Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 06:52 AM EST

PDB ID	:	3J7P
EMDB ID	:	EMD-2646
Title	:	Structure of the 80S mammalian ribosome bound to eEF2
Authors	:	Voorhees, R.M.; Fernandez, I.S.; Scheres, S.H.W.; Hegde, R.S.
Deposited on	:	2014-08-01
Resolution	:	3.50 Å(reported)
Based on initial models	:	3J3B, 3J3A, 3J3F, 3J3D

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:

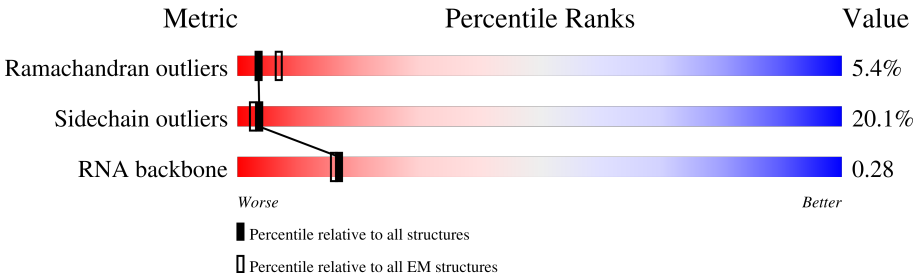
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	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	5	3664	5% 47% 40% 10%
2	7	120	69% 24% 6%
3	8	156	53% 33% 8% 5%
4	A	257	71% 18% 5% 5%
5	B	394	74% 21%
6	C	367	77% 19%
7	D	297	68% 25%
8	E	236	7% 64% 26% 9%

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Mol	Chain	Length	Quality of chain
9	F	225	72% 24%
10	G	266	5% 69% 18% 9%
11	H	192	73% 21% 5%
12	I	213	5% 72% 22% 5%
13	J	178	73% 20%
14	K	163	29% 51% 27% 12% 7%
15	L	211	73% 19% 6%
16	M	213	52% 11% 35%
17	N	204	70% 23% 5%
18	O	204	83% 12%
19	P	153	82% 14%
20	Q	188	74% 18% 6%
21	R	196	66% 20% 6% 8%
22	S	224	57% 16% 5% 22%
23	T	160	79% 18%
24	U	128	58% 16% 23%
25	V	140	74% 17% 6%
26	W	157	31% 7% 60%
27	X	156	62% 10% 24%
28	Y	145	67% 19% 6% 8%
29	Z	136	77% 19%
30	a	148	77% 17%
31	b	160	7% 33% 11% 53%
32	c	115	63% 15% 18%
33	d	125	56% 22% 8% 14%

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Mol	Chain	Length	Quality of chain
34	e	135	68% 23% 5%
35	f	110	78% 15% 5%
36	g	117	77% 19%
37	h	123	80% 12% 6%
38	i	105	76% 17%
39	j	86	73% 21% 6%
40	k	70	71% 27%
41	l	51	76% 18%
42	m	128	30% 10% 59%
43	n	25	72% 20% 8%
44	o	106	69% 23% 6%
45	p	91	82% 15%
46	q	202	15% 59% 28% 11%
47	r	125	74% 22%
48	4	856	22% 74% 20% 5%
49	S2	1742	5% 48% 41% 8%
50	SA	295	56% 14% 29%
51	SB	264	62% 15% 19%
52	SC	218	79% 17%
53	SD	243	9% 76% 14% 7%
54	SE	263	76% 20%
55	SF	204	15% 70% 23% 6%
56	SG	249	5% 77% 15% 5%
57	SH	194	5% 79% 15%
58	SI	208	7% 76% 19%

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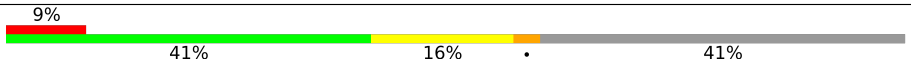
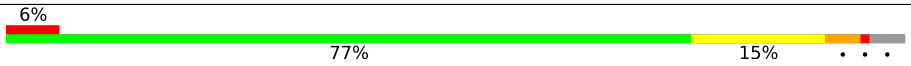
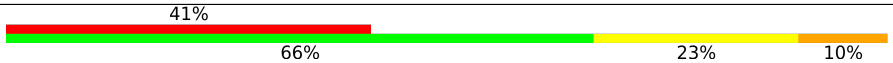
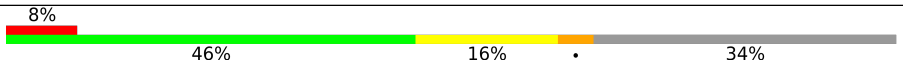
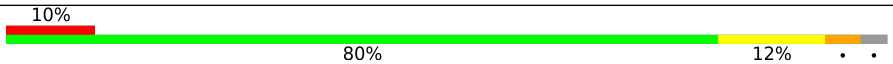
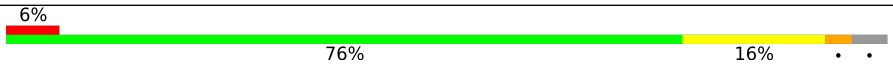
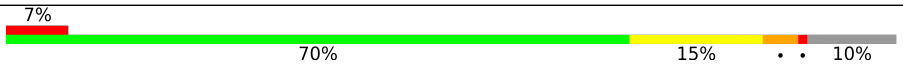
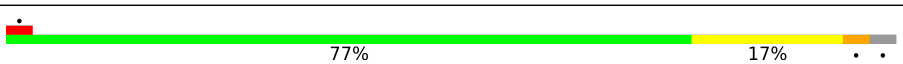
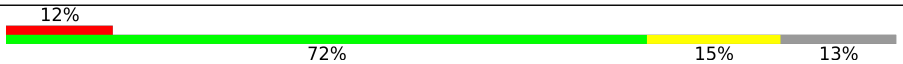
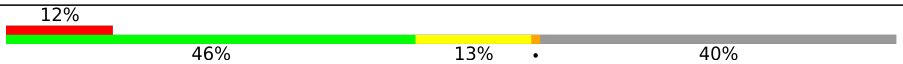
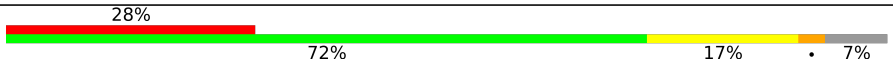
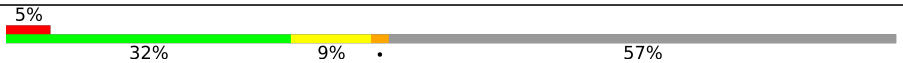
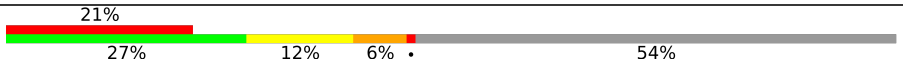
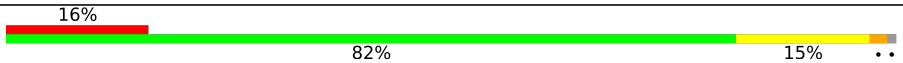
Mol	Chain	Length	Quality of chain
59	SJ	194	
60	SK	165	
61	SL	158	
62	SM	124	
63	SN	151	
64	SO	151	
65	SP	145	
66	SQ	146	
67	SR	135	
68	SS	152	
69	ST	145	
70	SU	119	
71	SV	83	
72	SW	130	
73	SX	143	
74	SY	132	
75	SZ	125	
76	Sa	115	
77	Sb	84	
78	Sc	69	
79	Sd	56	
80	Se	133	
81	Sf	156	
82	Sg	317	

2 Entry composition (i)

There are 84 unique types of molecules in this entry. The entry contains 221686 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	5	3662	78486	34947	14363	25515	3661	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	7	120	2558	1141	456	842	119	0	0

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	8	156	3314	1480	585	1094	155	0	0

- Molecule 4 is a protein called Ribosomal protein uL2.

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

- Molecule 5 is a protein called Ribosomal protein uL3.

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

- Molecule 6 is a protein called Ribosomal protein uL4.

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

- Molecule 7 is a protein called Ribosomal protein uL18.

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

- Molecule 8 is a protein called Ribosomal protein eL6.

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

- Molecule 9 is a protein called Ribosomal protein uL30.

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

- Molecule 10 is a protein called Ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	241	Total	C	N	O	S	0	0
			1934	1232	372	326	4		

- Molecule 11 is a protein called Ribosomal protein uL6.

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

- Molecule 12 is a protein called Ribosomal protein uL16.

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

- Molecule 13 is a protein called Ribosomal protein uL5.

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

- Molecule 14 is a protein called Ribosomal protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	151	Total	C	N	O	S	0	0
			1140	708	215	213	4		

- Molecule 15 is a protein called Ribosomal protein eL13.

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

- Molecule 16 is a protein called Ribosomal protein eL14.

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

- Molecule 17 is a protein called Ribosomal protein eL15.

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

- Molecule 18 is a protein called Ribosomal protein uL13.

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

- Molecule 19 is a protein called Ribosomal protein uL22.

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

- Molecule 20 is a protein called Ribosomal protein eL18.

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

- Molecule 21 is a protein called Ribosomal protein eL19.

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

- Molecule 22 is a protein called Ribosomal protein eL20.

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

- Molecule 23 is a protein called Ribosomal protein eL21.

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

- Molecule 24 is a protein called Ribosomal protein eL22.

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

- Molecule 25 is a protein called Ribosomal protein uL14.

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

- Molecule 26 is a protein called Ribosomal protein eL24.

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

- Molecule 27 is a protein called Ribosomal protein uL23.

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

- Molecule 28 is a protein called Ribosomal protein uL24.

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

- Molecule 29 is a protein called Ribosomal protein eL27.

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

- Molecule 30 is a protein called Ribosomal protein uL15.

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

- Molecule 31 is a protein called Ribosomal protein eL29.

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

- Molecule 32 is a protein called Ribosomal protein eL30.

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

- Molecule 33 is a protein called Ribosomal protein eL31.

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

- Molecule 34 is a protein called Ribosomal protein eL32.

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

- Molecule 35 is a protein called Ribosomal protein eL33.

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

- Molecule 36 is a protein called Ribosomal protein eL34.

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

- Molecule 37 is a protein called Ribosomal protein uL29.

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

- Molecule 38 is a protein called Ribosomal protein eL36.

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

- Molecule 39 is a protein called Ribosomal protein eL37.

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

- Molecule 40 is a protein called Ribosomal protein eL38.

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

- Molecule 41 is a protein called Ribosomal protein eL39.

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

- Molecule 42 is a protein called Ribosomal protein eL40.

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

- 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 eL42.

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

- Molecule 45 is a protein called Ribosomal protein eL43.

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

- Molecule 46 is a protein called Ribosomal protein uL10.

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

- Molecule 47 is a protein called Ribosomal protein eL28.

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

- Molecule 48 is a protein called Eukaryotic elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	4	856	Total	C	N	O	S	0	0
			6673	4234	1148	1247	44		

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

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

- Molecule 50 is a protein called Ribosomal protein uS2.

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

- Molecule 51 is a protein called Ribosomal protein eS1.

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

- Molecule 52 is a protein called Ribosomal protein uS5.

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

- Molecule 53 is a protein called Ribosomal protein uS3.

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

- Molecule 54 is a protein called Ribosomal protein eS4.

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

- Molecule 55 is a protein called Ribosomal protein uS7.

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

- Molecule 56 is a protein called Ribosomal protein eS6.

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

- Molecule 57 is a protein called Ribosomal protein eS7.

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

- Molecule 58 is a protein called Ribosomal protein eS8.

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

- Molecule 59 is a protein called Ribosomal protein uS4.

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

- Molecule 60 is a protein called Ribosomal protein eS10.

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

- Molecule 61 is a protein called Ribosomal protein uS17.

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

- Molecule 62 is a protein called Ribosomal protein eS12.

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

- Molecule 63 is a protein called Ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SN	150	Total	C	N	O	S	0	0
			1208	773	229	205	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 uS19.

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

- Molecule 66 is a protein called Ribosomal protein uS9.

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

- Molecule 67 is a protein called Ribosomal protein eS17.

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

- Molecule 68 is a protein called Ribosomal protein uS13.

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

- Molecule 69 is a protein called Ribosomal protein eS19.

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

- Molecule 70 is a protein called Ribosomal protein uS10.

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

- Molecule 71 is a protein called Ribosomal protein eS21.

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

- Molecule 72 is a protein called Ribosomal protein uS8.

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

- Molecule 73 is a protein called Ribosomal protein uS12.

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

- Molecule 74 is a protein called Ribosomal protein eS24.

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

- Molecule 75 is a protein called Ribosomal protein es25.

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

- Molecule 76 is a protein called Ribosomal protein eS26.

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

- Molecule 77 is a protein called Ribosomal protein eS27.

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

- Molecule 78 is a protein called Ribosomal protein eS28.

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

- Molecule 79 is a protein called Ribosomal protein uS14.

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

- Molecule 80 is a protein called Ribosomal protein eS30.

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

- Molecule 81 is a protein called Ribosomal protein eS31.

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

- Molecule 82 is a protein called Ribosomal protein RACK1.

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

- Molecule 83 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
83	5	118	Total	Mg	0
			118	118	
83	7	5	Total	Mg	0
			5	5	
83	8	4	Total	Mg	0
			4	4	

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Mol	Chain	Residues	Atoms	AltConf
83	P	1	Total Mg 1 1	0
83	V	1	Total Mg 1 1	0
83	4	1	Total Mg 1 1	0
83	S2	36	Total Mg 36 36	0

- Molecule 84 is ZINC ION (three-letter code: ZN) (formula: Zn).

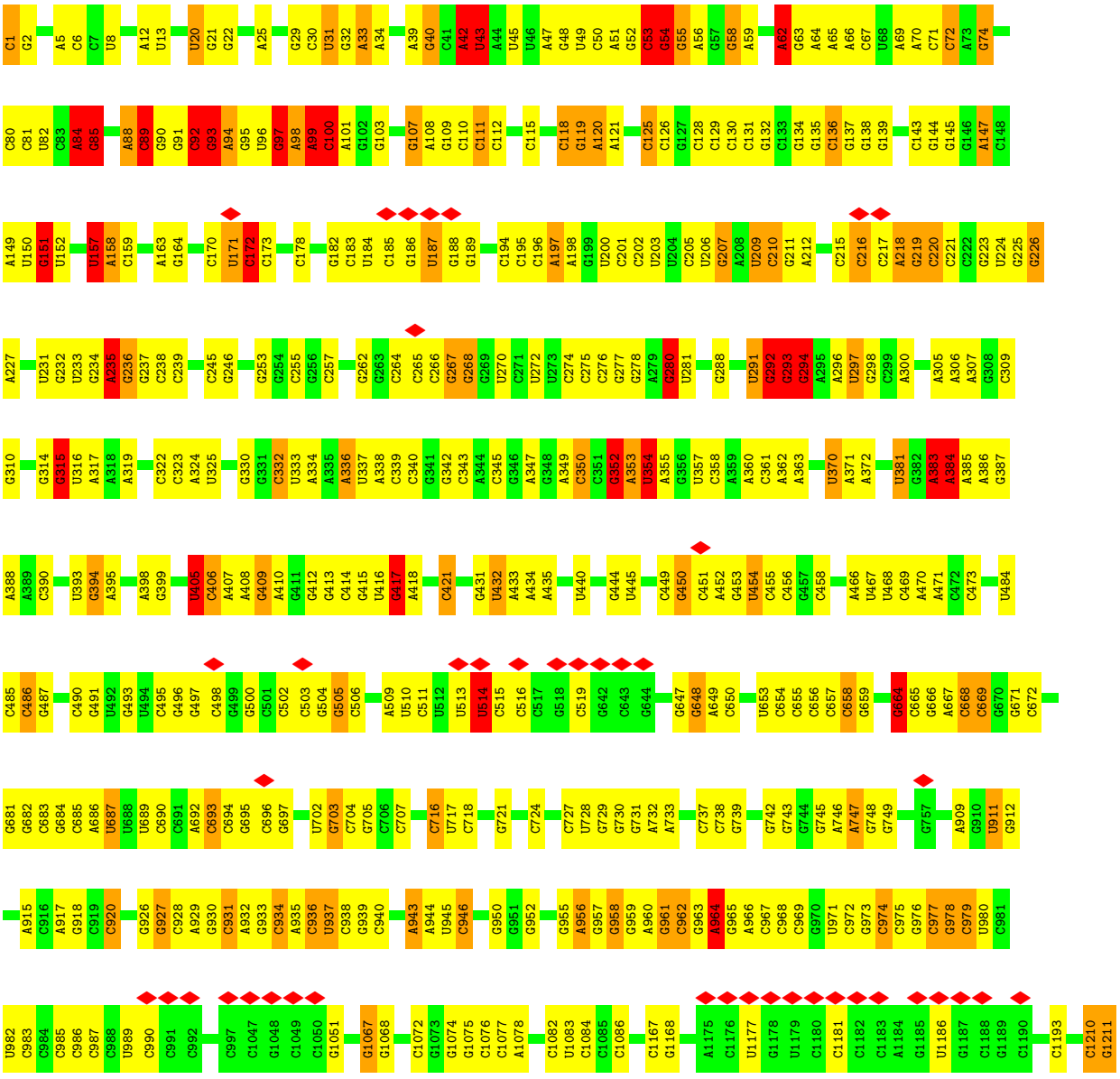
Mol	Chain	Residues	Atoms	AltConf
84	j	1	Total Zn 1 1	0
84	m	1	Total Zn 1 1	0
84	o	1	Total Zn 1 1	0
84	Sa	1	Total Zn 1 1	0

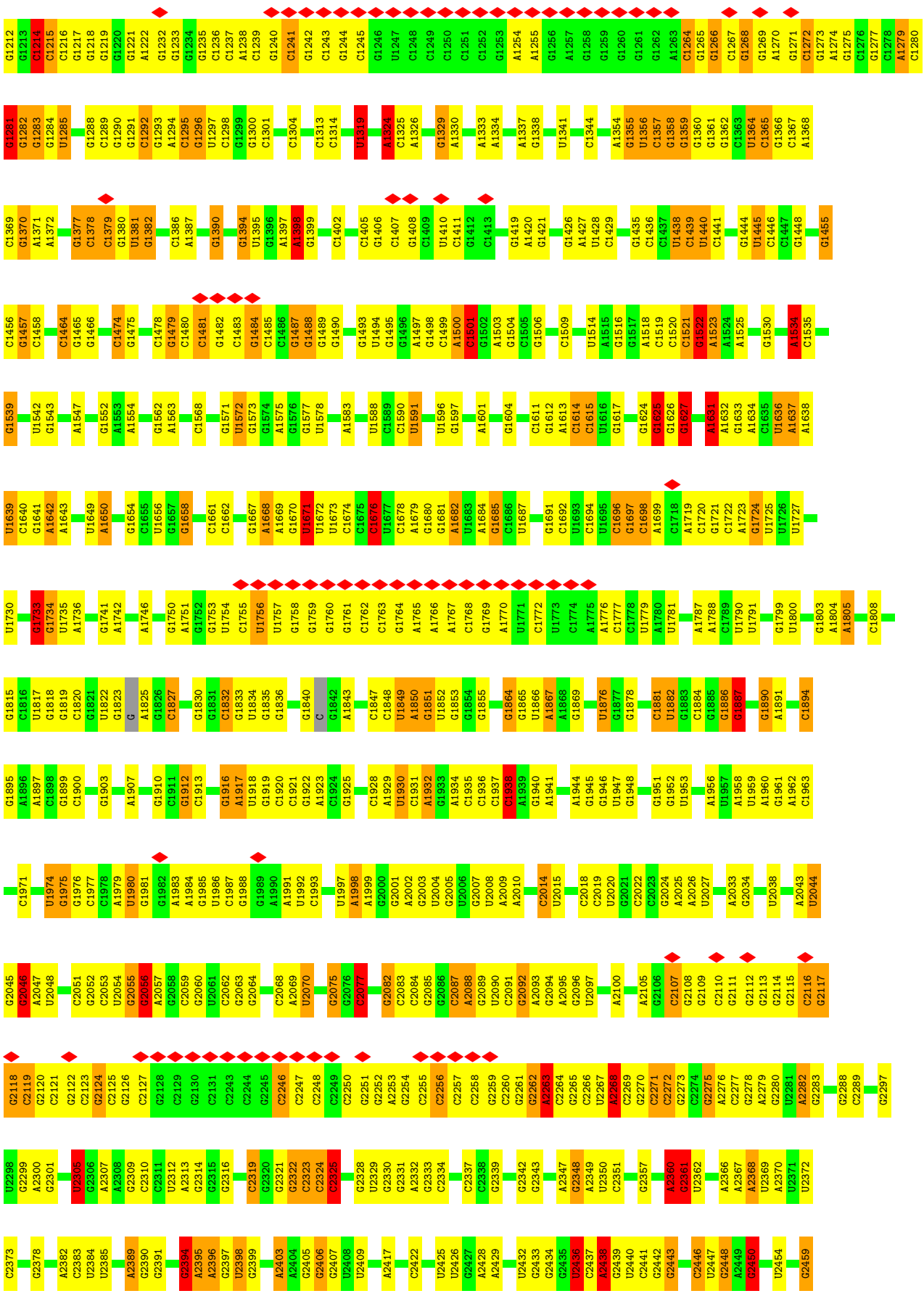
3 Residue-property plots (i)

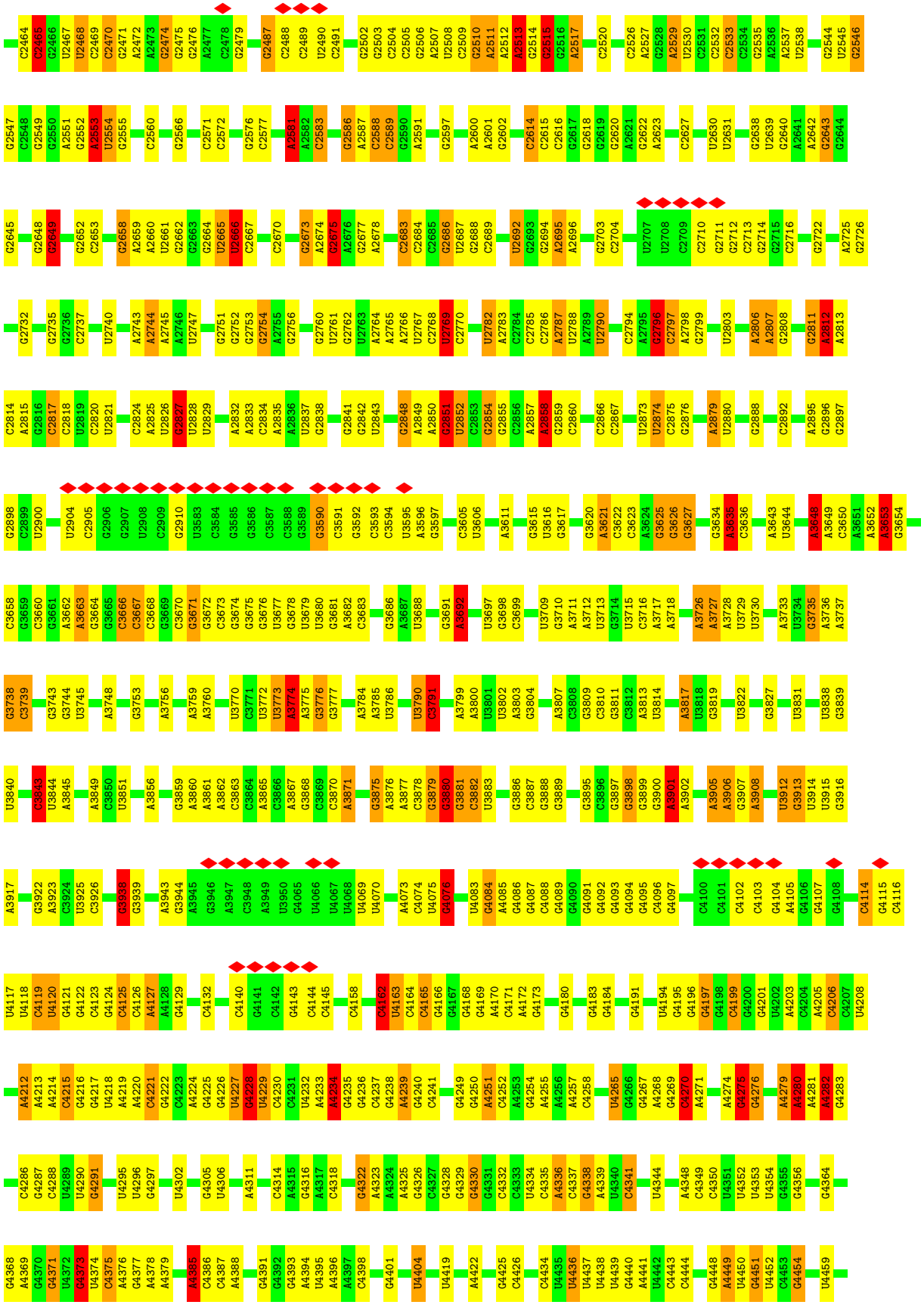
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

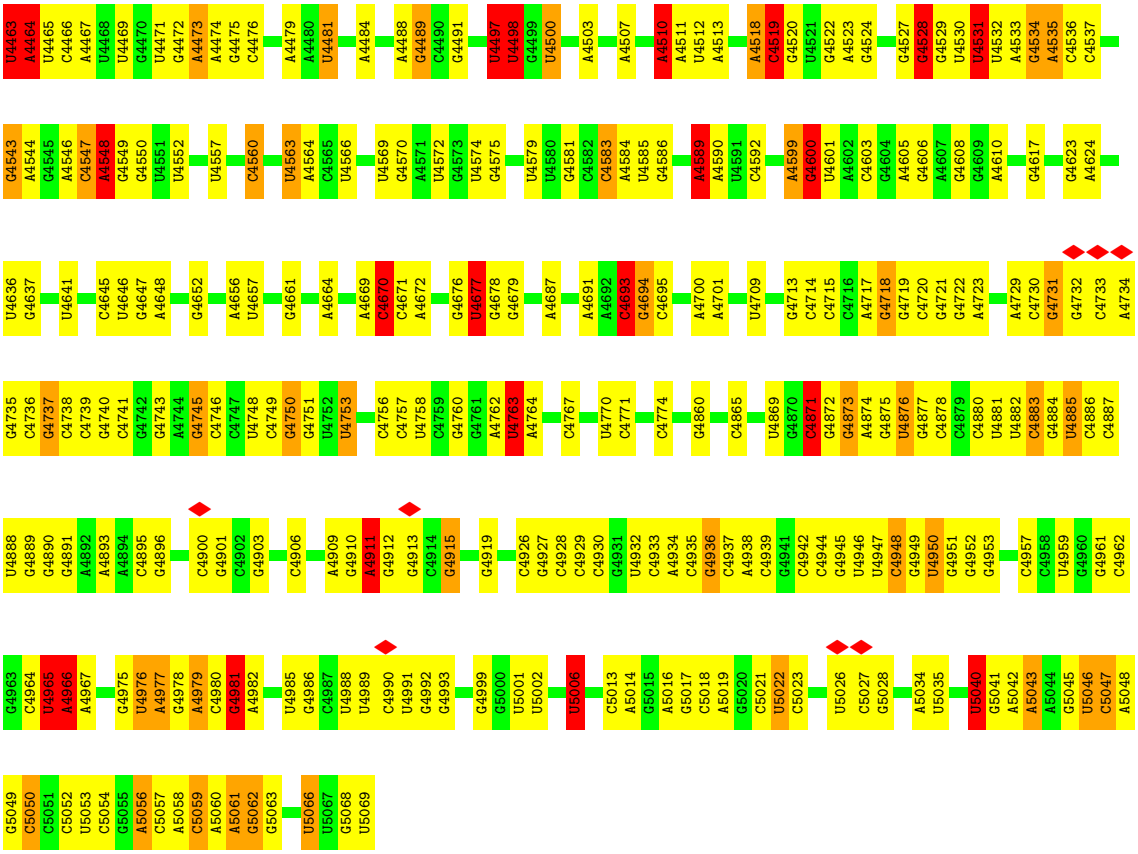
• Molecule 1: 28S ribosomal RNA

Chain 5:



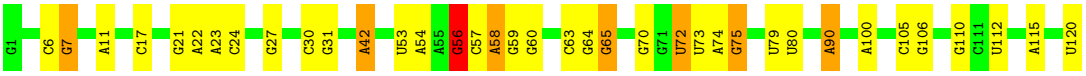






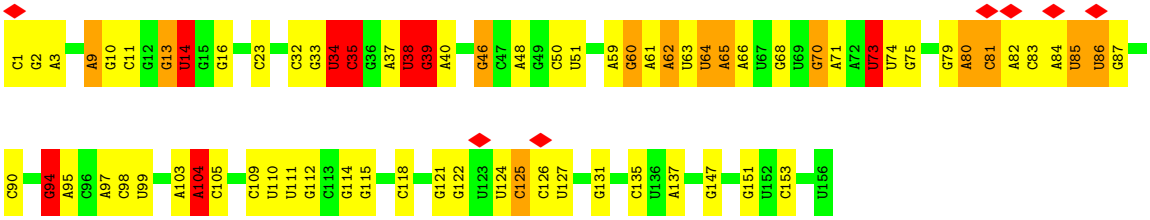
• Molecule 2: 5S ribosomal RNA

Chain 7:



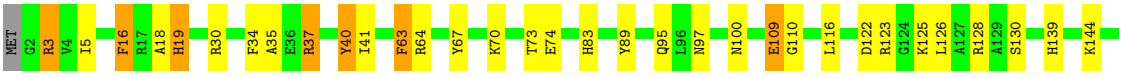
• Molecule 3: 5.8S ribosomal RNA

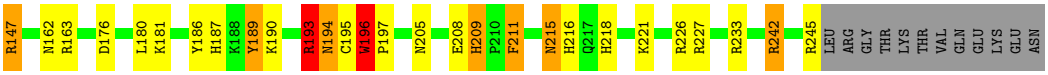
Chain 8:



• Molecule 4: Ribosomal protein uL2

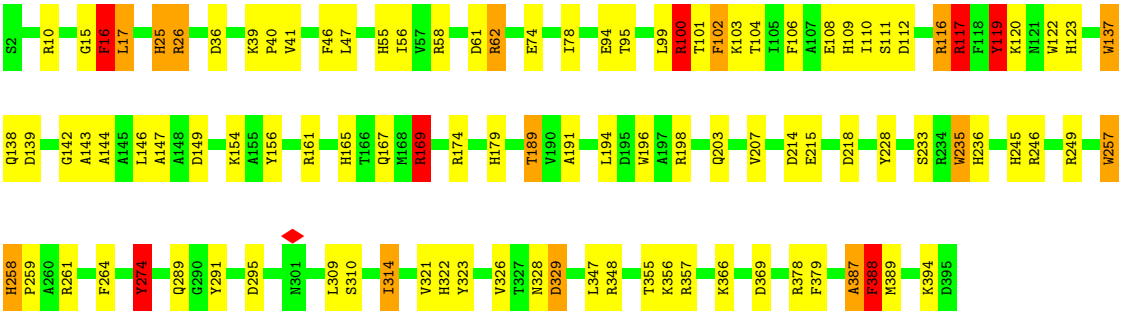
Chain A:





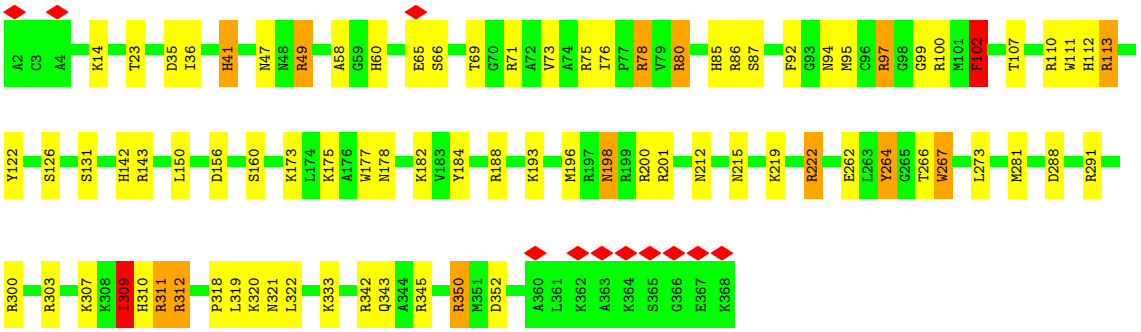
• Molecule 5: Ribosomal protein uL3

Chain B:



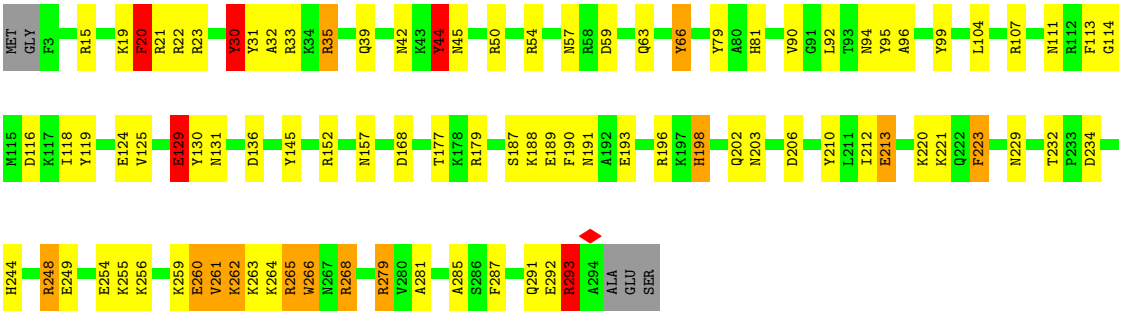
• Molecule 6: Ribosomal protein uL4

Chain C:



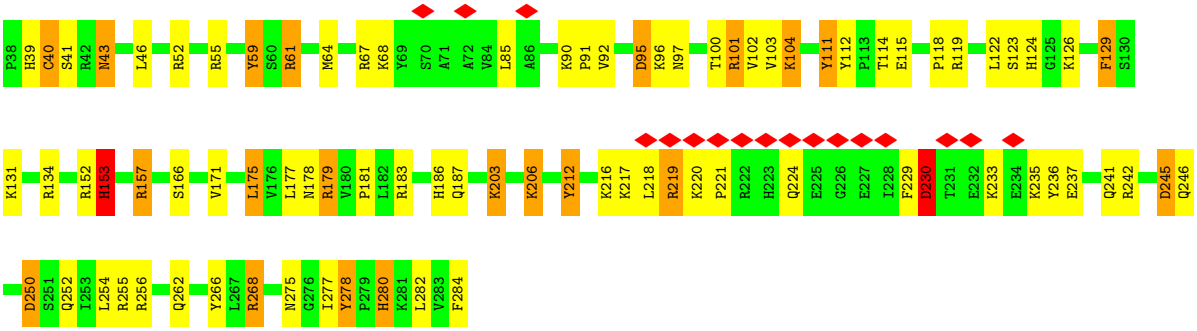
• Molecule 7: Ribosomal protein uL18

Chain D:

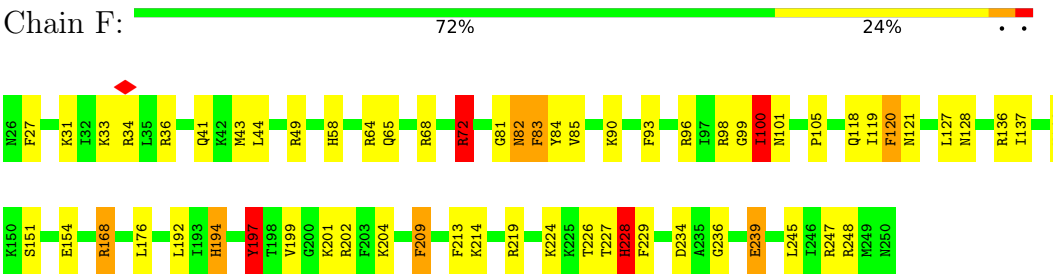


• Molecule 8: Ribosomal protein eL6

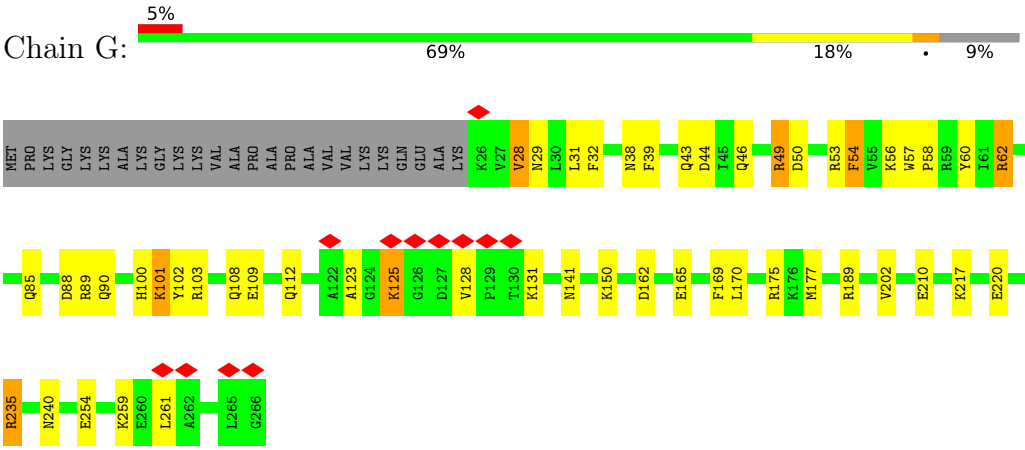
Chain E:



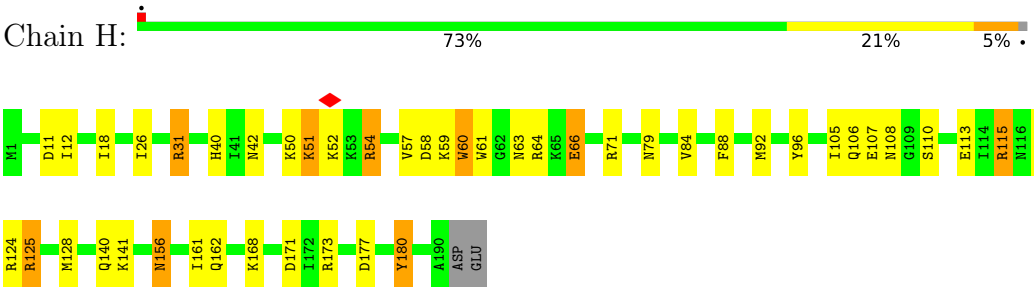
• Molecule 9: Ribosomal protein uL30



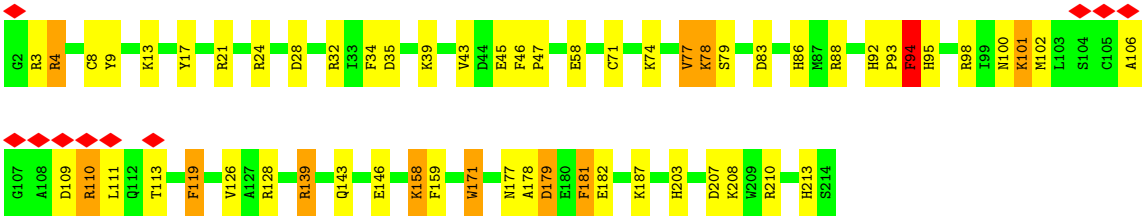
• Molecule 10: Ribosomal protein eL8



• Molecule 11: Ribosomal protein uL6

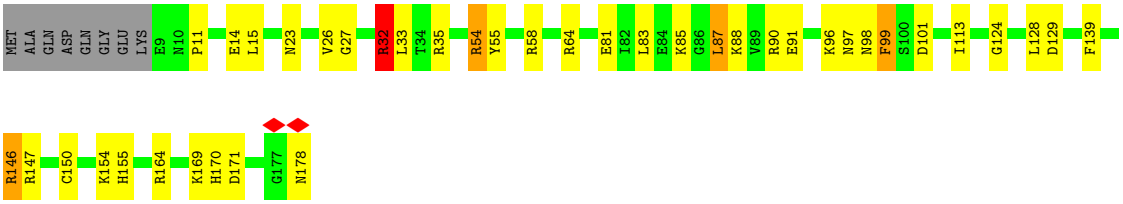


• Molecule 12: Ribosomal protein uL16



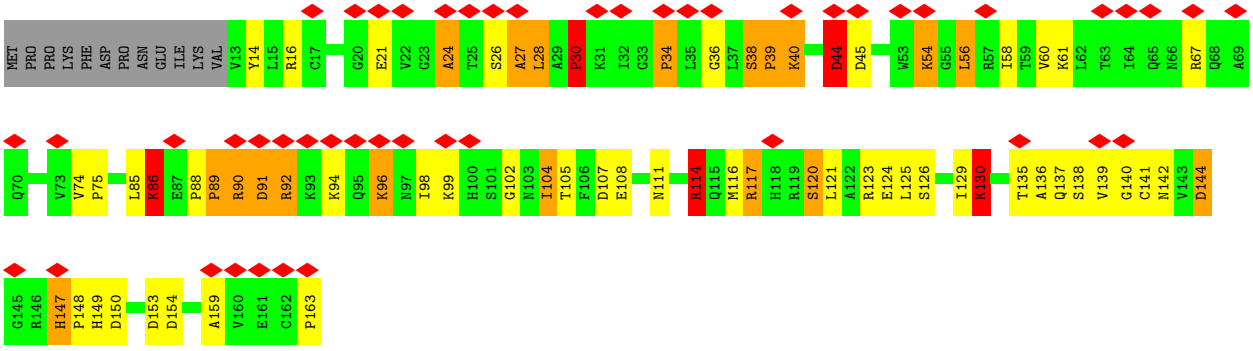
• Molecule 13: Ribosomal protein uL5

Chain J:



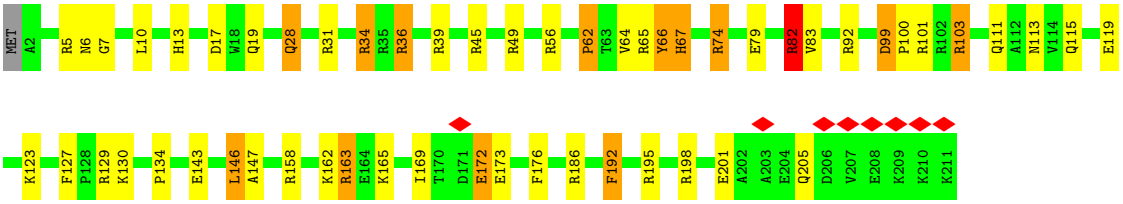
• Molecule 14: Ribosomal protein uL11

Chain K:



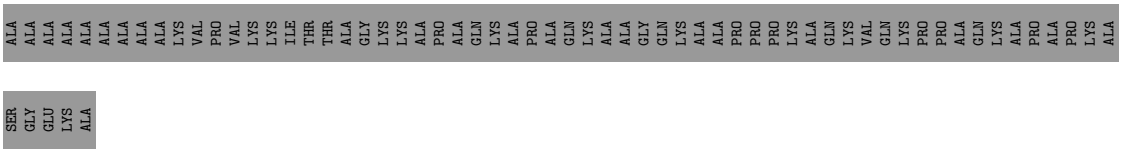
• Molecule 15: Ribosomal protein eL13

Chain L:



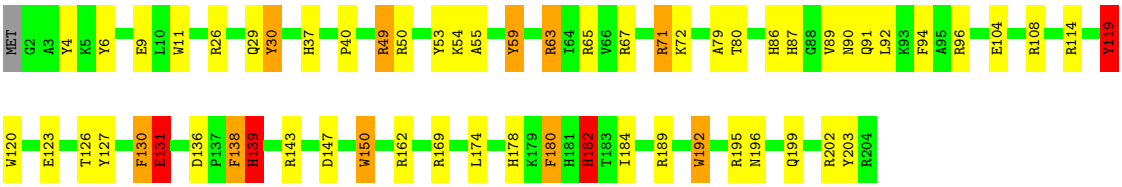
• Molecule 16: Ribosomal protein eL14

Chain M:



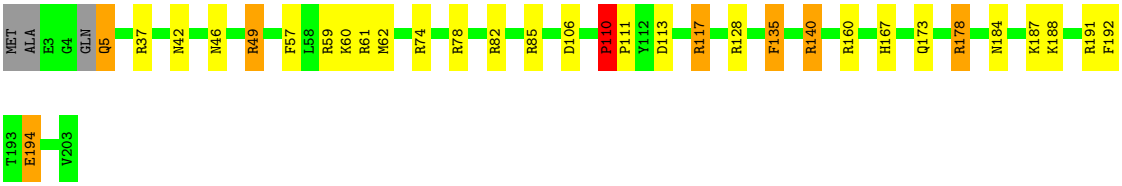
• Molecule 17: Ribosomal protein eL15

Chain N:



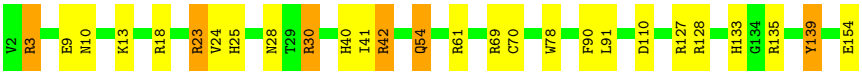
• Molecule 18: Ribosomal protein uL13

Chain O:



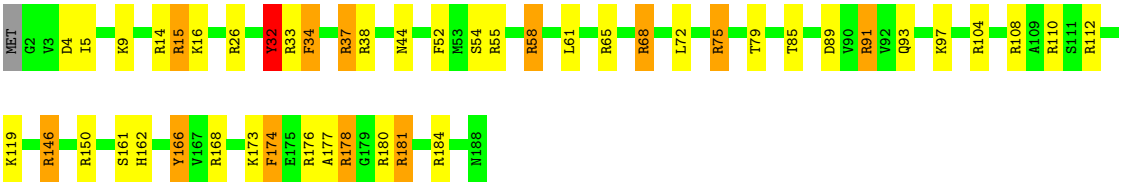
• Molecule 19: Ribosomal protein uL22

Chain P:



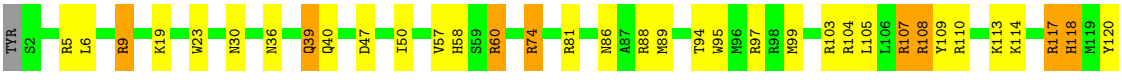
• Molecule 20: Ribosomal protein eL18

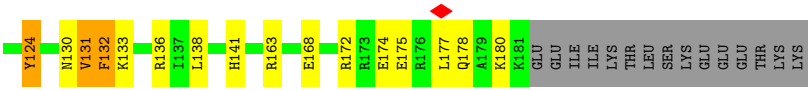
Chain Q:



• Molecule 21: Ribosomal protein eL19

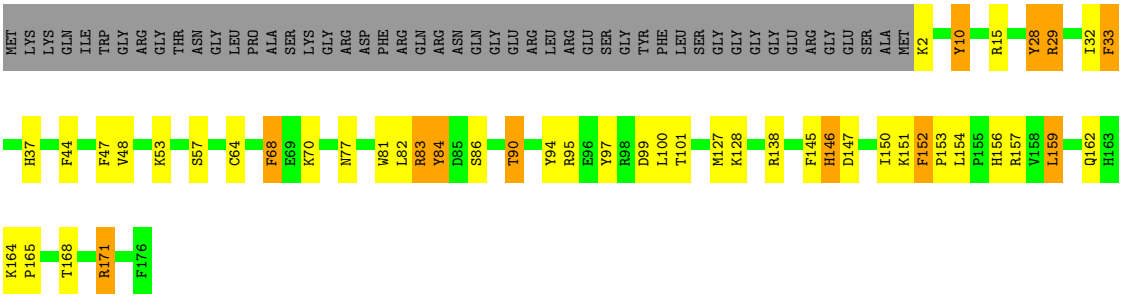
Chain R:





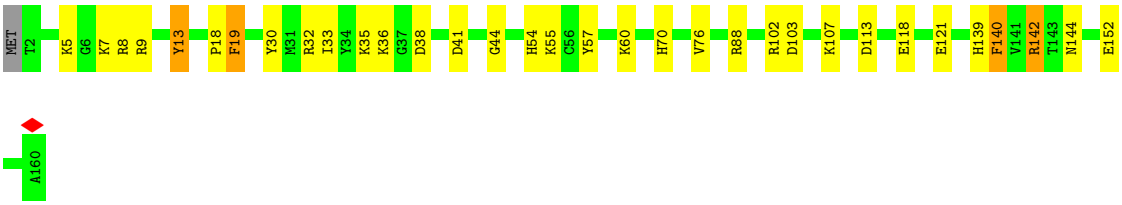
• Molecule 22: Ribosomal protein eL20

Chain S:



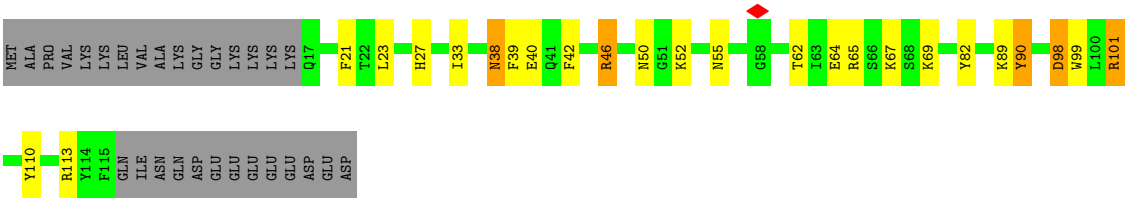
• Molecule 23: Ribosomal protein eL21

Chain T:



• Molecule 24: Ribosomal protein eL22

Chain U:

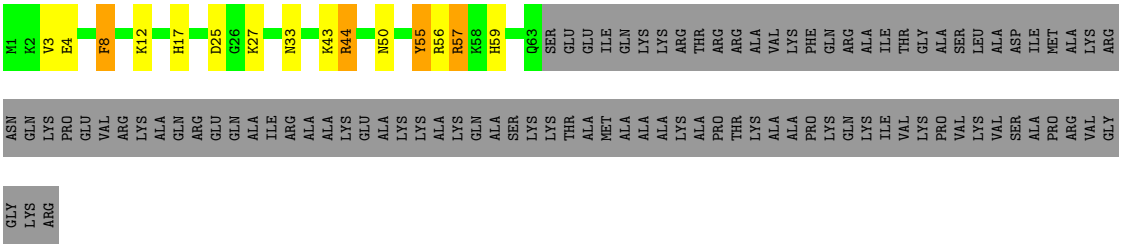


• Molecule 25: Ribosomal protein uL14

Chain V:

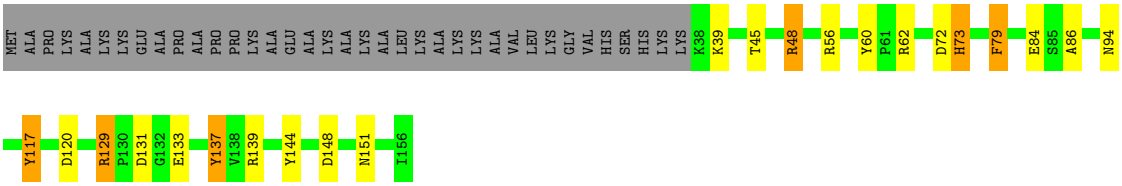
• Molecule 26: Ribosomal protein eL24

Chain W:



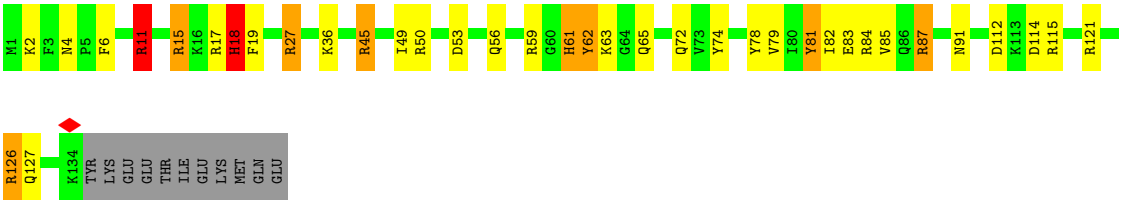
• Molecule 27: Ribosomal protein uL23

Chain X:



• Molecule 28: Ribosomal protein uL24

Chain Y:

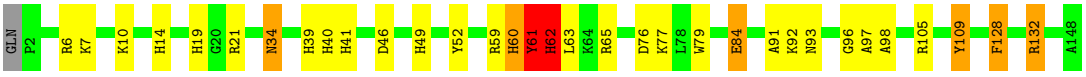


• Molecule 29: Ribosomal protein eL27

Chain Z:

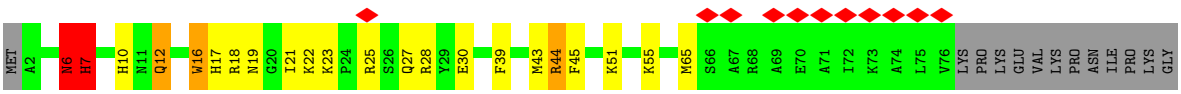
• Molecule 30: Ribosomal protein uL15

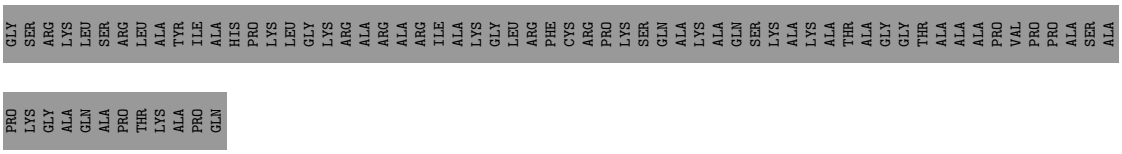
Chain a:



• Molecule 31: Ribosomal protein eL29

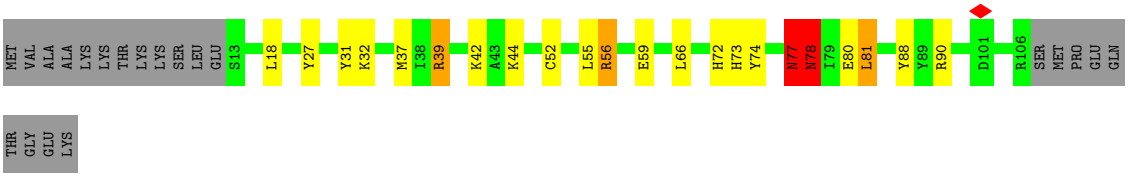
Chain b:





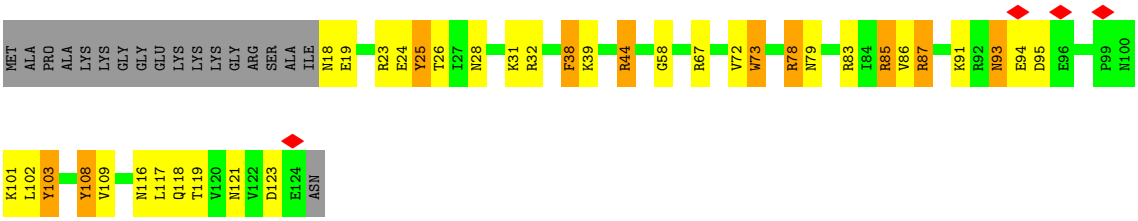
• Molecule 32: Ribosomal protein eL30

Chain c:



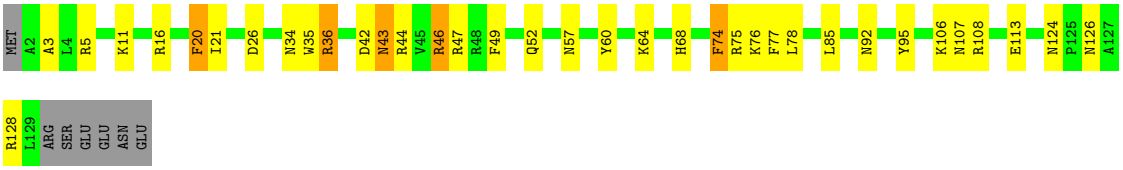
• Molecule 33: Ribosomal protein eL31

Chain d:



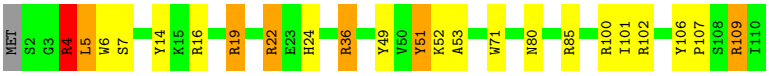
• Molecule 34: Ribosomal protein eL32

Chain e:



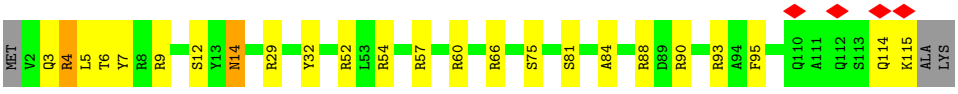
• Molecule 35: Ribosomal protein eL33

Chain f:



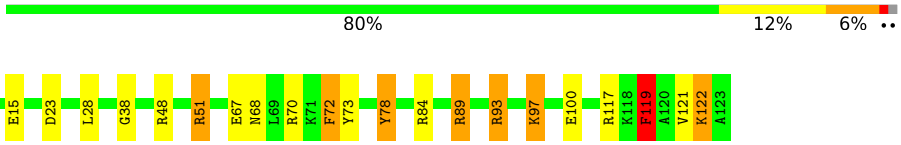
• Molecule 36: Ribosomal protein eL34

Chain g:



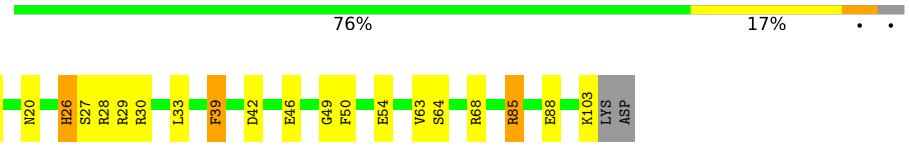
• Molecule 37: Ribosomal protein uL29

Chain h:



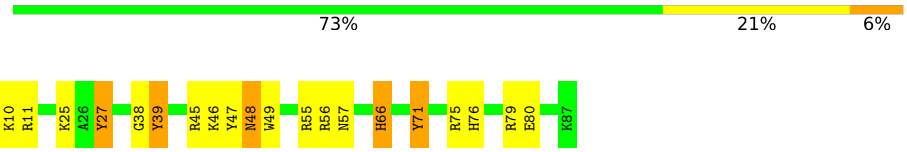
• Molecule 38: Ribosomal protein eL36

Chain i:



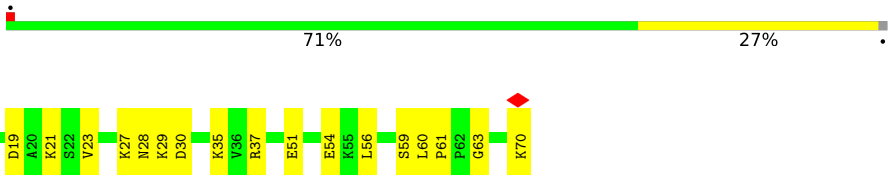
• Molecule 39: Ribosomal protein eL37

Chain j:



• Molecule 40: Ribosomal protein eL38

Chain k:

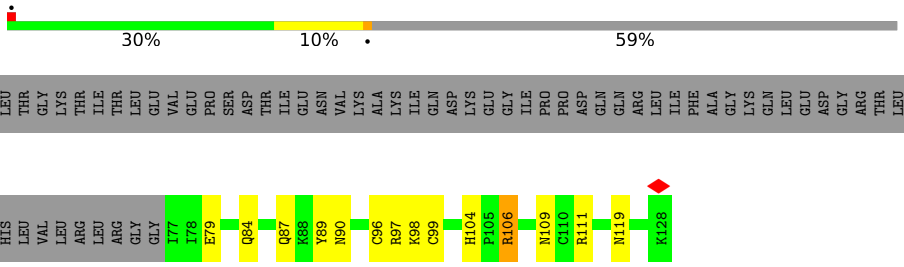


• Molecule 41: Ribosomal protein eL39

Chain l:

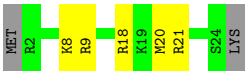
• Molecule 42: Ribosomal protein eL40

Chain m:



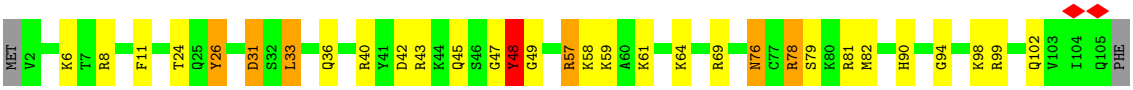
• Molecule 43: Ribosomal protein eL41

Chain n:



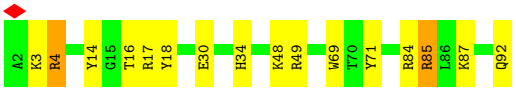
• Molecule 44: Ribosomal protein eL42

Chain o:



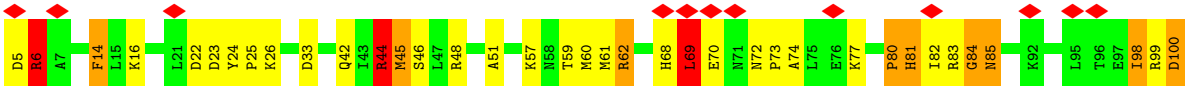
• Molecule 45: Ribosomal protein eL43

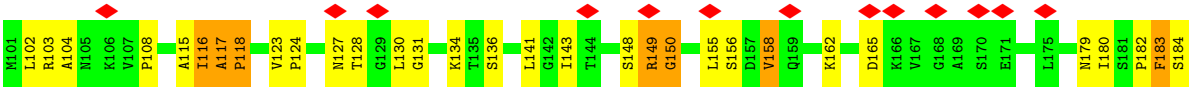
Chain p:



• Molecule 46: Ribosomal protein uL10

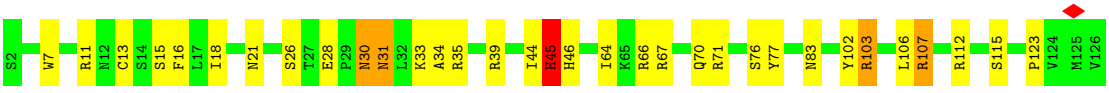
Chain q:





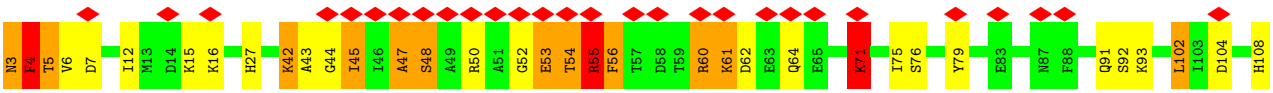
• Molecule 47: Ribosomal protein eL28

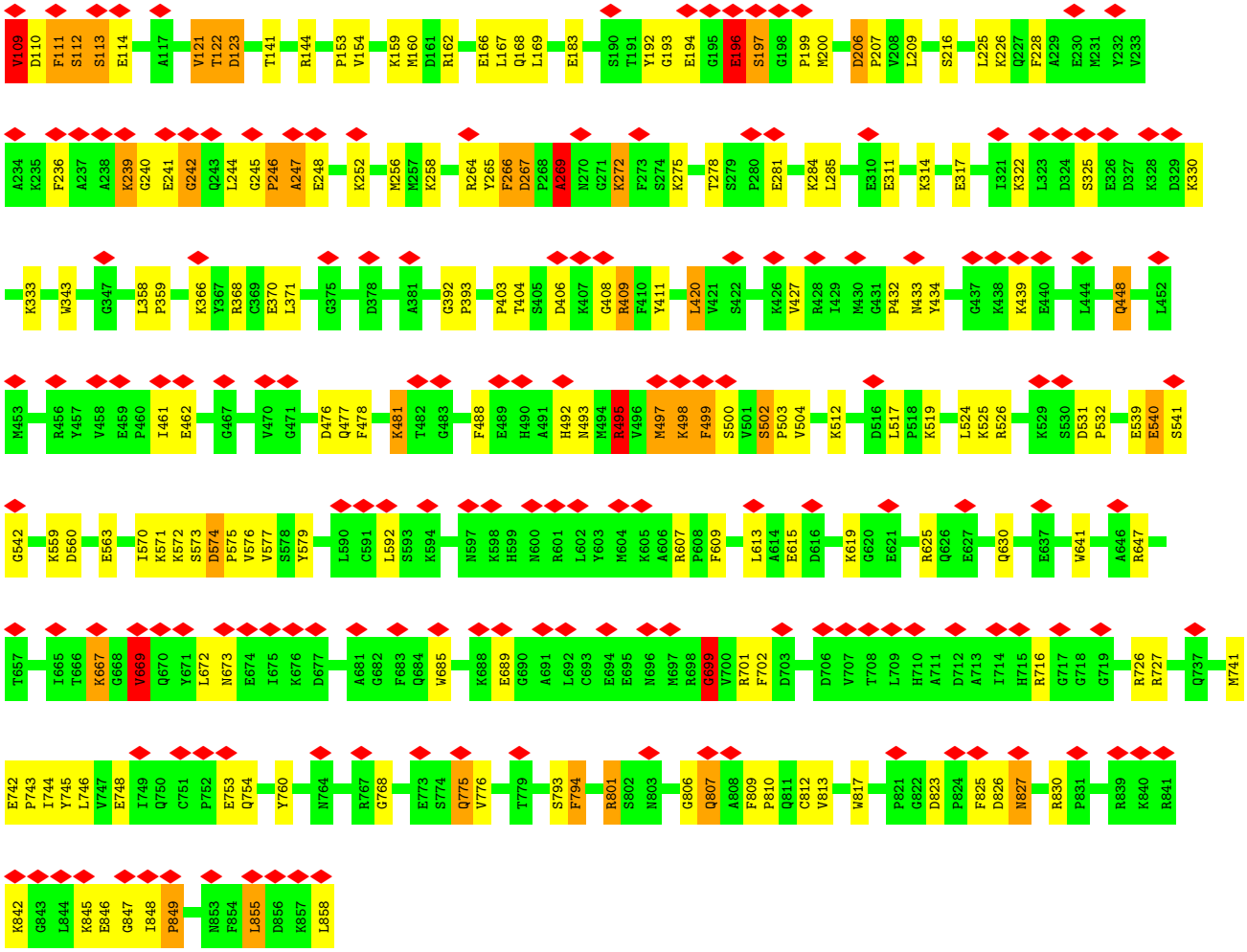
Chain r:



• Molecule 48: Eukaryotic elongation factor 2

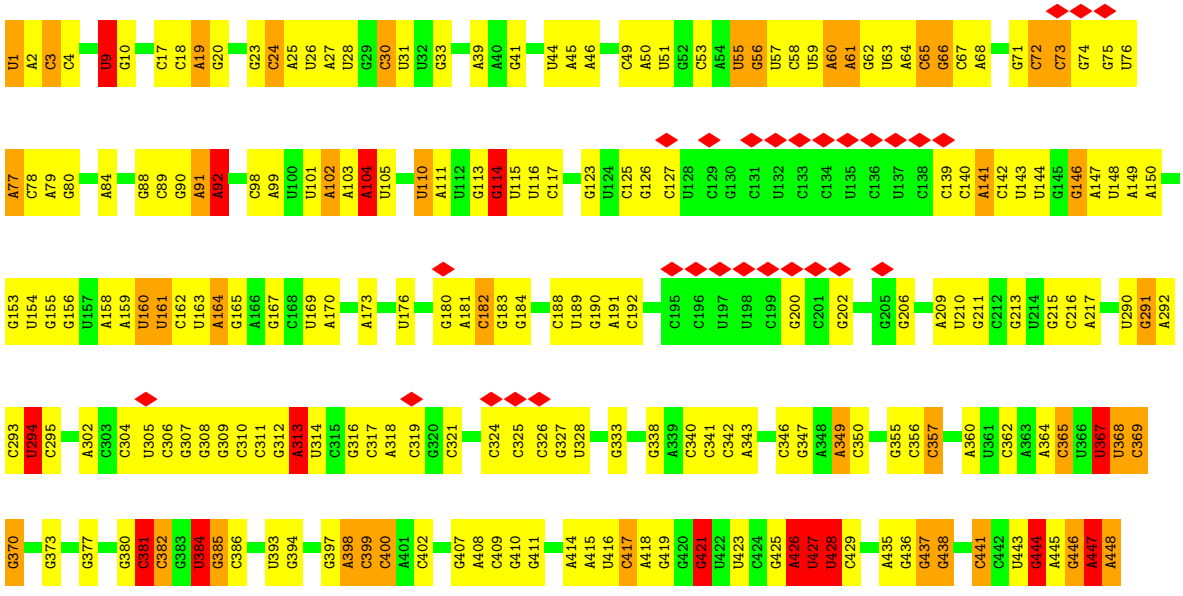
Chain 4:

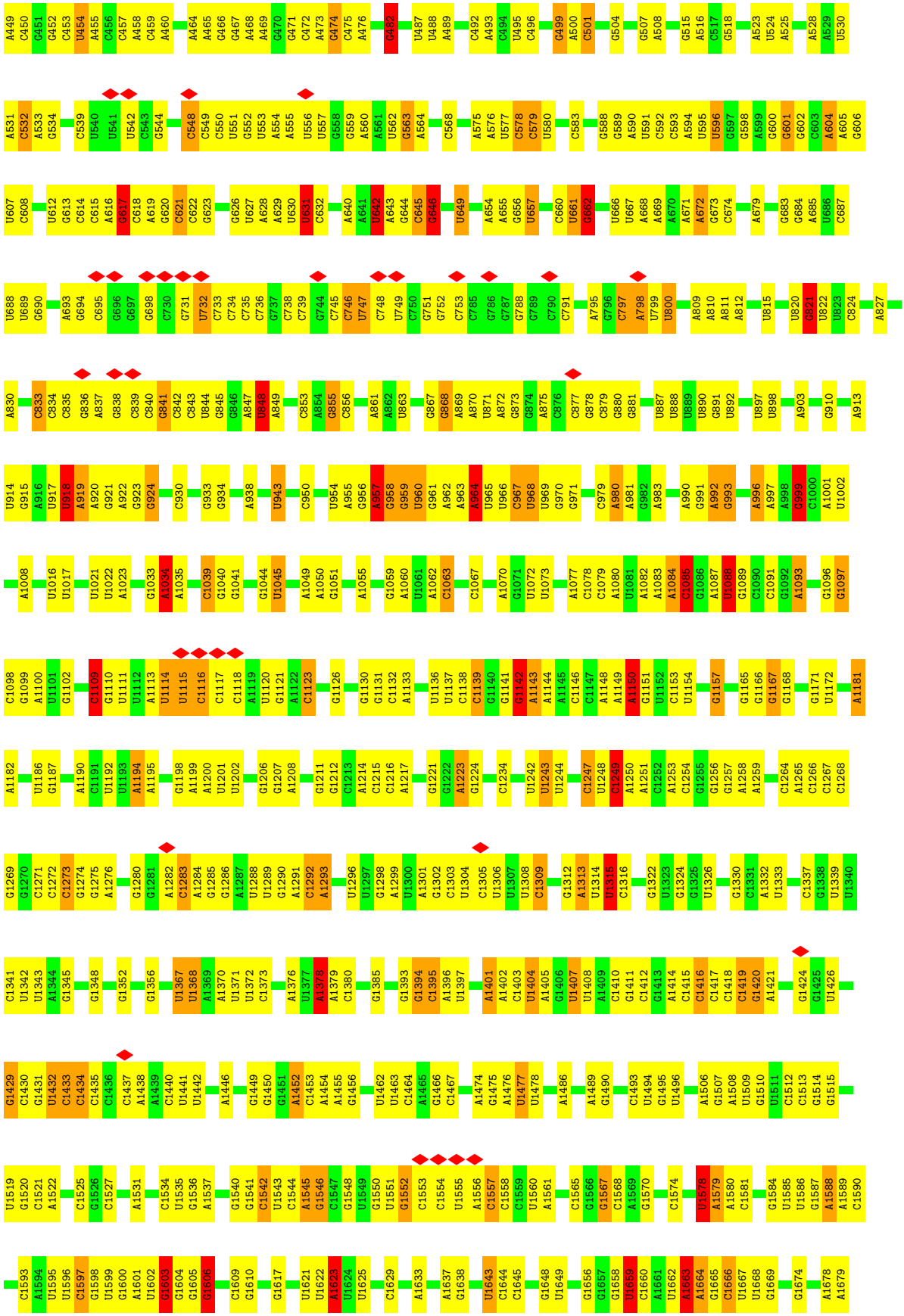


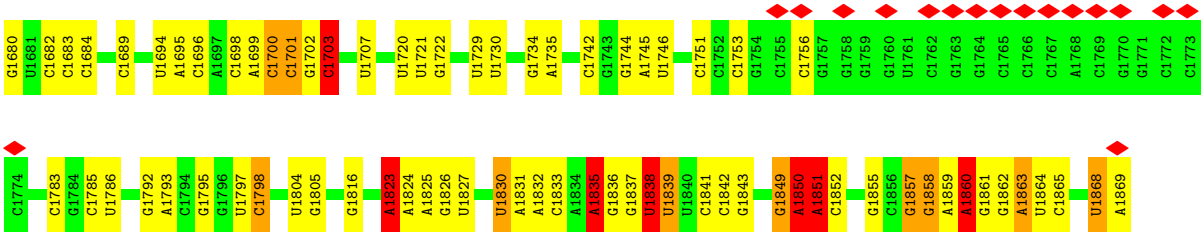


• Molecule 49: 18S ribosomal RNA

Chain S2:

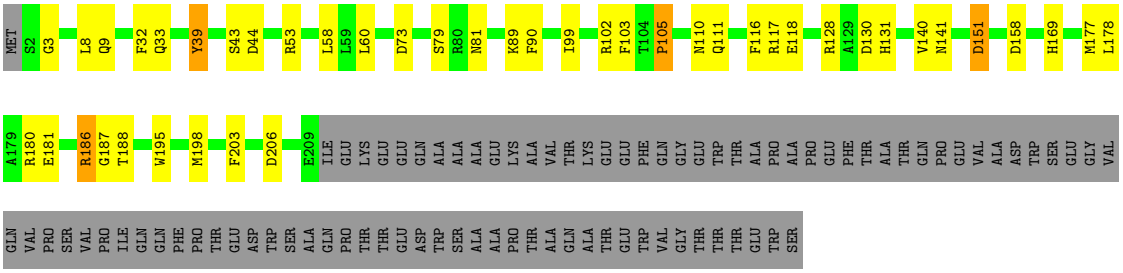






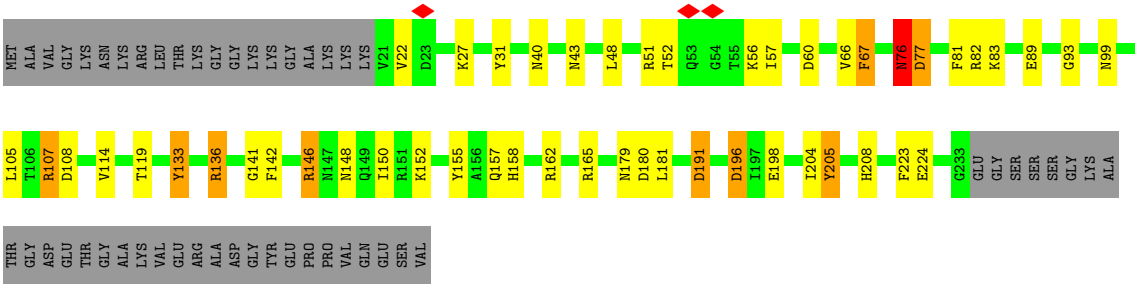
• Molecule 50: Ribosomal protein uS2

Chain SA:



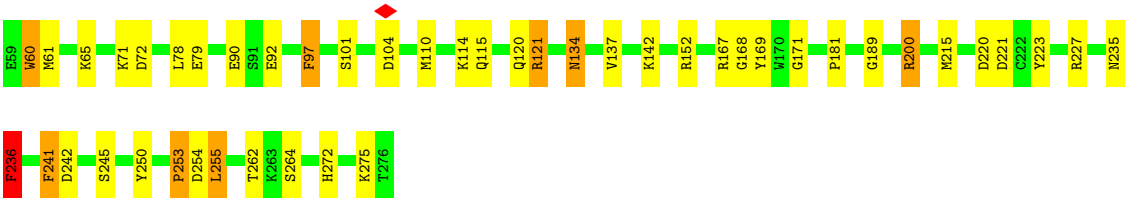
• Molecule 51: Ribosomal protein eS1

Chain SB:



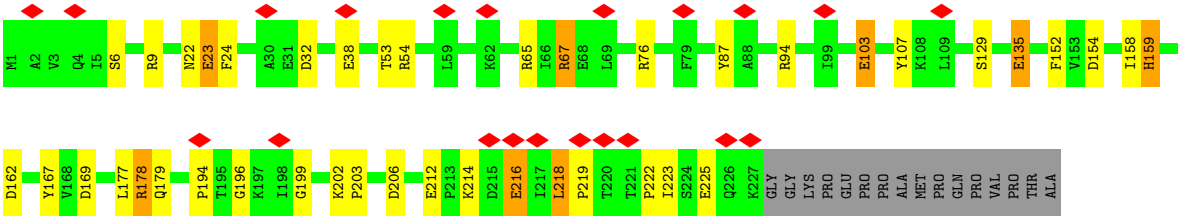
• Molecule 52: Ribosomal protein uS5

Chain SC:

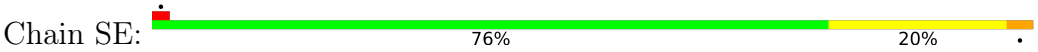


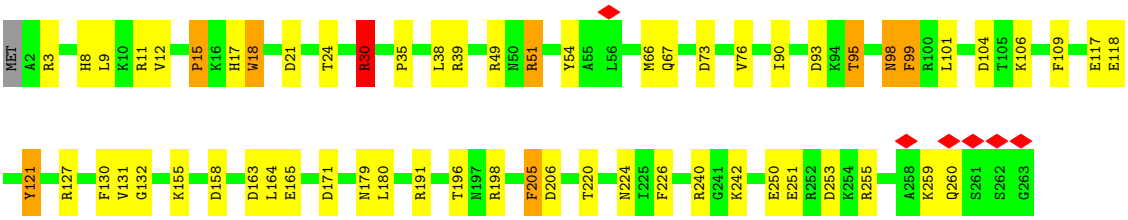
• Molecule 53: Ribosomal protein uS3

Chain SD:

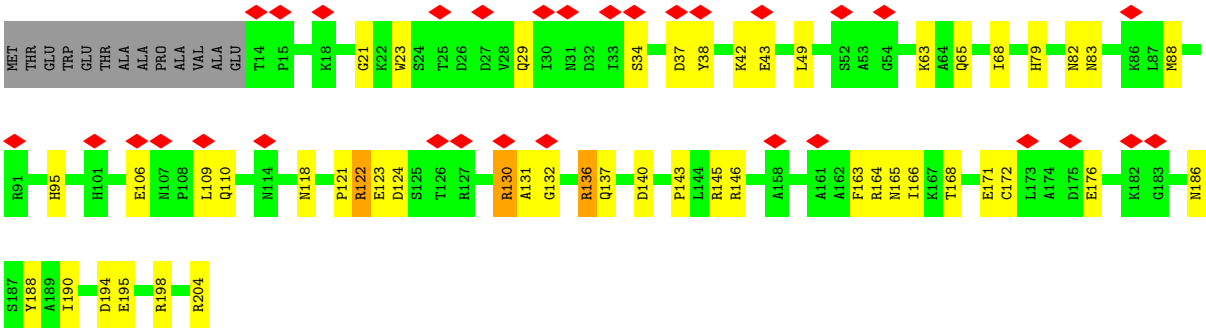


• Molecule 54: Ribosomal protein eS4

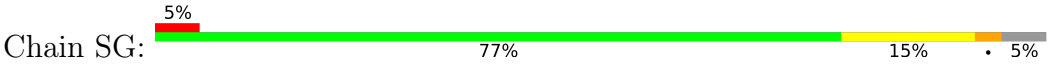


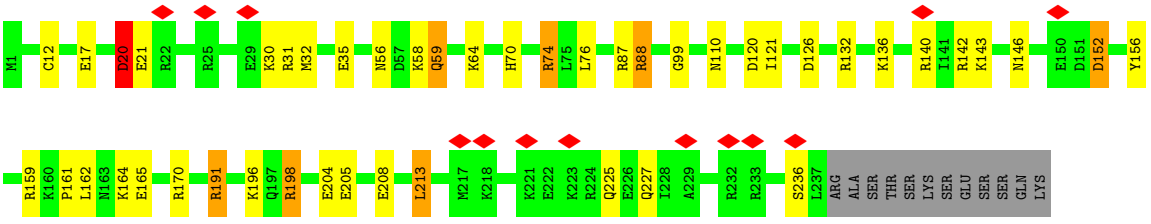


• Molecule 55: Ribosomal protein uS7

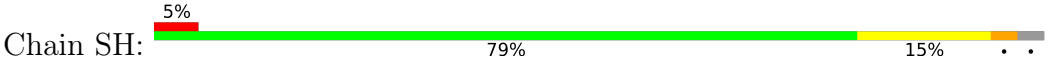


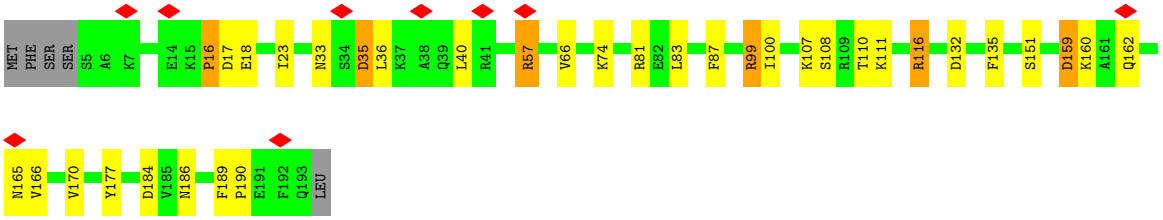
• Molecule 56: Ribosomal protein eS6



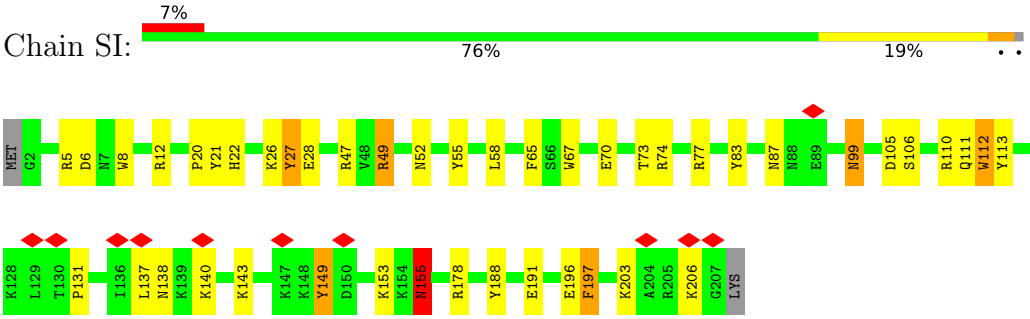


• Molecule 57: Ribosomal protein eS7

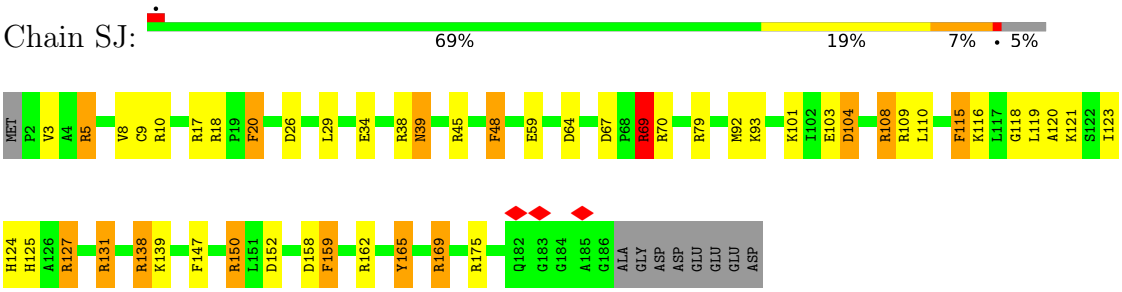




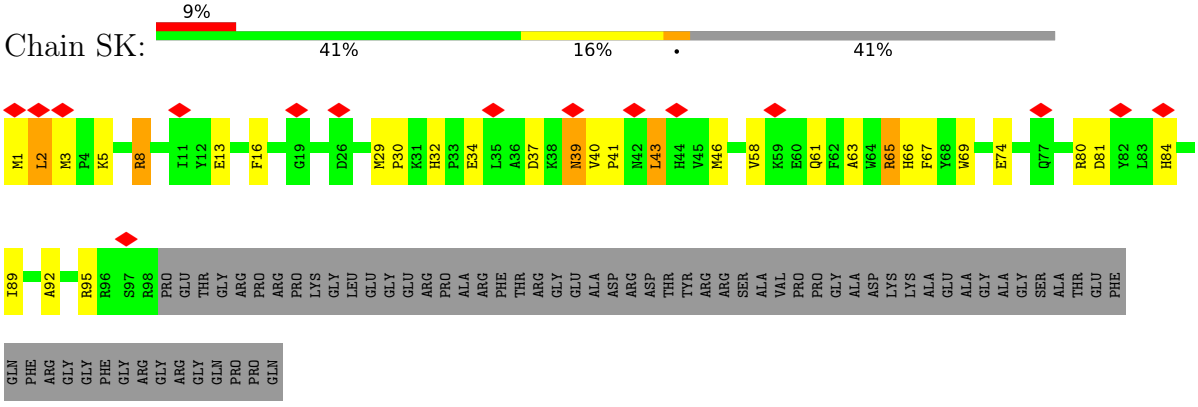
• Molecule 58: Ribosomal protein eS8



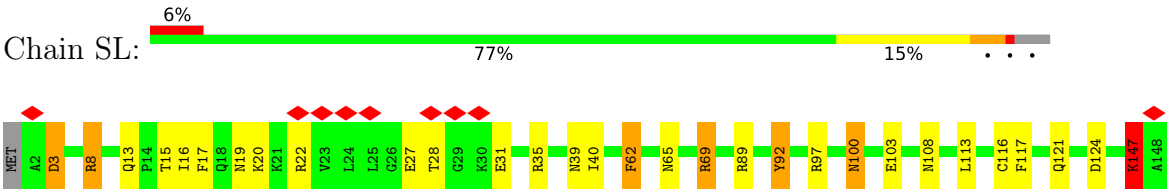
• Molecule 59: Ribosomal protein uS4

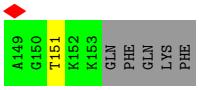


• Molecule 60: Ribosomal protein eS10



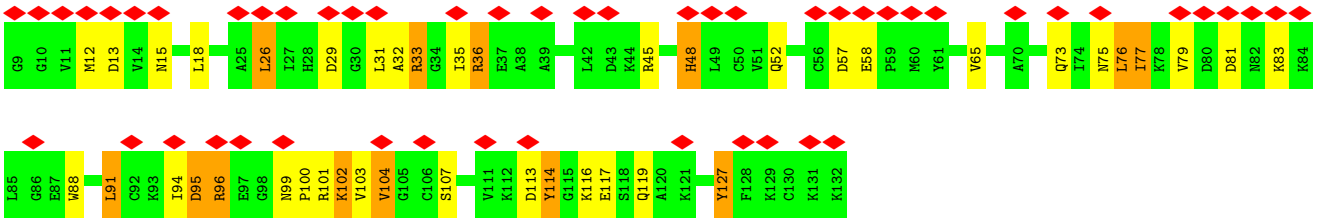
• Molecule 61: Ribosomal protein uS17





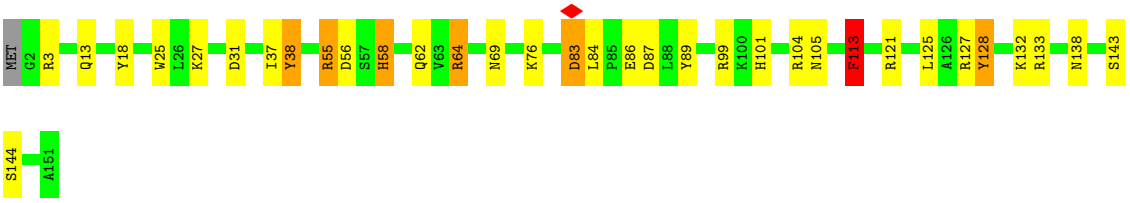
• Molecule 62: Ribosomal protein eS12

Chain SM:



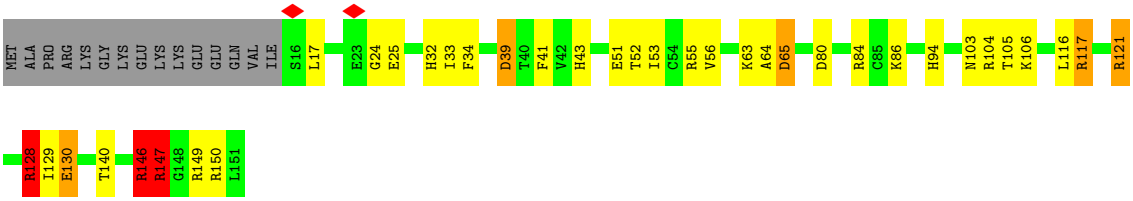
• Molecule 63: Ribosomal protein uS15

Chain SN:



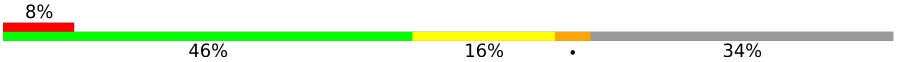
• Molecule 64: Ribosomal protein uS11

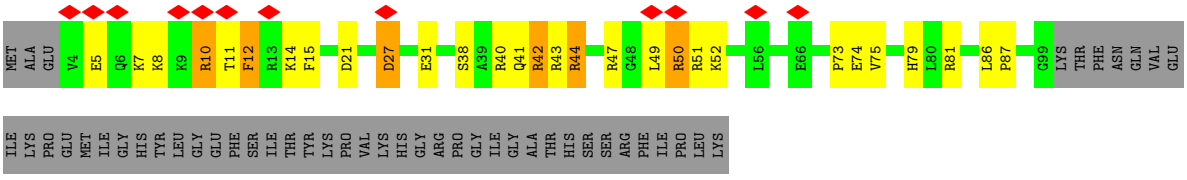
Chain SO:



• Molecule 65: Ribosomal protein uS19

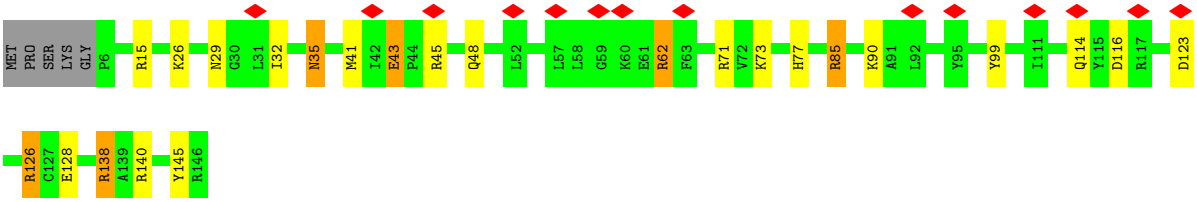
Chain SP:



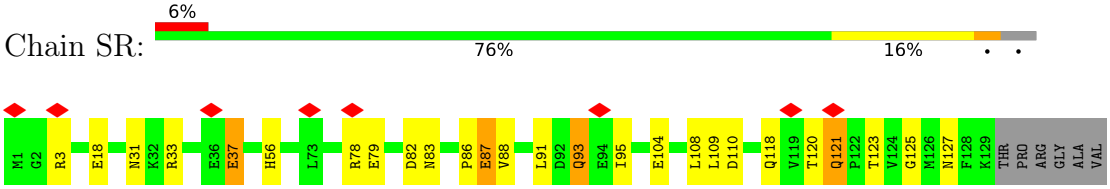


• Molecule 66: Ribosomal protein uS9

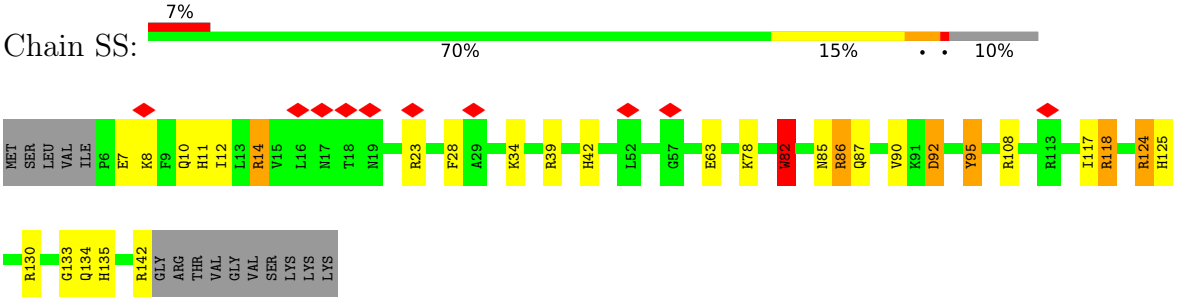
Chain SQ:



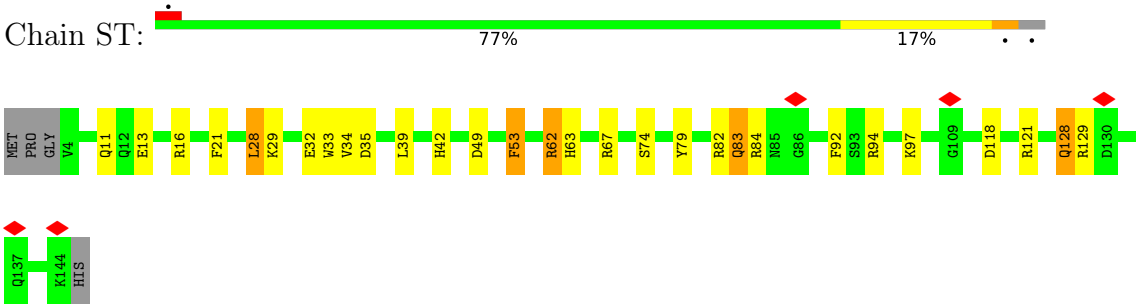
• Molecule 67: Ribosomal protein eS17



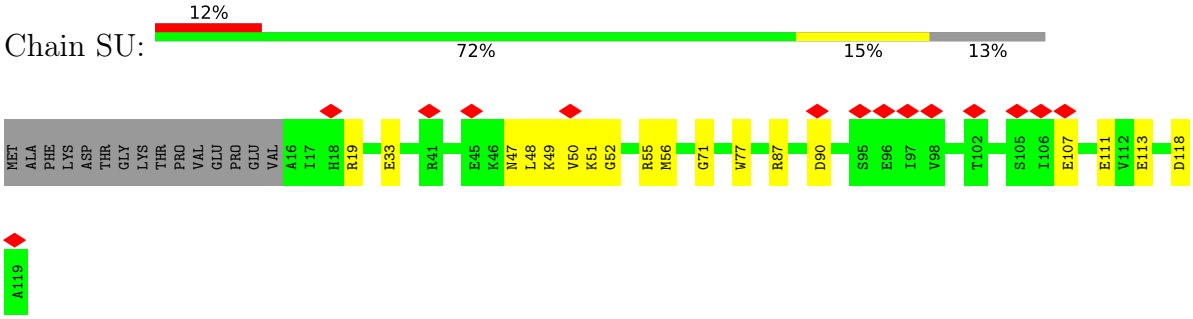
• Molecule 68: Ribosomal protein uS13



• Molecule 69: Ribosomal protein eS19

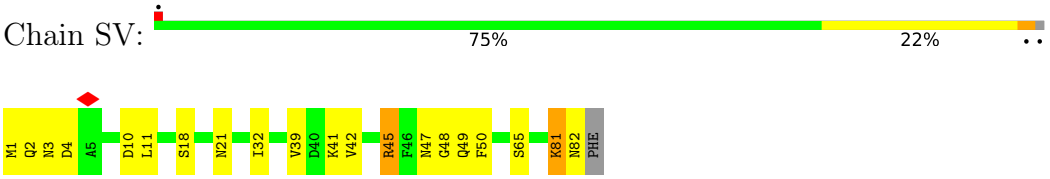


• Molecule 70: Ribosomal protein uS10



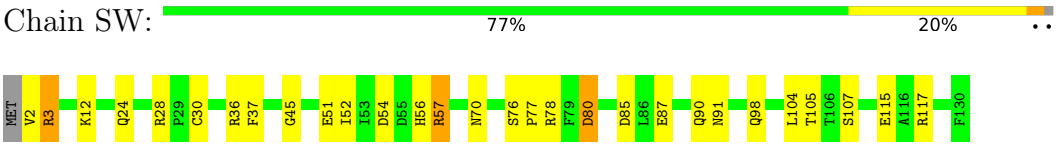
• Molecule 71: Ribosomal protein eS21

Chain SV:



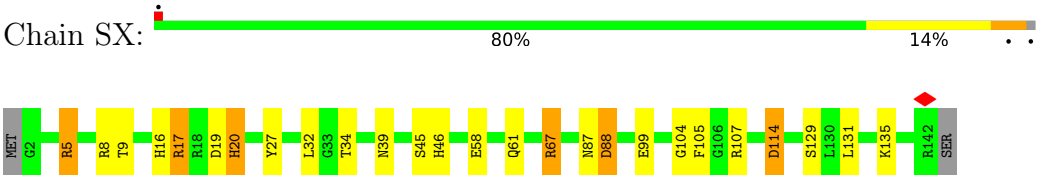
• Molecule 72: Ribosomal protein uS8

Chain SW:



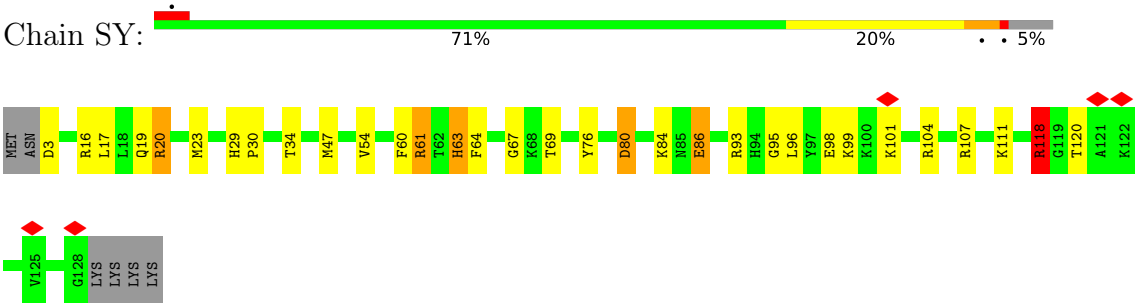
• Molecule 73: Ribosomal protein uS12

Chain SX:



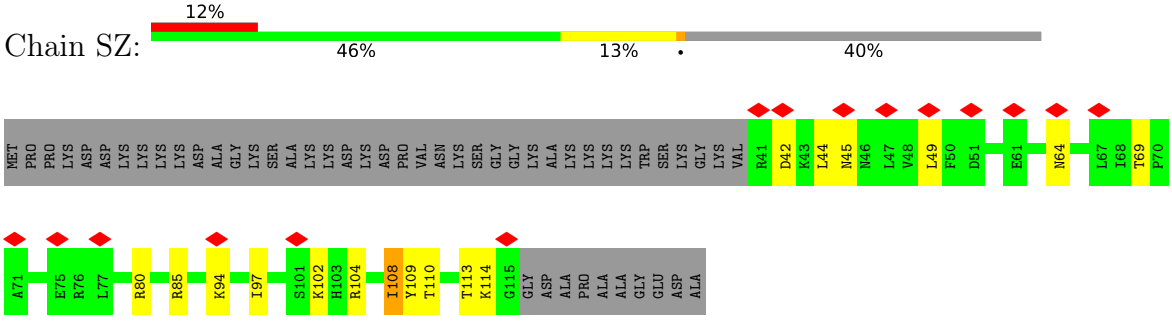
• Molecule 74: Ribosomal protein eS24

Chain SY:



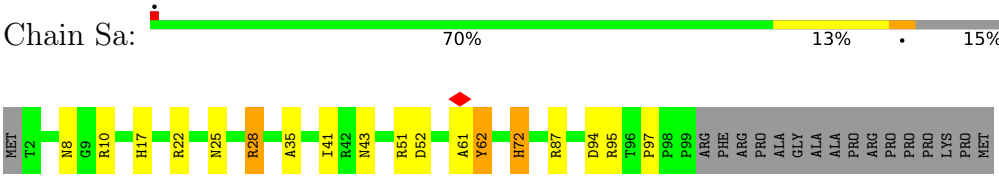
• Molecule 75: Ribosomal protein es25

Chain SZ:



• Molecule 76: Ribosomal protein eS26

Chain Sa:

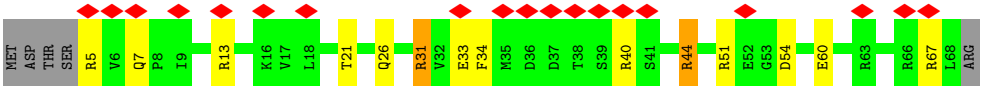


• Molecule 77: Ribosomal protein eS27

Chain Sb:

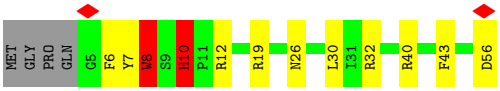
• Molecule 78: Ribosomal protein eS28

Chain Sc:



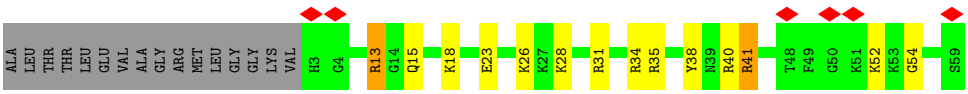
• Molecule 79: Ribosomal protein uS14

Chain Sd:



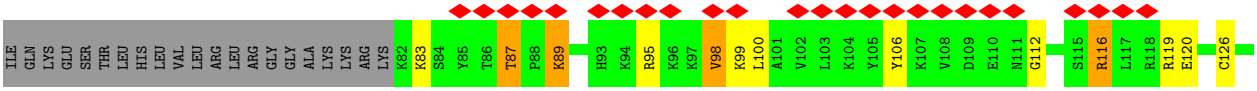
• Molecule 80: Ribosomal protein eS30

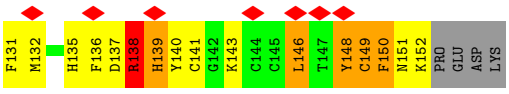
Chain Se:



• Molecule 81: Ribosomal protein eS31

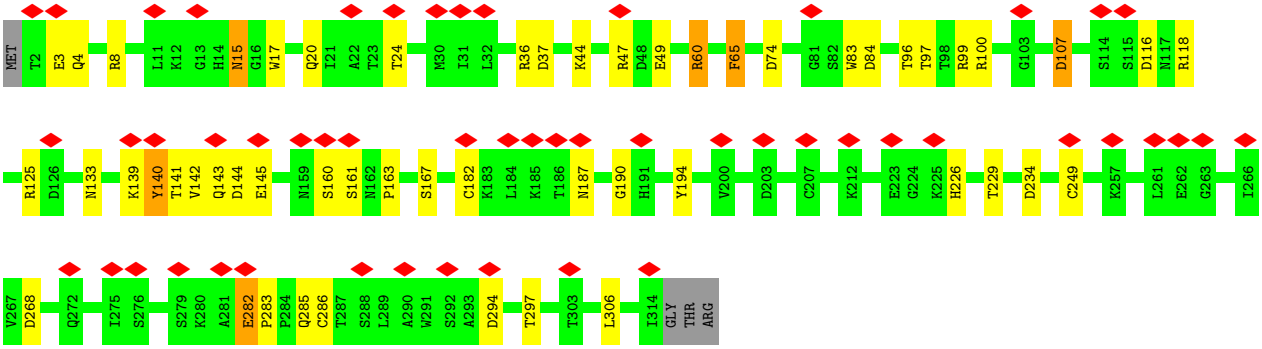
Chain Sf:





• Molecule 82: Ribosomal protein RACK1

Chain Sg:


MET T2 E3 Q4 R8 L11 K12 G13 H14 N15 G16 W17 Q20 I21 A22 T23 T24 M30 I31 L32 R36 D37 K44 R47 D48 E49 R60 F65 D74 G81 S82 W83 D84 T96 T97 T98 R99 R100 G103 D107 S114 S115 D116 N117 R118
R125 D126 N133 K139 Y140 T141 V142 Q143 D144 E145 N159 S160 S161 N162 P163 S167 C182 K183 L184 K185 T186 N187 G190 H191 Y194 V200 D203 C207 K212 E223 G224 K225 H226 T229 D234 C249 K257 L261 E262 G263 I266
V267 D268 Q272 I275 S276 S279 K280 A281 E282 P283 P284 Q285 C286 T287 S288 L289 A290 W291 S292 A293 D294 T297 T303 L306 I314 GLY THR ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	36667	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)	2500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.913	Depositor
Minimum map value	-0.580	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.065	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	5	0.64	75/87792 (0.1%)	1.12	729/136945 (0.5%)
2	7	0.54	1/2858 (0.0%)	0.96	9/4455 (0.2%)
3	8	0.68	3/3701 (0.1%)	1.19	42/5766 (0.7%)
4	A	0.80	3/1906 (0.2%)	1.26	21/2556 (0.8%)
5	B	0.81	8/3214 (0.2%)	1.16	25/4308 (0.6%)
6	C	0.73	3/2973 (0.1%)	1.12	18/3990 (0.5%)
7	D	0.73	2/2426 (0.1%)	1.23	26/3252 (0.8%)
8	E	0.73	5/1941 (0.3%)	1.21	20/2601 (0.8%)
9	F	0.80	2/1905 (0.1%)	1.27	27/2539 (1.1%)
10	G	0.76	4/1966 (0.2%)	1.09	14/2645 (0.5%)
11	H	0.77	3/1537 (0.2%)	1.17	10/2066 (0.5%)
12	I	0.66	1/1753 (0.1%)	1.11	12/2343 (0.5%)
13	J	0.63	1/1382 (0.1%)	1.04	12/1849 (0.6%)
14	K	1.04	11/1154 (1.0%)	1.78	54/1555 (3.5%)
15	L	0.70	2/1734 (0.1%)	1.12	15/2318 (0.6%)
16	M	0.76	2/1152 (0.2%)	1.11	5/1539 (0.3%)
17	N	0.84	4/1746 (0.2%)	1.33	23/2338 (1.0%)
18	O	0.72	3/1684 (0.2%)	1.10	12/2251 (0.5%)
19	P	0.74	2/1268 (0.2%)	1.10	9/1701 (0.5%)
20	Q	0.69	0/1530	1.35	31/2041 (1.5%)
21	R	0.79	3/1524 (0.2%)	1.27	20/2013 (1.0%)
22	S	0.95	8/1493 (0.5%)	1.30	19/2002 (0.9%)
23	T	0.67	1/1326 (0.1%)	1.04	7/1770 (0.4%)
24	U	0.63	1/822 (0.1%)	1.03	3/1103 (0.3%)
25	V	0.89	4/993 (0.4%)	1.11	7/1332 (0.5%)
26	W	0.71	0/541	1.23	5/720 (0.7%)
27	X	0.64	0/993	1.09	10/1334 (0.7%)
28	Y	0.72	0/1132	1.24	19/1504 (1.3%)
29	Z	0.63	0/1130	1.11	10/1507 (0.7%)
30	a	0.93	6/1192 (0.5%)	1.37	17/1591 (1.1%)
31	b	0.88	2/620 (0.3%)	1.17	5/819 (0.6%)
32	c	0.70	0/742	1.14	5/996 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	d	0.84	3/903 (0.3%)	1.37	16/1216 (1.3%)
34	e	0.90	3/1071 (0.3%)	1.23	15/1429 (1.0%)
35	f	1.01	2/895 (0.2%)	1.34	17/1198 (1.4%)
36	g	0.65	0/916	1.08	5/1220 (0.4%)
37	h	0.63	0/1023	1.21	14/1350 (1.0%)
38	i	0.63	0/843	1.20	8/1115 (0.7%)
39	j	0.97	1/721 (0.1%)	1.43	11/953 (1.2%)
40	k	0.59	0/575	0.97	1/761 (0.1%)
41	l	0.70	0/454	1.14	4/599 (0.7%)
42	m	0.55	0/435	0.95	1/575 (0.2%)
43	n	0.49	0/223	1.01	0/284
44	o	0.64	0/864	1.27	8/1140 (0.7%)
45	p	0.64	1/718 (0.1%)	1.01	3/953 (0.3%)
46	q	0.81	7/1580 (0.4%)	1.35	37/2133 (1.7%)
47	r	0.68	0/1017	1.12	8/1365 (0.6%)
48	4	0.99	20/6804 (0.3%)	1.41	93/9189 (1.0%)
49	S2	0.65	37/41243 (0.1%)	1.14	330/64257 (0.5%)
50	SA	0.94	4/1679 (0.2%)	1.06	6/2283 (0.3%)
51	SB	0.89	6/1753 (0.3%)	1.15	14/2350 (0.6%)
52	SC	0.99	8/1726 (0.5%)	1.11	9/2332 (0.4%)
53	SD	1.39	12/1793 (0.7%)	1.10	9/2414 (0.4%)
54	SE	0.83	8/2118 (0.4%)	0.98	7/2849 (0.2%)
55	SF	0.74	1/1531 (0.1%)	1.08	9/2059 (0.4%)
56	SG	0.97	9/1946 (0.5%)	1.03	9/2590 (0.3%)
57	SH	0.73	2/1544 (0.1%)	1.02	8/2068 (0.4%)
58	SI	0.97	8/1715 (0.5%)	1.12	12/2287 (0.5%)
59	SJ	1.07	12/1550 (0.8%)	1.28	16/2069 (0.8%)
60	SK	0.75	1/851 (0.1%)	1.00	3/1147 (0.3%)
61	SL	0.85	5/1259 (0.4%)	1.09	7/1684 (0.4%)
62	SM	2.22	2/970 (0.2%)	1.21	8/1300 (0.6%)
63	SN	0.82	4/1232 (0.3%)	1.15	10/1656 (0.6%)
64	SO	1.18	7/1029 (0.7%)	1.38	12/1380 (0.9%)
65	SP	1.52	6/816 (0.7%)	1.29	8/1084 (0.7%)
66	SQ	0.72	2/1142 (0.2%)	1.01	8/1528 (0.5%)
67	SR	0.81	5/1060 (0.5%)	1.02	2/1421 (0.1%)
68	SS	0.66	1/1157 (0.1%)	1.18	13/1548 (0.8%)
69	ST	0.67	2/1119 (0.2%)	1.08	7/1499 (0.5%)
70	SU	0.94	4/828 (0.5%)	0.96	1/1112 (0.1%)
71	SV	0.73	0/631	0.97	0/844
72	SW	1.06	6/1051 (0.6%)	1.22	5/1406 (0.4%)
73	SX	0.99	6/1118 (0.5%)	1.12	12/1493 (0.8%)
74	SY	1.63	5/1040 (0.5%)	1.11	9/1382 (0.7%)
75	SZ	0.56	0/604	0.87	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	Sa	0.81	1/794 (0.1%)	1.25	5/1065 (0.5%)
77	Sb	0.59	0/665	0.90	0/891
78	Sc	0.68	0/508	1.13	4/680 (0.6%)
79	Sd	0.79	0/445	1.12	1/589 (0.2%)
80	Se	0.72	1/458 (0.2%)	1.16	5/602 (0.8%)
81	Sf	1.08	6/593 (1.0%)	1.57	12/786 (1.5%)
82	Sg	0.80	11/2493 (0.4%)	0.89	8/3394 (0.2%)
All	All	0.75	379/237633 (0.2%)	1.15	2051/348088 (0.6%)

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	5	0	154
2	7	0	2
3	8	0	11
4	A	0	6
5	B	0	13
6	C	0	5
7	D	0	8
8	E	0	12
9	F	0	5
10	G	0	3
11	H	0	3
12	I	0	4
13	J	0	2
14	K	0	5
15	L	0	5
16	M	0	4
17	N	0	11
18	O	0	3
19	P	0	1
20	Q	0	5
21	R	0	6
22	S	0	11
23	T	0	2
24	U	0	2
25	V	0	3
26	W	0	1
27	X	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
28	Y	0	4
30	a	0	9
31	b	0	1
32	c	0	2
33	d	0	4
34	e	0	4
35	f	0	2
36	g	0	1
37	h	0	3
38	i	0	3
39	j	0	4
40	k	0	1
44	o	0	6
45	p	0	1
46	q	0	7
47	r	0	5
48	4	0	40
49	S2	1	66
50	SA	0	2
51	SB	0	4
52	SC	0	4
53	SD	0	3
54	SE	0	2
55	SF	0	1
57	SH	0	1
58	SI	0	6
59	SJ	0	2
60	SK	0	1
61	SL	0	4
62	SM	0	3
63	SN	0	1
64	SO	0	1
65	SP	0	1
66	SQ	0	1
67	SR	0	2
70	SU	0	1
71	SV	0	2
72	SW	0	2
73	SX	0	2
74	SY	0	1
75	SZ	0	1
76	Sa	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
77	Sb	0	1
79	Sd	0	2
81	Sf	0	4
All	All	1	507

All (379) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	SM	58	GLU	CD-OE1	64.43	1.96	1.25
53	SD	216	GLU	CD-OE1	43.67	1.73	1.25
1	5	1823	G	O3'-P	41.55	2.11	1.61
74	SY	86	GLU	CD-OE2	39.60	1.69	1.25
65	SP	21	ASP	CG-OD1	30.90	1.96	1.25
74	SY	86	GLU	CG-CD	22.60	1.85	1.51
56	SG	205	GLU	CD-OE1	21.22	1.49	1.25
64	SO	130	GLU	CD-OE1	17.40	1.44	1.25
72	SW	117	ARG	NE-CZ	16.50	1.54	1.33
10	G	109	GLU	CD-OE2	16.17	1.43	1.25
11	H	66	GLU	CD-OE1	15.81	1.43	1.25
59	SJ	59	GLU	CG-CD	15.74	1.75	1.51
35	f	6	TRP	CB-CG	-15.69	1.22	1.50
48	4	267	ASP	N-CA	15.35	1.77	1.46
54	SE	251	GLU	CD-OE1	14.43	1.41	1.25
50	SA	118	GLU	CG-CD	13.75	1.72	1.51
48	4	267	ASP	CA-C	13.58	1.88	1.52
31	b	16	TRP	CB-CG	-13.52	1.25	1.50
56	SG	205	GLU	CD-OE2	13.45	1.40	1.25
59	SJ	34	GLU	CG-CD	13.17	1.71	1.51
64	SO	130	GLU	CD-OE2	12.85	1.39	1.25
65	SP	31	GLU	CD-OE2	12.79	1.39	1.25
50	SA	151	ASP	CB-CG	12.77	1.78	1.51
65	SP	31	GLU	CD-OE1	12.46	1.39	1.25
50	SA	118	GLU	CD-OE2	12.23	1.39	1.25
64	SO	104	ARG	CZ-NH1	12.19	1.48	1.33
70	SU	33	GLU	CD-OE1	12.13	1.39	1.25
21	R	95	TRP	CB-CG	-12.07	1.28	1.50
25	V	97	TYR	CB-CG	-11.86	1.33	1.51
57	SH	132	ASP	CG-OD2	11.76	1.52	1.25
48	4	269	ALA	C-N	11.65	1.60	1.34
58	SI	111	GLN	CD-NE2	11.63	1.61	1.32
58	SI	188	TYR	CE1-CZ	11.54	1.53	1.38
14	K	163	PRO	C-O	-11.44	1.00	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	SC	90	GLU	CD-OE1	11.28	1.38	1.25
73	SX	58	GLU	CD-OE1	11.16	1.38	1.25
51	SB	198	GLU	CG-CD	11.03	1.68	1.51
54	SE	250	GLU	CD-OE2	10.89	1.37	1.25
74	SY	118	ARG	CZ-NH1	10.62	1.46	1.33
49	S2	1433	C	O3'-P	10.60	1.73	1.61
82	Sg	107	ASP	CB-CG	10.42	1.73	1.51
58	SI	188	TYR	CG-CD1	10.38	1.52	1.39
82	Sg	60	ARG	CZ-NH1	10.31	1.46	1.33
34	e	35	TRP	CB-CG	-10.24	1.31	1.50
73	SX	39	ASN	CG-ND2	10.24	1.58	1.32
64	SO	130	GLU	CG-CD	10.01	1.67	1.51
74	SY	80	ASP	CB-CG	9.94	1.72	1.51
10	G	54	PHE	CB-CG	-9.92	1.34	1.51
70	SU	90	ASP	CB-CG	9.83	1.72	1.51
58	SI	188	TYR	CG-CD2	9.80	1.51	1.39
53	SD	38	GLU	CD-OE2	9.79	1.36	1.25
73	SX	88	ASP	CG-OD2	9.60	1.47	1.25
49	S2	619	A	O3'-P	-9.53	1.49	1.61
53	SD	162	ASP	CG-OD1	9.48	1.47	1.25
58	SI	99	ASN	CG-OD1	9.45	1.44	1.24
52	SC	220	ASP	CG-OD2	9.39	1.47	1.25
52	SC	90	GLU	CG-CD	9.38	1.66	1.51
61	SL	100	ASN	CB-CG	9.36	1.72	1.51
70	SU	113	GLU	CD-OE2	9.35	1.35	1.25
17	N	192	TRP	CB-CG	-9.29	1.33	1.50
65	SP	21	ASP	CB-CG	9.25	1.71	1.51
14	K	114	ARG	CD-NE	9.14	1.61	1.46
52	SC	121	ARG	CZ-NH1	9.08	1.44	1.33
67	SR	87	GLU	CD-OE1	9.02	1.35	1.25
55	SF	130	ARG	CZ-NH1	8.96	1.44	1.33
16	M	6	PHE	CB-CG	-8.92	1.36	1.51
5	B	215	GLU	CD-OE1	8.83	1.35	1.25
59	SJ	64	ASP	CG-OD2	8.81	1.45	1.25
49	S2	1291	A	O3'-P	8.81	1.71	1.61
25	V	97	TYR	CA-CB	8.62	1.73	1.53
54	SE	250	GLU	CD-OE1	8.62	1.35	1.25
48	4	267	ASP	C-N	8.62	1.50	1.34
53	SD	216	GLU	CD-OE2	8.57	1.35	1.25
56	SG	208	GLU	CG-CD	8.48	1.64	1.51
8	E	278	TYR	CA-CB	8.48	1.72	1.53
30	a	109	TYR	CA-CB	8.40	1.72	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	SI	188	TYR	CE2-CZ	8.35	1.49	1.38
1	5	4547	C	O3'-P	8.29	1.71	1.61
61	SL	31	GLU	CD-OE1	8.28	1.34	1.25
81	Sf	120	GLU	CG-CD	8.28	1.64	1.51
59	SJ	158	ASP	CG-OD2	8.26	1.44	1.25
49	S2	1292	C	O3'-P	8.23	1.71	1.61
14	K	130	LYS	CA-CB	8.23	1.72	1.53
22	S	81	TRP	CA-CB	8.09	1.71	1.53
22	S	10	TYR	CB-CG	-8.07	1.39	1.51
53	SD	38	GLU	CG-CD	8.06	1.64	1.51
1	5	45	U	O3'-P	-8.04	1.51	1.61
1	5	3652	A	O3'-P	7.92	1.70	1.61
8	E	278	TYR	CB-CG	-7.87	1.39	1.51
21	R	132	PHE	CB-CG	-7.87	1.38	1.51
53	SD	135	GLU	CD-OE1	7.87	1.34	1.25
53	SD	23	GLU	CD-OE2	7.85	1.34	1.25
66	SQ	85	ARG	CZ-NH1	7.82	1.43	1.33
30	a	84	GLU	CD-OE1	7.82	1.34	1.25
59	SJ	38	ARG	CZ-NH1	7.77	1.43	1.33
49	S2	1309	C	O3'-P	7.73	1.70	1.61
56	SG	204	GLU	CD-OE1	7.71	1.34	1.25
53	SD	216	GLU	CG-CD	7.70	1.63	1.51
30	a	109	TYR	CB-CG	-7.62	1.40	1.51
48	4	76	SER	C-N	7.55	1.51	1.34
53	SD	162	ASP	CG-OD2	7.51	1.42	1.25
59	SJ	104	ASP	CG-OD2	7.47	1.42	1.25
49	S2	1142	G	O3'-P	7.45	1.70	1.61
56	SG	35	GLU	CD-OE1	7.38	1.33	1.25
1	5	4566	U	O3'-P	-7.35	1.52	1.61
35	f	6	TRP	CA-CB	7.35	1.70	1.53
54	SE	104	ASP	CG-OD2	7.30	1.42	1.25
49	S2	1378	A	O3'-P	7.24	1.69	1.61
1	5	2510	G	O3'-P	-7.22	1.52	1.61
76	Sa	22	ARG	CZ-NH1	7.20	1.42	1.33
67	SR	87	GLU	CD-OE2	7.18	1.33	1.25
59	SJ	158	ASP	CG-OD1	7.16	1.41	1.25
1	5	2361	G	O3'-P	7.15	1.69	1.61
50	SA	33	GLN	CD-NE2	7.06	1.50	1.32
56	SG	20	ASP	CG-OD2	7.04	1.41	1.25
6	C	267	TRP	CB-CG	-7.03	1.37	1.50
53	SD	135	GLU	CG-CD	7.00	1.62	1.51
22	S	81	TRP	CB-CG	-6.99	1.37	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	SP	27	ASP	CG-OD1	6.99	1.41	1.25
1	5	1851	G	O3'-P	-6.97	1.52	1.61
14	K	137	GLN	N-CA	6.97	1.60	1.46
1	5	1849	U	O3'-P	-6.92	1.52	1.61
5	B	119	TYR	CB-CG	-6.91	1.41	1.51
13	J	14	GLU	CD-OE1	6.88	1.33	1.25
49	S2	1839	U	O3'-P	6.83	1.69	1.61
72	SW	87	GLU	CD-OE1	6.83	1.33	1.25
30	a	128	PHE	CB-CG	-6.82	1.39	1.51
23	T	13	TYR	CB-CG	-6.82	1.41	1.51
1	5	4693	C	O3'-P	6.81	1.69	1.61
49	S2	1290	G	O3'-P	6.78	1.69	1.61
1	5	1364	U	O3'-P	6.76	1.69	1.61
39	j	49	TRP	CB-CG	-6.74	1.38	1.50
73	SX	88	ASP	CG-OD1	6.73	1.40	1.25
59	SJ	103	GLU	CD-OE2	6.73	1.33	1.25
82	Sg	83	TRP	CB-CG	-6.72	1.38	1.50
1	5	2692	U	O3'-P	-6.71	1.53	1.61
48	4	154	VAL	C-N	6.70	1.49	1.34
54	SE	104	ASP	CG-OD1	6.70	1.40	1.25
49	S2	1079	C	O3'-P	-6.69	1.53	1.61
1	5	514	U	O3'-P	6.69	1.69	1.61
5	B	274	TYR	CA-CB	6.68	1.68	1.53
61	SL	13	GLN	CD-NE2	6.68	1.49	1.32
1	5	2053	C	O3'-P	-6.67	1.53	1.61
14	K	130	LYS	CA-C	-6.65	1.35	1.52
72	SW	51	GLU	CD-OE1	6.64	1.32	1.25
1	5	964	A	O3'-P	6.63	1.69	1.61
33	d	25	TYR	CB-CG	-6.63	1.41	1.51
49	S2	1835	A	O3'-P	6.63	1.69	1.61
52	SC	220	ASP	CG-OD1	6.62	1.40	1.25
70	SU	33	GLU	CG-CD	6.61	1.61	1.51
67	SR	37	GLU	CG-CD	6.61	1.61	1.51
1	5	3692	A	O3'-P	6.59	1.69	1.61
12	I	171	TRP	CB-CG	-6.58	1.38	1.50
48	4	768	GLY	C-N	6.55	1.49	1.34
22	S	33	PHE	CB-CG	-6.52	1.40	1.51
1	5	1912	G	O3'-P	-6.51	1.53	1.61
82	Sg	187	ASN	CG-OD1	6.50	1.38	1.24
1	5	1522	G	O3'-P	6.49	1.69	1.61
48	4	56	PHE	CB-CG	6.49	1.62	1.51
1	5	4375	C	O3'-P	-6.48	1.53	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	ST	32	GLU	CD-OE2	6.48	1.32	1.25
6	C	111	TRP	CB-CG	-6.47	1.38	1.50
2	7	90	A	O3'-P	-6.47	1.53	1.61
1	5	2442	G	O3'-P	-6.45	1.53	1.61
18	O	194	GLU	CD-OE1	6.44	1.32	1.25
49	S2	646	G	O3'-P	6.43	1.68	1.61
73	SX	39	ASN	CG-OD1	6.43	1.38	1.24
49	S2	1833	C	O3'-P	-6.41	1.53	1.61
81	Sf	146	LEU	CA-CB	6.41	1.68	1.53
15	L	17	ASP	CG-OD2	6.40	1.40	1.25
61	SL	89	ARG	CZ-NH1	6.40	1.41	1.33
49	S2	1858	G	O3'-P	6.38	1.68	1.61
69	ST	32	GLU	CD-OE1	6.37	1.32	1.25
10	G	54	PHE	CA-CB	6.36	1.68	1.53
48	4	669	VAL	CA-CB	6.35	1.68	1.54
1	5	207	G	O3'-P	-6.30	1.53	1.61
8	E	101	ARG	CZ-NH2	6.29	1.41	1.33
7	D	213	GLU	CG-CD	6.26	1.61	1.51
1	5	1669	A	O3'-P	-6.26	1.53	1.61
63	SN	13	GLN	CD-NE2	6.25	1.48	1.32
22	S	10	TYR	CA-CB	6.22	1.67	1.53
18	O	106	ASP	CG-OD2	6.21	1.39	1.25
57	SH	177	TYR	CB-CG	-6.21	1.42	1.51
82	Sg	36	ARG	CZ-NH1	6.19	1.41	1.33
11	H	61	TRP	CB-CG	-6.17	1.39	1.50
1	5	1756	U	C4-O4	-6.17	1.18	1.23
48	4	825	PHE	CB-CG	-6.16	1.40	1.51
1	5	171	U	O3'-P	-6.16	1.53	1.61
49	S2	9	U	O3'-P	6.14	1.68	1.61
48	4	109	VAL	CA-CB	-6.13	1.41	1.54
9	F	120	PHE	CB-CG	-6.12	1.41	1.51
82	Sg	4	GLN	CD-OE1	6.12	1.37	1.24
46	q	205	ASP	C-N	6.09	1.48	1.34
59	SJ	48	PHE	CB-CG	-6.08	1.41	1.51
58	SI	99	ASN	CG-ND2	6.08	1.48	1.32
72	SW	115	GLU	CD-OE2	6.07	1.32	1.25
49	S2	1139	C	O3'-P	-6.06	1.53	1.61
48	4	111	PHE	CA-CB	6.05	1.67	1.53
1	5	1591	U	O3'-P	-6.05	1.53	1.61
7	D	44	TYR	CA-CB	6.05	1.67	1.53
1	5	1636	U	O3'-P	-6.04	1.53	1.61
1	5	2589	C	O3'-P	6.02	1.68	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	3901	A	O3'-P	-6.02	1.53	1.61
64	SO	104	ARG	NE-CZ	6.01	1.40	1.33
1	5	4464	A	O3'-P	5.99	1.68	1.61
49	S2	922	A	O3'-P	-5.97	1.53	1.61
49	S2	1055	A	O3'-P	-5.95	1.54	1.61
60	SK	34	GLU	CD-OE1	5.95	1.32	1.25
24	U	99	TRP	CB-CG	-5.94	1.39	1.50
54	SE	251	GLU	CD-OE2	5.94	1.32	1.25
63	SN	128	TYR	CG-CD2	-5.94	1.31	1.39
22	S	152	PHE	CB-CG	-5.93	1.41	1.51
49	S2	1838	U	O3'-P	5.92	1.68	1.61
81	Sf	150	PHE	CB-CG	5.92	1.61	1.51
51	SB	157	GLN	CG-CD	5.92	1.64	1.51
1	5	2520	C	O3'-P	-5.91	1.54	1.61
19	P	139	TYR	CB-CG	-5.88	1.42	1.51
54	SE	121	TYR	CB-CG	-5.88	1.42	1.51
33	d	73	TRP	CB-CG	-5.88	1.39	1.50
52	SC	236	PHE	CA-CB	5.87	1.66	1.53
31	b	16	TRP	CA-CB	5.86	1.66	1.53
14	K	137	GLN	CA-C	5.86	1.68	1.52
5	B	119	TYR	CA-CB	5.86	1.66	1.53
1	5	1395	U	O3'-P	-5.84	1.54	1.61
81	Sf	120	GLU	CD-OE1	-5.84	1.19	1.25
64	SO	147	ARG	CG-CD	5.84	1.66	1.51
51	SB	89	GLU	CD-OE2	5.83	1.32	1.25
82	Sg	145	GLU	CG-CD	5.83	1.60	1.51
53	SD	103	GLU	CD-OE1	5.82	1.32	1.25
19	P	139	TYR	CA-CB	5.82	1.66	1.53
14	K	114	ARG	C-N	-5.81	1.20	1.34
1	5	2811	G	O3'-P	5.81	1.68	1.61
59	SJ	48	PHE	CA-CB	5.81	1.66	1.53
5	B	274	TYR	CB-CG	-5.80	1.43	1.51
49	S2	1190	A	O3'-P	-5.80	1.54	1.61
52	SC	236	PHE	CB-CG	-5.79	1.41	1.51
49	S2	1798	C	O3'-P	-5.78	1.54	1.61
53	SD	38	GLU	CD-OE1	5.78	1.32	1.25
1	5	1357	C	O3'-P	5.77	1.68	1.61
49	S2	397	G	O3'-P	-5.76	1.54	1.61
67	SR	82	ASP	CG-OD1	5.75	1.38	1.25
48	4	794	PHE	CD1-CE1	-5.72	1.27	1.39
64	SO	25	GLU	CG-CD	5.72	1.60	1.51
45	p	18	TYR	CB-CG	-5.70	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	S2	798	A	O3'-P	5.70	1.68	1.61
25	V	97	TYR	CD2-CE2	-5.70	1.30	1.39
48	4	478	PHE	CD1-CE1	-5.70	1.27	1.39
14	K	114	ARG	CA-C	-5.68	1.38	1.52
15	L	173	GLU	CD-OE2	5.68	1.31	1.25
66	SQ	29	ASN	CG-ND2	5.67	1.47	1.32
1	5	2394	G	O3'-P	-5.66	1.54	1.61
1	5	90	G	O3'-P	-5.66	1.54	1.61
1	5	2325	C	O3'-P	5.66	1.68	1.61
56	SG	142	ARG	CZ-NH1	5.66	1.40	1.33
1	5	2055	G	O3'-P	5.66	1.68	1.61
1	5	32	G	O3'-P	-5.65	1.54	1.61
1	5	3635	A	O3'-P	5.64	1.68	1.61
33	d	25	TYR	CA-CB	5.63	1.66	1.53
63	SN	83	ASP	CB-CG	5.63	1.63	1.51
1	5	147	A	O3'-P	-5.63	1.54	1.61
5	B	235	TRP	CG-CD1	-5.63	1.28	1.36
51	SB	198	GLU	CD-OE2	5.63	1.31	1.25
1	5	2649	G	O3'-P	-5.63	1.54	1.61
49	S2	92	A	O3'-P	5.61	1.67	1.61
49	S2	1851	A	O3'-P	-5.61	1.54	1.61
46	q	62	ARG	N-CA	-5.61	1.35	1.46
1	5	1627	G	O3'-P	5.59	1.67	1.61
1	5	2051	C	O3'-P	5.58	1.67	1.61
17	N	119	TYR	CB-CG	-5.57	1.43	1.51
1	5	2535	G	O3'-P	-5.57	1.54	1.61
1	5	1282	G	O3'-P	-5.56	1.54	1.61
1	5	4239	A	O3'-P	5.56	1.67	1.61
72	SW	80	ASP	CB-CG	5.56	1.63	1.51
72	SW	115	GLU	CD-OE1	5.54	1.31	1.25
49	S2	657	U	O3'-P	-5.53	1.54	1.61
73	SX	58	GLU	CD-OE2	5.53	1.31	1.25
1	5	5001	U	O3'-P	-5.52	1.54	1.61
48	4	196	GLU	CG-CD	5.52	1.60	1.51
52	SC	241	PHE	CB-CG	-5.52	1.42	1.51
49	S2	640	A	O3'-P	-5.50	1.54	1.61
1	5	53	C	O3'-P	5.50	1.67	1.61
1	5	332	C	O3'-P	-5.50	1.54	1.61
30	a	79	TRP	CB-CG	-5.50	1.40	1.50
1	5	3875	G	O3'-P	5.49	1.67	1.61
1	5	4276	G	O3'-P	5.49	1.67	1.61
56	SG	204	GLU	CG-CD	5.49	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	109	GLU	CG-CD	5.48	1.60	1.51
49	S2	848	U	N3-C4	5.47	1.43	1.38
22	S	29	ARG	CG-CD	5.46	1.65	1.51
65	SP	27	ASP	CG-OD2	5.45	1.37	1.25
16	M	6	PHE	CA-CB	5.44	1.66	1.53
1	5	4326	G	O3'-P	-5.43	1.54	1.61
49	S2	1843	G	O3'-P	-5.42	1.54	1.61
63	SN	83	ASP	CG-OD1	5.41	1.37	1.25
1	5	1381	U	O3'-P	-5.40	1.54	1.61
48	4	801	ARG	NE-CZ	5.39	1.40	1.33
51	SB	224	GLU	CD-OE2	5.38	1.31	1.25
61	SL	3	ASP	CB-CG	5.38	1.63	1.51
3	8	64	U	O3'-P	5.38	1.67	1.61
81	Sf	151	ASN	CA-C	5.38	1.67	1.52
51	SB	205	TYR	CE2-CZ	5.38	1.45	1.38
56	SG	17	GLU	CD-OE2	5.37	1.31	1.25
46	q	25	PRO	N-CD	5.37	1.55	1.47
46	q	201	PRO	N-CD	5.36	1.55	1.47
1	5	372	A	O3'-P	-5.35	1.54	1.61
49	S2	357	C	O3'-P	5.35	1.67	1.61
80	Se	23	GLU	CG-CD	5.35	1.59	1.51
18	O	106	ASP	CG-OD1	5.33	1.37	1.25
1	5	89	C	O3'-P	-5.32	1.54	1.61
34	e	74	PHE	CB-CG	-5.32	1.42	1.51
48	4	266	PHE	C-N	5.32	1.46	1.34
67	SR	104	GLU	CD-OE2	5.30	1.31	1.25
1	5	937	U	O3'-P	-5.29	1.54	1.61
1	5	2297	G	O3'-P	-5.29	1.54	1.61
1	5	4548	A	O5'-C5'	5.28	1.52	1.44
8	E	250	ASP	CG-OD2	5.28	1.37	1.25
48	4	4	PHE	CD2-CE2	-5.28	1.28	1.39
1	5	4237	C	O3'-P	-5.27	1.54	1.61
59	SJ	104	ASP	CG-OD1	5.27	1.37	1.25
82	Sg	3	GLU	CD-OE2	5.27	1.31	1.25
1	5	943	A	O3'-P	-5.27	1.54	1.61
4	A	211	PHE	CA-CB	5.26	1.65	1.53
1	5	2043	A	O3'-P	-5.26	1.54	1.61
58	SI	27	TYR	CB-CG	-5.24	1.43	1.51
4	A	40	TYR	CA-CB	5.24	1.65	1.53
14	K	34	PRO	N-CD	5.24	1.55	1.47
1	5	2368	A	O3'-P	-5.22	1.54	1.61
1	5	1917	A	O3'-P	-5.21	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	97	ASN	CG-ND2	5.21	1.45	1.32
49	S2	1293	A	O3'-P	5.20	1.67	1.61
46	q	124	PRO	N-CD	5.20	1.55	1.47
1	5	4977	A	O3'-P	-5.20	1.54	1.61
5	B	137	TRP	CB-CG	-5.20	1.40	1.50
82	Sg	285	GLN	CD-NE2	5.19	1.45	1.32
21	R	132	PHE	CA-CB	5.19	1.65	1.53
25	V	98	PHE	CB-CG	-5.19	1.42	1.51
17	N	120	TRP	CE3-CZ3	-5.18	1.29	1.38
17	N	130	PHE	CB-CG	-5.17	1.42	1.51
46	q	68	HIS	C-N	5.17	1.46	1.34
48	4	478	PHE	CD2-CE2	-5.17	1.28	1.39
14	K	148	PRO	N-CD	5.16	1.55	1.47
4	A	209	HIS	CA-CB	5.16	1.65	1.53
74	SY	80	ASP	CG-OD2	5.15	1.37	1.25
82	Sg	116	ASP	CG-OD1	5.15	1.37	1.25
1	5	4275	G	O3'-P	5.15	1.67	1.61
11	H	66	GLU	CD-OE2	5.14	1.31	1.25
1	5	381	U	O3'-P	-5.14	1.54	1.61
68	SS	130	ARG	CZ-NH1	5.14	1.39	1.33
49	S2	999	G	O3'-P	5.13	1.67	1.61
1	5	4489	G	O3'-P	5.12	1.67	1.61
54	SE	251	GLU	CG-CD	5.12	1.59	1.51
1	5	1457	G	O3'-P	-5.11	1.55	1.61
82	Sg	60	ARG	NE-CZ	5.11	1.39	1.33
3	8	80	A	O3'-P	5.11	1.67	1.61
5	B	257	TRP	CE3-CZ3	-5.11	1.29	1.38
46	q	118	PRO	N-CD	5.10	1.54	1.47
34	e	35	TRP	CG-CD1	-5.09	1.29	1.36
1	5	1283	G	O3'-P	-5.09	1.55	1.61
9	F	228	HIS	CA-CB	5.09	1.65	1.53
48	4	794	PHE	CD2-CE2	-5.09	1.29	1.39
1	5	2406	G	O3'-P	5.09	1.67	1.61
49	S2	1039	C	O3'-P	5.08	1.67	1.61
1	5	97	G	O3'-P	5.08	1.67	1.61
62	SM	58	GLU	CD-OE2	5.08	1.31	1.25
1	5	1682	A	C6-N6	-5.07	1.29	1.33
1	5	2054	U	O3'-P	-5.07	1.55	1.61
49	S2	1552	G	O3'-P	5.07	1.67	1.61
14	K	30	PRO	CA-C	-5.06	1.42	1.52
49	S2	672	A	O3'-P	-5.05	1.55	1.61
1	5	4206	C	O3'-P	-5.05	1.55	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	102	PHE	CG-CD2	-5.05	1.31	1.38
22	S	152	PHE	CG-CD2	-5.04	1.31	1.38
49	S2	1168	G	O3'-P	-5.04	1.55	1.61
49	S2	957	A	O3'-P	-5.03	1.55	1.61
1	5	2324	C	O3'-P	5.03	1.67	1.61
30	a	79	TRP	CA-CB	5.03	1.65	1.53
59	SJ	108	ARG	CZ-NH1	5.03	1.39	1.33
81	Sf	149	CYS	N-CA	5.03	1.56	1.46
3	8	73	U	O3'-P	5.00	1.67	1.61

All (2051) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	4	699	GLY	CA-C-N	-32.10	46.58	117.20
48	4	699	GLY	C-N-CA	-28.33	50.88	121.70
48	4	768	GLY	O-C-N	21.39	156.93	122.70
72	SW	117	ARG	NE-CZ-NH2	-20.64	109.98	120.30
46	q	205	ASP	CA-C-N	-20.22	72.71	117.20
65	SP	21	ASP	CB-CG-OD1	-19.19	101.03	118.30
46	q	205	ASP	O-C-N	18.05	151.59	122.70
14	K	114	ARG	NE-CZ-NH1	17.38	128.99	120.30
81	Sf	146	LEU	CA-CB-CG	16.59	153.47	115.30
48	4	768	GLY	CA-C-N	-16.39	81.15	117.20
3	8	60	G	N9-C1'-C2'	16.18	135.04	114.00
48	4	154	VAL	CB-CA-C	16.12	142.02	111.40
14	K	114	ARG	CD-NE-CZ	16.11	146.16	123.60
64	SO	146	ARG	NE-CZ-NH1	15.24	127.92	120.30
76	Sa	28	ARG	NE-CZ-NH1	14.82	127.71	120.30
49	S2	1109	C	O4'-C1'-N1	14.31	119.65	108.20
48	4	266	PHE	O-C-N	-13.93	100.41	122.70
48	4	121	VAL	O-C-N	-13.86	100.52	122.70
49	S2	1823	A	N9-C1'-C2'	13.82	131.97	114.00
39	j	11	ARG	NE-CZ-NH2	-13.79	113.40	120.30
48	4	269	ALA	O-C-N	-13.70	100.78	122.70
64	SO	104	ARG	NE-CZ-NH2	-13.40	113.60	120.30
49	S2	1434	C	O5'-P-OP1	-12.95	94.05	105.70
14	K	111	ASN	N-CA-CB	12.81	133.66	110.60
20	Q	37	ARG	NE-CZ-NH2	12.80	126.70	120.30
14	K	130	LYS	CB-CA-C	-12.73	84.94	110.40
1	5	92	C	N1-C1'-C2'	-12.63	97.59	114.00
49	S2	1433	C	O5'-P-OP2	-12.40	94.54	105.70
49	S2	1838	U	O4'-C1'-N1	-12.39	98.28	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	S2	1109	C	N1-C1'-C2'	12.34	130.04	114.00
64	SO	146	ARG	NE-CZ-NH2	-12.34	114.13	120.30
12	I	139	ARG	CG-CD-NE	12.32	137.68	111.80
49	S2	1838	U	N1-C1'-C2'	12.03	129.64	114.00
1	5	1214	C	N1-C1'-C2'	11.94	129.52	114.00
48	4	278	THR	O-C-N	-11.86	103.72	122.70
4	A	3	ARG	NE-CZ-NH1	11.84	126.22	120.30
1	5	1	C	N1-C1'-C2'	11.83	129.38	114.00
14	K	24	ALA	O-C-N	-11.77	103.88	122.70
48	4	768	GLY	C-N-CA	-11.51	92.93	121.70
65	SP	21	ASP	CB-CG-OD2	11.41	128.57	118.30
33	d	44	ARG	NE-CZ-NH1	11.38	125.99	120.30
58	SI	49	ARG	NE-CZ-NH1	11.28	125.94	120.30
74	SY	80	ASP	CB-CG-OD2	-11.22	108.20	118.30
37	h	93	ARG	NE-CZ-NH1	11.18	125.89	120.30
1	5	4693	C	O4'-C1'-N1	-11.13	99.29	108.20
21	R	132	PHE	CB-CA-C	11.13	132.67	110.40
48	4	4	PHE	N-CA-C	11.12	141.03	111.00
7	D	265	ARG	NE-CZ-NH1	11.12	125.86	120.30
1	5	4373	G	N9-C1'-C2'	11.11	128.44	114.00
1	5	4275	G	N9-C1'-C2'	-11.10	99.57	114.00
61	SL	89	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	5	2361	G	N9-C1'-C2'	-10.98	99.73	114.00
30	a	61	TYR	CA-CB-CG	10.96	134.22	113.40
48	4	742	GLU	C-N-CD	-10.89	96.65	120.60
49	S2	1293	A	N9-C1'-C2'	10.87	128.13	114.00
21	R	108	ARG	NE-CZ-NH1	10.87	125.73	120.30
1	5	4871	C	N1-C1'-C2'	10.85	128.11	114.00
1	5	1938	C	N1-C1'-C2'	10.83	128.08	114.00
46	q	14	PHE	CB-CG-CD2	-10.81	113.23	120.80
16	M	6	PHE	CB-CG-CD2	-10.77	113.26	120.80
1	5	151	G	N9-C1'-C2'	-10.77	100.00	114.00
17	N	192	TRP	CA-CB-CG	10.62	133.87	113.70
28	Y	87	ARG	NE-CZ-NH2	10.61	125.61	120.30
30	a	132	ARG	NE-CZ-NH1	10.59	125.59	120.30
48	4	539	GLU	C-N-CA	-10.57	95.26	121.70
49	S2	848	U	N1-C1'-C2'	10.56	127.72	114.00
76	Sa	28	ARG	NE-CZ-NH2	-10.55	115.03	120.30
17	N	131	GLU	CA-CB-CG	10.55	136.60	113.40
48	4	111	PHE	CA-CB-CG	10.54	139.21	113.90
53	SD	216	GLU	CG-CD-OE1	-10.54	97.22	118.30
49	S2	642	U	C4'-C3'-O3'	10.53	134.07	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	4528	G	C2'-C3'-O3'	10.52	132.65	109.50
55	SF	130	ARG	NE-CZ-NH2	-10.51	115.04	120.30
1	5	2513	A	N9-C1'-C2'	10.51	127.66	114.00
49	S2	1378	A	N9-C1'-C2'	10.50	127.64	114.00
1	5	4163	U	C4'-C3'-O3'	10.48	133.95	113.00
48	4	154	VAL	CA-CB-CG1	10.46	126.58	110.90
49	S2	642	U	N1-C1'-C2'	-10.44	100.42	114.00
38	i	85	ARG	NE-CZ-NH1	10.39	125.49	120.30
49	S2	1114	U	N1-C1'-C2'	10.38	127.49	114.00
74	SY	118	ARG	NE-CZ-NH2	-10.36	115.12	120.30
3	8	34	U	C4'-C3'-O3'	-10.35	87.66	109.40
48	4	123	ASP	O-C-N	-10.34	105.62	123.20
1	5	1211	G	C2'-C3'-O3'	10.33	132.23	109.50
49	S2	1835	A	O4'-C1'-N9	-10.32	99.94	108.20
59	SJ	38	ARG	NE-CZ-NH2	-10.27	115.17	120.30
49	S2	24	C	C2'-C3'-O3'	10.27	132.09	109.50
62	SM	58	GLU	OE1-CD-OE2	10.24	135.59	123.30
30	a	109	TYR	CA-CB-CG	-10.22	93.98	113.40
1	5	62	A	N9-C1'-C2'	10.22	127.28	114.00
1	5	1329	G	C2'-C3'-O3'	10.21	131.97	109.50
44	o	78	ARG	NE-CZ-NH2	10.19	125.40	120.30
66	SQ	85	ARG	NE-CZ-NH2	-10.19	115.20	120.30
1	5	2436	U	N1-C1'-C2'	10.12	127.16	114.00
74	SY	86	GLU	CG-CD-OE2	-10.11	98.07	118.30
14	K	34	PRO	CA-N-CD	-10.10	97.36	111.50
1	5	2586	G	N9-C1'-C2'	10.09	127.12	114.00
1	5	664	G	O4'-C1'-N9	10.09	116.27	108.20
14	K	38	SER	C-N-CD	-10.08	98.42	120.60
1	5	1358	G	C4'-C3'-O3'	10.06	133.12	113.00
49	S2	645	C	N1-C1'-C2'	-10.05	100.93	114.00
11	H	54	ARG	NE-CZ-NH1	10.04	125.32	120.30
49	S2	92	A	N9-C1'-C2'	10.03	127.04	114.00
1	5	1890	G	N9-C1'-C2'	-10.02	100.97	114.00
1	5	4518	A	O5'-P-OP2	-10.02	96.68	105.70
1	5	2389	A	C2'-C3'-O3'	10.02	131.54	109.50
1	5	1887	G	N9-C1'-C2'	-10.00	101.00	112.00
33	d	25	TYR	CA-CB-CG	-9.99	94.41	113.40
50	SA	117	ARG	CG-CD-NE	9.98	132.76	111.80
10	G	54	PHE	CB-CG-CD1	-9.96	113.83	120.80
48	4	807	GLN	N-CA-C	-9.95	84.12	111.00
8	E	278	TYR	CA-CB-CG	-9.95	94.50	113.40
1	5	1974	U	N1-C1'-C2'	9.93	126.91	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1379	C	O4'-C1'-N1	9.92	116.14	108.20
76	Sa	22	ARG	NE-CZ-NH2	-9.84	115.38	120.30
49	S2	428	U	N1-C1'-C2'	9.83	126.78	114.00
1	5	2666	U	N1-C1'-C2'	-9.82	101.19	112.00
21	R	132	PHE	CB-CG-CD1	-9.80	113.94	120.80
14	K	30	PRO	CA-N-CD	-9.78	97.81	111.50
1	5	4693	C	N1-C1'-C2'	9.76	126.69	114.00
30	a	128	PHE	CB-CG-CD1	-9.73	113.99	120.80
1	5	2046	G	O4'-C1'-N9	9.72	115.98	108.20
26	W	44	ARG	NE-CZ-NH1	9.71	125.16	120.30
1	5	1398	A	N9-C1'-C2'	9.70	126.61	114.00
8	E	278	TYR	CB-CA-C	9.70	129.80	110.40
3	8	14	U	N1-C1'-C2'	9.68	126.58	114.00
49	S2	367	U	N1-C1'-C2'	-9.68	101.36	112.00
49	S2	291	G	C4'-C3'-O3'	-9.67	89.09	109.40
30	a	61	TYR	CB-CG-CD2	-9.67	115.20	121.00
49	S2	1063	C	N1-C1'-C2'	-9.66	101.38	112.00
1	5	4464	A	O4'-C1'-N9	-9.65	100.48	108.20
1	5	2394	G	N9-C1'-C2'	-9.64	101.40	112.00
52	SC	121	ARG	NE-CZ-NH2	-9.63	115.48	120.30
35	f	36	ARG	NE-CZ-NH1	9.63	125.12	120.30
64	SO	104	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	5	4750	G	N9-C1'-C2'	-9.62	101.42	112.00
68	SS	124	ARG	NE-CZ-NH1	9.60	125.10	120.30
49	S2	28	U	O5'-P-OP1	-9.60	97.06	105.70
59	SJ	131	ARG	NE-CZ-NH2	-9.59	115.50	120.30
1	5	4677	U	N1-C1'-C2'	-9.57	101.47	112.00
46	q	68	HIS	CA-C-O	-9.57	100.00	120.10
1	5	4162	C	N1-C1'-C2'	9.56	126.44	114.00
1	5	514	U	N1-C1'-C2'	-9.56	101.48	112.00
49	S2	1835	A	C2'-C3'-O3'	9.55	130.52	109.50
80	Se	13	ARG	NE-CZ-NH1	9.52	125.06	120.30
15	L	34	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	5	5040	U	N1-C1'-C2'	9.51	126.36	114.00
29	Z	36	ARG	NE-CZ-NH1	9.51	125.05	120.30
57	SH	177	TYR	CB-CG-CD2	-9.50	115.30	121.00
11	H	31	ARG	NE-CZ-NH1	9.50	125.05	120.30
49	S2	747	U	C2'-C3'-O3'	9.49	130.39	109.50
1	5	1501	C	O4'-C1'-N1	9.49	115.79	108.20
1	5	172	C	O4'-C1'-N1	9.49	115.79	108.20
39	j	66	HIS	N-CA-CB	9.46	127.62	110.60
1	5	2438	A	N9-C1'-C2'	-9.45	101.60	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	q	85	ASN	N-CA-CB	9.45	127.61	110.60
1	5	1501	C	N1-C1'-C2'	9.45	126.28	114.00
21	R	95	TRP	N-CA-CB	9.43	127.57	110.60
1	5	315	G	O4'-C1'-N9	9.42	115.74	108.20
7	D	54	ARG	CG-CD-NE	-9.41	92.04	111.80
1	5	42	A	O4'-C1'-N9	9.40	115.72	108.20
55	SF	130	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	5	294	G	O4'-C1'-N9	9.40	115.72	108.20
49	S2	447	A	O4'-C1'-N9	9.38	115.71	108.20
13	J	32	ARG	NE-CZ-NH2	-9.36	115.62	120.30
53	SD	67	ARG	NE-CZ-NH1	9.36	124.98	120.30
60	SK	2	LEU	CA-CB-CG	9.34	136.79	115.30
64	SO	147	ARG	CA-CB-CG	9.34	133.96	113.40
12	I	171	TRP	CA-CB-CG	-9.34	95.96	113.70
52	SC	200	ARG	NE-CZ-NH2	9.33	124.97	120.30
49	S2	1433	C	C4'-C3'-O3'	9.33	131.65	113.00
62	SM	33	ARG	NE-CZ-NH1	9.31	124.95	120.30
18	O	178	ARG	NE-CZ-NH1	9.29	124.94	120.30
17	N	49	ARG	NE-CZ-NH1	9.27	124.94	120.30
48	4	825	PHE	C-N-CA	-9.27	98.53	121.70
48	4	267	ASP	N-CA-C	9.26	136.01	111.00
1	5	5059	C	C2'-C3'-O3'	9.25	129.84	109.50
1	5	4280	A	N9-C1'-C2'	-9.25	101.83	112.00
14	K	75	PRO	CA-N-CD	-9.24	98.56	111.50
78	Sc	31	ARG	NE-CZ-NH1	9.23	124.92	120.30
46	q	68	HIS	O-C-N	9.22	137.45	122.70
48	4	206	ASP	C-N-CD	-9.22	100.32	120.60
28	Y	27	ARG	NE-CZ-NH2	9.22	124.91	120.30
1	5	1534	A	N9-C1'-C2'	9.18	125.93	114.00
46	q	204	LEU	O-C-N	9.18	137.39	122.70
20	Q	91	ARG	NE-CZ-NH2	9.17	124.89	120.30
49	S2	631	U	N1-C1'-C2'	9.17	125.92	114.00
1	5	280	G	O4'-C1'-N9	9.14	115.51	108.20
46	q	80	PRO	CA-N-CD	-9.14	98.70	111.50
1	5	4228	G	N9-C1'-C2'	-9.12	101.97	112.00
1	5	2406	G	N9-C1'-C2'	-9.11	101.97	112.00
49	S2	1552	G	C2'-C3'-O3'	9.11	129.53	109.50
1	5	1685	G	N9-C1'-C2'	9.10	125.83	114.00
69	ST	53	PHE	CB-CG-CD2	-9.09	114.44	120.80
1	5	2553	A	N9-C1'-C2'	9.09	125.81	114.00
5	B	100	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	5	1474	C	C2'-C3'-O3'	9.07	129.45	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	S2	1578	U	N1-C1'-C2'	9.07	125.79	114.00
46	q	14	PHE	CB-CG-CD1	9.06	127.14	120.80
5	B	119	TYR	CB-CG-CD1	-9.04	115.58	121.00
1	5	2658	G	N9-C1'-C2'	-9.03	102.07	112.00
33	d	85	ARG	NE-CZ-NH1	9.03	124.81	120.30
30	a	79	TRP	CA-CB-CG	-9.02	96.57	113.70
14	K	88	PRO	CA-N-CD	-9.00	98.90	111.50
28	Y	126	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	5	1882	U	O5'-P-OP1	-8.99	97.61	105.70
46	q	69	LEU	O-C-N	-8.97	108.35	122.70
69	ST	62	ARG	NE-CZ-NH2	8.97	124.78	120.30
25	V	97	TYR	CB-CG-CD2	-8.97	115.62	121.00
6	C	78	ARG	NE-CZ-NH1	8.96	124.78	120.30
34	e	46	ARG	NE-CZ-NH1	8.96	124.78	120.30
6	C	267	TRP	CA-CB-CG	8.96	130.72	113.70
38	i	4	ARG	NE-CZ-NH1	8.95	124.78	120.30
81	Sf	146	LEU	CB-CG-CD1	8.95	126.21	111.00
48	4	197	SER	C-N-CA	8.92	141.02	122.30
3	8	94	G	O4'-C1'-N9	-8.91	101.07	108.20
1	5	4911	A	O4'-C1'-N9	8.91	115.32	108.20
1	5	4385	A	N9-C1'-C2'	-8.90	102.21	112.00
1	5	4965	U	N1-C1'-C2'	-8.90	102.21	112.00
45	p	85	ARG	NE-CZ-NH1	8.89	124.75	120.30
49	S2	833	C	C2'-C3'-O3'	8.89	129.07	109.50
14	K	136	ALA	O-C-N	-8.88	108.50	122.70
1	5	125	C	C2'-C3'-O3'	8.87	129.02	109.50
33	d	25	TYR	CB-CA-C	8.86	128.13	110.40
49	S2	437	G	N9-C1'-C2'	8.85	125.50	114.00
1	5	1815	G	N9-C1'-C2'	8.82	125.46	114.00
49	S2	1088	U	N1-C1'-C2'	8.81	125.45	114.00
1	5	977	C	C2'-C3'-O3'	8.80	128.86	109.50
1	5	1998	A	N9-C1'-C2'	8.80	125.44	114.00
82	Sg	60	ARG	NE-CZ-NH2	-8.79	115.90	120.30
8	E	119	ARG	NE-CZ-NH1	8.79	124.69	120.30
65	SP	10	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	5	2268	A	N9-C1'-C2'	8.77	125.41	114.00
1	5	1356	U	C2'-C3'-O3'	8.77	128.78	109.50
49	S2	313	A	O4'-C1'-N9	8.77	115.21	108.20
1	5	1668	A	N9-C1'-C2'	8.76	125.39	114.00
18	O	135	PHE	N-CA-C	8.76	134.65	111.00
23	T	13	TYR	CB-CG-CD2	-8.75	115.75	121.00
72	SW	57	ARG	NE-CZ-NH1	8.75	124.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1534	A	O4'-C1'-N9	-8.74	101.20	108.20
1	5	978	G	C2'-C3'-O3'	8.73	128.71	109.50
14	K	163	PRO	CA-N-CD	-8.73	99.28	111.50
1	5	1359	G	C2'-C3'-O3'	8.73	128.71	109.50
1	5	31	U	N1-C1'-C2'	8.72	125.34	114.00
1	5	4976	U	O4'-C1'-N1	-8.72	101.22	108.20
22	S	81	TRP	CB-CA-C	8.72	127.84	110.40
49	S2	1859	A	C8-N9-C1'	-8.72	112.00	127.70
6	C	311	ARG	NE-CZ-NH2	-8.71	115.94	120.30
49	S2	3	C	N1-C1'-C2'	8.70	125.31	114.00
49	S2	1429	G	C2'-C3'-O3'	8.70	128.63	109.50
20	Q	58	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	5	4234	A	N9-C1'-C2'	8.68	125.28	114.00
19	P	54	GLN	CA-CB-CG	8.68	132.49	113.40
14	K	104	ILE	CG1-CB-CG2	8.67	130.47	111.40
29	Z	121	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	5	2305	U	O4'-C1'-N1	-8.65	101.28	108.20
1	5	2517	A	N9-C1'-C2'	8.65	125.25	114.00
1	5	2446	C	N1-C1'-C2'	8.65	125.24	114.00
22	S	81	TRP	CA-CB-CG	-8.65	97.27	113.70
10	G	62	ARG	NE-CZ-NH2	-8.64	115.98	120.30
82	Sg	60	ARG	NE-CZ-NH1	8.64	124.62	120.30
37	h	117	ARG	CG-CD-NE	-8.62	93.70	111.80
4	A	193	ARG	CG-CD-NE	-8.62	93.71	111.80
1	5	4221	C	N1-C1'-C2'	-8.60	102.54	112.00
1	5	4404	U	N1-C1'-C2'	-8.60	102.54	112.00
1	5	1637	A	N9-C1'-C2'	-8.59	102.55	112.00
44	o	31	ASP	CB-CA-C	8.59	127.57	110.40
81	Sf	138	ARG	NE-CZ-NH1	8.58	124.59	120.30
18	O	140	ARG	NE-CZ-NH2	8.58	124.59	120.30
2	7	56	G	N9-C1'-C2'	8.57	125.14	114.00
49	S2	110	U	C2'-C3'-O3'	8.56	128.34	109.50
1	5	1980	U	O4'-C1'-N1	8.56	115.05	108.20
48	4	794	PHE	CB-CA-C	8.56	127.52	110.40
51	SB	165	ARG	NE-CZ-NH2	8.56	124.58	120.30
1	5	2851	G	N9-C1'-C2'	-8.55	102.60	112.00
68	SS	95	TYR	CA-CB-CG	8.54	129.62	113.40
14	K	111	ASN	CB-CA-C	-8.54	93.33	110.40
1	5	352	G	N9-C1'-C2'	-8.52	102.62	112.00
49	S2	1859	A	C4-N9-C1'	8.52	141.63	126.30
1	5	1733	G	N9-C1'-C2'	-8.49	102.66	112.00
1	5	1439	C	C4'-C3'-O3'	-8.49	91.58	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	3790	U	N1-C1'-C2'	8.49	125.03	114.00
1	5	1296	G	O4'-C1'-N9	8.48	114.98	108.20
15	L	74	ARG	NE-CZ-NH1	8.47	124.54	120.30
48	4	392	GLY	C-N-CD	-8.46	101.98	120.60
27	X	73	HIS	CB-CA-C	8.46	127.32	110.40
1	5	4563	U	N1-C1'-C2'	8.45	124.99	114.00
34	e	35	TRP	CA-CB-CG	-8.44	97.66	113.70
49	S2	798	A	C2'-C3'-O3'	8.44	128.07	109.50
4	A	67	TYR	CA-CB-CG	8.43	129.42	113.40
58	SI	197	PHE	CB-CA-C	-8.42	93.55	110.40
73	SX	67	ARG	NE-CZ-NH2	8.41	124.50	120.30
49	S2	622	C	N1-C1'-C2'	-8.41	102.75	112.00
1	5	1937	C	N1-C1'-C2'	8.40	124.92	114.00
9	F	120	PHE	CB-CA-C	8.40	127.21	110.40
3	8	85	U	C2'-C3'-O3'	8.40	127.98	109.50
1	5	4119	C	C2'-C3'-O3'	8.39	127.97	109.50
14	K	89	PRO	CA-N-CD	-8.39	99.75	111.50
22	S	29	ARG	CA-CB-CG	8.39	131.85	113.40
59	SJ	127	ARG	NE-CZ-NH1	8.39	124.49	120.30
49	S2	421	G	N9-C1'-C2'	8.37	124.88	114.00
37	h	78	TYR	CA-CB-CG	-8.37	97.50	113.40
21	R	74	ARG	NE-CZ-NH1	-8.36	116.12	120.30
57	SH	177	TYR	CB-CA-C	-8.36	93.69	110.40
44	o	48	TYR	CB-CA-C	8.35	127.10	110.40
14	K	102	GLY	N-CA-C	8.33	133.93	113.10
57	SH	177	TYR	CA-CB-CG	8.32	129.22	113.40
8	E	268	ARG	NE-CZ-NH1	8.32	124.46	120.30
49	S2	294	U	N1-C1'-C2'	8.30	124.79	114.00
49	S2	1835	A	C4-N9-C1'	-8.29	111.38	126.30
80	Se	41	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	5	292	G	N9-C1'-C2'	8.28	124.76	114.00
49	S2	1407	U	N1-C1'-C2'	8.28	124.76	114.00
68	SS	86	ARG	NE-CZ-NH1	-8.28	116.16	120.30
1	5	958	G	C2'-C3'-O3'	8.26	127.67	109.50
37	h	78	TYR	CB-CA-C	8.26	126.92	110.40
3	8	70	G	N9-C1'-C2'	-8.25	102.92	112.00
10	G	53	ARG	NE-CZ-NH2	-8.23	116.18	120.30
22	S	29	ARG	CG-CD-NE	-8.23	94.52	111.80
22	S	10	TYR	CA-CB-CG	-8.22	97.78	113.40
1	5	2087	C	N1-C1'-C2'	-8.21	102.97	112.00
1	5	3938	G	N9-C1'-C2'	8.21	124.67	114.00
1	5	3879	G	N9-C1'-C2'	-8.20	102.98	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	R	132	PHE	N-CA-C	-8.20	88.86	111.00
1	5	3653	A	N9-C1'-C2'	-8.19	102.99	112.00
50	SA	151	ASP	CB-CG-OD2	8.19	125.67	118.30
1	5	93	G	N9-C1'-C2'	8.18	124.64	114.00
49	S2	594	A	N9-C1'-C2'	-8.18	103.00	112.00
1	5	2553	A	O4'-C1'-N9	8.18	114.74	108.20
49	S2	1623	A	C2'-C3'-O3'	8.17	127.48	109.50
35	f	85	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	5	4498	U	N1-C1'-C2'	-8.16	103.02	112.00
1	5	2797	C	N1-C1'-C2'	-8.15	103.03	112.00
49	S2	1408	U	N1-C1'-C2'	8.15	124.60	114.00
31	b	44	ARG	NE-CZ-NH1	8.15	124.37	120.30
7	D	268	ARG	NE-CZ-NH1	8.14	124.37	120.30
18	O	37	ARG	NE-CZ-NH2	-8.13	116.23	120.30
49	S2	381	C	N1-C1'-C2'	8.13	124.57	114.00
35	f	4	ARG	CA-CB-CG	8.12	131.28	113.40
1	5	2465	C	N1-C1'-C2'	8.12	124.56	114.00
1	5	2246	C	C2'-C3'-O3'	8.11	127.34	109.50
1	5	4723	A	C4-N9-C1'	8.11	140.89	126.30
1	5	2806	A	N9-C1'-C2'	-8.10	103.08	112.00
3	8	34	U	C2'-C3'-O3'	8.10	127.33	109.50
44	o	57	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	5	3635	A	N9-C1'-C2'	-8.10	103.09	112.00
1	5	1867	A	N9-C1'-C2'	8.09	124.52	114.00
9	F	58	HIS	CB-CA-C	-8.09	94.23	110.40
1	5	3735	G	C2'-C3'-O3'	8.07	127.26	109.50
66	SQ	126	ARG	NE-CZ-NH2	8.07	124.34	120.30
14	K	24	ALA	CA-C-N	8.06	134.94	117.20
1	5	3773	U	C4'-C3'-O3'	8.06	129.12	113.00
25	V	98	PHE	CB-CG-CD1	-8.05	115.16	120.80
1	5	235	A	O4'-C1'-N9	8.05	114.64	108.20
3	8	94	G	C2'-C3'-O3'	8.04	127.19	109.50
7	D	44	TYR	CB-CA-C	8.04	126.49	110.40
1	5	2683	C	C2'-C3'-O3'	8.04	127.19	109.50
1	5	3908	A	N9-C1'-C2'	8.03	124.44	114.00
35	f	22	ARG	NE-CZ-NH1	8.03	124.31	120.30
7	D	248	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	5	3905	A	C2'-C3'-O3'	8.02	127.15	109.50
17	N	139	HIS	N-CA-CB	8.01	125.02	110.60
1	5	4600	G	N9-C1'-C2'	-8.01	103.19	112.00
3	8	34	U	C5'-C4'-O4'	8.01	118.71	109.10
64	SO	147	ARG	CG-CD-NE	-8.00	95.00	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	62	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	5	4497	U	N1-C1'-C2'	-8.00	103.20	112.00
55	SF	136	ARG	NE-CZ-NH1	7.99	124.29	120.30
17	N	143	ARG	CG-CD-NE	-7.98	95.04	111.80
48	4	285	LEU	C-N-CD	-7.98	103.05	120.60
48	4	278	THR	CA-C-N	7.97	134.73	117.20
1	5	4885	U	C2'-C3'-O3'	7.97	127.03	109.50
5	B	169	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	5	2394	G	O4'-C1'-N9	7.95	114.56	108.20
1	5	3692	A	C2'-C3'-O3'	7.95	126.99	109.50
48	4	267	ASP	CA-C-N	7.95	139.34	117.10
20	Q	174	PHE	CB-CA-C	7.93	126.27	110.40
18	O	110	PRO	C-N-CD	-7.93	103.15	120.60
49	S2	964	A	N9-C1'-C2'	7.93	124.31	114.00
1	5	4163	U	N1-C1'-C2'	-7.93	103.28	112.00
12	I	119	PHE	CB-CG-CD1	7.92	126.35	120.80
19	P	3	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	5	315	G	C1'-O4'-C4'	-7.92	103.57	109.90
49	S2	1292	C	C4'-C3'-O3'	7.92	128.83	113.00
49	S2	399	C	N1-C1'-C2'	-7.91	103.30	112.00
1	5	4723	A	C8-N9-C1'	-7.90	113.48	127.70
4	A	193	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	5	4371	G	O4'-C1'-N9	7.90	114.52	108.20
49	S2	968	U	N1-C1'-C2'	-7.89	103.31	112.00
51	SB	146	ARG	NE-CZ-NH2	-7.88	116.36	120.30
68	SS	42	HIS	CB-CA-C	-7.88	94.65	110.40
1	5	2263	A	O4'-C1'-N9	-7.87	101.91	108.20
14	K	39	PRO	CA-N-CD	-7.86	100.49	111.50
67	SR	82	ASP	CB-CG-OD2	-7.86	111.22	118.30
1	5	668	C	C2'-C3'-O3'	7.86	126.78	109.50
1	5	2263	A	C5'-C4'-O4'	7.86	118.53	109.10
78	Sc	44	ARG	NE-CZ-NH2	7.85	124.22	120.30
49	S2	1703	C	N1-C1'-C2'	-7.84	103.37	112.00
49	S2	1835	A	C5'-C4'-O4'	7.84	118.51	109.10
66	SQ	126	ARG	NE-CZ-NH1	-7.84	116.38	120.30
4	A	37	ARG	NE-CZ-NH2	-7.84	116.38	120.30
48	4	76	SER	O-C-N	7.84	135.24	122.70
1	5	716	C	C2'-C3'-O3'	7.83	126.72	109.50
1	5	353	A	N9-C1'-C2'	-7.82	103.39	112.00
16	M	119	ARG	NE-CZ-NH2	7.82	124.21	120.30
1	5	1805	A	N9-C1'-C2'	7.82	124.17	114.00
1	5	962	C	N1-C1'-C2'	7.81	124.15	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	Y	11	ARG	NE-CZ-NH2	-7.80	116.40	120.30
3	8	64	U	N1-C1'-C2'	7.80	124.14	114.00
49	S2	164	A	N9-C1'-C2'	-7.80	103.42	112.00
1	5	964	A	C4'-C3'-O3'	7.78	128.56	113.00
23	T	13	TYR	N-CA-CB	-7.78	96.60	110.60
73	SX	67	ARG	NE-CZ-NH1	-7.76	116.42	120.30
1	5	4463	U	N1-C1'-C2'	-7.75	103.47	112.00
1	5	43	U	N1-C1'-C2'	-7.75	103.47	112.00
1	5	157	U	O4'-C1'-N1	7.74	114.40	108.20
7	D	198	HIS	CB-CA-C	7.74	125.89	110.40
1	5	4282	A	N9-C1'-C2'	7.73	124.05	114.00
48	4	495	ARG	O-C-N	-7.72	110.35	122.70
1	5	5066	U	N1-C1'-C2'	7.72	124.03	114.00
9	F	168	ARG	CG-CD-NE	-7.71	95.61	111.80
52	SC	241	PHE	N-CA-CB	7.70	124.46	110.60
1	5	4194	U	N1-C1'-C2'	-7.69	103.54	112.00
30	a	128	PHE	CB-CA-C	7.67	125.75	110.40
1	5	4238	G	N9-C1'-C2'	-7.67	103.57	112.00
1	5	294	G	C1'-O4'-C4'	-7.66	103.77	109.90
59	SJ	48	PHE	N-CA-CB	7.66	124.38	110.60
1	5	292	G	O4'-C1'-N9	-7.65	102.08	108.20
1	5	1522	G	N9-C1'-C2'	-7.65	103.59	112.00
35	f	4	ARG	CG-CD-NE	-7.64	95.75	111.80
49	S2	1701	C	N1-C1'-C2'	7.64	123.94	114.00
4	A	211	PHE	CB-CA-C	7.63	125.66	110.40
14	K	30	PRO	CB-CA-C	7.63	131.08	112.00
5	B	116	ARG	CG-CD-NE	7.63	127.82	111.80
63	SN	83	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	5	53	C	C2'-C3'-O3'	7.62	126.25	109.50
1	5	2790	U	N1-C1'-C2'	7.62	123.90	114.00
49	S2	1395	C	C2'-C3'-O3'	7.62	126.26	109.50
3	8	94	G	C5'-C4'-O4'	7.61	118.23	109.10
7	D	210	TYR	CA-CB-CG	-7.60	98.96	113.40
72	SW	117	ARG	NH1-CZ-NH2	7.60	127.76	119.40
9	F	36	ARG	NE-CZ-NH2	7.60	124.10	120.30
49	S2	349	A	C2'-C3'-O3'	7.59	126.21	109.50
1	5	1916	G	N9-C1'-C2'	7.59	123.87	114.00
73	SX	8	ARG	NE-CZ-NH1	-7.59	116.50	120.30
37	h	119	PHE	CB-CA-C	-7.59	95.22	110.40
52	SC	236	PHE	N-CA-CB	7.58	124.25	110.60
63	SN	113	PHE	CB-CA-C	-7.58	95.23	110.40
1	5	4464	A	C5'-C4'-O4'	7.58	118.19	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1575	A	N9-C1'-C2'	7.57	123.84	114.00
48	4	104	ASP	CB-CA-C	7.57	125.54	110.40
70	SU	90	ASP	CB-CG-OD1	7.56	125.11	118.30
12	I	4	ARG	CG-CD-NE	-7.56	95.93	111.80
1	5	4583	C	N1-C1'-C2'	-7.55	103.69	112.00
1	5	1377	G	C2'-C3'-O3'	7.55	126.11	109.50
1	5	4548	A	O4'-C1'-N9	-7.55	102.16	108.20
1	5	4911	A	C1'-O4'-C4'	-7.55	103.86	109.90
49	S2	1114	U	O4'-C1'-N1	7.54	114.24	108.20
1	5	158	A	N9-C1'-C2'	-7.54	103.70	112.00
49	S2	1664	A	C2'-C3'-O3'	7.54	126.09	109.50
3	8	38	U	O4'-C1'-N1	7.53	114.22	108.20
14	K	104	ILE	CA-CB-CG2	-7.53	95.84	110.90
1	5	2588	C	C4'-C3'-O3'	7.52	128.04	113.00
1	5	5046	U	C2'-C3'-O3'	7.52	126.05	109.50
7	D	35	ARG	NE-CZ-NH1	7.52	124.06	120.30
46	q	44	ARG	NE-CZ-NH1	7.52	124.06	120.30
3	8	104	A	O4'-C1'-N9	-7.52	102.19	108.20
1	5	354	U	N1-C1'-C2'	-7.51	103.73	112.00
14	K	130	LYS	CA-CB-CG	7.51	129.93	113.40
9	F	228	HIS	N-CA-CB	7.51	124.12	110.60
30	a	79	TRP	CB-CA-C	7.51	125.42	110.40
49	S2	1835	A	C4'-C3'-O3'	-7.51	93.63	109.40
1	5	4737	G	N9-C1'-C2'	7.51	123.76	114.00
49	S2	1863	A	N9-C1'-C2'	7.51	123.76	114.00
1	5	1881	C	N1-C1'-C2'	7.50	123.75	114.00
12	I	171	TRP	N-CA-CB	7.50	124.09	110.60
82	Sg	125	ARG	NE-CZ-NH2	-7.49	116.55	120.30
1	5	1724	G	O4'-C4'-C3'	-7.49	96.51	104.00
38	i	28	ARG	CG-CD-NE	-7.49	96.08	111.80
46	q	80	PRO	C-N-CA	-7.49	102.99	121.70
6	C	222	ARG	NE-CZ-NH1	7.48	124.04	120.30
49	S2	1142	G	N9-C1'-C2'	-7.48	103.77	112.00
49	S2	732	U	C2'-C3'-O3'	7.48	125.95	109.50
1	5	1382	G	N9-C1'-C2'	7.47	123.72	114.00
49	S2	9	U	N1-C1'-C2'	-7.47	103.78	112.00
1	5	3868	G	N9-C1'-C2'	-7.47	103.78	112.00
8	E	179	ARG	NE-CZ-NH1	7.47	124.03	120.30
14	K	137	GLN	N-CA-C	7.47	131.16	111.00
1	5	4693	C	C5'-C4'-O4'	7.46	118.05	109.10
58	SI	113	TYR	CA-CB-CG	7.46	127.57	113.40
17	N	131	GLU	CB-CG-CD	-7.46	94.06	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	157	U	N1-C1'-C2'	-7.46	103.80	112.00
1	5	1378	C	N1-C1'-C2'	7.45	123.69	114.00
49	S2	1542	C	N1-C1'-C2'	7.45	123.69	114.00
1	5	4535	A	C2'-C3'-O3'	7.44	125.87	109.50
48	4	123	ASP	CA-C-N	7.44	131.09	116.20
73	SX	88	ASP	CB-CG-OD2	-7.44	111.60	118.30
49	S2	1113	A	N9-C1'-C2'	7.44	123.67	114.00
1	5	4212	A	N9-C1'-C2'	7.44	123.67	114.00
1	5	2092	G	N9-C1'-C2'	7.44	123.67	114.00
20	Q	34	PHE	N-CA-CB	7.43	123.97	110.60
49	S2	384	U	N1-C1'-C2'	-7.43	103.83	112.00
5	B	117	ARG	NE-CZ-NH2	-7.43	116.59	120.30
49	S2	1	U	C5'-C4'-O4'	7.43	118.01	109.10
1	5	1266	G	C2'-C3'-O3'	7.42	125.83	109.50
1	5	1445	U	C2'-C3'-O3'	7.42	125.82	109.50
1	5	4120	U	N1-C1'-C2'	-7.42	103.84	112.00
49	S2	427	U	N1-C1'-C2'	7.41	123.64	114.00
1	5	2046	G	C1'-O4'-C4'	-7.41	103.97	109.90
1	5	1521	C	N1-C1'-C2'	-7.41	103.85	112.00
1	5	4322	G	N9-C1'-C2'	-7.41	103.86	112.00
81	Sf	143	LYS	CD-CE-NZ	7.41	128.73	111.70
81	Sf	116	ARG	NE-CZ-NH1	7.40	124.00	120.30
17	N	180	PHE	CB-CA-C	7.39	125.19	110.40
49	S2	1606	G	N9-C1'-C2'	-7.39	103.86	112.00
7	D	223	PHE	CB-CG-CD2	-7.39	115.62	120.80
30	a	34	ASN	CB-CA-C	7.39	125.19	110.40
1	5	4464	A	N9-C1'-C2'	7.39	123.60	114.00
1	5	394	G	N9-C1'-C2'	-7.38	103.88	112.00
1	5	3938	G	O4'-C1'-N9	-7.38	102.30	108.20
4	A	242	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	5	4981	G	N9-C1'-C2'	-7.38	103.89	112.00
1	5	2124	G	C2'-C3'-O3'	7.37	125.72	109.50
1	5	3871	A	N9-C1'-C2'	7.37	123.58	114.00
1	5	55	G	N9-C1'-C2'	-7.37	103.89	112.00
1	5	450	G	N9-C1'-C2'	-7.37	103.89	112.00
3	8	73	U	N1-C1'-C2'	-7.37	103.89	112.00
7	D	210	TYR	N-CA-CB	7.37	123.86	110.60
1	5	4251	A	N9-C1'-C2'	7.36	123.57	114.00
68	SS	86	ARG	CG-CD-NE	-7.36	96.33	111.80
1	5	5061	A	C2'-C3'-O3'	7.36	125.69	109.50
1	5	1370	G	N9-C1'-C2'	7.36	123.57	114.00
1	5	3843	C	N1-C1'-C2'	7.36	123.57	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	S2	1249	C	N1-C1'-C2'	-7.36	103.91	112.00
51	SB	136	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	5	1440	U	C2'-C3'-O3'	7.36	125.69	109.50
59	SJ	69	ARG	NE-CZ-NH2	7.36	123.98	120.30
4	A	189	TYR	CA-CB-CG	7.35	127.36	113.40
1	5	974	C	C2'-C3'-O3'	7.34	125.66	109.50
1	5	4531	U	N1-C1'-C2'	7.34	123.54	114.00
49	S2	1623	A	N9-C1'-C2'	-7.34	103.93	112.00
49	S2	1659	U	N1-C1'-C2'	-7.34	103.93	112.00
1	5	979	C	C2'-C3'-O3'	7.33	125.63	109.50
1	5	2769	U	N1-C1'-C2'	-7.33	103.94	112.00
49	S2	1115	U	N1-C1'-C2'	7.33	123.52	114.00
49	S2	1486	A	N9-C1'-C2'	-7.32	103.95	112.00
57	SH	99	ARG	NE-CZ-NH2	7.30	123.95	120.30
53	SD	159	HIS	CB-CA-C	7.30	124.99	110.40
1	5	147	A	N9-C1'-C2'	7.29	123.48	114.00
1	5	406	C	C2'-C3'-O3'	7.29	125.55	109.50
1	5	1601	A	N9-C1'-C2'	-7.29	103.98	112.00
1	5	2848	G	N9-C1'-C2'	-7.29	103.98	112.00
1	5	1379	C	C1'-O4'-C4'	-7.29	104.07	109.90
1	5	97	G	N9-C1'-C2'	-7.29	103.98	112.00
1	5	486	C	C2'-C3'-O3'	7.29	125.54	109.50
14	K	74	VAL	C-N-CD	-7.29	104.57	120.60
13	J	64	ARG	NE-CZ-NH2	7.29	123.94	120.30
14	K	130	LYS	CB-CG-CD	7.28	130.53	111.60
1	5	4084	G	C2'-C3'-O3'	7.28	125.50	109.50
1	5	4519	C	N1-C1'-C2'	-7.27	104.00	112.00
1	5	2280	G	N9-C1'-C2'	7.27	123.45	114.00
10	G	235	ARG	NE-CZ-NH1	7.26	123.93	120.30
51	SB	82	ARG	CG-CD-NE	-7.26	96.55	111.80
1	5	2796	G	N9-C1'-C2'	7.25	123.43	114.00
1	5	4750	G	O4'-C1'-N9	7.25	114.00	108.20
1	5	1481	C	C2'-C3'-O3'	7.25	125.45	109.50
27	X	48	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	5	4966	A	N9-C1'-C2'	7.24	123.41	114.00
1	5	2812	A	N9-C1'-C2'	7.23	123.40	114.00
1	5	664	G	C1'-O4'-C4'	-7.22	104.13	109.90
49	S2	1419	C	N1-C1'-C2'	-7.21	104.07	112.00
46	q	84	GLY	N-CA-C	7.20	131.10	113.10
39	j	11	ARG	NE-CZ-NH1	7.20	123.90	120.30
49	S2	24	C	N1-C1'-C2'	-7.20	104.08	112.00
1	5	100	C	N1-C1'-C2'	-7.20	104.08	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	4	269	ALA	C-N-CA	-7.20	103.71	121.70
49	S2	1339	U	N1-C1'-C2'	-7.19	104.09	112.00
59	SJ	115	PHE	CB-CG-CD2	-7.19	115.77	120.80
37	h	89	ARG	NE-CZ-NH1	7.19	123.89	120.30
39	j	71	TYR	CA-CB-CG	7.18	127.05	113.40
30	a	109	TYR	CB-CA-C	7.18	124.76	110.40
1	5	1534	A	C5'-C4'-O4'	7.18	117.71	109.10
1	5	2511	A	C4'-C3'-O3'	-7.17	94.34	109.40
53	SD	216	GLU	CG-CD-OE2	7.17	132.63	118.30
4	A	3	ARG	NE-CZ-NH2	-7.16	116.72	120.30
33	d	73	TRP	N-CA-CB	-7.16	97.71	110.60
14	K	28	LEU	CB-CG-CD1	7.16	123.17	111.00
49	S2	1404	U	C4'-C3'-O3'	-7.16	94.36	109.40
1	5	1359	G	C4'-C3'-O3'	-7.16	94.36	109.40
1	5	4279	A	N9-C1'-C2'	-7.16	104.13	112.00
49	S2	798	A	N9-C1'-C2'	-7.16	104.13	112.00
49	S2	402	C	N1-C1'-C2'	-7.16	104.13	112.00
6	C	41	HIS	N-CA-CB	7.14	123.46	110.60
38	i	39	PHE	N-CA-CB	7.14	123.44	110.60
59	SJ	115	PHE	CB-CG-CD1	7.13	125.79	120.80
1	5	157	U	C1'-O4'-C4'	-7.13	104.20	109.90
1	5	350	C	N1-C1'-C2'	7.13	123.26	114.00
14	K	114	ARG	CG-CD-NE	7.12	126.76	111.80
73	SX	20	HIS	CB-CA-C	7.12	124.65	110.40
1	5	383	A	C1'-C2'-O2'	-7.12	89.23	110.60
22	S	28	TYR	CB-CG-CD1	7.12	125.27	121.00
15	L	82	ARG	NE-CZ-NH2	-7.11	116.74	120.30
30	a	62	HIS	N-CA-CB	7.11	123.40	110.60
55	SF	122	ARG	NE-CZ-NH1	7.11	123.86	120.30
54	SE	104	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	5	29	G	N9-C1'-C2'	7.11	123.24	114.00
49	S2	1645	C	N1-C1'-C2'	7.11	123.24	114.00
1	5	1500	A	C4'-C3'-O3'	7.10	127.20	113.00
37	h	51	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	5	2324	C	C2'-C3'-O3'	7.10	125.12	109.50
3	8	38	U	C1'-O4'-C4'	-7.10	104.22	109.90
1	5	669	C	O4'-C1'-N1	7.09	113.87	108.20
1	5	4500	U	O5'-P-OP1	-7.09	99.32	105.70
39	j	27	TYR	CA-CB-CG	-7.09	99.92	113.40
3	8	94	G	N9-C1'-C2'	7.09	123.21	114.00
9	F	194	HIS	CB-CA-C	-7.09	96.23	110.40
1	5	4750	G	C1'-O4'-C4'	-7.08	104.23	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	X	48	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	5	4341	C	N1-C1'-C2'	-7.08	104.22	112.00
1	5	4464	A	C2'-C3'-O3'	7.07	125.06	109.50
1	5	30	C	N1-C1'-C2'	7.07	123.19	114.00
1	5	4519	C	O4'-C1'-N1	7.06	113.85	108.20
1	5	1355	G	N9-C1'-C2'	7.06	123.18	114.00
26	W	8	PHE	CB-CG-CD1	7.05	125.74	120.80
48	4	495	ARG	C-N-CA	-7.05	104.08	121.70
1	5	291	U	N1-C1'-C2'	7.05	123.16	114.00
11	H	156	ASN	N-CA-CB	7.04	123.27	110.60
48	4	113	SER	N-CA-C	-7.04	91.99	111.00
49	S2	384	U	C2'-C3'-O3'	7.04	124.98	109.50
1	5	2046	G	C2'-C3'-O3'	7.03	124.97	109.50
49	S2	863	U	N1-C1'-C2'	7.03	123.14	114.00
1	5	1479	G	N9-C1'-C2'	7.03	123.14	114.00
1	5	1552	G	N9-C1'-C2'	-7.03	104.27	112.00
8	E	219	ARG	NE-CZ-NH1	7.03	123.81	120.30
18	O	49	ARG	NE-CZ-NH1	7.03	123.81	120.30
33	d	25	TYR	CB-CG-CD1	-7.03	116.78	121.00
49	S2	821	G	O4'-C1'-N9	-7.03	102.58	108.20
51	SB	205	TYR	CA-CB-CG	-7.03	100.05	113.40
1	5	1455	G	C2'-C3'-O3'	7.02	124.95	109.50
1	5	514	U	C2'-C3'-O3'	7.02	124.94	109.50
53	SD	67	ARG	NE-CZ-NH2	-7.02	116.79	120.30
49	S2	1378	A	O4'-C1'-N9	-7.01	102.59	108.20
66	SQ	85	ARG	CG-CD-NE	-7.01	97.07	111.80
3	8	34	U	O4'-C1'-N1	-7.01	102.59	108.20
1	5	2695	A	C2'-C3'-O3'	7.00	124.91	109.50
1	5	3817	A	N9-C1'-C2'	7.00	123.10	114.00
49	S2	1157	G	N9-C1'-C2'	-7.00	104.30	112.00
1	5	235	A	N9-C1'-C2'	-7.00	104.30	112.00
1	5	4531	U	O4'-C1'-N1	-7.00	102.60	108.20
1	5	4510	A	O4'-C1'-N9	-7.00	102.60	108.20
48	4	741	MET	CA-CB-CG	7.00	125.19	113.30
49	S2	427	U	O4'-C1'-N1	-7.00	102.60	108.20
1	5	42	A	C1'-O4'-C4'	-6.99	104.31	109.90
48	4	801	ARG	N-CA-CB	6.99	123.19	110.60
1	5	4589	A	O4'-C1'-N9	-6.99	102.61	108.20
6	C	35	ASP	CB-CG-OD1	6.99	124.59	118.30
1	5	1676	C	C1'-C2'-O2'	-6.99	89.64	110.60
9	F	197	TYR	CB-CA-C	-6.99	96.42	110.40
49	S2	1839	U	C2-N1-C1'	6.98	126.08	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	o	48	TYR	CA-CB-CG	-6.98	100.14	113.40
48	4	701	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	5	2851	G	C2'-C3'-O3'	6.97	124.85	113.70
1	5	4265	U	N1-C1'-C2'	6.97	123.06	114.00
48	4	54	THR	N-CA-C	6.97	129.81	111.00
1	5	332	C	N1-C1'-C2'	6.97	123.06	114.00
1	5	4270	C	N1-C1'-C2'	-6.96	104.34	112.00
80	Se	13	ARG	NE-CZ-NH2	-6.96	116.82	120.30
49	S2	448	A	N9-C1'-C2'	-6.96	104.34	112.00
1	5	1625	G	N9-C1'-C2'	6.96	123.05	114.00
1	5	2589	C	C2'-C3'-O3'	6.96	124.83	113.70
49	S2	104	A	C2'-C3'-O3'	6.96	124.83	113.70
34	e	74	PHE	CB-CG-CD1	-6.95	115.93	120.80
59	SJ	138	ARG	NE-CZ-NH1	6.95	123.78	120.30
49	S2	1022	U	O4'-C1'-N1	6.95	113.76	108.20
37	h	93	ARG	NE-CZ-NH2	-6.95	116.83	120.30
49	S2	617	G	N9-C1'-C2'	-6.95	104.36	112.00
1	5	209	U	O4'-C1'-N1	6.95	113.76	108.20
13	J	32	ARG	NE-CZ-NH1	6.95	123.77	120.30
13	J	146	ARG	CG-CD-NE	-6.95	97.21	111.80
25	V	97	TYR	N-CA-C	-6.94	92.25	111.00
48	4	121	VAL	C-N-CA	6.94	139.06	121.70
1	5	4589	A	N9-C1'-C2'	6.94	123.02	114.00
21	R	74	ARG	NE-CZ-NH2	6.93	123.77	120.30
49	S2	1143	A	O5'-P-OP1	-6.92	99.47	105.70
5	B	100	ARG	NE-CZ-NH1	6.90	123.75	120.30
9	F	219	ARG	NE-CZ-NH1	6.90	123.75	120.30
21	R	88	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	5	54	G	N9-C1'-C2'	-6.89	104.42	112.00
10	G	49	ARG	NE-CZ-NH2	-6.89	116.85	120.30
49	S2	104	A	N9-C1'-C2'	-6.88	104.43	112.00
11	H	156	ASN	N-CA-C	-6.88	92.42	111.00
35	f	4	ARG	N-CA-CB	6.88	122.99	110.60
49	S2	923	G	C2'-C3'-O3'	6.88	124.71	113.70
1	5	454	U	C2'-C3'-O3'	6.87	124.70	113.70
49	S2	55	U	N1-C1'-C2'	6.87	122.94	114.00
1	5	1832	C	C2'-C3'-O3'	6.87	124.69	113.70
48	4	427	VAL	CB-CA-C	-6.87	98.34	111.40
20	Q	75	ARG	NE-CZ-NH1	6.87	123.73	120.30
49	S2	77	A	N9-C1'-C2'	-6.87	104.44	112.00
1	5	226	G	N9-C1'-C2'	-6.86	104.45	112.00
49	S2	674	C	O5'-P-OP2	-6.86	99.52	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	943	A	N9-C1'-C2'	-6.86	104.45	112.00
1	5	1631	A	O4'-C1'-N9	-6.86	102.71	108.20
8	E	179	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	5	5001	U	N1-C1'-C2'	6.86	122.91	114.00
5	B	274	TYR	CA-CB-CG	-6.85	100.39	113.40
1	5	1319	U	N1-C1'-C2'	-6.84	104.47	112.00
58	SI	197	PHE	CB-CG-CD2	-6.84	116.01	120.80
35	f	85	ARG	NE-CZ-NH1	6.83	123.72	120.30
49	S2	182	C	C2'-C3'-O3'	6.83	124.63	113.70
1	5	1815	G	O4'-C1'-N9	6.83	113.66	108.20
49	S2	73	C	O4'-C1'-N1	6.83	113.66	108.20
1	5	2271	C	N1-C1'-C2'	6.83	122.87	114.00
49	S2	1039	C	C2'-C3'-O3'	6.83	124.62	113.70
49	S2	1247	C	N1-C1'-C2'	6.83	122.87	114.00
1	5	3625	G	C2'-C3'-O3'	6.82	124.61	113.70
48	4	285	LEU	O-C-N	-6.82	108.14	121.10
20	Q	37	ARG	NE-CZ-NH1	-6.82	116.89	120.30
3	8	64	U	C2'-C3'-O3'	6.82	124.61	113.70
1	5	964	A	O4'-C1'-C2'	-6.81	98.99	105.80
1	5	5047	C	O5'-P-OP2	-6.81	99.57	105.70
46	q	6	ARG	N-CA-C	6.81	129.38	111.00
49	S2	992	A	N9-C1'-C2'	-6.80	104.52	112.00
63	SN	18	TYR	N-CA-CB	6.80	122.85	110.60
17	N	49	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	5	4518	A	O5'-P-OP1	6.80	118.86	110.70
1	5	1	C	O4'-C1'-N1	6.79	113.64	108.20
1	5	2319	C	N1-C1'-C2'	6.79	122.83	114.00
62	SM	127	TYR	CA-CB-CG	6.79	126.30	113.40
19	P	42	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	5	3611	A	N9-C1'-C2'	6.78	122.81	114.00
2	7	72	U	C2'-C3'-O3'	6.78	124.55	113.70
29	Z	65	ARG	CG-CD-NE	-6.78	97.57	111.80
10	G	73	ARG	NE-CZ-NH1	6.78	123.69	120.30
25	V	97	TYR	CA-CB-CG	-6.78	100.53	113.40
1	5	1292	C	C2'-C3'-O3'	6.77	124.53	113.70
13	J	99	PHE	CB-CA-C	6.77	123.94	110.40
48	4	825	PHE	N-CA-C	6.76	129.24	111.00
48	4	42	LYS	CA-C-N	-6.75	102.35	117.20
49	S2	61	A	C4'-C3'-O3'	-6.75	95.22	109.40
49	S2	1198	G	C2'-C3'-O3'	6.75	124.50	113.70
20	Q	33	ARG	CG-CD-NE	-6.74	97.64	111.80
49	S2	1114	U	C1'-O4'-C4'	-6.74	104.51	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	2395	A	N9-C1'-C2'	-6.74	104.59	112.00
49	S2	1838	U	O4'-C4'-C3'	-6.74	97.26	104.00
20	Q	15	ARG	NE-CZ-NH2	-6.74	116.93	120.30
10	G	54	PHE	CB-CG-CD2	-6.73	116.09	120.80
49	S2	596	U	N1-C1'-C2'	6.73	122.75	114.00
48	4	76	SER	CA-C-N	-6.72	102.41	117.20
8	E	101	ARG	NE-CZ-NH1	-6.72	116.94	120.30
1	5	1364	U	C2'-C3'-O3'	6.72	124.45	113.70
1	5	3875	G	N9-C1'-C2'	-6.72	104.61	112.00
1	5	4936	G	N9-C1'-C2'	-6.72	104.61	112.00
8	E	278	TYR	N-CA-C	-6.72	92.87	111.00
1	5	4230	C	O5'-P-OP1	-6.71	99.66	105.70
1	5	4197	G	N9-C1'-C2'	-6.71	104.62	112.00
49	S2	313	A	C1'-O4'-C4'	-6.71	104.53	109.90
49	S2	1433	C	C5'-C4'-C3'	6.71	126.73	116.00
1	5	84	A	O4'-C1'-N9	-6.71	102.83	108.20
1	5	58	G	N9-C1'-C2'	6.70	122.71	114.00
48	4	197	SER	CA-C-N	-6.70	102.80	116.20
14	K	111	ASN	CA-CB-CG	6.70	128.14	113.40
52	SC	200	ARG	NE-CZ-NH1	-6.70	116.95	120.30
49	S2	983	A	C8-N9-C1'	-6.70	115.64	127.70
1	5	2305	U	N1-C1'-C2'	6.70	122.70	114.00
14	K	26	SER	C-N-CA	6.70	138.44	121.70
59	SJ	108	ARG	NE-CZ-NH2	-6.69	116.96	120.30
49	S2	983	A	C4-N9-C1'	6.69	138.33	126.30
49	S2	824	C	N1-C1'-C2'	6.68	122.69	114.00
62	SM	33	ARG	CG-CD-NE	6.68	125.83	111.80
1	5	2675	G	N9-C1'-C2'	-6.68	104.66	112.00
29	Z	38	TYR	CB-CA-C	6.67	123.75	110.40
9	F	168	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	5	4280	A	C2'-C3'-O3'	6.67	124.37	113.70
49	S2	1201	U	N1-C1'-C2'	-6.67	104.67	112.00
33	d	87	ARG	N-CA-C	-6.67	93.00	111.00
46	q	204	LEU	CA-C-N	-6.67	102.54	117.20
48	4	122	THR	N-CA-CB	-6.66	97.64	110.30
49	S2	1838	U	C5'-C4'-O4'	6.66	117.10	109.10
1	5	3901	A	O4'-C1'-N9	-6.66	102.87	108.20
48	4	801	ARG	NE-CZ-NH2	-6.66	116.97	120.30
49	S2	918	U	N1-C1'-C2'	6.66	122.65	114.00
1	5	3882	C	N1-C1'-C2'	6.65	122.65	114.00
49	S2	415	A	C4-N9-C1'	-6.65	114.33	126.30
31	b	7	HIS	CB-CA-C	-6.65	97.10	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	d	73	TRP	CA-CB-CG	6.65	126.34	113.70
11	H	125	ARG	NE-CZ-NH1	6.65	123.62	120.30
57	SH	116	ARG	NE-CZ-NH2	-6.65	116.98	120.30
62	SM	33	ARG	NE-CZ-NH2	-6.64	116.98	120.30
49	S2	532	C	C2'-C3'-O3'	6.64	124.33	113.70
49	S2	1663	A	O4'-C1'-N9	6.64	113.51	108.20
1	5	1631	A	N9-C1'-C2'	6.64	122.63	114.00
1	5	4693	C	C2'-C3'-O3'	6.64	124.32	113.70
49	S2	620	G	O5'-P-OP1	6.63	118.66	110.70
49	S2	1667	U	N1-C1'-C2'	6.63	122.62	114.00
1	5	5022	U	C2'-C3'-O3'	6.63	124.31	113.70
1	5	336	A	O4'-C1'-N9	6.63	113.50	108.20
74	SY	76	TYR	CA-CB-CG	-6.63	100.81	113.40
1	5	3790	U	O4'-C1'-N1	-6.62	102.90	108.20
1	5	2827	G	O4'-C1'-N9	-6.61	102.91	108.20
1	5	4325	A	N9-C1'-C2'	6.61	122.60	114.00
1	5	4518	A	C2'-C3'-O3'	-6.61	94.96	109.50
49	S2	1452	A	N9-C1'-C2'	6.61	122.59	114.00
49	S2	1401	A	C2'-C3'-O3'	6.60	124.26	113.70
3	8	1	C	C5'-C4'-O4'	6.60	117.02	109.10
3	8	81	C	C1'-O4'-C4'	-6.59	104.62	109.90
1	5	514	U	C5'-C4'-O4'	6.59	117.01	109.10
1	5	964	A	N9-C1'-C2'	-6.59	104.75	112.00
1	5	3883	U	N1-C1'-C2'	6.59	122.57	114.00
5	B	26	ARG	CG-CD-NE	-6.59	97.96	111.80
69	ST	62	ARG	NE-CZ-NH1	-6.59	117.01	120.30
49	S2	631	U	O4'-C1'-N1	-6.59	102.93	108.20
1	5	927	G	C2'-C3'-O3'	6.58	124.23	113.70
28	Y	81	TYR	CA-CB-CG	-6.58	100.89	113.40
1	5	314	G	N9-C1'-C2'	-6.57	104.77	112.00
49	S2	1434	C	N1-C1'-C2'	6.57	122.55	114.00
49	S2	1835	A	O4'-C4'-C3'	-6.57	97.43	104.00
1	5	505	G	C2'-C3'-O3'	6.56	124.20	113.70
49	S2	415	A	C8-N9-C1'	6.56	139.51	127.70
1	5	2782	U	C4'-C3'-O3'	6.56	126.12	113.00
49	S2	1394	G	C2'-C3'-O3'	6.56	124.20	113.70
1	5	1930	U	N1-C1'-C2'	6.56	122.52	114.00
35	f	109	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	5	4336	A	N9-C1'-C2'	-6.55	104.79	112.00
1	5	187	U	C2'-C3'-O3'	6.55	124.18	113.70
49	S2	160	U	C2'-C3'-O3'	6.55	124.18	113.70
62	SM	26	LEU	CB-CG-CD2	6.55	122.14	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	j	27	TYR	CB-CG-CD1	-6.55	117.07	121.00
48	4	122	THR	CB-CA-C	6.55	129.28	111.60
17	N	150	TRP	CA-CB-CG	6.54	126.14	113.70
50	SA	9	GLN	CA-CB-CG	6.54	127.80	113.40
53	SD	162	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	5	1671	U	O4'-C1'-C2'	-6.54	99.26	105.80
49	S2	1830	U	N1-C1'-C2'	-6.54	104.81	112.00
19	P	23	ARG	NE-CZ-NH1	6.54	123.57	120.30
36	g	14	ASN	N-CA-CB	6.54	122.36	110.60
1	5	3827	G	N9-C1'-C2'	-6.53	104.81	112.00
33	d	85	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	5	1215	C	O5'-P-OP2	-6.53	99.83	105.70
1	5	1650	A	O4'-C1'-N9	-6.53	102.98	108.20
1	5	384	A	N9-C1'-C2'	6.52	122.48	114.00
1	5	119	G	O4'-C4'-C3'	-6.52	97.48	104.00
48	4	154	VAL	N-CA-C	-6.52	93.40	111.00
58	SI	55	TYR	CA-CB-CG	-6.52	101.02	113.40
16	M	109	ARG	NE-CZ-NH2	6.51	123.56	120.30
1	5	2075	G	C2'-C3'-O3'	6.51	124.11	113.70
1	5	5043	A	N9-C1'-C2'	6.50	122.45	114.00
1	5	432	U	N1-C1'-C2'	-6.50	104.85	112.00
49	S2	499	G	C2'-C3'-O3'	6.50	124.10	113.70
49	S2	1272	C	O5'-P-OP1	-6.50	99.85	105.70
1	5	946	C	O4'-C1'-N1	6.50	113.40	108.20
1	5	98	A	N9-C1'-C2'	-6.49	104.86	112.00
1	5	1887	G	C2'-C3'-O3'	6.49	124.09	113.70
73	SX	27	TYR	CA-CB-CG	6.49	125.73	113.40
1	5	4227	U	C2'-C3'-O3'	6.49	124.08	113.70
10	G	223	ARG	NE-CZ-NH1	6.49	123.54	120.30
19	P	25	HIS	CB-CA-C	6.48	123.37	110.40
56	SG	88	ARG	NE-CZ-NH1	6.48	123.54	120.30
49	S2	149	A	N9-C1'-C2'	6.48	122.43	114.00
1	5	209	U	C4'-C3'-O3'	6.48	125.95	113.00
49	S2	1838	U	C2-N1-C1'	-6.47	109.93	117.70
49	S2	427	U	C5'-C4'-O4'	6.47	116.87	109.10
50	SA	186	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	5	1379	C	N1-C1'-C2'	6.47	122.41	114.00
48	4	269	ALA	CA-C-N	6.47	131.43	117.20
1	5	2118	G	C4'-C3'-O3'	6.46	125.93	113.00
9	F	209	PHE	N-CA-CB	6.46	122.23	110.60
1	5	307	A	N9-C1'-C2'	6.46	122.40	114.00
3	8	86	U	O4'-C1'-C2'	-6.46	99.34	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
63	SN	18	TYR	CA-CB-CG	-6.46	101.13	113.40
1	5	136	C	N1-C1'-C2'	-6.46	104.90	112.00
64	SO	147	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	5	1853	G	N9-C1'-C2'	-6.46	104.90	112.00
68	SS	14	ARG	NE-CZ-NH1	6.46	123.53	120.30
3	8	64	U	C5'-C4'-O4'	6.45	116.84	109.10
49	S2	1291	A	P-O3'-C3'	6.45	127.44	119.70
1	5	4076	G	N9-C1'-C2'	-6.45	104.90	112.00
1	5	4199	C	C4'-C3'-O3'	6.45	125.89	113.00
1	5	1573	G	N9-C1'-C2'	6.44	122.37	114.00
20	Q	181	ARG	CA-CB-CG	6.44	127.57	113.40
49	S2	1850	A	N9-C1'-C2'	6.44	122.37	114.00
30	a	109	TYR	CB-CG-CD2	-6.44	117.14	121.00
49	S2	1116	C	O5'-P-OP1	-6.44	99.91	105.70
1	5	1572	U	N1-C1'-C2'	6.44	122.37	114.00
14	K	129	ILE	O-C-N	-6.43	112.41	122.70
23	T	13	TYR	CA-CB-CG	6.43	125.62	113.40
49	S2	1059	G	N9-C1'-C2'	6.43	122.36	114.00
63	SN	64	ARG	NE-CZ-NH2	-6.43	117.09	120.30
49	S2	848	U	C2-N1-C1'	6.43	125.41	117.70
47	r	31	ASN	N-CA-CB	6.42	122.16	110.60
49	S2	427	U	P-O5'-C5'	6.42	131.18	120.90
49	S2	1860	A	N9-C1'-C2'	-6.42	104.94	112.00
78	Sc	44	ARG	CG-CD-NE	6.42	125.28	111.80
1	5	4338	G	N9-C1'-C2'	-6.42	104.94	112.00
64	SO	147	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	5	2665	U	C2'-C3'-O3'	6.41	123.95	113.70
46	q	45	MET	CA-CB-CG	-6.41	102.41	113.30
1	5	4976	U	N1-C1'-C2'	6.41	122.33	114.00
1	5	4534	G	N9-C1'-C2'	-6.40	104.96	112.00
7	D	293	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	5	4127	A	O4'-C1'-N9	6.40	113.32	108.20
1	5	2546	G	C4'-C3'-O3'	6.40	125.80	113.00
1	5	2649	G	N9-C1'-C2'	6.40	122.32	114.00
48	4	278	THR	C-N-CA	6.40	137.69	121.70
1	5	2088	A	C2'-C3'-O3'	6.39	123.93	113.70
3	8	35	C	N1-C1'-C2'	6.39	122.31	114.00
49	S2	654	A	N9-C1'-C2'	-6.39	104.97	112.00
18	O	37	ARG	NE-CZ-NH1	6.39	123.50	120.30
9	F	168	ARG	CB-CG-CD	6.39	128.21	111.60
1	5	1980	U	C1'-O4'-C4'	-6.39	104.79	109.90
26	W	8	PHE	CB-CG-CD2	-6.39	116.33	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	Y	81	TYR	CB-CA-C	6.38	123.17	110.40
7	D	223	PHE	CB-CG-CD1	6.38	125.27	120.80
4	A	37	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	5	1724	G	C4'-C3'-O3'	-6.38	96.00	109.40
49	S2	1082	A	N9-C1'-C2'	6.38	122.29	114.00
49	S2	1249	C	C2'-C3'-O3'	6.38	123.91	113.70
1	5	1241	C	C2'-C3'-O3'	6.37	123.90	113.70
48	4	404	THR	N-CA-CB	6.37	122.41	110.30
49	S2	1851	A	N9-C1'-C2'	6.37	122.28	114.00
1	5	336	A	C1'-O4'-C4'	-6.36	104.81	109.90
48	4	497	MET	C-N-CA	6.36	137.61	121.70
1	5	1642	A	C4'-C3'-O3'	-6.36	96.05	109.40
6	C	143	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	5	1272	C	O4'-C1'-N1	6.36	113.28	108.20
4	A	63	PHE	CB-CG-CD1	6.36	125.25	120.80
49	S2	1109	C	C1'-O4'-C4'	-6.36	104.81	109.90
1	5	417	G	O4'-C1'-N9	6.35	113.28	108.20
1	5	2554	U	C2'-C3'-O3'	6.34	123.85	113.70
49	S2	1584	G	N9-C1'-C2'	6.34	122.24	114.00
49	S2	91	A	N9-C1'-C2'	-6.34	105.03	112.00
1	5	1615	C	C2'-C3'-O3'	6.34	123.84	113.70
1	5	4519	C	C2'-C3'-O3'	6.34	123.84	113.70
1	5	2511	A	O4'-C1'-N9	-6.33	103.13	108.20
1	5	3901	A	C5'-C4'-O4'	6.33	116.70	109.10
9	F	36	ARG	NE-CZ-NH1	-6.33	117.13	120.30
1	5	294	G	N9-C1'-C2'	6.33	122.23	114.00
1	5	2581	A	N9-C1'-C2'	6.33	122.23	114.00
1	5	84	A	N9-C1'-C2'	6.33	122.23	114.00
28	Y	78	TYR	CB-CA-C	6.33	123.05	110.40
46	q	44	ARG	CD-NE-CZ	6.33	132.46	123.60
1	5	4911	A	O5'-P-OP2	-6.32	100.01	105.70
49	S2	1292	C	P-O5'-C5'	6.32	131.01	120.90
1	5	4519	C	O4'-C4'-C3'	-6.32	97.69	104.00
49	S2	960	U	C2'-C3'-O3'	6.32	123.80	113.70
19	P	139	TYR	CA-CB-CG	-6.31	101.41	113.40
9	F	136	ARG	NE-CZ-NH2	-6.31	117.14	120.30
10	G	235	ARG	CG-CD-NE	6.30	125.04	111.80
12	I	34	PHE	CB-CG-CD1	-6.30	116.39	120.80
49	S2	1597	C	N1-C1'-C2'	6.30	122.19	114.00
1	5	3671	G	N9-C1'-C2'	6.29	122.18	114.00
49	S2	1194	A	N9-C1'-C2'	-6.29	105.08	112.00
1	5	1282	G	O5'-P-OP1	-6.29	100.04	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1724	G	N9-C1'-C2'	6.29	122.17	114.00
7	D	35	ARG	CG-CD-NE	6.29	125.00	111.80
1	5	1672	U	C2-N1-C1'	6.28	125.24	117.70
3	8	104	A	N9-C1'-C2'	6.28	122.17	114.00
66	SQ	138	ARG	NE-CZ-NH1	6.28	123.44	120.30
14	K	129	ILE	C-N-CA	6.28	137.40	121.70
49	S2	1519	U	N1-C1'-C2'	6.28	122.16	114.00
7	D	145	TYR	CB-CA-C	6.28	122.95	110.40
1	5	3653	A	O5'-P-OP1	-6.27	100.05	105.70
11	H	31	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	5	219	G	O5'-P-OP2	-6.27	100.06	105.70
22	S	83	ARG	CG-CD-NE	6.27	124.97	111.80
1	5	2827	G	N9-C1'-C2'	6.27	122.15	114.00
1	5	2511	A	C2'-C3'-O3'	6.27	123.73	113.70
1	5	4519	C	C4'-C3'-C2'	-6.27	96.33	102.60
49	S2	475	C	O5'-P-OP1	-6.26	100.06	105.70
7	D	30	TYR	CB-CA-C	6.26	122.92	110.40
1	5	3648	A	O4'-C1'-N9	6.25	113.20	108.20
49	S2	1669	G	N9-C1'-C2'	6.25	122.13	114.00
34	e	5	ARG	NE-CZ-NH1	6.25	123.42	120.30
3	8	62	A	C8-N9-C1'	6.25	138.95	127.70
1	5	3880	G	N9-C1'-C2'	6.25	122.12	114.00
20	Q	33	ARG	NE-CZ-NH2	-6.25	117.18	120.30
49	S2	1855	G	O5'-P-OP2	-6.25	100.08	105.70
1	5	1279	A	C2'-C3'-O3'	6.25	123.69	113.70
49	S2	841	G	O4'-C1'-C2'	-6.25	99.56	105.80
1	5	2874	U	O4'-C1'-N1	-6.24	103.21	108.20
1	5	2673	G	O4'-C1'-C2'	-6.24	99.56	105.80
49	S2	41	G	N9-C1'-C2'	-6.24	105.14	112.00
49	S2	66	G	N9-C1'-C2'	-6.24	105.14	112.00
1	5	4548	A	P-O5'-C5'	6.24	130.88	120.90
1	5	4718	G	N9-C1'-C2'	-6.24	105.14	112.00
55	SF	165	ASN	N-CA-CB	6.24	121.83	110.60
1	5	2403	A	N9-C1'-C2'	6.24	122.11	114.00
81	Sf	148	TYR	CA-CB-CG	6.23	125.24	113.40
82	Sg	140	TYR	CA-CB-CG	-6.23	101.56	113.40
1	5	5056	A	N9-C1'-C2'	6.23	122.10	114.00
49	S2	1022	U	C1'-O4'-C4'	-6.23	104.92	109.90
65	SP	44	ARG	NE-CZ-NH1	6.23	123.42	120.30
26	W	55	TYR	CB-CG-CD1	6.23	124.74	121.00
76	Sa	10	ARG	CG-CD-NE	-6.23	98.72	111.80
1	5	4677	U	C3'-C2'-C1'	6.22	106.48	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	L	192	PHE	N-CA-CB	6.22	121.80	110.60
62	SM	127	TYR	CB-CG-CD1	6.22	124.73	121.00
1	5	220	C	C2'-C3'-O3'	6.22	123.66	113.70
1	5	3791	C	O4'-C1'-N1	-6.22	103.22	108.20
49	S2	1	U	C5'-C4'-C3'	6.22	125.95	116.00
6	C	80	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	5	409	G	N9-C1'-C2'	-6.22	105.16	112.00
1	5	2082	G	N9-C1'-C2'	6.22	122.08	114.00
51	SB	165	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	5	1934	A	N9-C1'-C2'	-6.21	105.16	112.00
7	D	44	TYR	CA-CB-CG	-6.21	101.60	113.40
10	G	54	PHE	CB-CA-C	6.21	122.82	110.40
55	SF	146	ARG	NE-CZ-NH1	6.21	123.41	120.30
49	S2	1420	G	O5'-P-OP2	-6.21	100.11	105.70
49	S2	980	A	C2'-C3'-O3'	6.21	123.63	113.70
5	B	137	TRP	CA-CB-CG	-6.20	101.92	113.70
6	C	311	ARG	NE-CZ-NH1	6.20	123.40	120.30
39	j	11	ARG	CG-CD-NE	-6.20	98.79	111.80
49	S2	1453	C	O4'-C1'-N1	6.20	113.16	108.20
49	S2	1857	G	N9-C1'-C2'	-6.20	105.19	112.00
49	S2	1617	G	N9-C1'-C2'	-6.19	105.19	112.00
61	SL	89	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	5	4560	C	O4'-C1'-N1	-6.19	103.25	108.20
20	Q	4	ASP	CB-CA-C	6.19	122.78	110.40
26	W	57	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	5	747	A	C2'-C3'-O3'	6.19	123.60	113.70
37	h	89	ARG	CG-CD-NE	6.19	124.79	111.80
15	L	82	ARG	NE-CZ-NH1	6.19	123.39	120.30
32	c	90	ARG	CA-CB-CG	6.19	127.01	113.40
46	q	150	GLY	C-N-CA	-6.18	106.24	121.70
48	4	806	GLY	C-N-CA	-6.18	106.24	121.70
1	5	3727	A	N9-C1'-C2'	6.18	122.04	114.00
49	S2	963	A	N9-C1'-C2'	6.18	122.04	114.00
14	K	136	ALA	CA-C-N	6.18	130.80	117.20
36	g	90	ARG	CG-CD-NE	-6.18	98.82	111.80
35	f	19	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	5	2666	U	C4'-C3'-C2'	-6.18	96.42	102.60
81	Sf	146	LEU	N-CA-CB	6.18	122.75	110.40
1	5	99	A	N9-C1'-C2'	-6.17	105.21	112.00
1	5	219	G	O4'-C1'-C2'	-6.17	99.62	105.80
1	5	962	C	C4'-C3'-O3'	-6.17	96.43	109.40
28	Y	126	ARG	NE-CZ-NH2	-6.17	117.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	o	78	ARG	NE-CZ-NH1	-6.17	117.21	120.30
49	S2	1668	U	N1-C1'-C2'	6.17	122.02	114.00
9	F	98	ARG	NE-CZ-NH2	-6.17	117.22	120.30
30	a	61	TYR	CB-CG-CD1	6.17	124.70	121.00
48	4	432	PRO	C-N-CA	-6.17	106.28	121.70
9	F	239	GLU	CA-CB-CG	6.16	126.96	113.40
18	O	117	ARG	NE-CZ-NH1	6.16	123.38	120.30
49	S2	1839	U	C6-N1-C1'	-6.16	112.58	121.20
1	5	5006	U	N1-C1'-C2'	-6.16	105.23	112.00
46	q	6	ARG	C-N-CA	6.16	137.10	121.70
1	5	2470	C	O4'-C1'-C2'	-6.16	99.64	105.80
1	5	4579	U	C2-N1-C1'	6.16	125.09	117.70
9	F	168	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	5	2107	C	C2'-C3'-O3'	6.15	123.54	113.70
1	5	4976	U	C5'-C4'-O4'	6.15	116.48	109.10
1	5	2854	G	N9-C1'-C2'	-6.15	105.24	112.00
32	c	39	ARG	CG-CD-NE	-6.15	98.89	111.80
1	5	1379	C	C5'-C4'-O4'	6.14	116.47	109.10
1	5	1379	C	P-O5'-C5'	6.14	130.73	120.90
3	8	62	A	C4-N9-C1'	-6.14	115.24	126.30
6	C	35	ASP	CB-CG-OD2	-6.14	112.77	118.30
48	4	793	SER	C-N-CA	-6.14	106.34	121.70
49	S2	1603	G	O4'-C1'-N9	-6.14	103.29	108.20
1	5	4239	A	C2'-C3'-O3'	6.14	123.52	113.70
47	r	45	HIS	CB-CA-C	-6.14	98.12	110.40
33	d	87	ARG	CA-CB-CG	6.13	126.89	113.40
28	Y	15	ARG	NE-CZ-NH1	-6.13	117.23	120.30
49	S2	1123	C	O5'-P-OP1	-6.13	100.18	105.70
1	5	4451	G	N9-C1'-C2'	6.13	121.97	114.00
49	S2	1021	U	N1-C1'-C2'	6.13	121.97	114.00
73	SX	8	ARG	NE-CZ-NH2	6.13	123.36	120.30
49	S2	1735	A	N9-C1'-C2'	6.12	121.96	114.00
46	q	69	LEU	CA-C-N	6.12	130.67	117.20
21	R	9	ARG	NE-CZ-NH1	6.12	123.36	120.30
49	S2	1223	A	N9-C1'-C2'	-6.12	105.27	112.00
55	SF	164	ARG	CG-CD-NE	-6.12	98.95	111.80
1	5	2854	G	C2'-C3'-O3'	6.12	123.48	113.70
49	S2	19	A	C2'-C3'-O3'	6.12	123.48	113.70
1	5	4880	C	N1-C1'-C2'	6.11	121.95	114.00
49	S2	1545	A	N9-C1'-C2'	6.11	121.95	114.00
17	N	96	ARG	NE-CZ-NH1	-6.11	117.24	120.30
60	SK	8	ARG	NE-CZ-NH1	6.11	123.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1614	C	C2'-C3'-O3'	6.11	123.47	113.70
3	8	66	A	N9-C1'-C2'	6.11	121.94	114.00
3	8	81	C	O4'-C1'-N1	6.11	113.08	108.20
48	4	153	PRO	O-C-N	6.10	132.46	122.70
5	B	102	PHE	CB-CA-C	-6.10	98.20	110.40
8	E	59	TYR	N-CA-C	-6.10	94.53	111.00
21	R	107	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	5	514	U	C4'-C3'-C2'	-6.10	96.50	102.60
7	D	145	TYR	CA-CB-CG	-6.10	101.81	113.40
63	SN	128	TYR	CB-CG-CD1	6.09	124.66	121.00
80	Se	41	ARG	CG-CD-NE	6.09	124.60	111.80
49	S2	531	A	C2'-C3'-O3'	6.09	123.45	113.70
14	K	85	LEU	C-N-CA	6.09	136.93	121.70
1	5	4876	U	N1-C1'-C2'	6.09	121.92	114.00
33	d	87	ARG	CG-CD-NE	-6.09	99.01	111.80
49	S2	313	A	N9-C1'-C2'	6.09	121.92	114.00
1	5	1488	G	C2'-C3'-O3'	6.09	123.44	113.70
21	R	108	ARG	NE-CZ-NH2	-6.08	117.26	120.30
15	L	36	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	5	1214	C	O4'-C1'-N1	-6.08	103.34	108.20
1	5	5040	U	C4'-C3'-O3'	-6.08	96.64	109.40
1	5	2119	C	O4'-C1'-N1	6.07	113.06	108.20
1	5	1649	U	N1-C1'-C2'	6.07	121.89	114.00
1	5	3738	G	N9-C1'-C2'	-6.07	105.33	112.00
59	SJ	20	PHE	CB-CG-CD1	6.07	125.05	120.80
1	5	4948	C	C2'-C3'-O3'	6.06	123.40	113.70
48	4	531	ASP	C-N-CD	6.06	141.13	128.40
48	4	760	TYR	CB-CG-CD2	-6.06	117.36	121.00
49	S2	1552	G	N9-C1'-C2'	-6.06	105.33	112.00
14	K	130	LYS	CD-CE-NZ	6.06	125.63	111.70
4	A	83	HIS	N-CA-C	-6.05	94.65	111.00
39	j	39	TYR	CB-CA-C	-6.05	98.30	110.40
49	S2	9	U	C2'-C3'-O3'	6.05	123.38	113.70
49	S2	943	U	C2-N1-C1'	6.05	124.96	117.70
17	N	71	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	5	4270	C	C2'-C3'-O3'	6.04	123.37	113.70
1	5	4519	C	C1'-O4'-C4'	-6.04	105.07	109.90
20	Q	181	ARG	CG-CD-NE	-6.04	99.11	111.80
20	Q	58	ARG	NE-CZ-NH2	-6.04	117.28	120.30
49	S2	959	G	C2'-C3'-O3'	6.04	123.36	113.70
1	5	235	A	C1'-O4'-C4'	-6.04	105.07	109.90
69	ST	53	PHE	CB-CG-CD1	6.04	125.03	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	f	36	ARG	NE-CZ-NH2	-6.03	117.28	120.30
49	S2	1433	C	C4'-C3'-C2'	-6.03	96.57	102.60
49	S2	1419	C	C2'-C3'-O3'	6.03	123.35	113.70
49	S2	1588	A	N9-C1'-C2'	6.03	121.84	114.00
1	5	4986	G	N9-C1'-C2'	6.03	121.84	114.00
14	K	30	PRO	CA-C-O	-6.03	105.73	120.20
6	C	78	ARG	NE-CZ-NH2	-6.03	117.29	120.30
49	S2	398	A	N9-C1'-C2'	-6.03	105.37	112.00
1	5	3843	C	O4'-C1'-N1	-6.02	103.38	108.20
46	q	81	HIS	CB-CA-C	6.02	122.44	110.40
8	E	157	ARG	NE-CZ-NH1	-6.01	117.29	120.30
49	S2	1433	C	O4'-C4'-C3'	-6.01	97.99	104.00
1	5	1210	C	N1-C1'-C2'	6.01	121.81	114.00
1	5	4599	A	N9-C1'-C2'	6.01	121.81	114.00
32	c	56	ARG	NE-CZ-NH1	6.01	123.31	120.30
49	S2	1858	G	C2'-C3'-O3'	6.01	123.31	113.70
51	SB	107	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	5	4731	G	O4'-C1'-N9	6.00	113.00	108.20
14	K	28	LEU	N-CA-CB	6.00	122.41	110.40
44	o	40	ARG	NE-CZ-NH1	6.00	123.30	120.30
6	C	312	ARG	CG-CD-NE	-6.00	99.20	111.80
19	P	127	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	5	67	C	N1-C1'-C2'	-6.00	105.40	112.00
66	SQ	62	ARG	NE-CZ-NH1	6.00	123.30	120.30
3	8	13	G	N9-C1'-C2'	6.00	121.80	114.00
2	7	58	A	N9-C1'-C2'	-6.00	105.41	112.00
38	i	85	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	5	4694	G	O5'-P-OP1	-5.99	100.31	105.70
49	S2	918	U	C1'-O4'-C4'	-5.99	105.11	109.90
49	S2	400	C	N1-C1'-C2'	-5.99	105.41	112.00
1	5	1658	G	N9-C1'-C2'	5.99	121.78	114.00
1	5	3739	C	O4'-C1'-C2'	-5.99	99.81	105.80
1	5	3913	G	C2'-C3'-O3'	5.99	123.28	113.70
1	5	2744	A	N9-C1'-C2'	5.98	121.78	114.00
3	8	64	U	C2-N1-C1'	5.98	124.88	117.70
1	5	1697	G	O5'-P-OP2	5.98	117.88	110.70
49	S2	1084	A	N9-C1'-C2'	-5.98	105.42	112.00
49	S2	855	G	N9-C1'-C2'	-5.98	105.42	112.00
37	h	84	ARG	CG-CD-NE	-5.98	99.25	111.80
1	5	52	G	C2'-C3'-O3'	5.97	123.26	113.70
1	5	1523	A	O5'-P-OP1	-5.97	100.32	105.70
1	5	4979	A	N9-C1'-C2'	5.97	121.77	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	7	58	A	C2'-C3'-O3'	5.97	123.25	113.70
1	5	1495	G	N9-C1'-C2'	5.97	121.76	114.00
1	5	4871	C	O4'-C1'-N1	-5.97	103.42	108.20
14	K	124	GLU	N-CA-C	-5.97	94.89	111.00
51	SB	82	ARG	NE-CZ-NH1	-5.96	117.32	120.30
7	D	54	ARG	CB-CG-CD	5.96	127.10	111.60
47	r	103	ARG	NE-CZ-NH1	5.96	123.28	120.30
65	SP	42	ARG	NE-CZ-NH1	5.96	123.28	120.30
56	SG	191	ARG	NE-CZ-NH1	5.96	123.28	120.30
48	4	267	ASP	C-N-CD	5.96	140.92	128.40
20	Q	166	TYR	CB-CG-CD1	5.96	124.58	121.00
30	a	65	ARG	CG-CD-NE	-5.96	99.28	111.80
1	5	4473	A	C4-N9-C1'	5.96	137.02	126.30
34	e	46	ARG	NE-CZ-NH2	-5.96	117.32	120.30
49	S2	73	C	N1-C1'-C2'	5.96	121.74	114.00
49	S2	1420	G	C2'-C3'-O3'	5.95	123.22	113.70
16	M	90	ARG	CG-CD-NE	-5.95	99.31	111.80
1	5	2307	A	N9-C1'-C2'	5.95	121.73	114.00
63	SN	55	ARG	CG-CD-NE	5.95	124.28	111.80
49	S2	1114	U	C2'-C3'-O3'	5.94	123.21	113.70
1	5	2323	C	N1-C1'-C2'	-5.94	105.46	112.00
14	K	85	LEU	CD1-CG-CD2	5.94	128.33	110.50
1	5	231	U	C4'-C3'-O3'	-5.94	96.92	109.40
30	a	132	ARG	NE-CZ-NH2	-5.94	117.33	120.30
5	B	258	HIS	N-CA-C	5.94	127.03	111.00
48	4	71	LYS	C-N-CA	-5.94	106.85	121.70
1	5	2070	U	N1-C1'-C2'	5.94	121.72	114.00
1	5	669	C	C1'-O4'-C4'	-5.93	105.16	109.90
23	T	57	TYR	CA-CB-CG	5.93	124.67	113.40
1	5	3774	A	N9-C1'-C2'	5.93	121.71	114.00
6	C	102	PHE	N-CA-CB	5.93	121.27	110.60
49	S2	482	G	N9-C1'-C2'	-5.92	105.48	112.00
1	5	936	C	C4'-C3'-O3'	5.92	124.84	113.00
15	L	82	ARG	CG-CD-NE	-5.92	99.37	111.80
49	S2	1416	C	C2'-C3'-O3'	5.92	123.17	113.70
14	K	86	LYS	CB-CA-C	-5.92	98.56	110.40
1	5	2515	G	N9-C1'-C2'	-5.92	105.49	112.00
1	5	4291	G	N9-C1'-C2'	5.92	121.69	114.00
1	5	4479	A	N9-C1'-C2'	-5.92	105.49	112.00
49	S2	417	C	C2'-C3'-O3'	5.92	123.17	113.70
49	S2	1823	A	C2'-C3'-O3'	5.92	123.17	113.70
49	S2	1857	G	C2'-C3'-O3'	5.92	123.17	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	S2	795	A	N9-C1'-C2'	5.92	121.69	114.00
61	SL	92	TYR	CA-CB-CG	5.92	124.64	113.40
1	5	1894	C	N1-C1'-C2'	5.91	121.69	114.00
34	e	20	PHE	CB-CG-CD1	-5.91	116.66	120.80
1	5	4449	A	N9-C1'-C2'	-5.91	105.50	112.00
16	M	6	PHE	CB-CA-C	5.91	122.22	110.40
49	S2	848	U	C2-N3-C4	-5.91	123.45	127.00
49	S2	65	C	O4'-C1'-N1	5.91	112.93	108.20
49	S2	1309	C	C4'-C3'-O3'	5.90	124.81	113.00
1	5	1930	U	O4'-C1'-N1	-5.90	103.48	108.20
32	c	56	ARG	CD-NE-CZ	5.90	131.86	123.60
49	S2	446	G	C2'-C3'-O3'	5.90	123.14	113.70
1	5	1398	A	O5'-P-OP2	-5.90	100.39	105.70
1	5	2305	U	O4'-C4'-C3'	-5.90	98.10	104.00
1	5	2373	C	N1-C1'-C2'	5.90	121.67	114.00
1	5	33	A	N9-C1'-C2'	5.90	121.66	114.00
66	SQ	71	ARG	NE-CZ-NH1	5.90	123.25	120.30
33	d	78	ARG	NE-CZ-NH1	5.89	123.25	120.30
49	S2	474	G	C2'-C3'-O3'	5.89	123.13	113.70
48	4	196	GLU	N-CA-C	-5.89	95.10	111.00
1	5	4510	A	N9-C1'-C2'	5.89	121.65	114.00
1	5	2305	U	C5'-C4'-O4'	5.89	116.16	109.10
1	5	2322	G	C2'-C3'-O3'	5.89	123.12	113.70
1	5	4201	G	N9-C1'-C2'	5.89	121.65	114.00
1	5	1324	A	N9-C1'-C2'	5.88	121.65	114.00
49	S2	365	C	N1-C1'-C2'	-5.88	105.53	112.00
73	SX	17	ARG	CG-CD-NE	-5.88	99.44	111.80
49	S2	993	G	C5'-C4'-O4'	5.88	116.16	109.10
1	5	4670	C	O4'-C1'-N1	-5.88	103.50	108.20
8	E	275	ASN	N-CA-CB	5.88	121.19	110.60
49	S2	1273	C	N1-C1'-C2'	-5.88	105.53	112.00
1	5	53	C	N1-C1'-C2'	-5.88	105.53	112.00
1	5	4763	U	O4'-C1'-N1	5.88	112.90	108.20
61	SL	62	PHE	CB-CA-C	5.88	122.15	110.40
49	S2	1477	U	C2'-C3'-O3'	5.88	123.10	113.70
72	SW	3	ARG	CG-CD-NE	-5.87	99.47	111.80
1	5	1487	G	C2'-C3'-O3'	5.87	123.09	113.70
49	S2	1313	A	N9-C1'-C2'	5.87	121.63	114.00
1	5	2642	A	N9-C1'-C2'	-5.87	105.55	112.00
49	S2	26	U	C2'-C3'-O3'	5.87	123.08	113.70
56	SG	213	LEU	CA-CB-CG	5.86	128.79	115.30
1	5	4074	C	N1-C1'-C2'	5.86	121.62	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	S2	1367	U	C2'-C3'-O3'	5.86	123.08	113.70
1	5	1815	G	C1'-O4'-C4'	-5.86	105.21	109.90
53	SD	67	ARG	CG-CD-NE	5.86	124.11	111.80
48	4	247	ALA	N-CA-CB	5.86	118.30	110.10
1	5	4199	C	O4'-C1'-C2'	-5.86	99.94	105.80
51	SB	67	PHE	N-CA-CB	-5.85	100.06	110.60
48	4	432	PRO	O-C-N	-5.85	113.34	122.70
49	S2	1868	U	N1-C1'-C2'	5.85	121.61	114.00
11	H	54	ARG	NE-CZ-NH2	-5.85	117.38	120.30
48	4	60	ARG	NE-CZ-NH1	-5.85	117.38	120.30
49	S2	1356	G	N9-C1'-C2'	5.85	121.60	114.00
59	SJ	45	ARG	NE-CZ-NH2	-5.85	117.38	120.30
15	L	34	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	5	920	C	C5'-C4'-O4'	5.84	116.11	109.10
74	SY	76	TYR	CB-CG-CD1	-5.84	117.50	121.00
1	5	657	C	C2'-C3'-O3'	5.84	123.04	113.70
49	S2	30	C	N1-C1'-C2'	5.84	121.59	114.00
1	5	40	G	N9-C1'-C2'	5.83	121.58	114.00
1	5	2448	G	N9-C1'-C2'	5.83	121.58	114.00
1	5	72	C	C1'-O4'-C4'	-5.83	105.23	109.90
1	5	2586	G	O4'-C1'-N9	5.83	112.86	108.20
1	5	4481	U	C5'-C4'-O4'	5.83	116.10	109.10
12	I	119	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	5	4215	C	O4'-C1'-C2'	-5.82	99.98	105.80
46	q	68	HIS	N-CA-CB	5.82	121.08	110.60
49	S2	441	C	C4'-C3'-O3'	-5.82	97.17	109.40
1	5	934	C	O4'-C1'-N1	-5.82	103.55	108.20
7	D	265	ARG	NE-CZ-NH2	-5.82	117.39	120.30
49	S2	92	A	O4'-C1'-N9	-5.82	103.55	108.20
59	SJ	108	ARG	NE-CZ-NH1	5.82	123.21	120.30
49	S2	1835	A	N9-C1'-C2'	5.81	121.56	114.00
1	5	85	G	N9-C1'-C2'	-5.81	105.61	112.00
49	S2	1658	G	N9-C1'-C2'	-5.81	105.61	112.00
49	S2	548	C	C2'-C3'-O3'	5.81	123.00	113.70
1	5	2268	A	O4'-C1'-N9	-5.81	103.55	108.20
1	5	4463	U	O4'-C1'-N1	5.81	112.85	108.20
49	S2	454	U	N1-C1'-C2'	5.80	121.55	114.00
54	SE	121	TYR	CA-CB-CG	-5.80	102.37	113.40
59	SJ	48	PHE	CB-CG-CD1	-5.80	116.74	120.80
12	I	94	PHE	CB-CG-CD2	-5.80	116.74	120.80
34	e	60	TYR	CB-CA-C	5.80	122.00	110.40
4	A	63	PHE	CB-CG-CD2	-5.80	116.74	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	S2	918	U	O4'-C1'-N1	5.80	112.84	108.20
1	5	1341	U	N1-C1'-C2'	5.79	121.53	114.00
1	5	4548	A	C5'-C4'-O4'	5.79	116.05	109.10
22	S	84	TYR	CB-CG-CD1	5.79	124.48	121.00
49	S2	649	U	O5'-P-OP1	-5.79	100.49	105.70
1	5	1506	G	N9-C1'-C2'	-5.79	105.63	112.00
1	5	1650	A	C4-N9-C1'	-5.79	115.88	126.30
1	5	4473	A	C8-N9-C1'	-5.79	117.28	127.70
49	S2	563	G	N9-C1'-C2'	-5.79	105.63	112.00
3	8	34	U	C3'-C2'-C1'	5.79	106.13	101.50
52	SC	241	PHE	CB-CG-CD2	-5.79	116.75	120.80
58	SI	112	TRP	CA-CB-CG	5.79	124.69	113.70
49	S2	621	C	N1-C1'-C2'	-5.78	105.64	112.00
1	5	4481	U	N1-C1'-C2'	5.78	121.51	114.00
4	A	147	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	5	197	A	N9-C1'-C2'	5.78	121.51	114.00
3	8	81	C	C5'-C4'-C3'	5.78	125.24	116.00
5	B	117	ARG	CG-CD-NE	-5.77	99.67	111.80
48	4	5	THR	C-N-CA	-5.77	107.27	121.70
1	5	2807	A	C2'-C3'-O3'	5.77	122.94	113.70
28	Y	121	ARG	NE-CZ-NH1	5.77	123.19	120.30
45	p	14	TYR	CB-CA-C	5.77	121.94	110.40
51	SB	205	TYR	CB-CG-CD1	-5.77	117.54	121.00
3	8	115	G	C2'-C3'-O3'	5.77	122.93	113.70
17	N	30	TYR	N-CA-CB	-5.77	100.22	110.60
1	5	292	G	C4-N9-C1'	-5.77	119.00	126.50
51	SB	133	TYR	CA-CB-CG	5.76	124.35	113.40
35	f	6	TRP	N-CA-C	-5.76	95.45	111.00
1	5	2769	U	O4'-C1'-N1	5.76	112.81	108.20
1	5	3691	G	N9-C1'-C2'	5.76	121.48	114.00
22	S	97	TYR	CA-CB-CG	-5.75	102.47	113.40
7	D	35	ARG	NE-CZ-NH2	-5.75	117.42	120.30
49	S2	662	G	O4'-C1'-N9	-5.75	103.60	108.20
49	S2	848	U	C6-N1-C1'	-5.75	113.14	121.20
57	SH	189	PHE	CB-CA-C	5.75	121.91	110.40
48	4	685	TRP	CB-CG-CD2	-5.75	119.12	126.60
79	Sd	40	ARG	NE-CZ-NH1	5.75	123.17	120.30
68	SS	86	ARG	NE-CZ-NH2	5.75	123.17	120.30
49	S2	495	U	C1'-C2'-O2'	-5.75	93.36	110.60
54	SE	99	PHE	CB-CG-CD1	5.75	124.82	120.80
20	Q	32	TYR	CA-CB-CG	5.74	124.31	113.40
49	S2	855	G	C2'-C3'-O3'	5.74	122.89	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	S2	1832	A	O5'-P-OP2	-5.74	100.53	105.70
1	5	1398	A	O5'-P-OP1	5.74	117.58	110.70
48	4	3	ASN	N-CA-C	-5.74	95.51	111.00
76	Sa	87	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	5	2405	G	N9-C1'-C2'	-5.74	105.69	112.00
1	5	111	C	N1-C1'-C2'	-5.73	105.70	112.00
49	S2	662	G	N9-C1'-C2'	5.73	121.45	114.00
49	S2	594	A	C8-N9-C1'	-5.73	117.39	127.70
1	5	2360	A	N9-C1'-C2'	5.72	121.44	114.00
28	Y	18	HIS	N-CA-CB	5.72	120.90	110.60
54	SE	18	TRP	CB-CA-C	5.72	121.85	110.40
1	5	88	A	N9-C1'-C2'	5.72	121.44	114.00
68	SS	82	TRP	CA-CB-CG	5.72	124.57	113.70
1	5	4385	A	C2'-C3'-O3'	-5.72	96.92	109.50
8	E	278	TYR	CB-CG-CD1	-5.72	117.57	121.00
1	5	703	G	C1'-O4'-C4'	-5.72	105.33	109.90
1	5	1438	U	C2'-C3'-O3'	5.72	122.85	113.70
3	8	79	G	N9-C1'-C2'	5.71	121.43	114.00
1	5	1285	U	O4'-C1'-N1	5.71	112.77	108.20
37	h	119	PHE	CB-CG-CD2	-5.71	116.80	120.80
1	5	236	G	N9-C1'-C2'	5.71	121.42	114.00
48	4	669	VAL	CB-CA-C	5.71	122.25	111.40
1	5	1696	C	C2'-C3'-O3'	5.71	122.83	113.70
1	5	2119	C	C1'-O4'-C4'	-5.71	105.33	109.90
1	5	2643	G	C2'-C3'-O3'	5.71	122.83	113.70
1	5	4125	C	C4'-C3'-O3'	-5.71	97.41	109.40
9	F	136	ARG	CG-CD-NE	-5.71	99.81	111.80
68	SS	130	ARG	NE-CZ-NH2	-5.71	117.45	120.30
74	SY	63	HIS	N-CA-CB	5.71	120.87	110.60
49	S2	146	G	N9-C1'-C2'	-5.70	105.73	112.00
1	5	2553	A	C1'-O4'-C4'	-5.70	105.34	109.90
3	8	135	C	N1-C1'-C2'	5.70	121.41	114.00
9	F	100	ILE	CG1-CB-CG2	5.70	123.94	111.40
4	A	34	PHE	N-CA-CB	5.70	120.85	110.60
22	S	10	TYR	CB-CG-CD1	-5.70	117.58	121.00
1	5	3686	G	N9-C1'-C2'	-5.69	105.74	112.00
1	5	84	A	C4-N9-C1'	-5.69	116.06	126.30
1	5	1281	G	C5'-C4'-O4'	5.69	115.93	109.10
28	Y	61	HIS	N-CA-CB	5.69	120.84	110.60
1	5	2118	G	O4'-C4'-C3'	-5.69	98.31	104.00
82	Sg	83	TRP	CA-CB-CG	-5.68	102.90	113.70
49	S2	1842	C	N1-C1'-C2'	5.68	121.39	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1642	A	P-O3'-C3'	5.68	126.52	119.70
1	5	1849	U	O5'-P-OP1	5.68	117.52	110.70
1	5	1494	U	N1-C1'-C2'	5.68	121.38	114.00
48	4	420	LEU	CB-CG-CD2	-5.68	101.34	111.00
21	R	110	ARG	NE-CZ-NH1	5.68	123.14	120.30
31	b	17	HIS	CB-CA-C	-5.68	99.05	110.40
2	7	7	G	C5'-C4'-O4'	5.67	115.91	109.10
4	A	37	ARG	CG-CD-NE	-5.67	99.89	111.80
8	E	268	ARG	NE-CZ-NH2	-5.67	117.46	120.30
49	S2	504	G	N9-C1'-C2'	5.67	121.38	114.00
56	SG	156	TYR	CA-CB-CG	-5.67	102.62	113.40
1	5	2282	A	N9-C1'-C2'	5.67	121.37	114.00
54	SE	99	PHE	CB-CG-CD2	-5.67	116.83	120.80
49	S2	369	C	N1-C1'-C2'	5.67	121.36	114.00
49	S2	1546	G	N9-C1'-C2'	5.67	121.36	114.00
1	5	85	G	O4'-C1'-C2'	-5.66	100.14	105.80
1	5	1264	C	C2'-C3'-O3'	5.66	122.76	113.70
41	l	12	PHE	CB-CG-CD2	-5.66	116.84	120.80
48	4	358	LEU	C-N-CD	-5.66	108.14	120.60
1	5	100	C	C5'-C4'-O4'	5.66	115.89	109.10
20	Q	32	TYR	CB-CG-CD2	-5.66	117.60	121.00
49	S2	1243	U	C2'-C3'-O3'	5.66	122.76	113.70
8	E	101	ARG	NE-CZ-NH2	5.66	123.13	120.30
48	4	112	SER	CA-C-N	-5.66	104.75	117.20
21	R	97	ARG	CG-CD-NE	-5.66	99.92	111.80
49	S2	1291	A	C3'-C2'-C1'	5.66	106.03	101.50
1	5	1398	A	O4'-C1'-N9	5.66	112.72	108.20
1	5	3776	G	N9-C1'-C2'	-5.66	105.78	112.00
1	5	2088	A	N9-C1'-C2'	-5.65	105.78	112.00
1	5	2383	C	N1-C1'-C2'	5.65	121.34	114.00
61	SL	89	ARG	CG-CD-NE	-5.65	99.93	111.80
1	5	4693	C	O4'-C4'-C3'	-5.65	98.35	104.00
6	C	200	ARG	NE-CZ-NH2	-5.65	117.48	120.30
34	e	75	ARG	CG-CD-NE	-5.65	99.94	111.80
1	5	4966	A	C8-N9-C1'	-5.64	117.54	127.70
49	S2	1395	C	O4'-C1'-C2'	-5.64	100.16	105.80
11	H	180	TYR	CA-CB-CG	5.64	124.12	113.40
74	SY	61	ARG	CG-CD-NE	-5.64	99.95	111.80
5	B	246	ARG	NE-CZ-NH1	5.64	123.12	120.30
27	X	137	TYR	CB-CG-CD1	5.64	124.38	121.00
49	S2	382	C	N1-C1'-C2'	5.64	121.33	114.00
20	Q	104	ARG	NE-CZ-NH1	5.64	123.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1639	U	N1-C1'-C2'	5.63	121.32	114.00
48	4	56	PHE	N-CA-CB	5.63	120.74	110.60
49	S2	746	C	C2'-C3'-O3'	5.63	122.72	113.70
1	5	1876	U	C2'-C3'-O3'	5.63	122.71	113.70
73	SX	17	ARG	NE-CZ-NH1	-5.63	117.48	120.30
20	Q	176	ARG	CG-CD-NE	-5.63	99.97	111.80
39	j	27	TYR	N-CA-CB	5.63	120.74	110.60
1	5	514	U	C4'-C3'-O3'	5.63	124.26	113.00
1	5	370	U	N1-C1'-C2'	5.63	121.32	114.00
1	5	118	C	C2'-C3'-O3'	5.63	122.70	113.70
1	5	5062	G	P-O5'-C5'	5.63	129.90	120.90
5	B	169	ARG	CG-CD-NE	5.62	123.61	111.80
46	q	24	TYR	C-N-CD	5.62	140.21	128.40
49	S2	1085	C	N1-C1'-C2'	5.62	121.31	114.00
1	5	3773	U	N1-C1'-C2'	-5.62	105.81	112.00
6	C	311	ARG	CG-CD-NE	-5.62	99.99	111.80
49	S2	649	U	N1-C1'-C2'	5.62	121.31	114.00
49	S2	943	U	C5'-C4'-O4'	5.62	115.84	109.10
1	5	2686	G	N9-C1'-C2'	-5.62	105.82	112.00
49	S2	60	A	C1'-C2'-O2'	-5.62	93.74	110.60
68	SS	124	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	5	2077	C	N1-C1'-C2'	-5.61	105.83	112.00
6	C	350	ARG	NE-CZ-NH2	-5.61	117.49	120.30
48	4	478	PHE	CB-CA-C	5.61	121.63	110.40
1	5	4753	U	C2'-C3'-O3'	5.61	122.68	113.70
15	L	7	GLY	N-CA-C	-5.61	99.07	113.10
1	5	1539	G	C2'-C3'-O3'	5.61	122.67	113.70
14	K	147	HIS	C-N-CD	5.61	140.18	128.40
22	S	94	TYR	CA-CB-CG	-5.61	102.74	113.40
39	j	66	HIS	CA-CB-CG	-5.61	104.07	113.60
10	G	57	TRP	CA-CB-CG	-5.61	103.05	113.70
1	5	1932	A	N9-C1'-C2'	5.60	121.28	114.00
20	Q	68	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	5	2857	A	C1'-C2'-O2'	-5.60	93.80	110.60
49	S2	821	G	O4'-C4'-C3'	-5.60	98.40	104.00
1	5	2450	G	N9-C1'-C2'	-5.60	105.84	112.00
47	r	21	ASN	CB-CA-C	5.60	121.59	110.40
64	SO	121	ARG	NE-CZ-NH1	5.60	123.10	120.30
65	SP	81	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	5	2665	U	N1-C1'-C2'	-5.59	105.85	112.00
1	5	2474	G	C2'-C3'-O3'	5.59	122.64	113.70
1	5	2487	G	C2'-C3'-O3'	5.59	122.64	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	8	39	G	N9-C1'-C2'	-5.59	105.85	112.00
1	5	85	G	O4'-C1'-N9	5.59	112.67	108.20
1	5	977	C	C4'-C3'-C2'	-5.59	97.01	102.60
1	5	1295	C	N1-C1'-C2'	5.59	121.26	114.00
36	g	9	ARG	CG-CD-NE	-5.58	100.07	111.80
1	5	4114	C	N1-C1'-C2'	5.58	121.26	114.00
46	q	200	ASN	C-N-CD	5.58	140.13	128.40
1	5	1501	C	C1'-O4'-C4'	-5.58	105.43	109.90
29	Z	121	ARG	NE-CZ-NH2	-5.58	117.51	120.30
5	B	169	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	5	490	C	N1-C1'-C2'	5.58	121.25	114.00
15	L	6	ASN	N-CA-CB	5.58	120.64	110.60
49	S2	26	U	O4'-C1'-C2'	-5.58	100.22	105.80
57	SH	116	ARG	NE-CZ-NH1	5.58	123.09	120.30
80	Se	38	TYR	CA-CB-CG	5.58	124.00	113.40
1	5	1632	A	O4'-C1'-N9	5.57	112.66	108.20
49	S2	1376	A	C2'-C3'-O3'	5.57	122.62	113.70
1	5	3773	U	C4'-C3'-C2'	-5.57	97.03	102.60
20	Q	178	ARG	CG-CD-NE	-5.57	100.10	111.80
15	L	163	ARG	NE-CZ-NH1	5.57	123.08	120.30
51	SB	196	ASP	CB-CG-OD1	5.57	123.31	118.30
1	5	4950	U	N1-C1'-C2'	5.57	121.24	114.00
12	I	213	HIS	CB-CA-C	5.57	121.53	110.40
9	F	72	ARG	NE-CZ-NH2	-5.56	117.52	120.30
46	q	123	VAL	C-N-CD	5.56	140.07	128.40
1	5	1521	C	C2'-C3'-O3'	5.56	122.59	113.70
1	5	4076	G	C1'-O4'-C4'	-5.56	105.45	109.90
1	5	4767	C	C2'-C3'-O3'	5.56	122.59	113.70
54	SE	51	ARG	NE-CZ-NH1	-5.56	117.52	120.30
59	SJ	150	ARG	NE-CZ-NH1	5.56	123.08	120.30
49	S2	642	U	O5'-P-OP2	-5.55	100.70	105.70
11	H	115	ARG	CG-CD-NE	-5.55	100.14	111.80
1	5	1614	C	N1-C1'-C2'	-5.55	105.90	112.00
17	N	182	HIS	N-CA-CB	5.55	120.59	110.60
1	5	1631	A	C5'-C4'-O4'	5.55	115.76	109.10
7	D	210	TYR	CB-CG-CD1	-5.55	117.67	121.00
29	Z	28	ASN	N-CA-C	-5.55	96.03	111.00
48	4	855	LEU	C-N-CA	5.54	135.56	121.70
49	S2	661	U	N1-C1'-C2'	-5.54	105.90	112.00
1	5	2396	A	N9-C1'-C2'	5.54	121.20	114.00
1	5	4723	A	C5'-C4'-O4'	5.54	115.75	109.10
1	5	1672	U	C6-N1-C1'	-5.54	113.45	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	p	18	TYR	CA-CB-CG	5.54	123.92	113.40
9	F	98	ARG	NE-CZ-NH1	5.54	123.07	120.30
49	S2	457	C	N1-C1'-C2'	-5.54	105.91	112.00
1	5	956	A	N9-C1'-C2'	-5.53	105.91	112.00
1	5	1398	A	C2'-C3'-O3'	5.53	122.56	113.70
48	4	52	GLY	C-N-CA	5.53	135.53	121.70
1	5	687	U	N1-C1'-C2'	-5.53	105.92	112.00
1	5	2468	U	C4'-C3'-O3'	5.53	124.06	113.00
1	5	4975	G	O4'-C1'-N9	5.53	112.62	108.20
2	7	75	G	O4'-C1'-N9	5.53	112.62	108.20
34	e	35	TRP	CB-CG-CD1	-5.53	119.81	127.00
1	5	3735	G	C4'-C3'-O3'	-5.53	97.79	109.40
49	S2	844	U	C1'-O4'-C4'	-5.53	105.48	109.90
49	S2	393	U	O4'-C1'-N1	5.53	112.62	108.20
1	5	4944	C	N1-C1'-C2'	5.52	121.18	114.00
1	5	1359	G	N9-C1'-C2'	5.52	121.18	114.00
24	U	90	TYR	CB-CA-C	-5.52	99.36	110.40
56	SG	191	ARG	NE-CZ-NH2	-5.52	117.54	120.30
20	Q	184	ARG	CB-CG-CD	5.52	125.95	111.60
30	a	61	TYR	N-CA-C	-5.52	96.10	111.00
49	S2	924	G	N9-C1'-C2'	-5.52	105.93	112.00
1	5	2385	U	N1-C1'-C2'	5.52	121.17	114.00
34	e	47	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	5	2398	U	C2'-C3'-O3'	5.52	122.53	113.70
14	K	44	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	5	4326	G	N9-C1'-C2'	5.51	121.17	114.00
51	SB	198	GLU	OE1-CD-OE2	-5.51	116.69	123.30
1	5	1282	G	O5'-P-OP2	5.51	117.31	110.70
55	SF	204	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	5	3663	A	O4'-C1'-N9	-5.51	103.79	108.20
8	E	278	TYR	CB-CG-CD2	-5.51	117.69	121.00
1	5	421	C	C2'-C3'-O3'	5.51	122.51	113.70
49	S2	839	C	N1-C1'-C2'	5.51	121.16	114.00
65	SP	47	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	5	1534	A	P-O5'-C5'	5.50	129.70	120.90
1	5	3667	C	C2'-C3'-O3'	5.50	122.51	113.70
14	K	85	LEU	N-CA-CB	5.50	121.41	110.40
47	r	45	HIS	N-CA-CB	-5.50	100.70	110.60
1	5	2583	C	C2'-C3'-O3'	5.50	122.50	113.70
1	5	2754	G	N9-C1'-C2'	-5.50	105.95	112.00
1	5	1827	C	N1-C1'-C2'	5.50	121.15	114.00
24	U	101	ARG	NE-CZ-NH1	5.50	123.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	3905	A	N9-C1'-C2'	-5.49	105.96	112.00
1	5	4909	A	C1'-O4'-C4'	-5.49	105.50	109.90
1	5	4978	G	N9-C1'-C2'	5.49	121.14	114.00
20	Q	26	ARG	NE-CZ-NH1	5.49	123.05	120.30
8	E	153	HIS	N-CA-CB	-5.49	100.72	110.60
1	5	2852	U	O4'-C1'-C2'	-5.49	100.31	105.80
48	4	267	ASP	CA-C-O	-5.49	108.57	120.10
49	S2	447	A	C1'-O4'-C4'	-5.49	105.51	109.90
1	5	3634	G	C2'-C3'-O3'	5.49	122.48	113.70
10	G	235	ARG	NE-CZ-NH2	-5.48	117.56	120.30
32	c	78	ASN	N-CA-CB	5.48	120.47	110.60
49	S2	1292	C	O4'-C4'-C3'	-5.48	98.52	104.00
1	5	1734	G	N9-C1'-C2'	-5.48	105.97	112.00
20	Q	75	ARG	NE-CZ-NH2	-5.48	117.56	120.30
49	S2	1432	U	N1-C1'-C2'	5.48	121.12	114.00
1	5	210	C	N1-C1'-C2'	5.48	121.12	114.00
1	5	3912	U	C1'-C2'-O2'	-5.48	94.17	110.60
1	5	4731	G	N9-C1'-C2'	5.48	121.12	114.00
35	f	6	TRP	CB-CA-C	5.48	121.36	110.40
68	SS	11	HIS	CB-CA-C	5.48	121.35	110.40
1	5	2268	A	C2'-C3'-O3'	5.47	122.46	113.70
1	5	2858	A	N9-C1'-C2'	5.47	121.12	114.00
1	5	1211	G	N9-C1'-C2'	-5.47	105.98	112.00
1	5	2360	A	O4'-C1'-N9	-5.47	103.82	108.20
1	5	4713	G	C2'-C3'-O3'	5.47	122.46	113.70
14	K	114	ARG	NE-CZ-NH2	-5.47	117.56	120.30
49	S2	868	G	N9-C1'-C2'	-5.47	105.98	112.00
52	SC	97	PHE	CB-CG-CD2	-5.47	116.97	120.80
1	5	2056	G	N9-C1'-C2'	-5.47	105.98	112.00
21	R	60	ARG	NE-CZ-NH1	5.47	123.04	120.30
4	A	211	PHE	CB-CG-CD2	-5.47	116.97	120.80
49	S2	1419	C	O5'-P-OP2	-5.47	100.78	105.70
1	5	3886	G	N9-C1'-C2'	-5.47	105.98	112.00
1	5	4873	G	N9-C1'-C2'	5.46	121.10	114.00
49	S2	381	C	C3'-C2'-C1'	5.46	105.87	101.50
1	5	2117	G	O4'-C4'-C3'	-5.46	98.54	104.00
1	5	3906	A	N9-C1'-C2'	-5.46	105.99	112.00
63	SN	64	ARG	NE-CZ-NH1	5.46	123.03	120.30
64	SO	128	ARG	NE-CZ-NH2	-5.46	117.57	120.30
41	l	45	ARG	CB-CG-CD	5.46	125.79	111.60
1	5	1626	G	N9-C1'-C2'	-5.46	106.00	112.00
1	5	4909	A	O4'-C1'-N9	5.46	112.56	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	SD	65	ARG	NE-CZ-NH1	5.46	123.03	120.30
22	S	152	PHE	CB-CG-CD2	-5.45	116.98	120.80
49	S2	31	U	N1-C1'-C2'	5.45	121.09	114.00
49	S2	1698	C	N1-C1'-C2'	5.45	121.08	114.00
1	5	977	C	C5'-C4'-O4'	5.45	115.64	109.10
49	S2	604	A	C2'-C3'-O3'	5.45	122.42	113.70
27	X	129	ARG	NE-CZ-NH2	5.45	123.02	120.30
34	e	43	ASN	CB-CA-C	5.44	121.29	110.40
1	5	1464	C	N1-C1'-C2'	-5.44	106.01	112.00
1	5	4076	G	O4'-C1'-N9	5.44	112.56	108.20
38	i	26	HIS	N-CA-CB	5.44	120.39	110.60
49	S2	1315	U	C2'-C3'-O3'	5.44	122.40	113.70
22	S	171	ARG	CG-CD-NE	5.44	123.22	111.80
1	5	2054	U	C1'-O4'-C4'	-5.44	105.55	109.90
34	e	36	ARG	NE-CZ-NH1	-5.44	117.58	120.30
49	S2	619	A	C3'-C2'-C1'	-5.44	97.15	101.50
5	B	117	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	5	1852	U	N1-C1'-C2'	-5.43	106.02	112.00
1	5	2673	G	C1'-O4'-C4'	-5.43	105.55	109.90
14	K	28	LEU	N-CA-C	-5.43	96.33	111.00
1	5	372	A	N9-C1'-C2'	5.43	121.06	114.00
1	5	398	A	N9-C1'-C2'	5.43	121.06	114.00
4	A	16	PHE	CB-CA-C	5.43	121.26	110.40
14	K	114	ARG	NH1-CZ-NH2	-5.43	113.42	119.40
27	X	117	TYR	CB-CA-C	5.43	121.27	110.40
34	e	36	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	5	1365	C	C4'-C3'-O3'	5.43	123.86	113.00
1	5	3875	G	C2'-C3'-O3'	5.43	122.39	113.70
61	SL	100	ASN	N-CA-C	5.43	125.66	111.00
38	i	29	ARG	NE-CZ-NH1	5.43	123.01	120.30
47	r	103	ARG	NE-CZ-NH2	-5.43	117.59	120.30
49	S2	1557	C	N1-C1'-C2'	-5.43	106.03	112.00
1	5	2325	C	O4'-C1'-C2'	-5.42	100.38	105.80
1	5	4579	U	C6-N1-C1'	-5.42	113.61	121.20
1	5	4745	G	N9-C1'-C2'	5.42	121.05	114.00
5	B	119	TYR	CB-CA-C	5.42	121.25	110.40
1	5	1724	G	C8-N9-C1'	-5.42	119.95	127.00
37	h	70	ARG	NE-CZ-NH2	5.42	123.01	120.30
8	E	129	PHE	CB-CG-CD1	5.42	124.60	120.80
46	q	69	LEU	C-N-CA	5.42	135.25	121.70
1	5	280	G	C1'-O4'-C4'	-5.42	105.56	109.90
1	5	4915	G	C2'-C3'-O3'	5.42	122.37	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	S2	579	C	N1-C1'-C2'	-5.42	106.04	112.00
22	S	28	TYR	CA-CB-CG	5.41	123.69	113.40
1	5	1667	G	C2'-C3'-O3'	5.41	122.36	113.70
1	5	3898	G	C2'-C3'-O3'	5.41	122.36	113.70
18	O	128	ARG	NE-CZ-NH2	5.41	123.01	120.30
25	V	14	PHE	CB-CG-CD2	-5.41	117.01	120.80
64	SO	117	ARG	NE-CZ-NH1	-5.41	117.59	120.30
1	5	4481	U	C2-N1-C1'	5.41	124.19	117.70
31	b	6	ASN	CB-CA-C	5.41	121.22	110.40
1	5	1272	C	O4'-C1'-C2'	-5.41	100.39	105.80
1	5	2014	C	C2'-C3'-O3'	5.41	122.35	113.70
10	G	49	ARG	CG-CD-NE	-5.40	100.45	111.80
48	4	760	TYR	CB-CA-C	-5.40	99.59	110.40
1	5	3648	A	C1'-O4'-C4'	-5.40	105.58	109.90
44	o	26	TYR	CB-CG-CD1	5.40	124.24	121.00
1	5	693	C	C2'-C3'-O3'	5.39	122.33	113.70
1	5	4280	A	C4'-C3'-C2'	-5.39	97.21	102.60
21	R	108	ARG	CD-NE-CZ	5.39	131.15	123.60
49	S2	1643	U	C1'-C2'-O2'	-5.39	94.43	110.60
1	5	293	G	C2'-C3'-O3'	5.39	122.32	113.70
49	S2	578	C	C2'-C3'-O3'	5.39	122.32	113.70
19	P	42	ARG	CG-CD-NE	5.38	123.11	111.80
49	S2	444	G	O4'-C1'-C2'	-5.38	100.42	105.80
49	S2	1662	U	N1-C1'-C2'	-5.38	106.08	112.00
1	5	2348	G	O4'-C1'-N9	-5.38	103.89	108.20
42	m	106	ARG	NE-CZ-NH1	5.38	122.99	120.30
17	N	192	TRP	N-CA-CB	-5.38	100.92	110.60
20	Q	174	PHE	CB-CG-CD1	-5.38	117.04	120.80
49	S2	1415	C	N1-C1'-C2'	5.38	120.99	114.00
1	5	2272	C	C1'-C2'-O2'	-5.37	94.48	110.60
69	ST	67	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	5	1588	U	N1-C1'-C2'	5.37	120.98	114.00
1	5	4975	G	N9-C1'-C2'	-5.37	106.09	112.00
3	8	68	G	N9-C1'-C2'	5.37	120.97	114.00
13	J	32	ARG	CG-CD-NE	-5.37	100.53	111.80
22	S	81	TRP	N-CA-C	-5.37	96.51	111.00
2	7	59	G	N9-C1'-C2'	-5.36	106.10	112.00
8	E	236	TYR	CA-CB-CG	-5.36	103.21	113.40
38	i	39	PHE	CB-CG-CD1	-5.36	117.05	120.80
49	S2	426	A	C4'-C3'-O3'	5.36	123.72	113.00
1	5	1975	G	O4'-C1'-N9	-5.36	103.91	108.20
1	5	3625	G	C4'-C3'-O3'	-5.36	98.15	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	SJ	64	ASP	CB-CG-OD1	-5.36	113.48	118.30
4	A	19	HIS	N-CA-CB	-5.35	100.96	110.60
49	S2	1567	G	C1'-O4'-C4'	-5.35	105.62	109.90
49	S2	1292	C	C5'-C4'-C3'	5.35	124.56	116.00
1	5	3590	G	C2'-C3'-O3'	5.35	122.26	113.70
1	5	4228	G	O4'-C1'-N9	5.35	112.48	108.20
49	S2	1136	U	N1-C1'-C2'	5.35	120.95	114.00
1	5	703	G	N9-C1'-C2'	-5.34	106.12	112.00
1	5	82	U	N1-C1'-C2'	-5.34	106.12	112.00
3	8	34	U	C2-N1-C1'	-5.34	111.29	117.70
49	S2	56	G	N9-C1'-C2'	5.34	120.94	114.00
1	5	1390	G	N9-C1'-C2'	-5.34	106.13	112.00
1	5	3626	G	N9-C1'-C2'	-5.34	106.13	112.00
1	5	4302	U	N1-C1'-C2'	-5.34	106.13	112.00
11	H	115	ARG	CA-CB-CG	5.34	125.15	113.40
1	5	911	U	C2'-C3'-O3'	5.34	122.24	113.70
1	5	4883	C	O4'-C1'-N1	5.33	112.47	108.20
7	D	20	PHE	CB-CA-C	5.33	121.06	110.40
12	I	139	ARG	CB-CG-CD	-5.33	97.73	111.60
63	SN	55	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	5	416	U	N1-C1'-C2'	5.33	120.93	114.00
5	B	62	ARG	NE-CZ-NH2	-5.33	117.63	120.30
40	k	16	ARG	NE-CZ-NH1	5.33	122.97	120.30
49	S2	438	G	N9-C1'-C2'	5.33	120.93	114.00
49	S2	1666	C	N1-C1'-C2'	5.33	120.93	114.00
1	5	215	C	C4'-C3'-O3'	-5.33	98.22	109.40
1	5	3726	A	N9-C1'-C2'	5.33	120.92	114.00
23	T	140	PHE	CB-CA-C	-5.33	99.75	110.40
81	Sf	148	TYR	C-N-CA	5.33	135.02	121.70
9	F	136	ARG	CA-CB-CG	5.32	125.11	113.40
74	SY	20	ARG	NE-CZ-NH2	5.32	122.96	120.30
73	SX	17	ARG	NE-CZ-NH2	5.32	122.96	120.30
37	h	72	PHE	CB-CG-CD2	-5.32	117.08	120.80
49	S2	553	U	N1-C1'-C2'	5.32	120.92	114.00
78	Sc	44	ARG	CD-NE-CZ	5.32	131.05	123.60
27	X	79	PHE	CB-CG-CD1	5.32	124.52	120.80
67	SR	33	ARG	CG-CD-NE	-5.32	100.64	111.80
7	D	66	TYR	CB-CG-CD1	5.32	124.19	121.00
46	q	165	ASP	CB-CG-OD2	5.31	123.08	118.30
49	S2	1034	A	N9-C1'-C2'	5.31	120.91	114.00
17	N	192	TRP	CB-CG-CD1	-5.31	120.10	127.00
49	S2	646	G	N9-C1'-C2'	-5.31	106.16	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	E	212	TYR	CA-CB-CG	5.31	123.49	113.40
12	I	98	ARG	NE-CZ-NH2	5.31	122.95	120.30
25	V	97	TYR	CB-CA-C	5.31	121.02	110.40
13	J	147	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	5	1632	A	N9-C1'-C2'	-5.30	106.17	112.00
14	K	44	ASP	CB-CG-OD1	5.30	123.07	118.30
17	N	143	ARG	NE-CZ-NH2	-5.30	117.65	120.30
47	r	77	TYR	CB-CG-CD2	-5.30	117.82	121.00
48	4	55	ARG	C-N-CA	5.30	134.95	121.70
62	SM	26	LEU	CA-CB-CG	5.30	127.49	115.30
1	5	2056	G	P-O5'-C5'	-5.30	112.42	120.90
1	5	4528	G	O4'-C1'-C2'	-5.30	100.50	105.80
15	L	198	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	5	3753	G	C2'-C3'-O3'	5.29	122.17	113.70
50	SA	39	TYR	CA-CB-CG	5.29	123.46	113.40
1	5	212	A	N9-C1'-C2'	5.29	120.88	114.00
48	4	826	ASP	N-CA-C	-5.29	96.70	111.00
49	S2	1202	U	C2'-C3'-O3'	5.29	122.17	113.70
41	l	45	ARG	CG-CD-NE	-5.29	100.69	111.80
69	ST	83	GLN	CA-CB-CG	5.29	125.04	113.40
52	SC	236	PHE	CB-CG-CD1	-5.29	117.10	120.80
58	SI	49	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	5	2817	C	C2'-C3'-O3'	5.29	122.16	113.70
6	C	110	ARG	NE-CZ-NH1	5.29	122.94	120.30
49	S2	114	G	N9-C1'-C2'	-5.29	106.19	112.00
20	Q	75	ARG	CG-CD-NE	5.28	122.89	111.80
61	SL	17	PHE	N-CA-CB	5.28	120.11	110.60
1	5	3692	A	N9-C1'-C2'	-5.28	106.19	112.00
49	S2	983	A	C5'-C4'-O4'	5.28	115.44	109.10
1	5	3739	C	C2'-C3'-O3'	5.28	122.15	113.70
49	S2	800	U	O4'-C4'-C3'	-5.28	98.72	104.00
1	5	2263	A	C2'-C3'-O3'	5.28	122.14	113.70
9	F	228	HIS	CA-CB-CG	-5.28	104.63	113.60
5	B	246	ARG	NE-CZ-NH2	-5.28	117.66	120.30
82	Sg	15	ASN	CB-CA-C	5.28	120.95	110.40
5	B	274	TYR	CB-CG-CD1	-5.27	117.84	121.00
27	X	137	TYR	CA-CB-CG	5.27	123.42	113.40
33	d	44	ARG	NE-CZ-NH2	-5.27	117.66	120.30
48	4	409	ARG	CB-CA-C	5.27	120.94	110.40
60	SK	43	LEU	CA-CB-CG	5.27	127.42	115.30
63	SN	55	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	5	1211	G	C4'-C3'-C2'	-5.27	97.33	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1390	G	C2'-C3'-O3'	5.27	122.13	113.70
1	5	4497	U	C2'-C3'-O3'	5.27	122.13	113.70
13	J	54	ARG	NE-CZ-NH1	5.26	122.93	120.30
35	f	102	ARG	NE-CZ-NH1	5.26	122.93	120.30
49	S2	1243	U	O5'-P-OP2	-5.26	100.96	105.70
74	SY	86	GLU	CB-CG-CD	-5.26	99.99	114.20
35	f	19	ARG	CG-CD-NE	-5.26	100.75	111.80
46	q	204	LEU	C-N-CA	-5.26	108.55	121.70
1	5	4736	C	N1-C1'-C2'	5.26	120.84	114.00
13	J	147	ARG	NE-CZ-NH1	5.26	122.93	120.30
49	S2	1097	G	C2'-C3'-O3'	5.26	122.11	113.70
9	F	136	ARG	NE-CZ-NH1	5.25	122.93	120.30
46	q	22	ASP	CB-CG-OD2	5.25	123.03	118.30
1	5	216	C	C2'-C3'-O3'	5.25	122.10	113.70
48	4	542	GLY	N-CA-C	-5.25	99.98	113.10
51	SB	67	PHE	CB-CG-CD2	-5.25	117.13	120.80
1	5	4463	U	O4'-C1'-C2'	-5.25	100.55	105.80
25	V	128	LEU	CA-CB-CG	5.25	127.37	115.30
58	SI	188	TYR	CB-CG-CD1	-5.24	117.86	121.00
48	4	102	LEU	N-CA-C	-5.24	96.85	111.00
5	B	119	TYR	CA-CB-CG	-5.24	103.45	113.40
49	S2	943	U	C6-N1-C1'	-5.24	113.86	121.20
17	N	114	ARG	NE-CZ-NH2	-5.24	117.68	120.30
49	S2	501	C	O4'-C1'-C2'	-5.24	100.56	105.80
56	SG	198	ARG	NE-CZ-NH1	5.24	122.92	120.30
36	g	14	ASN	N-CA-C	-5.24	96.86	111.00
19	P	30	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	5	2753	G	C2'-C3'-O3'	5.23	122.07	113.70
1	5	3666	C	N1-C1'-C2'	-5.23	106.24	112.00
46	q	117	ALA	C-N-CD	5.23	139.39	128.40
48	4	47	ALA	O-C-N	5.23	131.07	122.70
69	ST	53	PHE	N-CA-CB	-5.23	101.18	110.60
28	Y	87	ARG	CD-NE-CZ	5.23	130.92	123.60
49	S2	368	U	C2'-C3'-O3'	5.23	122.07	113.70
56	SG	74	ARG	NE-CZ-NH1	5.23	122.92	120.30
35	f	19	ARG	CA-CB-CG	5.23	124.90	113.40
48	4	123	ASP	C-N-CA	5.22	133.27	122.30
49	S2	1578	U	O4'-C1'-N1	-5.22	104.02	108.20
49	S2	1663	A	C1'-O4'-C4'	-5.22	105.72	109.90
1	5	4328	G	N9-C1'-C2'	-5.22	106.26	112.00
5	B	25	HIS	CB-CA-C	5.22	120.84	110.40
1	5	1886	G	N9-C1'-C2'	-5.22	106.26	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	4966	A	C4-N9-C1'	5.22	135.69	126.30
4	A	89	TYR	CB-CA-C	5.22	120.84	110.40
9	F	58	HIS	N-CA-CB	5.22	120.00	110.60
49	S2	1093	A	C5'-C4'-O4'	5.22	115.36	109.10
1	5	2325	C	C2'-C3'-O3'	5.22	122.05	113.70
1	5	1	C	C3'-C2'-C1'	-5.22	97.33	101.50
14	K	144	ASP	CB-CG-OD2	5.22	123.00	118.30
20	Q	38	ARG	NE-CZ-NH2	-5.21	117.69	120.30
49	S2	1542	C	C1'-C2'-O2'	-5.21	94.96	110.60
28	Y	45	ARG	NE-CZ-NH1	5.21	122.91	120.30
49	S2	65	C	C2'-C3'-O3'	5.21	122.04	113.70
1	5	1484	G	O4'-C4'-C3'	-5.21	98.79	104.00
49	S2	1167	G	N9-C1'-C2'	5.21	120.78	114.00
1	5	223	G	N9-C1'-C2'	-5.21	106.27	112.00
1	5	2262	G	N9-C1'-C2'	5.21	120.77	114.00
1	5	1642	A	C5'-C4'-O4'	5.21	115.35	109.10
33	d	24	GLU	CA-CB-CG	5.21	124.86	113.40
1	5	2467	U	N1-C1'-C2'	-5.20	106.28	112.00
21	R	108	ARG	CG-CD-NE	5.20	122.73	111.80
56	SG	156	TYR	CB-CA-C	5.20	120.81	110.40
1	5	931	C	N1-C1'-C2'	5.20	120.76	114.00
20	Q	168	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	5	1698	C	O5'-P-OP1	-5.20	101.02	105.70
46	q	72	ASN	C-N-CD	-5.20	109.16	120.60
1	5	267	G	C2'-C3'-O3'	5.20	122.02	113.70
28	Y	87	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	5	2310	C	C2'-C3'-O3'	5.20	122.01	113.70
18	O	178	ARG	NE-CZ-NH2	-5.20	117.70	120.30
49	S2	1579	A	C2'-C3'-O3'	5.20	122.01	113.70
54	SE	30	ARG	NE-CZ-NH1	5.20	122.90	120.30
68	SS	124	ARG	CG-CD-NE	5.20	122.71	111.80
21	R	124	TYR	CA-CB-CG	5.19	123.27	113.40
1	5	63	G	N9-C1'-C2'	5.19	120.75	114.00
1	5	1394	G	N9-C1'-C2'	5.19	120.75	114.00
14	K	154	ASP	CB-CG-OD2	5.19	122.97	118.30
49	S2	672	A	C3'-C2'-C1'	-5.19	97.35	101.50
1	5	272	U	N1-C1'-C2'	5.18	120.74	114.00
17	N	63	ARG	NE-CZ-NH2	-5.18	117.71	120.30
48	4	196	GLU	N-CA-CB	5.18	119.93	110.60
49	S2	594	A	C4'-C3'-O3'	5.18	123.37	113.00
14	K	44	ASP	CA-C-O	-5.18	109.22	120.10
35	f	51	TYR	CA-CB-CG	5.18	123.25	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	q	118	PRO	CA-N-CD	-5.18	104.24	111.50
68	SS	95	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	5	194	C	N1-C1'-C2'	-5.18	106.30	112.00
48	4	794	PHE	N-CA-C	-5.18	97.02	111.00
49	S2	1292	C	C5'-C4'-O4'	5.18	115.31	109.10
1	5	172	C	O4'-C1'-C2'	-5.18	100.62	105.80
17	N	65	ARG	NE-CZ-NH2	5.18	122.89	120.30
53	SD	159	HIS	CA-CB-CG	-5.18	104.80	113.60
39	j	76	HIS	CB-CA-C	5.17	120.75	110.40
41	l	21	ARG	NE-CZ-NH1	5.17	122.89	120.30
49	S2	919	A	C2'-C3'-O3'	-5.17	98.12	109.50
1	5	268	G	C2'-C3'-O3'	5.17	121.97	113.70
1	5	2443	G	N9-C1'-C2'	5.17	120.72	114.00
15	L	99	ASP	CB-CG-OD1	-5.17	113.65	118.30
55	SF	188	TYR	CA-CB-CG	-5.17	103.58	113.40
1	5	4165	C	C2'-C3'-O3'	5.17	121.97	113.70
1	5	4543	G	N9-C1'-C2'	5.17	120.72	114.00
10	G	53	ARG	NE-CZ-NH1	5.17	122.88	120.30
22	S	29	ARG	CB-CA-C	5.17	120.74	110.40
49	S2	1150	A	N9-C1'-C2'	5.17	120.72	114.00
1	5	2597	G	N9-C1'-C2'	5.16	120.71	114.00
21	R	103	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	5	2256	C	N1-C1'-C2'	5.16	120.71	114.00
17	N	59	TYR	CA-CB-CG	5.16	123.21	113.40
1	5	961	G	C4'-C3'-O3'	5.16	123.32	113.00
2	7	6	C	C2'-C3'-O3'	5.16	121.96	113.70
2	7	65	G	C2'-C3'-O3'	5.16	121.95	113.70
7	D	268	ARG	CG-CD-NE	5.16	122.64	111.80
1	5	664	G	C4'-C3'-O3'	5.16	123.32	113.00
3	8	1	C	C5'-C4'-C3'	5.16	124.25	116.00
35	f	6	TRP	CA-CB-CG	-5.16	103.90	113.70
48	4	448	GLN	CB-CA-C	-5.16	100.08	110.40
23	T	8	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	5	2323	C	C2'-C3'-O3'	5.16	121.95	113.70
7	D	130	TYR	CA-CB-CG	-5.16	103.60	113.40
46	q	131	GLY	C-N-CD	5.16	139.23	128.40
81	Sf	138	ARG	CD-NE-CZ	5.15	130.81	123.60
30	a	6	ARG	NE-CZ-NH1	5.15	122.88	120.30
58	SI	188	TYR	CD1-CG-CD2	5.15	123.56	117.90
22	S	77	ASN	CB-CA-C	5.15	120.70	110.40
1	5	2879	A	N9-C1'-C2'	5.14	120.69	114.00
9	F	197	TYR	N-CA-CB	5.14	119.86	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	S2	1394	G	O4'-C1'-C2'	-5.14	100.66	105.80
1	5	4436	U	N1-C1'-C2'	-5.14	106.34	112.00
1	5	1850	A	N9-C1'-C2'	5.14	120.68	114.00
49	S2	1603	G	N9-C1'-C2'	5.14	120.68	114.00
20	Q	68	ARG	CG-CD-NE	-5.14	101.01	111.80
1	5	107	G	N9-C1'-C2'	-5.14	106.35	112.00
1	5	2044	U	C3'-C2'-C1'	5.14	105.61	101.50
1	5	4163	U	C4'-C3'-C2'	-5.14	97.46	102.60
1	5	2785	C	N1-C1'-C2'	5.13	120.67	114.00
1	5	2787	A	N9-C1'-C2'	-5.13	106.35	112.00
1	5	405	U	C2'-C3'-O3'	5.13	121.91	113.70
34	e	47	ARG	N-CA-C	-5.13	97.14	111.00
48	4	272	LYS	C-N-CA	5.13	134.53	121.70
1	5	703	G	O4'-C1'-N9	5.13	112.30	108.20
1	5	1577	G	N9-C1'-C2'	-5.13	106.36	112.00
18	O	140	ARG	NE-CZ-NH1	-5.13	117.73	120.30
5	B	161	ARG	NE-CZ-NH1	5.13	122.86	120.30
31	b	45	PHE	CB-CG-CD1	-5.13	117.21	120.80
49	S2	996	A	C4-N9-C1'	-5.13	117.07	126.30
3	8	46	G	N9-C1'-C2'	5.12	120.66	114.00
17	N	130	PHE	CB-CA-C	5.12	120.65	110.40
48	4	699	GLY	O-C-N	5.12	130.90	122.70
1	5	2529	A	O4'-C1'-N9	5.12	112.30	108.20
7	D	248	ARG	NE-CZ-NH1	5.12	122.86	120.30
81	Sf	138	ARG	CG-CD-NE	5.12	122.56	111.80
1	5	1615	C	N1-C1'-C2'	-5.12	106.37	112.00
15	L	99	ASP	N-CA-C	-5.12	97.18	111.00
36	g	4	ARG	NE-CZ-NH2	-5.12	117.74	120.30
46	q	205	ASP	CB-CG-OD2	5.12	122.91	118.30
49	S2	1567	G	N9-C1'-C2'	5.12	120.65	114.00
29	Z	51	ARG	NE-CZ-NH1	5.12	122.86	120.30
47	r	77	TYR	N-CA-CB	-5.12	101.39	110.60
1	5	648	G	C2'-C3'-O3'	5.11	121.88	113.70
1	5	658	C	C2'-C3'-O3'	5.11	121.88	113.70
1	5	2075	G	N9-C1'-C2'	-5.11	106.37	112.00
49	S2	102	A	C2'-C3'-O3'	5.11	121.88	113.70
22	S	10	TYR	CB-CA-C	5.11	120.62	110.40
29	Z	36	ARG	NE-CZ-NH2	-5.11	117.74	120.30
49	S2	797	C	O4'-C1'-C2'	-5.11	100.69	105.80
21	R	9	ARG	CG-CD-NE	5.11	122.53	111.80
49	S2	141	A	C2'-C3'-O3'	5.11	121.88	113.70
29	Z	51	ARG	NE-CZ-NH2	-5.11	117.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	S2	72	C	O4'-C1'-N1	5.11	112.29	108.20
1	5	297	U	N1-C1'-C2'	-5.11	106.38	112.00
1	5	3880	G	C1'-C2'-O2'	-5.11	95.28	110.60
1	5	2538	U	O5'-P-OP1	-5.11	101.11	105.70
1	5	4276	G	N9-C1'-C2'	-5.11	106.38	112.00
65	SP	10	ARG	NE-CZ-NH2	-5.11	117.75	120.30
14	K	91	ASP	N-CA-C	5.10	124.78	111.00
46	q	45	MET	CB-CA-C	5.10	120.61	110.40
6	C	143	ARG	NE-CZ-NH1	5.10	122.85	120.30
46	q	68	HIS	C-N-CA	5.10	134.45	121.70
48	4	539	GLU	O-C-N	-5.10	114.54	122.70
33	d	85	ARG	CG-CD-NE	5.10	122.50	111.80
48	4	239	LYS	CD-CE-NZ	-5.10	99.98	111.70
50	SA	9	GLN	CB-CG-CD	-5.10	98.35	111.60
82	Sg	36	ARG	NE-CZ-NH2	-5.10	117.75	120.30
21	R	117	ARG	CB-CA-C	5.10	120.59	110.40
48	4	433	ASN	CB-CA-C	5.09	120.59	110.40
56	SG	205	GLU	OE1-CD-OE2	5.09	129.41	123.30
1	5	3666	C	C2'-C3'-O3'	5.09	121.84	113.70
3	8	125	C	O4'-C1'-N1	-5.09	104.13	108.20
14	K	153	ASP	CB-CG-OD2	5.09	122.88	118.30
9	F	72	ARG	NE-CZ-NH1	5.09	122.84	120.30
33	d	87	ARG	N-CA-CB	5.09	119.76	110.60
1	5	2117	G	C1'-O4'-C4'	-5.08	105.83	109.90
1	5	218	A	N9-C1'-C2'	-5.08	106.41	112.00
1	5	3870	C	N1-C1'-C2'	5.08	120.61	114.00
3	8	104	A	P-O5'-C5'	5.08	129.03	120.90
24	U	46	ARG	NE-CZ-NH1	5.08	122.84	120.30
49	S2	73	C	O4'-C1'-C2'	-5.08	100.72	105.80
49	S2	853	C	C2'-C3'-O3'	5.08	121.83	113.70
1	5	1361	G	C2'-C3'-O3'	5.08	121.83	113.70
1	5	3667	C	N1-C1'-C2'	-5.08	106.41	112.00
14	K	45	ASP	CB-CG-OD2	5.08	122.87	118.30
28	Y	126	ARG	CD-NE-CZ	5.08	130.71	123.60
28	Y	126	ARG	CG-CD-NE	5.08	122.46	111.80
49	S2	1700	C	N1-C1'-C2'	-5.08	106.42	112.00
27	X	137	TYR	CB-CG-CD2	-5.07	117.96	121.00
28	Y	87	ARG	CG-CD-NE	5.07	122.45	111.80
1	5	1359	G	O4'-C4'-C3'	-5.07	98.93	104.00
1	5	4975	G	C1'-O4'-C4'	-5.07	105.84	109.90
1	5	2614	C	N1-C1'-C2'	-5.07	106.42	112.00
15	L	103	ARG	CA-CB-CG	5.07	124.56	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	S2	524	U	C2'-C3'-O3'	5.07	121.81	113.70
1	5	3627	G	C2'-C3'-O3'	5.07	121.81	113.70
49	S2	410	G	O5'-P-OP1	-5.07	101.14	105.70
1	5	336	A	N9-C1'-C2'	-5.07	106.43	112.00
29	Z	36	ARG	CG-CD-NE	5.07	122.44	111.80
49	S2	1080	A	O4'-C1'-N9	5.07	112.25	108.20
1	5	3804	G	N9-C1'-C2'	-5.06	106.43	112.00
1	5	3863	C	N1-C1'-C2'	5.06	120.58	114.00
1	5	4936	G	C4'-C3'-O3'	5.06	123.12	113.00
1	5	1887	G	C4'-C3'-C2'	-5.06	97.54	102.60
1	5	4563	U	C2-N1-C1'	5.06	123.77	117.70
46	q	23	ASP	CB-CG-OD2	5.06	122.85	118.30
13	J	170	HIS	CB-CA-C	5.06	120.52	110.40
14	K	150	ASP	CB-CG-OD2	5.06	122.85	118.30
49	S2	798	A	C4'-C3'-C2'	-5.06	97.54	102.60
1	5	1672	U	N1-C1'-C2'	5.06	120.57	114.00
1	5	4404	U	C3'-C2'-C1'	5.06	105.54	101.50
17	N	143	ARG	CB-CG-CD	5.06	124.75	111.60
28	Y	74	TYR	N-CA-CB	5.06	119.70	110.60
1	5	2459	G	N9-C1'-C2'	-5.05	106.44	112.00
14	K	27	ALA	N-CA-C	5.05	124.65	111.00
59	SJ	175	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	5	4670	C	P-O5'-C5'	5.05	128.99	120.90
20	Q	33	ARG	CB-CG-CD	5.05	124.74	111.60
1	5	1268	G	N9-C1'-C2'	5.05	120.57	114.00
1	5	1895	G	N9-C1'-C2'	5.05	120.57	114.00
1	5	2054	U	N1-C1'-C2'	5.05	120.57	114.00
1	5	54	G	C2'-C3'-O3'	5.05	121.78	113.70
1	5	4498	U	C1'-C2'-O2'	5.05	125.75	110.60
4	A	209	HIS	CA-CB-CG	-5.05	105.02	113.60
49	S2	1368	U	N1-C1'-C2'	-5.05	106.45	112.00
48	4	242	GLY	C-N-CA	5.05	134.32	121.70
82	Sg	125	ARG	CG-CD-NE	-5.04	101.21	111.80
1	5	20	U	N1-C1'-C2'	-5.04	106.45	112.00
1	5	3773	U	O4'-C4'-C3'	-5.04	98.96	104.00
5	B	257	TRP	N-CA-CB	5.04	119.68	110.60
12	I	181	PHE	CB-CG-CD1	5.04	124.33	120.80
72	SW	57	ARG	CG-CD-NE	5.04	122.39	111.80
1	5	4398	C	C2'-C3'-O3'	5.04	121.76	113.70
13	J	99	PHE	CB-CG-CD2	-5.04	117.27	120.80
58	SI	28	GLU	N-CA-C	-5.04	97.39	111.00
1	5	1067	G	C2'-C3'-O3'	5.04	121.76	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	88	A	C1'-C2'-O2'	-5.04	95.49	110.60
23	T	19	PHE	CB-CA-C	-5.04	100.33	110.40
1	5	74	G	N9-C1'-C2'	5.03	120.54	114.00
1	5	2361	G	P-O3'-C3'	5.03	125.74	119.70
81	Sf	146	LEU	N-CA-C	-5.03	97.41	111.00
14	K	44	ASP	CA-CB-CG	5.03	124.47	113.40
57	SH	99	ARG	CG-CD-NE	5.03	122.37	111.80
1	5	1398	A	C3'-C2'-C1'	-5.03	97.48	101.50
1	5	2116	C	C2'-C3'-O3'	5.03	121.75	113.70
49	S2	385	G	N9-C1'-C2'	5.03	120.54	114.00
58	SI	5	ARG	NE-CZ-NH1	5.03	122.81	120.30
73	SX	20	HIS	CA-CB-CG	-5.03	105.05	113.60
1	5	4373	G	C3'-C2'-C1'	-5.03	97.48	101.50
27	X	56	ARG	CG-CD-NE	-5.03	101.24	111.80
1	5	2275	G	C2'-C3'-O3'	5.03	121.74	113.70
64	SO	55	ARG	NE-CZ-NH2	-5.03	117.79	120.30
34	e	44	ARG	NE-CZ-NH1	5.03	122.81	120.30
81	Sf	150	PHE	CB-CG-CD1	5.03	124.32	120.80
1	5	514	U	O4'-C4'-C3'	-5.02	98.98	104.00
1	5	1216	C	C2'-C3'-O3'	5.02	121.73	113.70
13	J	146	ARG	NE-CZ-NH1	-5.02	117.79	120.30
22	S	28	TYR	CB-CG-CD2	-5.02	117.99	121.00
73	SX	5	ARG	NE-CZ-NH2	5.02	122.81	120.30
1	5	352	G	C3'-C2'-C1'	5.02	105.51	101.50
1	5	1953	U	N1-C1'-C2'	5.02	120.52	114.00
1	5	2533	C	N1-C1'-C2'	5.01	120.52	114.00
17	N	6	TYR	CA-CB-CG	-5.01	103.87	113.40
49	S2	370	G	O5'-P-OP1	-5.01	101.19	105.70
1	5	2827	G	O4'-C4'-C3'	-5.01	98.99	104.00
20	Q	33	ARG	N-CA-CB	5.01	119.62	110.60
1	5	1281	G	C3'-C2'-C1'	5.01	105.51	101.50
1	5	1591	U	N1-C1'-C2'	5.01	120.52	114.00
1	5	4224	A	N9-C1'-C2'	-5.01	106.49	112.00
52	SC	223	TYR	CB-CG-CD1	-5.01	117.99	121.00
1	5	1272	C	C5'-C4'-O4'	5.01	115.11	109.10
1	5	1864	G	C2'-C3'-O3'	5.01	121.71	113.70
49	S2	161	U	N1-C1'-C2'	5.01	120.51	114.00
58	SI	77	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	5	1440	U	C4'-C3'-C2'	-5.01	97.59	102.60
18	O	117	ARG	NE-CZ-NH2	-5.01	117.80	120.30
66	SQ	138	ARG	CG-CD-NE	5.01	122.31	111.80
9	F	83	PHE	N-CA-CB	-5.00	101.59	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1479	G	C1'-C2'-O2'	-5.00	95.59	110.60
1	5	1398	A	P-O3'-C3'	5.00	125.70	119.70
1	5	4454	G	C2'-C3'-O3'	5.00	121.70	113.70
37	h	72	PHE	CB-CG-CD1	5.00	124.30	120.80
49	S2	28	U	C4'-C3'-O3'	5.00	123.00	113.00
49	S2	967	C	N1-C1'-C2'	-5.00	106.50	112.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
49	S2	1109	C	C1'

All (507) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
48	4	102	LEU	Mainchain
48	4	108	HIS	Peptide
48	4	111	PHE	Sidechain
48	4	112	SER	Mainchain,Peptide
48	4	121	VAL	Mainchain
48	4	123	ASP	Mainchain
48	4	193	GLY	Mainchain
48	4	196	GLU	Peptide
48	4	197	SER	Peptide
48	4	199	PRO	Peptide
48	4	242	GLY	Mainchain,Peptide
48	4	245	GLY	Peptide
48	4	246	PRO	Peptide
48	4	247	ALA	Peptide
48	4	266	PHE	Mainchain,Peptide
48	4	269	ALA	Mainchain
48	4	272	LYS	Peptide
48	4	325	SER	Peptide
48	4	4	PHE	Peptide
48	4	403	PRO	Peptide
48	4	406	ASP	Peptide
48	4	408	GLY	Peptide
48	4	42	LYS	Mainchain
48	4	495	ARG	Mainchain,Peptide
48	4	540	GLU	Peptide
48	4	55	ARG	Peptide
48	4	573	SER	Peptide

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Mol	Chain	Res	Type	Group
48	4	574	ASP	Peptide
48	4	575	PRO	Mainchain
48	4	667	LYS	Peptide
48	4	669	VAL	Peptide
48	4	699	GLY	Mainchain
48	4	702	PHE	Sidechain
48	4	775	GLN	Peptide
48	4	827	ASN	Peptide
48	4	847	GLY	Peptide
1	5	100	C	Sidechain
1	5	103	G	Sidechain
1	5	1167	C	Sidechain
1	5	120	A	Sidechain
1	5	1214	C	Sidechain
1	5	1281	G	Sidechain
1	5	1319	U	Sidechain
1	5	1324	A	Sidechain
1	5	1355	G	Sidechain
1	5	1398	A	Sidechain
1	5	147	A	Sidechain
1	5	1501	C	Sidechain
1	5	151	G	Sidechain
1	5	1522	G	Sidechain
1	5	1534	A	Sidechain
1	5	157	U	Sidechain
1	5	1625	G	Sidechain
1	5	1627	G	Sidechain
1	5	1631	A	Sidechain
1	5	1658	G	Sidechain
1	5	1668	A	Sidechain
1	5	1671	U	Sidechain
1	5	1676	C	Sidechain
1	5	172	C	Sidechain
1	5	1733	G	Sidechain
1	5	1887	G	Sidechain
1	5	1894	C	Sidechain
1	5	1938	C	Sidechain
1	5	2046	G	Sidechain
1	5	2056	G	Sidechain
1	5	2077	C	Sidechain
1	5	2082	G	Sidechain
1	5	2087	C	Sidechain

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Mol	Chain	Res	Type	Group
1	5	22	G	Sidechain
1	5	2263	A	Sidechain
1	5	2268	A	Sidechain
1	5	2271	C	Sidechain
1	5	2305	U	Sidechain
1	5	2325	C	Sidechain
1	5	235	A	Sidechain
1	5	2360	A	Sidechain
1	5	2361	G	Sidechain
1	5	2394	G	Sidechain
1	5	2403	A	Sidechain
1	5	2406	G	Sidechain
1	5	2436	U	Sidechain
1	5	2438	A	Sidechain
1	5	2446	C	Sidechain
1	5	2450	G	Sidechain
1	5	2465	C	Sidechain
1	5	2513	A	Sidechain
1	5	2515	G	Sidechain
1	5	2517	A	Sidechain
1	5	2553	A	Sidechain
1	5	2581	A	Sidechain
1	5	2649	G	Sidechain
1	5	2666	U	Sidechain
1	5	2675	G	Sidechain
1	5	2769	U	Sidechain
1	5	2796	G	Sidechain
1	5	280	G	Sidechain
1	5	2812	A	Sidechain
1	5	2827	G	Sidechain
1	5	2851	G	Sidechain
1	5	2858	A	Sidechain
1	5	291	U	Sidechain
1	5	292	G	Sidechain
1	5	293	G	Sidechain
1	5	294	G	Sidechain
1	5	31	U	Sidechain
1	5	315	G	Sidechain
1	5	332	C	Sidechain
1	5	336	A	Sidechain
1	5	352	G	Sidechain
1	5	354	U	Sidechain

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Mol	Chain	Res	Type	Group
1	5	3621	A	Sidechain
1	5	3635	A	Sidechain
1	5	3648	A	Sidechain
1	5	3653	A	Sidechain
1	5	3692	A	Sidechain
1	5	3726	A	Sidechain
1	5	3774	A	Sidechain
1	5	3790	U	Sidechain
1	5	3791	C	Sidechain
1	5	383	A	Sidechain
1	5	384	A	Sidechain
1	5	3843	C	Sidechain
1	5	3844	U	Sidechain
1	5	3871	A	Sidechain
1	5	3880	G	Sidechain
1	5	3881	G	Sidechain
1	5	3901	A	Sidechain
1	5	3938	G	Sidechain
1	5	405	U	Sidechain
1	5	4076	G	Sidechain
1	5	4162	C	Sidechain
1	5	417	G	Sidechain
1	5	42	A	Sidechain
1	5	4228	G	Sidechain
1	5	4229	U	Sidechain
1	5	4234	A	Sidechain
1	5	4270	C	Sidechain
1	5	4275	G	Sidechain
1	5	4280	A	Sidechain
1	5	4282	A	Sidechain
1	5	43	U	Sidechain
1	5	4330	G	Sidechain
1	5	4341	C	Sidechain
1	5	4371	G	Sidechain
1	5	4373	G	Sidechain
1	5	4385	A	Sidechain
1	5	4404	U	Sidechain
1	5	4463	U	Sidechain
1	5	4464	A	Sidechain
1	5	4497	U	Sidechain
1	5	4498	U	Sidechain
1	5	4510	A	Sidechain

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Mol	Chain	Res	Type	Group
1	5	4519	C	Sidechain
1	5	4528	G	Sidechain
1	5	4531	U	Sidechain
1	5	4548	A	Sidechain
1	5	4563	U	Sidechain
1	5	4564	A	Sidechain
1	5	4589	A	Sidechain
1	5	4600	G	Sidechain
1	5	4670	C	Sidechain
1	5	4677	U	Sidechain
1	5	4693	C	Sidechain
1	5	4763	U	Sidechain
1	5	4871	C	Sidechain
1	5	4911	A	Sidechain
1	5	4965	U	Sidechain
1	5	4966	A	Sidechain
1	5	4976	U	Sidechain
1	5	4981	G	Sidechain
1	5	5006	U	Sidechain
1	5	5040	U	Sidechain
1	5	5043	A	Sidechain
1	5	5050	C	Sidechain
1	5	5066	U	Sidechain
1	5	514	U	Sidechain
1	5	53	C	Sidechain
1	5	54	G	Sidechain
1	5	62	A	Sidechain
1	5	664	G	Sidechain
1	5	84	A	Sidechain
1	5	85	G	Sidechain
1	5	89	C	Sidechain
1	5	92	C	Sidechain
1	5	93	G	Sidechain
1	5	94	A	Sidechain
1	5	964	A	Sidechain
1	5	97	G	Sidechain
1	5	99	A	Sidechain
2	7	42	A	Sidechain
2	7	56	G	Sidechain
3	8	104	A	Sidechain
3	8	14	U	Sidechain
3	8	34	U	Sidechain

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Mol	Chain	Res	Type	Group
3	8	35	C	Sidechain
3	8	38	U	Sidechain
3	8	39	G	Sidechain
3	8	60	G	Sidechain
3	8	65	A	Sidechain
3	8	73	U	Sidechain
3	8	9	A	Sidechain
3	8	94	G	Sidechain
4	A	18	ALA	Peptide
4	A	194	ASN	Peptide
4	A	196	TRP	Peptide
4	A	209	HIS	Sidechain
4	A	211	PHE	Sidechain
4	A	215	ASN	Peptide
5	B	100	ARG	Sidechain
5	B	102	PHE	Peptide
5	B	117	ARG	Sidechain
5	B	119	TYR	Sidechain
5	B	142	GLY	Peptide
5	B	15	GLY	Peptide
5	B	16	PHE	Peptide
5	B	179	HIS	Sidechain
5	B	274	TYR	Sidechain
5	B	322	HIS	Peptide
5	B	379	PHE	Peptide
5	B	387	ALA	Peptide
5	B	388	PHE	Peptide
6	C	102	PHE	Sidechain
6	C	113	ARG	Peptide
6	C	264	TYR	Peptide
6	C	309	ILE	Peptide
6	C	41	HIS	Sidechain
7	D	129	GLU	Peptide
7	D	190	PHE	Peptide
7	D	198	HIS	Sidechain
7	D	20	PHE	Peptide
7	D	261	VAL	Peptide
7	D	266	TRP	Peptide
7	D	30	TYR	Peptide
7	D	44	TYR	Sidechain
8	E	102	VAL	Peptide
8	E	103	VAL	Peptide

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Mol	Chain	Res	Type	Group
8	E	111	TYR	Peptide
8	E	123	SER	Peptide
8	E	152	ARG	Peptide
8	E	177	LEU	Peptide
8	E	216	LYS	Peptide
8	E	224	GLN	Peptide
8	E	230	ASP	Peptide
8	E	235	LYS	Peptide
8	E	278	TYR	Sidechain
8	E	41	SER	Peptide
9	F	127	LEU	Peptide
9	F	197	TYR	Peptide
9	F	228	HIS	Sidechain
9	F	81	GLY	Peptide
9	F	82	ASN	Peptide
10	G	101	LYS	Peptide
10	G	261	LEU	Peptide
10	G	54	PHE	Sidechain
11	H	156	ASN	Sidechain,Peptide
11	H	50	LYS	Peptide
12	I	113	THR	Peptide
12	I	139	ARG	Sidechain
12	I	77	VAL	Peptide
12	I	93	PRO	Peptide
13	J	87	LEU	Peptide
13	J	99	PHE	Sidechain
14	K	114	ARG	Mainchain
14	K	130	LYS	Mainchain
14	K	27	ALA	Peptide
14	K	44	ASP	Mainchain
14	K	86	LYS	Peptide
15	L	146	LEU	Peptide
15	L	147	ALA	Peptide
15	L	192	PHE	Sidechain
15	L	62	PRO	Peptide
15	L	66	TYR	Peptide
16	M	6	PHE	Sidechain
16	M	65	PRO	Peptide
16	M	79	LYS	Peptide
16	M	94	LYS	Peptide
17	N	119	TYR	Sidechain
17	N	130	PHE	Sidechain

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Mol	Chain	Res	Type	Group
17	N	131	GLU	Sidechain
17	N	138	PHE	Peptide
17	N	139	HIS	Sidechain
17	N	180	PHE	Sidechain
17	N	184	ILE	Peptide
17	N	202	ARG	Peptide
17	N	37	HIS	Sidechain
17	N	90	ASN	Peptide
17	N	94	PHE	Sidechain
18	O	110	PRO	Peptide
18	O	117	ARG	Peptide
18	O	135	PHE	Sidechain
19	P	139	TYR	Sidechain
20	Q	161	SER	Peptide
20	Q	162	HIS	Peptide
20	Q	174	PHE	Sidechain
20	Q	32	TYR	Peptide
20	Q	34	PHE	Sidechain
21	R	118	HIS	Sidechain
21	R	132	PHE	Sidechain
21	R	174	GLU	Peptide
21	R	19	LYS	Peptide
21	R	57	VAL	Peptide
21	R	94	THR	Peptide
22	S	10	TYR	Sidechain
22	S	145	PHE	Sidechain,Peptide
22	S	152	PHE	Peptide
22	S	154	LEU	Peptide
22	S	159	LEU	Peptide
22	S	164	LYS	Peptide
22	S	32	ILE	Peptide
22	S	33	PHE	Peptide
22	S	68	PHE	Peptide
22	S	90	THR	Peptide
49	S2	1034	A	Sidechain
49	S2	104	A	Sidechain
49	S2	1045	U	Sidechain
49	S2	1063	C	Sidechain
49	S2	1085	C	Sidechain
49	S2	1088	U	Sidechain
49	S2	1109	C	Sidechain
49	S2	114	G	Sidechain

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Mol	Chain	Res	Type	Group
49	S2	1142	G	Sidechain
49	S2	1150	A	Sidechain
49	S2	1167	G	Sidechain
49	S2	1181	A	Sidechain
49	S2	1249	C	Sidechain
49	S2	1283	C	Sidechain
49	S2	1315	U	Sidechain
49	S2	1378	A	Sidechain
49	S2	1565	C	Sidechain
49	S2	1578	U	Sidechain
49	S2	1603	G	Sidechain
49	S2	1606	G	Sidechain
49	S2	1623	A	Sidechain
49	S2	1659	U	Sidechain
49	S2	1663	A	Sidechain
49	S2	1703	C	Sidechain
49	S2	1823	A	Sidechain
49	S2	1835	A	Sidechain
49	S2	1838	U	Sidechain
49	S2	1849	G	Sidechain
49	S2	1850	A	Sidechain
49	S2	1851	A	Sidechain
49	S2	1860	A	Sidechain
49	S2	294	U	Sidechain
49	S2	30	C	Sidechain
49	S2	313	A	Sidechain
49	S2	367	U	Sidechain
49	S2	381	C	Sidechain
49	S2	384	U	Sidechain
49	S2	399	C	Sidechain
49	S2	421	G	Sidechain
49	S2	423	U	Sidechain
49	S2	426	A	Sidechain
49	S2	427	U	Sidechain
49	S2	428	U	Sidechain
49	S2	437	G	Sidechain
49	S2	444	G	Sidechain
49	S2	447	A	Sidechain
49	S2	482	G	Sidechain
49	S2	601	G	Sidechain
49	S2	617	G	Sidechain
49	S2	631	U	Sidechain

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Mol	Chain	Res	Type	Group
49	S2	642	U	Sidechain
49	S2	645	C	Sidechain
49	S2	646	G	Sidechain
49	S2	661	U	Sidechain
49	S2	662	G	Sidechain
49	S2	685	A	Sidechain
49	S2	821	G	Sidechain
49	S2	848	U	Sidechain
49	S2	849	A	Sidechain
49	S2	9	U	Sidechain
49	S2	918	U	Sidechain
49	S2	92	A	Sidechain
49	S2	957	A	Sidechain
49	S2	958	G	Sidechain
49	S2	964	A	Sidechain
49	S2	999	G	Sidechain
50	SA	103	PHE	Sidechain
50	SA	131	HIS	Peptide
51	SB	141	GLY	Peptide
51	SB	40	ASN	Peptide
51	SB	66	VAL	Peptide
51	SB	76	ASN	Peptide
52	SC	168	GLY	Peptide
52	SC	236	PHE	Sidechain
52	SC	241	PHE	Sidechain
52	SC	60	TRP	Peptide
53	SD	159	HIS	Sidechain
53	SD	196	GLY	Peptide
53	SD	203	PRO	Peptide
54	SE	17	HIS	Peptide
54	SE	205	PHE	Peptide
55	SF	43	GLU	Peptide
57	SH	108	SER	Peptide
58	SI	149	TYR	Peptide
58	SI	153	LYS	Peptide
58	SI	155	ASN	Peptide
58	SI	26	LYS	Peptide
58	SI	65	PHE	Peptide
58	SI	99	ASN	Sidechain
59	SJ	165	TYR	Peptide
59	SJ	48	PHE	Sidechain
60	SK	29	MET	Peptide

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Mol	Chain	Res	Type	Group
61	SL	147	LYS	Peptide
61	SL	15	THR	Peptide
61	SL	151	THR	Peptide
61	SL	62	PHE	Sidechain
62	SM	100	PRO	Peptide
62	SM	107	SER	Peptide
62	SM	32	ALA	Peptide
63	SN	113	PHE	Peptide
64	SO	147	ARG	Sidechain
65	SP	11	THR	Peptide
66	SQ	43	GLU	Peptide
67	SR	108	LEU	Peptide
67	SR	125	GLY	Peptide
70	SU	71	GLY	Peptide
71	SV	32	ILE	Peptide
71	SV	48	GLY	Peptide
72	SW	54	ASP	Peptide
72	SW	76	SER	Peptide
73	SX	16	HIS	Sidechain
73	SX	20	HIS	Sidechain
74	SY	86	GLU	Sidechain
75	SZ	108	ILE	Peptide
76	Sa	17	HIS	Sidechain
77	Sb	81	ARG	Peptide
79	Sd	10	HIS	Peptide
79	Sd	8	TRP	Peptide
81	Sf	132	MET	Peptide
81	Sf	135	HIS	Peptide
81	Sf	138	ARG	Peptide
81	Sf	139	HIS	Peptide
23	T	140	PHE	Sidechain
23	T	142	ARG	Peptide
24	U	110	TYR	Peptide
24	U	55	ASN	Peptide
25	V	108	ASN	Peptide
25	V	97	TYR	Sidechain
25	V	98	PHE	Sidechain
26	W	27	LYS	Peptide
27	X	73	HIS	Sidechain
28	Y	18	HIS	Sidechain
28	Y	61	HIS	Sidechain
28	Y	62	TYR	Peptide

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Mol	Chain	Res	Type	Group
28	Y	81	TYR	Sidechain
30	a	109	TYR	Sidechain
30	a	128	PHE	Sidechain
30	a	34	ASN	Sidechain
30	a	39	HIS	Peptide
30	a	60	HIS	Sidechain
30	a	61	TYR	Sidechain,Peptide
30	a	62	HIS	Sidechain
30	a	91	ALA	Peptide
31	b	6	ASN	Sidechain
32	c	77	ASN	Peptide
32	c	78	ASN	Sidechain
33	d	103	TYR	Peptide
33	d	108	TYR	Peptide
33	d	25	TYR	Sidechain
33	d	72	VAL	Peptide
34	e	20	PHE	Sidechain
34	e	3	ALA	Peptide
34	e	74	PHE	Sidechain
34	e	76	LYS	Peptide
35	f	100	ARG	Peptide
35	f	53	ALA	Peptide
36	g	6	THR	Peptide
37	h	121	VAL	Peptide
37	h	78	TYR	Sidechain
37	h	97	LYS	Peptide
38	i	26	HIS	Sidechain
38	i	39	PHE	Sidechain
38	i	49	GLY	Peptide
39	j	46	LYS	Peptide
39	j	48	ASN	Peptide
39	j	66	HIS	Sidechain
39	j	8	PHE	Sidechain
40	k	28	ASN	Peptide
44	o	31	ASP	Sidechain,Peptide
44	o	43	ARG	Peptide
44	o	47	GLY	Peptide
44	o	48	TYR	Sidechain
44	o	76	ASN	Peptide
45	p	17	ARG	Peptide
46	q	108	PRO	Peptide
46	q	148	SER	Peptide

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Mol	Chain	Res	Type	Group
46	q	205	ASP	Mainchain,Peptide
46	q	44	ARG	Sidechain
46	q	6	ARG	Peptide
46	q	99	ARG	Sidechain
47	r	30	ASN	Peptide
47	r	31	ASN	Sidechain
47	r	45	HIS	Sidechain
47	r	70	GLN	Peptide
47	r	76	SER	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
4	A	242/257 (94%)	203 (84%)	30 (12%)	9 (4%)	3 26
5	B	392/394 (100%)	319 (81%)	40 (10%)	33 (8%)	1 9
6	C	365/367 (100%)	304 (83%)	46 (13%)	15 (4%)	3 23
7	D	290/297 (98%)	235 (81%)	33 (11%)	22 (8%)	1 10
8	E	232/236 (98%)	150 (65%)	51 (22%)	31 (13%)	0 4
9	F	223/225 (99%)	190 (85%)	23 (10%)	10 (4%)	2 21
10	G	239/266 (90%)	200 (84%)	32 (13%)	7 (3%)	4 31
11	H	188/192 (98%)	164 (87%)	20 (11%)	4 (2%)	7 38
12	I	211/213 (99%)	166 (79%)	31 (15%)	14 (7%)	1 13
13	J	168/178 (94%)	137 (82%)	23 (14%)	8 (5%)	2 20
14	K	147/163 (90%)	83 (56%)	31 (21%)	33 (22%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	L	208/211 (99%)	172 (83%)	25 (12%)	11 (5%)	2	17
16	M	136/213 (64%)	118 (87%)	16 (12%)	2 (2%)	10	45
17	N	201/204 (98%)	172 (86%)	23 (11%)	6 (3%)	4	30
18	O	199/204 (98%)	182 (92%)	14 (7%)	3 (2%)	10	45
19	P	151/153 (99%)	140 (93%)	9 (6%)	2 (1%)	12	48
20	Q	185/188 (98%)	160 (86%)	20 (11%)	5 (3%)	5	33
21	R	178/196 (91%)	153 (86%)	21 (12%)	4 (2%)	6	37
22	S	173/224 (77%)	146 (84%)	24 (14%)	3 (2%)	9	42
23	T	157/160 (98%)	128 (82%)	26 (17%)	3 (2%)	8	40
24	U	97/128 (76%)	74 (76%)	21 (22%)	2 (2%)	7	38
25	V	129/140 (92%)	112 (87%)	14 (11%)	3 (2%)	6	36
26	W	61/157 (39%)	57 (93%)	3 (5%)	1 (2%)	9	43
27	X	117/156 (75%)	108 (92%)	7 (6%)	2 (2%)	9	42
28	Y	132/145 (91%)	112 (85%)	14 (11%)	6 (4%)	2	21
29	Z	133/136 (98%)	113 (85%)	15 (11%)	5 (4%)	3	25
30	a	145/148 (98%)	111 (77%)	26 (18%)	8 (6%)	2	17
31	b	73/160 (46%)	58 (80%)	11 (15%)	4 (6%)	2	17
32	c	92/115 (80%)	78 (85%)	10 (11%)	4 (4%)	2	22
33	d	105/125 (84%)	85 (81%)	16 (15%)	4 (4%)	3	25
34	e	126/135 (93%)	110 (87%)	15 (12%)	1 (1%)	19	58
35	f	107/110 (97%)	95 (89%)	7 (6%)	5 (5%)	2	20
36	g	112/117 (96%)	103 (92%)	7 (6%)	2 (2%)	8	41
37	h	120/123 (98%)	102 (85%)	15 (12%)	3 (2%)	5	34
38	i	100/105 (95%)	91 (91%)	7 (7%)	2 (2%)	7	39
39	j	84/86 (98%)	67 (80%)	13 (16%)	4 (5%)	2	20
40	k	67/70 (96%)	55 (82%)	7 (10%)	5 (8%)	1	11
41	l	48/51 (94%)	42 (88%)	4 (8%)	2 (4%)	3	23
42	m	50/128 (39%)	44 (88%)	6 (12%)	0	100	100
43	n	21/25 (84%)	21 (100%)	0	0	100	100
44	o	102/106 (96%)	85 (83%)	11 (11%)	6 (6%)	1	15
45	p	89/91 (98%)	79 (89%)	9 (10%)	1 (1%)	14	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
46	q	200/202 (99%)	133 (66%)	27 (14%)	40 (20%)	0 1
47	r	123/125 (98%)	97 (79%)	20 (16%)	6 (5%)	2 19
48	4	854/856 (100%)	754 (88%)	58 (7%)	42 (5%)	2 19
50	SA	206/295 (70%)	176 (85%)	24 (12%)	6 (3%)	4 31
51	SB	211/264 (80%)	170 (81%)	27 (13%)	14 (7%)	1 13
52	SC	216/218 (99%)	189 (88%)	19 (9%)	8 (4%)	3 26
53	SD	225/243 (93%)	170 (76%)	44 (20%)	11 (5%)	2 19
54	SE	260/263 (99%)	202 (78%)	41 (16%)	17 (6%)	1 14
55	SF	189/204 (93%)	160 (85%)	19 (10%)	10 (5%)	2 17
56	SG	235/249 (94%)	194 (83%)	35 (15%)	6 (3%)	5 33
57	SH	187/194 (96%)	143 (76%)	29 (16%)	15 (8%)	1 10
58	SI	204/208 (98%)	176 (86%)	21 (10%)	7 (3%)	3 28
59	SJ	183/194 (94%)	145 (79%)	24 (13%)	14 (8%)	1 10
60	SK	96/165 (58%)	60 (62%)	26 (27%)	10 (10%)	0 7
61	SL	150/158 (95%)	122 (81%)	21 (14%)	7 (5%)	2 20
62	SM	122/124 (98%)	77 (63%)	25 (20%)	20 (16%)	0 2
63	SN	148/151 (98%)	115 (78%)	28 (19%)	5 (3%)	3 28
64	SO	134/151 (89%)	102 (76%)	18 (13%)	14 (10%)	0 7
65	SP	94/145 (65%)	65 (69%)	18 (19%)	11 (12%)	0 5
66	SQ	139/146 (95%)	112 (81%)	21 (15%)	6 (4%)	2 22
67	SR	127/135 (94%)	95 (75%)	24 (19%)	8 (6%)	1 14
68	SS	135/152 (89%)	104 (77%)	23 (17%)	8 (6%)	1 15
69	ST	139/145 (96%)	116 (84%)	17 (12%)	6 (4%)	2 22
70	SU	102/119 (86%)	80 (78%)	18 (18%)	4 (4%)	3 25
71	SV	80/83 (96%)	63 (79%)	10 (12%)	7 (9%)	1 8
72	SW	127/130 (98%)	112 (88%)	11 (9%)	4 (3%)	4 30
73	SX	139/143 (97%)	116 (84%)	18 (13%)	5 (4%)	3 26
74	SY	124/132 (94%)	92 (74%)	23 (18%)	9 (7%)	1 11
75	SZ	73/125 (58%)	54 (74%)	13 (18%)	6 (8%)	1 9
76	Sa	96/115 (84%)	74 (77%)	15 (16%)	7 (7%)	1 11
77	Sb	81/84 (96%)	61 (75%)	15 (18%)	5 (6%)	1 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
78	Sc	62/69 (90%)	46 (74%)	16 (26%)	0	100 100
79	Sd	50/56 (89%)	38 (76%)	9 (18%)	3 (6%)	1 15
80	Se	55/133 (41%)	40 (73%)	14 (26%)	1 (2%)	8 41
81	Sf	69/156 (44%)	39 (56%)	21 (30%)	9 (13%)	0 4
82	Sg	311/317 (98%)	250 (80%)	45 (14%)	16 (5%)	2 19
All	All	12341/13747 (90%)	10066 (82%)	1613 (13%)	662 (5%)	3 17

All (662) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	19	HIS
4	A	197	PRO
5	B	16	PHE
5	B	40	PRO
5	B	108	GLU
5	B	109	HIS
5	B	111	SER
5	B	120	LYS
5	B	138	GLN
5	B	143	ALA
5	B	169	ARG
5	B	191	ALA
5	B	196	TRP
5	B	388	PHE
5	B	389	MET
6	C	69	THR
6	C	99	GLY
6	C	309	ILE
6	C	318	PRO
6	C	319	LEU
7	D	19	LYS
7	D	212	ILE
7	D	262	LYS
7	D	285	ALA
8	E	55	ARG
8	E	59	TYR
8	E	96	LYS
8	E	131	LYS
8	E	175	LEU
8	E	221	PRO

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Mol	Chain	Res	Type
8	E	230	ASP
8	E	280	HIS
9	F	72	ARG
9	F	128	ASN
9	F	236	GLY
10	G	128	VAL
11	H	60	TRP
12	I	78	LYS
12	I	79	SER
12	I	178	ALA
12	I	179	ASP
12	I	187	LYS
13	J	91	GLU
14	K	28	LEU
14	K	30	PRO
14	K	38	SER
14	K	39	PRO
14	K	58	ILE
14	K	86	LYS
14	K	89	PRO
14	K	92	ARG
14	K	98	ILE
14	K	105	THR
14	K	117	ARG
14	K	120	SER
14	K	126	SER
14	K	135	THR
14	K	141	CYS
14	K	142	ASN
14	K	144	ASP
14	K	149	HIS
14	K	159	ALA
15	L	62	PRO
15	L	64	VAL
15	L	67	HIS
15	L	82	ARG
15	L	83	VAL
15	L	134	PRO
16	M	7	VAL
17	N	30	TYR
17	N	89	VAL
18	O	5	GLN

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Mol	Chain	Res	Type
18	O	111	PRO
19	P	41	ILE
20	Q	177	ALA
21	R	36	ASN
22	S	146	HIS
22	S	165	PRO
25	V	14	PHE
25	V	99	GLU
27	X	131	ASP
30	a	76	ASP
30	a	92	LYS
30	a	96	GLY
31	b	7	HIS
31	b	12	GLN
35	f	4	ARG
36	g	7	TYR
37	h	119	PHE
38	i	64	SER
40	k	23	VAL
40	k	59	SER
41	l	22	PRO
44	o	90	HIS
44	o	94	GLY
46	q	51	ALA
46	q	60	MET
46	q	69	LEU
46	q	70	GLU
46	q	73	PRO
46	q	74	ALA
46	q	98	ILE
46	q	100	ASP
46	q	104	ALA
46	q	118	PRO
46	q	136	SER
46	q	149	ARG
46	q	150	GLY
46	q	182	PRO
46	q	183	PHE
46	q	184	SER
46	q	185	PHE
47	r	34	ALA
47	r	45	HIS

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Mol	Chain	Res	Type
47	r	107	ARG
48	4	4	PHE
48	4	43	ALA
48	4	44	GLY
48	4	45	ILE
48	4	47	ALA
48	4	61	LYS
48	4	71	LYS
48	4	206	ASP
48	4	207	PRO
48	4	240	GLY
48	4	241	GLU
48	4	481	LYS
48	4	498	LYS
48	4	499	PHE
48	4	500	SER
48	4	504	VAL
48	4	576	VAL
48	4	577	VAL
48	4	716	ARG
48	4	743	PRO
48	4	744	ILE
48	4	753	GLU
48	4	776	VAL
48	4	812	CYS
48	4	813	VAL
48	4	849	PRO
50	SA	3	GLY
51	SB	57	ILE
51	SB	179	ASN
51	SB	191	ASP
51	SB	223	PHE
52	SC	253	PRO
52	SC	254	ASP
53	SD	54	ARG
53	SD	202	LYS
53	SD	223	ILE
54	SE	12	VAL
54	SE	95	THR
54	SE	101	LEU
54	SE	196	THR
55	SF	34	SER

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Mol	Chain	Res	Type
55	SF	37	ASP
57	SH	16	PRO
57	SH	17	ASP
57	SH	18	GLU
57	SH	66	VAL
57	SH	116	ARG
57	SH	170	VAL
57	SH	190	PRO
58	SI	155	ASN
59	SJ	3	VAL
59	SJ	69	ARG
59	SJ	70	ARG
59	SJ	119	LEU
59	SJ	121	LYS
59	SJ	159	PHE
60	SK	30	PRO
60	SK	58	VAL
61	SL	19	ASN
61	SL	100	ASN
62	SM	15	ASN
62	SM	77	ILE
62	SM	91	LEU
62	SM	96	ARG
62	SM	102	LYS
62	SM	114	TYR
63	SN	143	SER
64	SO	56	VAL
64	SO	65	ASP
64	SO	140	THR
65	SP	14	LYS
65	SP	38	SER
66	SQ	48	GLN
66	SQ	77	HIS
67	SR	88	VAL
68	SS	12	ILE
68	SS	90	VAL
68	SS	118	ARG
69	ST	29	LYS
70	SU	50	VAL
70	SU	107	GLU
71	SV	41	LYS
71	SV	65	SER

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Mol	Chain	Res	Type
72	SW	77	PRO
72	SW	107	SER
73	SX	34	THR
73	SX	129	SER
75	SZ	113	THR
81	Sf	89	LYS
81	Sf	98	VAL
81	Sf	137	ASP
82	Sg	96	THR
82	Sg	142	VAL
82	Sg	161	SER
82	Sg	182	CYS
82	Sg	282	GLU
4	A	110	GLY
5	B	47	LEU
5	B	147	ALA
5	B	274	TYR
5	B	314	ILE
5	B	394	LYS
6	C	58	ALA
6	C	66	SER
6	C	320	LYS
7	D	21	ARG
7	D	57	ASN
7	D	96	ALA
7	D	220	LYS
7	D	260	GLU
7	D	279	ARG
7	D	281	ALA
7	D	293	ARG
8	E	43	ASN
8	E	91	PRO
8	E	181	PRO
8	E	220	LYS
9	F	31	LYS
9	F	168	ARG
9	F	229	PHE
10	G	28	VAL
11	H	64	ARG
12	I	101	LYS
12	I	158	LYS
12	I	210	ARG

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Mol	Chain	Res	Type
13	J	26	VAL
13	J	88	LYS
13	J	169	LYS
14	K	24	ALA
14	K	34	PRO
14	K	60	VAL
14	K	94	LYS
14	K	140	GLY
15	L	143	GLU
16	M	87	ALA
17	N	79	ALA
20	Q	178	ARG
21	R	39	GLN
23	T	18	PRO
23	T	44	GLY
23	T	55	LYS
27	X	86	ALA
28	Y	6	PHE
29	Z	91	LEU
30	a	60	HIS
30	a	62	HIS
30	a	97	ALA
32	c	32	LYS
32	c	80	GLU
32	c	81	LEU
33	d	93	ASN
34	e	34	ASN
37	h	122	LYS
40	k	61	PRO
44	o	33	LEU
44	o	98	LYS
46	q	46	SER
46	q	84	GLY
46	q	128	THR
46	q	158	VAL
46	q	179	ASN
46	q	180	ILE
46	q	202	GLU
46	q	203	VAL
47	r	123	PRO
48	4	48	SER
48	4	53	GLU

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Mol	Chain	Res	Type
48	4	54	THR
48	4	62	ASP
48	4	532	PRO
50	SA	110	ASN
50	SA	187	GLY
51	SB	83	LYS
51	SB	108	ASP
51	SB	152	LYS
51	SB	204	ILE
52	SC	134	ASN
52	SC	255	LEU
53	SD	219	PRO
54	SE	76	VAL
54	SE	98	ASN
54	SE	109	PHE
55	SF	21	GLY
55	SF	121	PRO
56	SG	99	GLY
57	SH	160	LYS
58	SI	126	GLY
58	SI	137	LEU
58	SI	138	ASN
59	SJ	5	ARG
59	SJ	118	GLY
61	SL	3	ASP
62	SM	35	ILE
62	SM	48	HIS
62	SM	79	VAL
63	SN	38	TYR
64	SO	32	HIS
64	SO	33	ILE
64	SO	64	ALA
64	SO	105	THR
64	SO	129	ILE
64	SO	146	ARG
65	SP	12	PHE
66	SQ	32	ILE
66	SQ	35	ASN
67	SR	93	GLN
67	SR	95	ILE
67	SR	110	ASP
67	SR	123	THR

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Mol	Chain	Res	Type
68	SS	7	GLU
68	SS	133	GLY
69	ST	28	LEU
69	ST	34	VAL
69	ST	39	LEU
69	ST	49	ASP
72	SW	45	GLY
73	SX	99	GLU
74	SY	60	PHE
74	SY	84	LYS
74	SY	118	ARG
74	SY	120	THR
75	SZ	42	ASP
75	SZ	102	LYS
75	SZ	104	ARG
75	SZ	108	ILE
76	Sa	8	ASN
76	Sa	25	ASN
77	Sb	6	ASP
77	Sb	59	CYS
81	Sf	112	GLY
82	Sg	97	THR
82	Sg	139	LYS
82	Sg	141	THR
4	A	180	LEU
4	A	196	TRP
5	B	295	ASP
6	C	73	VAL
6	C	97	ARG
6	C	266	THR
6	C	273	LEU
7	D	129	GLU
7	D	152	ARG
7	D	187	SER
7	D	188	LYS
8	E	61	ARG
8	E	92	VAL
8	E	95	ASP
8	E	104	LYS
8	E	153	HIS
8	E	206	LYS
8	E	218	LEU

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Mol	Chain	Res	Type
8	E	255	ARG
9	F	105	PRO
12	I	94	PHE
12	I	106	ALA
13	J	124	GLY
14	K	56	LEU
14	K	67	ARG
14	K	90	ARG
14	K	139	VAL
15	L	172	GLU
19	P	54	GLN
20	Q	52	PHE
20	Q	146	ARG
21	R	130	ASN
22	S	153	PRO
24	U	38	ASN
28	Y	11	ARG
28	Y	18	HIS
29	Z	8	GLY
29	Z	33	THR
30	a	93	ASN
33	d	38	PHE
35	f	80	ASN
35	f	107	PRO
41	l	47	THR
44	o	49	GLY
46	q	115	ALA
48	4	269	ALA
48	4	434	TYR
48	4	810	PRO
50	SA	105	PRO
51	SB	43	ASN
52	SC	264	SER
53	SD	178	ARG
53	SD	179	GLN
54	SE	24	THR
54	SE	163	ASP
54	SE	171	ASP
55	SF	163	PHE
57	SH	107	LYS
57	SH	110	THR
58	SI	143	LYS

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Mol	Chain	Res	Type
60	SK	63	ALA
60	SK	92	ALA
61	SL	28	THR
62	SM	36	ARG
62	SM	65	VAL
62	SM	95	ASP
62	SM	103	VAL
62	SM	116	LYS
62	SM	117	GLU
64	SO	128	ARG
65	SP	50	ARG
65	SP	73	PRO
65	SP	74	GLU
65	SP	87	PRO
67	SR	127	ASN
68	SS	92	ASP
69	ST	128	GLN
71	SV	3	ASN
72	SW	30	CYS
73	SX	114	ASP
74	SY	104	ARG
75	SZ	80	ARG
76	Sa	61	ALA
76	Sa	62	TYR
76	Sa	97	PRO
79	Sd	7	TYR
81	Sf	83	LYS
81	Sf	99	LYS
81	Sf	100	LEU
82	Sg	65	PHE
82	Sg	144	ASP
82	Sg	283	PRO
4	A	35	ALA
4	A	109	GLU
4	A	193	ARG
5	B	117	ARG
5	B	189	THR
5	B	310	SER
5	B	329	ASP
6	C	23	THR
6	C	49	ARG
7	D	20	PHE

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Mol	Chain	Res	Type
7	D	32	ALA
8	E	85	LEU
8	E	118	PRO
8	E	122	LEU
8	E	183	ARG
8	E	203	LYS
8	E	254	LEU
10	G	43	GLN
10	G	165	GLU
11	H	51	LYS
12	I	77	VAL
12	I	109	ASP
14	K	40	LYS
14	K	54	LYS
17	N	182	HIS
20	Q	55	ARG
21	R	131	VAL
24	U	98	ASP
25	V	110	GLY
26	W	43	LYS
30	a	98	ALA
31	b	10	HIS
32	c	77	ASN
33	d	58	GLY
33	d	102	LEU
35	f	5	LEU
40	k	29	LYS
44	o	8	ARG
46	q	61	MET
46	q	130	LEU
46	q	134	LYS
46	q	156	SER
46	q	191	GLN
46	q	199	TYR
46	q	201	PRO
48	4	502	SER
50	SA	188	THR
51	SB	77	ASP
53	SD	218	LEU
54	SE	132	GLY
55	SF	131	ALA
55	SF	132	GLY

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Mol	Chain	Res	Type
55	SF	143	PRO
56	SG	146	ASN
56	SG	152	ASP
57	SH	35	ASP
57	SH	57	ARG
57	SH	111	LYS
59	SJ	39	ASN
59	SJ	92	MET
59	SJ	120	ALA
59	SJ	125	HIS
60	SK	3	MET
60	SK	65	ARG
61	SL	8	ARG
62	SM	76	LEU
62	SM	119	GLN
65	SP	8	LYS
65	SP	75	VAL
66	SQ	116	ASP
71	SV	10	ASP
74	SY	30	PRO
74	SY	34	THR
76	Sa	35	ALA
77	Sb	75	GLU
79	Sd	8	TRP
81	Sf	87	THR
82	Sg	37	ASP
82	Sg	160	SER
82	Sg	286	CYS
4	A	130	SER
5	B	137	TRP
5	B	139	ASP
5	B	194	LEU
5	B	387	ALA
7	D	125	VAL
7	D	263	LYS
8	E	229	PHE
8	E	245	ASP
9	F	99	GLY
10	G	123	ALA
10	G	125	LYS
11	H	110	SER
13	J	11	PRO

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Mol	Chain	Res	Type
13	J	32	ARG
14	K	36	GLY
14	K	96	LYS
17	N	40	PRO
17	N	55	ALA
28	Y	85	VAL
29	Z	124	THR
31	b	21	ILE
35	f	106	TYR
36	g	84	ALA
39	j	5	THR
39	j	38	GLY
45	p	4	ARG
46	q	82	ILE
48	4	246	PRO
48	4	574	ASP
51	SB	76	ASN
51	SB	93	GLY
52	SC	181	PRO
52	SC	189	GLY
53	SD	199	GLY
53	SD	214	LYS
54	SE	38	LEU
55	SF	68	ILE
56	SG	20	ASP
57	SH	100	ILE
57	SH	159	ASP
60	SK	39	ASN
60	SK	67	PHE
60	SK	69	TRP
61	SL	147	LYS
62	SM	81	ASP
63	SN	58	HIS
63	SN	138	ASN
64	SO	39	ASP
64	SO	149	ARG
66	SQ	43	GLU
68	SS	82	TRP
70	SU	118	ASP
71	SV	42	VAL
71	SV	45	ARG
76	Sa	72	HIS

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Mol	Chain	Res	Type
79	Sd	10	HIS
81	Sf	138	ARG
5	B	17	LEU
5	B	112	ASP
5	B	144	ALA
6	C	198	ASN
8	E	40	CYS
8	E	100	THR
12	I	110	ARG
13	J	27	GLY
14	K	138	SER
15	L	169	ILE
18	O	110	PRO
28	Y	63	LYS
28	Y	79	VAL
29	Z	4	PHE
39	j	9	GLY
39	j	75	ARG
46	q	85	ASN
46	q	198	ILE
47	r	103	ARG
48	4	7	ASP
48	4	503	PRO
50	SA	43	SER
51	SB	22	VAL
53	SD	222	PRO
54	SE	30	ARG
54	SE	35	PRO
56	SG	59	GLN
58	SI	131	PRO
60	SK	41	PRO
61	SL	69	ARG
65	SP	27	ASP
65	SP	49	LEU
67	SR	121	GLN
68	SS	117	ILE
71	SV	81	LYS
73	SX	104	GLY
77	Sb	48	SER
5	B	110	ILE
5	B	259	PRO
7	D	114	GLY

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Mol	Chain	Res	Type
40	k	63	GLY
46	q	196	GLY
48	4	517	LEU
48	4	699	GLY
52	SC	171	GLY
55	SF	166	ILE
74	SY	95	GLY
82	Sg	190	GLY
15	L	100	PRO
46	q	80	PRO
46	q	116	ILE
48	4	109	VAL
54	SE	15	PRO
56	SG	161	PRO
63	SN	37	ILE
80	Se	54	GLY
7	D	261	VAL
12	I	47	PRO
37	h	38	GLY
53	SD	194	PRO
54	SE	131	VAL
59	SJ	8	VAL
59	SJ	169	ARG
62	SM	94	ILE
67	SR	86	PRO
70	SU	52	GLY
74	SY	67	GLY
77	Sb	58	GLY
82	Sg	163	PRO
5	B	321	VAL
8	E	90	LYS
9	F	100	ILE
10	G	58	PRO
15	L	28	GLN
38	i	63	VAL
47	r	44	ILE
51	SB	114	VAL
54	SE	90	ILE
62	SM	104	VAL
64	SO	24	GLY
64	SO	53	ILE
9	F	199	VAL

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Mol	Chain	Res	Type
46	q	117	ALA
58	SI	20	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	A	187/199 (94%)	139 (74%)	48 (26%)	0 3
5	B	335/335 (100%)	265 (79%)	70 (21%)	1 6
6	C	305/305 (100%)	239 (78%)	66 (22%)	1 5
7	D	246/250 (98%)	178 (72%)	68 (28%)	0 3
8	E	209/209 (100%)	158 (76%)	51 (24%)	0 4
9	F	194/194 (100%)	145 (75%)	49 (25%)	0 3
10	G	206/226 (91%)	158 (77%)	48 (23%)	1 4
11	H	169/171 (99%)	125 (74%)	44 (26%)	0 3
12	I	180/180 (100%)	135 (75%)	45 (25%)	0 4
13	J	143/149 (96%)	115 (80%)	28 (20%)	1 7
14	K	124/136 (91%)	98 (79%)	26 (21%)	1 5
15	L	176/177 (99%)	135 (77%)	41 (23%)	1 4
16	M	116/160 (72%)	95 (82%)	21 (18%)	1 9
17	N	171/172 (99%)	129 (75%)	42 (25%)	0 4
18	O	172/174 (99%)	146 (85%)	26 (15%)	3 17
19	P	134/134 (100%)	112 (84%)	22 (16%)	2 13
20	Q	163/164 (99%)	132 (81%)	31 (19%)	1 8
21	R	159/175 (91%)	120 (76%)	39 (24%)	0 4
22	S	156/192 (81%)	121 (78%)	35 (22%)	1 4
23	T	139/140 (99%)	112 (81%)	27 (19%)	1 7
24	U	89/114 (78%)	67 (75%)	22 (25%)	0 4
25	V	101/107 (94%)	77 (76%)	24 (24%)	0 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
26	W	55/126 (44%)	42 (76%)	13 (24%)	1 4
27	X	107/133 (80%)	89 (83%)	18 (17%)	2 12
28	Y	124/135 (92%)	96 (77%)	28 (23%)	1 4
29	Z	117/118 (99%)	94 (80%)	23 (20%)	1 7
30	a	119/120 (99%)	102 (86%)	17 (14%)	3 19
31	b	63/123 (51%)	45 (71%)	18 (29%)	0 3
32	c	79/97 (81%)	60 (76%)	19 (24%)	0 4
33	d	98/110 (89%)	66 (67%)	32 (33%)	0 2
34	e	114/121 (94%)	89 (78%)	25 (22%)	1 5
35	f	88/89 (99%)	73 (83%)	15 (17%)	2 12
36	g	98/100 (98%)	79 (81%)	19 (19%)	1 7
37	h	109/110 (99%)	92 (84%)	17 (16%)	2 16
38	i	86/89 (97%)	71 (83%)	15 (17%)	2 11
39	j	73/73 (100%)	60 (82%)	13 (18%)	2 10
40	k	64/65 (98%)	52 (81%)	12 (19%)	1 8
41	l	47/48 (98%)	39 (83%)	8 (17%)	2 12
42	m	48/116 (41%)	34 (71%)	14 (29%)	0 2
43	n	22/24 (92%)	17 (77%)	5 (23%)	1 4
44	o	92/94 (98%)	70 (76%)	22 (24%)	0 4
45	p	74/74 (100%)	61 (82%)	13 (18%)	2 10
46	q	170/170 (100%)	133 (78%)	37 (22%)	1 5
47	r	109/109 (100%)	86 (79%)	23 (21%)	1 5
48	4	728/728 (100%)	586 (80%)	142 (20%)	1 7
50	SA	174/245 (71%)	141 (81%)	33 (19%)	1 8
51	SB	194/231 (84%)	164 (84%)	30 (16%)	2 16
52	SC	184/184 (100%)	148 (80%)	36 (20%)	1 7
53	SD	190/202 (94%)	163 (86%)	27 (14%)	3 19
54	SE	224/225 (100%)	180 (80%)	44 (20%)	1 7
55	SF	161/170 (95%)	128 (80%)	33 (20%)	1 6
56	SG	207/218 (95%)	171 (83%)	36 (17%)	2 11
57	SH	169/174 (97%)	149 (88%)	20 (12%)	5 25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
58	SI	178/180 (99%)	148 (83%)	30 (17%)	2 12
59	SJ	161/168 (96%)	128 (80%)	33 (20%)	1 6
60	SK	89/136 (65%)	68 (76%)	21 (24%)	1 4
61	SL	136/142 (96%)	116 (85%)	20 (15%)	3 18
62	SM	104/104 (100%)	76 (73%)	28 (27%)	0 3
63	SN	130/131 (99%)	101 (78%)	29 (22%)	1 4
64	SO	106/119 (89%)	83 (78%)	23 (22%)	1 5
65	SP	88/130 (68%)	73 (83%)	15 (17%)	2 12
66	SQ	117/121 (97%)	100 (86%)	17 (14%)	3 18
67	SR	117/121 (97%)	102 (87%)	15 (13%)	4 22
68	SS	119/132 (90%)	97 (82%)	22 (18%)	1 8
69	ST	112/115 (97%)	89 (80%)	23 (20%)	1 6
70	SU	94/107 (88%)	84 (89%)	10 (11%)	6 30
71	SV	66/67 (98%)	53 (80%)	13 (20%)	1 7
72	SW	112/113 (99%)	93 (83%)	19 (17%)	2 12
73	SX	113/115 (98%)	97 (86%)	16 (14%)	3 19
74	SY	108/114 (95%)	86 (80%)	22 (20%)	1 6
75	SZ	66/103 (64%)	55 (83%)	11 (17%)	2 12
76	Sa	85/98 (87%)	76 (89%)	9 (11%)	6 30
77	Sb	75/76 (99%)	64 (85%)	11 (15%)	3 18
78	Sc	57/62 (92%)	43 (75%)	14 (25%)	0 4
79	Sd	45/48 (94%)	35 (78%)	10 (22%)	1 5
80	Se	46/105 (44%)	35 (76%)	11 (24%)	0 4
81	Sf	64/140 (46%)	45 (70%)	19 (30%)	0 2
82	Sg	272/275 (99%)	242 (89%)	30 (11%)	6 29
All	All	10721/11706 (92%)	8570 (80%)	2151 (20%)	3 6

All (2151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	ARG
4	A	5	ILE
4	A	16	PHE

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Mol	Chain	Res	Type
4	A	30	ARG
4	A	37	ARG
4	A	40	TYR
4	A	41	ILE
4	A	63	PHE
4	A	64	ARG
4	A	70	LYS
4	A	73	THR
4	A	74	GLU
4	A	95	GLN
4	A	97	ASN
4	A	100	ASN
4	A	109	GLU
4	A	116	LEU
4	A	122	ASP
4	A	123	ARG
4	A	125	LYS
4	A	126	LEU
4	A	128	ARG
4	A	139	HIS
4	A	144	LYS
4	A	147	ARG
4	A	162	ASN
4	A	163	ARG
4	A	176	ASP
4	A	181	LYS
4	A	186	TYR
4	A	187	HIS
4	A	189	TYR
4	A	190	LYS
4	A	193	ARG
4	A	194	ASN
4	A	195	CYS
4	A	196	TRP
4	A	205	ASN
4	A	208	GLU
4	A	215	ASN
4	A	216	HIS
4	A	218	HIS
4	A	221	LYS
4	A	226	ARG
4	A	227	ARG

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Mol	Chain	Res	Type
4	A	233	ARG
4	A	242	ARG
4	A	245	ARG
5	B	10	ARG
5	B	16	PHE
5	B	17	LEU
5	B	25	HIS
5	B	26	ARG
5	B	36	ASP
5	B	39	LYS
5	B	41	VAL
5	B	46	PHE
5	B	55	HIS
5	B	56	ILE
5	B	58	ARG
5	B	61	ASP
5	B	62	ARG
5	B	74	GLU
5	B	78	ILE
5	B	94	GLU
5	B	95	THR
5	B	99	LEU
5	B	100	ARG
5	B	101	THR
5	B	103	LYS
5	B	104	THR
5	B	106	PHE
5	B	116	ARG
5	B	117	ARG
5	B	119	TYR
5	B	122	TRP
5	B	123	HIS
5	B	146	LEU
5	B	149	ASP
5	B	154	LYS
5	B	156	TYR
5	B	165	HIS
5	B	167	GLN
5	B	169	ARG
5	B	174	ARG
5	B	189	THR
5	B	198	ARG

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Mol	Chain	Res	Type
5	B	203	GLN
5	B	207	VAL
5	B	214	ASP
5	B	218	ASP
5	B	228	TYR
5	B	233	SER
5	B	235	TRP
5	B	236	HIS
5	B	245	HIS
5	B	249	ARG
5	B	257	TRP
5	B	258	HIS
5	B	261	ARG
5	B	264	PHE
5	B	289	GLN
5	B	291	TYR
5	B	309	LEU
5	B	314	ILE
5	B	323	TYR
5	B	326	VAL
5	B	328	ASN
5	B	329	ASP
5	B	347	LEU
5	B	348	ARG
5	B	355	THR
5	B	356	LYS
5	B	357	ARG
5	B	366	LYS
5	B	369	ASP
5	B	378	ARG
5	B	388	PHE
6	C	14	LYS
6	C	36	ILE
6	C	47	ASN
6	C	49	ARG
6	C	60	HIS
6	C	65	GLU
6	C	71	ARG
6	C	75	ARG
6	C	76	ILE
6	C	78	ARG
6	C	80	ARG

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Mol	Chain	Res	Type
6	C	85	HIS
6	C	86	ARG
6	C	87	SER
6	C	92	PHE
6	C	94	ASN
6	C	95	MET
6	C	97	ARG
6	C	100	ARG
6	C	102	PHE
6	C	107	THR
6	C	112	HIS
6	C	113	ARG
6	C	122	TYR
6	C	126	SER
6	C	131	SER
6	C	142	HIS
6	C	150	LEU
6	C	156	ASP
6	C	160	SER
6	C	173	LYS
6	C	175	LYS
6	C	177	TRP
6	C	178	ASN
6	C	182	LYS
6	C	184	TYR
6	C	188	ARG
6	C	193	LYS
6	C	196	MET
6	C	198	ASN
6	C	201	ARG
6	C	212	ASN
6	C	215	ASN
6	C	219	LYS
6	C	222	ARG
6	C	262	GLU
6	C	264	TYR
6	C	267	TRP
6	C	281	MET
6	C	288	ASP
6	C	291	ARG
6	C	300	ARG
6	C	303	ARG

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Mol	Chain	Res	Type
6	C	307	LYS
6	C	309	ILE
6	C	310	HIS
6	C	311	ARG
6	C	312	ARG
6	C	321	ASN
6	C	322	LEU
6	C	333	LYS
6	C	342	ARG
6	C	343	GLN
6	C	345	ARG
6	C	350	ARG
6	C	352	ASP
7	D	15	ARG
7	D	22	ARG
7	D	23	ARG
7	D	30	TYR
7	D	31	TYR
7	D	33	ARG
7	D	35	ARG
7	D	39	GLN
7	D	42	ASN
7	D	44	TYR
7	D	45	ASN
7	D	50	ARG
7	D	59	ASP
7	D	63	GLN
7	D	66	TYR
7	D	79	TYR
7	D	81	HIS
7	D	90	VAL
7	D	92	LEU
7	D	94	ASN
7	D	95	TYR
7	D	99	TYR
7	D	104	LEU
7	D	107	ARG
7	D	111	ASN
7	D	113	PHE
7	D	116	ASP
7	D	118	ILE
7	D	119	TYR

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Mol	Chain	Res	Type
7	D	124	GLU
7	D	129	GLU
7	D	131	ASN
7	D	136	ASP
7	D	157	ASN
7	D	168	ASP
7	D	177	THR
7	D	179	ARG
7	D	189	GLU
7	D	191	ASN
7	D	193	GLU
7	D	196	ARG
7	D	202	GLN
7	D	203	ASN
7	D	206	ASP
7	D	213	GLU
7	D	221	LYS
7	D	223	PHE
7	D	229	ASN
7	D	232	THR
7	D	234	ASP
7	D	244	HIS
7	D	248	ARG
7	D	249	GLU
7	D	254	GLU
7	D	255	LYS
7	D	256	LYS
7	D	259	LYS
7	D	260	GLU
7	D	262	LYS
7	D	264	LYS
7	D	265	ARG
7	D	266	TRP
7	D	268	ARG
7	D	279	ARG
7	D	287	PHE
7	D	291	GLN
7	D	292	GLU
7	D	293	ARG
8	E	39	HIS
8	E	40	CYS
8	E	43	ASN

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Mol	Chain	Res	Type
8	E	46	LEU
8	E	52	ARG
8	E	61	ARG
8	E	64	MET
8	E	67	ARG
8	E	68	LYS
8	E	95	ASP
8	E	101	ARG
8	E	104	LYS
8	E	111	TYR
8	E	112	TYR
8	E	114	THR
8	E	115	GLU
8	E	124	HIS
8	E	126	LYS
8	E	129	PHE
8	E	134	ARG
8	E	153	HIS
8	E	157	ARG
8	E	166	SER
8	E	171	VAL
8	E	175	LEU
8	E	178	ASN
8	E	179	ARG
8	E	186	HIS
8	E	187	GLN
8	E	203	LYS
8	E	206	LYS
8	E	212	TYR
8	E	217	LYS
8	E	219	ARG
8	E	230	ASP
8	E	233	LYS
8	E	237	GLU
8	E	241	GLN
8	E	242	ARG
8	E	245	ASP
8	E	246	GLN
8	E	250	ASP
8	E	252	GLN
8	E	256	ARG
8	E	262	GLN

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Mol	Chain	Res	Type
8	E	266	TYR
8	E	268	ARG
8	E	277	ILE
8	E	280	HIS
8	E	282	LEU
8	E	284	PHE
9	F	27	PHE
9	F	33	LYS
9	F	34	ARG
9	F	41	GLN
9	F	43	MET
9	F	44	LEU
9	F	49	ARG
9	F	64	ARG
9	F	65	GLN
9	F	68	ARG
9	F	72	ARG
9	F	82	ASN
9	F	83	PHE
9	F	84	TYR
9	F	85	VAL
9	F	90	LYS
9	F	93	PHE
9	F	96	ARG
9	F	100	ILE
9	F	101	ASN
9	F	118	GLN
9	F	119	ILE
9	F	120	PHE
9	F	121	ASN
9	F	137	ILE
9	F	146	TYR
9	F	148	ASN
9	F	149	LEU
9	F	151	SER
9	F	154	GLU
9	F	176	LEU
9	F	192	LEU
9	F	194	HIS
9	F	197	TYR
9	F	201	LYS
9	F	202	ARG

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Mol	Chain	Res	Type
9	F	204	LYS
9	F	209	PHE
9	F	213	PHE
9	F	214	LYS
9	F	224	LYS
9	F	226	THR
9	F	227	THR
9	F	228	HIS
9	F	234	ASP
9	F	239	GLU
9	F	245	LEU
9	F	247	ARG
9	F	248	ARG
10	G	28	VAL
10	G	29	ASN
10	G	31	LEU
10	G	32	PHE
10	G	38	ASN
10	G	39	PHE
10	G	44	ASP
10	G	46	GLN
10	G	49	ARG
10	G	50	ASP
10	G	56	LYS
10	G	60	TYR
10	G	62	ARG
10	G	67	ARG
10	G	71	TYR
10	G	73	ARG
10	G	85	GLN
10	G	88	ASP
10	G	89	ARG
10	G	90	GLN
10	G	100	HIS
10	G	101	LYS
10	G	102	TYR
10	G	103	ARG
10	G	108	GLN
10	G	112	GLN
10	G	125	LYS
10	G	131	LYS
10	G	141	ASN

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Mol	Chain	Res	Type
10	G	150	LYS
10	G	162	ASP
10	G	169	PHE
10	G	170	LEU
10	G	175	ARG
10	G	177	MET
10	G	189	ARG
10	G	202	VAL
10	G	210	GLU
10	G	217	LYS
10	G	220	GLU
10	G	223	ARG
10	G	227	ASN
10	G	230	TYR
10	G	231	ASN
10	G	235	ARG
10	G	240	ASN
10	G	254	GLU
10	G	259	LYS
11	H	11	ASP
11	H	12	ILE
11	H	18	ILE
11	H	26	ILE
11	H	31	ARG
11	H	40	HIS
11	H	42	ASN
11	H	51	LYS
11	H	52	LYS
11	H	54	ARG
11	H	57	VAL
11	H	58	ASP
11	H	59	LYS
11	H	60	TRP
11	H	63	ASN
11	H	66	GLU
11	H	71	ARG
11	H	79	ASN
11	H	84	VAL
11	H	88	PHE
11	H	92	MET
11	H	96	TYR
11	H	105	ILE

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Mol	Chain	Res	Type
11	H	106	GLN
11	H	107	GLU
11	H	108	ASN
11	H	113	GLU
11	H	115	ARG
11	H	117	PHE
11	H	118	LEU
11	H	122	TYR
11	H	123	ILE
11	H	124	ARG
11	H	125	ARG
11	H	128	MET
11	H	140	GLN
11	H	141	LYS
11	H	161	ILE
11	H	162	GLN
11	H	168	LYS
11	H	171	ASP
11	H	173	ARG
11	H	177	ASP
11	H	180	TYR
12	I	3	ARG
12	I	4	ARG
12	I	8	CYS
12	I	9	TYR
12	I	13	LYS
12	I	17	TYR
12	I	21	ARG
12	I	24	ARG
12	I	28	ASP
12	I	32	ARG
12	I	35	ASP
12	I	39	LYS
12	I	43	VAL
12	I	45	GLU
12	I	46	PHE
12	I	58	GLU
12	I	71	CYS
12	I	74	LYS
12	I	78	LYS
12	I	83	ASP
12	I	86	HIS

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Mol	Chain	Res	Type
12	I	88	ARG
12	I	92	HIS
12	I	94	PHE
12	I	95	HIS
12	I	100	ASN
12	I	101	LYS
12	I	102	MET
12	I	110	ARG
12	I	111	LEU
12	I	119	PHE
12	I	126	VAL
12	I	128	ARG
12	I	143	GLN
12	I	146	GLU
12	I	158	LYS
12	I	159	PHE
12	I	171	TRP
12	I	177	ASN
12	I	179	ASP
12	I	181	PHE
12	I	182	GLU
12	I	203	HIS
12	I	207	ASP
12	I	208	LYS
13	J	15	LEU
13	J	23	ASN
13	J	32	ARG
13	J	33	LEU
13	J	35	ARG
13	J	54	ARG
13	J	55	TYR
13	J	58	ARG
13	J	81	GLU
13	J	83	LEU
13	J	85	LYS
13	J	87	LEU
13	J	90	ARG
13	J	96	LYS
13	J	97	ASN
13	J	98	ASN
13	J	101	ASP
13	J	113	ILE

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Mol	Chain	Res	Type
13	J	128	LEU
13	J	129	ASP
13	J	139	PHE
13	J	146	ARG
13	J	150	CYS
13	J	154	LYS
13	J	155	HIS
13	J	164	ARG
13	J	171	ASP
13	J	178	ASN
14	K	14	TYR
14	K	16	ARG
14	K	21	GLU
14	K	30	PRO
14	K	40	LYS
14	K	44	ASP
14	K	54	LYS
14	K	56	LEU
14	K	61	LYS
14	K	90	ARG
14	K	91	ASP
14	K	92	ARG
14	K	96	LYS
14	K	99	LYS
14	K	104	ILE
14	K	107	ASP
14	K	108	GLU
14	K	114	ARG
14	K	116	MET
14	K	117	ARG
14	K	120	SER
14	K	121	LEU
14	K	123	ARG
14	K	125	LEU
14	K	130	LYS
14	K	147	HIS
15	L	5	ARG
15	L	10	LEU
15	L	13	HIS
15	L	19	GLN
15	L	28	GLN
15	L	31	ARG

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Mol	Chain	Res	Type
15	L	34	ARG
15	L	36	ARG
15	L	39	ARG
15	L	45	ARG
15	L	49	ARG
15	L	56	ARG
15	L	65	ARG
15	L	66	TYR
15	L	67	HIS
15	L	74	ARG
15	L	79	GLU
15	L	82	ARG
15	L	92	ARG
15	L	99	ASP
15	L	101	ARG
15	L	103	ARG
15	L	111	GLN
15	L	113	ASN
15	L	115	GLN
15	L	119	GLU
15	L	123	LYS
15	L	127	PHE
15	L	129	ARG
15	L	130	LYS
15	L	146	LEU
15	L	158	ARG
15	L	162	LYS
15	L	163	ARG
15	L	165	LYS
15	L	172	GLU
15	L	176	PHE
15	L	186	ARG
15	L	195	ARG
15	L	201	GLU
15	L	205	GLN
16	M	8	GLU
16	M	11	ARG
16	M	17	PHE
16	M	29	ASP
16	M	32	ASP
16	M	33	GLN
16	M	34	ASN

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Mol	Chain	Res	Type
16	M	38	VAL
16	M	47	ARG
16	M	56	GLN
16	M	57	LEU
16	M	59	ASP
16	M	61	ILE
16	M	66	HIS
16	M	70	GLN
16	M	79	LYS
16	M	89	THR
16	M	90	ARG
16	M	91	TRP
16	M	98	ARG
16	M	119	ARG
17	N	4	TYR
17	N	9	GLU
17	N	11	TRP
17	N	26	ARG
17	N	29	GLN
17	N	49	ARG
17	N	50	ARG
17	N	53	TYR
17	N	54	LYS
17	N	59	TYR
17	N	63	ARG
17	N	67	ARG
17	N	71	ARG
17	N	72	LYS
17	N	80	THR
17	N	86	HIS
17	N	87	HIS
17	N	91	GLN
17	N	92	LEU
17	N	104	GLU
17	N	108	ARG
17	N	119	TYR
17	N	123	GLU
17	N	126	THR
17	N	127	TYR
17	N	131	GLU
17	N	136	ASP
17	N	138	PHE

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Mol	Chain	Res	Type
17	N	139	HIS
17	N	147	ASP
17	N	150	TRP
17	N	162	ARG
17	N	169	ARG
17	N	174	LEU
17	N	178	HIS
17	N	182	HIS
17	N	189	ARG
17	N	192	TRP
17	N	195	ARG
17	N	196	ASN
17	N	199	GLN
17	N	203	TYR
18	O	5	GLN
18	O	42	ASN
18	O	46	ASN
18	O	49	ARG
18	O	57	PHE
18	O	59	ARG
18	O	60	LYS
18	O	61	ARG
18	O	62	MET
18	O	74	ARG
18	O	78	ARG
18	O	82	ARG
18	O	85	ARG
18	O	110	PRO
18	O	113	ASP
18	O	140	ARG
18	O	160	ARG
18	O	167	HIS
18	O	173	GLN
18	O	178	ARG
18	O	184	ASN
18	O	187	LYS
18	O	188	LYS
18	O	191	ARG
18	O	192	PHE
18	O	194	GLU
19	P	3	ARG
19	P	9	GLU

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Mol	Chain	Res	Type
19	P	10	ASN
19	P	13	LYS
19	P	18	ARG
19	P	23	ARG
19	P	24	VAL
19	P	28	ASN
19	P	30	ARG
19	P	40	HIS
19	P	42	ARG
19	P	61	ARG
19	P	69	ARG
19	P	70	CYS
19	P	78	TRP
19	P	90	PHE
19	P	91	LEU
19	P	110	ASP
19	P	128	ARG
19	P	133	HIS
19	P	135	ARG
19	P	154	GLU
20	Q	5	ILE
20	Q	9	LYS
20	Q	14	ARG
20	Q	15	ARG
20	Q	16	LYS
20	Q	32	TYR
20	Q	37	ARG
20	Q	44	ASN
20	Q	54	SER
20	Q	58	ARG
20	Q	61	LEU
20	Q	65	ARG
20	Q	68	ARG
20	Q	72	LEU
20	Q	75	ARG
20	Q	79	THR
20	Q	85	THR
20	Q	89	ASP
20	Q	91	ARG
20	Q	93	GLN
20	Q	97	LYS
20	Q	108	ARG

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Mol	Chain	Res	Type
20	Q	110	ARG
20	Q	112	ARG
20	Q	119	LYS
20	Q	146	ARG
20	Q	150	ARG
20	Q	166	TYR
20	Q	173	LYS
20	Q	180	ARG
20	Q	181	ARG
21	R	5	ARG
21	R	6	LEU
21	R	9	ARG
21	R	23	TRP
21	R	30	ASN
21	R	39	GLN
21	R	40	GLN
21	R	47	ASP
21	R	50	ILE
21	R	58	HIS
21	R	60	ARG
21	R	74	ARG
21	R	81	ARG
21	R	86	ASN
21	R	89	MET
21	R	99	MET
21	R	104	ARG
21	R	105	LEU
21	R	107	ARG
21	R	108	ARG
21	R	109	TYR
21	R	113	LYS
21	R	114	LYS
21	R	117	ARG
21	R	118	HIS
21	R	120	TYR
21	R	124	TYR
21	R	131	VAL
21	R	133	LYS
21	R	136	ARG
21	R	138	LEU
21	R	141	HIS
21	R	163	ARG

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Mol	Chain	Res	Type
21	R	168	GLU
21	R	172	ARG
21	R	175	GLU
21	R	177	LEU
21	R	178	GLN
21	R	180	LYS
22	S	2	LYS
22	S	15	ARG
22	S	28	TYR
22	S	29	ARG
22	S	37	HIS
22	S	44	PHE
22	S	47	PHE
22	S	48	VAL
22	S	53	LYS
22	S	57	SER
22	S	64	CYS
22	S	68	PHE
22	S	70	LYS
22	S	82	LEU
22	S	83	ARG
22	S	84	TYR
22	S	86	SER
22	S	90	THR
22	S	95	ARG
22	S	99	ASP
22	S	100	LEU
22	S	101	THR
22	S	127	MET
22	S	128	LYS
22	S	138	ARG
22	S	146	HIS
22	S	147	ASP
22	S	150	ILE
22	S	151	LYS
22	S	156	HIS
22	S	157	ARG
22	S	159	LEU
22	S	162	GLN
22	S	168	THR
22	S	171	ARG
23	T	5	LYS

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Mol	Chain	Res	Type
23	T	7	LYS
23	T	9	ARG
23	T	13	TYR
23	T	19	PHE
23	T	30	TYR
23	T	32	ARG
23	T	33	ILE
23	T	35	LYS
23	T	36	LYS
23	T	38	ASP
23	T	41	ASP
23	T	54	HIS
23	T	60	LYS
23	T	70	HIS
23	T	76	VAL
23	T	88	ARG
23	T	102	ARG
23	T	103	ASP
23	T	107	LYS
23	T	113	ASP
23	T	118	GLU
23	T	121	GLU
23	T	139	HIS
23	T	142	ARG
23	T	144	ASN
23	T	152	GLU
24	U	21	PHE
24	U	23	LEU
24	U	27	HIS
24	U	33	ILE
24	U	38	ASN
24	U	39	PHE
24	U	40	GLU
24	U	42	PHE
24	U	46	ARG
24	U	50	ASN
24	U	52	LYS
24	U	62	THR
24	U	64	GLU
24	U	65	ARG
24	U	67	LYS
24	U	69	LYS

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Mol	Chain	Res	Type
24	U	82	TYR
24	U	89	LYS
24	U	90	TYR
24	U	98	ASP
24	U	101	ARG
24	U	113	ARG
25	V	13	LYS
25	V	14	PHE
25	V	15	ARG
25	V	18	LEU
25	V	27	ASN
25	V	30	ASP
25	V	36	ASN
25	V	46	LYS
25	V	48	ARG
25	V	50	ASN
25	V	51	ARG
25	V	59	ASP
25	V	60	MET
25	V	73	ARG
25	V	77	HIS
25	V	84	GLN
25	V	91	LYS
25	V	98	PHE
25	V	100	ASP
25	V	107	ASN
25	V	109	LYS
25	V	111	GLU
25	V	123	LYS
25	V	128	LEU
26	W	3	VAL
26	W	4	GLU
26	W	8	PHE
26	W	12	LYS
26	W	17	HIS
26	W	25	ASP
26	W	33	ASN
26	W	44	ARG
26	W	50	ASN
26	W	55	TYR
26	W	56	ARG
26	W	57	ARG

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Mol	Chain	Res	Type
26	W	59	HIS
27	X	39	LYS
27	X	45	THR
27	X	48	ARG
27	X	60	TYR
27	X	62	ARG
27	X	72	ASP
27	X	79	PHE
27	X	84	GLU
27	X	94	ASN
27	X	117	TYR
27	X	120	ASP
27	X	129	ARG
27	X	133	GLU
27	X	137	TYR
27	X	139	ARG
27	X	144	TYR
27	X	148	ASP
27	X	151	ASN
28	Y	2	LYS
28	Y	4	ASN
28	Y	11	ARG
28	Y	15	ARG
28	Y	17	ARG
28	Y	18	HIS
28	Y	19	PHE
28	Y	27	ARG
28	Y	36	LYS
28	Y	45	ARG
28	Y	49	ILE
28	Y	50	ARG
28	Y	53	ASP
28	Y	56	GLN
28	Y	59	ARG
28	Y	62	TYR
28	Y	65	GLN
28	Y	72	GLN
28	Y	82	ILE
28	Y	83	GLU
28	Y	84	ARG
28	Y	87	ARG
28	Y	91	ASN

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Mol	Chain	Res	Type
28	Y	112	ASP
28	Y	114	ASP
28	Y	115	ARG
28	Y	126	ARG
28	Y	127	GLN
29	Z	4	PHE
29	Z	17	ARG
29	Z	21	ARG
29	Z	27	LYS
29	Z	30	ASP
29	Z	36	ARG
29	Z	38	TYR
29	Z	54	THR
29	Z	57	MET
29	Z	60	LYS
29	Z	64	LYS
29	Z	78	ASN
29	Z	88	ASP
29	Z	92	ASP
29	Z	93	LYS
29	Z	98	LYS
29	Z	102	ARG
29	Z	108	ARG
29	Z	109	LYS
29	Z	112	ARG
29	Z	121	ARG
29	Z	122	TYR
29	Z	136	PHE
30	a	7	LYS
30	a	10	LYS
30	a	14	HIS
30	a	19	HIS
30	a	21	ARG
30	a	40	HIS
30	a	41	HIS
30	a	46	ASP
30	a	49	HIS
30	a	52	TYR
30	a	59	ARG
30	a	61	TYR
30	a	63	LEU
30	a	77	LYS

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Mol	Chain	Res	Type
30	a	84	GLU
30	a	105	ARG
30	a	132	ARG
31	b	6	ASN
31	b	7	HIS
31	b	12	GLN
31	b	16	TRP
31	b	18	ARG
31	b	19	ASN
31	b	22	LYS
31	b	23	LYS
31	b	25	ARG
31	b	27	GLN
31	b	28	ARG
31	b	30	GLU
31	b	39	PHE
31	b	43	MET
31	b	44	ARG
31	b	51	LYS
31	b	55	LYS
31	b	65	MET
32	c	18	LEU
32	c	27	TYR
32	c	31	TYR
32	c	37	MET
32	c	39	ARG
32	c	42	LYS
32	c	44	LYS
32	c	52	CYS
32	c	55	LEU
32	c	56	ARG
32	c	59	GLU
32	c	66	LEU
32	c	72	HIS
32	c	73	HIS
32	c	74	TYR
32	c	77	ASN
32	c	78	ASN
32	c	81	LEU
32	c	88	TYR
33	d	18	ASN
33	d	19	GLU

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Mol	Chain	Res	Type
33	d	23	ARG
33	d	26	THR
33	d	28	ASN
33	d	31	LYS
33	d	32	ARG
33	d	38	PHE
33	d	39	LYS
33	d	44	ARG
33	d	67	ARG
33	d	73	TRP
33	d	78	ARG
33	d	79	ASN
33	d	83	ARG
33	d	85	ARG
33	d	86	VAL
33	d	87	ARG
33	d	91	LYS
33	d	93	ASN
33	d	94	GLU
33	d	95	ASP
33	d	101	LYS
33	d	103	TYR
33	d	108	TYR
33	d	109	VAL
33	d	116	ASN
33	d	117	LEU
33	d	118	GLN
33	d	119	THR
33	d	121	ASN
33	d	123	ASP
34	e	11	LYS
34	e	16	ARG
34	e	21	ILE
34	e	26	ASP
34	e	36	ARG
34	e	42	ASP
34	e	43	ASN
34	e	46	ARG
34	e	49	PHE
34	e	52	GLN
34	e	57	ASN
34	e	64	LYS

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Mol	Chain	Res	Type
34	e	68	HIS
34	e	77	PHE
34	e	78	LEU
34	e	85	LEU
34	e	92	ASN
34	e	95	TYR
34	e	106	LYS
34	e	107	ASN
34	e	108	ARG
34	e	113	GLU
34	e	124	ASN
34	e	126	ASN
34	e	128	ARG
35	f	4	ARG
35	f	5	LEU
35	f	7	SER
35	f	14	TYR
35	f	16	ARG
35	f	19	ARG
35	f	22	ARG
35	f	24	HIS
35	f	36	ARG
35	f	49	TYR
35	f	51	TYR
35	f	52	LYS
35	f	71	TRP
35	f	101	ILE
35	f	109	ARG
36	g	3	GLN
36	g	4	ARG
36	g	5	LEU
36	g	12	SER
36	g	14	ASN
36	g	29	ARG
36	g	32	TYR
36	g	52	ARG
36	g	54	ARG
36	g	57	ARG
36	g	60	ARG
36	g	66	ARG
36	g	75	SER
36	g	81	SER

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Mol	Chain	Res	Type
36	g	88	ARG
36	g	93	ARG
36	g	95	PHE
36	g	114	GLN
36	g	115	LYS
37	h	8	ASP
37	h	10	ARG
37	h	15	GLU
37	h	23	ASP
37	h	28	LEU
37	h	48	ARG
37	h	51	ARG
37	h	67	GLU
37	h	68	ASN
37	h	72	PHE
37	h	73	TYR
37	h	89	ARG
37	h	93	ARG
37	h	97	LYS
37	h	100	GLU
37	h	119	PHE
37	h	122	LYS
38	i	3	LEU
38	i	4	ARG
38	i	12	ASN
38	i	20	ASN
38	i	27	SER
38	i	30	ARG
38	i	33	LEU
38	i	42	ASP
38	i	46	GLU
38	i	50	PHE
38	i	54	GLU
38	i	68	ARG
38	i	85	ARG
38	i	88	GLU
38	i	103	LYS
39	j	10	LYS
39	j	25	LYS
39	j	27	TYR
39	j	39	TYR
39	j	45	ARG

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Mol	Chain	Res	Type
39	j	47	TYR
39	j	48	ASN
39	j	55	ARG
39	j	56	ARG
39	j	57	ASN
39	j	71	TYR
39	j	79	ARG
39	j	80	GLU
40	k	14	THR
40	k	19	ASP
40	k	21	LYS
40	k	27	LYS
40	k	30	ASP
40	k	35	LYS
40	k	37	ARG
40	k	51	GLU
40	k	54	GLU
40	k	56	LEU
40	k	60	LEU
40	k	70	LYS
41	l	11	ARG
41	l	12	PHE
41	l	16	LYS
41	l	17	GLN
41	l	21	ARG
41	l	36	ARG
41	l	46	ARG
41	l	49	LEU
42	m	79	GLU
42	m	84	GLN
42	m	87	GLN
42	m	89	TYR
42	m	90	ASN
42	m	96	CYS
42	m	97	ARG
42	m	98	LYS
42	m	99	CYS
42	m	104	HIS
42	m	106	ARG
42	m	109	ASN
42	m	111	ARG
42	m	119	ASN

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Mol	Chain	Res	Type
43	n	8	LYS
43	n	9	ARG
43	n	18	ARG
43	n	20	MET
43	n	21	ARG
44	o	6	LYS
44	o	11	PHE
44	o	24	THR
44	o	26	TYR
44	o	33	LEU
44	o	36	GLN
44	o	42	ASP
44	o	45	GLN
44	o	48	TYR
44	o	57	ARG
44	o	58	LYS
44	o	59	LYS
44	o	61	LYS
44	o	64	LYS
44	o	69	ARG
44	o	76	ASN
44	o	78	ARG
44	o	79	SER
44	o	81	ARG
44	o	82	MET
44	o	99	ARG
44	o	102	GLN
45	p	3	LYS
45	p	4	ARG
45	p	16	THR
45	p	30	GLU
45	p	34	HIS
45	p	48	LYS
45	p	49	ARG
45	p	69	TRP
45	p	71	TYR
45	p	84	ARG
45	p	85	ARG
45	p	87	LYS
45	p	92	GLN
46	q	5	ASP
46	q	6	ARG

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Mol	Chain	Res	Type
46	q	14	PHE
46	q	16	LYS
46	q	26	LYS
46	q	33	ASP
46	q	42	GLN
46	q	44	ARG
46	q	45	MET
46	q	48	ARG
46	q	57	LYS
46	q	59	THR
46	q	62	ARG
46	q	69	LEU
46	q	77	LYS
46	q	81	HIS
46	q	83	ARG
46	q	98	ILE
46	q	100	ASP
46	q	102	LEU
46	q	103	ARG
46	q	116	ILE
46	q	127	ASN
46	q	141	LEU
46	q	143	ILE
46	q	149	ARG
46	q	155	LEU
46	q	158	VAL
46	q	162	LYS
46	q	183	PHE
46	q	185	PHE
46	q	191	GLN
46	q	194	ASP
46	q	197	SER
46	q	202	GLU
46	q	203	VAL
46	q	206	ILE
47	r	7	TRP
47	r	11	ARG
47	r	13	CYS
47	r	15	SER
47	r	16	PHE
47	r	18	ILE
47	r	26	SER

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Mol	Chain	Res	Type
47	r	28	GLU
47	r	30	ASN
47	r	33	LYS
47	r	35	ARG
47	r	39	ARG
47	r	46	HIS
47	r	64	ILE
47	r	66	ARG
47	r	67	ARG
47	r	71	ARG
47	r	83	ASN
47	r	102	TYR
47	r	106	LEU
47	r	107	ARG
47	r	112	ARG
47	r	115	SER
48	4	3	ASN
48	4	4	PHE
48	4	5	THR
48	4	6	VAL
48	4	12	ILE
48	4	15	LYS
48	4	16	LYS
48	4	27	HIS
48	4	45	ILE
48	4	48	SER
48	4	50	ARG
48	4	53	GLU
48	4	55	ARG
48	4	56	PHE
48	4	60	ARG
48	4	61	LYS
48	4	64	GLN
48	4	71	LYS
48	4	75	ILE
48	4	79	TYR
48	4	91	GLN
48	4	92	SER
48	4	93	LYS
48	4	109	VAL
48	4	110	ASP
48	4	113	SER

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Mol	Chain	Res	Type
48	4	114	GLU
48	4	122	THR
48	4	141	THR
48	4	144	ARG
48	4	159	LYS
48	4	160	MET
48	4	162	ARG
48	4	166	GLU
48	4	167	LEU
48	4	168	GLN
48	4	169	LEU
48	4	183	GLU
48	4	192	TYR
48	4	194	GLU
48	4	196	GLU
48	4	200	MET
48	4	209	LEU
48	4	216	SER
48	4	225	LEU
48	4	226	LYS
48	4	228	PHE
48	4	236	PHE
48	4	239	LYS
48	4	244	LEU
48	4	248	GLU
48	4	252	LYS
48	4	256	MET
48	4	258	LYS
48	4	264	ARG
48	4	265	TYR
48	4	267	ASP
48	4	275	LYS
48	4	281	GLU
48	4	284	LYS
48	4	311	GLU
48	4	314	LYS
48	4	317	GLU
48	4	322	LYS
48	4	330	LYS
48	4	333	LYS
48	4	343	TRP
48	4	359	PRO

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Mol	Chain	Res	Type
48	4	366	LYS
48	4	368	ARG
48	4	370	GLU
48	4	371	LEU
48	4	393	PRO
48	4	409	ARG
48	4	411	TYR
48	4	420	LEU
48	4	439	LYS
48	4	448	GLN
48	4	461	ILE
48	4	462	GLU
48	4	476	ASP
48	4	477	GLN
48	4	481	LYS
48	4	488	PHE
48	4	492	HIS
48	4	493	ASN
48	4	495	ARG
48	4	497	MET
48	4	498	LYS
48	4	499	PHE
48	4	502	SER
48	4	512	LYS
48	4	519	LYS
48	4	524	LEU
48	4	525	LYS
48	4	526	ARG
48	4	540	GLU
48	4	541	SER
48	4	559	LYS
48	4	560	ASP
48	4	563	GLU
48	4	570	ILE
48	4	571	LYS
48	4	572	LYS
48	4	579	TYR
48	4	592	LEU
48	4	607	ARG
48	4	609	PHE
48	4	613	LEU
48	4	615	GLU

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Mol	Chain	Res	Type
48	4	619	LYS
48	4	625	ARG
48	4	630	GLN
48	4	641	TRP
48	4	647	ARG
48	4	667	LYS
48	4	669	VAL
48	4	672	LEU
48	4	673	ASN
48	4	689	GLU
48	4	726	ARG
48	4	727	ARG
48	4	745	TYR
48	4	746	LEU
48	4	748	GLU
48	4	754	GLN
48	4	775	GLN
48	4	794	PHE
48	4	801	ARG
48	4	807	GLN
48	4	809	PHE
48	4	817	TRP
48	4	823	ASP
48	4	827	ASN
48	4	830	ARG
48	4	842	LYS
48	4	845	LYS
48	4	846	GLU
48	4	848	ILE
48	4	849	PRO
48	4	855	LEU
48	4	858	LEU
50	SA	8	LEU
50	SA	32	PHE
50	SA	39	TYR
50	SA	44	ASP
50	SA	53	ARG
50	SA	58	LEU
50	SA	60	LEU
50	SA	73	ASP
50	SA	79	SER
50	SA	81	ASN

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Mol	Chain	Res	Type
50	SA	89	LYS
50	SA	90	PHE
50	SA	99	ILE
50	SA	102	ARG
50	SA	105	PRO
50	SA	111	GLN
50	SA	116	PHE
50	SA	128	ARG
50	SA	130	ASP
50	SA	140	VAL
50	SA	141	ASN
50	SA	151	ASP
50	SA	158	ASP
50	SA	169	HIS
50	SA	177	MET
50	SA	178	LEU
50	SA	180	ARG
50	SA	181	GLU
50	SA	186	ARG
50	SA	195	TRP
50	SA	198	MET
50	SA	203	PHE
50	SA	206	ASP
51	SB	27	LYS
51	SB	31	TYR
51	SB	48	LEU
51	SB	51	ARG
51	SB	52	THR
51	SB	56	LYS
51	SB	60	ASP
51	SB	67	PHE
51	SB	76	ASN
51	SB	77	ASP
51	SB	81	PHE
51	SB	99	ASN
51	SB	105	LEU
51	SB	107	ARG
51	SB	119	THR
51	SB	133	TYR
51	SB	136	ARG
51	SB	142	PHE
51	SB	146	ARG

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Mol	Chain	Res	Type
51	SB	148	ASN
51	SB	150	ILE
51	SB	155	TYR
51	SB	158	HIS
51	SB	162	ARG
51	SB	180	ASP
51	SB	181	LEU
51	SB	191	ASP
51	SB	196	ASP
51	SB	205	TYR
51	SB	208	HIS
52	SC	60	TRP
52	SC	61	MET
52	SC	65	LYS
52	SC	71	LYS
52	SC	72	ASP
52	SC	78	LEU
52	SC	79	GLU
52	SC	92	GLU
52	SC	97	PHE
52	SC	101	SER
52	SC	104	ASP
52	SC	110	MET
52	SC	114	LYS
52	SC	115	GLN
52	SC	120	GLN
52	SC	121	ARG
52	SC	134	ASN
52	SC	137	VAL
52	SC	142	LYS
52	SC	152	ARG
52	SC	167	ARG
52	SC	169	TYR
52	SC	200	ARG
52	SC	215	MET
52	SC	221	ASP
52	SC	227	ARG
52	SC	235	ASN
52	SC	236	PHE
52	SC	242	ASP
52	SC	245	SER
52	SC	250	TYR

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Mol	Chain	Res	Type
52	SC	253	PRO
52	SC	255	LEU
52	SC	262	THR
52	SC	272	HIS
52	SC	275	LYS
53	SD	6	SER
53	SD	9	ARG
53	SD	22	ASN
53	SD	23	GLU
53	SD	24	PHE
53	SD	32	ASP
53	SD	53	THR
53	SD	67	ARG
53	SD	76	ARG
53	SD	87	TYR
53	SD	94	ARG
53	SD	103	GLU
53	SD	107	TYR
53	SD	129	SER
53	SD	135	GLU
53	SD	152	PHE
53	SD	154	ASP
53	SD	158	ILE
53	SD	167	TYR
53	SD	169	ASP
53	SD	177	LEU
53	SD	178	ARG
53	SD	206	ASP
53	SD	212	GLU
53	SD	216	GLU
53	SD	218	LEU
53	SD	225	GLU
54	SE	3	ARG
54	SE	8	HIS
54	SE	9	LEU
54	SE	11	ARG
54	SE	15	PRO
54	SE	18	TRP
54	SE	21	ASP
54	SE	30	ARG
54	SE	39	ARG
54	SE	49	ARG

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Mol	Chain	Res	Type
54	SE	51	ARG
54	SE	54	TYR
54	SE	66	MET
54	SE	67	GLN
54	SE	73	ASP
54	SE	93	ASP
54	SE	95	THR
54	SE	98	ASN
54	SE	99	PHE
54	SE	106	LYS
54	SE	117	GLU
54	SE	118	GLU
54	SE	121	TYR
54	SE	127	ARG
54	SE	130	PHE
54	SE	155	LYS
54	SE	158	ASP
54	SE	164	LEU
54	SE	165	GLU
54	SE	179	ASN
54	SE	180	LEU
54	SE	191	ARG
54	SE	198	ARG
54	SE	205	PHE
54	SE	206	ASP
54	SE	220	THR
54	SE	224	ASN
54	SE	226	PHE
54	SE	240	ARG
54	SE	242	LYS
54	SE	253	ASP
54	SE	255	ARG
54	SE	259	LYS
54	SE	260	GLN
55	SF	23	TRP
55	SF	29	GLN
55	SF	38	TYR
55	SF	42	LYS
55	SF	49	LEU
55	SF	63	LYS
55	SF	65	GLN
55	SF	79	HIS

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Mol	Chain	Res	Type
55	SF	82	ASN
55	SF	83	ASN
55	SF	88	MET
55	SF	95	HIS
55	SF	106	GLU
55	SF	109	LEU
55	SF	110	GLN
55	SF	118	ASN
55	SF	122	ARG
55	SF	123	GLU
55	SF	124	ASP
55	SF	130	ARG
55	SF	136	ARG
55	SF	137	GLN
55	SF	140	ASP
55	SF	145	ARG
55	SF	168	THR
55	SF	171	GLU
55	SF	172	CYS
55	SF	176	GLU
55	SF	186	ASN
55	SF	190	ILE
55	SF	194	ASP
55	SF	195	GLU
55	SF	198	ARG
56	SG	12	CYS
56	SG	20	ASP
56	SG	21	GLU
56	SG	30	LYS
56	SG	31	ARG
56	SG	32	MET
56	SG	56	ASN
56	SG	58	LYS
56	SG	59	GLN
56	SG	64	LYS
56	SG	70	HIS
56	SG	74	ARG
56	SG	76	LEU
56	SG	87	ARG
56	SG	88	ARG
56	SG	110	ASN
56	SG	120	ASP

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Mol	Chain	Res	Type
56	SG	121	ILE
56	SG	126	ASP
56	SG	132	ARG
56	SG	136	LYS
56	SG	140	ARG
56	SG	143	LYS
56	SG	152	ASP
56	SG	159	ARG
56	SG	162	LEU
56	SG	164	LYS
56	SG	165	GLU
56	SG	170	ARG
56	SG	191	ARG
56	SG	196	LYS
56	SG	198	ARG
56	SG	213	LEU
56	SG	225	GLN
56	SG	227	GLN
56	SG	236	SER
57	SH	16	PRO
57	SH	23	ILE
57	SH	33	ASN
57	SH	35	ASP
57	SH	36	LEU
57	SH	40	LEU
57	SH	57	ARG
57	SH	74	LYS
57	SH	81	ARG
57	SH	83	LEU
57	SH	87	PHE
57	SH	99	ARG
57	SH	135	PHE
57	SH	151	SER
57	SH	159	ASP
57	SH	162	GLN
57	SH	165	ASN
57	SH	166	VAL
57	SH	184	ASP
57	SH	186	ASN
58	SI	6	ASP
58	SI	8	TRP
58	SI	12	ARG

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Mol	Chain	Res	Type
58	SI	21	TYR
58	SI	22	HIS
58	SI	27	TYR
58	SI	47	ARG
58	SI	49	ARG
58	SI	52	ASN
58	SI	58	LEU
58	SI	67	TRP
58	SI	70	GLU
58	SI	73	THR
58	SI	74	ARG
58	SI	83	TYR
58	SI	87	ASN
58	SI	105	ASP
58	SI	106	SER
58	SI	110	ARG
58	SI	112	TRP
58	SI	123	ARG
58	SI	140	LYS
58	SI	149	TYR
58	SI	155	ASN
58	SI	178	ARG
58	SI	191	GLU
58	SI	196	GLU
58	SI	197	PHE
58	SI	203	LYS
58	SI	206	LYS
59	SJ	5	ARG
59	SJ	9	CYS
59	SJ	10	ARG
59	SJ	17	ARG
59	SJ	18	ARG
59	SJ	20	PHE
59	SJ	26	ASP
59	SJ	29	LEU
59	SJ	39	ASN
59	SJ	67	ASP
59	SJ	69	ARG
59	SJ	79	ARG
59	SJ	93	LYS
59	SJ	101	LYS
59	SJ	104	ASP

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Mol	Chain	Res	Type
59	SJ	108	ARG
59	SJ	109	ARG
59	SJ	110	LEU
59	SJ	115	PHE
59	SJ	116	LYS
59	SJ	123	ILE
59	SJ	124	HIS
59	SJ	127	ARG
59	SJ	131	ARG
59	SJ	138	ARG
59	SJ	139	LYS
59	SJ	147	PHE
59	SJ	150	ARG
59	SJ	152	ASP
59	SJ	159	PHE
59	SJ	162	ARG
59	SJ	165	TYR
59	SJ	169	ARG
60	SK	1	MET
60	SK	2	LEU
60	SK	5	LYS
60	SK	8	ARG
60	SK	13	GLU
60	SK	16	PHE
60	SK	32	HIS
60	SK	37	ASP
60	SK	39	ASN
60	SK	40	VAL
60	SK	43	LEU
60	SK	46	MET
60	SK	61	GLN
60	SK	65	ARG
60	SK	66	HIS
60	SK	74	GLU
60	SK	80	ARG
60	SK	81	ASP
60	SK	84	HIS
60	SK	89	ILE
60	SK	95	ARG
61	SL	8	ARG
61	SL	16	ILE
61	SL	20	LYS

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Mol	Chain	Res	Type
61	SL	22	ARG
61	SL	27	GLU
61	SL	35	ARG
61	SL	39	ASN
61	SL	40	ILE
61	SL	65	ASN
61	SL	69	ARG
61	SL	92	TYR
61	SL	97	ARG
61	SL	103	GLU
61	SL	108	ASN
61	SL	113	LEU
61	SL	116	CYS
61	SL	117	PHE
61	SL	121	GLN
61	SL	124	ASP
61	SL	147	LYS
62	SM	12	MET
62	SM	13	ASP
62	SM	18	LEU
62	SM	26	LEU
62	SM	29	ASP
62	SM	31	LEU
62	SM	33	ARG
62	SM	36	ARG
62	SM	45	ARG
62	SM	48	HIS
62	SM	52	GLN
62	SM	57	ASP
62	SM	73	GLN
62	SM	75	ASN
62	SM	76	LEU
62	SM	77	ILE
62	SM	83	LYS
62	SM	88	TRP
62	SM	91	LEU
62	SM	95	ASP
62	SM	96	ARG
62	SM	99	ASN
62	SM	101	ARG
62	SM	102	LYS
62	SM	104	VAL

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Mol	Chain	Res	Type
62	SM	113	ASP
62	SM	114	TYR
62	SM	127	TYR
63	SN	3	ARG
63	SN	25	TRP
63	SN	27	LYS
63	SN	31	ASP
63	SN	38	TYR
63	SN	55	ARG
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	83	ASP
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	104	ARG
63	SN	105	ASN
63	SN	113	PHE
63	SN	121	ARG
63	SN	125	LEU
63	SN	127	ARG
63	SN	128	TYR
63	SN	132	LYS
63	SN	133	ARG
63	SN	144	SER
64	SO	17	LEU
64	SO	34	PHE
64	SO	39	ASP
64	SO	41	PHE
64	SO	43	HIS
64	SO	51	GLU
64	SO	52	THR
64	SO	63	LYS
64	SO	65	ASP
64	SO	80	ASP

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Mol	Chain	Res	Type
64	SO	84	ARG
64	SO	86	LYS
64	SO	94	HIS
64	SO	103	ASN
64	SO	106	LYS
64	SO	116	LEU
64	SO	117	ARG
64	SO	121	ARG
64	SO	128	ARG
64	SO	130	GLU
64	SO	146	ARG
64	SO	147	ARG
64	SO	150	ARG
65	SP	5	GLU
65	SP	7	LYS
65	SP	10	ARG
65	SP	12	PHE
65	SP	15	PHE
65	SP	40	ARG
65	SP	41	GLN
65	SP	42	ARG
65	SP	43	ARG
65	SP	44	ARG
65	SP	50	ARG
65	SP	51	ARG
65	SP	52	LYS
65	SP	79	HIS
65	SP	86	LEU
66	SQ	15	ARG
66	SQ	26	LYS
66	SQ	35	ASN
66	SQ	41	MET
66	SQ	45	ARG
66	SQ	62	ARG
66	SQ	73	LYS
66	SQ	85	ARG
66	SQ	90	LYS
66	SQ	99	TYR
66	SQ	114	GLN
66	SQ	123	ASP
66	SQ	126	ARG
66	SQ	128	GLU

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Mol	Chain	Res	Type
66	SQ	138	ARG
66	SQ	140	ARG
66	SQ	145	TYR
67	SR	3	ARG
67	SR	18	GLU
67	SR	31	ASN
67	SR	37	GLU
67	SR	56	HIS
67	SR	78	ARG
67	SR	79	GLU
67	SR	83	ASN
67	SR	87	GLU
67	SR	91	LEU
67	SR	93	GLN
67	SR	109	LEU
67	SR	118	GLN
67	SR	120	THR
67	SR	121	GLN
68	SS	8	LYS
68	SS	10	GLN
68	SS	14	ARG
68	SS	23	ARG
68	SS	28	PHE
68	SS	34	LYS
68	SS	39	ARG
68	SS	63	GLU
68	SS	78	LYS
68	SS	82	TRP
68	SS	85	ASN
68	SS	86	ARG
68	SS	87	GLN
68	SS	92	ASP
68	SS	95	TYR
68	SS	108	ARG
68	SS	118	ARG
68	SS	124	ARG
68	SS	125	HIS
68	SS	134	GLN
68	SS	135	HIS
68	SS	142	ARG
69	ST	11	GLN
69	ST	13	GLU

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Mol	Chain	Res	Type
69	ST	16	ARG
69	ST	21	PHE
69	ST	28	LEU
69	ST	33	TRP
69	ST	35	ASP
69	ST	42	HIS
69	ST	53	PHE
69	ST	62	ARG
69	ST	63	HIS
69	ST	74	SER
69	ST	79	TYR
69	ST	82	ARG
69	ST	83	GLN
69	ST	84	ARG
69	ST	92	PHE
69	ST	94	ARG
69	ST	97	LYS
69	ST	118	ASP
69	ST	121	ARG
69	ST	128	GLN
69	ST	129	ARG
70	SU	19	ARG
70	SU	47	ASN
70	SU	48	LEU
70	SU	49	LYS
70	SU	51	LYS
70	SU	55	ARG
70	SU	56	MET
70	SU	77	TRP
70	SU	87	ARG
70	SU	111	GLU
71	SV	1	MET
71	SV	2	GLN
71	SV	4	ASP
71	SV	11	LEU
71	SV	18	SER
71	SV	21	ASN
71	SV	39	VAL
71	SV	45	ARG
71	SV	47	ASN
71	SV	49	GLN
71	SV	50	PHE

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Mol	Chain	Res	Type
71	SV	81	LYS
71	SV	82	ASN
72	SW	2	VAL
72	SW	3	ARG
72	SW	12	LYS
72	SW	24	GLN
72	SW	28	ARG
72	SW	36	ARG
72	SW	37	PHE
72	SW	52	ILE
72	SW	56	HIS
72	SW	57	ARG
72	SW	70	ASN
72	SW	78	ARG
72	SW	80	ASP
72	SW	85	ASP
72	SW	90	GLN
72	SW	91	ASN
72	SW	98	GLN
72	SW	104	LEU
72	SW	105	THR
73	SX	5	ARG
73	SX	9	THR
73	SX	17	ARG
73	SX	19	ASP
73	SX	32	LEU
73	SX	45	SER
73	SX	46	HIS
73	SX	61	GLN
73	SX	67	ARG
73	SX	87	ASN
73	SX	88	ASP
73	SX	105	PHE
73	SX	107	ARG
73	SX	114	ASP
73	SX	131	LEU
73	SX	135	LYS
74	SY	3	ASP
74	SY	16	ARG
74	SY	17	LEU
74	SY	19	GLN
74	SY	20	ARG

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Mol	Chain	Res	Type
74	SY	23	MET
74	SY	29	HIS
74	SY	47	MET
74	SY	54	VAL
74	SY	61	ARG
74	SY	63	HIS
74	SY	64	PHE
74	SY	69	THR
74	SY	80	ASP
74	SY	93	ARG
74	SY	96	LEU
74	SY	98	GLU
74	SY	99	LYS
74	SY	101	LYS
74	SY	107	ARG
74	SY	111	LYS
74	SY	118	ARG
75	SZ	44	LEU
75	SZ	45	ASN
75	SZ	49	LEU
75	SZ	64	ASN
75	SZ	69	THR
75	SZ	85	ARG
75	SZ	94	LYS
75	SZ	97	ILE
75	SZ	109	TYR
75	SZ	110	THR
75	SZ	114	LYS
76	Sa	28	ARG
76	Sa	41	ILE
76	Sa	43	ASN
76	Sa	51	ARG
76	Sa	52	ASP
76	Sa	62	TYR
76	Sa	72	HIS
76	Sa	94	ASP
76	Sa	95	ARG
77	Sb	14	GLU
77	Sb	17	ARG
77	Sb	26	GLN
77	Sb	34	ASP
77	Sb	37	CYS

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Mol	Chain	Res	Type
77	Sb	47	PHE
77	Sb	59	CYS
77	Sb	72	ARG
77	Sb	78	SER
77	Sb	83	GLN
77	Sb	84	HIS
78	Sc	5	ARG
78	Sc	7	GLN
78	Sc	13	ARG
78	Sc	21	THR
78	Sc	26	GLN
78	Sc	31	ARG
78	Sc	33	GLU
78	Sc	34	PHE
78	Sc	40	ARG
78	Sc	44	ARG
78	Sc	51	ARG
78	Sc	54	ASP
78	Sc	60	GLU
78	Sc	67	ARG
79	Sd	6	PHE
79	Sd	8	TRP
79	Sd	10	HIS
79	Sd	12	ARG
79	Sd	19	ARG
79	Sd	26	ASN
79	Sd	30	LEU
79	Sd	32	ARG
79	Sd	43	PHE
79	Sd	56	ASP
80	Se	13	ARG
80	Se	15	GLN
80	Se	18	LYS
80	Se	26	LYS
80	Se	28	LYS
80	Se	31	ARG
80	Se	34	ARG
80	Se	35	ARG
80	Se	40	ARG
80	Se	41	ARG
80	Se	52	LYS
81	Sf	87	THR

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Mol	Chain	Res	Type
81	Sf	89	LYS
81	Sf	95	ARG
81	Sf	98	VAL
81	Sf	106	TYR
81	Sf	116	ARG
81	Sf	119	ARG
81	Sf	126	CYS
81	Sf	131	PHE
81	Sf	136	PHE
81	Sf	138	ARG
81	Sf	139	HIS
81	Sf	140	TYR
81	Sf	141	CYS
81	Sf	146	LEU
81	Sf	148	TYR
81	Sf	149	CYS
81	Sf	150	PHE
81	Sf	152	LYS
82	Sg	8	ARG
82	Sg	15	ASN
82	Sg	17	TRP
82	Sg	20	GLN
82	Sg	24	THR
82	Sg	44	LYS
82	Sg	47	ARG
82	Sg	49	GLU
82	Sg	60	ARG
82	Sg	65	PHE
82	Sg	74	ASP
82	Sg	84	ASP
82	Sg	99	ARG
82	Sg	100	ARG
82	Sg	107	ASP
82	Sg	118	ARG
82	Sg	133	ASN
82	Sg	140	TYR
82	Sg	143	GLN
82	Sg	167	SER
82	Sg	194	TYR
82	Sg	226	HIS
82	Sg	229	THR
82	Sg	234	ASP

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Mol	Chain	Res	Type
82	Sg	249	CYS
82	Sg	268	ASP
82	Sg	282	GLU
82	Sg	294	ASP
82	Sg	297	THR
82	Sg	306	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (296) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	19	HIS
4	A	100	ASN
4	A	132	ASN
4	A	194	ASN
4	A	209	HIS
4	A	215	ASN
5	B	123	HIS
5	B	167	GLN
5	B	179	HIS
5	B	203	GLN
5	B	258	HIS
5	B	275	HIS
5	B	276	HIS
5	B	301	ASN
5	B	302	ASN
5	B	322	HIS
5	B	380	GLN
6	C	50	GLN
6	C	85	HIS
6	C	94	ASN
6	C	112	HIS
6	C	142	HIS
6	C	178	ASN
6	C	198	ASN
6	C	203	GLN
6	C	223	ASN
6	C	286	ASN
6	C	338	ASN
6	C	343	GLN
7	D	45	ASN
7	D	94	ASN
7	D	111	ASN

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Mol	Chain	Res	Type
7	D	122	GLN
7	D	131	ASN
7	D	157	ASN
7	D	191	ASN
7	D	195	HIS
7	D	198	HIS
7	D	202	GLN
7	D	244	HIS
7	D	250	ASN
7	D	282	GLN
8	E	124	HIS
8	E	153	HIS
8	E	178	ASN
8	E	186	HIS
8	E	224	GLN
8	E	246	GLN
9	F	58	HIS
9	F	82	ASN
9	F	153	ASN
9	F	165	ASN
9	F	174	ASN
9	F	194	HIS
9	F	237	ASN
9	F	250	ASN
10	G	29	ASN
10	G	64	GLN
10	G	81	ASN
10	G	108	GLN
10	G	112	GLN
10	G	153	GLN
10	G	227	ASN
10	G	231	ASN
11	H	40	HIS
11	H	63	ASN
11	H	106	GLN
12	I	59	GLN
12	I	100	ASN
12	I	144	ASN
12	I	163	GLN
12	I	213	HIS
13	J	155	HIS
14	K	149	HIS

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Mol	Chain	Res	Type
15	L	6	ASN
15	L	28	GLN
15	L	104	ASN
15	L	113	ASN
15	L	159	ASN
16	M	33	GLN
16	M	34	ASN
16	M	48	GLN
16	M	66	HIS
17	N	8	GLN
17	N	90	ASN
17	N	178	HIS
17	N	181	HIS
17	N	182	HIS
17	N	196	ASN
17	N	201	HIS
18	O	65	ASN
18	O	96	GLN
18	O	173	GLN
19	P	25	HIS
19	P	28	ASN
19	P	54	GLN
19	P	64	ASN
19	P	72	GLN
19	P	80	GLN
19	P	97	ASN
19	P	133	HIS
19	P	145	HIS
20	Q	7	HIS
20	Q	40	ASN
20	Q	57	ASN
21	R	66	ASN
21	R	75	HIS
21	R	118	HIS
21	R	143	HIS
22	S	37	HIS
22	S	91	HIS
22	S	92	ASN
22	S	122	HIS
22	S	125	GLN
22	S	163	HIS
23	T	58	HIS

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Mol	Chain	Res	Type
23	T	70	HIS
23	T	139	HIS
24	U	55	ASN
25	V	36	ASN
26	W	17	HIS
26	W	59	HIS
27	X	93	ASN
27	X	111	GLN
28	Y	24	HIS
28	Y	56	GLN
28	Y	72	GLN
28	Y	86	GLN
28	Y	100	HIS
28	Y	127	GLN
29	Z	79	HIS
30	a	41	HIS
30	a	62	HIS
30	a	66	ASN
30	a	67	GLN
31	b	6	ASN
31	b	7	HIS
31	b	12	GLN
31	b	19	ASN
31	b	27	GLN
31	b	42	ASN
32	c	19	GLN
32	c	40	GLN
32	c	73	HIS
32	c	77	ASN
33	d	30	HIS
33	d	93	ASN
33	d	100	ASN
34	e	24	GLN
34	e	43	ASN
34	e	126	ASN
35	f	21	GLN
35	f	24	HIS
35	f	55	ASN
35	f	80	ASN
36	g	18	ASN
36	g	110	GLN
36	g	112	GLN

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Mol	Chain	Res	Type
37	h	68	ASN
37	h	98	HIS
39	j	16	HIS
39	j	48	ASN
41	l	19	GLN
42	m	84	GLN
42	m	87	GLN
42	m	109	ASN
44	o	21	HIS
44	o	25	GLN
44	o	45	GLN
44	o	76	ASN
44	o	90	HIS
46	q	41	GLN
46	q	58	ASN
46	q	68	HIS
46	q	126	GLN
46	q	139	GLN
46	q	191	GLN
46	q	200	ASN
47	r	6	GLN
47	r	12	ASN
47	r	21	ASN
47	r	31	ASN
47	r	36	ASN
47	r	41	ASN
47	r	70	GLN
47	r	83	ASN
48	4	3	ASN
48	4	21	ASN
48	4	27	HIS
48	4	64	GLN
48	4	158	ASN
48	4	168	GLN
48	4	179	GLN
48	4	448	GLN
48	4	477	GLN
48	4	493	ASN
48	4	684	GLN
48	4	705	HIS
48	4	710	HIS
48	4	715	HIS

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Mol	Chain	Res	Type
48	4	737	GLN
48	4	803	ASN
48	4	807	GLN
48	4	811	GLN
48	4	816	HIS
48	4	827	ASN
50	SA	24	HIS
50	SA	33	GLN
50	SA	84	GLN
50	SA	141	ASN
50	SA	169	HIS
51	SB	40	ASN
51	SB	99	ASN
51	SB	118	GLN
51	SB	124	HIS
51	SB	148	ASN
52	SC	113	GLN
52	SC	115	GLN
52	SC	120	GLN
52	SC	134	ASN
52	SC	272	HIS
53	SD	4	GLN
53	SD	22	ASN
53	SD	159	HIS
54	SE	36	HIS
54	SE	138	HIS
54	SE	161	GLN
55	SF	29	GLN
55	SF	65	GLN
55	SF	82	ASN
55	SF	95	HIS
55	SF	137	GLN
55	SF	186	ASN
55	SF	203	ASN
56	SG	59	GLN
56	SG	65	GLN
56	SG	110	ASN
58	SI	9	HIS
58	SI	44	HIS
58	SI	155	ASN
58	SI	165	GLN
59	SJ	111	GLN

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Mol	Chain	Res	Type
59	SJ	177	ASN
60	SK	28	HIS
60	SK	39	ASN
61	SL	19	ASN
61	SL	106	HIS
61	SL	141	ASN
62	SM	19	GLN
62	SM	48	HIS
62	SM	99	ASN
63	SN	5	HIS
63	SN	69	ASN
65	SP	41	GLN
65	SP	46	ASN
65	SP	79	HIS
66	SQ	48	GLN
66	SQ	114	GLN
66	SQ	142	GLN
67	SR	83	ASN
68	SS	10	GLN
68	SS	17	ASN
68	SS	42	HIS
68	SS	120	HIS
68	SS	125	HIS
68	SS	135	HIS
69	ST	51	ASN
69	ST	63	HIS
70	SU	47	ASN
71	SV	29	HIS
71	SV	47	ASN
71	SV	49	GLN
72	SW	64	ASN
72	SW	82	GLN
72	SW	98	GLN
73	SX	20	HIS
73	SX	23	HIS
73	SX	61	GLN
73	SX	87	ASN
73	SX	97	ASN
74	SY	85	ASN
74	SY	94	HIS
75	SZ	103	HIS
76	Sa	17	HIS

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Mol	Chain	Res	Type
76	Sa	72	HIS
77	Sb	19	HIS
78	Sc	7	GLN
78	Sc	24	GLN
78	Sc	26	GLN
79	Sd	10	HIS
79	Sd	26	ASN
79	Sd	28	HIS
81	Sf	111	ASN
82	Sg	119	GLN
82	Sg	181	ASN
82	Sg	215	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3647/3664 (99%)	1616 (44%)	621 (17%)
2	7	119/120 (99%)	31 (26%)	9 (7%)
3	8	155/156 (99%)	61 (39%)	22 (14%)
49	S2	1717/1742 (98%)	745 (43%)	269 (15%)
All	All	5638/5682 (99%)	2453 (43%)	921 (16%)

All (2453) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	2	G
1	5	5	A
1	5	6	C
1	5	8	U
1	5	12	A
1	5	13	U
1	5	20	U
1	5	21	G
1	5	25	A
1	5	33	A
1	5	34	A
1	5	39	A
1	5	40	G
1	5	42	A
1	5	43	U
1	5	47	A

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Mol	Chain	Res	Type
1	5	48	G
1	5	49	U
1	5	50	C
1	5	51	A
1	5	54	G
1	5	55	G
1	5	56	A
1	5	58	G
1	5	59	A
1	5	64	A
1	5	65	A
1	5	66	A
1	5	69	A
1	5	70	A
1	5	71	C
1	5	72	C
1	5	74	G
1	5	80	C
1	5	81	C
1	5	84	A
1	5	85	G
1	5	88	A
1	5	89	C
1	5	91	G
1	5	92	C
1	5	93	G
1	5	94	A
1	5	95	G
1	5	96	U
1	5	98	A
1	5	99	A
1	5	101	A
1	5	107	G
1	5	108	A
1	5	109	G
1	5	110	C
1	5	111	C
1	5	112	C
1	5	115	C
1	5	118	C
1	5	119	G
1	5	120	A

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Mol	Chain	Res	Type
1	5	121	A
1	5	126	C
1	5	128	C
1	5	129	C
1	5	130	C
1	5	131	C
1	5	132	G
1	5	134	G
1	5	135	G
1	5	136	C
1	5	137	G
1	5	138	G
1	5	139	G
1	5	143	C
1	5	144	G
1	5	145	G
1	5	150	U
1	5	152	U
1	5	157	U
1	5	158	A
1	5	159	C
1	5	164	G
1	5	170	C
1	5	171	U
1	5	172	C
1	5	173	C
1	5	178	C
1	5	182	G
1	5	183	C
1	5	184	U
1	5	185	C
1	5	186	G
1	5	187	U
1	5	188	G
1	5	189	G
1	5	195	C
1	5	196	C
1	5	197	A
1	5	198	A
1	5	200	U
1	5	201	C
1	5	202	C

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Mol	Chain	Res	Type
1	5	203	U
1	5	205	C
1	5	206	U
1	5	210	C
1	5	211	G
1	5	216	C
1	5	217	C
1	5	218	A
1	5	219	G
1	5	220	C
1	5	221	C
1	5	224	U
1	5	225	G
1	5	226	G
1	5	227	A
1	5	232	G
1	5	233	U
1	5	234	G
1	5	235	A
1	5	236	G
1	5	238	C
1	5	239	C
1	5	245	C
1	5	246	G
1	5	255	C
1	5	257	C
1	5	262	G
1	5	264	C
1	5	265	C
1	5	266	C
1	5	267	G
1	5	270	U
1	5	274	C
1	5	275	C
1	5	276	C
1	5	277	G
1	5	278	G
1	5	280	G
1	5	281	U
1	5	288	G
1	5	292	G
1	5	293	G

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Mol	Chain	Res	Type
1	5	294	G
1	5	296	A
1	5	297	U
1	5	300	A
1	5	305	A
1	5	306	A
1	5	309	C
1	5	310	G
1	5	315	G
1	5	316	U
1	5	317	A
1	5	319	A
1	5	322	C
1	5	323	C
1	5	324	A
1	5	325	U
1	5	330	G
1	5	334	A
1	5	337	U
1	5	338	A
1	5	339	C
1	5	340	C
1	5	342	G
1	5	343	C
1	5	345	C
1	5	347	A
1	5	349	A
1	5	350	C
1	5	352	G
1	5	353	A
1	5	354	U
1	5	355	A
1	5	357	U
1	5	358	C
1	5	360	A
1	5	361	C
1	5	362	A
1	5	363	A
1	5	370	U
1	5	381	U
1	5	383	A
1	5	384	A

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Mol	Chain	Res	Type
1	5	385	A
1	5	386	A
1	5	387	G
1	5	388	A
1	5	390	C
1	5	395	A
1	5	399	G
1	5	406	C
1	5	407	A
1	5	408	A
1	5	409	G
1	5	410	A
1	5	412	G
1	5	413	G
1	5	414	C
1	5	415	G
1	5	417	G
1	5	418	A
1	5	431	G
1	5	432	U
1	5	433	A
1	5	434	A
1	5	440	U
1	5	444	G
1	5	445	U
1	5	449	C
1	5	450	G
1	5	451	C
1	5	452	A
1	5	453	G
1	5	454	U
1	5	455	C
1	5	456	C
1	5	458	C
1	5	466	A
1	5	467	U
1	5	468	U
1	5	469	C
1	5	470	A
1	5	471	A
1	5	473	C
1	5	484	U

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Mol	Chain	Res	Type
1	5	485	C
1	5	486	C
1	5	487	G
1	5	491	G
1	5	496	G
1	5	498	C
1	5	500	G
1	5	502	C
1	5	503	C
1	5	504	G
1	5	506	C
1	5	509	A
1	5	510	U
1	5	511	C
1	5	513	U
1	5	514	U
1	5	515	C
1	5	516	C
1	5	519	C
1	5	647	G
1	5	648	G
1	5	649	A
1	5	650	C
1	5	653	U
1	5	654	C
1	5	656	C
1	5	658	C
1	5	664	G
1	5	665	C
1	5	666	G
1	5	667	A
1	5	668	C
1	5	669	C
1	5	671	G
1	5	672	C
1	5	681	G
1	5	682	G
1	5	683	C
1	5	684	G
1	5	685	C
1	5	686	A
1	5	687	U

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Mol	Chain	Res	Type
1	5	689	U
1	5	690	C
1	5	692	A
1	5	694	C
1	5	695	G
1	5	696	C
1	5	697	G
1	5	702	U
1	5	703	G
1	5	704	C
1	5	705	G
1	5	707	C
1	5	716	C
1	5	717	U
1	5	718	C
1	5	721	G
1	5	724	C
1	5	727	C
1	5	728	U
1	5	729	G
1	5	730	G
1	5	731	G
1	5	732	A
1	5	737	C
1	5	739	G
1	5	742	G
1	5	743	G
1	5	745	G
1	5	746	A
1	5	747	A
1	5	748	G
1	5	749	G
1	5	912	G
1	5	915	A
1	5	917	A
1	5	918	G
1	5	926	G
1	5	927	G
1	5	928	C
1	5	929	A
1	5	930	G
1	5	931	C

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Mol	Chain	Res	Type
1	5	932	A
1	5	933	G
1	5	934	C
1	5	935	A
1	5	936	C
1	5	937	U
1	5	938	C
1	5	939	G
1	5	940	C
1	5	944	A
1	5	945	U
1	5	946	C
1	5	950	G
1	5	952	G
1	5	955	G
1	5	956	A
1	5	957	G
1	5	958	G
1	5	959	G
1	5	960	A
1	5	961	G
1	5	962	C
1	5	963	G
1	5	964	A
1	5	965	G
1	5	966	A
1	5	967	C
1	5	968	C
1	5	969	C
1	5	971	U
1	5	972	C
1	5	973	G
1	5	974	C
1	5	975	C
1	5	976	G
1	5	977	C
1	5	978	G
1	5	979	C
1	5	980	U
1	5	982	U
1	5	983	C
1	5	985	C

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Mol	Chain	Res	Type
1	5	990	C
1	5	1051	G
1	5	1072	C
1	5	1075	G
1	5	1076	C
1	5	1077	C
1	5	1078	A
1	5	1082	C
1	5	1083	U
1	5	1084	C
1	5	1086	C
1	5	1168	G
1	5	1177	U
1	5	1181	C
1	5	1193	C
1	5	1210	C
1	5	1211	G
1	5	1212	G
1	5	1214	C
1	5	1215	C
1	5	1218	G
1	5	1219	G
1	5	1221	G
1	5	1222	A
1	5	1233	G
1	5	1235	G
1	5	1236	C
1	5	1237	C
1	5	1238	A
1	5	1239	C
1	5	1240	G
1	5	1242	G
1	5	1243	C
1	5	1244	G
1	5	1245	C
1	5	1255	A
1	5	1264	C
1	5	1265	G
1	5	1266	G
1	5	1267	C
1	5	1268	G
1	5	1269	G

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Mol	Chain	Res	Type
1	5	1270	A
1	5	1271	G
1	5	1272	C
1	5	1273	G
1	5	1274	A
1	5	1275	G
1	5	1277	G
1	5	1279	A
1	5	1280	C
1	5	1282	G
1	5	1283	G
1	5	1284	G
1	5	1285	U
1	5	1288	G
1	5	1289	C
1	5	1290	G
1	5	1291	G
1	5	1292	C
1	5	1293	G
1	5	1294	A
1	5	1295	C
1	5	1296	G
1	5	1297	U
1	5	1298	C
1	5	1300	G
1	5	1301	C
1	5	1304	C
1	5	1313	C
1	5	1314	C
1	5	1319	U
1	5	1325	C
1	5	1326	A
1	5	1330	A
1	5	1333	A
1	5	1337	A
1	5	1338	G
1	5	1344	C
1	5	1354	A
1	5	1357	C
1	5	1358	G
1	5	1359	G
1	5	1360	G

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Mol	Chain	Res	Type
1	5	1362	G
1	5	1364	U
1	5	1365	C
1	5	1366	G
1	5	1367	C
1	5	1368	A
1	5	1369	C
1	5	1370	G
1	5	1371	A
1	5	1372	A
1	5	1377	G
1	5	1378	C
1	5	1379	C
1	5	1380	G
1	5	1381	U
1	5	1382	G
1	5	1387	A
1	5	1390	G
1	5	1394	G
1	5	1397	A
1	5	1398	A
1	5	1399	G
1	5	1402	C
1	5	1407	C
1	5	1408	G
1	5	1410	U
1	5	1411	C
1	5	1420	A
1	5	1421	G
1	5	1426	G
1	5	1427	A
1	5	1428	U
1	5	1429	C
1	5	1435	G
1	5	1436	C
1	5	1439	C
1	5	1440	U
1	5	1441	C
1	5	1444	G
1	5	1445	U
1	5	1446	C
1	5	1448	G

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Mol	Chain	Res	Type
1	5	1455	G
1	5	1456	C
1	5	1457	G
1	5	1458	C
1	5	1465	G
1	5	1466	G
1	5	1474	C
1	5	1475	G
1	5	1478	C
1	5	1479	G
1	5	1480	C
1	5	1481	C
1	5	1482	G
1	5	1483	C
1	5	1484	G
1	5	1485	C
1	5	1487	G
1	5	1488	G
1	5	1489	G
1	5	1490	G
1	5	1493	G
1	5	1497	A
1	5	1498	G
1	5	1499	C
1	5	1500	A
1	5	1501	C
1	5	1503	A
1	5	1504	G
1	5	1514	U
1	5	1516	G
1	5	1518	A
1	5	1519	C
1	5	1520	C
1	5	1522	G
1	5	1523	A
1	5	1525	A
1	5	1530	G
1	5	1534	A
1	5	1535	C
1	5	1542	U
1	5	1543	G
1	5	1547	A

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Mol	Chain	Res	Type
1	5	1562	G
1	5	1563	A
1	5	1568	C
1	5	1571	G
1	5	1572	U
1	5	1578	U
1	5	1583	A
1	5	1590	C
1	5	1591	U
1	5	1596	U
1	5	1597	G
1	5	1604	G
1	5	1611	C
1	5	1612	G
1	5	1613	A
1	5	1614	C
1	5	1624	G
1	5	1625	G
1	5	1631	A
1	5	1633	G
1	5	1634	A
1	5	1636	U
1	5	1637	A
1	5	1638	A
1	5	1639	U
1	5	1640	C
1	5	1641	G
1	5	1642	A
1	5	1643	A
1	5	1650	A
1	5	1654	G
1	5	1656	U
1	5	1661	C
1	5	1662	C
1	5	1670	G
1	5	1671	U
1	5	1673	U
1	5	1674	C
1	5	1676	C
1	5	1678	C
1	5	1679	A
1	5	1680	G

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Mol	Chain	Res	Type
1	5	1681	G
1	5	1684	A
1	5	1685	G
1	5	1687	U
1	5	1691	G
1	5	1692	C
1	5	1694	C
1	5	1696	C
1	5	1697	G
1	5	1698	C
1	5	1699	A
1	5	1719	A
1	5	1720	C
1	5	1721	G
1	5	1722	C
1	5	1723	A
1	5	1724	G
1	5	1725	U
1	5	1727	U
1	5	1730	U
1	5	1733	G
1	5	1734	G
1	5	1735	U
1	5	1736	A
1	5	1741	G
1	5	1742	A
1	5	1746	A
1	5	1750	G
1	5	1751	A
1	5	1753	G
1	5	1754	U
1	5	1755	C
1	5	1756	U
1	5	1757	U
1	5	1758	G
1	5	1759	G
1	5	1760	G
1	5	1761	G
1	5	1762	C
1	5	1764	G
1	5	1765	A
1	5	1766	A

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Mol	Chain	Res	Type
1	5	1767	A
1	5	1768	C
1	5	1769	G
1	5	1770	A
1	5	1772	C
1	5	1776	A
1	5	1777	C
1	5	1779	U
1	5	1781	U
1	5	1787	A
1	5	1788	A
1	5	1790	U
1	5	1791	U
1	5	1799	G
1	5	1800	U
1	5	1803	G
1	5	1804	A
1	5	1805	A
1	5	1817	U
1	5	1818	G
1	5	1819	G
1	5	1820	C
1	5	1822	U
1	5	1825	A
1	5	1827	C
1	5	1830	G
1	5	1832	C
1	5	1833	G
1	5	1834	U
1	5	1835	G
1	5	1836	G
1	5	1840	G
1	5	1843	A
1	5	1847	C
1	5	1848	C
1	5	1849	U
1	5	1850	A
1	5	1851	G
1	5	1855	G
1	5	1864	G
1	5	1866	U
1	5	1867	A

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Mol	Chain	Res	Type
1	5	1869	G
1	5	1878	G
1	5	1881	C
1	5	1882	U
1	5	1886	G
1	5	1890	G
1	5	1891	A
1	5	1897	A
1	5	1899	G
1	5	1900	C
1	5	1903	G
1	5	1907	A
1	5	1910	G
1	5	1912	G
1	5	1913	C
1	5	1916	G
1	5	1917	A
1	5	1918	U
1	5	1919	G
1	5	1920	C
1	5	1921	C
1	5	1922	G
1	5	1923	A
1	5	1925	G
1	5	1929	A
1	5	1930	U
1	5	1931	C
1	5	1932	A
1	5	1935	C
1	5	1936	C
1	5	1938	C
1	5	1940	G
1	5	1941	A
1	5	1944	A
1	5	1945	G
1	5	1946	G
1	5	1947	U
1	5	1948	G
1	5	1951	G
1	5	1952	G
1	5	1956	A
1	5	1958	A

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Mol	Chain	Res	Type
1	5	1959	U
1	5	1960	A
1	5	1961	G
1	5	1962	A
1	5	1963	C
1	5	1971	C
1	5	1974	U
1	5	1975	G
1	5	1976	G
1	5	1977	C
1	5	1979	A
1	5	1980	U
1	5	1981	G
1	5	1983	A
1	5	1984	A
1	5	1985	G
1	5	1986	U
1	5	1987	C
1	5	1988	G
1	5	1991	A
1	5	1992	U
1	5	1993	C
1	5	1997	U
1	5	1998	A
1	5	1999	A
1	5	2001	G
1	5	2002	A
1	5	2003	G
1	5	2004	U
1	5	2005	G
1	5	2007	G
1	5	2008	U
1	5	2009	A
1	5	2010	A
1	5	2015	U
1	5	2018	C
1	5	2019	C
1	5	2020	U
1	5	2022	C
1	5	2024	G
1	5	2025	A
1	5	2026	A

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Mol	Chain	Res	Type
1	5	2027	U
1	5	2033	A
1	5	2034	G
1	5	2038	U
1	5	2044	U
1	5	2045	G
1	5	2046	G
1	5	2047	A
1	5	2048	U
1	5	2052	G
1	5	2055	G
1	5	2056	G
1	5	2057	A
1	5	2059	C
1	5	2060	G
1	5	2062	C
1	5	2063	G
1	5	2064	G
1	5	2069	A
1	5	2070	U
1	5	2077	C
1	5	2083	C
1	5	2084	C
1	5	2085	G
1	5	2088	A
1	5	2089	G
1	5	2090	U
1	5	2091	C
1	5	2092	G
1	5	2093	A
1	5	2094	G
1	5	2095	A
1	5	2096	G
1	5	2097	U
1	5	2100	A
1	5	2105	A
1	5	2107	C
1	5	2108	G
1	5	2109	G
1	5	2110	C
1	5	2111	G
1	5	2112	G

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Mol	Chain	Res	Type
1	5	2113	G
1	5	2114	G
1	5	2115	G
1	5	2116	C
1	5	2117	G
1	5	2118	G
1	5	2119	C
1	5	2120	G
1	5	2121	C
1	5	2122	G
1	5	2123	C
1	5	2124	G
1	5	2125	C
1	5	2126	G
1	5	2127	C
1	5	2247	C
1	5	2248	C
1	5	2250	C
1	5	2251	G
1	5	2252	G
1	5	2253	A
1	5	2254	G
1	5	2255	C
1	5	2256	C
1	5	2257	C
1	5	2258	C
1	5	2259	G
1	5	2260	C
1	5	2261	G
1	5	2262	G
1	5	2263	A
1	5	2264	C
1	5	2265	G
1	5	2266	C
1	5	2267	U
1	5	2268	A
1	5	2269	C
1	5	2270	G
1	5	2273	G
1	5	2275	G
1	5	2277	C
1	5	2279	A

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Mol	Chain	Res	Type
1	5	2282	A
1	5	2283	G
1	5	2288	G
1	5	2289	C
1	5	2299	G
1	5	2300	A
1	5	2301	G
1	5	2305	U
1	5	2309	G
1	5	2312	U
1	5	2313	A
1	5	2314	G
1	5	2316	G
1	5	2319	C
1	5	2321	G
1	5	2322	G
1	5	2324	C
1	5	2325	C
1	5	2328	G
1	5	2329	U
1	5	2330	G
1	5	2331	G
1	5	2332	A
1	5	2333	G
1	5	2334	C
1	5	2337	C
1	5	2339	G
1	5	2342	G
1	5	2343	G
1	5	2347	A
1	5	2348	G
1	5	2349	A
1	5	2350	U
1	5	2351	C
1	5	2357	G
1	5	2360	A
1	5	2361	G
1	5	2362	U
1	5	2366	A
1	5	2367	A
1	5	2368	A
1	5	2369	U

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Mol	Chain	Res	Type
1	5	2370	A
1	5	2372	U
1	5	2378	G
1	5	2382	A
1	5	2384	U
1	5	2389	A
1	5	2390	G
1	5	2391	G
1	5	2395	A
1	5	2396	A
1	5	2397	G
1	5	2398	U
1	5	2399	G
1	5	2407	G
1	5	2409	U
1	5	2417	A
1	5	2422	C
1	5	2425	U
1	5	2426	U
1	5	2428	A
1	5	2429	A
1	5	2432	U
1	5	2433	G
1	5	2434	G
1	5	2437	C
1	5	2438	A
1	5	2439	G
1	5	2440	U
1	5	2441	C
1	5	2443	G
1	5	2447	U
1	5	2448	G
1	5	2450	G
1	5	2454	U
1	5	2464	C
1	5	2465	C
1	5	2468	U
1	5	2469	C
1	5	2470	C
1	5	2471	G
1	5	2472	A
1	5	2474	G

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Mol	Chain	Res	Type
1	5	2475	G
1	5	2476	G
1	5	2487	G
1	5	2488	C
1	5	2489	C
1	5	2490	U
1	5	2491	C
1	5	2502	G
1	5	2503	G
1	5	2504	C
1	5	2505	C
1	5	2506	G
1	5	2507	A
1	5	2508	U
1	5	2509	C
1	5	2510	G
1	5	2511	A
1	5	2512	A
1	5	2513	A
1	5	2514	G
1	5	2526	C
1	5	2527	A
1	5	2529	A
1	5	2530	U
1	5	2532	C
1	5	2537	A
1	5	2544	G
1	5	2545	U
1	5	2546	G
1	5	2547	G
1	5	2549	G
1	5	2551	A
1	5	2552	G
1	5	2553	A
1	5	2554	U
1	5	2555	G
1	5	2560	C
1	5	2566	G
1	5	2571	C
1	5	2572	C
1	5	2577	C
1	5	2581	A

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Mol	Chain	Res	Type
1	5	2583	C
1	5	2586	G
1	5	2587	A
1	5	2588	C
1	5	2589	C
1	5	2600	A
1	5	2601	A
1	5	2602	G
1	5	2615	C
1	5	2616	C
1	5	2620	G
1	5	2623	A
1	5	2627	C
1	5	2630	U
1	5	2631	U
1	5	2638	G
1	5	2639	U
1	5	2640	G
1	5	2643	G
1	5	2645	G
1	5	2648	G
1	5	2649	G
1	5	2653	C
1	5	2658	G
1	5	2659	A
1	5	2660	A
1	5	2661	U
1	5	2662	G
1	5	2664	G
1	5	2666	U
1	5	2667	C
1	5	2670	C
1	5	2673	G
1	5	2674	A
1	5	2675	G
1	5	2678	A
1	5	2684	C
1	5	2687	U
1	5	2688	G
1	5	2689	C
1	5	2692	U
1	5	2694	G

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Mol	Chain	Res	Type
1	5	2696	A
1	5	2704	C
1	5	2710	C
1	5	2711	G
1	5	2712	G
1	5	2713	C
1	5	2714	G
1	5	2716	C
1	5	2722	G
1	5	2725	A
1	5	2726	G
1	5	2735	G
1	5	2737	C
1	5	2740	U
1	5	2743	A
1	5	2744	A
1	5	2745	A
1	5	2747	U
1	5	2751	G
1	5	2752	G
1	5	2754	G
1	5	2756	G
1	5	2760	G
1	5	2762	G
1	5	2764	A
1	5	2765	A
1	5	2766	A
1	5	2767	U
1	5	2768	C
1	5	2769	U
1	5	2770	C
1	5	2783	A
1	5	2786	C
1	5	2787	A
1	5	2788	U
1	5	2790	U
1	5	2794	C
1	5	2796	G
1	5	2797	C
1	5	2798	A
1	5	2799	G
1	5	2806	A

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Mol	Chain	Res	Type
1	5	2807	A
1	5	2808	G
1	5	2812	A
1	5	2813	A
1	5	2814	C
1	5	2815	A
1	5	2818	C
1	5	2820	C
1	5	2821	U
1	5	2824	C
1	5	2826	U
1	5	2827	G
1	5	2828	U
1	5	2829	U
1	5	2832	A
1	5	2833	A
1	5	2834	C
1	5	2835	A
1	5	2838	G
1	5	2841	G
1	5	2842	G
1	5	2848	G
1	5	2849	A
1	5	2850	A
1	5	2852	U
1	5	2854	G
1	5	2855	G
1	5	2858	A
1	5	2859	G
1	5	2860	C
1	5	2866	C
1	5	2867	C
1	5	2873	U
1	5	2874	U
1	5	2875	C
1	5	2876	G
1	5	2879	A
1	5	2880	U
1	5	2888	G
1	5	2892	C
1	5	2897	G
1	5	2898	G

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Mol	Chain	Res	Type
1	5	2900	U
1	5	2904	U
1	5	2905	C
1	5	2910	G
1	5	3591	C
1	5	3592	G
1	5	3594	C
1	5	3595	U
1	5	3596	A
1	5	3597	G
1	5	3605	C
1	5	3606	U
1	5	3615	G
1	5	3616	U
1	5	3617	G
1	5	3620	G
1	5	3621	A
1	5	3623	C
1	5	3625	G
1	5	3626	G
1	5	3627	G
1	5	3635	A
1	5	3636	C
1	5	3643	A
1	5	3644	U
1	5	3649	A
1	5	3650	C
1	5	3658	C
1	5	3660	C
1	5	3662	A
1	5	3663	A
1	5	3664	G
1	5	3667	C
1	5	3668	C
1	5	3670	C
1	5	3671	G
1	5	3672	G
1	5	3673	C
1	5	3674	G
1	5	3675	G
1	5	3677	U
1	5	3678	G

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Mol	Chain	Res	Type
1	5	3679	U
1	5	3680	U
1	5	3681	G
1	5	3682	A
1	5	3688	U
1	5	3692	A
1	5	3698	G
1	5	3699	C
1	5	3709	U
1	5	3710	G
1	5	3711	A
1	5	3712	A
1	5	3713	U
1	5	3715	U
1	5	3716	C
1	5	3717	A
1	5	3718	A
1	5	3727	A
1	5	3728	A
1	5	3729	U
1	5	3733	A
1	5	3735	G
1	5	3736	A
1	5	3737	A
1	5	3738	G
1	5	3739	C
1	5	3743	G
1	5	3744	G
1	5	3745	U
1	5	3748	A
1	5	3756	A
1	5	3759	A
1	5	3760	A
1	5	3770	U
1	5	3772	U
1	5	3773	U
1	5	3774	A
1	5	3775	A
1	5	3776	G
1	5	3777	G
1	5	3784	A
1	5	3785	A

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Mol	Chain	Res	Type
1	5	3786	U
1	5	3791	C
1	5	3799	A
1	5	3800	A
1	5	3802	U
1	5	3803	A
1	5	3807	A
1	5	3809	G
1	5	3810	C
1	5	3811	G
1	5	3813	A
1	5	3814	U
1	5	3817	A
1	5	3819	G
1	5	3822	U
1	5	3831	U
1	5	3838	U
1	5	3839	G
1	5	3840	U
1	5	3843	C
1	5	3849	A
1	5	3851	U
1	5	3859	G
1	5	3861	A
1	5	3865	A
1	5	3867	A
1	5	3876	A
1	5	3877	A
1	5	3878	C
1	5	3879	G
1	5	3880	G
1	5	3881	G
1	5	3882	C
1	5	3887	C
1	5	3889	G
1	5	3895	G
1	5	3897	G
1	5	3898	G
1	5	3899	G
1	5	3900	G
1	5	3901	A
1	5	3902	A

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Mol	Chain	Res	Type
1	5	3905	A
1	5	3906	A
1	5	3907	G
1	5	3908	A
1	5	3912	U
1	5	3913	G
1	5	3914	U
1	5	3915	U
1	5	3916	G
1	5	3917	A
1	5	3923	A
1	5	3925	U
1	5	3926	C
1	5	3938	G
1	5	3939	G
1	5	3943	A
1	5	4069	U
1	5	4070	U
1	5	4073	A
1	5	4075	U
1	5	4076	G
1	5	4083	U
1	5	4084	G
1	5	4085	A
1	5	4086	G
1	5	4087	G
1	5	4088	C
1	5	4089	G
1	5	4091	G
1	5	4092	G
1	5	4093	G
1	5	4094	G
1	5	4095	G
1	5	4097	G
1	5	4104	G
1	5	4105	A
1	5	4107	G
1	5	4114	C
1	5	4115	G
1	5	4116	C
1	5	4117	U
1	5	4118	U

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Mol	Chain	Res	Type
1	5	4119	C
1	5	4120	U
1	5	4121	G
1	5	4122	G
1	5	4125	C
1	5	4126	C
1	5	4127	A
1	5	4129	G
1	5	4132	C
1	5	4140	C
1	5	4143	G
1	5	4145	C
1	5	4158	C
1	5	4162	C
1	5	4164	C
1	5	4166	G
1	5	4168	G
1	5	4169	G
1	5	4171	C
1	5	4172	A
1	5	4173	G
1	5	4180	G
1	5	4183	G
1	5	4184	G
1	5	4191	G
1	5	4195	G
1	5	4196	G
1	5	4197	G
1	5	4199	C
1	5	4203	A
1	5	4205	A
1	5	4206	C
1	5	4208	U
1	5	4212	A
1	5	4213	A
1	5	4214	A
1	5	4215	C
1	5	4216	G
1	5	4217	G
1	5	4218	U
1	5	4219	A
1	5	4220	A

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Mol	Chain	Res	Type
1	5	4221	C
1	5	4222	G
1	5	4225	G
1	5	4226	G
1	5	4228	G
1	5	4229	U
1	5	4232	U
1	5	4233	A
1	5	4234	A
1	5	4235	G
1	5	4236	G
1	5	4239	A
1	5	4241	C
1	5	4249	G
1	5	4251	A
1	5	4252	C
1	5	4254	G
1	5	4255	A
1	5	4257	A
1	5	4258	C
1	5	4265	U
1	5	4267	G
1	5	4268	A
1	5	4271	A
1	5	4274	A
1	5	4276	G
1	5	4279	A
1	5	4280	A
1	5	4281	A
1	5	4282	A
1	5	4283	G
1	5	4286	C
1	5	4287	G
1	5	4288	C
1	5	4290	U
1	5	4291	G
1	5	4296	U
1	5	4297	G
1	5	4305	G
1	5	4306	U
1	5	4311	A
1	5	4314	C

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Mol	Chain	Res	Type
1	5	4316	G
1	5	4318	C
1	5	4323	A
1	5	4329	G
1	5	4330	G
1	5	4332	C
1	5	4335	C
1	5	4336	A
1	5	4337	C
1	5	4339	A
1	5	4344	U
1	5	4348	A
1	5	4349	C
1	5	4350	C
1	5	4352	U
1	5	4353	U
1	5	4354	U
1	5	4356	G
1	5	4364	G
1	5	4368	G
1	5	4369	A
1	5	4373	G
1	5	4374	U
1	5	4375	C
1	5	4376	A
1	5	4377	G
1	5	4378	A
1	5	4379	A
1	5	4385	A
1	5	4386	C
1	5	4387	C
1	5	4388	A
1	5	4391	G
1	5	4393	G
1	5	4394	A
1	5	4395	U
1	5	4396	A
1	5	4401	G
1	5	4419	U
1	5	4422	A
1	5	4425	G
1	5	4426	C

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Mol	Chain	Res	Type
1	5	4434	C
1	5	4436	U
1	5	4437	U
1	5	4438	U
1	5	4439	U
1	5	4440	G
1	5	4441	A
1	5	4443	C
1	5	4444	C
1	5	4448	G
1	5	4449	A
1	5	4450	U
1	5	4451	G
1	5	4452	U
1	5	4454	G
1	5	4459	U
1	5	4463	U
1	5	4464	A
1	5	4465	U
1	5	4466	C
1	5	4467	A
1	5	4469	U
1	5	4471	U
1	5	4472	G
1	5	4473	A
1	5	4475	G
1	5	4476	C
1	5	4484	A
1	5	4488	A
1	5	4489	G
1	5	4491	G
1	5	4498	U
1	5	4500	U
1	5	4503	A
1	5	4510	A
1	5	4511	A
1	5	4512	U
1	5	4513	A
1	5	4518	A
1	5	4519	C
1	5	4520	G
1	5	4522	G

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Mol	Chain	Res	Type
1	5	4523	A
1	5	4524	G
1	5	4528	G
1	5	4529	G
1	5	4530	U
1	5	4531	U
1	5	4532	U
1	5	4534	G
1	5	4536	C
1	5	4537	C
1	5	4543	G
1	5	4544	A
1	5	4546	A
1	5	4548	A
1	5	4549	G
1	5	4550	G
1	5	4552	U
1	5	4557	U
1	5	4560	C
1	5	4569	U
1	5	4570	G
1	5	4572	U
1	5	4574	U
1	5	4575	G
1	5	4581	G
1	5	4583	C
1	5	4584	A
1	5	4585	U
1	5	4586	G
1	5	4589	A
1	5	4590	A
1	5	4592	C
1	5	4599	A
1	5	4600	G
1	5	4601	U
1	5	4603	C
1	5	4605	A
1	5	4606	G
1	5	4608	G
1	5	4617	G
1	5	4623	G
1	5	4624	A

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Mol	Chain	Res	Type
1	5	4636	U
1	5	4637	G
1	5	4641	U
1	5	4646	U
1	5	4647	G
1	5	4648	A
1	5	4652	G
1	5	4656	A
1	5	4657	U
1	5	4661	G
1	5	4664	A
1	5	4669	A
1	5	4670	C
1	5	4671	C
1	5	4672	A
1	5	4676	G
1	5	4677	U
1	5	4678	G
1	5	4679	G
1	5	4687	A
1	5	4693	C
1	5	4694	G
1	5	4695	C
1	5	4700	A
1	5	4701	A
1	5	4709	U
1	5	4714	C
1	5	4715	C
1	5	4717	A
1	5	4718	G
1	5	4719	G
1	5	4720	C
1	5	4721	G
1	5	4722	G
1	5	4729	A
1	5	4730	C
1	5	4731	G
1	5	4732	G
1	5	4733	C
1	5	4734	A
1	5	4735	G
1	5	4737	G

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Mol	Chain	Res	Type
1	5	4738	C
1	5	4741	C
1	5	4743	G
1	5	4745	G
1	5	4746	C
1	5	4748	U
1	5	4749	C
1	5	4750	G
1	5	4751	G
1	5	4753	U
1	5	4756	C
1	5	4757	C
1	5	4758	U
1	5	4760	G
1	5	4763	U
1	5	4764	A
1	5	4770	U
1	5	4771	C
1	5	4774	C
1	5	4860	G
1	5	4865	C
1	5	4869	U
1	5	4871	C
1	5	4872	G
1	5	4873	G
1	5	4874	A
1	5	4875	G
1	5	4876	U
1	5	4877	G
1	5	4878	C
1	5	4881	U
1	5	4882	U
1	5	4883	C
1	5	4884	G
1	5	4885	U
1	5	4886	C
1	5	4888	U
1	5	4889	G
1	5	4890	G
1	5	4891	G
1	5	4893	A
1	5	4895	C

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Mol	Chain	Res	Type
1	5	4896	G
1	5	4900	C
1	5	4901	G
1	5	4903	G
1	5	4906	C
1	5	4910	G
1	5	4911	A
1	5	4912	G
1	5	4913	G
1	5	4915	G
1	5	4919	G
1	5	4926	C
1	5	4927	G
1	5	4928	C
1	5	4929	C
1	5	4930	C
1	5	4932	U
1	5	4933	C
1	5	4934	A
1	5	4936	G
1	5	4937	C
1	5	4938	A
1	5	4939	C
1	5	4942	C
1	5	4945	G
1	5	4946	U
1	5	4947	U
1	5	4948	C
1	5	4949	G
1	5	4950	U
1	5	4951	G
1	5	4952	G
1	5	4953	G
1	5	4957	C
1	5	4959	U
1	5	4961	G
1	5	4962	C
1	5	4964	C
1	5	4965	U
1	5	4966	A
1	5	4967	A
1	5	4977	A

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Mol	Chain	Res	Type
1	5	4979	A
1	5	4980	C
1	5	4981	G
1	5	4982	A
1	5	4985	U
1	5	4988	U
1	5	4989	U
1	5	4990	C
1	5	4991	U
1	5	4992	G
1	5	4993	G
1	5	4999	G
1	5	5002	U
1	5	5006	U
1	5	5013	C
1	5	5014	A
1	5	5016	A
1	5	5017	G
1	5	5018	C
1	5	5019	A
1	5	5021	C
1	5	5023	C
1	5	5026	U
1	5	5027	C
1	5	5028	G
1	5	5034	A
1	5	5035	U
1	5	5040	U
1	5	5041	G
1	5	5042	A
1	5	5045	G
1	5	5047	C
1	5	5048	A
1	5	5049	G
1	5	5050	C
1	5	5052	C
1	5	5053	U
1	5	5054	C
1	5	5056	A
1	5	5057	C
1	5	5058	A
1	5	5060	A

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Mol	Chain	Res	Type
1	5	5061	A
1	5	5062	G
1	5	5063	G
1	5	5069	U
2	7	7	G
2	7	11	A
2	7	17	C
2	7	21	G
2	7	22	A
2	7	23	A
2	7	24	C
2	7	27	G
2	7	30	C
2	7	31	G
2	7	42	A
2	7	53	U
2	7	54	A
2	7	57	C
2	7	60	G
2	7	63	C
2	7	64	G
2	7	65	G
2	7	70	G
2	7	73	U
2	7	74	A
2	7	79	U
2	7	80	U
2	7	90	A
2	7	100	A
2	7	105	C
2	7	106	G
2	7	110	G
2	7	112	U
2	7	115	A
2	7	120	U
3	8	2	G
3	8	3	A
3	8	9	A
3	8	11	C
3	8	13	G
3	8	16	G
3	8	23	C

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Mol	Chain	Res	Type
3	8	32	C
3	8	33	G
3	8	34	U
3	8	35	C
3	8	37	A
3	8	38	U
3	8	39	G
3	8	40	A
3	8	46	G
3	8	48	A
3	8	50	C
3	8	51	U
3	8	59	A
3	8	61	A
3	8	62	A
3	8	63	U
3	8	64	U
3	8	65	A
3	8	70	G
3	8	71	A
3	8	74	U
3	8	75	G
3	8	80	A
3	8	81	C
3	8	82	A
3	8	83	C
3	8	84	A
3	8	85	U
3	8	86	U
3	8	87	G
3	8	90	C
3	8	94	G
3	8	95	A
3	8	97	A
3	8	98	C
3	8	99	U
3	8	103	A
3	8	104	A
3	8	105	C
3	8	109	C
3	8	110	U
3	8	111	U

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Mol	Chain	Res	Type
3	8	112	G
3	8	114	G
3	8	118	C
3	8	121	G
3	8	122	G
3	8	125	C
3	8	126	C
3	8	127	U
3	8	137	A
3	8	147	G
3	8	151	G
3	8	153	C
49	S2	3	C
49	S2	4	C
49	S2	9	U
49	S2	10	G
49	S2	17	C
49	S2	18	C
49	S2	20	G
49	S2	23	G
49	S2	24	C
49	S2	25	A
49	S2	27	A
49	S2	33	G
49	S2	39	A
49	S2	44	U
49	S2	45	A
49	S2	46	A
49	S2	49	C
49	S2	51	U
49	S2	53	C
49	S2	56	G
49	S2	57	U
49	S2	58	C
49	S2	59	U
49	S2	60	A
49	S2	61	A
49	S2	62	G
49	S2	63	U
49	S2	64	A
49	S2	65	C
49	S2	66	G

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Mol	Chain	Res	Type
49	S2	67	C
49	S2	68	A
49	S2	71	G
49	S2	72	C
49	S2	73	C
49	S2	74	G
49	S2	75	G
49	S2	76	U
49	S2	77	A
49	S2	78	C
49	S2	79	A
49	S2	80	G
49	S2	84	A
49	S2	88	G
49	S2	89	C
49	S2	92	A
49	S2	98	C
49	S2	99	A
49	S2	101	U
49	S2	103	A
49	S2	105	U
49	S2	111	A
49	S2	113	G
49	S2	114	G
49	S2	115	U
49	S2	116	U
49	S2	117	C
49	S2	123	G
49	S2	125	C
49	S2	127	C
49	S2	139	C
49	S2	140	C
49	S2	141	A
49	S2	142	C
49	S2	143	U
49	S2	144	U
49	S2	146	G
49	S2	147	A
49	S2	148	U
49	S2	150	A
49	S2	153	G
49	S2	154	U

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Mol	Chain	Res	Type
49	S2	155	G
49	S2	156	G
49	S2	159	A
49	S2	160	U
49	S2	161	U
49	S2	162	C
49	S2	163	U
49	S2	164	A
49	S2	165	G
49	S2	167	G
49	S2	169	U
49	S2	170	A
49	S2	173	A
49	S2	176	U
49	S2	180	G
49	S2	181	A
49	S2	182	C
49	S2	183	G
49	S2	184	G
49	S2	188	C
49	S2	189	U
49	S2	191	A
49	S2	192	C
49	S2	200	G
49	S2	202	G
49	S2	206	G
49	S2	209	A
49	S2	210	U
49	S2	211	G
49	S2	213	G
49	S2	215	G
49	S2	216	C
49	S2	217	A
49	S2	290	U
49	S2	291	G
49	S2	292	A
49	S2	293	C
49	S2	295	C
49	S2	302	A
49	S2	305	U
49	S2	306	C
49	S2	307	G

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Mol	Chain	Res	Type
49	S2	308	G
49	S2	309	G
49	S2	310	C
49	S2	311	C
49	S2	312	G
49	S2	313	A
49	S2	314	U
49	S2	316	G
49	S2	317	C
49	S2	318	A
49	S2	319	C
49	S2	321	C
49	S2	324	C
49	S2	325	C
49	S2	326	C
49	S2	328	U
49	S2	338	G
49	S2	340	C
49	S2	341	C
49	S2	342	C
49	S2	343	A
49	S2	346	C
49	S2	347	G
49	S2	350	C
49	S2	355	G
49	S2	356	C
49	S2	357	C
49	S2	360	A
49	S2	362	C
49	S2	364	A
49	S2	365	C
49	S2	367	U
49	S2	368	U
49	S2	369	C
49	S2	370	G
49	S2	373	G
49	S2	377	G
49	S2	380	G
49	S2	381	C
49	S2	382	C
49	S2	384	U
49	S2	385	G

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Mol	Chain	Res	Type
49	S2	386	C
49	S2	394	G
49	S2	398	A
49	S2	400	C
49	S2	407	G
49	S2	408	A
49	S2	409	C
49	S2	411	G
49	S2	414	A
49	S2	416	U
49	S2	417	C
49	S2	418	A
49	S2	419	G
49	S2	425	G
49	S2	426	A
49	S2	427	U
49	S2	428	U
49	S2	429	C
49	S2	435	A
49	S2	436	G
49	S2	438	G
49	S2	441	C
49	S2	444	G
49	S2	445	A
49	S2	447	A
49	S2	448	A
49	S2	449	A
49	S2	450	C
49	S2	453	C
49	S2	454	U
49	S2	455	A
49	S2	459	C
49	S2	460	A
49	S2	464	A
49	S2	465	A
49	S2	466	G
49	S2	467	G
49	S2	468	A
49	S2	469	A
49	S2	471	G
49	S2	472	C
49	S2	473	A

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Mol	Chain	Res	Type
49	S2	474	G
49	S2	476	A
49	S2	482	G
49	S2	487	U
49	S2	488	U
49	S2	489	A
49	S2	492	C
49	S2	493	A
49	S2	496	C
49	S2	500	A
49	S2	501	C
49	S2	507	G
49	S2	508	A
49	S2	516	A
49	S2	518	G
49	S2	523	A
49	S2	525	A
49	S2	528	A
49	S2	530	U
49	S2	532	C
49	S2	533	A
49	S2	534	G
49	S2	542	U
49	S2	544	G
49	S2	548	C
49	S2	549	C
49	S2	550	C
49	S2	551	U
49	S2	552	G
49	S2	554	A
49	S2	555	A
49	S2	556	U
49	S2	557	U
49	S2	559	G
49	S2	560	A
49	S2	562	U
49	S2	563	G
49	S2	564	A
49	S2	568	C
49	S2	575	A
49	S2	576	A
49	S2	579	C

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Mol	Chain	Res	Type
49	S2	580	U
49	S2	583	C
49	S2	588	G
49	S2	589	G
49	S2	590	A
49	S2	591	U
49	S2	592	C
49	S2	593	C
49	S2	595	U
49	S2	596	U
49	S2	598	G
49	S2	600	G
49	S2	601	G
49	S2	602	G
49	S2	604	A
49	S2	605	A
49	S2	607	U
49	S2	608	C
49	S2	612	U
49	S2	614	C
49	S2	616	A
49	S2	617	G
49	S2	621	C
49	S2	623	G
49	S2	626	G
49	S2	627	U
49	S2	628	A
49	S2	629	A
49	S2	630	U
49	S2	631	U
49	S2	632	C
49	S2	643	A
49	S2	644	G
49	S2	646	G
49	S2	649	U
49	S2	655	A
49	S2	657	U
49	S2	660	C
49	S2	662	G
49	S2	666	U
49	S2	667	U
49	S2	668	A

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Mol	Chain	Res	Type
49	S2	669	A
49	S2	671	A
49	S2	672	A
49	S2	673	G
49	S2	679	A
49	S2	683	G
49	S2	684	G
49	S2	687	C
49	S2	688	U
49	S2	689	U
49	S2	690	G
49	S2	693	A
49	S2	694	G
49	S2	695	C
49	S2	698	G
49	S2	731	G
49	S2	733	C
49	S2	734	C
49	S2	735	C
49	S2	736	C
49	S2	738	C
49	S2	739	C
49	S2	745	C
49	S2	747	U
49	S2	748	C
49	S2	749	U
49	S2	751	G
49	S2	752	G
49	S2	753	C
49	S2	788	G
49	S2	791	C
49	S2	797	C
49	S2	798	A
49	S2	799	U
49	S2	800	U
49	S2	809	A
49	S2	810	A
49	S2	811	A
49	S2	812	A
49	S2	820	U
49	S2	821	G
49	S2	822	U

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Mol	Chain	Res	Type
49	S2	827	A
49	S2	830	A
49	S2	833	C
49	S2	834	C
49	S2	835	C
49	S2	836	G
49	S2	837	A
49	S2	838	G
49	S2	840	C
49	S2	841	G
49	S2	842	C
49	S2	843	C
49	S2	845	G
49	S2	847	A
49	S2	848	U
49	S2	856	C
49	S2	861	A
49	S2	867	G
49	S2	868	G
49	S2	869	A
49	S2	870	A
49	S2	871	U
49	S2	872	A
49	S2	873	G
49	S2	875	A
49	S2	877	C
49	S2	878	G
49	S2	879	C
49	S2	880	G
49	S2	881	G
49	S2	887	U
49	S2	888	U
49	S2	890	U
49	S2	891	G
49	S2	892	U
49	S2	897	U
49	S2	898	U
49	S2	903	A
49	S2	910	G
49	S2	913	A
49	S2	914	U
49	S2	915	G

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Mol	Chain	Res	Type
49	S2	917	U
49	S2	918	U
49	S2	919	A
49	S2	920	A
49	S2	921	G
49	S2	930	C
49	S2	933	G
49	S2	934	G
49	S2	938	A
49	S2	943	U
49	S2	954	U
49	S2	955	A
49	S2	956	G
49	S2	957	A
49	S2	958	G
49	S2	959	G
49	S2	960	U
49	S2	961	G
49	S2	962	A
49	S2	964	A
49	S2	965	U
49	S2	966	U
49	S2	968	U
49	S2	969	U
49	S2	970	G
49	S2	971	G
49	S2	979	C
49	S2	980	A
49	S2	981	A
49	S2	990	A
49	S2	991	G
49	S2	992	A
49	S2	996	A
49	S2	997	A
49	S2	999	G
49	S2	1001	A
49	S2	1002	U
49	S2	1008	A
49	S2	1017	U
49	S2	1023	A
49	S2	1033	G
49	S2	1034	A

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Mol	Chain	Res	Type
49	S2	1035	A
49	S2	1040	G
49	S2	1041	G
49	S2	1044	G
49	S2	1045	U
49	S2	1049	A
49	S2	1050	A
49	S2	1060	A
49	S2	1062	A
49	S2	1067	C
49	S2	1070	A
49	S2	1072	U
49	S2	1073	U
49	S2	1077	A
49	S2	1078	C
49	S2	1083	A
49	S2	1084	A
49	S2	1085	C
49	S2	1087	A
49	S2	1088	U
49	S2	1089	G
49	S2	1091	C
49	S2	1096	G
49	S2	1099	G
49	S2	1100	A
49	S2	1102	G
49	S2	1109	C
49	S2	1110	G
49	S2	1111	U
49	S2	1114	U
49	S2	1115	U
49	S2	1116	C
49	S2	1117	C
49	S2	1118	C
49	S2	1120	U
49	S2	1123	C
49	S2	1126	G
49	S2	1130	G
49	S2	1131	G
49	S2	1133	A
49	S2	1138	C
49	S2	1139	C

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Mol	Chain	Res	Type
49	S2	1143	A
49	S2	1144	A
49	S2	1146	C
49	S2	1148	A
49	S2	1149	A
49	S2	1150	A
49	S2	1151	G
49	S2	1153	C
49	S2	1154	U
49	S2	1157	G
49	S2	1165	G
49	S2	1166	G
49	S2	1171	G
49	S2	1172	U
49	S2	1181	A
49	S2	1182	A
49	S2	1186	U
49	S2	1187	G
49	S2	1192	U
49	S2	1194	A
49	S2	1195	A
49	S2	1199	A
49	S2	1200	A
49	S2	1207	G
49	S2	1208	A
49	S2	1211	G
49	S2	1212	G
49	S2	1214	A
49	S2	1215	C
49	S2	1216	C
49	S2	1217	A
49	S2	1221	G
49	S2	1224	G
49	S2	1234	C
49	S2	1242	U
49	S2	1243	U
49	S2	1244	U
49	S2	1247	C
49	S2	1248	U
49	S2	1250	A
49	S2	1251	A
49	S2	1253	A

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Mol	Chain	Res	Type
49	S2	1254	C
49	S2	1256	G
49	S2	1257	G
49	S2	1258	A
49	S2	1259	A
49	S2	1264	C
49	S2	1265	A
49	S2	1266	C
49	S2	1267	C
49	S2	1268	C
49	S2	1269	G
49	S2	1271	C
49	S2	1273	C
49	S2	1274	G
49	S2	1275	G
49	S2	1276	A
49	S2	1280	G
49	S2	1282	A
49	S2	1283	C
49	S2	1284	A
49	S2	1285	G
49	S2	1286	G
49	S2	1288	U
49	S2	1289	U
49	S2	1292	C
49	S2	1293	A
49	S2	1296	U
49	S2	1298	G
49	S2	1299	A
49	S2	1301	A
49	S2	1302	G
49	S2	1303	C
49	S2	1304	U
49	S2	1305	C
49	S2	1306	U
49	S2	1308	U
49	S2	1309	C
49	S2	1312	G
49	S2	1313	A
49	S2	1314	U
49	S2	1315	U
49	S2	1316	C

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Mol	Chain	Res	Type
49	S2	1322	G
49	S2	1324	G
49	S2	1326	U
49	S2	1330	G
49	S2	1332	A
49	S2	1333	U
49	S2	1337	C
49	S2	1342	U
49	S2	1343	U
49	S2	1345	G
49	S2	1348	G
49	S2	1352	G
49	S2	1367	U
49	S2	1370	A
49	S2	1371	U
49	S2	1372	U
49	S2	1373	C
49	S2	1378	A
49	S2	1379	A
49	S2	1380	C
49	S2	1385	G
49	S2	1394	G
49	S2	1395	C
49	S2	1396	A
49	S2	1397	U
49	S2	1401	A
49	S2	1402	A
49	S2	1403	C
49	S2	1404	U
49	S2	1405	A
49	S2	1407	U
49	S2	1410	C
49	S2	1411	G
49	S2	1412	C
49	S2	1414	A
49	S2	1417	C
49	S2	1418	C
49	S2	1419	C
49	S2	1420	G
49	S2	1424	G
49	S2	1426	U
49	S2	1430	C

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Mol	Chain	Res	Type
49	S2	1431	G
49	S2	1432	U
49	S2	1433	C
49	S2	1434	C
49	S2	1435	C
49	S2	1437	C
49	S2	1438	A
49	S2	1441	U
49	S2	1442	U
49	S2	1449	G
49	S2	1450	G
49	S2	1452	A
49	S2	1454	A
49	S2	1455	A
49	S2	1456	G
49	S2	1462	U
49	S2	1463	U
49	S2	1464	C
49	S2	1466	G
49	S2	1467	C
49	S2	1474	A
49	S2	1475	G
49	S2	1476	A
49	S2	1477	U
49	S2	1478	U
49	S2	1489	A
49	S2	1490	G
49	S2	1493	C
49	S2	1494	U
49	S2	1495	G
49	S2	1496	U
49	S2	1506	A
49	S2	1507	G
49	S2	1508	A
49	S2	1509	U
49	S2	1510	G
49	S2	1512	C
49	S2	1513	C
49	S2	1514	G
49	S2	1515	G
49	S2	1520	G
49	S2	1521	C

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Mol	Chain	Res	Type
49	S2	1522	A
49	S2	1525	C
49	S2	1527	C
49	S2	1531	A
49	S2	1534	C
49	S2	1535	U
49	S2	1536	G
49	S2	1537	A
49	S2	1541	G
49	S2	1542	C
49	S2	1543	U
49	S2	1544	C
49	S2	1545	A
49	S2	1546	G
49	S2	1548	G
49	S2	1550	G
49	S2	1551	U
49	S2	1552	G
49	S2	1553	C
49	S2	1554	C
49	S2	1555	U
49	S2	1556	A
49	S2	1557	C
49	S2	1558	C
49	S2	1560	U
49	S2	1567	G
49	S2	1568	C
49	S2	1570	G
49	S2	1574	C
49	S2	1578	U
49	S2	1579	A
49	S2	1580	A
49	S2	1581	C
49	S2	1585	U
49	S2	1586	U
49	S2	1587	G
49	S2	1588	A
49	S2	1589	A
49	S2	1590	C
49	S2	1593	C
49	S2	1595	U
49	S2	1596	U

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Mol	Chain	Res	Type
49	S2	1598	G
49	S2	1599	U
49	S2	1600	G
49	S2	1601	A
49	S2	1602	U
49	S2	1604	G
49	S2	1606	G
49	S2	1609	C
49	S2	1610	G
49	S2	1621	U
49	S2	1622	U
49	S2	1623	A
49	S2	1625	U
49	S2	1633	A
49	S2	1637	A
49	S2	1638	G
49	S2	1644	C
49	S2	1648	G
49	S2	1649	U
49	S2	1656	G
49	S2	1660	C
49	S2	1663	A
49	S2	1664	A
49	S2	1665	G
49	S2	1666	C
49	S2	1674	G
49	S2	1679	A
49	S2	1680	G
49	S2	1682	C
49	S2	1683	C
49	S2	1684	C
49	S2	1689	C
49	S2	1695	A
49	S2	1696	C
49	S2	1699	A
49	S2	1700	C
49	S2	1701	C
49	S2	1702	G
49	S2	1707	U
49	S2	1720	U
49	S2	1721	U
49	S2	1722	G

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Mol	Chain	Res	Type
49	S2	1729	U
49	S2	1730	U
49	S2	1734	G
49	S2	1742	C
49	S2	1745	A
49	S2	1746	U
49	S2	1751	C
49	S2	1753	C
49	S2	1783	C
49	S2	1785	C
49	S2	1786	U
49	S2	1792	G
49	S2	1793	A
49	S2	1795	G
49	S2	1797	U
49	S2	1798	C
49	S2	1804	U
49	S2	1805	G
49	S2	1816	G
49	S2	1823	A
49	S2	1824	A
49	S2	1825	A
49	S2	1826	G
49	S2	1827	U
49	S2	1831	A
49	S2	1835	A
49	S2	1836	G
49	S2	1837	G
49	S2	1838	U
49	S2	1839	U
49	S2	1841	C
49	S2	1849	G
49	S2	1850	A
49	S2	1851	A
49	S2	1852	C
49	S2	1860	A
49	S2	1861	G
49	S2	1862	G
49	S2	1863	A
49	S2	1864	U
49	S2	1865	C
49	S2	1868	U

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Mol	Chain	Res	Type
49	S2	1869	A

All (921) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	1	C
1	5	20	U
1	5	33	A
1	5	39	A
1	5	42	A
1	5	47	A
1	5	48	G
1	5	51	A
1	5	53	C
1	5	54	G
1	5	55	G
1	5	62	A
1	5	64	A
1	5	65	A
1	5	66	A
1	5	84	A
1	5	85	G
1	5	88	A
1	5	94	A
1	5	97	G
1	5	98	A
1	5	99	A
1	5	100	C
1	5	107	G
1	5	111	C
1	5	112	C
1	5	119	G
1	5	120	A
1	5	125	C
1	5	134	G
1	5	136	C
1	5	143	C
1	5	149	A
1	5	151	G
1	5	158	A
1	5	159	C
1	5	163	A

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Mol	Chain	Res	Type
1	5	170	C
1	5	172	C
1	5	183	C
1	5	186	G
1	5	187	U
1	5	197	A
1	5	207	G
1	5	209	U
1	5	216	C
1	5	218	A
1	5	219	G
1	5	226	G
1	5	235	A
1	5	237	G
1	5	245	C
1	5	253	G
1	5	265	C
1	5	266	C
1	5	268	G
1	5	275	C
1	5	276	C
1	5	280	G
1	5	292	G
1	5	293	G
1	5	296	A
1	5	298	G
1	5	315	G
1	5	333	U
1	5	337	U
1	5	340	C
1	5	349	A
1	5	353	A
1	5	354	U
1	5	360	A
1	5	361	C
1	5	362	A
1	5	371	A
1	5	385	A
1	5	387	G
1	5	388	A
1	5	393	U
1	5	394	G

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Mol	Chain	Res	Type
1	5	405	U
1	5	406	C
1	5	407	A
1	5	410	A
1	5	414	C
1	5	417	G
1	5	421	C
1	5	432	U
1	5	435	A
1	5	451	C
1	5	454	U
1	5	485	C
1	5	486	C
1	5	493	G
1	5	495	C
1	5	496	G
1	5	497	G
1	5	502	C
1	5	505	G
1	5	514	U
1	5	647	G
1	5	648	G
1	5	655	C
1	5	658	C
1	5	659	G
1	5	664	G
1	5	666	G
1	5	668	C
1	5	684	G
1	5	686	A
1	5	693	C
1	5	704	C
1	5	727	C
1	5	728	U
1	5	732	A
1	5	733	A
1	5	738	C
1	5	746	A
1	5	747	A
1	5	909	A
1	5	911	U
1	5	917	A

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Mol	Chain	Res	Type
1	5	920	C
1	5	927	G
1	5	930	G
1	5	931	C
1	5	932	A
1	5	936	C
1	5	943	A
1	5	946	C
1	5	956	A
1	5	957	G
1	5	958	G
1	5	961	G
1	5	962	C
1	5	965	G
1	5	968	C
1	5	974	C
1	5	977	C
1	5	978	G
1	5	979	C
1	5	986	C
1	5	987	C
1	5	989	U
1	5	1067	G
1	5	1068	G
1	5	1074	G
1	5	1076	C
1	5	1186	U
1	5	1210	C
1	5	1211	G
1	5	1214	C
1	5	1217	G
1	5	1221	G
1	5	1232	G
1	5	1235	G
1	5	1236	C
1	5	1237	C
1	5	1238	A
1	5	1239	C
1	5	1241	C
1	5	1243	C
1	5	1244	G
1	5	1254	A

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Mol	Chain	Res	Type
1	5	1264	C
1	5	1266	G
1	5	1268	G
1	5	1272	C
1	5	1274	A
1	5	1279	A
1	5	1280	C
1	5	1281	G
1	5	1293	G
1	5	1296	G
1	5	1319	U
1	5	1324	A
1	5	1325	C
1	5	1329	G
1	5	1334	A
1	5	1356	U
1	5	1357	C
1	5	1359	G
1	5	1364	U
1	5	1365	C
1	5	1368	A
1	5	1370	G
1	5	1371	A
1	5	1377	G
1	5	1378	C
1	5	1379	C
1	5	1380	G
1	5	1386	C
1	5	1398	A
1	5	1405	C
1	5	1406	G
1	5	1407	C
1	5	1410	U
1	5	1419	G
1	5	1420	A
1	5	1426	G
1	5	1428	U
1	5	1438	U
1	5	1439	C
1	5	1440	U
1	5	1445	U
1	5	1464	C

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Mol	Chain	Res	Type
1	5	1474	C
1	5	1479	G
1	5	1480	C
1	5	1481	C
1	5	1484	G
1	5	1488	G
1	5	1489	G
1	5	1500	A
1	5	1509	C
1	5	1521	C
1	5	1522	G
1	5	1539	G
1	5	1554	A
1	5	1596	U
1	5	1613	A
1	5	1614	C
1	5	1615	C
1	5	1617	G
1	5	1627	G
1	5	1633	G
1	5	1636	U
1	5	1640	C
1	5	1650	A
1	5	1654	G
1	5	1671	U
1	5	1676	C
1	5	1681	G
1	5	1682	A
1	5	1696	C
1	5	1697	G
1	5	1698	C
1	5	1724	G
1	5	1725	U
1	5	1742	A
1	5	1763	C
1	5	1764	G
1	5	1804	A
1	5	1808	C
1	5	1819	G
1	5	1835	G
1	5	1864	G
1	5	1865	G

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Mol	Chain	Res	Type
1	5	1869	G
1	5	1876	U
1	5	1881	C
1	5	1884	C
1	5	1887	G
1	5	1890	G
1	5	1891	A
1	5	1912	G
1	5	1919	G
1	5	1920	C
1	5	1921	C
1	5	1925	G
1	5	1928	C
1	5	1930	U
1	5	1935	C
1	5	1938	C
1	5	1959	U
1	5	1960	A
1	5	1974	U
1	5	1975	G
1	5	1980	U
1	5	1983	A
1	5	1998	A
1	5	2007	G
1	5	2008	U
1	5	2009	A
1	5	2014	C
1	5	2044	U
1	5	2046	G
1	5	2057	A
1	5	2068	C
1	5	2075	G
1	5	2077	C
1	5	2083	C
1	5	2088	A
1	5	2089	G
1	5	2090	U
1	5	2093	A
1	5	2094	G
1	5	2096	G
1	5	2107	C
1	5	2111	G

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Mol	Chain	Res	Type
1	5	2114	G
1	5	2116	C
1	5	2118	G
1	5	2119	C
1	5	2122	G
1	5	2123	C
1	5	2124	G
1	5	2126	G
1	5	2246	C
1	5	2248	C
1	5	2250	C
1	5	2251	G
1	5	2256	C
1	5	2257	C
1	5	2258	C
1	5	2260	C
1	5	2261	G
1	5	2262	G
1	5	2264	C
1	5	2265	G
1	5	2266	C
1	5	2267	U
1	5	2268	A
1	5	2269	C
1	5	2272	C
1	5	2276	A
1	5	2278	G
1	5	2289	C
1	5	2313	A
1	5	2321	G
1	5	2323	C
1	5	2324	C
1	5	2325	C
1	5	2328	G
1	5	2329	U
1	5	2331	G
1	5	2332	A
1	5	2347	A
1	5	2361	G
1	5	2362	U
1	5	2370	A
1	5	2389	A

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Mol	Chain	Res	Type
1	5	2394	G
1	5	2396	A
1	5	2398	U
1	5	2417	A
1	5	2436	U
1	5	2438	A
1	5	2447	U
1	5	2448	G
1	5	2459	G
1	5	2464	C
1	5	2468	U
1	5	2470	C
1	5	2474	G
1	5	2479	G
1	5	2487	G
1	5	2490	U
1	5	2502	G
1	5	2507	A
1	5	2509	C
1	5	2512	A
1	5	2513	A
1	5	2514	G
1	5	2515	G
1	5	2529	A
1	5	2533	C
1	5	2544	G
1	5	2545	U
1	5	2546	G
1	5	2553	A
1	5	2554	U
1	5	2576	G
1	5	2581	A
1	5	2583	C
1	5	2587	A
1	5	2588	C
1	5	2589	C
1	5	2591	A
1	5	2600	A
1	5	2614	C
1	5	2618	G
1	5	2622	G
1	5	2631	U

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Mol	Chain	Res	Type
1	5	2652	G
1	5	2658	G
1	5	2661	U
1	5	2665	U
1	5	2666	U
1	5	2673	G
1	5	2674	A
1	5	2677	G
1	5	2683	C
1	5	2686	G
1	5	2688	G
1	5	2695	A
1	5	2703	G
1	5	2711	G
1	5	2732	G
1	5	2744	A
1	5	2761	U
1	5	2768	C
1	5	2769	U
1	5	2782	U
1	5	2786	C
1	5	2787	A
1	5	2796	G
1	5	2803	U
1	5	2806	A
1	5	2811	G
1	5	2812	A
1	5	2817	C
1	5	2825	A
1	5	2827	G
1	5	2828	U
1	5	2833	A
1	5	2834	C
1	5	2837	U
1	5	2843	U
1	5	2848	G
1	5	2851	G
1	5	2858	A
1	5	2859	G
1	5	2879	A
1	5	2895	A
1	5	2896	G

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Mol	Chain	Res	Type
1	5	3590	G
1	5	3593	C
1	5	3615	G
1	5	3620	G
1	5	3622	C
1	5	3625	G
1	5	3626	G
1	5	3636	C
1	5	3648	A
1	5	3653	A
1	5	3654	G
1	5	3663	A
1	5	3666	C
1	5	3667	C
1	5	3671	G
1	5	3676	G
1	5	3679	U
1	5	3681	G
1	5	3683	C
1	5	3692	A
1	5	3697	U
1	5	3712	A
1	5	3717	A
1	5	3727	A
1	5	3730	U
1	5	3735	G
1	5	3736	A
1	5	3773	U
1	5	3774	A
1	5	3776	G
1	5	3784	A
1	5	3799	A
1	5	3802	U
1	5	3803	A
1	5	3809	G
1	5	3813	A
1	5	3817	A
1	5	3839	G
1	5	3845	A
1	5	3856	A
1	5	3860	A
1	5	3862	A

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Mol	Chain	Res	Type
1	5	3875	G
1	5	3876	A
1	5	3877	A
1	5	3879	G
1	5	3888	G
1	5	3905	A
1	5	3922	G
1	5	3938	G
1	5	3944	G
1	5	4069	U
1	5	4075	U
1	5	4084	G
1	5	4085	A
1	5	4086	G
1	5	4095	G
1	5	4096	C
1	5	4097	G
1	5	4102	C
1	5	4103	C
1	5	4115	G
1	5	4118	U
1	5	4119	C
1	5	4120	U
1	5	4121	G
1	5	4123	C
1	5	4124	G
1	5	4127	A
1	5	4144	C
1	5	4163	U
1	5	4165	C
1	5	4170	A
1	5	4173	G
1	5	4183	G
1	5	4195	G
1	5	4197	G
1	5	4219	A
1	5	4221	C
1	5	4227	U
1	5	4228	G
1	5	4229	U
1	5	4232	U
1	5	4233	A

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Mol	Chain	Res	Type
1	5	4239	A
1	5	4240	G
1	5	4250	G
1	5	4251	A
1	5	4254	G
1	5	4257	A
1	5	4269	G
1	5	4270	C
1	5	4275	G
1	5	4276	G
1	5	4280	A
1	5	4282	A
1	5	4283	G
1	5	4287	G
1	5	4291	G
1	5	4295	U
1	5	4297	G
1	5	4322	G
1	5	4330	G
1	5	4334	U
1	5	4338	G
1	5	4348	A
1	5	4349	C
1	5	4368	G
1	5	4374	U
1	5	4375	C
1	5	4378	A
1	5	4385	A
1	5	4395	U
1	5	4419	U
1	5	4425	G
1	5	4436	U
1	5	4440	G
1	5	4448	G
1	5	4449	A
1	5	4451	G
1	5	4454	G
1	5	4463	U
1	5	4464	A
1	5	4472	G
1	5	4474	A
1	5	4475	G

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Mol	Chain	Res	Type
1	5	4481	U
1	5	4488	A
1	5	4489	G
1	5	4497	U
1	5	4498	U
1	5	4507	A
1	5	4518	A
1	5	4519	C
1	5	4522	G
1	5	4527	G
1	5	4528	G
1	5	4531	U
1	5	4533	A
1	5	4535	A
1	5	4536	C
1	5	4543	G
1	5	4547	C
1	5	4548	A
1	5	4560	C
1	5	4574	U
1	5	4583	C
1	5	4600	G
1	5	4605	A
1	5	4610	A
1	5	4645	C
1	5	4647	G
1	5	4656	A
1	5	4670	C
1	5	4677	U
1	5	4678	G
1	5	4691	A
1	5	4693	C
1	5	4700	A
1	5	4718	G
1	5	4719	G
1	5	4720	C
1	5	4730	C
1	5	4731	G
1	5	4737	G
1	5	4739	C
1	5	4740	G
1	5	4745	G

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Mol	Chain	Res	Type
1	5	4756	C
1	5	4762	A
1	5	4763	U
1	5	4871	C
1	5	4872	G
1	5	4873	G
1	5	4874	A
1	5	4884	G
1	5	4885	U
1	5	4887	C
1	5	4888	U
1	5	4889	G
1	5	4900	C
1	5	4911	A
1	5	4926	C
1	5	4929	C
1	5	4935	C
1	5	4936	G
1	5	4938	A
1	5	4948	C
1	5	4949	G
1	5	4950	U
1	5	4951	G
1	5	4981	G
1	5	4990	C
1	5	4991	U
1	5	5022	U
1	5	5026	U
1	5	5027	C
1	5	5041	G
1	5	5046	U
1	5	5049	G
1	5	5056	A
1	5	5059	C
1	5	5060	A
1	5	5061	A
1	5	5062	G
1	5	5068	G
2	7	7	G
2	7	21	G
2	7	42	A
2	7	56	G

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Mol	Chain	Res	Type
2	7	58	A
2	7	60	G
2	7	63	C
2	7	72	U
2	7	75	G
3	8	2	G
3	8	9	A
3	8	10	G
3	8	14	U
3	8	33	G
3	8	34	U
3	8	37	A
3	8	64	U
3	8	70	G
3	8	73	U
3	8	81	C
3	8	83	C
3	8	85	U
3	8	94	G
3	8	95	A
3	8	98	C
3	8	110	U
3	8	111	U
3	8	124	U
3	8	125	C
3	8	126	C
3	8	131	G
49	S2	1	U
49	S2	2	A
49	S2	9	U
49	S2	19	A
49	S2	24	C
49	S2	50	A
49	S2	55	U
49	S2	60	A
49	S2	61	A
49	S2	65	C
49	S2	66	G
49	S2	67	C
49	S2	72	C
49	S2	73	C
49	S2	74	G

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Mol	Chain	Res	Type
49	S2	90	G
49	S2	91	A
49	S2	98	C
49	S2	102	A
49	S2	104	A
49	S2	110	U
49	S2	113	G
49	S2	126	G
49	S2	127	C
49	S2	139	C
49	S2	140	C
49	S2	141	A
49	S2	142	C
49	S2	158	A
49	S2	160	U
49	S2	163	U
49	S2	164	A
49	S2	180	G
49	S2	181	A
49	S2	182	C
49	S2	183	G
49	S2	190	G
49	S2	215	G
49	S2	291	G
49	S2	294	U
49	S2	304	C
49	S2	305	U
49	S2	312	G
49	S2	313	A
49	S2	327	G
49	S2	333	G
49	S2	340	C
49	S2	349	A
49	S2	355	G
49	S2	357	C
49	S2	360	A
49	S2	368	U
49	S2	369	C
49	S2	377	G
49	S2	381	C
49	S2	384	U
49	S2	385	G

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Mol	Chain	Res	Type
49	S2	409	C
49	S2	421	G
49	S2	427	U
49	S2	435	A
49	S2	443	U
49	S2	444	G
49	S2	446	G
49	S2	448	A
49	S2	452	G
49	S2	453	C
49	S2	458	A
49	S2	465	A
49	S2	468	A
49	S2	471	G
49	S2	473	A
49	S2	482	G
49	S2	492	C
49	S2	499	G
49	S2	515	G
49	S2	532	C
49	S2	539	C
49	S2	548	C
49	S2	550	C
49	S2	577	U
49	S2	578	C
49	S2	579	C
49	S2	601	G
49	S2	604	A
49	S2	606	G
49	S2	607	U
49	S2	613	G
49	S2	615	C
49	S2	618	C
49	S2	642	U
49	S2	646	G
49	S2	649	U
49	S2	656	G
49	S2	671	A
49	S2	687	C
49	S2	688	U
49	S2	732	U
49	S2	733	C

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Mol	Chain	Res	Type
49	S2	746	C
49	S2	747	U
49	S2	751	G
49	S2	752	G
49	S2	797	C
49	S2	798	A
49	S2	799	U
49	S2	800	U
49	S2	810	A
49	S2	815	U
49	S2	821	G
49	S2	827	A
49	S2	833	C
49	S2	841	G
49	S2	855	G
49	S2	867	G
49	S2	868	G
49	S2	869	A
49	S2	870	A
49	S2	871	U
49	S2	872	A
49	S2	918	U
49	S2	919	A
49	S2	924	G
49	S2	950	C
49	S2	956	G
49	S2	957	A
49	S2	958	G
49	S2	959	G
49	S2	960	U
49	S2	964	A
49	S2	967	C
49	S2	970	G
49	S2	980	A
49	S2	991	G
49	S2	992	A
49	S2	993	G
49	S2	999	G
49	S2	1001	A
49	S2	1016	U
49	S2	1039	C
49	S2	1050	A

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Mol	Chain	Res	Type
49	S2	1051	G
49	S2	1083	A
49	S2	1085	C
49	S2	1087	A
49	S2	1088	U
49	S2	1093	A
49	S2	1097	G
49	S2	1098	C
49	S2	1109	C
49	S2	1110	G
49	S2	1114	U
49	S2	1115	U
49	S2	1121	G
49	S2	1132	C
49	S2	1133	A
49	S2	1137	U
49	S2	1138	C
49	S2	1141	G
49	S2	1142	G
49	S2	1150	A
49	S2	1153	C
49	S2	1165	G
49	S2	1171	G
49	S2	1181	A
49	S2	1194	A
49	S2	1199	A
49	S2	1206	G
49	S2	1207	G
49	S2	1223	A
49	S2	1244	U
49	S2	1247	C
49	S2	1249	C
49	S2	1250	A
49	S2	1253	A
49	S2	1265	A
49	S2	1273	C
49	S2	1275	G
49	S2	1283	C
49	S2	1292	C
49	S2	1298	G
49	S2	1302	G
49	S2	1312	G

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Mol	Chain	Res	Type
49	S2	1313	A
49	S2	1315	U
49	S2	1341	C
49	S2	1367	U
49	S2	1368	U
49	S2	1372	U
49	S2	1393	G
49	S2	1395	C
49	S2	1396	A
49	S2	1401	A
49	S2	1404	U
49	S2	1416	C
49	S2	1417	C
49	S2	1418	C
49	S2	1419	C
49	S2	1421	A
49	S2	1429	G
49	S2	1433	C
49	S2	1434	C
49	S2	1440	C
49	S2	1441	U
49	S2	1442	U
49	S2	1446	A
49	S2	1454	A
49	S2	1462	U
49	S2	1463	U
49	S2	1474	A
49	S2	1475	G
49	S2	1477	U
49	S2	1489	A
49	S2	1493	C
49	S2	1494	U
49	S2	1506	A
49	S2	1512	C
49	S2	1521	C
49	S2	1522	A
49	S2	1534	C
49	S2	1537	A
49	S2	1540	G
49	S2	1542	C
49	S2	1543	U
49	S2	1552	G

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Mol	Chain	Res	Type
49	S2	1555	U
49	S2	1556	A
49	S2	1557	C
49	S2	1561	A
49	S2	1568	C
49	S2	1579	A
49	S2	1585	U
49	S2	1588	A
49	S2	1593	C
49	S2	1597	C
49	S2	1598	G
49	S2	1599	U
49	S2	1603	G
49	S2	1605	G
49	S2	1623	A
49	S2	1629	C
49	S2	1637	A
49	S2	1643	U
49	S2	1648	G
49	S2	1659	U
49	S2	1664	A
49	S2	1678	A
49	S2	1679	A
49	S2	1682	C
49	S2	1694	U
49	S2	1695	A
49	S2	1700	C
49	S2	1703	C
49	S2	1720	U
49	S2	1744	G
49	S2	1756	C
49	S2	1823	A
49	S2	1825	A
49	S2	1826	G
49	S2	1830	U
49	S2	1835	A
49	S2	1836	G
49	S2	1838	U
49	S2	1849	G
49	S2	1857	G
49	S2	1858	G
49	S2	1860	A

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Mol	Chain	Res	Type
49	S2	1863	A
49	S2	1868	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	5	13
49	S2	4
8	E	1
14	K	1
48	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	72:ALA	C	84:VAL	N	23.51
1	S2	753:C	O3'	785:C	P	22.68
1	S2	698:G	O3'	730:C	P	19.95
1	5	4776:G	O3'	4859:C	P	17.87
1	5	757:G	O3'	906:C	P	16.89
1	5	519:C	O3'	642:G	P	16.61
1	5	2910:G	O3'	3583:U	P	16.04
1	5	2131:C	O3'	2243:C	P	14.89
1	5	997:C	O3'	1047:C	P	13.99
1	5	3950:U	O3'	4065:G	P	13.97
1	5	1051:G	O3'	1064:G	P	9.59
1	S2	739:C	O3'	744:G	P	7.74
1	S2	225:G	O3'	287:U	P	6.54
1	5	1222:A	O3'	1232:G	P	3.97
1	5	1699:A	O3'	1718:C	P	3.33
1	5	1100:U	O3'	1167:C	P	3.02
1	5	4939:C	O3'	4941:G	P	2.74
1	5	4942:C	O3'	4944:C	P	2.72
1	K	154:ASP	C	155:ILE	N	2.32
1	4	269:ALA	C	270:ASN	N	1.60

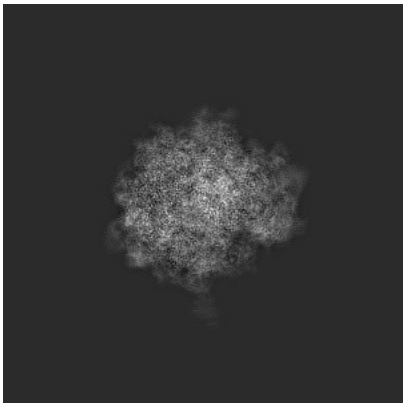
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2646. These allow visual inspection of the internal detail of the map and identification of artifacts.

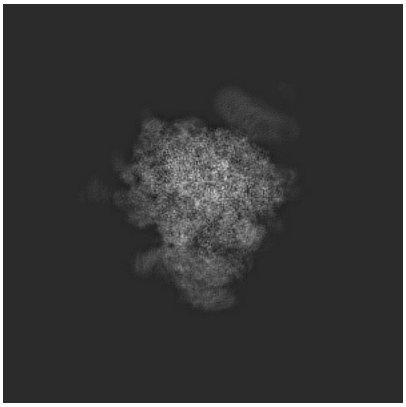
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

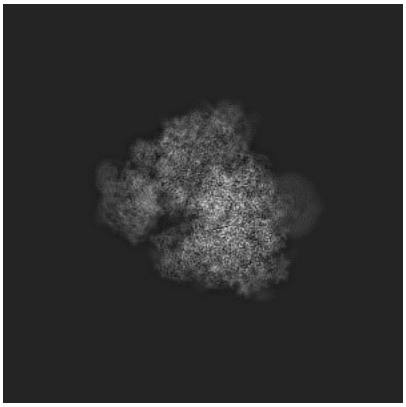
6.1.1 Primary map



X



Y

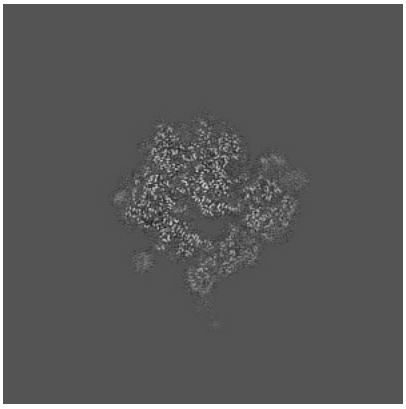


Z

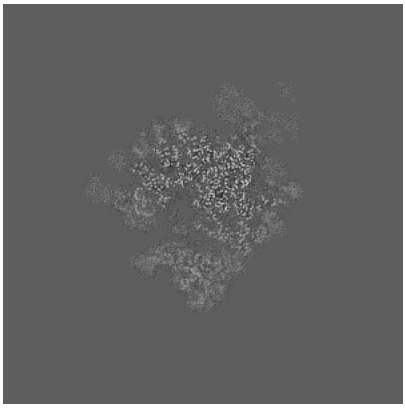
The images above show the map projected in three orthogonal directions.

6.2 Central slices

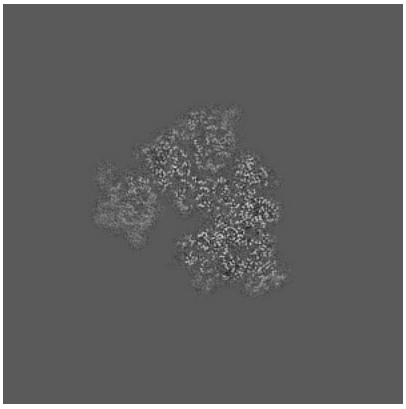
6.2.1 Primary map



X Index: 210



Y Index: 210

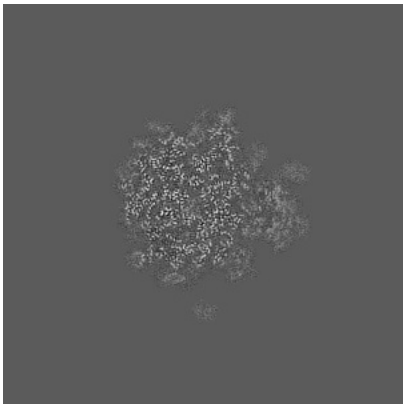


Z Index: 210

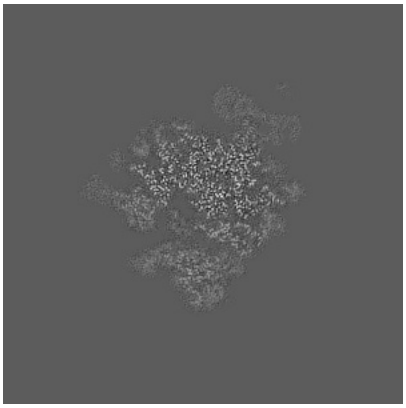
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

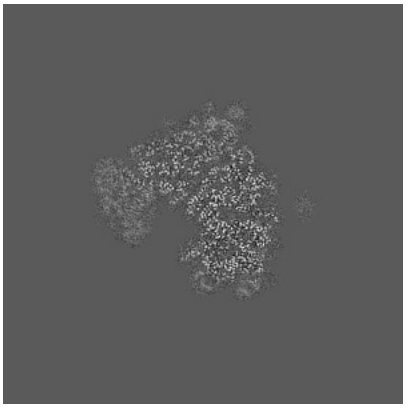
6.3.1 Primary map



X Index: 232



Y Index: 212

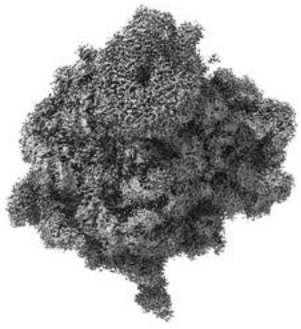


Z Index: 221

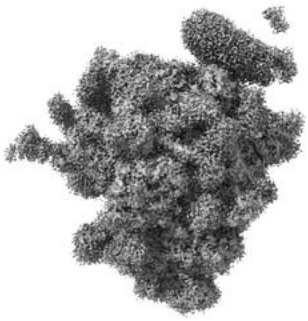
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

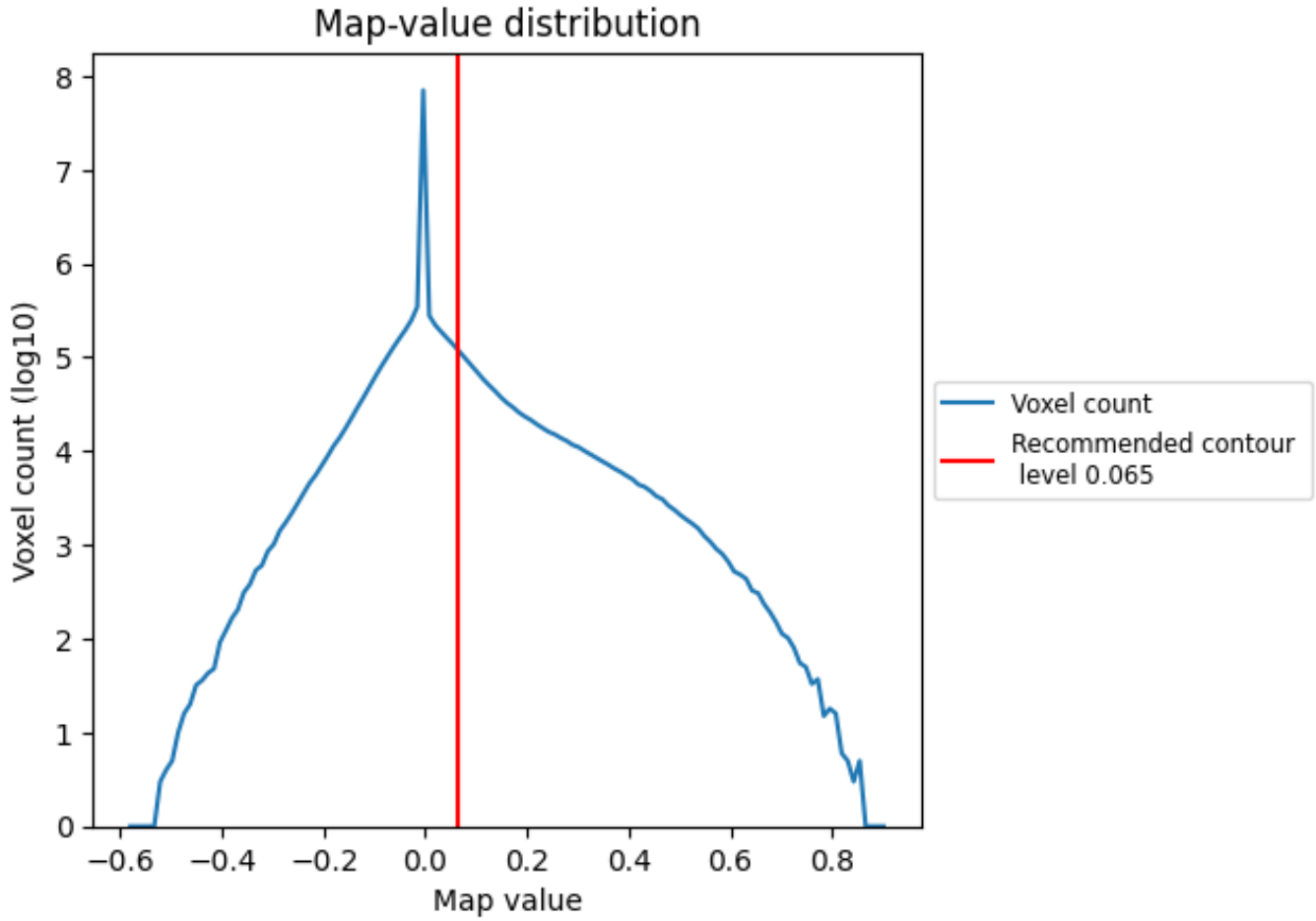
6.5 Mask visualisation (i)

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

7 Map analysis

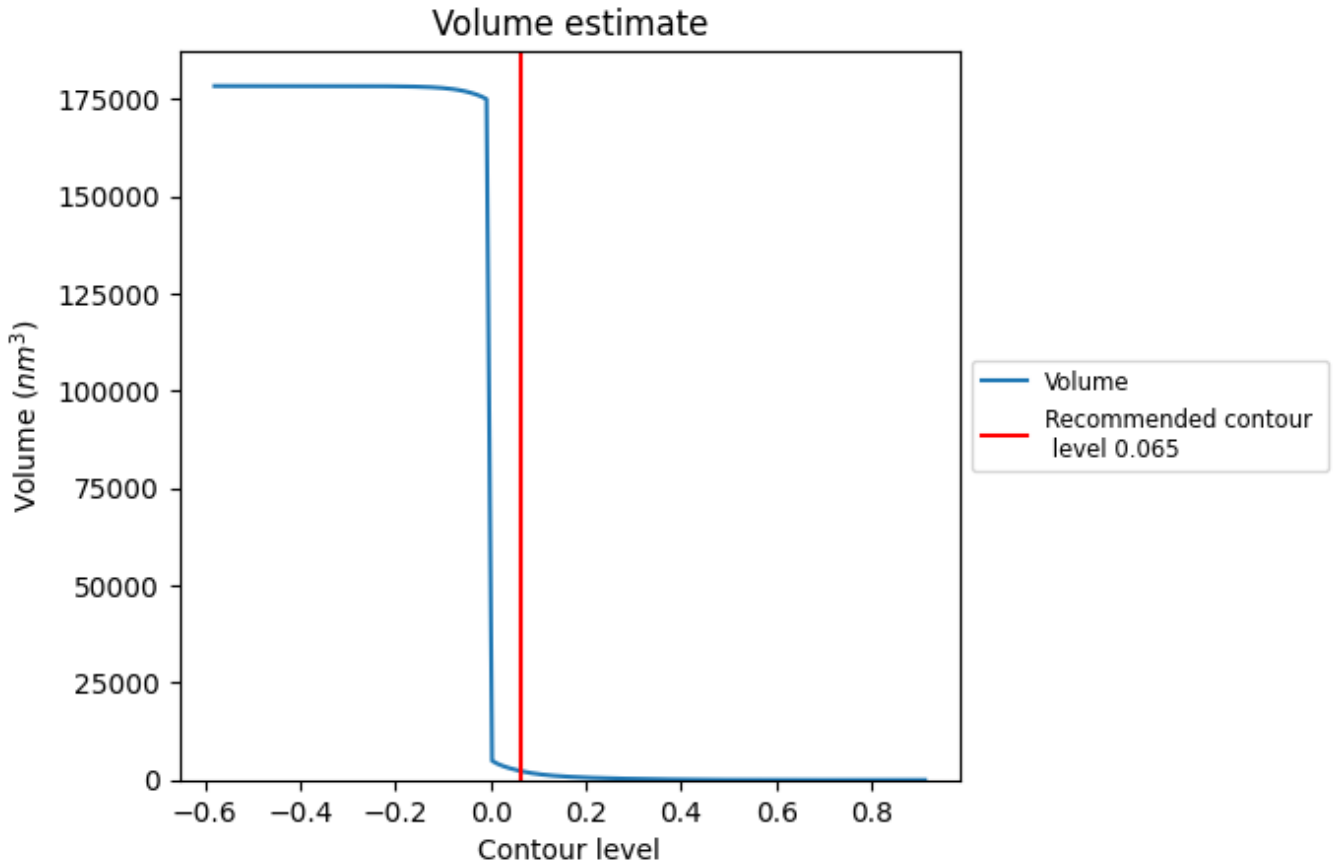
This section contains the results of statistical analysis of the map.

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.

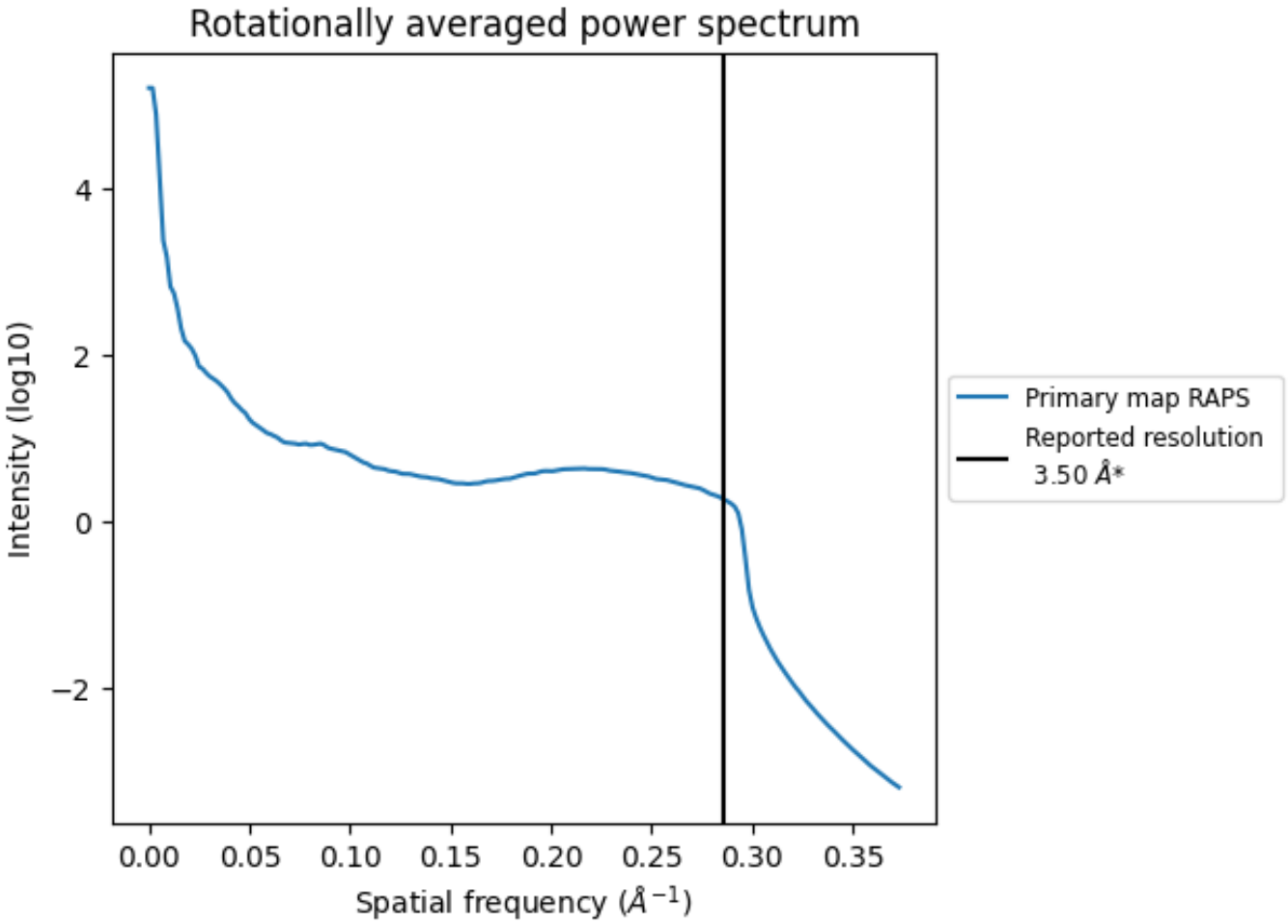
7.2 Volume estimate



The volume at the recommended contour level is 2236 nm^3; this corresponds to an approximate mass of 2020 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

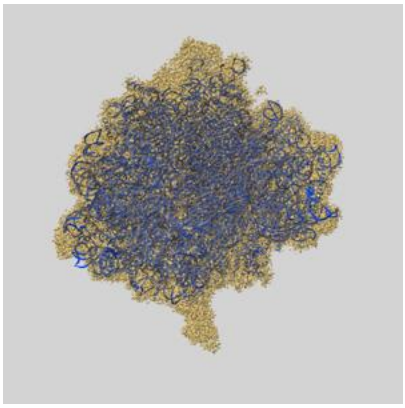
8 Fourier-Shell correlation

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

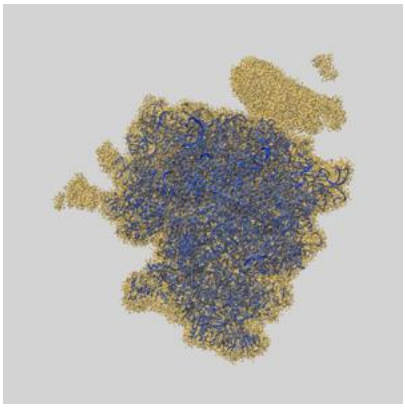
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2646 and PDB model 3J7P. Per-residue inclusion information can be found in section 3 on page 19.

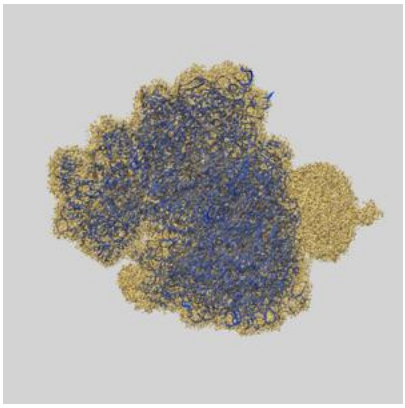
9.1 Map-model overlay



X



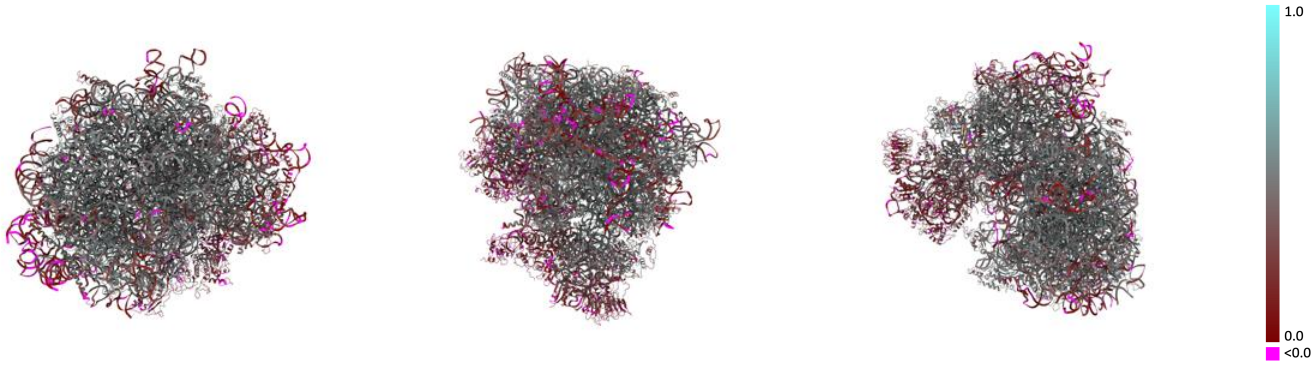
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

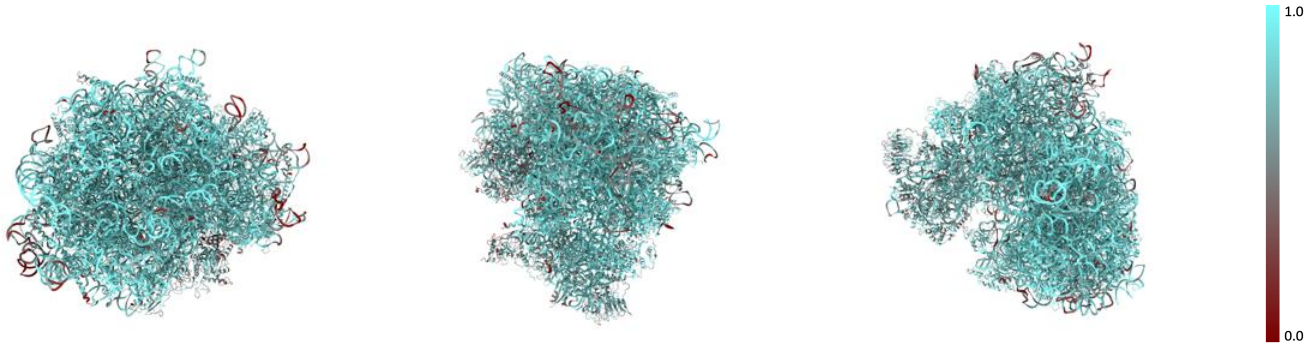
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

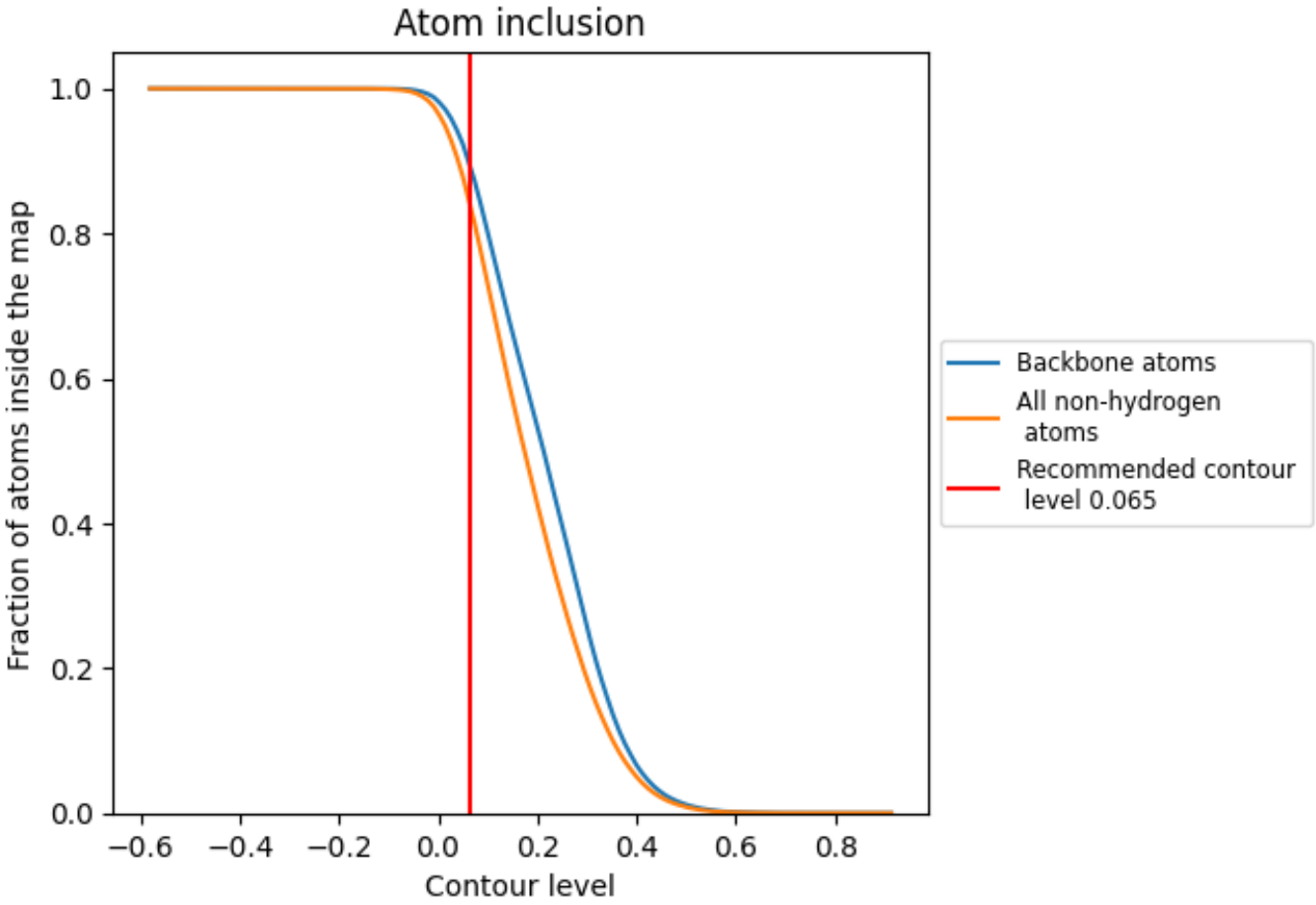
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.065).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8378	0.3940
4	0.5765	0.2090
5	0.8683	0.4020
7	0.9512	0.4630
8	0.8957	0.4310
A	0.8932	0.5000
B	0.8910	0.4950
C	0.8696	0.4840
D	0.8727	0.4340
E	0.8353	0.4260
F	0.8777	0.4820
G	0.8426	0.4340
H	0.8804	0.4840
I	0.8485	0.4640
J	0.8302	0.4140
K	0.5233	0.1450
L	0.8439	0.4520
M	0.8797	0.4790
N	0.9037	0.5080
O	0.8966	0.5060
P	0.8873	0.5030
Q	0.8974	0.5060
R	0.8480	0.4450
S	0.9100	0.4990
S2	0.8576	0.3530
SA	0.8826	0.4570
SB	0.8417	0.4280
SC	0.8890	0.4900
SD	0.7085	0.2870
SE	0.8444	0.4430
SF	0.6226	0.2060
SG	0.7240	0.2970
SH	0.7842	0.3730
SI	0.7812	0.3810
SJ	0.8512	0.4450

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Chain	Atom inclusion	Q-score
SK	0.6696	0.2230
SL	0.8188	0.4330
SM	0.4672	0.0930
SN	0.8720	0.4550
SO	0.8511	0.4440
SP	0.6490	0.2520
SQ	0.6912	0.2540
SR	0.7291	0.3230
SS	0.6953	0.2300
ST	0.7386	0.2670
SU	0.6976	0.2790
SV	0.8642	0.4650
SW	0.9158	0.5060
SX	0.8759	0.5020
SY	0.8077	0.3850
SZ	0.6106	0.1690
Sa	0.8699	0.4610
Sb	0.8779	0.4540
Sc	0.5412	0.2010
Sd	0.8317	0.3900
Se	0.7941	0.4090
Sf	0.4117	0.0550
Sg	0.6386	0.2040
T	0.8789	0.4820
U	0.7962	0.3830
V	0.8633	0.4870
W	0.8546	0.4750
X	0.8367	0.4700
Y	0.8599	0.4710
Z	0.8798	0.4690
a	0.8990	0.5040
b	0.7609	0.3830
c	0.8601	0.4600
d	0.8530	0.4540
e	0.8918	0.5010
f	0.9216	0.5060
g	0.8562	0.4830
h	0.8503	0.4650
i	0.8534	0.4570
j	0.9050	0.4880
k	0.8097	0.4220
l	0.8818	0.5080

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Chain	Atom inclusion	Q-score
m	0.8582	0.4980
n	0.8856	0.4620
o	0.8487	0.4690
p	0.8648	0.4870
q	0.6416	0.2130
r	0.8828	0.4930