.90
53	S2	1376	A	C2'-C3'-O3'	5.41	122.35	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	j	43	ARG	CG-CD-NE	5.40	123.15	111.80
32	5	663	G	C4'-C3'-O3'	5.40	123.80	113.00
32	5	4683	U	N1-C1'-C2'	5.40	121.02	114.00
50	4	15	C	N1-C1'-C2'	-5.40	106.06	112.00
76	SP	18	ARG	NE-CZ-NH2	-5.40	117.60	120.30
10	Q	14	ARG	NE-CZ-NH1	5.39	123.00	120.30
11	R	108	ARG	NE-CZ-NH2	-5.39	117.60	120.30
32	5	1395	U	N1-C1'-C2'	5.39	121.01	114.00
34	8	85	U	P-O3'-C3'	5.39	126.17	119.70
37	E	278	TYR	N-CA-C	-5.39	96.44	111.00
53	S2	28	U	C4'-C3'-O3'	5.39	123.78	113.00
53	S2	1860	A	N9-C1'-C2'	-5.39	106.07	112.00
12	S	44	PHE	N-CA-CB	5.39	120.30	110.60
32	5	4078	C	C2'-C3'-O3'	5.39	122.33	113.70
32	5	1660	U	N1-C1'-C2'	-5.39	106.07	112.00
36	C	67	TRP	CA-CB-CG	5.39	123.94	113.70
53	S2	73	C	C1'-O4'-C4'	-5.39	105.59	109.90
69	Sa	28	ARG	NE-CZ-NH2	-5.39	117.61	120.30
32	5	1616	U	O4'-C1'-C2'	-5.39	100.41	105.80
67	SX	14	ARG	NE-CZ-NH2	-5.39	117.61	120.30
32	5	4325	A	N9-C1'-C2'	5.39	121.00	114.00
32	5	4320	G	N9-C1'-C2'	5.38	121.00	114.00
33	7	42	A	O4'-C1'-C2'	-5.38	100.42	105.80
10	Q	75	ARG	NE-CZ-NH2	-5.38	117.61	120.30
12	S	97	TYR	CA-CB-CG	-5.38	103.18	113.40
37	E	42	ARG	N-CA-C	5.38	125.53	111.00
5	J	54	ARG	NE-CZ-NH2	-5.38	117.61	120.30
40	P	3	ARG	NE-CZ-NH2	-5.38	117.61	120.30
53	S2	105	U	C2'-C3'-O3'	5.38	122.30	113.70
53	S2	1292	C	O4'-C4'-C3'	-5.38	98.62	104.00
45	r	107	ARG	NE-CZ-NH2	-5.38	117.61	120.30
32	5	729	G	N9-C1'-C2'	5.37	120.98	114.00
32	5	3723	A	C5-C6-N6	-5.37	119.40	123.70
53	S2	800	U	O4'-C4'-C3'	-5.37	98.63	104.00
53	S2	1092	G	C2'-C3'-O3'	5.37	122.30	113.70
74	SK	57	TYR	CB-CA-C	5.37	121.14	110.40
80	ST	33	TRP	CB-CA-C	5.37	121.14	110.40
2	D	31	TYR	N-CA-C	-5.37	96.50	111.00
32	5	2272	C	C1'-C2'-O2'	-5.37	94.49	110.60
12	S	157	ARG	NE-CZ-NH2	-5.37	117.62	120.30
32	5	2117	G	C1'-O4'-C4'	-5.37	105.61	109.90
54	SA	39	TYR	CA-CB-CG	5.37	123.60	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	5	2256	C	N1-C1'-C2'	5.37	120.98	114.00
85	Sf	133	ALA	N-CA-C	5.37	125.48	111.00
32	5	745	G	N9-C1'-C2'	5.36	120.97	114.00
32	5	4909	A	O4'-C1'-N9	5.36	112.49	108.20
55	SB	165	ARG	CD-NE-CZ	5.36	131.11	123.60
32	5	4398	C	C2'-C3'-O3'	5.36	122.28	113.70
32	5	4731	G	C1'-O4'-C4'	-5.36	105.61	109.90
62	SL	105	ARG	NE-CZ-NH1	5.36	122.98	120.30
32	5	4330	G	N9-C1'-C2'	-5.36	106.11	112.00
53	S2	149	A	N9-C1'-C2'	5.36	120.96	114.00
32	5	1847	C	N1-C1'-C2'	5.35	120.96	114.00
54	SA	116	PHE	CB-CG-CD1	5.35	124.55	120.80
53	S2	1671	G	N9-C1'-C2'	5.35	120.96	114.00
56	SC	97	PHE	CB-CG-CD2	-5.35	117.05	120.80
4	H	125	ARG	CG-CD-NE	5.35	123.04	111.80
47	q	99	ARG	CD-NE-CZ	5.35	131.09	123.60
54	SA	117	ARG	CG-CD-NE	5.35	123.03	111.80
61	SJ	109	ARG	NE-CZ-NH1	5.35	122.97	120.30
10	Q	34	PHE	CB-CG-CD2	-5.35	117.06	120.80
32	5	2746	A	N9-C1'-C2'	5.35	120.95	114.00
64	SO	34	PHE	CB-CG-CD2	-5.35	117.06	120.80
56	SC	96	PHE	N-CA-CB	5.35	120.22	110.60
32	5	2056	G	N9-C1'-C2'	-5.34	106.12	112.00
32	5	3663	A	O4'-C4'-C3'	-5.34	98.66	104.00
1	A	193	ARG	NE-CZ-NH2	-5.34	117.63	120.30
32	5	2075	G	N9-C1'-C2'	-5.34	106.13	112.00
32	5	1642	A	C2'-C3'-O3'	5.33	122.24	113.70
32	5	2088	A	N9-C1'-C2'	-5.33	106.13	112.00
32	5	2250	C	P-O5'-C5'	5.33	129.43	120.90
32	5	2689	C	O4'-C1'-C2'	-5.33	100.47	105.80
53	S2	980	A	C4-N9-C1'	5.33	135.90	126.30
53	S2	1641	A	N9-C1'-C2'	5.33	120.93	114.00
32	5	1484	G	C4-N9-C1'	-5.33	119.57	126.50
11	R	103	ARG	NE-CZ-NH2	-5.33	117.64	120.30
32	5	922	C	C2'-C3'-O3'	5.33	122.23	113.70
32	5	4463	U	O4'-C1'-N1	5.33	112.46	108.20
10	Q	180	ARG	NE-CZ-NH2	5.33	122.96	120.30
9	O	140	ARG	NE-CZ-NH1	-5.33	117.64	120.30
53	S2	1146	C	N1-C1'-C2'	5.33	120.92	114.00
20	b	41	ARG	NE-CZ-NH2	-5.32	117.64	120.30
20	b	44	ARG	NE-CZ-NH2	-5.32	117.64	120.30
32	5	405	U	C2'-C3'-O3'	5.32	122.22	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	5	1264	C	C2'-C3'-O3'	5.32	122.22	113.70
32	5	2008	U	O4'-C4'-C3'	-5.32	98.68	104.00
32	5	4227	U	C2'-C3'-O3'	5.32	122.22	113.70
54	SA	158	ASP	CB-CG-OD2	5.32	123.09	118.30
32	5	2424	G	N9-C1'-C2'	5.32	120.92	114.00
13	T	140	PHE	CB-CA-C	-5.32	99.76	110.40
4	H	96	TYR	CA-CB-CG	5.32	123.50	113.40
40	P	42	ARG	CG-CD-NE	5.32	122.97	111.80
32	5	1880	G	N9-C1'-C2'	5.32	120.91	114.00
32	5	4533	A	N9-C1'-C2'	-5.32	106.15	112.00
10	Q	75	ARG	CG-CD-NE	5.31	122.95	111.80
32	5	381	U	N1-C1'-C2'	5.31	120.90	114.00
53	S2	1093	A	C5'-C4'-O4'	5.31	115.47	109.10
15	V	96	LEU	CA-CB-CG	5.31	127.51	115.30
32	5	2316	G	N9-C1'-C2'	5.31	120.90	114.00
59	SH	118	ARG	NE-CZ-NH2	-5.31	117.64	120.30
66	SW	97	ARG	NE-CZ-NH1	5.31	122.95	120.30
32	5	936	C	N1-C1'-C2'	-5.31	106.16	112.00
32	5	4497	U	C4'-C3'-C2'	-5.31	97.29	102.60
32	5	4750	G	N9-C1'-C2'	-5.31	106.16	112.00
53	S2	654	A	N9-C1'-C2'	-5.30	106.17	112.00
24	f	51	TYR	CB-CG-CD1	5.30	124.18	121.00
32	5	1211	G	O4'-C1'-C2'	-5.30	100.50	105.80
40	P	25	HIS	CB-CA-C	5.30	121.00	110.40
53	S2	167	G	N9-C1'-C2'	5.30	120.89	114.00
2	D	226	TYR	CA-CB-CG	-5.30	103.33	113.40
32	5	279	A	N9-C1'-C2'	5.30	120.89	114.00
32	5	5047	C	O5'-P-OP2	-5.30	100.93	105.70
63	SN	64	ARG	NE-CZ-NH1	5.30	122.95	120.30
32	5	703	G	C1'-O4'-C4'	-5.30	105.66	109.90
75	SM	127	TYR	CB-CG-CD1	5.30	124.18	121.00
1	A	189	TYR	N-CA-CB	5.29	120.13	110.60
17	Y	61	HIS	N-CA-CB	5.29	120.13	110.60
23	e	75	ARG	CG-CD-NE	-5.29	100.68	111.80
53	S2	843	C	N1-C1'-C2'	5.29	120.88	114.00
57	SE	103	TYR	N-CA-CB	5.29	120.13	110.60
5	J	147	ARG	NE-CZ-NH2	-5.29	117.65	120.30
75	SM	26	LEU	CB-CG-CD2	5.29	120.00	111.00
53	S2	1453	C	C4'-C3'-O3'	5.29	123.58	113.00
32	5	1313	C	O4'-C1'-N1	-5.29	103.97	108.20
34	8	34	U	O4'-C1'-N1	-5.29	103.97	108.20
35	B	179	HIS	CB-CA-C	5.29	120.98	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
61	SJ	38	ARG	NE-CZ-NH2	-5.29	117.66	120.30
32	5	2323	C	N1-C1'-C2'	-5.29	106.18	112.00
53	S2	957	A	C4'-C3'-O3'	-5.29	98.30	109.40
32	5	4723	A	C5'-C4'-O4'	5.29	115.44	109.10
10	Q	33	ARG	N-CA-C	-5.29	96.73	111.00
32	5	2361	G	O4'-C1'-N9	5.29	112.43	108.20
32	5	4234	A	C2'-C3'-O3'	5.29	122.16	113.70
17	Y	26	ARG	NE-CZ-NH2	-5.28	117.66	120.30
53	S2	1568	C	N1-C1'-C2'	5.28	120.87	114.00
85	Sf	148	TYR	C-N-CA	5.28	134.91	121.70
32	5	88	A	C1'-C2'-O2'	-5.28	94.76	110.60
34	8	73	U	C2'-C3'-O3'	5.28	122.15	113.70
32	5	2545	U	C5'-C4'-O4'	5.28	115.43	109.10
32	5	2889	G	N9-C1'-C2'	5.28	120.86	114.00
32	5	4763	U	O4'-C1'-N1	5.28	112.42	108.20
53	S2	1666	C	N1-C1'-C2'	5.28	120.86	114.00
32	5	4695	C	N1-C1'-C2'	5.28	120.86	114.00
2	D	157	ASN	CB-CA-C	5.27	120.95	110.40
8	N	96	ARG	NE-CZ-NH2	5.27	122.94	120.30
35	B	228	TYR	CB-CG-CD1	5.27	124.16	121.00
32	5	737	C	C2'-C3'-O3'	5.27	122.13	113.70
32	5	2737	C	N1-C1'-C2'	5.27	120.85	114.00
32	5	3905	A	O4'-C4'-C3'	-5.27	98.73	104.00
48	z	109	LEU	CA-CB-CG	5.26	127.41	115.30
76	SP	42	ARG	CG-CD-NE	-5.26	100.75	111.80
22	d	73	TRP	N-CA-CB	-5.26	101.13	110.60
66	SW	57	ARG	NE-CZ-NH2	-5.26	117.67	120.30
32	5	4761	G	N9-C1'-C2'	5.26	120.84	114.00
53	S2	1395	C	O4'-C1'-C2'	-5.26	100.54	105.80
32	5	333	U	N1-C1'-C2'	5.26	120.83	114.00
32	5	2436	U	O4'-C1'-N1	-5.25	104.00	108.20
33	7	114	U	N1-C1'-C2'	5.25	120.83	114.00
71	Se	41	ARG	NE-CZ-NH1	5.25	122.92	120.30
32	5	2858	A	N9-C1'-C2'	5.25	120.83	114.00
1	A	147	ARG	NE-CZ-NH1	5.25	122.92	120.30
32	5	2733	C	C2'-C3'-O3'	5.25	122.10	113.70
53	S2	457	C	N1-C1'-C2'	-5.25	106.23	112.00
53	S2	1522	A	O4'-C4'-C3'	-5.25	98.75	104.00
74	SK	68	TYR	CB-CA-C	5.25	120.90	110.40
32	5	2745	A	C1'-C2'-O2'	-5.25	94.86	110.60
32	5	1445	U	C2'-C3'-O3'	5.25	122.09	113.70
32	5	2586	G	O4'-C1'-N9	5.25	112.40	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	5	2665	U	C2'-C3'-O3'	5.25	122.09	113.70
53	S2	1080	A	O4'-C1'-N9	5.25	112.40	108.20
32	5	480	C	C2'-C3'-O3'	5.24	122.09	113.70
32	5	4556	U	C1'-O4'-C4'	-5.24	105.71	109.90
13	T	105	PHE	CB-CA-C	5.24	120.88	110.40
32	5	2725	A	N9-C1'-C2'	5.24	120.81	114.00
53	S2	428	U	O4'-C1'-N1	-5.24	104.01	108.20
2	D	66	TYR	CA-CB-CG	5.24	123.35	113.40
2	D	145	TYR	CB-CA-C	5.24	120.87	110.40
32	5	2753	G	C2'-C3'-O3'	5.24	122.08	113.70
53	S2	1420	G	C2'-C3'-O3'	5.24	122.08	113.70
24	f	22	ARG	NE-CZ-NH1	5.23	122.92	120.30
49	3	38	C	OP1-P-O3'	5.23	116.72	105.20
6	L	186	ARG	CG-CD-NE	-5.23	100.81	111.80
32	5	1266	G	C2'-C3'-O3'	5.23	122.07	113.70
32	5	1852	U	N1-C1'-C2'	-5.23	106.24	112.00
53	S2	367	U	C1'-C2'-O2'	5.23	126.30	110.60
32	5	4322	G	C2'-C3'-O3'	5.23	122.07	113.70
60	SI	197	PHE	N-CA-C	-5.23	96.88	111.00
10	Q	33	ARG	N-CA-CB	5.23	120.01	110.60
32	5	2089	G	O4'-C1'-N9	5.23	112.38	108.20
55	SB	136	ARG	NE-CZ-NH2	5.23	122.91	120.30
57	SE	18	TRP	CA-CB-CG	-5.23	103.77	113.70
5	J	147	ARG	NE-CZ-NH1	5.22	122.91	120.30
23	e	74	PHE	CB-CG-CD1	-5.22	117.14	120.80
53	S2	1675	A	N9-C1'-C2'	-5.22	106.25	112.00
64	SO	147	ARG	NE-CZ-NH1	5.22	122.91	120.30
71	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
34	8	46	G	N9-C1'-C2'	5.22	120.78	114.00
53	S2	1605	G	C2'-C3'-O3'	5.22	122.05	113.70
50	4	162	C	N3-C4-C5	-5.22	119.81	121.90
32	5	5043	A	C1'-C2'-O2'	-5.21	94.95	110.60
35	B	257	TRP	N-CA-CB	5.21	119.98	110.60
32	5	1885	G	C4'-C3'-O3'	5.21	123.42	113.00
42	j	66	HIS	CA-CB-CG	-5.21	104.74	113.60
21	c	56	ARG	NE-CZ-NH2	-5.21	117.69	120.30
53	S2	297	A	N9-C1'-C2'	-5.21	106.27	112.00
18	Z	38	TYR	CB-CA-C	5.21	120.82	110.40
32	5	2741	U	N1-C1'-C2'	5.21	120.77	114.00
32	5	3908	A	C3'-C2'-C1'	-5.21	97.33	101.50
44	p	85	ARG	CG-CD-NE	5.21	122.73	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
77	SQ	71	ARG	CG-CD-NE	5.21	122.73	111.80
32	5	4701	A	C4-N9-C1'	5.21	135.67	126.30
53	S2	1225	U	C2'-C3'-O3'	5.20	122.03	113.70
6	L	36	ARG	NE-CZ-NH1	5.20	122.90	120.30
32	5	210	C	N1-C1'-C2'	5.20	120.76	114.00
32	5	1697	G	O4'-C1'-N9	5.20	112.36	108.20
1	A	189	TYR	CB-CG-CD2	-5.20	117.88	121.00
11	R	155	LEU	CA-CB-CG	5.20	127.25	115.30
53	S2	631	U	C2'-C3'-O3'	5.20	122.02	113.70
53	S2	651	U	N1-C1'-C2'	5.20	120.76	114.00
32	5	1296	G	C1'-O4'-C4'	-5.20	105.74	109.90
62	SL	62	PHE	CB-CG-CD2	-5.20	117.16	120.80
67	SX	67	ARG	NE-CZ-NH1	-5.20	117.70	120.30
32	5	393	U	N1-C1'-C2'	-5.19	106.29	112.00
32	5	2665	U	N1-C1'-C2'	-5.19	106.29	112.00
32	5	4709	U	C5'-C4'-O4'	5.19	115.33	109.10
56	SC	68	ARG	NE-CZ-NH1	5.19	122.89	120.30
32	5	4670	C	O4'-C1'-N1	-5.19	104.05	108.20
32	5	4966	A	C8-N9-C1'	-5.19	118.36	127.70
32	5	468	U	N1-C1'-C2'	5.19	120.74	114.00
10	Q	168	ARG	NE-CZ-NH1	5.18	122.89	120.30
32	5	96	U	C2'-C3'-O3'	5.18	121.99	113.70
32	5	272	U	N1-C1'-C2'	5.18	120.74	114.00
32	5	2080	U	N1-C1'-C2'	5.18	120.74	114.00
4	H	88	PHE	CB-CG-CD2	-5.18	117.17	120.80
37	E	129	PHE	CB-CG-CD1	5.18	124.43	120.80
55	SB	100	PHE	N-CA-CB	5.18	119.92	110.60
17	Y	87	ARG	CD-NE-CZ	5.18	130.85	123.60
32	5	2089	G	C1'-O4'-C4'	-5.18	105.76	109.90
2	D	145	TYR	CA-CB-CG	-5.18	103.56	113.40
6	L	82	ARG	NE-CZ-NH2	-5.18	117.71	120.30
32	5	1832	C	C2'-C3'-O3'	5.18	121.98	113.70
53	S2	980	A	C8-N9-C1'	-5.18	118.38	127.70
61	SJ	127	ARG	NE-CZ-NH2	-5.18	117.71	120.30
32	5	931	C	N1-C1'-C2'	5.17	120.73	114.00
32	5	2328	G	C1'-C2'-O2'	-5.17	95.08	110.60
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
36	C	35	ASP	CB-CG-OD2	-5.17	113.65	118.30
32	5	2056	G	O4'-C1'-N9	5.17	112.33	108.20
53	S2	1522	A	N9-C1'-C2'	-5.17	106.31	112.00
50	4	183	A	P-O3'-C3'	-5.17	113.50	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	5	4589	A	O4'-C4'-C3'	-5.17	98.83	104.00
46	K	55	GLY	N-CA-C	-5.17	100.19	113.10
38	F	100	ILE	CG1-CB-CG2	5.16	122.76	111.40
53	S2	1823	A	C2'-C3'-O3'	5.16	121.96	113.70
27	i	41	ARG	NE-CZ-NH1	5.16	122.88	120.30
32	5	1609	U	C2'-C3'-O3'	5.16	121.96	113.70
32	5	1365	C	P-O3'-C3'	5.16	125.89	119.70
32	5	5002	U	N1-C1'-C2'	5.16	120.71	114.00
53	S2	600	G	N9-C1'-C2'	5.16	120.71	114.00
36	C	100	ARG	NE-CZ-NH1	5.16	122.88	120.30
42	j	27	TYR	CB-CG-CD1	-5.16	117.91	121.00
54	SA	204	TYR	CB-CG-CD1	5.16	124.09	121.00
3	G	73	ARG	NE-CZ-NH1	5.16	122.88	120.30
32	5	4280	A	C5'-C4'-O4'	5.16	115.29	109.10
36	C	143	ARG	NE-CZ-NH2	-5.16	117.72	120.30
45	r	45	HIS	CB-CA-C	-5.16	100.09	110.40
53	S2	1292	C	P-O3'-C3'	5.16	125.89	119.70
32	5	2077	C	N1-C1'-C2'	-5.15	106.33	112.00
53	S2	1386	A	C2'-C3'-O3'	5.15	121.95	113.70
53	S2	165	G	O4'-C4'-C3'	-5.15	98.85	104.00
53	S2	645	C	C2'-C3'-O3'	5.15	121.94	113.70
53	S2	1525	C	C2'-C3'-O3'	5.15	121.94	113.70
32	5	2802	C	N1-C1'-C2'	-5.15	106.33	112.00
32	5	4270	C	C5'-C4'-O4'	5.15	115.28	109.10
42	j	11	ARG	CG-CD-NE	-5.15	100.98	111.80
53	S2	61	A	C4'-C3'-O3'	-5.15	98.59	109.40
53	S2	957	A	C2'-C3'-O3'	5.15	121.94	113.70
53	S2	1049	A	C1'-O4'-C4'	-5.15	105.78	109.90
2	D	44	TYR	CA-CB-CG	-5.15	103.62	113.40
11	R	95	TRP	N-CA-C	-5.15	97.10	111.00
32	5	1444	G	N9-C1'-C2'	5.15	120.69	114.00
33	7	5	A	N9-C1'-C2'	-5.15	106.34	112.00
33	7	6	C	N1-C1'-C2'	-5.15	106.34	112.00
32	5	4234	A	C4-N9-C1'	-5.15	117.04	126.30
55	SB	82	ARG	N-CA-C	5.15	124.89	111.00
31	o	78	ARG	NE-CZ-NH1	-5.14	117.73	120.30
32	5	961	G	C4'-C3'-O3'	5.14	123.29	113.00
53	S2	844	U	O4'-C1'-N1	5.14	112.32	108.20
32	5	1793	A	C2'-C3'-O3'	5.14	121.93	113.70
60	SI	28	GLU	N-CA-C	-5.14	97.12	111.00
32	5	4337	C	N1-C1'-C2'	5.14	120.68	114.00
1	A	227	ARG	NE-CZ-NH1	5.14	122.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	SA	90	PHE	N-CA-CB	5.14	119.85	110.60
32	5	2787	A	O5'-P-OP1	5.13	116.86	110.70
33	7	22	A	C1'-O4'-C4'	-5.13	105.79	109.90
73	SF	48	TYR	CA-CB-CG	5.13	123.15	113.40
53	S2	638	C	N1-C1'-C2'	5.13	120.67	114.00
73	SF	152	TRP	N-CA-CB	5.13	119.83	110.60
32	5	514	U	C4'-C3'-O3'	5.13	123.26	113.00
32	5	2360	A	N9-C1'-C2'	5.13	120.67	114.00
32	5	148	C	N1-C1'-C2'	5.13	120.66	114.00
32	5	219	G	O4'-C1'-C2'	-5.13	100.67	105.80
10	Q	181	ARG	CG-CD-NE	-5.12	101.04	111.80
53	S2	603	C	C4'-C3'-O3'	5.12	123.25	113.00
53	S2	1142	G	C4'-C3'-C2'	-5.12	97.47	102.60
17	Y	87	ARG	NE-CZ-NH1	-5.12	117.74	120.30
32	5	1520	C	C2'-C3'-O3'	5.12	121.90	113.70
32	5	4239	A	C2'-C3'-O3'	5.12	121.90	113.70
77	SQ	71	ARG	CD-NE-CZ	5.12	130.77	123.60
32	5	58	G	O4'-C1'-N9	-5.12	104.10	108.20
2	D	175	HIS	N-CA-C	-5.12	97.18	111.00
32	5	3898	G	C2'-C3'-O3'	5.12	121.89	113.70
1	A	194	ASN	N-CA-CB	5.12	119.81	110.60
32	5	3719	A	C2'-C3'-O3'	5.12	121.89	113.70
32	5	3727	A	C1'-C2'-O2'	-5.12	95.25	110.60
33	7	57	C	C2'-C3'-O3'	5.12	121.89	113.70
70	Sb	31	TYR	CA-CB-CG	5.12	123.13	113.40
85	Sf	138	ARG	CD-NE-CZ	5.12	130.77	123.60
53	S2	619	A	C3'-C2'-C1'	-5.12	97.41	101.50
55	SB	81	PHE	CB-CG-CD1	-5.12	117.22	120.80
5	J	146	ARG	NE-CZ-NH2	5.12	122.86	120.30
32	5	5005	G	N9-C1'-C2'	-5.12	106.37	112.00
5	J	32	ARG	NE-CZ-NH2	-5.11	117.74	120.30
32	5	1947	U	C4'-C3'-O3'	5.11	123.23	113.00
53	S2	446	G	N9-C1'-C2'	-5.11	106.38	112.00
10	Q	33	ARG	CG-CD-NE	-5.11	101.06	111.80
53	S2	1391	C	C2'-C3'-O3'	5.11	121.88	113.70
32	5	107	G	N9-C1'-C2'	-5.11	106.38	112.00
32	5	21	G	C4'-C3'-O3'	5.11	123.22	113.00
53	S2	1481	G	N9-C1'-C2'	5.11	120.64	114.00
32	5	1271	G	C4'-C3'-O3'	5.11	123.21	113.00
53	S2	1097	G	C2'-C3'-O3'	5.11	121.87	113.70
20	b	16	TRP	CB-CA-C	5.10	120.61	110.40
32	5	394	G	C4'-C3'-C2'	-5.10	97.50	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	5	1341	U	N1-C1'-C2'	5.10	120.63	114.00
32	5	1447	C	O4'-C1'-N1	5.10	112.28	108.20
32	5	2127	C	N1-C1'-C2'	5.10	120.63	114.00
53	S2	839	C	N1-C1'-C2'	5.10	120.63	114.00
53	S2	56	G	N9-C1'-C2'	5.10	120.63	114.00
31	o	42	ASP	N-CA-CB	5.09	119.77	110.60
53	S2	381	C	P-O5'-C5'	5.09	129.05	120.90
32	5	4229	U	O4'-C1'-C2'	-5.09	100.71	105.80
32	5	4884	G	O4'-C1'-C2'	-5.09	100.71	105.80
35	B	117	ARG	CG-CD-NE	-5.09	101.11	111.80
53	S2	992	A	N9-C1'-C2'	-5.09	106.40	112.00
53	S2	1149	A	N9-C1'-C2'	-5.09	106.40	112.00
86	Sg	302	TYR	CB-CG-CD2	-5.09	117.94	121.00
36	C	201	ARG	NE-CZ-NH1	5.09	122.84	120.30
66	SW	28	ARG	NE-CZ-NH1	5.09	122.84	120.30
72	SD	106	ARG	NE-CZ-NH1	5.09	122.84	120.30
67	SX	17	ARG	CG-CD-NE	-5.08	101.12	111.80
22	d	44	ARG	NE-CZ-NH2	-5.08	117.76	120.30
32	5	4441	A	C2'-C3'-O3'	5.08	121.83	113.70
33	7	49	A	N9-C1'-C2'	-5.08	106.41	112.00
50	4	32	A	N9-C1'-C2'	-5.08	106.41	112.00
55	SB	107	ARG	NE-CZ-NH2	-5.08	117.76	120.30
32	5	209	U	O4'-C1'-N1	5.08	112.27	108.20
32	5	2782	U	P-O3'-C3'	5.08	125.80	119.70
53	S2	943	U	C5'-C4'-O4'	5.08	115.20	109.10
32	5	1365	C	O4'-C1'-N1	-5.08	104.14	108.20
32	5	4911	A	N9-C1'-C2'	-5.08	106.41	112.00
32	5	4975	G	C3'-C2'-C1'	5.08	105.56	101.50
5	J	35	ARG	NE-CZ-NH2	-5.08	117.76	120.30
53	S2	968	U	C2'-C3'-O3'	5.08	121.82	113.70
32	5	2264	C	C2'-C3'-O3'	5.08	121.82	113.70
53	S2	1036	A	C2'-C3'-O3'	5.08	121.82	113.70
53	S2	1604	G	C2'-C3'-O3'	5.08	121.82	113.70
77	SQ	138	ARG	CG-CD-NE	5.08	122.46	111.80
12	S	111	ARG	NE-CZ-NH2	5.07	122.84	120.30
53	S2	1703	C	N1-C1'-C2'	-5.07	106.42	112.00
32	5	1488	G	C2'-C3'-O3'	5.07	121.81	113.70
32	5	1980	U	O4'-C1'-N1	5.07	112.25	108.20
53	S2	798	A	C4'-C3'-C2'	-5.07	97.53	102.60
57	SE	235	TRP	CA-CB-CG	5.07	123.33	113.70
32	5	1267	C	N1-C1'-C2'	5.07	120.59	114.00
33	7	81	G	C2'-C3'-O3'	5.07	121.81	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	8	113	C	C2'-C3'-O3'	5.07	121.81	113.70
53	S2	1404	U	C4'-C3'-O3'	-5.07	98.76	109.40
56	SC	68	ARG	CG-CD-NE	5.07	122.44	111.80
4	H	124	ARG	NE-CZ-NH1	5.06	122.83	120.30
11	R	108	ARG	CG-CD-NE	5.06	122.43	111.80
53	S2	646	G	C2'-C3'-O3'	5.06	121.80	113.70
6	L	99	ASP	N-CA-C	-5.06	97.34	111.00
41	W	8	PHE	CB-CA-C	5.06	120.52	110.40
53	S2	1404	U	O4'-C1'-N1	-5.06	104.15	108.20
11	R	108	ARG	CD-NE-CZ	5.06	130.68	123.60
32	5	20	U	N1-C1'-C2'	-5.06	106.44	112.00
32	5	1522	G	C4'-C3'-C2'	-5.06	97.54	102.60
32	5	292	G	C4'-C3'-O3'	-5.05	98.79	109.40
32	5	383	A	C1'-C2'-O2'	-5.05	95.44	110.60
32	5	3740	G	O4'-C1'-C2'	-5.05	100.75	105.80
32	5	5044	A	C1'-C2'-O2'	-5.05	95.44	110.60
33	7	59	G	C2'-C3'-O3'	5.05	121.78	113.70
32	5	338	A	C2'-C3'-O3'	5.05	121.78	113.70
32	5	4094	G	C2'-C3'-O3'	5.05	121.78	113.70
39	I	147	HIS	CB-CA-C	5.05	120.50	110.40
32	5	1636	U	N1-C1'-C2'	5.05	120.56	114.00
53	S2	800	U	O4'-C1'-N1	5.05	112.24	108.20
27	i	85	ARG	CD-NE-CZ	5.05	130.66	123.60
32	5	2511	A	C5'-C4'-O4'	5.05	115.16	109.10
32	5	2545	U	C2'-C3'-O3'	5.05	121.78	113.70
53	S2	606	G	O4'-C1'-N9	5.05	112.24	108.20
53	S2	127	C	C4'-C3'-O3'	5.04	123.09	113.00
10	Q	52	PHE	N-CA-CB	-5.04	101.52	110.60
38	F	228	HIS	N-CA-CB	5.04	119.68	110.60
59	SH	135	PHE	CB-CG-CD1	5.04	124.33	120.80
10	Q	32	TYR	CA-CB-CG	5.04	122.98	113.40
36	C	350	ARG	NE-CZ-NH2	-5.04	117.78	120.30
87	S1	44	ASP	CB-CG-OD1	-5.04	113.76	118.30
53	S2	376	A	N9-C1'-C2'	-5.04	106.46	112.00
53	S2	1561	A	N9-C1'-C2'	-5.04	106.46	112.00
53	S2	1339	U	C3'-C2'-C1'	5.04	105.53	101.50
8	N	143	ARG	NE-CZ-NH2	-5.03	117.78	120.30
53	S2	504	G	N9-C1'-C2'	5.03	120.55	114.00
67	SX	5	ARG	NE-CZ-NH1	-5.03	117.78	120.30
30	m	111	ARG	NE-CZ-NH2	5.03	122.82	120.30
32	5	4539	U	N1-C1'-C2'	5.03	120.54	114.00
53	S2	1537	A	N9-C1'-C2'	-5.03	106.47	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	32	ARG	NE-CZ-NH1	5.03	122.82	120.30
32	5	4939	C	O4'-C1'-C2'	-5.03	100.77	105.80
34	8	70	G	C3'-C2'-C1'	5.03	105.53	101.50
53	S2	943	U	C2-N1-C1'	5.03	123.73	117.70
77	SQ	99	TYR	CB-CG-CD1	5.03	124.02	121.00
32	5	4463	U	O4'-C1'-C2'	-5.03	100.77	105.80
40	P	42	ARG	NE-CZ-NH2	-5.03	117.79	120.30
7	M	109	ARG	CA-CB-CG	5.02	124.45	113.40
48	z	281	ASP	CB-CG-OD2	-5.02	113.78	118.30
53	S2	1138	C	C1'-O4'-C4'	-5.02	105.88	109.90
77	SQ	71	ARG	NE-CZ-NH2	-5.02	117.79	120.30
32	5	84	A	O4'-C4'-C3'	-5.02	98.98	104.00
34	8	67	U	N1-C1'-C2'	5.02	120.52	114.00
53	S2	1416	C	C2'-C3'-O3'	5.02	121.73	113.70
32	5	3667	C	N1-C1'-C2'	-5.01	106.48	112.00
38	F	197	TYR	CB-CA-C	-5.01	100.37	110.40
32	5	2268	A	P-O3'-C3'	5.01	125.72	119.70
32	5	3881	G	O4'-C1'-N9	-5.01	104.19	108.20
32	5	4114	C	N1-C1'-C2'	5.01	120.52	114.00
32	5	4976	U	N1-C1'-C2'	5.01	120.51	114.00
79	SS	124	ARG	CG-CD-NE	5.01	122.32	111.80
32	5	4606	G	N9-C1'-C2'	5.01	120.51	114.00
32	5	2586	G	C3'-C2'-C1'	-5.01	97.49	101.50
32	5	4436	U	N1-C1'-C2'	-5.01	106.49	112.00
48	z	237	LYS	CD-CE-NZ	5.01	123.22	111.70
32	5	1397	A	C2'-C3'-O3'	5.01	121.71	113.70
53	S2	349	A	C4'-C3'-O3'	-5.01	98.89	109.40
53	S2	1830	U	N1-C1'-C2'	-5.00	106.50	112.00
13	T	19	PHE	CB-CA-C	-5.00	100.39	110.40
32	5	1733	G	C4'-C3'-O3'	5.00	123.01	113.00
32	5	2666	U	C5'-C4'-O4'	5.00	115.10	109.10
32	5	4519	C	C4'-C3'-C2'	-5.00	97.60	102.60
85	Sf	146	LEU	N-CA-CB	5.00	120.41	110.40

There are no chirality outliers.

All (525) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	5	100	C	Sidechain
32	5	120	A	Sidechain
32	5	1214	C	Sidechain
32	5	1319	U	Sidechain

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Mol	Chain	Res	Type	Group
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
32	5	2082	G	Sidechain
32	5	2087	C	Sidechain
32	5	22	G	Sidechain
32	5	2263	A	Sidechain

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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	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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
10	Q	51	LEU	Peptide
11	R	132	PHE	Sidechain,Peptide
11	R	174	GLU	Peptide
11	R	19	LYS	Peptide
11	R	23	TRP	Peptide
11	R	31	GLU	Peptide

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Mol	Chain	Res	Type	Group
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
87	S1	46	LEU	Peptide
87	S1	5	GLN	Peptide,Mainchain
87	S1	52	LYS	Peptide
53	S2	1036	A	Sidechain
53	S2	1063	C	Sidechain
53	S2	1085	C	Sidechain
53	S2	1088	U	Sidechain
53	S2	1142	G	Sidechain
53	S2	1167	G	Sidechain
53	S2	1168	G	Sidechain
53	S2	1221	G	Sidechain
53	S2	1247	C	Sidechain
53	S2	1249	C	Sidechain
53	S2	1378	A	Sidechain
53	S2	1408	U	Sidechain
53	S2	1452	A	Sidechain
53	S2	1453	C	Sidechain
53	S2	1537	A	Sidechain
53	S2	1552	G	Sidechain
53	S2	1578	U	Sidechain
53	S2	1603	G	Sidechain
53	S2	1606	G	Sidechain
53	S2	1623	A	Sidechain
53	S2	1659	U	Sidechain
53	S2	1835	A	Sidechain
53	S2	1838	U	Sidechain
53	S2	26	U	Sidechain
53	S2	27	A	Sidechain
53	S2	294	U	Sidechain
53	S2	3	C	Sidechain
53	S2	31	U	Sidechain
53	S2	313	A	Sidechain
53	S2	367	U	Sidechain

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Mol	Chain	Res	Type	Group
53	S2	381	C	Sidechain
53	S2	382	C	Sidechain
53	S2	399	C	Sidechain
53	S2	409	C	Sidechain
53	S2	421	G	Sidechain
53	S2	423	U	Sidechain
53	S2	426	A	Sidechain
53	S2	427	U	Sidechain
53	S2	428	U	Sidechain
53	S2	437	G	Sidechain
53	S2	447	A	Sidechain
53	S2	448	A	Sidechain
53	S2	482	G	Sidechain
53	S2	596	U	Sidechain
53	S2	617	G	Sidechain
53	S2	631	U	Sidechain
53	S2	642	U	Sidechain
53	S2	645	C	Sidechain
53	S2	648	A	Sidechain
53	S2	662	G	Sidechain
53	S2	821	G	Sidechain
53	S2	825	A	Sidechain
53	S2	841	G	Sidechain
53	S2	875	A	Sidechain
53	S2	876	C	Sidechain
53	S2	91	A	Sidechain
53	S2	92	A	Sidechain
53	S2	945	U	Sidechain
53	S2	999	G	Sidechain
54	SA	103	PHE	Sidechain
54	SA	115	ALA	Peptide
54	SA	163	CYS	Peptide
54	SA	2	SER	Peptide
54	SA	40	LYS	Peptide
55	SB	100	PHE	Sidechain
55	SB	205	TYR	Sidechain
55	SB	211	PHE	Peptide
55	SB	40	ASN	Peptide
55	SB	66	VAL	Peptide
55	SB	81	PHE	Sidechain,Peptide
56	SC	168	GLY	Peptide
56	SC	235	ASN	Peptide

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Mol	Chain	Res	Type	Group
56	SC	236	PHE	Sidechain
56	SC	240	THR	Peptide
56	SC	241	PHE	Sidechain
56	SC	60	TRP	Peptide
56	SC	96	PHE	Peptide
72	SD	159	HIS	Sidechain
72	SD	196	GLY	Peptide
72	SD	203	PRO	Peptide
57	SE	100	ARG	Peptide
57	SE	121	TYR	Sidechain
57	SE	17	HIS	Peptide
57	SE	205	PHE	Peptide
57	SE	41	CYS	Peptide
57	SE	86	PHE	Sidechain
73	SF	164	ARG	Peptide
73	SF	22	LYS	Peptide
73	SF	43	GLU	Peptide
73	SF	51	HIS	Sidechain
58	SG	57	ASP	Peptide
59	SH	108	SER	Peptide
59	SH	189	PHE	Peptide
60	SI	111	GLN	Peptide
60	SI	149	TYR	Peptide
60	SI	153	LYS	Peptide
60	SI	155	ASN	Peptide
60	SI	197	PHE	Peptide
60	SI	26	LYS	Peptide
60	SI	50	GLY	Peptide
60	SI	64	ASN	Peptide
60	SI	65	PHE	Peptide
61	SJ	18	ARG	Peptide
61	SJ	38	ARG	Peptide
61	SJ	93	LYS	Peptide
74	SK	60	GLU	Peptide
62	SL	15	THR	Peptide
62	SL	151	THR	Peptide
62	SL	62	PHE	Sidechain
75	SM	32	ALA	Peptide
75	SM	75	ASN	Peptide
63	SN	112	LYS	Peptide
63	SN	113	PHE	Peptide
63	SN	127	ARG	Peptide

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

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Mol	Chain	Res	Type	Group
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
31	o	47	GLY	Peptide
44	p	17	ARG	Peptide
47	q	116	ILE	Peptide
47	q	117	ALA	Peptide
47	q	132	PRO	Peptide
47	q	202	GLU	Peptide

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Mol	Chain	Res	Type	Group
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	Peptide,Mainchain
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%)	3 27
2	D	290/292 (99%)	228 (79%)	41 (14%)	21 (7%)	1 16
3	G	236/238 (99%)	188 (80%)	41 (17%)	7 (3%)	4 34
4	H	188/190 (99%)	162 (86%)	20 (11%)	6 (3%)	4 33
5	J	168/170 (99%)	126 (75%)	33 (20%)	9 (5%)	2 22
6	L	208/210 (99%)	166 (80%)	29 (14%)	13 (6%)	1 19
7	M	136/138 (99%)	111 (82%)	21 (15%)	4 (3%)	4 34
8	N	201/203 (99%)	159 (79%)	31 (15%)	11 (6%)	2 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
9	O	199/201 (99%)	177 (89%)	19 (10%)	3 (2%)	10 45
10	Q	185/187 (99%)	154 (83%)	24 (13%)	7 (4%)	3 29
11	R	178/180 (99%)	148 (83%)	23 (13%)	7 (4%)	3 28
12	S	173/175 (99%)	139 (80%)	27 (16%)	7 (4%)	3 28
13	T	157/159 (99%)	132 (84%)	20 (13%)	5 (3%)	4 33
14	U	97/99 (98%)	80 (82%)	14 (14%)	3 (3%)	4 33
15	V	129/131 (98%)	110 (85%)	14 (11%)	5 (4%)	3 28
16	X	117/119 (98%)	102 (87%)	12 (10%)	3 (3%)	5 36
17	Y	132/134 (98%)	105 (80%)	21 (16%)	6 (4%)	2 25
18	Z	133/135 (98%)	111 (84%)	15 (11%)	7 (5%)	2 22
19	a	145/147 (99%)	114 (79%)	24 (17%)	7 (5%)	2 24
20	b	73/75 (97%)	60 (82%)	10 (14%)	3 (4%)	3 27
21	c	92/94 (98%)	78 (85%)	10 (11%)	4 (4%)	2 26
22	d	105/107 (98%)	85 (81%)	16 (15%)	4 (4%)	3 29
23	e	126/128 (98%)	110 (87%)	14 (11%)	2 (2%)	9 44
24	f	107/109 (98%)	89 (83%)	11 (10%)	7 (6%)	1 19
25	g	112/114 (98%)	100 (89%)	10 (9%)	2 (2%)	8 42
26	h	120/122 (98%)	97 (81%)	21 (18%)	2 (2%)	9 43
27	i	100/102 (98%)	85 (85%)	13 (13%)	2 (2%)	7 41
28	k	67/69 (97%)	53 (79%)	11 (16%)	3 (4%)	2 25
29	l	48/50 (96%)	42 (88%)	5 (10%)	1 (2%)	7 40
30	m	50/52 (96%)	44 (88%)	6 (12%)	0	100 100
31	o	102/104 (98%)	79 (78%)	17 (17%)	6 (6%)	1 20
35	B	392/394 (100%)	309 (79%)	54 (14%)	29 (7%)	1 15
36	C	365/367 (100%)	292 (80%)	55 (15%)	18 (5%)	2 23
37	E	232/236 (98%)	144 (62%)	55 (24%)	33 (14%)	0 4
38	F	223/225 (99%)	180 (81%)	35 (16%)	8 (4%)	3 30
39	I	211/213 (99%)	170 (81%)	28 (13%)	13 (6%)	1 19
40	P	151/153 (99%)	134 (89%)	15 (10%)	2 (1%)	12 48
41	W	61/63 (97%)	57 (93%)	4 (7%)	0	100 100
42	j	84/86 (98%)	64 (76%)	18 (21%)	2 (2%)	6 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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 20
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 4
48	z	399/426 (94%)	348 (87%)	30 (8%)	21 (5%)	2 22
51	9	103/105 (98%)	96 (93%)	7 (7%)	0	100 100
52	6	175/179 (98%)	168 (96%)	7 (4%)	0	100 100
54	SA	206/208 (99%)	163 (79%)	29 (14%)	14 (7%)	1 17
55	SB	211/213 (99%)	154 (73%)	36 (17%)	21 (10%)	0 9
56	SC	216/218 (99%)	182 (84%)	27 (12%)	7 (3%)	4 33
57	SE	260/262 (99%)	198 (76%)	44 (17%)	18 (7%)	1 17
58	SG	235/237 (99%)	195 (83%)	32 (14%)	8 (3%)	3 32
59	SH	187/189 (99%)	140 (75%)	30 (16%)	17 (9%)	1 11
60	SI	204/206 (99%)	165 (81%)	30 (15%)	9 (4%)	2 25
61	SJ	183/185 (99%)	134 (73%)	34 (19%)	15 (8%)	1 12
62	SL	150/152 (99%)	122 (81%)	22 (15%)	6 (4%)	3 28
63	SN	147/149 (99%)	115 (78%)	28 (19%)	4 (3%)	5 35
64	SO	134/136 (98%)	99 (74%)	21 (16%)	14 (10%)	0 8
65	SV	80/82 (98%)	58 (72%)	15 (19%)	7 (9%)	1 11
66	SW	127/129 (98%)	108 (85%)	16 (13%)	3 (2%)	6 37
67	SX	139/141 (99%)	109 (78%)	26 (19%)	4 (3%)	4 34
68	SY	124/126 (98%)	101 (82%)	16 (13%)	7 (6%)	2 21
69	Sa	96/98 (98%)	69 (72%)	18 (19%)	9 (9%)	0 10
70	Sb	81/83 (98%)	61 (75%)	16 (20%)	4 (5%)	2 23
71	Se	55/57 (96%)	41 (74%)	12 (22%)	2 (4%)	3 30
72	SD	225/227 (99%)	174 (77%)	41 (18%)	10 (4%)	2 25
73	SF	189/191 (99%)	146 (77%)	33 (18%)	10 (5%)	2 22
74	SK	96/98 (98%)	58 (60%)	26 (27%)	12 (12%)	0 5
75	SM	122/124 (98%)	78 (64%)	24 (20%)	20 (16%)	0 3
76	SP	94/96 (98%)	67 (71%)	17 (18%)	10 (11%)	0 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
77	SQ	139/141 (99%)	111 (80%)	20 (14%)	8 (6%)	1 20
78	SR	127/129 (98%)	111 (87%)	11 (9%)	5 (4%)	3 28
79	SS	135/137 (98%)	114 (84%)	12 (9%)	9 (7%)	1 18
80	ST	139/141 (99%)	115 (83%)	18 (13%)	6 (4%)	2 26
81	SU	102/104 (98%)	83 (81%)	13 (13%)	6 (6%)	1 20
82	SZ	73/75 (97%)	59 (81%)	9 (12%)	5 (7%)	1 17
83	Sc	60/64 (94%)	47 (78%)	12 (20%)	1 (2%)	9 43
84	Sd	50/52 (96%)	36 (72%)	11 (22%)	3 (6%)	1 20
85	Sf	69/71 (97%)	42 (61%)	15 (22%)	12 (17%)	0 2
86	Sg	311/313 (99%)	240 (77%)	56 (18%)	15 (5%)	2 24
87	S1	72/74 (97%)	61 (85%)	6 (8%)	5 (7%)	1 17
88	S4	72/76 (95%)	68 (94%)	4 (6%)	0	100 100
All	All	12314/12513 (98%)	9837 (80%)	1799 (15%)	678 (6%)	3 21

All (678) 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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
48	z	360	MET
48	z	363	GLY
48	z	364	ASN
54	SA	44	ASP
54	SA	200	ASP
55	SB	53	GLN
55	SB	56	LYS
55	SB	59	SER
55	SB	147	ASN
55	SB	152	LYS
55	SB	179	ASN
55	SB	191	ASP
55	SB	223	PHE
56	SC	264	SER
57	SE	95	THR
57	SE	98	ASN
57	SE	101	LEU
57	SE	109	PHE
57	SE	196	THR

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Mol	Chain	Res	Type
58	SG	99	GLY
58	SG	146	ASN
59	SH	16	PRO
59	SH	17	ASP
59	SH	18	GLU
59	SH	66	VAL
59	SH	115	LYS
59	SH	116	ARG
59	SH	170	VAL
60	SI	52	ASN
60	SI	138	ASN
60	SI	155	ASN
61	SJ	3	VAL
61	SJ	22	LYS
61	SJ	119	LEU
61	SJ	121	LYS
62	SL	100	ASN
62	SL	147	LYS
63	SN	108	ASP
63	SN	143	SER
64	SO	56	VAL
64	SO	65	ASP
64	SO	105	THR
64	SO	140	THR
65	SV	41	LYS
65	SV	65	SER
66	SW	107	SER
67	SX	34	THR
68	SY	60	PHE
68	SY	95	GLY
69	Sa	72	HIS
70	Sb	4	ALA
72	SD	5	ILE
72	SD	202	LYS
72	SD	223	ILE
73	SF	34	SER
73	SF	68	ILE
74	SK	30	PRO
75	SM	15	ASN
75	SM	77	ILE
75	SM	91	LEU
75	SM	102	LYS

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
54	SA	3	GLY
54	SA	187	GLY
55	SB	54	GLY
55	SB	57	ILE
55	SB	83	LYS
55	SB	93	GLY
55	SB	151	ARG
56	SC	189	GLY
56	SC	255	LEU
57	SE	12	VAL
57	SE	76	VAL
57	SE	163	ASP
57	SE	164	LEU
57	SE	171	ASP
57	SE	195	ILE
58	SG	105	ASN

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Mol	Chain	Res	Type
58	SG	124	LEU
59	SH	160	LYS
60	SI	27	TYR
60	SI	126	GLY
60	SI	137	LEU
61	SJ	39	ASN
61	SJ	89	GLU
61	SJ	92	MET
61	SJ	118	GLY
64	SO	32	HIS
66	SW	77	PRO
67	SX	113	GLY
67	SX	129	SER
69	Sa	8	ASN
69	Sa	97	PRO
70	Sb	58	GLY
72	SD	178	ARG
72	SD	196	GLY
72	SD	219	PRO
73	SF	43	GLU
73	SF	121	PRO
73	SF	132	GLY
73	SF	166	ILE
74	SK	3	MET
74	SK	58	VAL
74	SK	63	ALA
74	SK	65	ARG
74	SK	92	ALA
75	SM	30	GLY
75	SM	35	ILE
75	SM	79	VAL
76	SP	12	PHE
76	SP	14	LYS
77	SQ	32	ILE
77	SQ	77	HIS
78	SR	95	ILE
78	SR	115	SER
80	ST	28	LEU
80	ST	39	LEU
81	SU	52	GLY
82	SZ	104	ARG
82	SZ	112	ASN

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Mol	Chain	Res	Type
84	Sd	10	HIS
85	Sf	89	LYS
85	Sf	100	LEU
85	Sf	137	ASP
85	Sf	148	TYR
86	Sg	65	PHE
86	Sg	142	VAL
86	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
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

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Mol	Chain	Res	Type
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
54	SA	105	PRO
54	SA	191	ARG
55	SB	24	PRO
55	SB	67	PHE
57	SE	38	LEU
57	SE	68	ARG
58	SG	20	ASP
58	SG	122	PRO
59	SH	112	ASN
59	SH	113	LYS
59	SH	159	ASP
59	SH	190	PRO
60	SI	143	LYS
61	SJ	4	ALA
62	SL	8	ARG
62	SL	19	ASN
62	SL	28	THR
64	SO	117	ARG
64	SO	128	ARG
64	SO	129	ILE
64	SO	147	ARG
65	SV	3	ASN
67	SX	99	GLU
68	SY	30	PRO
68	SY	84	LYS
68	SY	118	ARG
69	Sa	10	ARG
69	Sa	62	TYR

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Mol	Chain	Res	Type
70	Sb	59	CYS
73	SF	21	GLY
73	SF	143	PRO
74	SK	84	HIS
75	SM	85	LEU
75	SM	96	ARG
75	SM	116	LYS
76	SP	18	ARG
79	SS	7	GLU
81	SU	51	LYS
81	SU	118	ASP
84	Sd	7	TYR
84	Sd	8	TRP
85	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
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
26	h	119	PHE
26	h	122	LYS
27	i	25	ARG
31	o	98	LYS
35	B	189	THR
35	B	258	HIS
36	C	73	VAL

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Mol	Chain	Res	Type
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
54	SA	43	SER
54	SA	110	ASN
54	SA	186	ARG
54	SA	207	PRO
55	SB	190	PRO
55	SB	204	ILE
56	SC	171	GLY
56	SC	190	SER
58	SG	152	ASP
59	SH	107	LYS
60	SI	20	PRO
61	SJ	18	ARG
61	SJ	96	TYR
61	SJ	120	ALA
62	SL	69	ARG
64	SO	146	ARG
68	SY	103	SER
69	Sa	15	ARG
69	Sa	61	ALA
72	SD	48	ILE
72	SD	218	LEU
73	SF	163	PHE
74	SK	31	LYS
75	SM	117	GLU
75	SM	119	GLN
76	SP	75	VAL

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Mol	Chain	Res	Type
78	SR	127	ASN
79	SS	88	LYS
81	SU	106	ILE
85	Sf	83	LYS
85	Sf	87	THR
85	Sf	110	GLU
86	Sg	49	GLU
86	Sg	97	THR
86	Sg	163	PRO
86	Sg	172	LYS
86	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
6	L	82	ARG
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	58	LYS
31	o	77	CYS
35	B	38	SER
35	B	110	ILE
35	B	112	ASP
35	B	310	SER
35	B	329	ASP
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

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Mol	Chain	Res	Type
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
55	SB	86	LEU
55	SB	108	ASP
55	SB	207	LEU
56	SC	134	ASN
56	SC	256	TRP
57	SE	15	PRO
57	SE	30	ARG
59	SH	6	ALA
59	SH	100	ILE
60	SI	21	TYR
61	SJ	103	GLU
63	SN	28	LEU
64	SO	24	GLY
64	SO	33	ILE
65	SV	42	VAL
65	SV	45	ARG
65	SV	53	TYR
66	SW	29	PRO
69	Sa	46	GLU
70	Sb	48	SER
72	SD	130	GLY
74	SK	34	GLU
75	SM	94	ILE
76	SP	87	PRO
77	SQ	47	LEU
77	SQ	80	GLN
79	SS	92	ASP
80	ST	128	GLN
82	SZ	108	ILE
87	S1	45	ASP
2	D	263	LYS
4	H	40	HIS
6	L	10	LEU
6	L	169	ILE
11	R	19	LYS

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Mol	Chain	Res	Type
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
54	SA	42	LYS
59	SH	10	LYS
61	SJ	169	ARG
64	SO	54	CYS
64	SO	64	ALA
65	SV	10	ASP
68	SY	6	THR
71	Se	26	LYS
74	SK	43	LEU
75	SM	78	LYS
75	SM	81	ASP
76	SP	37	TYR
76	SP	54	HIS
78	SR	52	GLY
85	Sf	99	LYS
85	Sf	122	PRO
85	Sf	145	CYS
86	Sg	190	GLY
5	J	27	GLY
18	Z	95	VAL
48	z	158	PRO
48	z	213	GLN
54	SA	45	GLY
55	SB	22	VAL
57	SE	90	ILE
57	SE	131	VAL
59	SH	176	VAL
74	SK	41	PRO
74	SK	90	VAL
77	SQ	43	GLU
78	SR	121	GLN
79	SS	117	ILE
12	S	5	GLY

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Mol	Chain	Res	Type
35	B	259	PRO
47	q	142	GLY
58	SG	182	PRO
63	SN	52	VAL
72	SD	222	PRO
75	SM	65	VAL
75	SM	89	VAL
83	Sc	7	GLN
4	H	104	VAL
5	J	127	GLY
14	U	27	HIS
35	B	17	LEU
38	F	105	PRO
39	I	149	ILE
48	z	161	GLY
69	Sa	98	PRO
71	Se	54	GLY
75	SM	104	VAL
5	J	174	ILE
8	N	52	GLY
47	q	84	GLY
54	SA	106	GLY
54	SA	199	PRO
57	SE	64	ILE
61	SJ	36	GLY
73	SF	92	ILE
79	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 4
3	G	204/206 (99%)	150 (74%)	54 (26%)	0 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	H	169/169 (100%)	131 (78%)	38 (22%)	1 6
5	J	143/143 (100%)	108 (76%)	35 (24%)	0 5
6	L	176/176 (100%)	133 (76%)	43 (24%)	0 5
7	M	116/116 (100%)	88 (76%)	28 (24%)	0 5
8	N	171/171 (100%)	126 (74%)	45 (26%)	0 3
9	O	172/172 (100%)	138 (80%)	34 (20%)	1 9
10	Q	163/163 (100%)	126 (77%)	37 (23%)	1 6
11	R	159/159 (100%)	120 (76%)	39 (24%)	0 5
12	S	156/156 (100%)	124 (80%)	32 (20%)	1 8
13	T	139/139 (100%)	105 (76%)	34 (24%)	0 5
14	U	89/89 (100%)	65 (73%)	24 (27%)	0 3
15	V	101/101 (100%)	78 (77%)	23 (23%)	1 6
16	X	107/107 (100%)	89 (83%)	18 (17%)	2 14
17	Y	124/124 (100%)	94 (76%)	30 (24%)	0 5
18	Z	117/117 (100%)	93 (80%)	24 (20%)	1 8
19	a	119/119 (100%)	99 (83%)	20 (17%)	2 14
20	b	63/63 (100%)	48 (76%)	15 (24%)	0 5
21	c	79/79 (100%)	59 (75%)	20 (25%)	0 4
22	d	98/98 (100%)	65 (66%)	33 (34%)	0 1
23	e	114/114 (100%)	91 (80%)	23 (20%)	1 8
24	f	88/88 (100%)	73 (83%)	15 (17%)	2 14
25	g	98/98 (100%)	78 (80%)	20 (20%)	1 8
26	h	109/109 (100%)	91 (84%)	18 (16%)	2 14
27	i	86/86 (100%)	69 (80%)	17 (20%)	1 9
28	k	64/64 (100%)	51 (80%)	13 (20%)	1 8
29	l	47/47 (100%)	37 (79%)	10 (21%)	1 7
30	m	48/48 (100%)	33 (69%)	15 (31%)	0 1
31	o	92/92 (100%)	70 (76%)	22 (24%)	0 5
35	B	335/335 (100%)	260 (78%)	75 (22%)	1 6
36	C	305/305 (100%)	233 (76%)	72 (24%)	1 5
37	E	209/209 (100%)	163 (78%)	46 (22%)	1 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	F	194/194 (100%)	142 (73%)	52 (27%)	0	3
39	I	180/180 (100%)	126 (70%)	54 (30%)	0	2
40	P	134/134 (100%)	108 (81%)	26 (19%)	1	9
41	W	55/55 (100%)	38 (69%)	17 (31%)	0	2
42	j	73/73 (100%)	60 (82%)	13 (18%)	2	12
43	n	22/22 (100%)	16 (73%)	6 (27%)	0	3
44	p	74/74 (100%)	62 (84%)	12 (16%)	2	15
45	r	109/109 (100%)	83 (76%)	26 (24%)	0	5
46	K	136/136 (100%)	118 (87%)	18 (13%)	4	23
47	q	170/170 (100%)	134 (79%)	36 (21%)	1	7
48	z	340/340 (100%)	318 (94%)	22 (6%)	17	49
51	9	92/94 (98%)	88 (96%)	4 (4%)	29	58
52	6	157/157 (100%)	151 (96%)	6 (4%)	33	61
54	SA	174/174 (100%)	132 (76%)	42 (24%)	0	5
55	SB	194/194 (100%)	155 (80%)	39 (20%)	1	8
56	SC	184/184 (100%)	141 (77%)	43 (23%)	1	5
57	SE	224/224 (100%)	172 (77%)	52 (23%)	1	6
58	SG	207/207 (100%)	166 (80%)	41 (20%)	1	9
59	SH	169/169 (100%)	145 (86%)	24 (14%)	3	21
60	SI	178/178 (100%)	144 (81%)	34 (19%)	1	9
61	SJ	161/161 (100%)	117 (73%)	44 (27%)	0	3
62	SL	136/136 (100%)	104 (76%)	32 (24%)	1	5
63	SN	130/130 (100%)	103 (79%)	27 (21%)	1	7
64	SO	106/106 (100%)	74 (70%)	32 (30%)	0	2
65	SV	66/66 (100%)	50 (76%)	16 (24%)	0	5
66	SW	112/112 (100%)	90 (80%)	22 (20%)	1	9
67	SX	113/113 (100%)	95 (84%)	18 (16%)	2	16
68	SY	108/108 (100%)	85 (79%)	23 (21%)	1	7
69	Sa	85/85 (100%)	72 (85%)	13 (15%)	2	17
70	Sb	75/75 (100%)	58 (77%)	17 (23%)	1	6
71	Se	46/46 (100%)	35 (76%)	11 (24%)	0	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
72	SD	190/190 (100%)	149 (78%)	41 (22%)	1 7
73	SF	161/161 (100%)	123 (76%)	38 (24%)	1 5
74	SK	89/89 (100%)	68 (76%)	21 (24%)	1 5
75	SM	104/104 (100%)	74 (71%)	30 (29%)	0 2
76	SP	88/88 (100%)	70 (80%)	18 (20%)	1 8
77	SQ	117/117 (100%)	91 (78%)	26 (22%)	1 6
78	SR	117/117 (100%)	102 (87%)	15 (13%)	4 23
79	SS	119/119 (100%)	96 (81%)	23 (19%)	1 9
80	ST	112/112 (100%)	87 (78%)	25 (22%)	1 6
81	SU	94/94 (100%)	82 (87%)	12 (13%)	4 23
82	SZ	66/66 (100%)	57 (86%)	9 (14%)	3 22
83	Sc	57/57 (100%)	47 (82%)	10 (18%)	2 12
84	Sd	45/45 (100%)	36 (80%)	9 (20%)	1 8
85	Sf	64/64 (100%)	45 (70%)	19 (30%)	0 2
86	Sg	272/272 (100%)	235 (86%)	37 (14%)	3 22
87	S1	67/67 (100%)	59 (88%)	8 (12%)	5 26
88	S4	69/69 (100%)	60 (87%)	9 (13%)	4 23
All	All	10728/10733 (100%)	8471 (79%)	2257 (21%)	3 7

All (2257) 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
1	A	63	PHE
1	A	74	GLU
1	A	83	HIS
1	A	84	THR

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Mol	Chain	Res	Type
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
2	D	23	ARG
2	D	30	TYR
2	D	35	ARG
2	D	39	GLN

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Mol	Chain	Res	Type
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
2	D	225	GLN
2	D	229	ASN
2	D	232	THR
2	D	234	ASP

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Mol	Chain	Res	Type
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
3	G	101	LYS
3	G	102	TYR
3	G	103	ARG
3	G	106	THR

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Mol	Chain	Res	Type
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
4	H	60	TRP
4	H	63	ASN
4	H	66	GLU
4	H	71	ARG

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Mol	Chain	Res	Type
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
5	J	87	LEU
5	J	90	ARG
5	J	96	LYS
5	J	97	ASN

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Mol	Chain	Res	Type
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
6	L	113	ASN
6	L	115	GLN
6	L	121	ARG
6	L	123	LYS

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Mol	Chain	Res	Type
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	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
7	M	83	ASN
7	M	89	THR
7	M	90	ARG
7	M	91	TRP
7	M	98	ARG

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Mol	Chain	Res	Type
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
8	N	162	ARG
8	N	166	SER
8	N	169	ARG
8	N	174	LEU
8	N	178	HIS

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Mol	Chain	Res	Type
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
9	O	198	THR
9	O	199	HIS
9	O	202	LEU
10	Q	3	VAL
10	Q	4	ASP

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Mol	Chain	Res	Type
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
11	R	17	CYS
11	R	23	TRP
11	R	30	ASN
11	R	39	GLN
11	R	40	GLN

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Mol	Chain	Res	Type
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
12	S	47	PHE
12	S	48	VAL
12	S	53	LYS
12	S	64	CYS
12	S	68	PHE

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Mol	Chain	Res	Type
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
13	T	70	HIS
13	T	76	VAL
13	T	88	ARG
13	T	102	ARG
13	T	103	ASP

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Mol	Chain	Res	Type
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
14	U	113	ARG
15	V	13	LYS
15	V	14	PHE
15	V	15	ARG
15	V	18	LEU

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Mol	Chain	Res	Type
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	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
16	X	151	ASN
17	Y	2	LYS
17	Y	4	ASN
17	Y	17	ARG
17	Y	18	HIS
17	Y	19	PHE

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Mol	Chain	Res	Type
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
18	Z	78	ASN
18	Z	88	ASP
18	Z	91	LEU
18	Z	92	ASP
18	Z	93	LYS
18	Z	98	LYS

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Mol	Chain	Res	Type
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
20	b	41	ARG
20	b	43	MET
20	b	44	ARG
20	b	51	LYS
20	b	55	LYS
20	b	65	MET

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Mol	Chain	Res	Type
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
22	d	85	ARG
22	d	86	VAL
22	d	87	ARG
22	d	91	LYS
22	d	93	ASN
22	d	94	GLU

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Mol	Chain	Res	Type
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
24	f	19	ARG
24	f	24	HIS
24	f	25	THR
24	f	28	LEU
24	f	34	TYR
24	f	36	ARG

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Mol	Chain	Res	Type
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
26	h	72	PHE
26	h	73	TYR
26	h	89	ARG
26	h	93	ARG
26	h	97	LYS
26	h	100	GLU

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Mol	Chain	Res	Type
26	h	117	ARG
26	h	119	PHE
26	h	122	LYS
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
48	z	273	ILE
48	z	280	ASP
48	z	283	GLU
48	z	349	LEU
48	z	360	MET
48	z	362	LYS
48	z	383	ASN
48	z	412	VAL
48	z	427	PHE
51	9	72	TRP
51	9	77	GLN
51	9	79	ARG
51	9	89	GLU
52	6	84	ARG
52	6	91	ASN
52	6	108	ASP
52	6	122	ASP
52	6	129	TYR
52	6	142	ARG
54	SA	6	ASP
54	SA	8	LEU
54	SA	9	GLN
54	SA	32	PHE
54	SA	36	GLN
54	SA	39	TYR
54	SA	44	ASP
54	SA	53	ARG
54	SA	56	GLU
54	SA	58	LEU
54	SA	60	LEU
54	SA	70	ASN
54	SA	73	ASP
54	SA	75	SER
54	SA	81	ASN
54	SA	84	GLN
54	SA	89	LYS
54	SA	90	PHE
54	SA	97	THR
54	SA	99	ILE
54	SA	102	ARG
54	SA	105	PRO
54	SA	111	GLN

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Mol	Chain	Res	Type
54	SA	116	PHE
54	SA	117	ARG
54	SA	130	ASP
54	SA	131	HIS
54	SA	135	THR
54	SA	140	VAL
54	SA	141	ASN
54	SA	151	ASP
54	SA	158	ASP
54	SA	169	HIS
54	SA	181	GLU
54	SA	185	MET
54	SA	186	ARG
54	SA	195	TRP
54	SA	196	GLU
54	SA	203	PHE
54	SA	204	TYR
54	SA	206	ASP
54	SA	208	GLU
55	SB	27	LYS
55	SB	28	ARG
55	SB	30	TRP
55	SB	31	TYR
55	SB	32	ASP
55	SB	34	LYS
55	SB	43	ASN
55	SB	51	ARG
55	SB	52	THR
55	SB	53	GLN
55	SB	56	LYS
55	SB	65	ARG
55	SB	67	PHE
55	SB	68	GLU
55	SB	81	PHE
55	SB	88	THR
55	SB	100	PHE
55	SB	104	ASP
55	SB	105	LEU
55	SB	107	ARG
55	SB	111	CYS
55	SB	119	THR
55	SB	133	TYR

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Mol	Chain	Res	Type
55	SB	136	ARG
55	SB	138	PHE
55	SB	146	ARG
55	SB	148	ASN
55	SB	150	ILE
55	SB	151	ARG
55	SB	155	TYR
55	SB	158	HIS
55	SB	165	ARG
55	SB	181	LEU
55	SB	191	ASP
55	SB	196	ASP
55	SB	202	GLN
55	SB	205	TYR
55	SB	208	HIS
55	SB	223	PHE
56	SC	59	GLU
56	SC	60	TRP
56	SC	61	MET
56	SC	65	LYS
56	SC	68	ARG
56	SC	71	LYS
56	SC	72	ASP
56	SC	78	LEU
56	SC	79	GLU
56	SC	96	PHE
56	SC	97	PHE
56	SC	101	SER
56	SC	104	ASP
56	SC	110	MET
56	SC	114	LYS
56	SC	115	GLN
56	SC	120	GLN
56	SC	121	ARG
56	SC	123	ARG
56	SC	134	ASN
56	SC	137	VAL
56	SC	142	LYS
56	SC	143	CYS
56	SC	152	ARG
56	SC	167	ARG
56	SC	169	TYR

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Mol	Chain	Res	Type
56	SC	183	LYS
56	SC	192	LEU
56	SC	200	ARG
56	SC	206	SER
56	SC	215	MET
56	SC	220	ASP
56	SC	221	ASP
56	SC	223	TYR
56	SC	227	ARG
56	SC	242	ASP
56	SC	248	TYR
56	SC	250	TYR
56	SC	255	LEU
56	SC	261	PHE
56	SC	262	THR
56	SC	272	HIS
56	SC	275	LYS
57	SE	3	ARG
57	SE	8	HIS
57	SE	9	LEU
57	SE	11	ARG
57	SE	18	TRP
57	SE	21	ASP
57	SE	30	ARG
57	SE	39	ARG
57	SE	42	LEU
57	SE	49	ARG
57	SE	51	ARG
57	SE	54	TYR
57	SE	67	GLN
57	SE	73	ASP
57	SE	87	MET
57	SE	93	ASP
57	SE	95	THR
57	SE	98	ASN
57	SE	99	PHE
57	SE	100	ARG
57	SE	103	TYR
57	SE	106	LYS
57	SE	108	ARG
57	SE	112	HIS
57	SE	115	THR

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Mol	Chain	Res	Type
57	SE	117	GLU
57	SE	118	GLU
57	SE	121	TYR
57	SE	122	LYS
57	SE	130	PHE
57	SE	148	ARG
57	SE	155	LYS
57	SE	158	ASP
57	SE	164	LEU
57	SE	165	GLU
57	SE	179	ASN
57	SE	180	LEU
57	SE	188	ASN
57	SE	191	ARG
57	SE	198	ARG
57	SE	205	PHE
57	SE	220	THR
57	SE	221	ARG
57	SE	224	ASN
57	SE	226	PHE
57	SE	235	TRP
57	SE	240	ARG
57	SE	242	LYS
57	SE	245	ARG
57	SE	253	ASP
57	SE	259	LYS
57	SE	260	GLN
58	SG	20	ASP
58	SG	27	PHE
58	SG	29	GLU
58	SG	30	LYS
58	SG	31	ARG
58	SG	32	MET
58	SG	56	ASN
58	SG	58	LYS
58	SG	59	GLN
58	SG	64	LYS
58	SG	65	GLN
58	SG	70	HIS
58	SG	74	ARG
58	SG	76	LEU
58	SG	87	ARG

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Mol	Chain	Res	Type
58	SG	88	ARG
58	SG	98	ARG
58	SG	109	LEU
58	SG	110	ASN
58	SG	120	ASP
58	SG	126	ASP
58	SG	132	ARG
58	SG	133	LEU
58	SG	140	ARG
58	SG	143	LYS
58	SG	145	PHE
58	SG	152	ASP
58	SG	155	GLN
58	SG	159	ARG
58	SG	162	LEU
58	SG	164	LYS
58	SG	165	GLU
58	SG	170	ARG
58	SG	190	ARG
58	SG	191	ARG
58	SG	196	LYS
58	SG	198	ARG
58	SG	213	LEU
58	SG	224	ARG
58	SG	227	GLN
58	SG	236	SER
59	SH	12	ASN
59	SH	16	PRO
59	SH	23	ILE
59	SH	35	ASP
59	SH	36	LEU
59	SH	40	LEU
59	SH	46	THR
59	SH	57	ARG
59	SH	81	ARG
59	SH	83	LEU
59	SH	109	ARG
59	SH	126	HIS
59	SH	135	PHE
59	SH	137	SER
59	SH	138	GLU
59	SH	148	LEU

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Mol	Chain	Res	Type
59	SH	159	ASP
59	SH	160	LYS
59	SH	162	GLN
59	SH	166	VAL
59	SH	177	TYR
59	SH	184	ASP
59	SH	186	ASN
59	SH	190	PRO
60	SI	5	ARG
60	SI	6	ASP
60	SI	8	TRP
60	SI	12	ARG
60	SI	21	TYR
60	SI	22	HIS
60	SI	25	ARG
60	SI	27	TYR
60	SI	47	ARG
60	SI	52	ASN
60	SI	58	LEU
60	SI	65	PHE
60	SI	67	TRP
60	SI	72	CYS
60	SI	73	THR
60	SI	74	ARG
60	SI	83	TYR
60	SI	86	SER
60	SI	110	ARG
60	SI	111	GLN
60	SI	112	TRP
60	SI	113	TYR
60	SI	116	HIS
60	SI	123	ARG
60	SI	140	LYS
60	SI	149	TYR
60	SI	155	ASN
60	SI	174	CYS
60	SI	178	ARG
60	SI	188	TYR
60	SI	191	GLU
60	SI	196	GLU
60	SI	203	LYS
60	SI	206	LYS

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Mol	Chain	Res	Type
61	SJ	5	ARG
61	SJ	9	CYS
61	SJ	10	ARG
61	SJ	13	TYR
61	SJ	18	ARG
61	SJ	20	PHE
61	SJ	26	ASP
61	SJ	29	LEU
61	SJ	35	TYR
61	SJ	37	LEU
61	SJ	39	ASN
61	SJ	42	GLU
61	SJ	44	TRP
61	SJ	67	ASP
61	SJ	69	ARG
61	SJ	70	ARG
61	SJ	83	ARG
61	SJ	88	ASP
61	SJ	91	LYS
61	SJ	93	LYS
61	SJ	95	ASP
61	SJ	96	TYR
61	SJ	101	LYS
61	SJ	108	ARG
61	SJ	109	ARG
61	SJ	110	LEU
61	SJ	115	PHE
61	SJ	116	LYS
61	SJ	123	ILE
61	SJ	124	HIS
61	SJ	125	HIS
61	SJ	127	ARG
61	SJ	131	ARG
61	SJ	136	ARG
61	SJ	138	ARG
61	SJ	139	LYS
61	SJ	147	PHE
61	SJ	150	ARG
61	SJ	158	ASP
61	SJ	162	ARG
61	SJ	165	TYR
61	SJ	169	ARG

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Mol	Chain	Res	Type
61	SJ	172	ARG
61	SJ	174	LYS
62	SL	8	ARG
62	SL	13	GLN
62	SL	16	ILE
62	SL	20	LYS
62	SL	22	ARG
62	SL	25	LEU
62	SL	27	GLU
62	SL	35	ARG
62	SL	39	ASN
62	SL	40	ILE
62	SL	44	PHE
62	SL	57	ASP
62	SL	61	PRO
62	SL	65	ASN
62	SL	66	VAL
62	SL	69	ARG
62	SL	74	SER
62	SL	85	THR
62	SL	89	ARG
62	SL	90	ARG
62	SL	92	TYR
62	SL	97	ARG
62	SL	103	GLU
62	SL	108	ASN
62	SL	113	LEU
62	SL	117	PHE
62	SL	121	GLN
62	SL	124	ASP
62	SL	131	CYS
62	SL	132	ARG
62	SL	139	ARG
62	SL	147	LYS
63	SN	3	ARG
63	SN	13	GLN
63	SN	14	SER
63	SN	20	ARG
63	SN	27	LYS
63	SN	31	ASP
63	SN	38	TYR
63	SN	55	ARG

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Mol	Chain	Res	Type
63	SN	56	ASP
63	SN	58	HIS
63	SN	62	GLN
63	SN	64	ARG
63	SN	69	ASN
63	SN	76	LYS
63	SN	84	LEU
63	SN	86	GLU
63	SN	87	ASP
63	SN	89	TYR
63	SN	99	ARG
63	SN	101	HIS
63	SN	105	ASN
63	SN	113	PHE
63	SN	127	ARG
63	SN	128	TYR
63	SN	132	LYS
63	SN	139	TRP
63	SN	141	TYR
64	SO	17	LEU
64	SO	20	GLN
64	SO	26	ASN
64	SO	32	HIS
64	SO	34	PHE
64	SO	37	PHE
64	SO	39	ASP
64	SO	41	PHE
64	SO	43	HIS
64	SO	46	ASP
64	SO	50	LYS
64	SO	51	GLU
64	SO	60	MET
64	SO	63	LYS
64	SO	65	ASP
64	SO	66	ARG
64	SO	80	ASP
64	SO	84	ARG
64	SO	86	LYS
64	SO	94	HIS
64	SO	103	ASN
64	SO	106	LYS
64	SO	116	LEU

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Mol	Chain	Res	Type
64	SO	121	ARG
64	SO	128	ARG
64	SO	130	GLU
64	SO	131	ASP
64	SO	141	ARG
64	SO	146	ARG
64	SO	147	ARG
64	SO	149	ARG
64	SO	150	ARG
65	SV	1	MET
65	SV	2	GLN
65	SV	4	ASP
65	SV	11	LEU
65	SV	18	SER
65	SV	21	ASN
65	SV	39	VAL
65	SV	46	PHE
65	SV	47	ASN
65	SV	49	GLN
65	SV	50	PHE
65	SV	53	TYR
65	SV	66	ASP
65	SV	67	ASP
65	SV	81	LYS
65	SV	82	ASN
66	SW	12	LYS
66	SW	15	ASN
66	SW	18	GLU
66	SW	24	GLN
66	SW	28	ARG
66	SW	36	ARG
66	SW	37	PHE
66	SW	52	ILE
66	SW	55	ASP
66	SW	57	ARG
66	SW	70	ASN
66	SW	80	ASP
66	SW	83	LEU
66	SW	85	ASP
66	SW	98	GLN
66	SW	105	THR
66	SW	111	MET

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Mol	Chain	Res	Type
66	SW	113	HIS
66	SW	114	GLU
66	SW	117	ARG
66	SW	118	ARG
66	SW	120	HIS
67	SX	5	ARG
67	SX	9	THR
67	SX	17	ARG
67	SX	19	ASP
67	SX	32	LEU
67	SX	46	HIS
67	SX	61	GLN
67	SX	67	ARG
67	SX	84	PHE
67	SX	88	ASP
67	SX	105	PHE
67	SX	110	HIS
67	SX	114	ASP
67	SX	115	ILE
67	SX	131	LEU
67	SX	134	TYR
67	SX	135	LYS
67	SX	142	ARG
68	SY	16	ARG
68	SY	17	LEU
68	SY	19	GLN
68	SY	20	ARG
68	SY	22	GLN
68	SY	23	MET
68	SY	34	THR
68	SY	47	MET
68	SY	54	VAL
68	SY	61	ARG
68	SY	63	HIS
68	SY	69	THR
68	SY	72	PHE
68	SY	77	ASP
68	SY	81	TYR
68	SY	96	LEU
68	SY	97	TYR
68	SY	98	GLU
68	SY	99	LYS

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Mol	Chain	Res	Type
68	SY	107	ARG
68	SY	111	LYS
68	SY	118	ARG
68	SY	124	ASN
69	Sa	6	ARG
69	Sa	8	ASN
69	Sa	22	ARG
69	Sa	23	CYS
69	Sa	26	CYS
69	Sa	28	ARG
69	Sa	41	ILE
69	Sa	51	ARG
69	Sa	52	ASP
69	Sa	62	TYR
69	Sa	86	ASN
69	Sa	94	ASP
69	Sa	95	ARG
70	Sb	14	GLU
70	Sb	17	ARG
70	Sb	20	LYS
70	Sb	23	ARG
70	Sb	31	TYR
70	Sb	32	PHE
70	Sb	33	MET
70	Sb	34	ASP
70	Sb	37	CYS
70	Sb	47	PHE
70	Sb	51	GLN
70	Sb	72	ARG
70	Sb	75	GLU
70	Sb	78	SER
70	Sb	80	ARG
70	Sb	83	GLN
70	Sb	84	HIS
71	Se	13	ARG
71	Se	15	GLN
71	Se	18	LYS
71	Se	26	LYS
71	Se	28	LYS
71	Se	31	ARG
71	Se	34	ARG
71	Se	37	GLN

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Mol	Chain	Res	Type
71	Se	40	ARG
71	Se	41	ARG
71	Se	52	LYS
72	SD	4	GLN
72	SD	5	ILE
72	SD	6	SER
72	SD	9	ARG
72	SD	17	PHE
72	SD	22	ASN
72	SD	24	PHE
72	SD	28	GLU
72	SD	32	ASP
72	SD	40	ARG
72	SD	42	THR
72	SD	53	THR
72	SD	56	GLN
72	SD	67	ARG
72	SD	76	ARG
72	SD	87	TYR
72	SD	94	ARG
72	SD	103	GLU
72	SD	106	ARG
72	SD	107	TYR
72	SD	113	LEU
72	SD	135	GLU
72	SD	141	LYS
72	SD	152	PHE
72	SD	156	LEU
72	SD	158	ILE
72	SD	159	HIS
72	SD	162	ASP
72	SD	163	PRO
72	SD	167	TYR
72	SD	169	ASP
72	SD	177	LEU
72	SD	178	ARG
72	SD	192	TRP
72	SD	206	ASP
72	SD	207	HIS
72	SD	212	GLU
72	SD	216	GLU
72	SD	218	LEU

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Mol	Chain	Res	Type
72	SD	225	GLU
72	SD	226	GLN
73	SF	23	TRP
73	SF	27	ASP
73	SF	29	GLN
73	SF	35	LEU
73	SF	37	ASP
73	SF	42	LYS
73	SF	43	GLU
73	SF	49	LEU
73	SF	55	ARG
73	SF	63	LYS
73	SF	79	HIS
73	SF	82	ASN
73	SF	83	ASN
73	SF	88	MET
73	SF	94	LYS
73	SF	101	HIS
73	SF	106	GLU
73	SF	110	GLN
73	SF	114	ASN
73	SF	118	ASN
73	SF	122	ARG
73	SF	123	GLU
73	SF	130	ARG
73	SF	136	ARG
73	SF	137	GLN
73	SF	140	ASP
73	SF	145	ARG
73	SF	152	TRP
73	SF	164	ARG
73	SF	168	THR
73	SF	171	GLU
73	SF	172	CYS
73	SF	184	SER
73	SF	186	ASN
73	SF	187	SER
73	SF	190	ILE
73	SF	194	ASP
73	SF	198	ARG
74	SK	1	MET
74	SK	2	LEU

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Mol	Chain	Res	Type
74	SK	5	LYS
74	SK	8	ARG
74	SK	16	PHE
74	SK	32	HIS
74	SK	37	ASP
74	SK	39	ASN
74	SK	43	LEU
74	SK	46	MET
74	SK	54	SER
74	SK	61	GLN
74	SK	65	ARG
74	SK	66	HIS
74	SK	70	TYR
74	SK	74	GLU
74	SK	80	ARG
74	SK	81	ASP
74	SK	89	ILE
74	SK	95	ARG
74	SK	96	ARG
75	SM	12	MET
75	SM	18	LEU
75	SM	20	GLU
75	SM	26	LEU
75	SM	29	ASP
75	SM	31	LEU
75	SM	33	ARG
75	SM	43	ASP
75	SM	45	ARG
75	SM	48	HIS
75	SM	49	LEU
75	SM	52	GLN
75	SM	57	ASP
75	SM	61	TYR
75	SM	72	HIS
75	SM	73	GLN
75	SM	77	ILE
75	SM	81	ASP
75	SM	83	LYS
75	SM	88	TRP
75	SM	91	LEU
75	SM	92	CYS
75	SM	95	ASP

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Mol	Chain	Res	Type
75	SM	96	ARG
75	SM	99	ASN
75	SM	101	ARG
75	SM	102	LYS
75	SM	113	ASP
75	SM	114	TYR
75	SM	127	TYR
76	SP	5	GLU
76	SP	7	LYS
76	SP	10	ARG
76	SP	15	PHE
76	SP	18	ARG
76	SP	27	ASP
76	SP	30	TYR
76	SP	40	ARG
76	SP	41	GLN
76	SP	42	ARG
76	SP	43	ARG
76	SP	44	ARG
76	SP	50	ARG
76	SP	51	ARG
76	SP	52	LYS
76	SP	81	ARG
76	SP	82	ASP
76	SP	86	LEU
77	SQ	15	ARG
77	SQ	26	LYS
77	SQ	27	ARG
77	SQ	33	LYS
77	SQ	35	ASN
77	SQ	41	MET
77	SQ	45	ARG
77	SQ	50	LYS
77	SQ	63	PHE
77	SQ	69	ARG
77	SQ	71	ARG
77	SQ	73	LYS
77	SQ	77	HIS
77	SQ	90	LYS
77	SQ	99	TYR
77	SQ	107	GLU
77	SQ	114	GLN

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Mol	Chain	Res	Type
77	SQ	115	TYR
77	SQ	116	ASP
77	SQ	117	ARG
77	SQ	119	LEU
77	SQ	123	ASP
77	SQ	128	GLU
77	SQ	138	ARG
77	SQ	140	ARG
77	SQ	145	TYR
78	SR	1	MET
78	SR	3	ARG
78	SR	6	THR
78	SR	28	PHE
78	SR	31	ASN
78	SR	33	ARG
78	SR	37	GLU
78	SR	49	LYS
78	SR	56	HIS
78	SR	58	MET
78	SR	99	ASP
78	SR	102	THR
78	SR	105	MET
78	SR	116	ASN
78	SR	127	ASN
79	SS	8	LYS
79	SS	10	GLN
79	SS	14	ARG
79	SS	34	LYS
79	SS	39	ARG
79	SS	42	HIS
79	SS	55	ARG
79	SS	63	GLU
79	SS	72	GLN
79	SS	78	LYS
79	SS	81	ASP
79	SS	82	TRP
79	SS	85	ASN
79	SS	86	ARG
79	SS	87	GLN
79	SS	92	ASP
79	SS	95	TYR
79	SS	108	ARG

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Mol	Chain	Res	Type
79	SS	113	ARG
79	SS	118	ARG
79	SS	124	ARG
79	SS	134	GLN
79	SS	135	HIS
80	ST	8	ASP
80	ST	11	GLN
80	ST	16	ARG
80	ST	21	PHE
80	ST	28	LEU
80	ST	35	ASP
80	ST	42	HIS
80	ST	52	TRP
80	ST	53	PHE
80	ST	56	ARG
80	ST	62	ARG
80	ST	63	HIS
80	ST	74	SER
80	ST	79	TYR
80	ST	82	ARG
80	ST	84	ARG
80	ST	90	SER
80	ST	92	PHE
80	ST	94	ARG
80	ST	97	LYS
80	ST	102	ARG
80	ST	118	ASP
80	ST	121	ARG
80	ST	123	LEU
80	ST	128	GLN
81	SU	19	ARG
81	SU	47	ASN
81	SU	48	LEU
81	SU	55	ARG
81	SU	56	MET
81	SU	62	ARG
81	SU	64	THR
81	SU	79	ARG
81	SU	84	ILE
81	SU	87	ARG
81	SU	93	SER
81	SU	111	GLU

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Mol	Chain	Res	Type
82	SZ	44	LEU
82	SZ	45	ASN
82	SZ	51	ASP
82	SZ	64	ASN
82	SZ	94	LYS
82	SZ	97	ILE
82	SZ	109	TYR
82	SZ	110	THR
82	SZ	114	LYS
83	Sc	5	ARG
83	Sc	7	GLN
83	Sc	13	ARG
83	Sc	21	THR
83	Sc	26	GLN
83	Sc	51	ARG
83	Sc	54	ASP
83	Sc	60	GLU
83	Sc	62	GLU
83	Sc	67	ARG
84	Sd	6	PHE
84	Sd	8	TRP
84	Sd	9	SER
84	Sd	12	ARG
84	Sd	26	ASN
84	Sd	30	LEU
84	Sd	34	TYR
84	Sd	43	PHE
84	Sd	56	ASP
85	Sf	87	THR
85	Sf	89	LYS
85	Sf	95	ARG
85	Sf	104	LYS
85	Sf	106	TYR
85	Sf	116	ARG
85	Sf	119	ARG
85	Sf	121	CYS
85	Sf	126	CYS
85	Sf	131	PHE
85	Sf	138	ARG
85	Sf	139	HIS
85	Sf	140	TYR
85	Sf	141	CYS

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Mol	Chain	Res	Type
85	Sf	146	LEU
85	Sf	147	THR
85	Sf	148	TYR
85	Sf	149	CYS
85	Sf	150	PHE
86	Sg	8	ARG
86	Sg	15	ASN
86	Sg	17	TRP
86	Sg	20	GLN
86	Sg	24	THR
86	Sg	36	ARG
86	Sg	44	LYS
86	Sg	47	ARG
86	Sg	48	ASP
86	Sg	49	GLU
86	Sg	59	LEU
86	Sg	65	PHE
86	Sg	84	ASP
86	Sg	100	ARG
86	Sg	107	ASP
86	Sg	118	ARG
86	Sg	143	GLN
86	Sg	172	LYS
86	Sg	186	THR
86	Sg	187	ASN
86	Sg	194	TYR
86	Sg	213	ASP
86	Sg	215	GLN
86	Sg	226	HIS
86	Sg	229	THR
86	Sg	234	ASP
86	Sg	240	CYS
86	Sg	247	TRP
86	Sg	268	ASP
86	Sg	269	GLU
86	Sg	273	GLU
86	Sg	289	LEU
86	Sg	294	ASP
86	Sg	299	PHE
86	Sg	302	TYR
86	Sg	306	LEU
86	Sg	310	TRP

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Mol	Chain	Res	Type
87	S1	9	GLU
87	S1	18	TYR
87	S1	32	ARG
87	S1	35	ASP
87	S1	43	THR
87	S1	46	LEU
87	S1	54	ASP
87	S1	63	GLU
88	S4	21	ARG
88	S4	32	LYS
88	S4	34	ASP
88	S4	56	CYS
88	S4	77	ASN
88	S4	85	ASN
88	S4	92	ASP
88	S4	94	LEU
88	S4	95	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (271) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	50	HIS
1	A	100	ASN
1	A	187	HIS
1	A	194	ASN
1	A	209	HIS
1	A	215	ASN
2	D	45	ASN
2	D	94	ASN
2	D	111	ASN
2	D	122	GLN
2	D	195	HIS
2	D	202	GLN
2	D	244	HIS
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	124	HIS
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
40	P	80	GLN
40	P	133	HIS
40	P	145	HIS
41	W	17	HIS
41	W	59	HIS
42	j	16	HIS

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Mol	Chain	Res	Type
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	429	GLN
54	SA	33	GLN
54	SA	36	GLN
54	SA	70	ASN
54	SA	84	GLN
54	SA	132	GLN
54	SA	169	HIS
55	SB	40	ASN
55	SB	53	GLN
55	SB	75	GLN
55	SB	99	ASN
55	SB	124	HIS
55	SB	148	ASN
55	SB	158	HIS
55	SB	232	HIS
56	SC	113	GLN
56	SC	115	GLN
56	SC	120	GLN
56	SC	134	ASN
57	SE	36	HIS
57	SE	138	HIS
57	SE	142	HIS

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Mol	Chain	Res	Type
57	SE	188	ASN
58	SG	59	GLN
58	SG	65	GLN
58	SG	81	HIS
58	SG	110	ASN
59	SH	112	ASN
59	SH	114	GLN
60	SI	44	HIS
60	SI	64	ASN
60	SI	155	ASN
60	SI	165	GLN
60	SI	168	GLN
61	SJ	111	GLN
62	SL	19	ASN
62	SL	65	ASN
62	SL	106	HIS
63	SN	5	HIS
63	SN	69	ASN
64	SO	26	ASN
64	SO	43	HIS
65	SV	47	ASN
66	SW	64	ASN
66	SW	82	GLN
66	SW	91	ASN
66	SW	98	GLN
66	SW	113	HIS
67	SX	20	HIS
67	SX	23	HIS
68	SY	112	ASN
70	Sb	9	HIS
70	Sb	26	GLN
71	Se	37	GLN
72	SD	4	GLN
72	SD	22	ASN
72	SD	56	GLN
73	SF	29	GLN
73	SF	65	GLN
73	SF	83	ASN
73	SF	101	HIS
73	SF	107	ASN
73	SF	137	GLN
73	SF	186	ASN

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Mol	Chain	Res	Type
73	SF	203	ASN
74	SK	28	HIS
74	SK	32	HIS
74	SK	39	ASN
74	SK	66	HIS
75	SM	19	GLN
75	SM	48	HIS
75	SM	99	ASN
77	SQ	24	HIS
77	SQ	80	GLN
77	SQ	142	GLN
78	SR	48	ASN
78	SR	74	GLN
78	SR	83	ASN
78	SR	118	GLN
78	SR	121	GLN
79	SS	10	GLN
79	SS	17	ASN
79	SS	19	ASN
79	SS	120	HIS
79	SS	125	HIS
79	SS	135	HIS
80	ST	11	GLN
80	ST	63	HIS
81	SU	47	ASN
82	SZ	46	ASN
82	SZ	89	GLN
82	SZ	103	HIS
83	Sc	7	GLN
83	Sc	45	ASN
84	Sd	26	ASN
86	Sg	64	HIS
86	Sg	187	ASN
86	Sg	191	HIS
86	Sg	215	GLN
86	Sg	237	ASN
87	S1	3	GLN
87	S1	5	GLN
88	S4	80	GLN
88	S4	85	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	5	3642/3658 (99%)	1674 (45%)	665 (18%)
33	7	119/120 (99%)	38 (31%)	13 (10%)
34	8	155/156 (99%)	63 (40%)	29 (18%)
49	3	73/76 (96%)	27 (36%)	5 (6%)
50	4	197/206 (95%)	43 (21%)	10 (5%)
53	S2	1714/1742 (98%)	830 (48%)	303 (17%)
All	All	5900/5958 (99%)	2675 (45%)	1025 (17%)

All (2675) 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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
32	5	4332	C
32	5	4334	U
32	5	4335	C
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
49	3	2	U
49	3	6	C
49	3	8	U
49	3	9	A
49	3	17	G
49	3	18	G
49	3	19	U
49	3	20	U
49	3	21	A
49	3	22	U
49	3	33	U
49	3	37	A
49	3	39	G
49	3	40	C
49	3	42	A
49	3	46	G
49	3	48	C
49	3	51	C
49	3	52	G
49	3	59	A
49	3	60	A

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Mol	Chain	Res	Type
49	3	61	C
49	3	69	A
49	3	73	A
49	3	74	C
49	3	75	C
49	3	76	A
50	4	4	G
50	4	12	U
50	4	24	G
50	4	28	U
50	4	29	C
50	4	32	A
50	4	33	G
50	4	35	U
50	4	36	A
50	4	38	U
50	4	39	C
50	4	40	G
50	4	47	U
50	4	48	G
50	4	53	U
50	4	54	G
50	4	65	U
50	4	287	A
50	4	115	A
50	4	116	C
50	4	120	G
50	4	139	A
50	4	144	C
50	4	151	C
50	4	170	C
50	4	172	A
50	4	173	A
50	4	174	G
50	4	175	G
50	4	176	A
50	4	177	G
50	4	178	G
50	4	183	A
50	4	186	C
50	4	190	C
50	4	191	C

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Mol	Chain	Res	Type
50	4	206	G
50	4	212	C
50	4	215	A
50	4	227	G
50	4	234	A
50	4	235	G
50	4	236	U
53	S2	3	C
53	S2	4	C
53	S2	5	U
53	S2	9	U
53	S2	10	G
53	S2	17	C
53	S2	18	C
53	S2	20	G
53	S2	21	U
53	S2	26	U
53	S2	28	U
53	S2	33	G
53	S2	37	C
53	S2	42	A
53	S2	44	U
53	S2	46	A
53	S2	49	C
53	S2	51	U
53	S2	53	C
53	S2	54	A
53	S2	56	G
53	S2	57	U
53	S2	58	C
53	S2	59	U
53	S2	60	A
53	S2	61	A
53	S2	62	G
53	S2	63	U
53	S2	64	A
53	S2	65	C
53	S2	66	G
53	S2	67	C
53	S2	68	A
53	S2	72	C
53	S2	73	C

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Mol	Chain	Res	Type
53	S2	74	G
53	S2	75	G
53	S2	77	A
53	S2	78	C
53	S2	79	A
53	S2	80	G
53	S2	81	U
53	S2	84	A
53	S2	89	C
53	S2	92	A
53	S2	93	U
53	S2	98	C
53	S2	99	A
53	S2	101	U
53	S2	103	A
53	S2	104	A
53	S2	105	U
53	S2	111	A
53	S2	113	G
53	S2	114	G
53	S2	115	U
53	S2	116	U
53	S2	123	G
53	S2	124	U
53	S2	125	C
53	S2	126	G
53	S2	127	C
53	S2	139	C
53	S2	140	C
53	S2	141	A
53	S2	142	C
53	S2	144	U
53	S2	146	G
53	S2	147	A
53	S2	148	U
53	S2	153	G
53	S2	154	U
53	S2	155	G
53	S2	159	A
53	S2	160	U
53	S2	161	U
53	S2	162	C

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Mol	Chain	Res	Type
53	S2	163	U
53	S2	164	A
53	S2	165	G
53	S2	167	G
53	S2	168	C
53	S2	169	U
53	S2	170	A
53	S2	171	A
53	S2	172	U
53	S2	173	A
53	S2	180	G
53	S2	181	A
53	S2	182	C
53	S2	183	G
53	S2	184	G
53	S2	188	C
53	S2	189	U
53	S2	191	A
53	S2	192	C
53	S2	200	G
53	S2	202	G
53	S2	206	G
53	S2	208	G
53	S2	209	A
53	S2	213	G
53	S2	214	U
53	S2	215	G
53	S2	216	C
53	S2	217	A
53	S2	290	U
53	S2	291	G
53	S2	292	A
53	S2	293	C
53	S2	294	U
53	S2	295	C
53	S2	297	A
53	S2	302	A
53	S2	305	U
53	S2	306	C
53	S2	307	G
53	S2	308	G
53	S2	309	G

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Mol	Chain	Res	Type
53	S2	310	C
53	S2	311	C
53	S2	312	G
53	S2	313	A
53	S2	314	U
53	S2	315	C
53	S2	317	C
53	S2	319	C
53	S2	321	C
53	S2	323	C
53	S2	324	C
53	S2	325	C
53	S2	326	C
53	S2	327	G
53	S2	328	U
53	S2	334	C
53	S2	335	G
53	S2	338	G
53	S2	340	C
53	S2	341	C
53	S2	342	C
53	S2	343	A
53	S2	346	C
53	S2	347	G
53	S2	350	C
53	S2	355	G
53	S2	356	C
53	S2	357	C
53	S2	360	A
53	S2	361	U
53	S2	362	C
53	S2	364	A
53	S2	365	C
53	S2	366	U
53	S2	367	U
53	S2	368	U
53	S2	369	C
53	S2	370	G
53	S2	372	U
53	S2	373	G
53	S2	380	G
53	S2	381	C

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Mol	Chain	Res	Type
53	S2	382	C
53	S2	383	G
53	S2	384	U
53	S2	385	G
53	S2	386	C
53	S2	387	C
53	S2	394	G
53	S2	395	G
53	S2	398	A
53	S2	399	C
53	S2	400	C
53	S2	401	A
53	S2	407	G
53	S2	408	A
53	S2	409	C
53	S2	411	G
53	S2	416	U
53	S2	417	C
53	S2	418	A
53	S2	419	G
53	S2	421	G
53	S2	422	U
53	S2	425	G
53	S2	426	A
53	S2	427	U
53	S2	428	U
53	S2	429	C
53	S2	435	A
53	S2	436	G
53	S2	437	G
53	S2	438	G
53	S2	441	C
53	S2	442	C
53	S2	444	G
53	S2	445	A
53	S2	446	G
53	S2	447	A
53	S2	448	A
53	S2	449	A
53	S2	450	C
53	S2	453	C
53	S2	454	U

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Mol	Chain	Res	Type
53	S2	455	A
53	S2	458	A
53	S2	459	C
53	S2	460	A
53	S2	464	A
53	S2	465	A
53	S2	466	G
53	S2	467	G
53	S2	469	A
53	S2	471	G
53	S2	472	C
53	S2	473	A
53	S2	474	G
53	S2	476	A
53	S2	482	G
53	S2	485	A
53	S2	487	U
53	S2	489	A
53	S2	492	C
53	S2	493	A
53	S2	496	C
53	S2	504	G
53	S2	507	G
53	S2	508	A
53	S2	516	A
53	S2	518	G
53	S2	523	A
53	S2	525	A
53	S2	528	A
53	S2	530	U
53	S2	532	C
53	S2	533	A
53	S2	534	G
53	S2	540	U
53	S2	542	U
53	S2	544	G
53	S2	548	C
53	S2	549	C
53	S2	550	C
53	S2	551	U
53	S2	552	G
53	S2	554	A

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Mol	Chain	Res	Type
53	S2	556	U
53	S2	557	U
53	S2	559	G
53	S2	560	A
53	S2	563	G
53	S2	564	A
53	S2	568	C
53	S2	569	A
53	S2	575	A
53	S2	576	A
53	S2	579	C
53	S2	580	U
53	S2	583	C
53	S2	588	G
53	S2	589	G
53	S2	590	A
53	S2	591	U
53	S2	592	C
53	S2	593	C
53	S2	595	U
53	S2	596	U
53	S2	597	G
53	S2	598	G
53	S2	600	G
53	S2	601	G
53	S2	602	G
53	S2	604	A
53	S2	605	A
53	S2	607	U
53	S2	608	C
53	S2	612	U
53	S2	613	G
53	S2	614	C
53	S2	616	A
53	S2	617	G
53	S2	620	G
53	S2	621	C
53	S2	623	G
53	S2	624	C
53	S2	626	G
53	S2	627	U
53	S2	628	A

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Mol	Chain	Res	Type
53	S2	629	A
53	S2	630	U
53	S2	631	U
53	S2	634	A
53	S2	639	C
53	S2	640	A
53	S2	642	U
53	S2	643	A
53	S2	644	G
53	S2	646	G
53	S2	647	U
53	S2	649	U
53	S2	651	U
53	S2	655	A
53	S2	656	G
53	S2	657	U
53	S2	660	C
53	S2	664	A
53	S2	666	U
53	S2	668	A
53	S2	669	A
53	S2	671	A
53	S2	672	A
53	S2	673	G
53	S2	679	A
53	S2	682	U
53	S2	683	G
53	S2	684	G
53	S2	687	C
53	S2	688	U
53	S2	689	U
53	S2	690	G
53	S2	693	A
53	S2	694	G
53	S2	698	G
53	S2	731	G
53	S2	733	C
53	S2	735	C
53	S2	738	C
53	S2	739	C
53	S2	747	U
53	S2	748	C

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Mol	Chain	Res	Type
53	S2	749	U
53	S2	751	G
53	S2	752	G
53	S2	753	C
53	S2	788	G
53	S2	791	C
53	S2	793	G
53	S2	794	A
53	S2	797	C
53	S2	798	A
53	S2	799	U
53	S2	800	U
53	S2	807	G
53	S2	810	A
53	S2	811	A
53	S2	812	A
53	S2	820	U
53	S2	821	G
53	S2	822	U
53	S2	825	A
53	S2	827	A
53	S2	830	A
53	S2	833	C
53	S2	834	C
53	S2	835	C
53	S2	836	G
53	S2	837	A
53	S2	838	G
53	S2	839	C
53	S2	840	C
53	S2	841	G
53	S2	842	C
53	S2	843	C
53	S2	845	G
53	S2	846	G
53	S2	847	A
53	S2	848	U
53	S2	853	C
53	S2	859	G
53	S2	862	A
53	S2	864	A
53	S2	867	G

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Mol	Chain	Res	Type
53	S2	868	G
53	S2	869	A
53	S2	870	A
53	S2	871	U
53	S2	872	A
53	S2	873	G
53	S2	875	A
53	S2	876	C
53	S2	877	C
53	S2	878	G
53	S2	879	C
53	S2	880	G
53	S2	881	G
53	S2	887	U
53	S2	888	U
53	S2	890	U
53	S2	891	G
53	S2	892	U
53	S2	893	U
53	S2	897	U
53	S2	898	U
53	S2	903	A
53	S2	913	A
53	S2	914	U
53	S2	918	U
53	S2	919	A
53	S2	920	A
53	S2	921	G
53	S2	930	C
53	S2	933	G
53	S2	934	G
53	S2	938	A
53	S2	943	U
53	S2	946	U
53	S2	955	A
53	S2	956	G
53	S2	957	A
53	S2	958	G
53	S2	959	G
53	S2	960	U
53	S2	961	G
53	S2	962	A

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Mol	Chain	Res	Type
53	S2	964	A
53	S2	965	U
53	S2	968	U
53	S2	969	U
53	S2	971	G
53	S2	974	C
53	S2	975	G
53	S2	979	C
53	S2	980	A
53	S2	981	A
53	S2	989	C
53	S2	990	A
53	S2	991	G
53	S2	992	A
53	S2	994	C
53	S2	996	A
53	S2	997	A
53	S2	999	G
53	S2	1001	A
53	S2	1002	U
53	S2	1008	A
53	S2	1016	U
53	S2	1017	U
53	S2	1018	U
53	S2	1023	A
53	S2	1024	A
53	S2	1030	A
53	S2	1033	G
53	S2	1034	A
53	S2	1035	A
53	S2	1039	C
53	S2	1040	G
53	S2	1041	G
53	S2	1042	A
53	S2	1044	G
53	S2	1045	U
53	S2	1049	A
53	S2	1050	A
53	S2	1060	A
53	S2	1062	A
53	S2	1070	A
53	S2	1072	U

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Mol	Chain	Res	Type
53	S2	1073	U
53	S2	1077	A
53	S2	1078	C
53	S2	1083	A
53	S2	1084	A
53	S2	1085	C
53	S2	1087	A
53	S2	1088	U
53	S2	1089	G
53	S2	1093	A
53	S2	1096	G
53	S2	1099	G
53	S2	1100	A
53	S2	1108	G
53	S2	1109	C
53	S2	1110	G
53	S2	1111	U
53	S2	1113	A
53	S2	1114	U
53	S2	1115	U
53	S2	1116	C
53	S2	1118	C
53	S2	1120	U
53	S2	1121	G
53	S2	1123	C
53	S2	1124	C
53	S2	1130	G
53	S2	1131	G
53	S2	1133	A
53	S2	1138	C
53	S2	1139	C
53	S2	1143	A
53	S2	1144	A
53	S2	1146	C
53	S2	1148	A
53	S2	1149	A
53	S2	1150	A
53	S2	1151	G
53	S2	1153	C
53	S2	1154	U
53	S2	1157	G
53	S2	1165	G

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Mol	Chain	Res	Type
53	S2	1166	G
53	S2	1180	C
53	S2	1182	A
53	S2	1191	C
53	S2	1194	A
53	S2	1195	A
53	S2	1199	A
53	S2	1200	A
53	S2	1201	U
53	S2	1203	G
53	S2	1204	A
53	S2	1205	C
53	S2	1206	G
53	S2	1207	G
53	S2	1208	A
53	S2	1210	G
53	S2	1211	G
53	S2	1214	A
53	S2	1215	C
53	S2	1216	C
53	S2	1217	A
53	S2	1221	G
53	S2	1222	G
53	S2	1224	G
53	S2	1234	C
53	S2	1240	A
53	S2	1242	U
53	S2	1243	U
53	S2	1245	G
53	S2	1247	C
53	S2	1248	U
53	S2	1249	C
53	S2	1250	A
53	S2	1251	A
53	S2	1252	C
53	S2	1253	A
53	S2	1254	C
53	S2	1256	G
53	S2	1257	G
53	S2	1258	A
53	S2	1259	A
53	S2	1264	C

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Mol	Chain	Res	Type
53	S2	1265	A
53	S2	1266	C
53	S2	1267	C
53	S2	1268	C
53	S2	1269	G
53	S2	1271	C
53	S2	1273	C
53	S2	1274	G
53	S2	1275	G
53	S2	1276	A
53	S2	1280	G
53	S2	1282	A
53	S2	1283	C
53	S2	1284	A
53	S2	1285	G
53	S2	1286	G
53	S2	1288	U
53	S2	1289	U
53	S2	1292	C
53	S2	1293	A
53	S2	1296	U
53	S2	1298	G
53	S2	1299	A
53	S2	1301	A
53	S2	1302	G
53	S2	1303	C
53	S2	1304	U
53	S2	1305	C
53	S2	1306	U
53	S2	1308	U
53	S2	1309	C
53	S2	1312	G
53	S2	1313	A
53	S2	1314	U
53	S2	1315	U
53	S2	1316	C
53	S2	1322	G
53	S2	1324	G
53	S2	1326	U
53	S2	1331	C
53	S2	1332	A
53	S2	1337	C

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Mol	Chain	Res	Type
53	S2	1339	U
53	S2	1340	U
53	S2	1341	C
53	S2	1342	U
53	S2	1343	U
53	S2	1344	A
53	S2	1345	G
53	S2	1347	U
53	S2	1348	G
53	S2	1349	G
53	S2	1351	G
53	S2	1352	G
53	S2	1353	A
53	S2	1354	G
53	S2	1355	C
53	S2	1356	G
53	S2	1357	A
53	S2	1358	U
53	S2	1364	U
53	S2	1367	U
53	S2	1368	U
53	S2	1370	A
53	S2	1371	U
53	S2	1372	U
53	S2	1373	C
53	S2	1374	C
53	S2	1378	A
53	S2	1379	A
53	S2	1380	C
53	S2	1385	G
53	S2	1394	G
53	S2	1395	C
53	S2	1396	A
53	S2	1397	U
53	S2	1398	G
53	S2	1401	A
53	S2	1402	A
53	S2	1403	C
53	S2	1404	U
53	S2	1405	A
53	S2	1407	U
53	S2	1408	U

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Mol	Chain	Res	Type
53	S2	1410	C
53	S2	1411	G
53	S2	1412	C
53	S2	1413	G
53	S2	1414	A
53	S2	1417	C
53	S2	1418	C
53	S2	1419	C
53	S2	1420	G
53	S2	1423	C
53	S2	1424	G
53	S2	1425	G
53	S2	1426	U
53	S2	1430	C
53	S2	1432	U
53	S2	1433	C
53	S2	1434	C
53	S2	1435	C
53	S2	1437	C
53	S2	1438	A
53	S2	1439	A
53	S2	1441	U
53	S2	1442	U
53	S2	1444	U
53	S2	1449	G
53	S2	1452	A
53	S2	1453	C
53	S2	1454	A
53	S2	1455	A
53	S2	1462	U
53	S2	1463	U
53	S2	1464	C
53	S2	1465	A
53	S2	1466	G
53	S2	1473	G
53	S2	1475	G
53	S2	1476	A
53	S2	1477	U
53	S2	1478	U
53	S2	1488	C
53	S2	1489	A
53	S2	1490	G

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Mol	Chain	Res	Type
53	S2	1493	C
53	S2	1494	U
53	S2	1495	G
53	S2	1496	U
53	S2	1497	G
53	S2	1501	C
53	S2	1507	G
53	S2	1508	A
53	S2	1509	U
53	S2	1510	G
53	S2	1511	U
53	S2	1512	C
53	S2	1513	C
53	S2	1514	G
53	S2	1515	G
53	S2	1520	G
53	S2	1521	C
53	S2	1522	A
53	S2	1523	C
53	S2	1525	C
53	S2	1527	C
53	S2	1531	A
53	S2	1533	A
53	S2	1534	C
53	S2	1535	U
53	S2	1537	A
53	S2	1540	G
53	S2	1541	G
53	S2	1543	U
53	S2	1544	C
53	S2	1545	A
53	S2	1546	G
53	S2	1547	C
53	S2	1548	G
53	S2	1550	G
53	S2	1551	U
53	S2	1552	G
53	S2	1553	C
53	S2	1555	U
53	S2	1556	A
53	S2	1557	C
53	S2	1558	C

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Mol	Chain	Res	Type
53	S2	1560	U
53	S2	1563	G
53	S2	1567	G
53	S2	1568	C
53	S2	1570	G
53	S2	1574	C
53	S2	1578	U
53	S2	1579	A
53	S2	1580	A
53	S2	1581	C
53	S2	1582	C
53	S2	1585	U
53	S2	1586	U
53	S2	1587	G
53	S2	1588	A
53	S2	1589	A
53	S2	1590	C
53	S2	1593	C
53	S2	1594	A
53	S2	1595	U
53	S2	1598	G
53	S2	1599	U
53	S2	1600	G
53	S2	1601	A
53	S2	1602	U
53	S2	1604	G
53	S2	1606	G
53	S2	1607	A
53	S2	1609	C
53	S2	1610	G
53	S2	1621	U
53	S2	1622	U
53	S2	1623	A
53	S2	1625	U
53	S2	1632	G
53	S2	1633	A
53	S2	1634	A
53	S2	1637	A
53	S2	1638	G
53	S2	1641	A
53	S2	1644	C
53	S2	1645	C

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Mol	Chain	Res	Type
53	S2	1646	C
53	S2	1647	A
53	S2	1648	G
53	S2	1649	U
53	S2	1654	G
53	S2	1659	U
53	S2	1660	C
53	S2	1663	A
53	S2	1664	A
53	S2	1665	G
53	S2	1666	C
53	S2	1667	U
53	S2	1668	U
53	S2	1669	G
53	S2	1674	G
53	S2	1679	A
53	S2	1680	G
53	S2	1682	C
53	S2	1683	C
53	S2	1684	C
53	S2	1688	C
53	S2	1689	C
53	S2	1695	A
53	S2	1698	C
53	S2	1700	C
53	S2	1701	C
53	S2	1702	G
53	S2	1714	U
53	S2	1720	U
53	S2	1721	U
53	S2	1722	G
53	S2	1724	A
53	S2	1725	U
53	S2	1729	U
53	S2	1730	U
53	S2	1734	G
53	S2	1737	G
53	S2	1745	A
53	S2	1746	U
53	S2	1751	C
53	S2	1753	C
53	S2	1757	G

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Mol	Chain	Res	Type
53	S2	1760	G
53	S2	1761	U
53	S2	1779	G
53	S2	1783	C
53	S2	1784	G
53	S2	1785	C
53	S2	1786	U
53	S2	1792	G
53	S2	1795	G
53	S2	1797	U
53	S2	1798	C
53	S2	1805	G
53	S2	1810	U
53	S2	1817	G
53	S2	1819	A
53	S2	1823	A
53	S2	1824	A
53	S2	1825	A
53	S2	1826	G
53	S2	1827	U
53	S2	1831	A
53	S2	1835	A
53	S2	1836	G
53	S2	1838	U
53	S2	1839	U
53	S2	1840	U
53	S2	1841	C
53	S2	1844	U
53	S2	1847	G
53	S2	1850	A
53	S2	1852	C
53	S2	1860	A
53	S2	1861	G
53	S2	1862	G
53	S2	1863	A
53	S2	1864	U
53	S2	1865	C
53	S2	1868	U
53	S2	1869	A

All (1025) 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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	2083	C
32	5	2087	C
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	42	A
33	7	49	A
33	7	56	G
33	7	57	C

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Mol	Chain	Res	Type
33	7	58	A
33	7	59	G
33	7	60	G
33	7	72	U
33	7	75	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	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
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
49	3	9	A
49	3	17	G
49	3	19	U
49	3	60	A
49	3	75	C
50	4	10	G
50	4	35	U
50	4	37	C

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Mol	Chain	Res	Type
50	4	38	U
50	4	39	C
50	4	45	G
50	4	47	U
50	4	176	A
50	4	234	A
50	4	235	G
53	S2	2	A
53	S2	3	C
53	S2	9	U
53	S2	19	A
53	S2	25	A
53	S2	27	A
53	S2	37	C
53	S2	55	U
53	S2	61	A
53	S2	65	C
53	S2	67	C
53	S2	72	C
53	S2	73	C
53	S2	74	G
53	S2	91	A
53	S2	98	C
53	S2	102	A
53	S2	104	A
53	S2	105	U
53	S2	110	U
53	S2	113	G
53	S2	126	G
53	S2	127	C
53	S2	139	C
53	S2	140	C
53	S2	141	A
53	S2	158	A
53	S2	160	U
53	S2	163	U
53	S2	171	A
53	S2	180	G
53	S2	181	A
53	S2	182	C
53	S2	183	G
53	S2	190	G

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Mol	Chain	Res	Type
53	S2	215	G
53	S2	291	G
53	S2	294	U
53	S2	297	A
53	S2	305	U
53	S2	312	G
53	S2	313	A
53	S2	325	C
53	S2	327	G
53	S2	334	C
53	S2	340	C
53	S2	357	C
53	S2	360	A
53	S2	366	U
53	S2	367	U
53	S2	368	U
53	S2	369	C
53	S2	376	A
53	S2	377	G
53	S2	384	U
53	S2	393	U
53	S2	394	G
53	S2	398	A
53	S2	399	C
53	S2	402	C
53	S2	409	C
53	S2	413	G
53	S2	421	G
53	S2	426	A
53	S2	428	U
53	S2	437	G
53	S2	442	C
53	S2	443	U
53	S2	444	G
53	S2	446	G
53	S2	447	A
53	S2	448	A
53	S2	452	G
53	S2	453	C
53	S2	457	C
53	S2	465	A
53	S2	468	A

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Mol	Chain	Res	Type
53	S2	470	G
53	S2	473	A
53	S2	474	G
53	S2	499	G
53	S2	505	G
53	S2	515	G
53	S2	532	C
53	S2	550	C
53	S2	559	G
53	S2	577	U
53	S2	578	C
53	S2	579	C
53	S2	596	U
53	S2	604	A
53	S2	607	U
53	S2	608	C
53	S2	613	G
53	S2	617	G
53	S2	639	C
53	S2	641	A
53	S2	642	U
53	S2	643	A
53	S2	645	C
53	S2	649	U
53	S2	650	A
53	S2	656	G
53	S2	687	C
53	S2	688	U
53	S2	732	U
53	S2	734	C
53	S2	746	C
53	S2	747	U
53	S2	752	G
53	S2	797	C
53	S2	798	A
53	S2	799	U
53	S2	800	U
53	S2	802	A
53	S2	807	G
53	S2	810	A
53	S2	811	A
53	S2	815	U

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Mol	Chain	Res	Type
53	S2	818	A
53	S2	821	G
53	S2	822	U
53	S2	829	C
53	S2	833	C
53	S2	841	G
53	S2	842	C
53	S2	868	G
53	S2	870	A
53	S2	871	U
53	S2	875	A
53	S2	913	A
53	S2	914	U
53	S2	918	U
53	S2	919	A
53	S2	920	A
53	S2	924	G
53	S2	955	A
53	S2	959	G
53	S2	960	U
53	S2	962	A
53	S2	964	A
53	S2	967	C
53	S2	968	U
53	S2	975	G
53	S2	980	A
53	S2	991	G
53	S2	993	G
53	S2	999	G
53	S2	1001	A
53	S2	1016	U
53	S2	1036	A
53	S2	1037	G
53	S2	1050	A
53	S2	1063	C
53	S2	1087	A
53	S2	1088	U
53	S2	1092	G
53	S2	1093	A
53	S2	1096	G
53	S2	1098	C
53	S2	1099	G

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Mol	Chain	Res	Type
53	S2	1107	G
53	S2	1109	C
53	S2	1110	G
53	S2	1113	A
53	S2	1114	U
53	S2	1115	U
53	S2	1121	G
53	S2	1132	C
53	S2	1137	U
53	S2	1141	G
53	S2	1142	G
53	S2	1153	C
53	S2	1165	G
53	S2	1194	A
53	S2	1199	A
53	S2	1204	A
53	S2	1207	G
53	S2	1221	G
53	S2	1223	A
53	S2	1224	G
53	S2	1225	U
53	S2	1226	G
53	S2	1244	U
53	S2	1247	C
53	S2	1249	C
53	S2	1250	A
53	S2	1253	A
53	S2	1265	A
53	S2	1273	C
53	S2	1274	G
53	S2	1283	C
53	S2	1288	U
53	S2	1289	U
53	S2	1292	C
53	S2	1298	G
53	S2	1302	G
53	S2	1312	G
53	S2	1313	A
53	S2	1315	U
53	S2	1341	C
53	S2	1342	U
53	S2	1350	U

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Mol	Chain	Res	Type
53	S2	1352	G
53	S2	1355	C
53	S2	1362	U
53	S2	1363	C
53	S2	1367	U
53	S2	1368	U
53	S2	1370	A
53	S2	1372	U
53	S2	1373	C
53	S2	1378	A
53	S2	1379	A
53	S2	1386	A
53	S2	1391	C
53	S2	1395	C
53	S2	1396	A
53	S2	1401	A
53	S2	1418	C
53	S2	1419	C
53	S2	1421	A
53	S2	1423	C
53	S2	1429	G
53	S2	1430	C
53	S2	1433	C
53	S2	1438	A
53	S2	1440	C
53	S2	1441	U
53	S2	1442	U
53	S2	1446	A
53	S2	1452	A
53	S2	1454	A
53	S2	1462	U
53	S2	1463	U
53	S2	1474	A
53	S2	1475	G
53	S2	1477	U
53	S2	1480	A
53	S2	1488	C
53	S2	1489	A
53	S2	1495	G
53	S2	1512	C
53	S2	1515	G
53	S2	1521	C

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Mol	Chain	Res	Type
53	S2	1522	A
53	S2	1524	G
53	S2	1533	A
53	S2	1534	C
53	S2	1537	A
53	S2	1540	G
53	S2	1543	U
53	S2	1546	G
53	S2	1551	U
53	S2	1552	G
53	S2	1556	A
53	S2	1568	C
53	S2	1571	G
53	S2	1578	U
53	S2	1579	A
53	S2	1581	C
53	S2	1591	C
53	S2	1597	C
53	S2	1598	G
53	S2	1599	U
53	S2	1601	A
53	S2	1603	G
53	S2	1605	G
53	S2	1617	G
53	S2	1621	U
53	S2	1623	A
53	S2	1629	C
53	S2	1637	A
53	S2	1639	G
53	S2	1641	A
53	S2	1644	C
53	S2	1645	C
53	S2	1657	G
53	S2	1659	U
53	S2	1664	A
53	S2	1668	U
53	S2	1678	A
53	S2	1679	A
53	S2	1682	C
53	S2	1695	A
53	S2	1697	A
53	S2	1700	C

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Mol	Chain	Res	Type
53	S2	1726	G
53	S2	1804	U
53	S2	1821	U
53	S2	1823	A
53	S2	1824	A
53	S2	1825	A
53	S2	1826	G
53	S2	1830	U
53	S2	1837	G
53	S2	1838	U
53	S2	1843	G
53	S2	1849	G
53	S2	1857	G
53	S2	1858	G
53	S2	1863	A
53	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

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
53	S2	6
48	z	5
50	4	3
49	3	3
46	K	2
37	E	1
88	S4	1
52	6	1
83	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	141.53
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	S2	698:G	O3'	730:C	P	20.30
1	z	465:UNK	C	477:UNK	N	19.07
1	z	434:MET	C	455:UNK	N	18.79
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	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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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	3.44
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

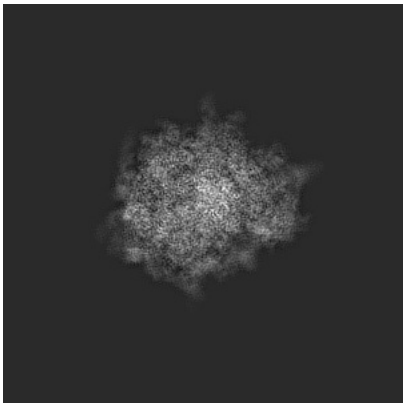
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3045. These allow visual inspection of the internal detail of the map and identification of artifacts.

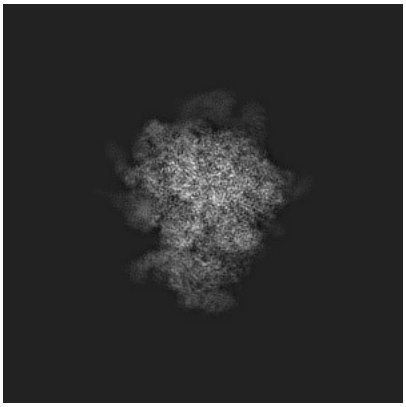
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

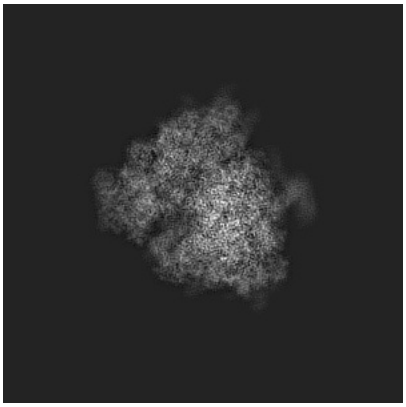
6.1.1 Primary map



X



Y

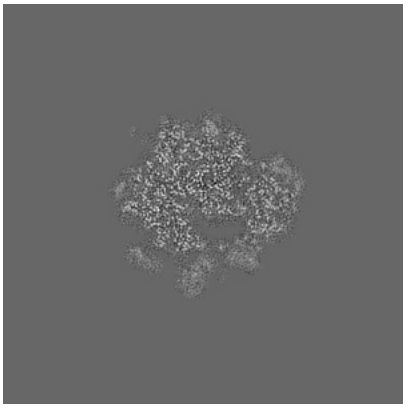


Z

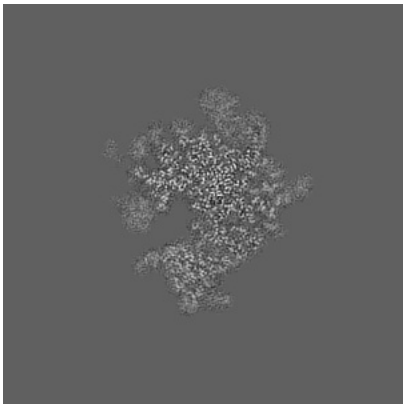
The images above show the map projected in three orthogonal directions.

6.2 Central slices

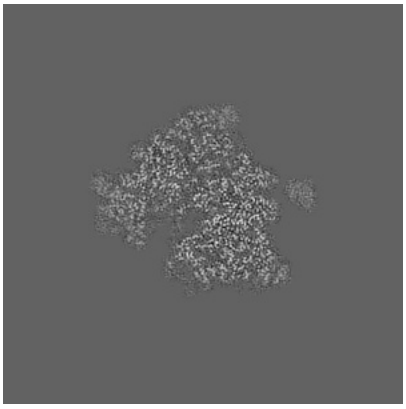
6.2.1 Primary map



X Index: 210



Y Index: 210

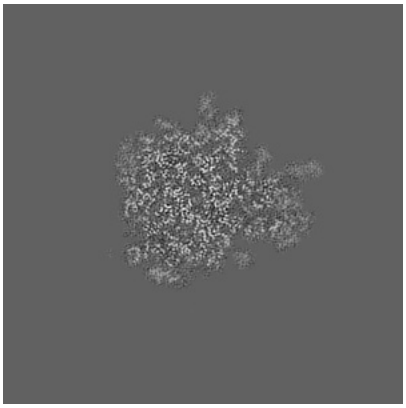


Z Index: 210

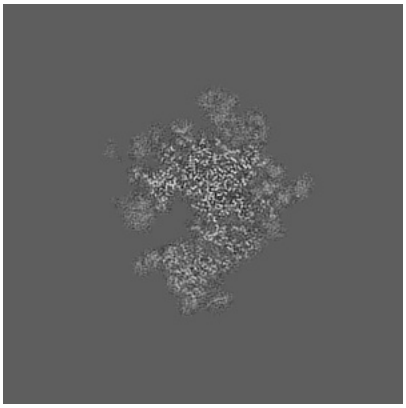
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

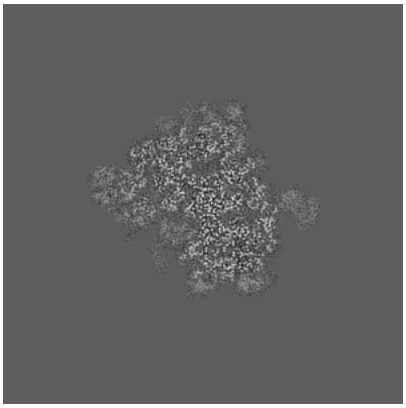
6.3.1 Primary map



X Index: 230



Y Index: 211

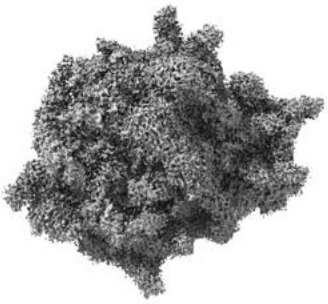


Z Index: 227

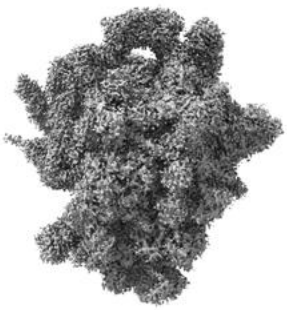
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

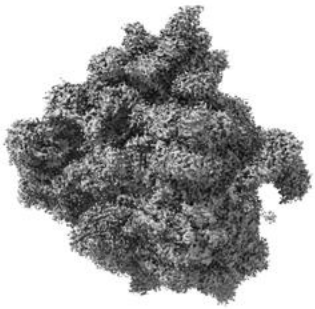
6.4.1 Primary map



X



Y



Z

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

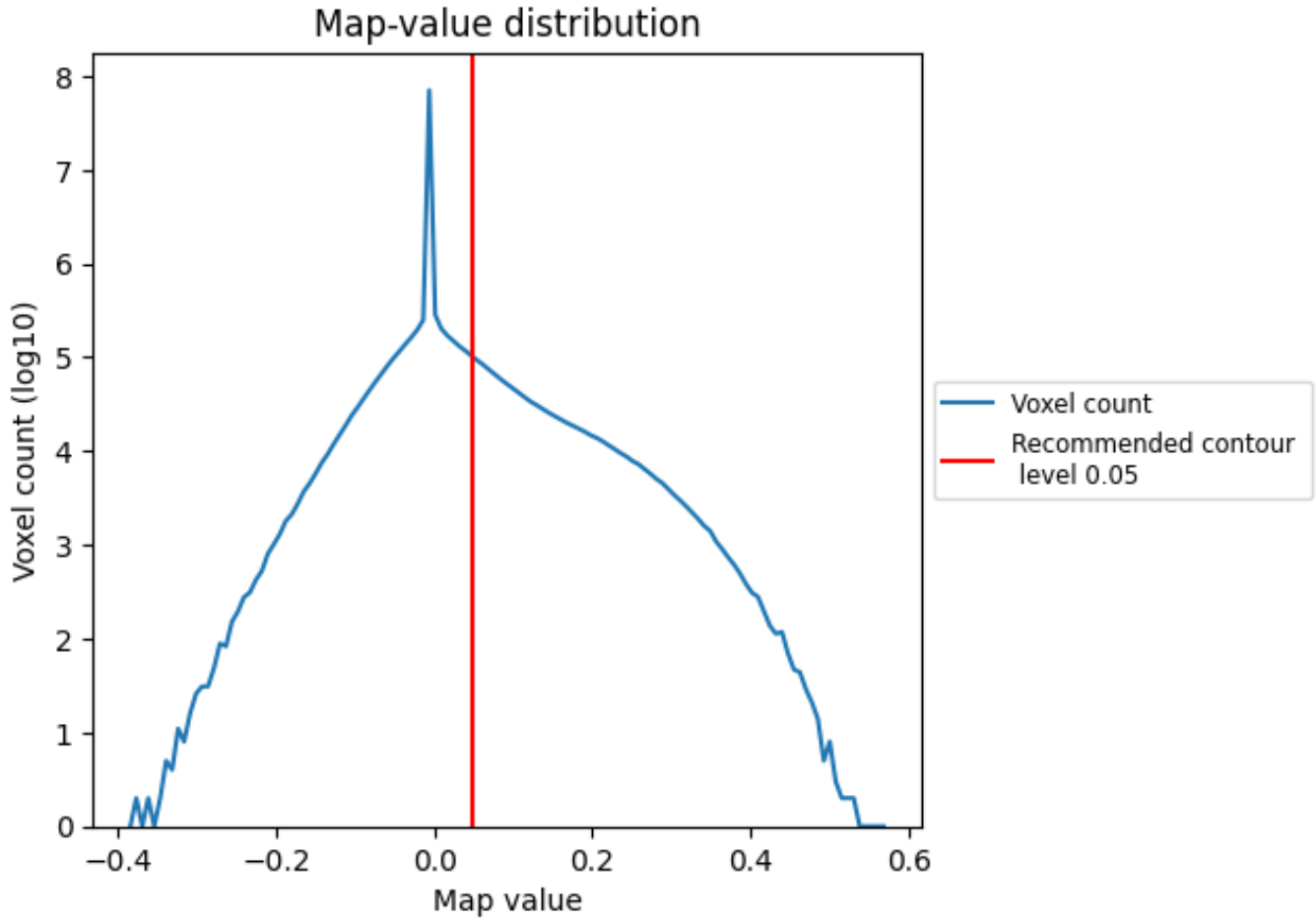
6.5 Mask visualisation (i)

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

7 Map analysis

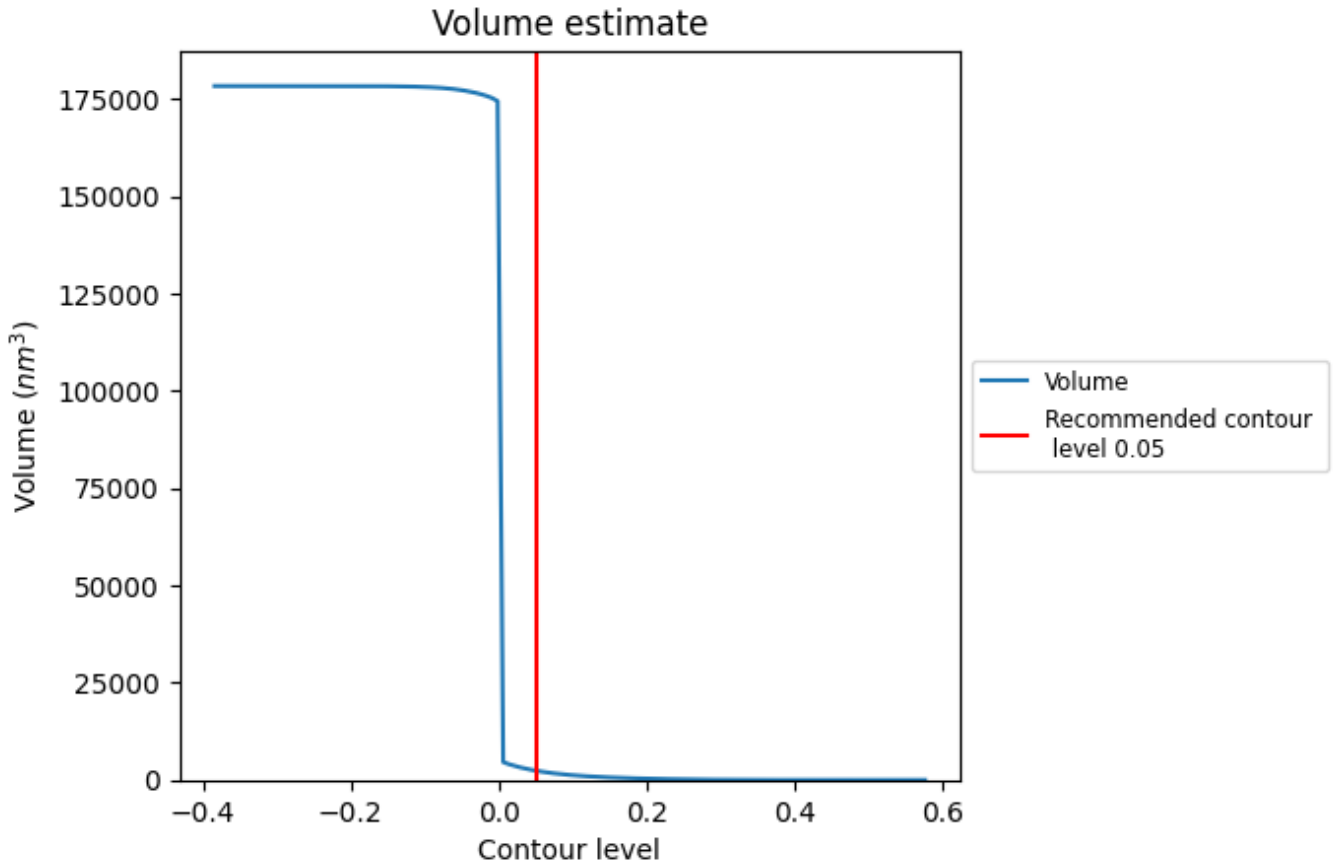
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

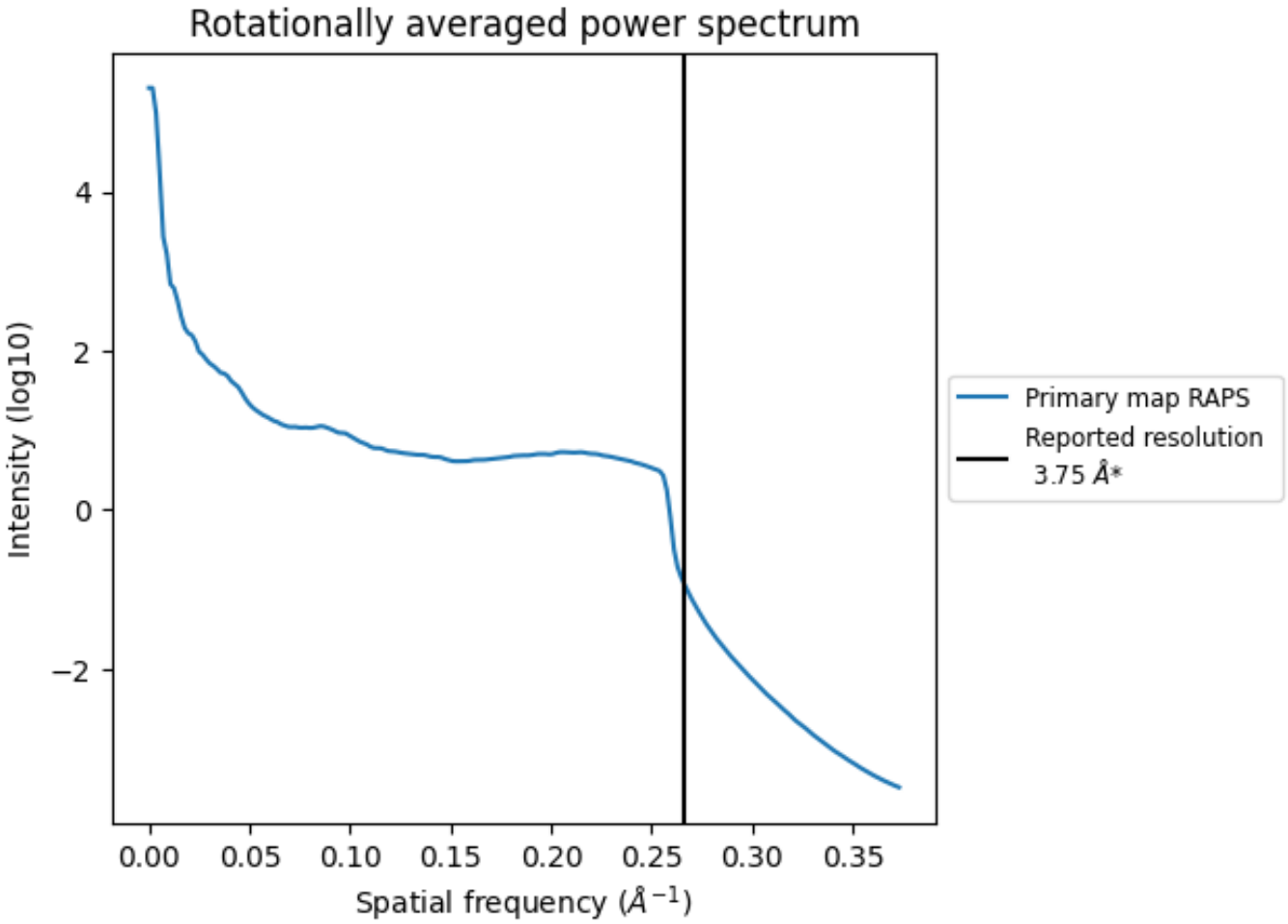
7.2 Volume estimate



The volume at the recommended contour level is 2397 nm^3; this corresponds to an approximate mass of 2166 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.267 Å^{-1}

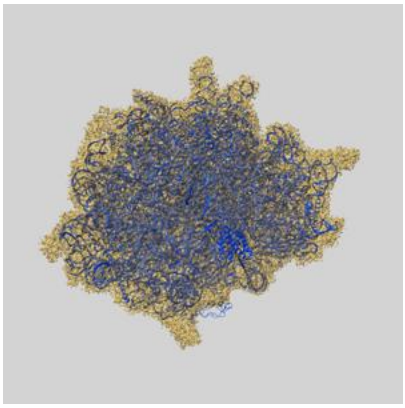
8 Fourier-Shell correlation

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

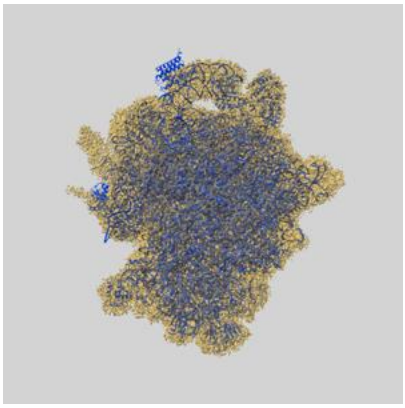
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3045 and PDB model 3JAN. Per-residue inclusion information can be found in section 3 on page 21.

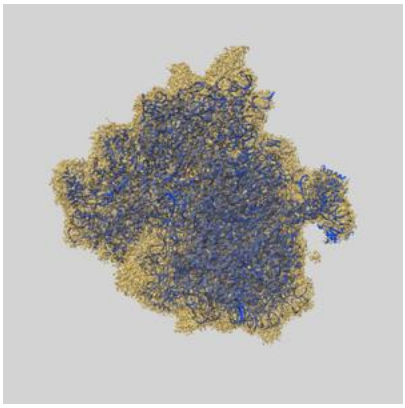
9.1 Map-model overlay



X



Y



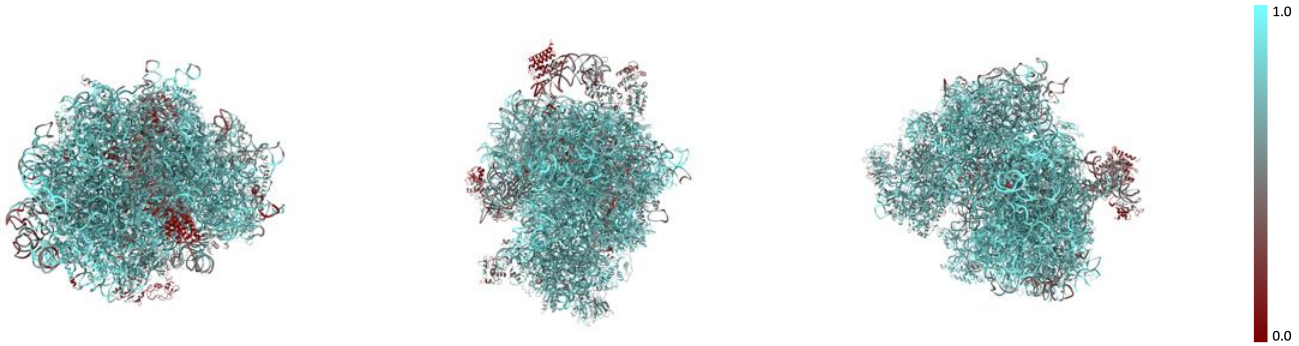
Z

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

This section was not generated.

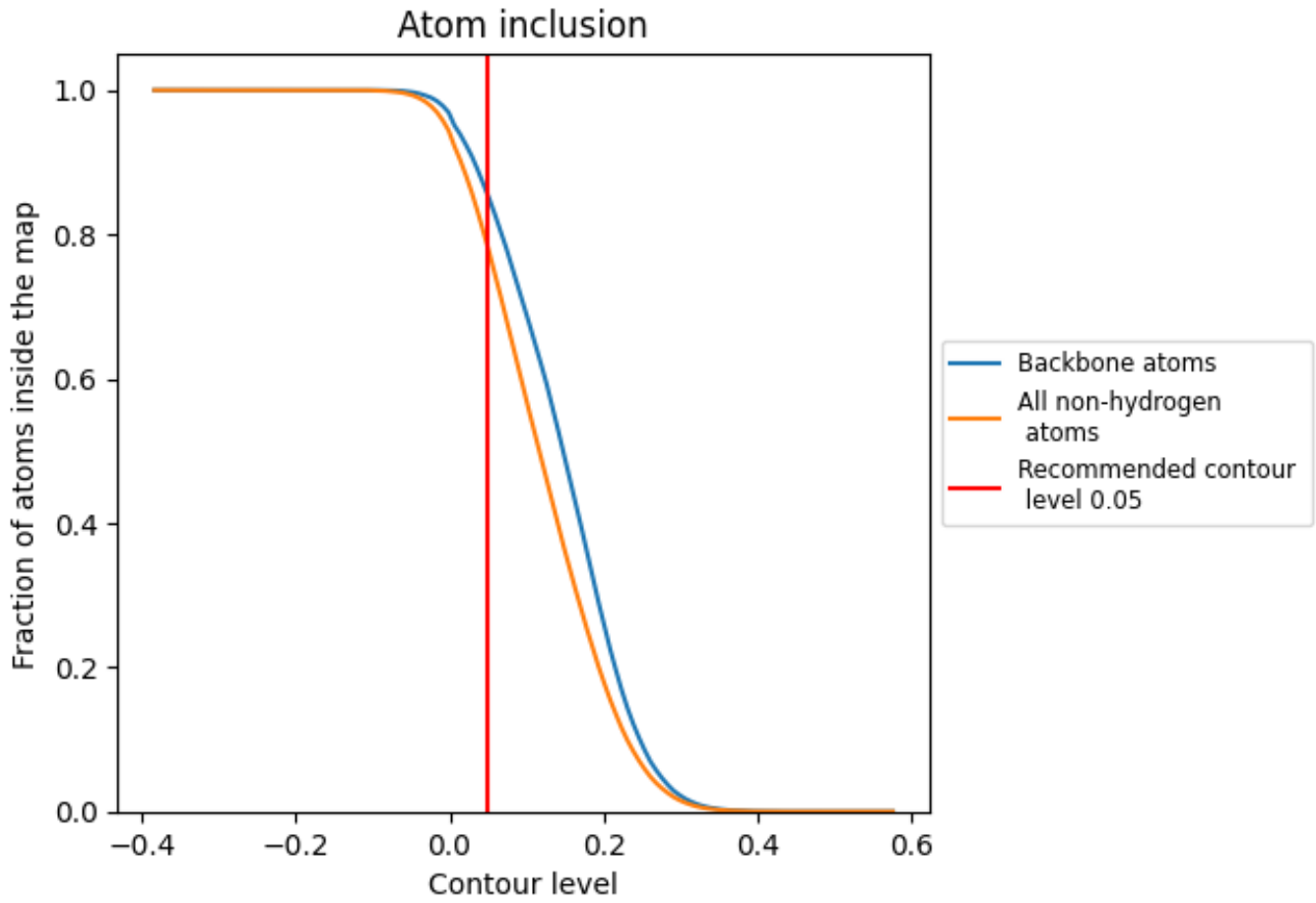
9.3 Atom inclusion mapped to coordinate model



X Y Z

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

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 78% 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
All	0.7812
3	0.6095
4	0.4715
5	0.8338
6	0.1320
7	0.9188
8	0.8527
9	0.2293
A	0.8069
B	0.8298
C	0.8150
D	0.8157
E	0.7535
F	0.8196
G	0.7648
H	0.8108
I	0.8106
J	0.7923
K	0.2845
L	0.8017
M	0.8113
N	0.8241
O	0.8202
P	0.8085
Q	0.8351
R	0.7759
S	0.8450
S1	0.4958
S2	0.8388
S4	0.5346
SA	0.7926
SB	0.7832
SC	0.8070
SD	0.6841
SE	0.7956

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Chain	Atom inclusion
SF	0.6792
SG	0.6992
SH	0.7118
SI	0.7646
SJ	0.8082
SK	0.6522
SL	0.7490
SM	0.3467
SN	0.7967
SO	0.7923
SP	0.6361
SQ	0.7298
SR	0.6948
SS	0.7381
ST	0.7544
SU	0.6901
SV	0.7905
SW	0.8188
SX	0.8078
SY	0.7462
SZ	0.6964
Sa	0.8353
Sb	0.7778
Sc	0.6626
Sd	0.7812
Se	0.6979
Sf	0.3375
Sg	0.6315
T	0.8100
U	0.7392
V	0.8038
W	0.7898
X	0.7808
Y	0.7755
Z	0.8034
a	0.8361
b	0.7357
c	0.7888
d	0.7853
e	0.8319
f	0.8409
g	0.7747

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Chain	Atom inclusion
h	0.7648
i	0.8195
j	0.8561
k	0.7397
l	0.7730
m	0.8341
n	0.7910
o	0.8184
p	0.7936
q	0.2154
r	0.8382
z	0.4252