



Full wwPDB EM Validation Report ⓘ

Nov 13, 2024 – 04:42 PM EST

PDB ID : 3J7R
EMDB ID : EMD-2644
Title : Structure of the translating mammalian ribosome-Sec61 complex
Authors : Voorhees, R.M.; Fernandez, I.S.; Scheres, S.H.W.; Hegde, R.S.
Deposited on : 2014-08-01
Resolution : 3.90 Å (reported)
Based on initial models : 3J3D, 3J3B, 3J3A, 3J3F

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

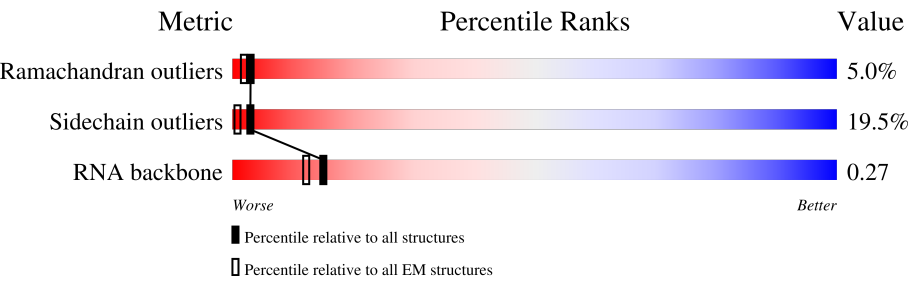
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) :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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 Å.

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













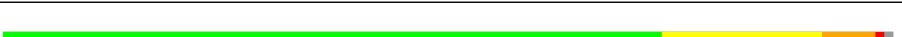


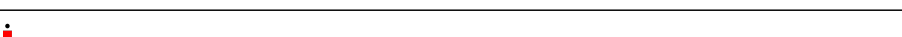
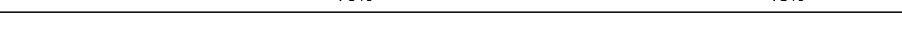
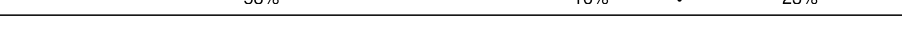



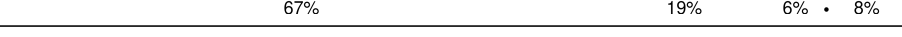





Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	5	3722	<div><div>6%</div><div>47%</div><div>40%</div><div>10%</div><div>.</div></div>
2	7	120	<div><div>.</div><div>69%</div><div>24%</div><div>6%</div><div>.</div></div>
3	8	156	<div><div>5%</div><div>53%</div><div>33%</div><div>8%</div><div>5%</div></div>
4	A	257	<div><div>.</div><div>71%</div><div>18%</div><div>5%</div><div>5%</div></div>
5	B	394	<div><div>74%</div><div>21%</div><div>.</div><div>.</div></div>
6	C	367	<div><div>.</div><div>77%</div><div>19%</div><div>.</div><div>.</div></div>
7	D	297	<div><div>.</div><div>68%</div><div>24%</div><div>5%</div><div>.</div><div>.</div></div>
8	E	236	<div><div>6%</div><div>64%</div><div>25%</div><div>9%</div><div>.</div></div>









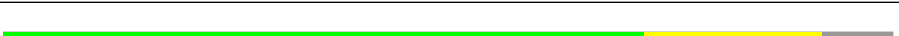

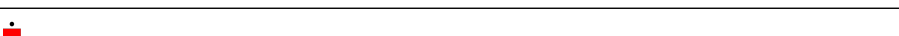
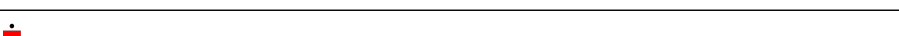

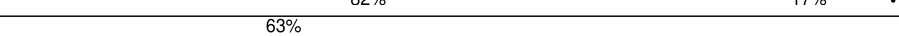
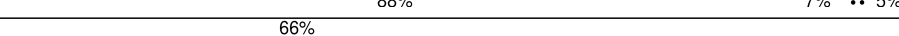
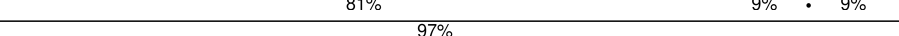
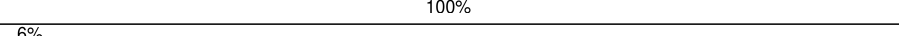








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Mol	Chain	Length	Quality of chain
9	F	225	
10	G	266	
11	H	192	
12	I	213	
13	J	178	
14	L	211	
15	M	213	
16	N	204	
17	O	201	
18	P	153	
19	Q	188	
20	R	196	
21	S	224	
22	T	160	
23	U	128	
24	V	140	
25	W	157	
26	X	156	
27	Y	145	
28	Z	136	
29	a	148	
30	b	160	
31	c	115	
32	d	125	
33	e	135	

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Mol	Chain	Length	Quality of chain
34	f	110	
35	g	117	
36	h	123	
37	i	105	
38	j	86	
39	k	70	
40	l	51	
41	m	128	
42	n	25	
43	o	106	
44	p	91	
45	r	125	
46	z	217	
47	1	393	
48	2	68	
49	3	36	
50	S2	1742	
51	SA	295	
52	SB	264	
53	SC	218	
54	SD	243	
55	SE	263	
56	SF	204	
57	SG	249	
58	SH	194	

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Mol	Chain	Length	Quality of chain
59	SI	208	
60	SJ	194	
61	SK	165	
62	SL	158	
63	SM	124	
64	SN	151	
65	SO	151	
66	SP	145	
67	SQ	146	
68	SR	135	
69	SS	152	
70	ST	145	
71	SU	119	
72	SV	83	
73	SW	130	
74	SX	143	
75	SY	132	
76	SZ	125	
77	Sa	115	
78	Sb	84	
79	Sc	69	
80	Sd	56	
81	Se	133	
82	Sf	156	
83	Sg	317	

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Mol	Chain	Length	Quality of chain
84	S4	10	<div><div></div><div>10%</div><div></div><div>90%</div></div>
85	S5	74	<div><div></div><div>26%</div><div></div><div>32%</div><div></div><div>66%</div><div></div><div></div></div>
86	S6	76	<div><div></div><div>11%</div><div></div><div>29%</div><div></div><div>70%</div><div></div><div></div></div>

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 222336 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
1	5	3720	Total	C	N	O	P	0	0
			79736	35504	14597	25916	3719		

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

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

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

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

- Molecule 4 is a protein called Ribosomal protein uL2.

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

- Molecule 5 is a protein called Ribosomal protein uL3.

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

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ILE	VAL	conflict	UNP A0A480L253
B	86	VAL	ILE	conflict	UNP A0A480L253
B	140	ALA	GLU	conflict	UNP A0A480L253

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Chain	Residue	Modelled	Actual	Comment	Reference
B	141	ALA	ASP	conflict	UNP A0A480L253
B	143	ALA	LYS	conflict	UNP A0A480L253
B	144	ALA	LYS	conflict	UNP A0A480L253
B	145	ALA	GLN	conflict	UNP A0A480L253
B	147	ALA	GLU	conflict	UNP A0A480L253
B	148	ALA	ARG	conflict	UNP A0A480L253
B	155	ALA	LYS	conflict	UNP A0A480L253

- Molecule 6 is a protein called Ribosomal protein uL4.

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	354	ALA	-	insertion	UNP A0A287AE76
C	355	ALA	-	insertion	UNP A0A287AE76
C	356	ALA	-	insertion	UNP A0A287AE76

- 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		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	62	MET	LYS	conflict	UNP Q2YGT9
E	64	MET	LEU	conflict	UNP Q2YGT9
E	?	-	LYS	deletion	UNP Q2YGT9
E	?	-	SER	deletion	UNP Q2YGT9
E	?	-	LYS	deletion	UNP Q2YGT9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	VAL	deletion	UNP Q2YGT9
E	?	-	GLU	deletion	UNP Q2YGT9
E	?	-	LYS	deletion	UNP Q2YGT9
E	?	-	LYS	deletion	UNP Q2YGT9
E	?	-	LYS	deletion	UNP Q2YGT9
E	?	-	LYS	deletion	UNP Q2YGT9
E	?	-	VAL	deletion	UNP Q2YGT9
E	?	-	ARG	deletion	UNP Q2YGT9
E	176	VAL	SER	conflict	UNP Q2YGT9
E	206	LYS	GLU	conflict	UNP Q2YGT9

- 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		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	31	LYS	ARG	conflict	UNP A0A480W0U3

- 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		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	53	ARG	CYS	conflict	UNP A0A4X1W808
G	172	ALA	SER	conflict	UNP A0A4X1W808
G	185	LYS	ASN	conflict	UNP A0A4X1W808
G	231	ASN	ASP	conflict	UNP A0A4X1W808

- 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		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	49	GLY	CYS	conflict	UNP Q29195
I	82	ARG	LYS	conflict	UNP Q29195
I	87	MET	ILE	conflict	UNP Q29195
I	145	GLU	LYS	conflict	UNP Q29195
I	187	LYS	GLU	conflict	UNP Q29195
I	189	CYS	ARG	conflict	UNP Q29195
I	200	VAL	ILE	conflict	UNP Q29195
I	203	HIS	ARG	conflict	UNP Q29195
I	211	VAL	ALA	conflict	UNP Q29195

- 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 eL13.

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

- Molecule 15 is a protein called Ribosomal protein eL14.

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

- Molecule 16 is a protein called Ribosomal protein eL15.

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

- Molecule 17 is a protein called Ribosomal protein uL13.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	3	GLU	-	variant	UNP A0A480L469
O	4	GLY	-	variant	UNP A0A480L469

- Molecule 18 is a protein called Ribosomal protein uL22.

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

- Molecule 19 is a protein called Ribosomal protein eL18.

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

- Molecule 20 is a protein called Ribosomal protein eL19.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	1	TYR	-	variant	UNP A0A480VXS3

- Molecule 21 is a protein called Ribosomal protein eL20.

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

- Molecule 22 is a protein called Ribosomal protein eL21.

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

- Molecule 23 is a protein called Ribosomal protein eL22.

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

- Molecule 24 is a protein called Ribosomal protein uL14.

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

- Molecule 25 is a protein called Ribosomal protein eL24.

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

- Molecule 26 is a protein called Ribosomal protein uL23.

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

- Molecule 27 is a protein called Ribosomal protein uL24.

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

- Molecule 28 is a protein called Ribosomal protein eL27.

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

- Molecule 29 is a protein called Ribosomal protein uL15.

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

- Molecule 30 is a protein called Ribosomal protein eL29.

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

- Molecule 31 is a protein called Ribosomal protein eL30.

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

- Molecule 32 is a protein called Ribosomal protein eL31.

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

- Molecule 33 is a protein called Ribosomal protein eL32.

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

- Molecule 34 is a protein called Ribosomal protein eL33.

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

- Molecule 35 is a protein called Ribosomal protein eL34.

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

- Molecule 36 is a protein called Ribosomal protein uL29.

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

- Molecule 37 is a protein called Ribosomal protein eL36.

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

- Molecule 38 is a protein called Ribosomal protein eL37.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j	82	ILE	THR	conflict	UNP A0A480UVT3

- Molecule 39 is a protein called Ribosomal protein eL38.

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

- Molecule 40 is a protein called Ribosomal protein eL39.

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

- Molecule 41 is a protein called Ribosomal protein eL40.

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

- Molecule 42 is a protein called Ribosomal protein eL41.

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

- Molecule 43 is a protein called Ribosomal protein eL42.

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

- Molecule 44 is a protein called Ribosomal protein eL43.

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

- Molecule 45 is a protein called Ribosomal protein eL28.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	64	ILE	MET	conflict	UNP A0A480YX24

- Molecule 46 is a protein called Ribosomal protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	z	217	Total	C	N	O	S	0	0
			1741	1113	312	307	9		

- Molecule 47 is a protein called Sec61 alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	1	375	Total	C	N	O	S	0	0
			2914	1919	469	508	18		

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	?	-	GLN	deletion	UNP A0A4X1TV07

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Chain	Residue	Modelled	Actual	Comment	Reference
1	?	-	ILE	deletion	UNP A0A4X1TV07
1	?	-	PRO	deletion	UNP A0A4X1TV07
1	?	-	LEU	deletion	UNP A0A4X1TV07
1	?	-	PHE	deletion	UNP A0A4X1TV07
1	?	-	GLY	deletion	UNP A0A4X1TV07
1	?	-	ILE	deletion	UNP A0A4X1TV07
1	?	-	MET	deletion	UNP A0A4X1TV07
1	?	-	SER	deletion	UNP A0A4X1TV07
1	?	-	SER	deletion	UNP A0A4X1TV07
1	?	-	ASP	deletion	UNP A0A4X1TV07
1	?	-	THR	deletion	UNP A0A4X1TV07
1	?	-	GLY	deletion	UNP A0A4X1TV07
1	?	-	MET	deletion	UNP A0A4X1TV07
1	?	-	TYR	deletion	UNP A0A4X1TV07
1	?	-	GLY	deletion	UNP A0A4X1TV07
1	?	-	ASP	deletion	UNP A0A4X1TV07
1	?	-	PRO	deletion	UNP A0A4X1TV07
1	?	-	SER	deletion	UNP A0A4X1TV07
1	?	-	GLU	deletion	UNP A0A4X1TV07
1	?	-	MET	deletion	UNP A0A4X1TV07
1	?	-	GLY	deletion	UNP A0A4X1TV07
1	?	-	ALA	deletion	UNP A0A4X1TV07
1	?	-	GLY	deletion	UNP A0A4X1TV07
1	?	-	ILE	deletion	UNP A0A4X1TV07
1	?	-	SER	deletion	UNP A0A4X1TV07
1	?	-	GLY	deletion	UNP A0A4X1TV07
1	?	-	ASN	deletion	UNP A0A4X1TV07
1	?	-	LEU	deletion	UNP A0A4X1TV07
1	?	-	LEU	deletion	UNP A0A4X1TV07
1	?	-	VAL	deletion	UNP A0A4X1TV07
1	?	-	SER	deletion	UNP A0A4X1TV07
1	?	-	LEU	deletion	UNP A0A4X1TV07
1	?	-	LEU	deletion	UNP A0A4X1TV07
1	?	-	GLY	deletion	UNP A0A4X1TV07
1	?	-	THR	deletion	UNP A0A4X1TV07
1	?	-	TRP	deletion	UNP A0A4X1TV07
1	?	-	SER	deletion	UNP A0A4X1TV07
1	?	-	ASP	deletion	UNP A0A4X1TV07
1	?	-	THR	deletion	UNP A0A4X1TV07
1	?	-	SER	deletion	UNP A0A4X1TV07
1	?	-	SER	deletion	UNP A0A4X1TV07
1	?	-	GLY	deletion	UNP A0A4X1TV07

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Chain	Residue	Modelled	Actual	Comment	Reference
1	?	-	GLY	deletion	UNP A0A4X1TV07
1	?	-	PRO	deletion	UNP A0A4X1TV07
1	?	-	ALA	deletion	UNP A0A4X1TV07
1	?	-	ARG	deletion	UNP A0A4X1TV07
1	?	-	ALA	deletion	UNP A0A4X1TV07
1	?	-	TYR	deletion	UNP A0A4X1TV07
1	343	HIS	TYR	conflict	UNP A0A4X1TV07

- Molecule 48 is a protein called Sec61 gamma subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	2	62	Total	C	N	O	S	0	0
			494	326	86	79	3		

- Molecule 49 is a protein called Sec61 beta subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	3	36	Total	C	N	O	0	0
			180	108	36	36		

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

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

There are 658 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S2	1	U	-	variant	GB 37956930
S2	2	A	-	variant	GB 37956930
S2	3	C	-	variant	GB 37956930
S2	4	C	-	variant	GB 37956930
S2	5	U	-	variant	GB 37956930
S2	6	G	-	variant	GB 37956930
S2	7	G	-	variant	GB 37956930
S2	8	U	-	variant	GB 37956930
S2	9	U	-	variant	GB 37956930
S2	10	G	-	variant	GB 37956930
S2	11	A	-	variant	GB 37956930
S2	12	U	-	variant	GB 37956930
S2	13	C	-	variant	GB 37956930

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Chain	Residue	Modelled	Actual	Comment	Reference
S2	14	C	-	variant	GB 37956930
S2	15	U	-	variant	GB 37956930
S2	16	G	-	variant	GB 37956930
S2	17	C	-	variant	GB 37956930
S2	18	C	-	variant	GB 37956930
S2	19	A	-	variant	GB 37956930
S2	20	G	-	variant	GB 37956930
S2	21	U	-	variant	GB 37956930
S2	22	A	-	variant	GB 37956930
S2	23	G	-	variant	GB 37956930
S2	24	C	-	variant	GB 37956930
S2	25	A	-	variant	GB 37956930
S2	26	U	-	variant	GB 37956930
S2	27	A	-	variant	GB 37956930
S2	28	U	-	variant	GB 37956930
S2	29	G	-	variant	GB 37956930
S2	30	C	-	variant	GB 37956930
S2	31	U	-	variant	GB 37956930
S2	32	U	-	variant	GB 37956930
S2	33	G	-	variant	GB 37956930
S2	34	U	-	variant	GB 37956930
S2	35	C	-	variant	GB 37956930
S2	36	U	-	variant	GB 37956930
S2	37	C	-	variant	GB 37956930
S2	38	A	-	variant	GB 37956930
S2	39	A	-	variant	GB 37956930
S2	40	A	-	variant	GB 37956930
S2	41	G	-	variant	GB 37956930
S2	42	A	-	variant	GB 37956930
S2	43	U	-	variant	GB 37956930
S2	44	U	-	variant	GB 37956930
S2	45	A	-	variant	GB 37956930
S2	46	A	-	variant	GB 37956930
S2	47	G	-	variant	GB 37956930
S2	48	C	-	variant	GB 37956930
S2	49	C	-	variant	GB 37956930
S2	50	A	-	variant	GB 37956930
S2	51	U	-	variant	GB 37956930
S2	52	G	-	variant	GB 37956930
S2	53	C	-	variant	GB 37956930
S2	54	A	-	variant	GB 37956930
S2	55	U	-	variant	GB 37956930

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Chain	Residue	Modelled	Actual	Comment	Reference
S2	56	G	-	variant	GB 37956930
S2	57	U	-	variant	GB 37956930
S2	58	C	-	variant	GB 37956930
S2	59	U	-	variant	GB 37956930
S2	60	A	-	variant	GB 37956930
S2	61	A	-	variant	GB 37956930
S2	62	G	-	variant	GB 37956930
S2	63	U	-	variant	GB 37956930
S2	64	A	-	variant	GB 37956930
S2	65	C	-	variant	GB 37956930
S2	66	G	-	variant	GB 37956930
S2	67	C	-	variant	GB 37956930
S2	68	A	-	variant	GB 37956930
S2	69	C	-	variant	GB 37956930
S2	70	G	-	variant	GB 37956930
S2	71	G	-	variant	GB 37956930
S2	72	C	-	variant	GB 37956930
S2	73	C	-	variant	GB 37956930
S2	74	G	-	variant	GB 37956930
S2	75	G	-	variant	GB 37956930
S2	76	U	-	variant	GB 37956930
S2	77	A	-	variant	GB 37956930
S2	78	C	-	variant	GB 37956930
S2	79	A	-	variant	GB 37956930
S2	80	G	-	variant	GB 37956930
S2	81	U	-	variant	GB 37956930
S2	82	G	-	variant	GB 37956930
S2	83	A	-	variant	GB 37956930
S2	84	A	-	variant	GB 37956930
S2	85	A	-	variant	GB 37956930
S2	86	C	-	variant	GB 37956930
S2	87	U	-	variant	GB 37956930
S2	88	G	-	variant	GB 37956930
S2	89	C	-	variant	GB 37956930
S2	90	G	-	variant	GB 37956930
S2	91	A	-	variant	GB 37956930
S2	92	A	-	variant	GB 37956930
S2	93	U	-	variant	GB 37956930
S2	94	G	-	variant	GB 37956930
S2	95	G	-	variant	GB 37956930
S2	96	C	-	variant	GB 37956930
S2	97	U	-	variant	GB 37956930

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Chain	Residue	Modelled	Actual	Comment	Reference
S2	98	C	-	variant	GB 37956930
S2	99	A	-	variant	GB 37956930
S2	100	U	-	variant	GB 37956930
S2	101	U	-	variant	GB 37956930
S2	102	A	-	variant	GB 37956930
S2	103	A	-	variant	GB 37956930
S2	104	A	-	variant	GB 37956930
S2	105	U	-	variant	GB 37956930
S2	106	C	-	variant	GB 37956930
S2	107	A	-	variant	GB 37956930
S2	108	G	-	variant	GB 37956930
S2	109	U	-	variant	GB 37956930
S2	110	U	-	variant	GB 37956930
S2	111	A	-	variant	GB 37956930
S2	112	U	-	variant	GB 37956930
S2	113	G	-	variant	GB 37956930
S2	114	G	-	variant	GB 37956930
S2	115	U	-	variant	GB 37956930
S2	116	U	-	variant	GB 37956930
S2	117	C	-	variant	GB 37956930
S2	118	C	-	variant	GB 37956930
S2	119	U	-	variant	GB 37956930
S2	120	U	-	variant	GB 37956930
S2	121	U	-	variant	GB 37956930
S2	122	G	-	variant	GB 37956930
S2	123	G	-	variant	GB 37956930
S2	124	U	-	variant	GB 37956930
S2	125	C	-	variant	GB 37956930
S2	126	G	-	variant	GB 37956930
S2	127	C	-	variant	GB 37956930
S2	128	U	-	variant	GB 37956930
S2	129	C	-	variant	GB 37956930
S2	130	G	-	variant	GB 37956930
S2	131	C	-	variant	GB 37956930
S2	132	U	-	variant	GB 37956930
S2	133	C	-	variant	GB 37956930
S2	134	C	-	variant	GB 37956930
S2	135	U	-	variant	GB 37956930
S2	136	C	-	variant	GB 37956930
S2	137	U	-	variant	GB 37956930
S2	138	C	-	variant	GB 37956930
S2	139	C	-	variant	GB 37956930

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Chain	Residue	Modelled	Actual	Comment	Reference
S2	140	C	-	variant	GB 37956930
S2	141	A	-	variant	GB 37956930
S2	142	C	-	variant	GB 37956930
S2	143	U	-	variant	GB 37956930
S2	144	U	-	variant	GB 37956930
S2	145	G	-	variant	GB 37956930
S2	146	G	-	variant	GB 37956930
S2	147	A	-	variant	GB 37956930
S2	148	U	-	variant	GB 37956930
S2	149	A	-	variant	GB 37956930
S2	150	A	-	variant	GB 37956930
S2	151	C	-	variant	GB 37956930
S2	152	U	-	variant	GB 37956930
S2	153	G	-	variant	GB 37956930
S2	154	U	-	variant	GB 37956930
S2	155	G	-	variant	GB 37956930
S2	156	G	-	variant	GB 37956930
S2	157	U	-	variant	GB 37956930
S2	158	A	-	variant	GB 37956930
S2	159	A	-	variant	GB 37956930
S2	160	U	-	variant	GB 37956930
S2	161	U	-	variant	GB 37956930
S2	162	C	-	variant	GB 37956930
S2	163	U	-	variant	GB 37956930
S2	164	A	-	variant	GB 37956930
S2	165	G	-	variant	GB 37956930
S2	166	A	-	variant	GB 37956930
S2	167	G	-	variant	GB 37956930
S2	168	C	-	variant	GB 37956930
S2	169	U	-	variant	GB 37956930
S2	170	A	-	variant	GB 37956930
S2	171	A	-	variant	GB 37956930
S2	172	U	-	variant	GB 37956930
S2	173	A	-	variant	GB 37956930
S2	174	C	-	variant	GB 37956930
S2	175	A	-	variant	GB 37956930
S2	176	U	-	variant	GB 37956930
S2	177	G	-	variant	GB 37956930
S2	178	C	-	variant	GB 37956930
S2	179	C	-	variant	GB 37956930
S2	180	G	-	variant	GB 37956930
S2	181	A	-	variant	GB 37956930

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Chain	Residue	Modelled	Actual	Comment	Reference
S2	182	C	-	variant	GB 37956930
S2	183	G	-	variant	GB 37956930
S2	184	G	-	variant	GB 37956930
S2	185	G	-	variant	GB 37956930
S2	186	C	-	variant	GB 37956930
S2	187	G	-	variant	GB 37956930
S2	188	C	-	variant	GB 37956930
S2	189	U	-	variant	GB 37956930
S2	190	G	-	variant	GB 37956930
S2	191	A	-	variant	GB 37956930
S2	192	C	-	variant	GB 37956930
S2	193	C	-	variant	GB 37956930
S2	194	C	-	variant	GB 37956930
S2	195	C	-	variant	GB 37956930
S2	196	C	-	variant	GB 37956930
S2	197	U	-	variant	GB 37956930
S2	198	U	-	variant	GB 37956930
S2	199	C	-	variant	GB 37956930
S2	200	G	-	variant	GB 37956930
S2	201	C	-	variant	GB 37956930
S2	202	G	-	variant	GB 37956930
S2	203	G	-	variant	GB 37956930
S2	204	G	-	variant	GB 37956930
S2	205	G	-	variant	GB 37956930
S2	206	G	-	variant	GB 37956930
S2	207	G	-	variant	GB 37956930
S2	208	G	-	variant	GB 37956930
S2	209	A	-	variant	GB 37956930
S2	210	U	-	variant	GB 37956930
S2	211	G	-	variant	GB 37956930
S2	212	C	-	variant	GB 37956930
S2	213	G	-	variant	GB 37956930
S2	214	U	-	variant	GB 37956930
S2	215	G	-	variant	GB 37956930
S2	216	C	-	variant	GB 37956930
S2	217	A	-	variant	GB 37956930
S2	218	U	-	variant	GB 37956930
S2	219	U	-	variant	GB 37956930
S2	220	U	-	variant	GB 37956930
S2	221	A	-	variant	GB 37956930
S2	222	U	-	variant	GB 37956930
S2	223	C	-	variant	GB 37956930

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Chain	Residue	Modelled	Actual	Comment	Reference
S2	224	A	-	variant	GB 37956930
S2	225	G	-	variant	GB 37956930
S2	287	U	-	variant	GB 37956930
S2	288	G	-	variant	GB 37956930
S2	289	G	-	variant	GB 37956930
S2	290	U	-	variant	GB 37956930
S2	291	G	-	variant	GB 37956930
S2	292	A	-	variant	GB 37956930
S2	293	C	-	variant	GB 37956930
S2	294	U	-	variant	GB 37956930
S2	295	C	-	variant	GB 37956930
S2	296	U	-	variant	GB 37956930
S2	297	A	-	variant	GB 37956930
S2	298	G	-	variant	GB 37956930
S2	299	A	-	variant	GB 37956930
S2	300	U	-	variant	GB 37956930
S2	301	A	-	variant	GB 37956930
S2	302	A	-	variant	GB 37956930
S2	303	C	-	variant	GB 37956930
S2	304	C	-	variant	GB 37956930
S2	305	U	-	variant	GB 37956930
S2	306	C	-	variant	GB 37956930
S2	307	G	-	variant	GB 37956930
S2	308	G	-	variant	GB 37956930
S2	309	G	-	variant	GB 37956930
S2	310	C	-	variant	GB 37956930
S2	311	C	-	variant	GB 37956930
S2	312	G	-	variant	GB 37956930
S2	313	A	-	variant	GB 37956930
S2	314	U	-	variant	GB 37956930
S2	315	C	-	variant	GB 37956930
S2	316	G	-	variant	GB 37956930
S2	317	C	-	variant	GB 37956930
S2	318	A	-	variant	GB 37956930
S2	319	C	-	variant	GB 37956930
S2	320	G	-	variant	GB 37956930
S2	321	C	-	variant	GB 37956930
S2	322	C	-	variant	GB 37956930
S2	323	C	-	variant	GB 37956930
S2	324	C	-	variant	GB 37956930
S2	325	C	-	variant	GB 37956930
S2	326	C	-	variant	GB 37956930

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Chain	Residue	Modelled	Actual	Comment	Reference
S2	327	G	-	variant	GB 37956930
S2	328	U	-	variant	GB 37956930
S2	329	G	-	variant	GB 37956930
S2	330	G	-	variant	GB 37956930
S2	331	C	-	variant	GB 37956930
S2	332	G	-	variant	GB 37956930
S2	333	G	-	variant	GB 37956930
S2	334	C	-	variant	GB 37956930
S2	335	G	-	variant	GB 37956930
S2	336	A	-	variant	GB 37956930
S2	337	C	-	variant	GB 37956930
S2	338	G	-	variant	GB 37956930
S2	339	A	-	variant	GB 37956930
S2	340	C	-	variant	GB 37956930
S2	341	C	-	variant	GB 37956930
S2	342	C	-	variant	GB 37956930
S2	343	A	-	variant	GB 37956930
S2	344	U	-	variant	GB 37956930
S2	345	U	-	variant	GB 37956930
S2	346	C	-	variant	GB 37956930
S2	347	G	-	variant	GB 37956930
S2	348	A	-	variant	GB 37956930
S2	349	A	-	variant	GB 37956930
S2	350	C	-	variant	GB 37956930
S2	351	G	-	variant	GB 37956930
S2	352	U	-	variant	GB 37956930
S2	353	C	-	variant	GB 37956930
S2	354	U	-	variant	GB 37956930
S2	355	G	-	variant	GB 37956930
S2	356	C	-	variant	GB 37956930
S2	357	C	-	variant	GB 37956930
S2	358	C	-	variant	GB 37956930
S2	359	U	-	variant	GB 37956930
S2	360	A	-	variant	GB 37956930
S2	361	U	-	variant	GB 37956930
S2	362	C	-	variant	GB 37956930
S2	363	A	-	variant	GB 37956930
S2	364	A	-	variant	GB 37956930
S2	365	C	-	variant	GB 37956930
S2	366	U	-	variant	GB 37956930
S2	367	U	-	variant	GB 37956930
S2	368	U	-	variant	GB 37956930

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Chain	Residue	Modelled	Actual	Comment	Reference
S2	369	C	-	variant	GB 37956930
S2	370	G	-	variant	GB 37956930
S2	371	A	-	variant	GB 37956930
S2	372	U	-	variant	GB 37956930
S2	373	G	-	variant	GB 37956930
S2	374	G	-	variant	GB 37956930
S2	375	U	-	variant	GB 37956930
S2	376	A	-	variant	GB 37956930
S2	377	G	-	variant	GB 37956930
S2	378	U	-	variant	GB 37956930
S2	379	C	-	variant	GB 37956930
S2	380	G	-	variant	GB 37956930
S2	381	C	-	variant	GB 37956930
S2	382	C	-	variant	GB 37956930
S2	383	G	-	variant	GB 37956930
S2	384	U	-	variant	GB 37956930
S2	385	G	-	variant	GB 37956930
S2	386	C	-	variant	GB 37956930
S2	387	C	-	variant	GB 37956930
S2	388	U	-	variant	GB 37956930
S2	389	A	-	variant	GB 37956930
S2	390	C	-	variant	GB 37956930
S2	391	C	-	variant	GB 37956930
S2	392	A	-	variant	GB 37956930
S2	393	U	-	variant	GB 37956930
S2	394	G	-	variant	GB 37956930
S2	395	G	-	variant	GB 37956930
S2	396	U	-	variant	GB 37956930
S2	397	G	-	variant	GB 37956930
S2	398	A	-	variant	GB 37956930
S2	399	C	-	variant	GB 37956930
S2	400	C	-	variant	GB 37956930
S2	401	A	-	variant	GB 37956930
S2	402	C	-	variant	GB 37956930
S2	403	G	-	variant	GB 37956930
S2	404	G	-	variant	GB 37956930
S2	405	G	-	variant	GB 37956930
S2	406	U	-	variant	GB 37956930
S2	407	G	-	variant	GB 37956930
S2	408	A	-	variant	GB 37956930
S2	409	C	-	variant	GB 37956930
S2	410	G	-	variant	GB 37956930

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Chain	Residue	Modelled	Actual	Comment	Reference
S2	411	G	-	variant	GB 37956930
S2	412	G	-	variant	GB 37956930
S2	413	G	-	variant	GB 37956930
S2	414	A	-	variant	GB 37956930
S2	415	A	-	variant	GB 37956930
S2	416	U	-	variant	GB 37956930
S2	417	C	-	variant	GB 37956930
S2	418	A	-	variant	GB 37956930
S2	419	G	-	variant	GB 37956930
S2	420	G	-	variant	GB 37956930
S2	421	G	-	variant	GB 37956930
S2	422	U	-	variant	GB 37956930
S2	423	U	-	variant	GB 37956930
S2	424	C	-	variant	GB 37956930
S2	425	G	-	variant	GB 37956930
S2	426	A	-	variant	GB 37956930
S2	427	U	-	variant	GB 37956930
S2	428	U	-	variant	GB 37956930
S2	429	C	-	variant	GB 37956930
S2	430	C	-	variant	GB 37956930
S2	431	G	-	variant	GB 37956930
S2	432	G	-	variant	GB 37956930
S2	433	A	-	variant	GB 37956930
S2	434	G	-	variant	GB 37956930
S2	435	A	-	variant	GB 37956930
S2	436	G	-	variant	GB 37956930
S2	437	G	-	variant	GB 37956930
S2	438	G	-	variant	GB 37956930
S2	439	A	-	variant	GB 37956930
S2	440	G	-	variant	GB 37956930
S2	441	C	-	variant	GB 37956930
S2	442	C	-	variant	GB 37956930
S2	443	U	-	variant	GB 37956930
S2	444	G	-	variant	GB 37956930
S2	445	A	-	variant	GB 37956930
S2	446	G	-	variant	GB 37956930
S2	447	A	-	variant	GB 37956930
S2	448	A	-	variant	GB 37956930
S2	449	A	-	variant	GB 37956930
S2	450	C	-	variant	GB 37956930
S2	451	G	-	variant	GB 37956930
S2	452	G	-	variant	GB 37956930

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Chain	Residue	Modelled	Actual	Comment	Reference
S2	453	C	-	variant	GB 37956930
S2	454	U	-	variant	GB 37956930
S2	455	A	-	variant	GB 37956930
S2	456	C	-	variant	GB 37956930
S2	457	C	-	variant	GB 37956930
S2	458	A	-	variant	GB 37956930
S2	459	C	-	variant	GB 37956930
S2	460	A	-	variant	GB 37956930
S2	461	U	-	variant	GB 37956930
S2	462	C	-	variant	GB 37956930
S2	463	C	-	variant	GB 37956930
S2	464	A	-	variant	GB 37956930
S2	465	A	-	variant	GB 37956930
S2	466	G	-	variant	GB 37956930
S2	467	G	-	variant	GB 37956930
S2	468	A	-	variant	GB 37956930
S2	469	A	-	variant	GB 37956930
S2	470	G	-	variant	GB 37956930
S2	471	G	-	variant	GB 37956930
S2	472	C	-	variant	GB 37956930
S2	473	A	-	variant	GB 37956930
S2	474	G	-	variant	GB 37956930
S2	475	C	-	variant	GB 37956930
S2	476	A	-	variant	GB 37956930
S2	477	G	-	variant	GB 37956930
S2	478	G	-	variant	GB 37956930
S2	479	C	-	variant	GB 37956930
S2	480	G	-	variant	GB 37956930
S2	481	C	-	variant	GB 37956930
S2	482	G	-	variant	GB 37956930
S2	483	C	-	variant	GB 37956930
S2	484	A	-	variant	GB 37956930
S2	485	A	-	variant	GB 37956930
S2	486	A	-	variant	GB 37956930
S2	487	U	-	variant	GB 37956930
S2	488	U	-	variant	GB 37956930
S2	489	A	-	variant	GB 37956930
S2	490	C	-	variant	GB 37956930
S2	491	C	-	variant	GB 37956930
S2	492	C	-	variant	GB 37956930
S2	493	A	-	variant	GB 37956930
S2	494	C	-	variant	GB 37956930

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Chain	Residue	Modelled	Actual	Comment	Reference
S2	495	U	-	variant	GB 37956930
S2	496	C	-	variant	GB 37956930
S2	497	C	-	variant	GB 37956930
S2	498	C	-	variant	GB 37956930
S2	499	G	-	variant	GB 37956930
S2	500	A	-	variant	GB 37956930
S2	501	C	-	variant	GB 37956930
S2	502	C	-	variant	GB 37956930
S2	503	C	-	variant	GB 37956930
S2	504	G	-	variant	GB 37956930
S2	505	G	-	variant	GB 37956930
S2	506	G	-	variant	GB 37956930
S2	507	G	-	variant	GB 37956930
S2	508	A	-	variant	GB 37956930
S2	509	G	-	variant	GB 37956930
S2	510	G	-	variant	GB 37956930
S2	511	U	-	variant	GB 37956930
S2	512	A	-	variant	GB 37956930
S2	513	G	-	variant	GB 37956930
S2	514	U	-	variant	GB 37956930
S2	515	G	-	variant	GB 37956930
S2	516	A	-	variant	GB 37956930
S2	517	C	-	variant	GB 37956930
S2	518	G	-	variant	GB 37956930
S2	519	A	-	variant	GB 37956930
S2	520	A	-	variant	GB 37956930
S2	521	A	-	variant	GB 37956930
S2	522	A	-	variant	GB 37956930
S2	523	A	-	variant	GB 37956930
S2	524	U	-	variant	GB 37956930
S2	525	A	-	variant	GB 37956930
S2	526	A	-	variant	GB 37956930
S2	527	C	-	variant	GB 37956930
S2	528	A	-	variant	GB 37956930
S2	529	A	-	variant	GB 37956930
S2	530	U	-	variant	GB 37956930
S2	531	A	-	variant	GB 37956930
S2	532	C	-	variant	GB 37956930
S2	533	A	-	variant	GB 37956930
S2	534	G	-	variant	GB 37956930
S2	535	G	-	variant	GB 37956930
S2	536	A	-	variant	GB 37956930

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Chain	Residue	Modelled	Actual	Comment	Reference
S2	537	C	-	variant	GB 37956930
S2	538	U	-	variant	GB 37956930
S2	539	C	-	variant	GB 37956930
S2	540	U	-	variant	GB 37956930
S2	541	U	-	variant	GB 37956930
S2	542	U	-	variant	GB 37956930
S2	543	C	-	variant	GB 37956930
S2	544	G	-	variant	GB 37956930
S2	545	A	-	variant	GB 37956930
S2	546	G	-	variant	GB 37956930
S2	547	G	-	variant	GB 37956930
S2	548	C	-	variant	GB 37956930
S2	549	C	-	variant	GB 37956930
S2	550	C	-	variant	GB 37956930
S2	551	U	-	variant	GB 37956930
S2	552	G	-	variant	GB 37956930
S2	553	U	-	variant	GB 37956930
S2	554	A	-	variant	GB 37956930
S2	555	A	-	variant	GB 37956930
S2	556	U	-	variant	GB 37956930
S2	557	U	-	variant	GB 37956930
S2	558	G	-	variant	GB 37956930
S2	559	G	-	variant	GB 37956930
S2	560	A	-	variant	GB 37956930
S2	561	A	-	variant	GB 37956930
S2	562	U	-	variant	GB 37956930
S2	563	G	-	variant	GB 37956930
S2	564	A	-	variant	GB 37956930
S2	565	G	-	variant	GB 37956930
S2	566	U	-	variant	GB 37956930
S2	567	C	-	variant	GB 37956930
S2	568	C	-	variant	GB 37956930
S2	569	A	-	variant	GB 37956930
S2	570	C	-	variant	GB 37956930
S2	571	U	-	variant	GB 37956930
S2	572	U	-	variant	GB 37956930
S2	573	U	-	variant	GB 37956930
S2	574	A	-	variant	GB 37956930
S2	575	A	-	variant	GB 37956930
S2	576	A	-	variant	GB 37956930
S2	577	U	-	variant	GB 37956930
S2	578	C	-	variant	GB 37956930

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Chain	Residue	Modelled	Actual	Comment	Reference
S2	579	C	-	variant	GB 37956930
S2	580	U	-	variant	GB 37956930
S2	581	U	-	variant	GB 37956930
S2	582	C	-	variant	GB 37956930
S2	583	C	-	variant	GB 37956930
S2	584	G	-	variant	GB 37956930
S2	585	C	-	variant	GB 37956930
S2	586	G	-	variant	GB 37956930
S2	587	A	-	variant	GB 37956930
S2	588	G	-	variant	GB 37956930
S2	589	G	-	variant	GB 37956930
S2	590	A	-	variant	GB 37956930
S2	591	U	-	variant	GB 37956930
S2	592	C	-	variant	GB 37956930
S2	593	C	-	variant	GB 37956930
S2	594	A	-	variant	GB 37956930
S2	595	U	-	variant	GB 37956930
S2	596	U	-	variant	GB 37956930
S2	597	G	-	variant	GB 37956930
S2	598	G	-	variant	GB 37956930
S2	599	A	-	variant	GB 37956930
S2	600	G	-	variant	GB 37956930
S2	601	G	-	variant	GB 37956930
S2	602	G	-	variant	GB 37956930
S2	603	C	-	variant	GB 37956930
S2	604	A	-	variant	GB 37956930
S2	605	A	-	variant	GB 37956930
S2	606	G	-	variant	GB 37956930
S2	607	U	-	variant	GB 37956930
S2	608	C	-	variant	GB 37956930
S2	609	U	-	variant	GB 37956930
S2	610	G	-	variant	GB 37956930
S2	611	G	-	variant	GB 37956930
S2	612	U	-	variant	GB 37956930
S2	613	G	-	variant	GB 37956930
S2	614	C	-	variant	GB 37956930
S2	615	C	-	variant	GB 37956930
S2	616	A	-	variant	GB 37956930
S2	617	G	-	variant	GB 37956930
S2	618	C	-	variant	GB 37956930
S2	619	A	-	variant	GB 37956930
S2	620	G	-	variant	GB 37956930

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Chain	Residue	Modelled	Actual	Comment	Reference
S2	621	C	-	variant	GB 37956930
S2	622	C	-	variant	GB 37956930
S2	623	G	-	variant	GB 37956930
S2	624	C	-	variant	GB 37956930
S2	625	G	-	variant	GB 37956930
S2	626	G	-	variant	GB 37956930
S2	627	U	-	variant	GB 37956930
S2	628	A	-	variant	GB 37956930
S2	629	A	-	variant	GB 37956930
S2	630	U	-	variant	GB 37956930
S2	631	U	-	variant	GB 37956930
S2	632	C	-	variant	GB 37956930
S2	633	C	-	variant	GB 37956930
S2	634	A	-	variant	GB 37956930
S2	635	G	-	variant	GB 37956930
S2	636	C	-	variant	GB 37956930
S2	637	U	-	variant	GB 37956930
S2	638	C	-	variant	GB 37956930
S2	639	C	-	variant	GB 37956930
S2	640	A	-	variant	GB 37956930
S2	641	A	-	variant	GB 37956930
S2	642	U	-	variant	GB 37956930
S2	643	A	-	variant	GB 37956930
S2	644	G	-	variant	GB 37956930
S2	645	C	-	variant	GB 37956930
S2	646	G	-	variant	GB 37956930
S2	647	U	-	variant	GB 37956930
S2	648	A	-	variant	GB 37956930
S2	649	U	-	variant	GB 37956930
S2	650	A	-	variant	GB 37956930
S2	651	U	-	variant	GB 37956930
S2	652	U	-	variant	GB 37956930
S2	653	A	-	variant	GB 37956930
S2	654	A	-	variant	GB 37956930
S2	655	A	-	variant	GB 37956930
S2	656	G	-	variant	GB 37956930
S2	657	U	-	variant	GB 37956930
S2	658	U	-	variant	GB 37956930
S2	659	G	-	variant	GB 37956930
S2	660	C	-	variant	GB 37956930
S2	661	U	-	variant	GB 37956930
S2	662	G	-	variant	GB 37956930

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Chain	Residue	Modelled	Actual	Comment	Reference
S2	663	C	-	variant	GB 37956930
S2	664	A	-	variant	GB 37956930
S2	665	G	-	variant	GB 37956930
S2	666	U	-	variant	GB 37956930
S2	667	U	-	variant	GB 37956930
S2	668	A	-	variant	GB 37956930
S2	669	A	-	variant	GB 37956930
S2	670	A	-	variant	GB 37956930
S2	671	A	-	variant	GB 37956930
S2	672	A	-	variant	GB 37956930
S2	673	G	-	variant	GB 37956930
S2	674	C	-	variant	GB 37956930
S2	675	U	-	variant	GB 37956930
S2	676	C	-	variant	GB 37956930
S2	677	G	-	variant	GB 37956930
S2	678	U	-	variant	GB 37956930
S2	679	A	-	variant	GB 37956930
S2	680	G	-	variant	GB 37956930
S2	681	U	-	variant	GB 37956930
S2	682	U	-	variant	GB 37956930
S2	683	G	-	variant	GB 37956930
S2	684	G	-	variant	GB 37956930
S2	685	A	-	variant	GB 37956930
S2	686	U	-	variant	GB 37956930
S2	687	C	-	variant	GB 37956930
S2	688	U	-	variant	GB 37956930
S2	689	U	-	variant	GB 37956930
S2	690	G	-	variant	GB 37956930
S2	691	G	-	variant	GB 37956930
S2	692	G	-	variant	GB 37956930
S2	693	A	-	variant	GB 37956930
S2	694	G	-	variant	GB 37956930
S2	695	C	-	variant	GB 37956930
S2	696	G	-	variant	GB 37956930
S2	697	G	-	variant	GB 37956930
S2	698	G	-	variant	GB 37956930
S2	730	C	-	variant	GB 37956930
S2	731	G	-	variant	GB 37956930
S2	732	U	-	variant	GB 37956930
S2	733	C	-	variant	GB 37956930
S2	734	C	-	variant	GB 37956930
S2	735	C	-	variant	GB 37956930

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Chain	Residue	Modelled	Actual	Comment	Reference
S2	736	C	-	variant	GB 37956930
S2	737	G	-	variant	GB 37956930
S2	738	C	-	variant	GB 37956930
S2	739	C	-	variant	GB 37956930
S2	744	G	-	variant	GB 37956930
S2	745	C	-	variant	GB 37956930
S2	746	C	-	variant	GB 37956930
S2	747	U	-	variant	GB 37956930
S2	748	C	-	variant	GB 37956930
S2	749	U	-	variant	GB 37956930
S2	750	C	-	variant	GB 37956930
S2	751	G	-	variant	GB 37956930
S2	752	G	-	variant	GB 37956930
S2	753	C	-	variant	GB 37956930
S2	798	A	G	conflict	GB 37956930

- Molecule 51 is a protein called Ribosomal protein uS2.

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

- Molecule 52 is a protein called Ribosomal protein eS1.

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

- Molecule 53 is a protein called Ribosomal protein uS5.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SC	61	MET	LEU	conflict	UNP I3LJ87

- Molecule 54 is a protein called Ribosomal protein uS3.

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

- Molecule 55 is a protein called Ribosomal protein eS4.

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

- Molecule 56 is a protein called Ribosomal protein uS7.

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

- Molecule 57 is a protein called Ribosomal protein eS6.

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

- Molecule 58 is a protein called Ribosomal protein eS7.

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

- Molecule 59 is a protein called Ribosomal protein eS8.

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

- Molecule 60 is a protein called Ribosomal protein uS4.

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

- Molecule 61 is a protein called Ribosomal protein eS10.

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

- Molecule 62 is a protein called Ribosomal protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SL	156	Total	C	N	O	S	0	0
			1276	813	239	218	6		

- Molecule 63 is a protein called Ribosomal protein eS12.

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SM	52	GLN	LEU	conflict	UNP P46405
SM	69	LEU	CYS	conflict	UNP P46405
SM	99	ASN	LYS	conflict	UNP P46405

- Molecule 64 is a protein called Ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SN	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 65 is a protein called Ribosomal protein uS11.

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

- Molecule 66 is a protein called Ribosomal protein uS19.

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

- Molecule 67 is a protein called Ribosomal protein uS9.

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

- Molecule 68 is a protein called Ribosomal protein eS17.

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

- Molecule 69 is a protein called Ribosomal protein uS13.

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

- Molecule 70 is a protein called Ribosomal protein eS19.

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

- Molecule 71 is a protein called Ribosomal protein uS10.

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

- Molecule 72 is a protein called Ribosomal protein eS21.

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

- Molecule 73 is a protein called Ribosomal protein uS8.

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

- Molecule 74 is a protein called Ribosomal protein uS12.

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

- Molecule 75 is a protein called Ribosomal protein eS24.

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

- Molecule 76 is a protein called Ribosomal protein es25.

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

- Molecule 77 is a protein called Ribosomal protein eS26.

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

- Molecule 78 is a protein called Ribosomal protein eS27.

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

- Molecule 79 is a protein called Ribosomal protein eS28.

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

- Molecule 80 is a protein called Ribosomal protein uS14.

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

- Molecule 81 is a protein called Ribosomal protein eS30.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Se	-33	VAL	LEU	conflict	UNP A0A480W155
Se	-23	GLU	ASP	conflict	UNP A0A480W155
Se	-21	THR	ILE	conflict	UNP A0A480W155
Se	-11	THR	ARG	conflict	UNP A0A480W155

- Molecule 82 is a protein called Ribosomal protein eS31.

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

- Molecule 83 is a protein called Ribosomal protein RACK1.

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

- Molecule 84 is a RNA chain called Messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	S4	10	Total	C	N	O	P	0	0
			201	91	23	78	9		

- Molecule 85 is a RNA chain called A/P tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	S5	74	Total	C	N	O	P	0	0
			1579	705	285	516	73		

- Molecule 86 is a RNA chain called P/E tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	S6	76	Total	C	N	O	P	0	0
			1622	723	291	532	76		

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
87	5	120	Total 120	Mg 120	0
87	7	5	Total 5	Mg 5	0
87	8	3	Total 3	Mg 3	0
87	P	1	Total 1	Mg 1	0
87	V	1	Total 1	Mg 1	0
87	S2	36	Total 36	Mg 36	0

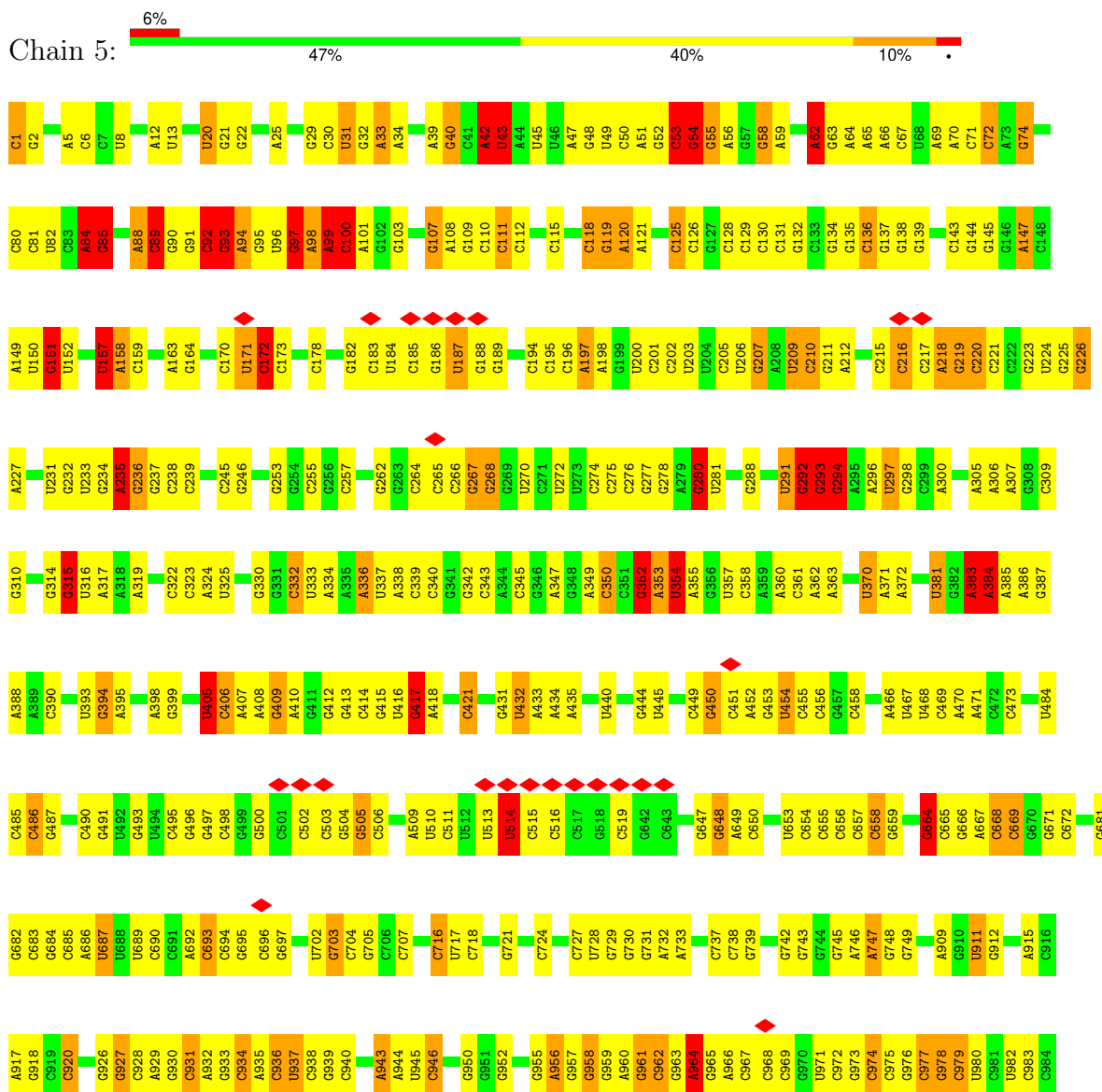
- Molecule 88 is ZINC ION (three-letter code: ZN) (formula: Zn).

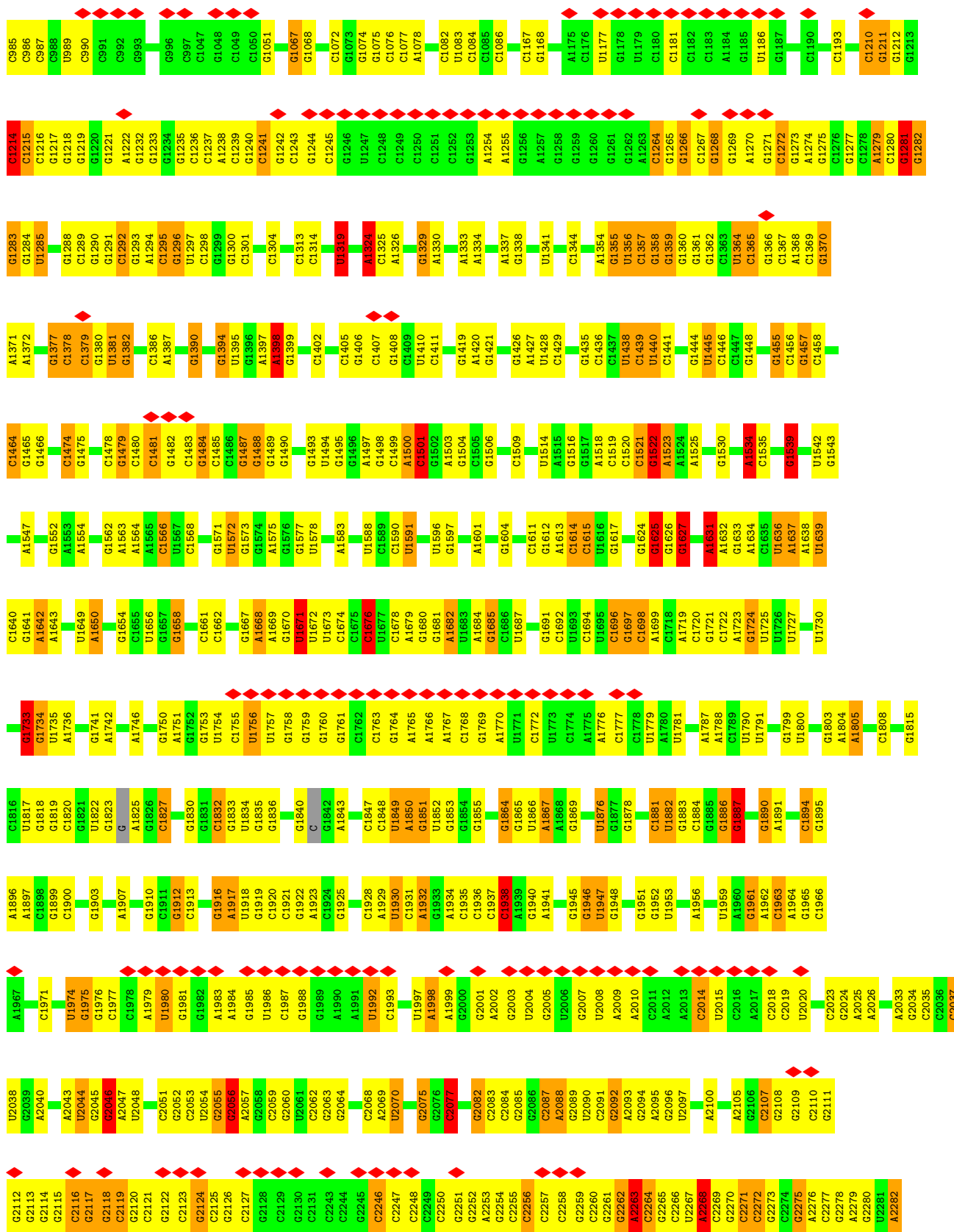
Mol	Chain	Residues	Atoms		AltConf
88	j	1	Total 1	Zn 1	0
88	m	1	Total 1	Zn 1	0
88	o	1	Total 1	Zn 1	0
88	Sa	1	Total 1	Zn 1	0

3 Residue-property plots [i](#)

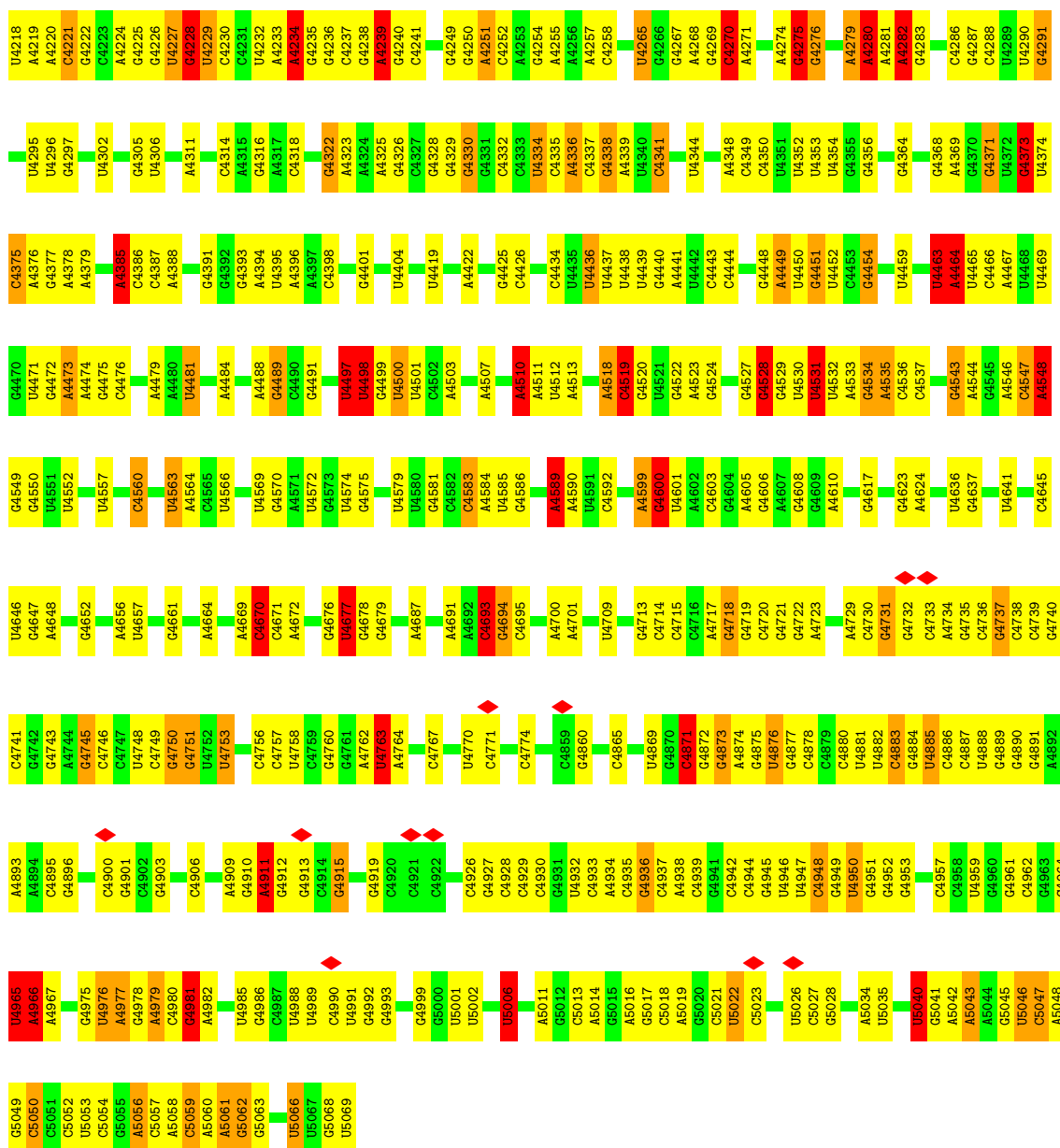
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 28S ribosomal RNA





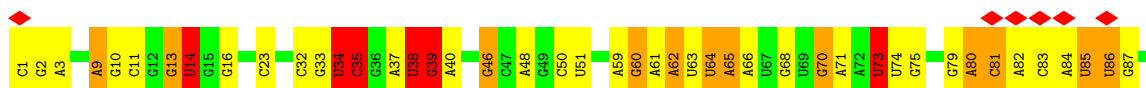




• Molecule 2: 5S ribosomal RNA

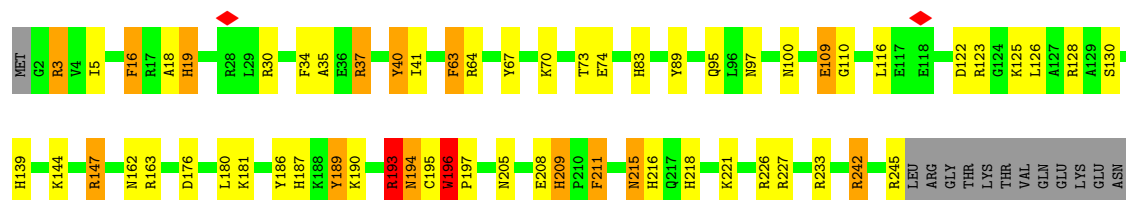


• Molecule 3: 5.8S ribosomal RNA

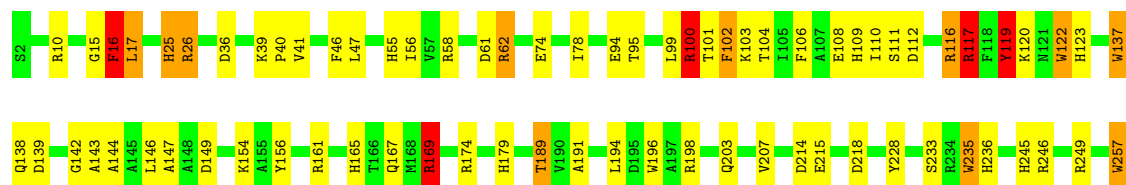




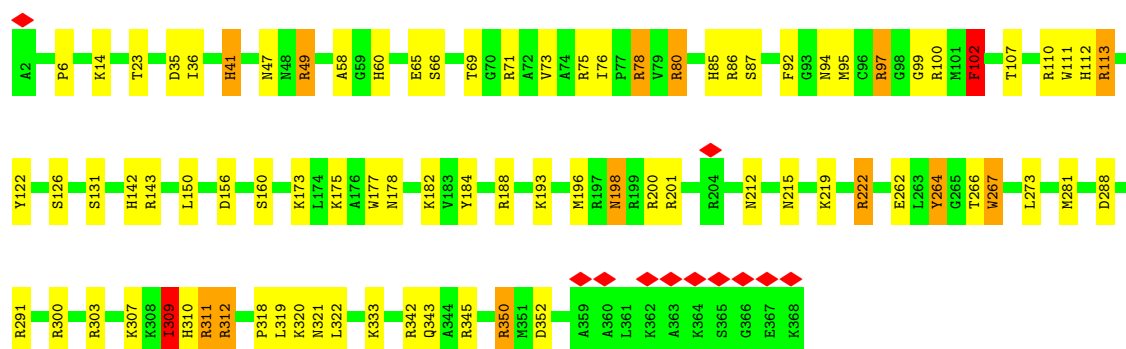
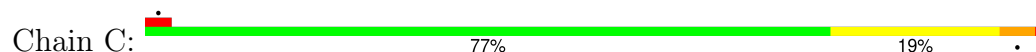
• Molecule 4: Ribosomal protein uL2



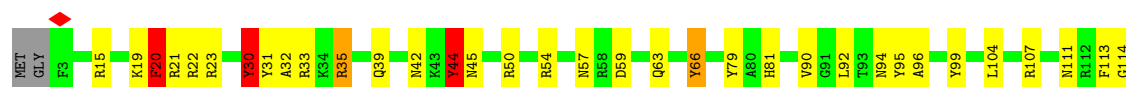
• Molecule 5: Ribosomal protein uL3

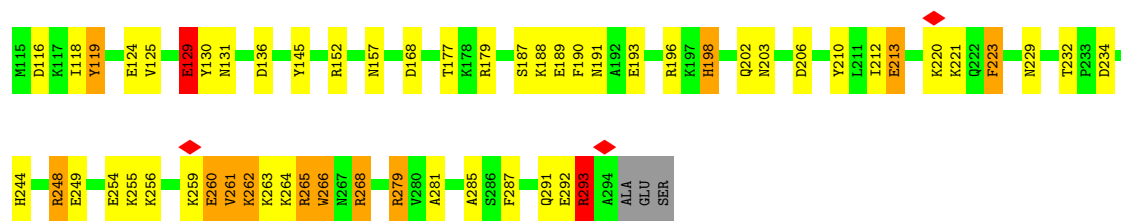


• Molecule 6: Ribosomal protein uL4

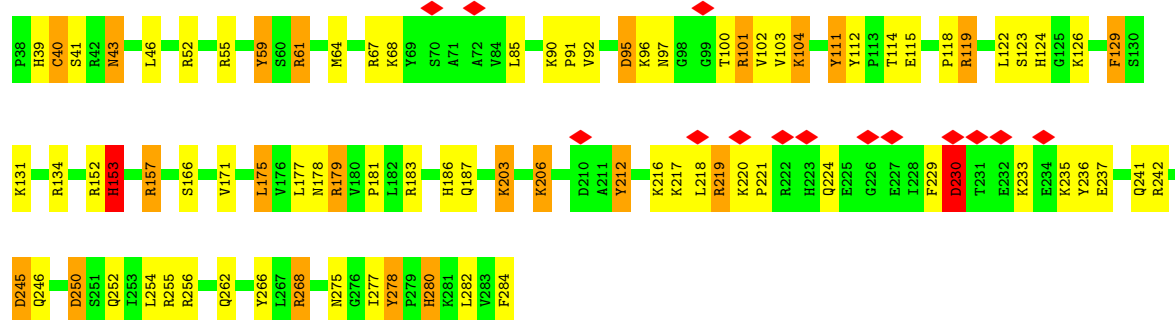


• Molecule 7: Ribosomal protein uL18

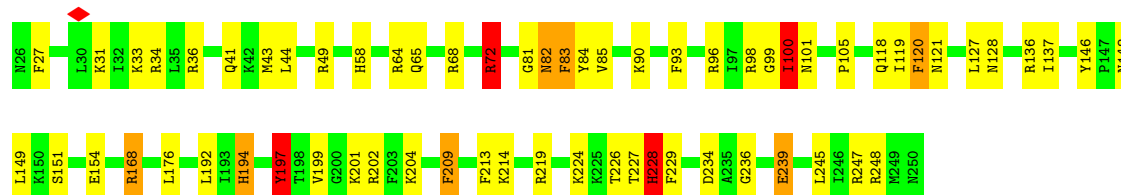




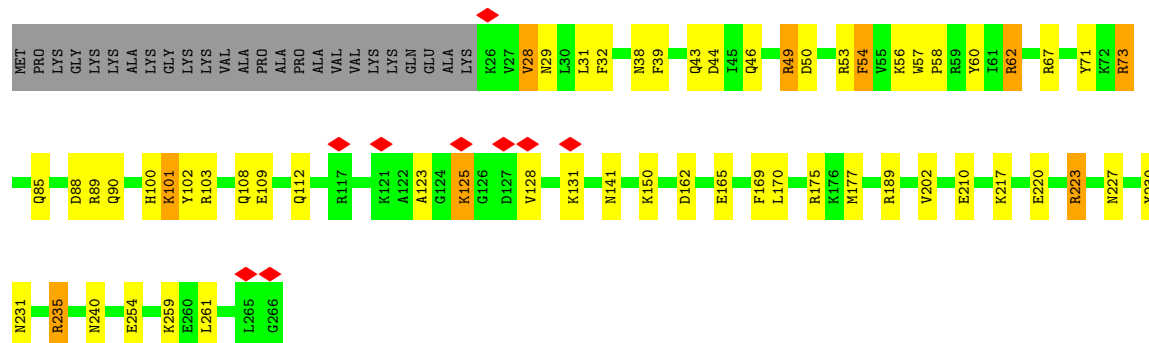
• Molecule 8: Ribosomal protein eL6



• Molecule 9: Ribosomal protein uL30

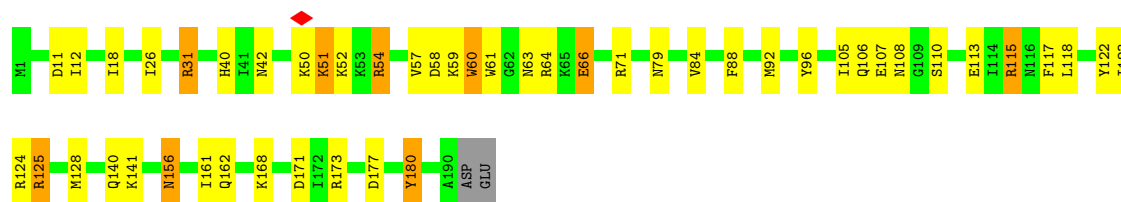


• Molecule 10: Ribosomal protein eL8

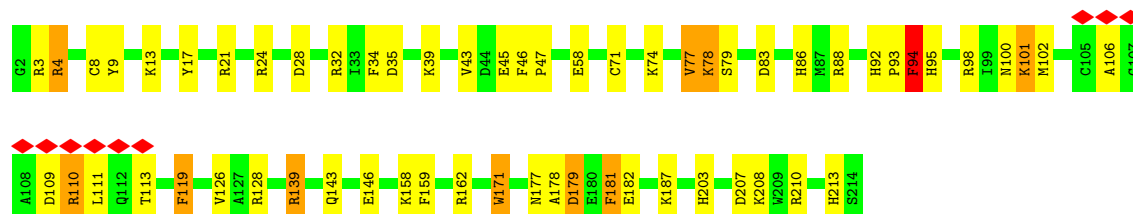


• Molecule 11: Ribosomal protein uL6

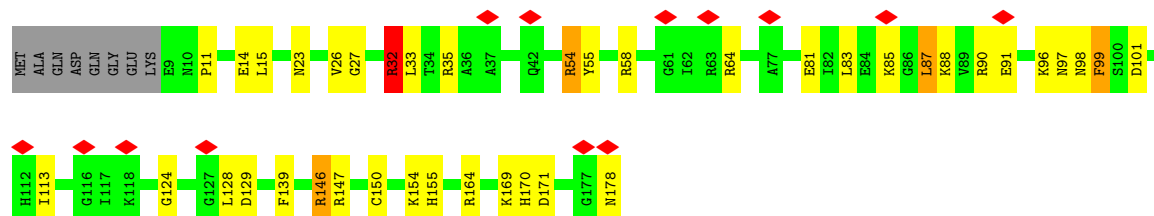




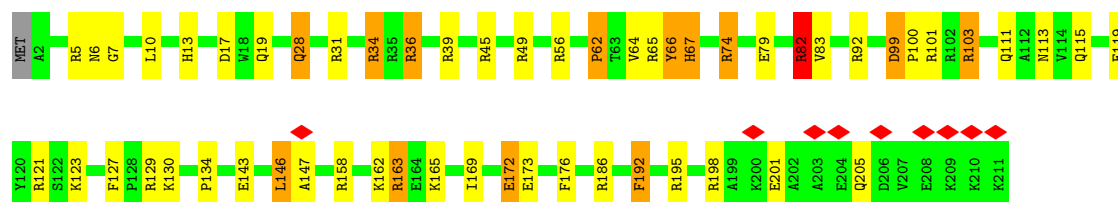
• Molecule 12: Ribosomal protein uL16



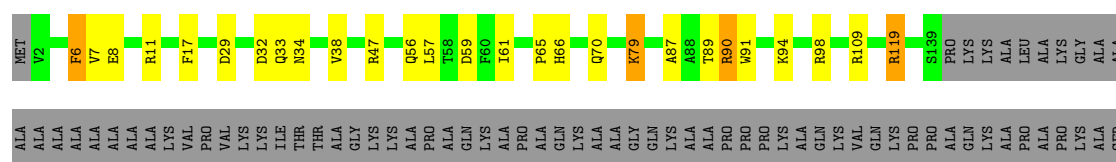
• Molecule 13: Ribosomal protein uL5



• Molecule 14: Ribosomal protein eL13



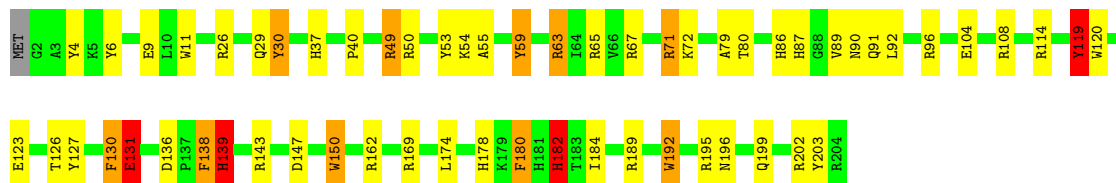
• Molecule 15: Ribosomal protein eL14




GLY
GLU
LYS
ALA

• Molecule 16: Ribosomal protein eL15

Chain N:  71% 22% 5% •




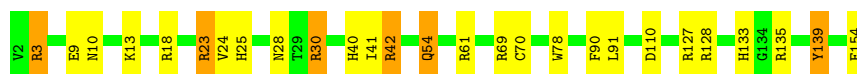
• Molecule 17: Ribosomal protein uL13

Chain O:  84% 12% •



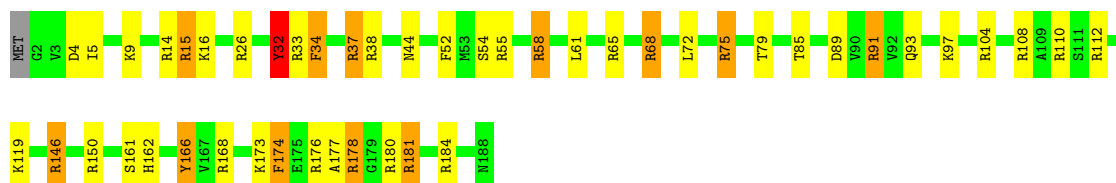
• Molecule 18: Ribosomal protein uL22

Chain P:  82% 14% •



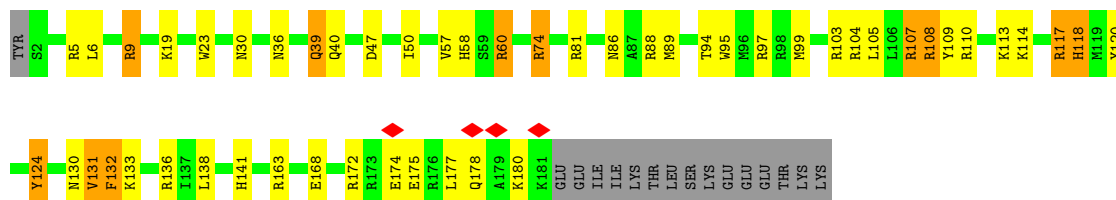
• Molecule 19: Ribosomal protein eL18

Chain Q:  74% 18% 6% ••

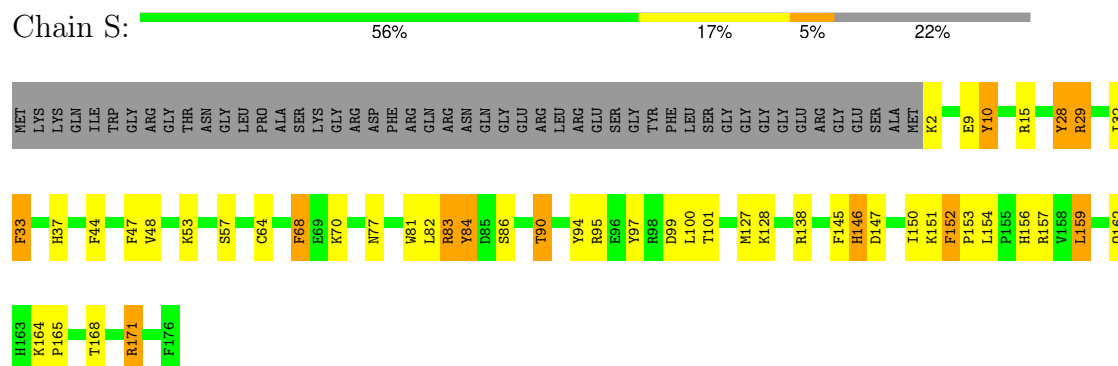


• Molecule 20: Ribosomal protein eL19

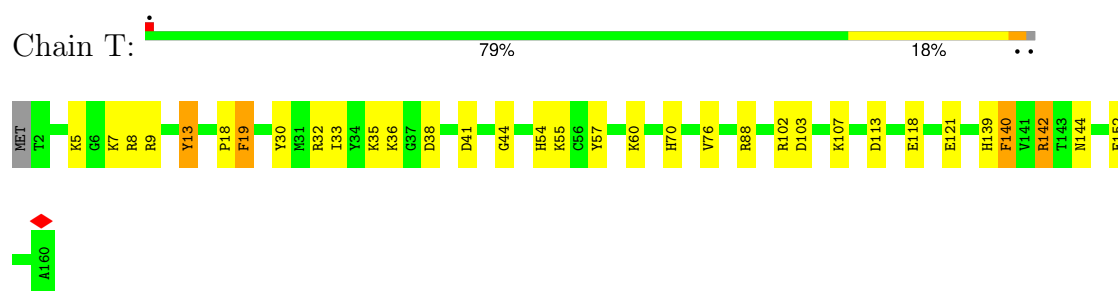
Chain R:  66% 20% 6% 8%



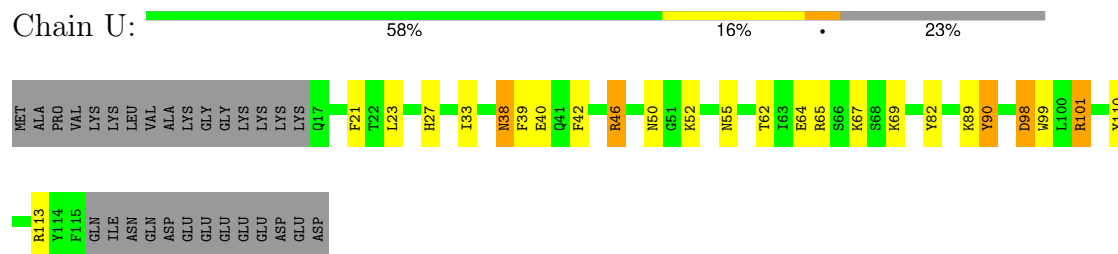
• Molecule 21: Ribosomal protein eL20



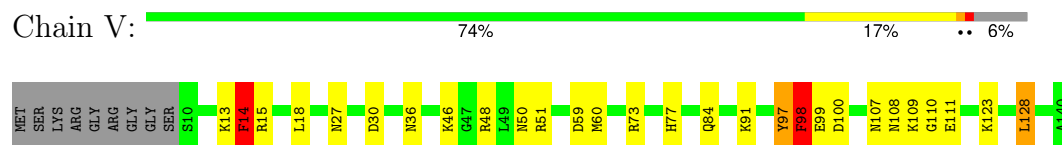
• Molecule 22: Ribosomal protein eL21



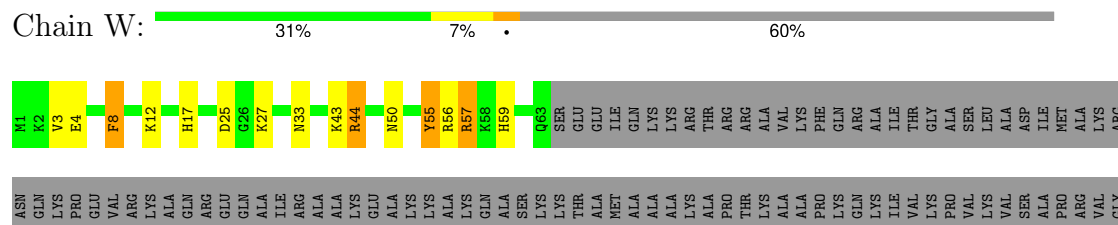
• Molecule 23: Ribosomal protein eL22



• Molecule 24: Ribosomal protein uL14



• Molecule 25: Ribosomal protein eL24



LYS
GLY
ALA
GLN
ALA
PRO
THR
LYS
ALA
PRO
GLN

• Molecule 31: Ribosomal protein eL30

Chain c:  63% 15% 18%

MET VAL ALA ALA LYS LYS THR LYS LYS SER LEU GLU S13 L18 Y27 Y31 K32 M37 I38 R39 K42 A43 K44 C52 L55 R56 E59 L66 H72 H73 Y74 M77 M78 I79 E80 L81 Y88 Y89 R90 D101 R106 SER MET PRO GLU GLN

THR GLY GLU LYS

• Molecule 32: Ribosomal protein eL31

Chain d:  56% 22% 8% 14%

MET ALA PRO ALA LYS LYS GLY GLY LYS LYS LYS GLY ARG SER ALA ILE N18 E19 R23 E24 Y25 T26 I27 N28 K31 R32 F38 K39 R44 G58 R67 V72 M73 R78 M79 R83 I84 R85 V86 R87 K91 R92 N93 E94 D95 E96 D97 K101

L102 Y103 Y108 Y109 N116 L117 Q118 T119 V120 N121 V122 D123 E124 ASN

• Molecule 33: Ribosomal protein eL32

Chain e:  69% 22% 5%

MET A2 A3 L4 R5 K11 R16 F20 I21 D26 N34 W35 R36 D42 M43 R46 R47 R48 F49 Q52 N57 Y60 K64 H68 F74 R75 K76 F77 L78 L85 N92 Y95 K106 N107 R108 E113 N124 P125 N126 A127 R128


L129 ARG SER GLU ASN GLU

• Molecule 34: Ribosomal protein eL33

Chain f:  78% 15% 5% 2%

MET S2 G3 R4 L5 W6 S7 Y14 R15 R16 R19 R22 E23 H24 R36 Y49 V50 Y51 K52 A53 W71 N80 R85 R100 I101 R102 Y106 P107 S108 R109 I110

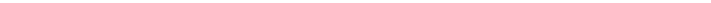
• Molecule 35: Ribosomal protein eL34

Chain g:  6% 77% 19% 2%

MET V2 Q3 R4 L5 T6 Y7 R8 R9 S12 Y13 N14 R29 Y32 Y36 R52 R53 L54 R55 R57 R60 R66 S75 S81 A84 R88 D89 R90 R93 A94 F95 K108 A109 Q110 A111 Q112 S113 Q114 K115 ALA LYS

• Molecule 36: Ribosomal protein uL29

Bar chart showing the distribution of 20 amino acids. The x-axis represents the count of each amino acid, ranging from 0 to 20. The y-axis lists the amino acids: MET, A2, D8, L9, R10, E15, D23, L28, G38, R48, R51, E67, M68, L69, R70, K71, F72, Y73, Y78, R84, R89, R93, K97, E100, R117, K118, F119, A120, V121, K122, A123, and A124. The bars are colored in a repeating pattern of yellow, orange, and red. MET and A2 are marked with red diamonds above them.

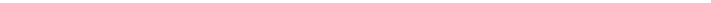
- Chain i:  76% 17% . .

- Chain j:  73% 21% 6%

T2	T5	F8	G9	K10	R11	K25	A26	Y27	G38	Y39	R45	K46	Y47	N48	W49	R55	R56	N57	H66	Y71	R75	H76	R79	E80	K87
----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain k:  71% 27%

Category	Count
NET	100
P2	100
T14	100
A15	100
R16	100
D19	100
A20	100
K21	100
S22	100
V23	100
K27	100
N28	100
K29	100
D30	100
K35	100
V36	100
R37	100
E51	100
E54	100
K55	100
L56	100
S59	100
L60	100
P61	100
P62	100
G63	100
K70	100

- Chain 1:  76% 20%

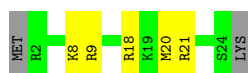
A vertical bar chart showing the distribution of 150 samples across 15 categories. The categories are MET, S2, R11, F12, K16, Q17, R21, P22, K34, I35, R36, R45, R46, T47, K48, L49, G50, and L51. The bars are colored in a repeating pattern of grey, green, yellow, and orange. Red diamonds are placed above the bars for K34 and G50.

- Chain m: 

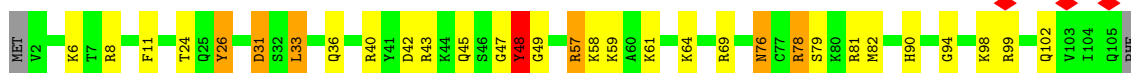
MET	GLN	ILE	PHE	VAL	LYS	THR	LEU	THR	GLY	LYS	THR	ILE	THR	LEU	GLU	VAL	GLU	GLU	PRO	SER	ASP	THR	ILE	GLU	ASN	VAL	LYS	LYS	ILE	GLN	ASP	LYS	GLY	ILE	PRO	PRO	ASP	GLN	GLN	ARG	LEU	ILE	PHE	LEU	GLU	LEU	ASP	GLY	LYS	GLN	THR	ARG	GLY	LEU	ASP	SER	THR	TYR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

[illegible]

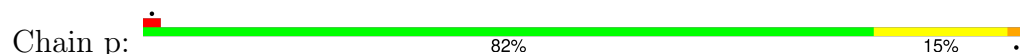
- Chain n:  72% 20% 8%



- Molecule 43: Ribosomal protein eL42



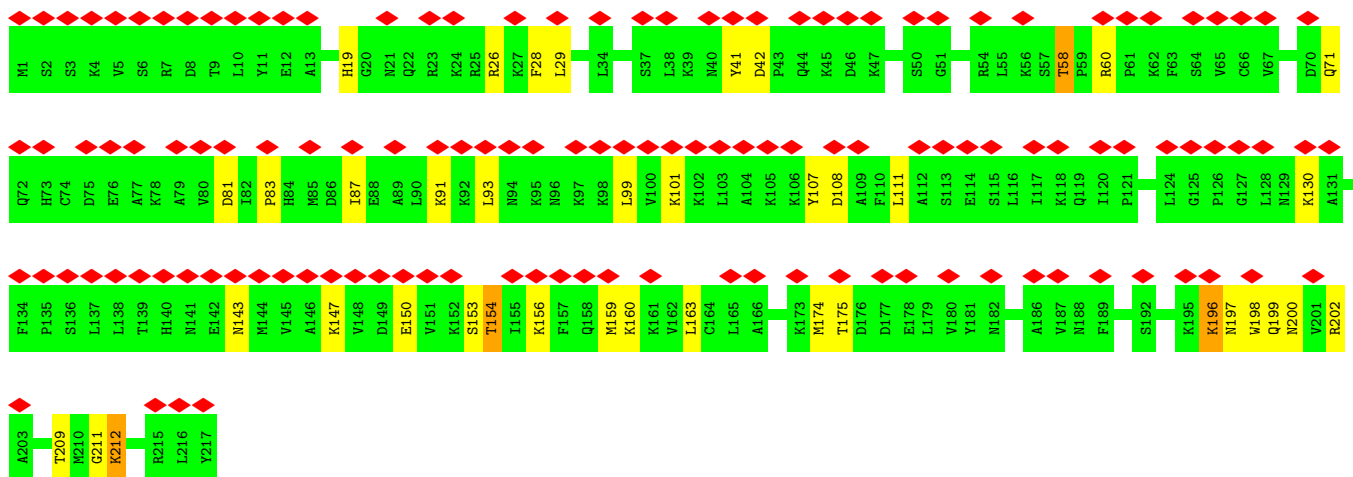
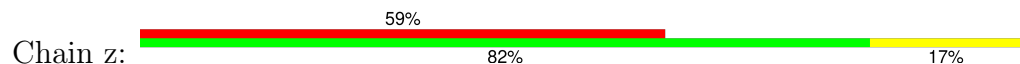
- Molecule 44: Ribosomal protein eL43




- Molecule 45: Ribosomal protein eL28

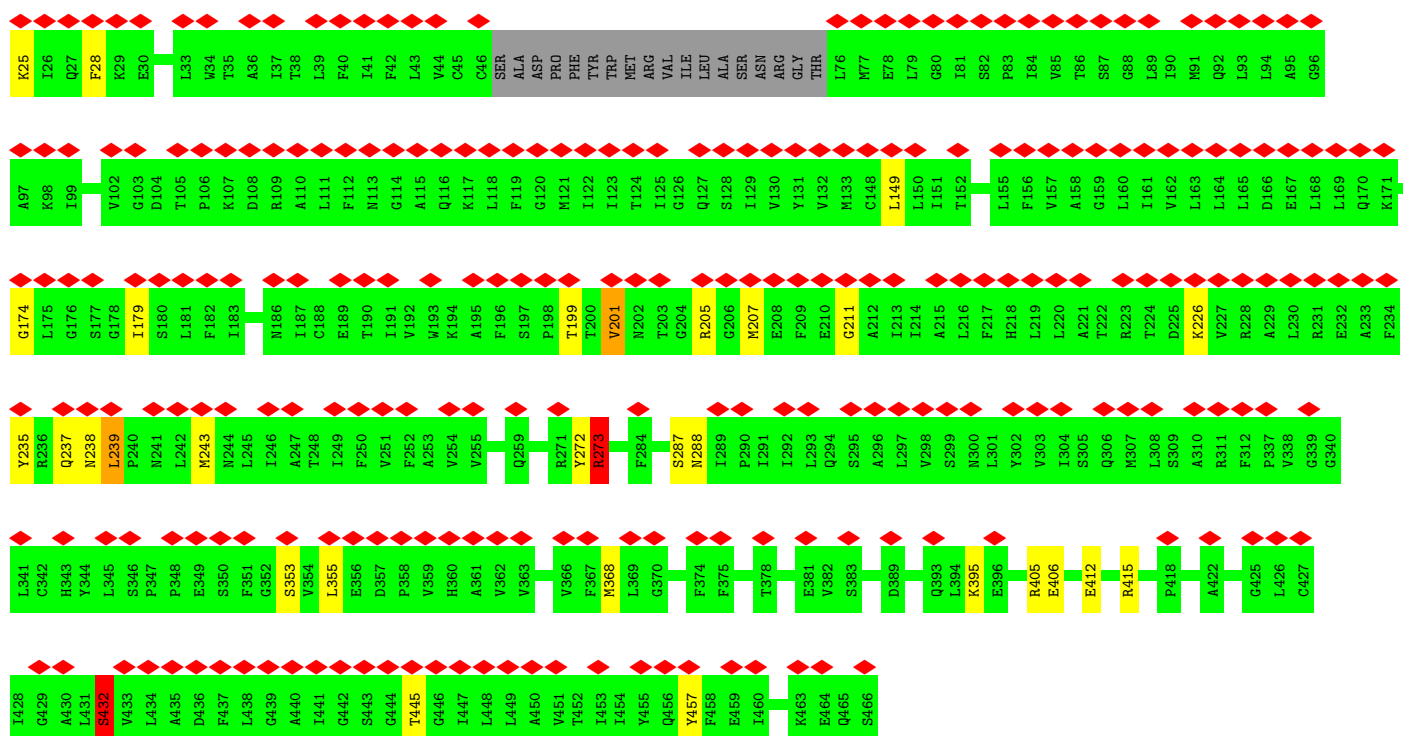


- Molecule 46: Ribosomal protein uL1




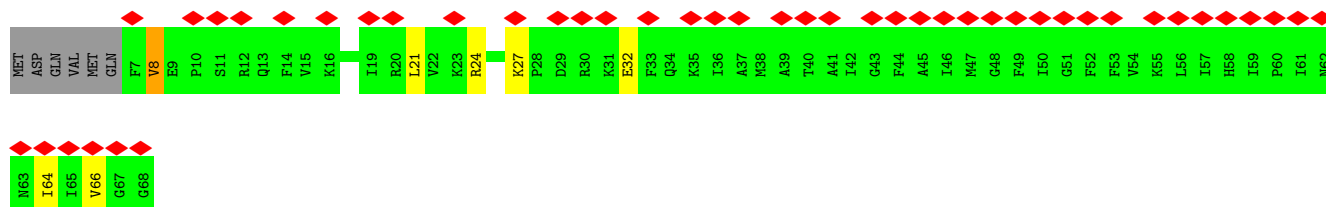
- Molecule 47: Sec61 alpha subunit

Chain 1: 



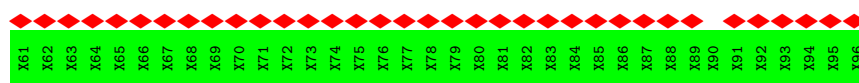
• Molecule 48: Sec61 gamma subunit

Chain 2: 



• Molecule 49: Sec61 beta subunit

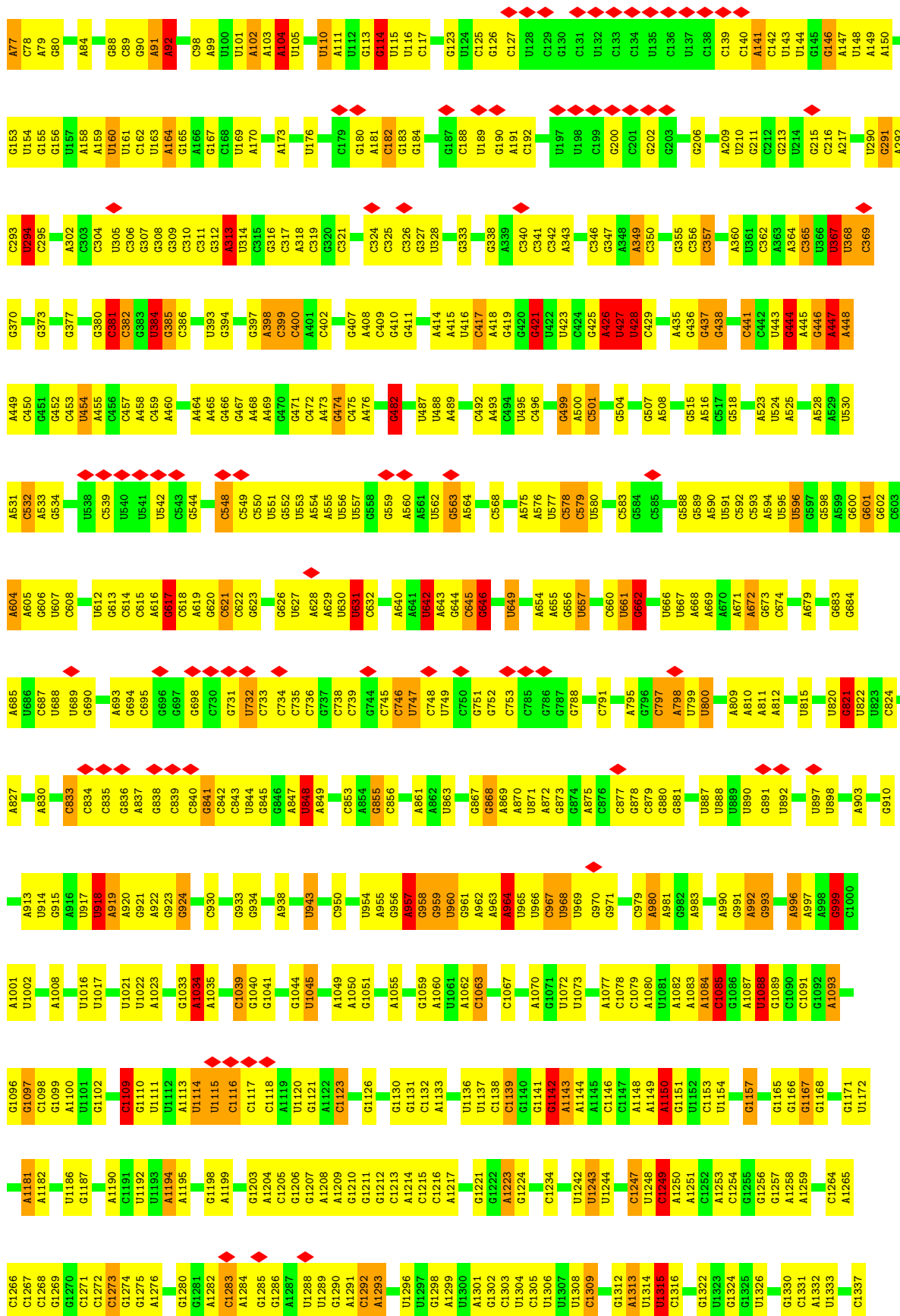
Chain 3: 

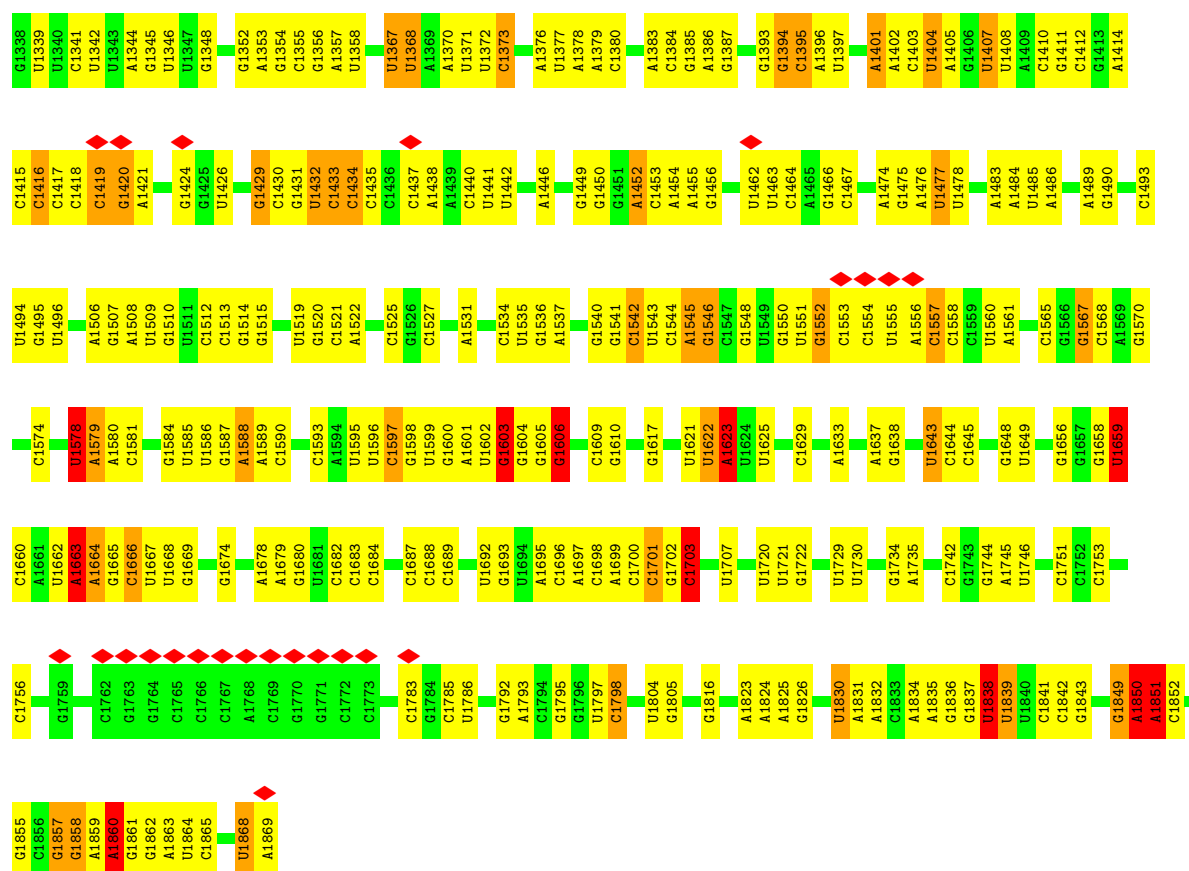


• Molecule 50: 18S ribosomal RNA

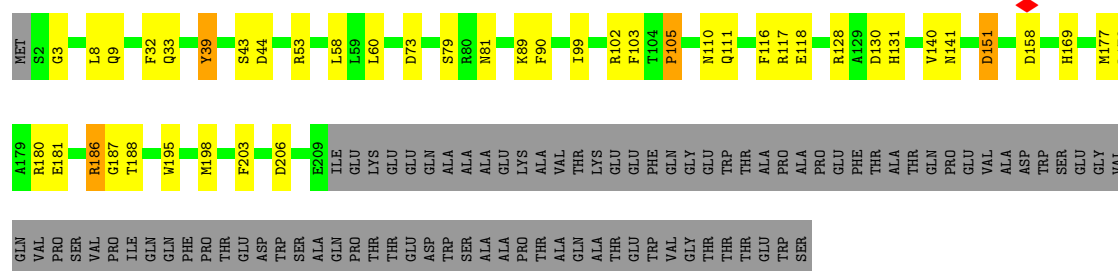
Chain S2: 



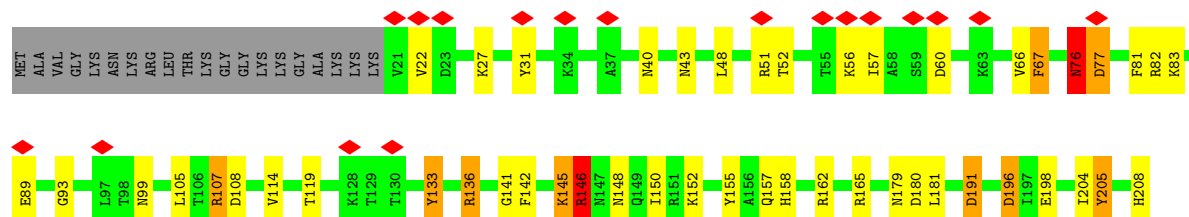


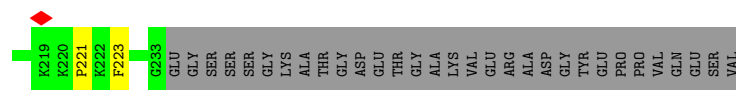


• Molecule 51: Ribosomal protein uS2

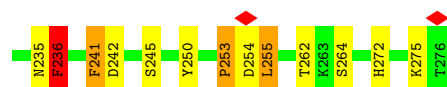
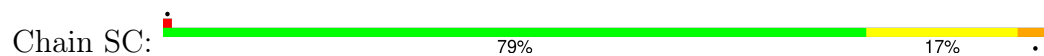


• Molecule 52: Ribosomal protein eS1

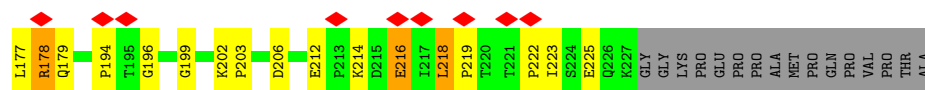
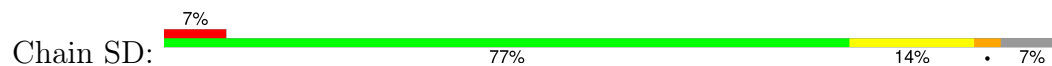




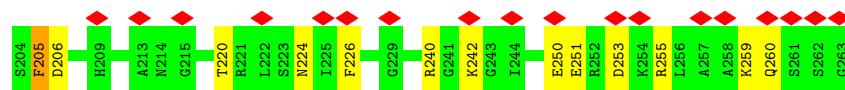
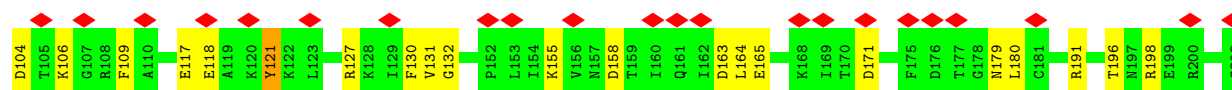
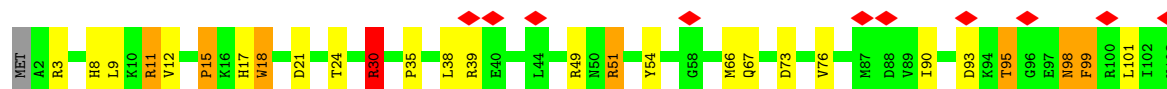
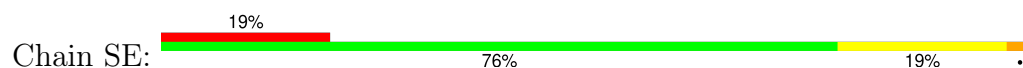
• Molecule 53: Ribosomal protein uS5



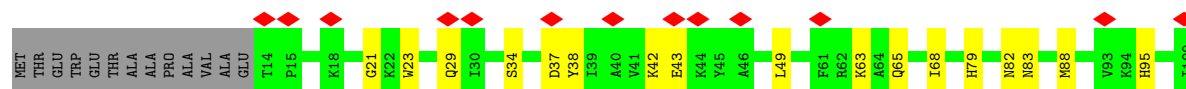
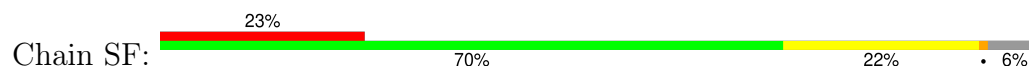
• Molecule 54: Ribosomal protein uS3

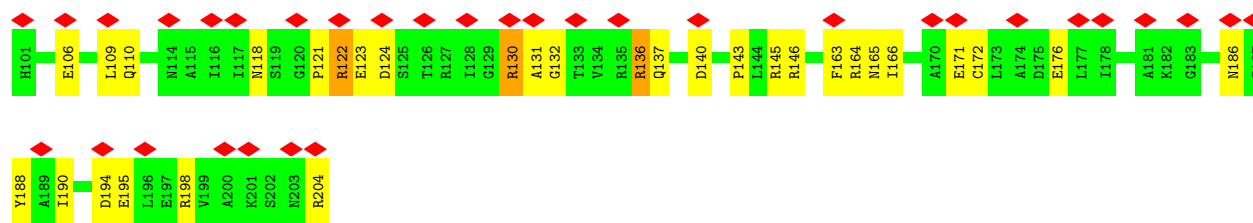


• Molecule 55: Ribosomal protein eS4

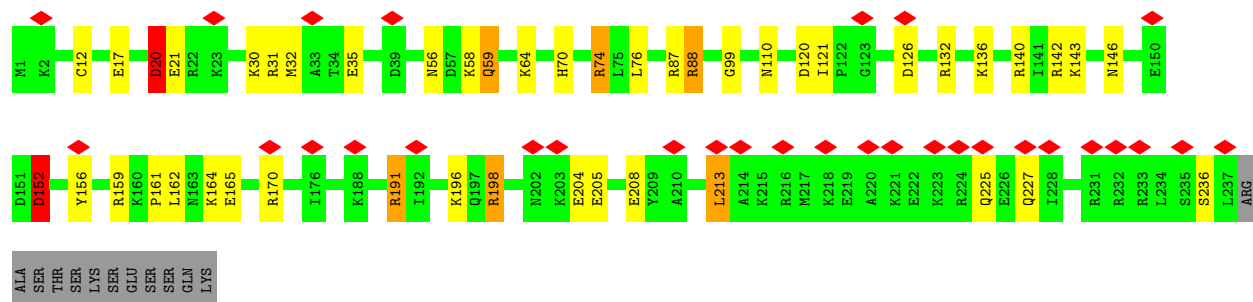
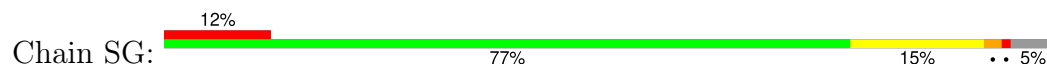


• Molecule 56: Ribosomal protein uS7

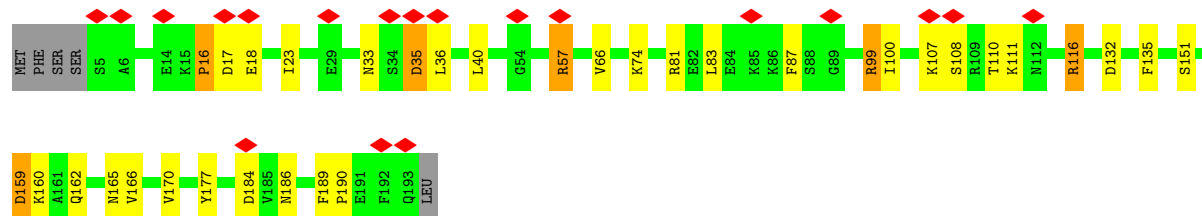
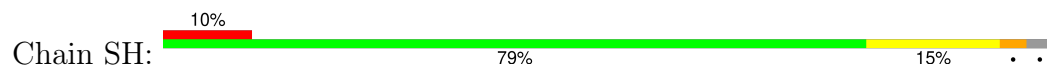




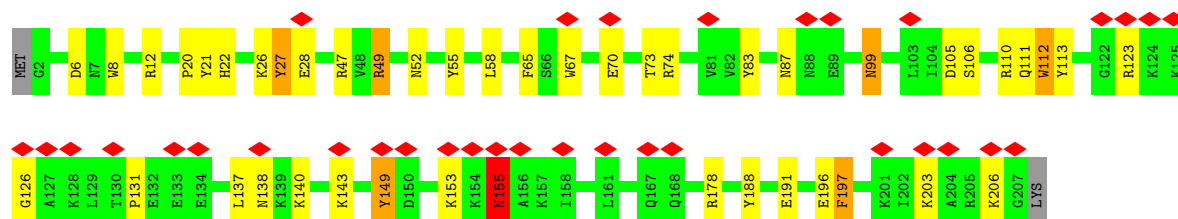
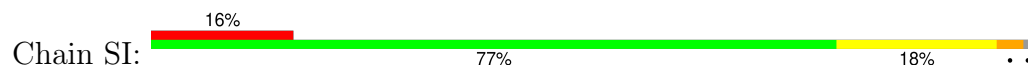
• Molecule 57: Ribosomal protein eS6



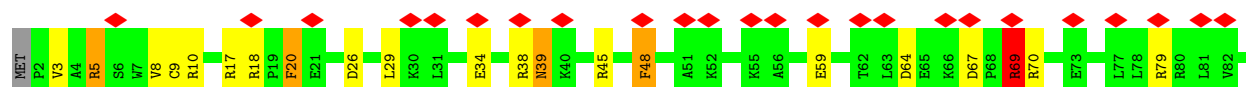
• Molecule 58: Ribosomal protein eS7

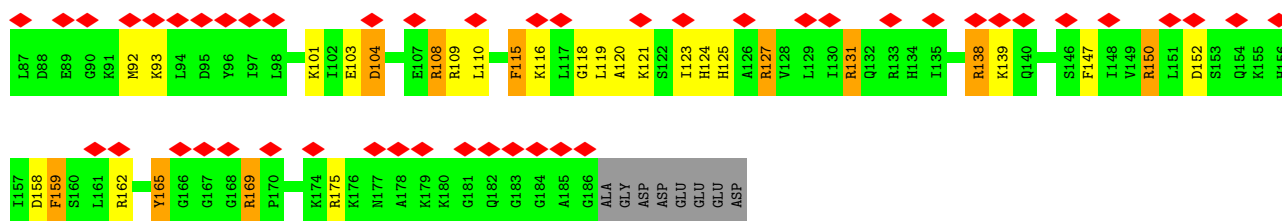


• Molecule 59: Ribosomal protein eS8

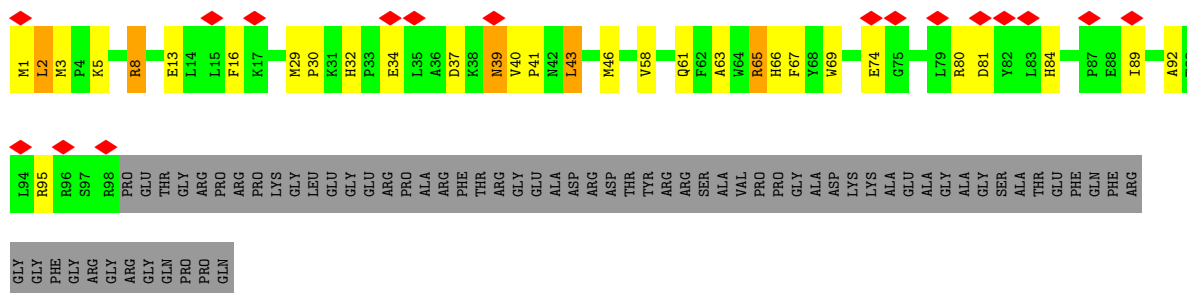


• Molecule 60: Ribosomal protein uS4

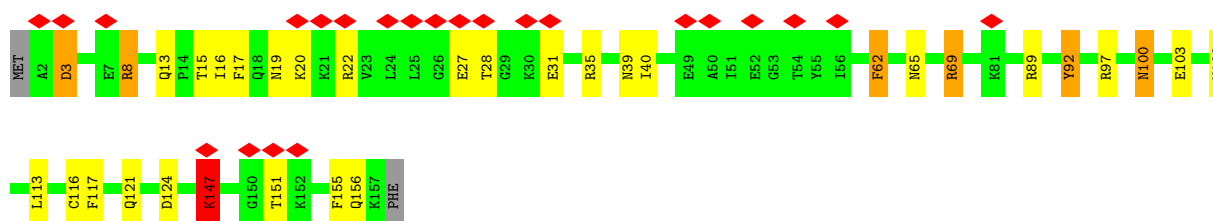
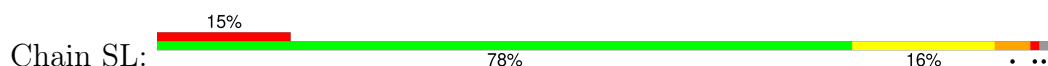




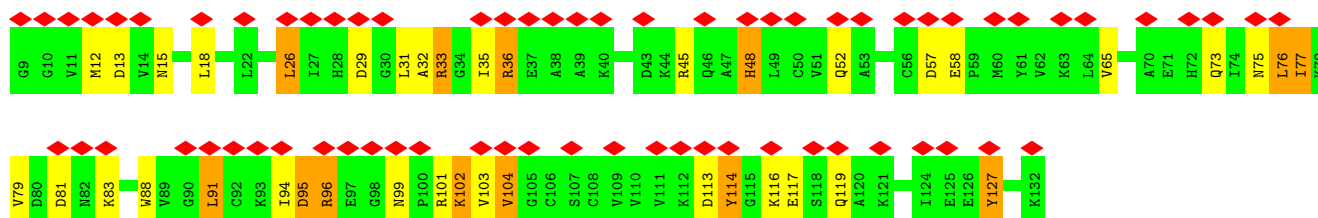
• Molecule 61: Ribosomal protein eS10



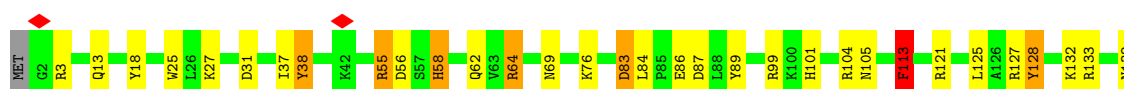
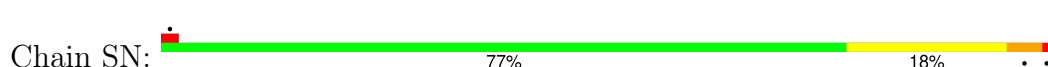
• Molecule 62: Ribosomal protein uS17

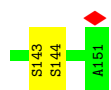


• Molecule 63: Ribosomal protein eS12

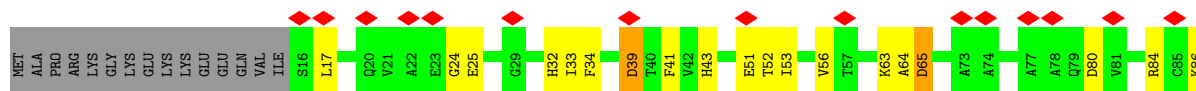


• Molecule 64: Ribosomal protein uS15

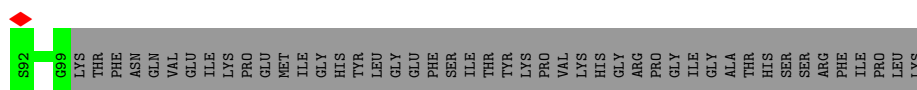
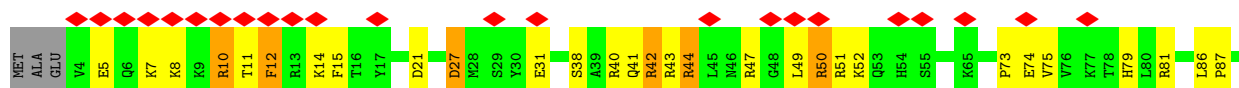




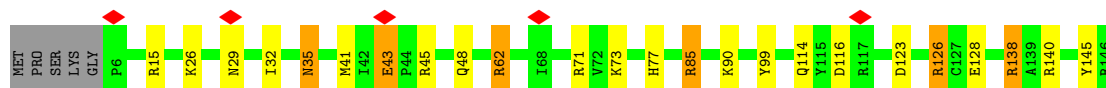
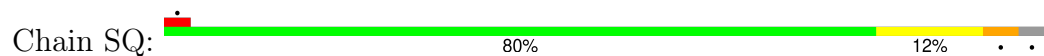
• Molecule 65: Ribosomal protein uS11



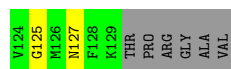
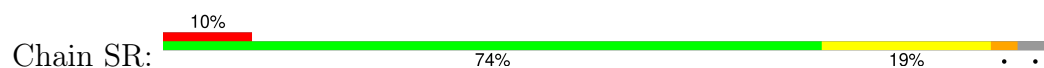
• Molecule 66: Ribosomal protein uS19



• Molecule 67: Ribosomal protein uS9

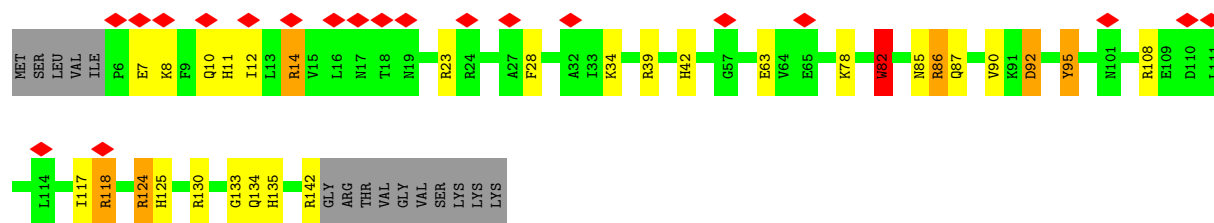


• Molecule 68: Ribosomal protein eS17

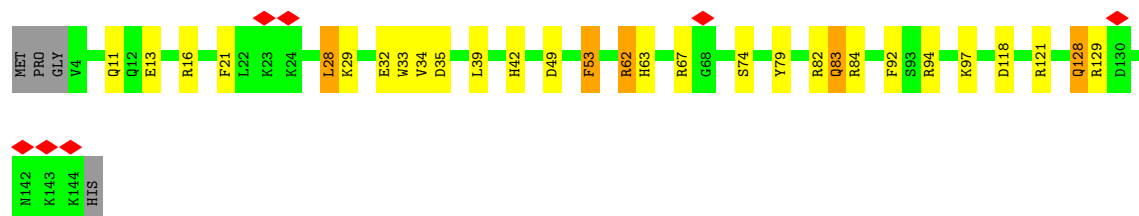
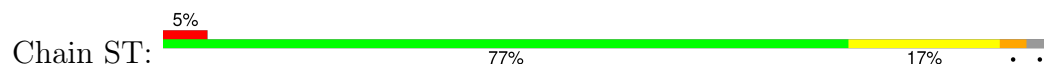


• Molecule 69: Ribosomal protein uS13

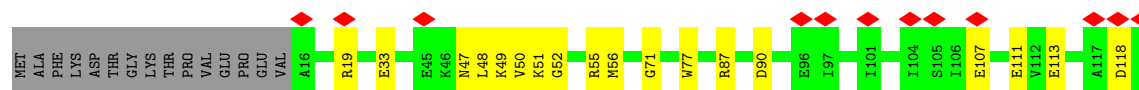
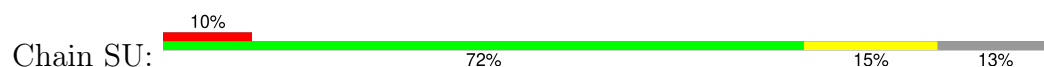




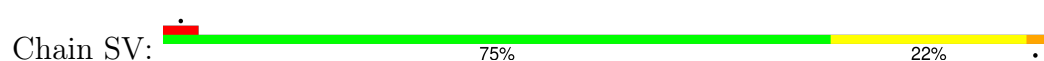
- Molecule 70: Ribosomal protein eS19



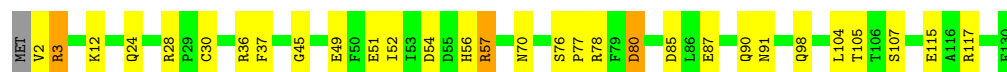
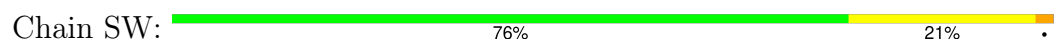
- Molecule 71: Ribosomal protein uS10



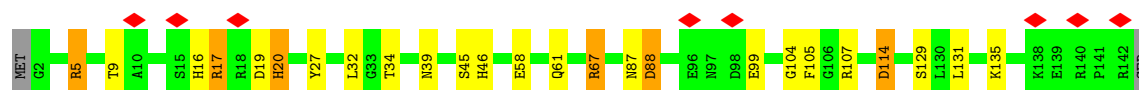
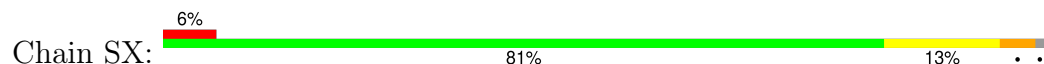
- Molecule 72: Ribosomal protein eS21



- Molecule 73: Ribosomal protein uS8

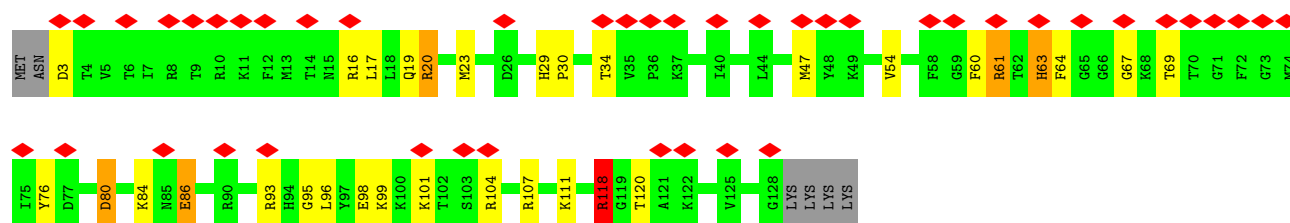


- Molecule 74: Ribosomal protein uS12



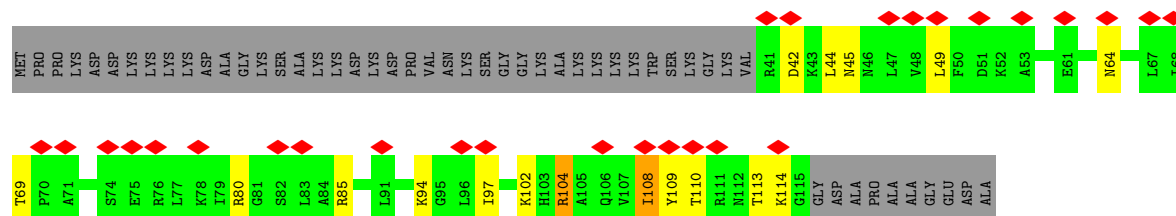
- Molecule 75: Ribosomal protein eS24

Chain SY: 



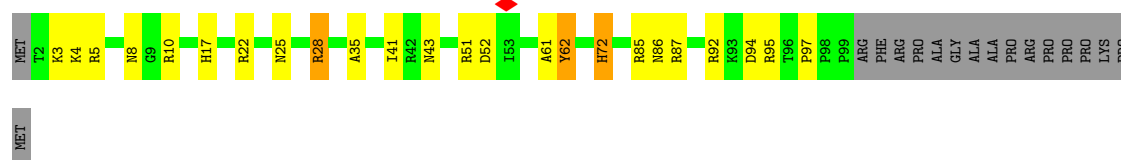
- Molecule 76: Ribosomal protein es25

Chain SZ: 




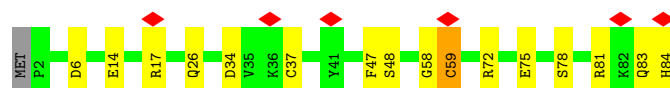
- Molecule 77: Ribosomal protein eS26

Chain Sa: 




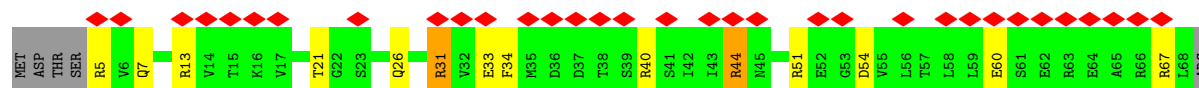
- Molecule 78: Ribosomal protein eS27

Chain Sb: 



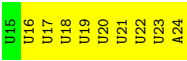
- Molecule 79: Ribosomal protein eS28

Chain Sc: 

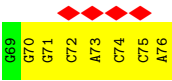
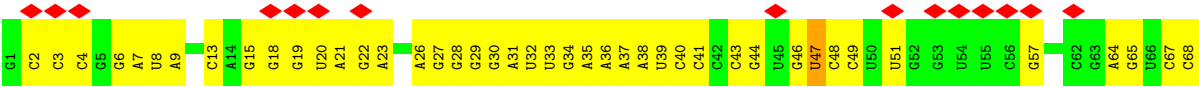


- Molecule 80: Ribosomal protein uS14

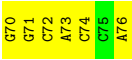
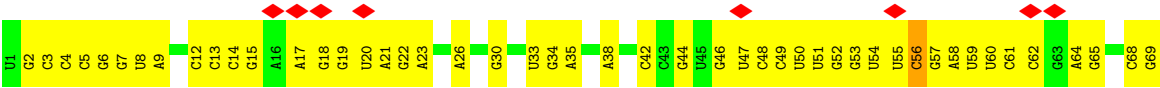
Chain Sd: 



● Molecule 85: A/P tRNA



● Molecule 86: P/E tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	14723	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	27	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.675	Depositor
Minimum map value	-0.394	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.065	Depositor
Map size (\AA)	562.8, 562.8, 562.8	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.3399999, 1.3399999, 1.3399999	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	5	0.70	83/89191 (0.1%)	1.13	754/139124 (0.5%)
2	7	0.54	1/2858 (0.0%)	0.96	9/4455 (0.2%)
3	8	0.68	3/3701 (0.1%)	1.20	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	26/4308 (0.6%)
6	C	0.73	4/2973 (0.1%)	1.12	18/3990 (0.5%)
7	D	0.73	2/2426 (0.1%)	1.23	27/3252 (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	13/2645 (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	13/2343 (0.6%)
13	J	0.63	1/1382 (0.1%)	1.04	10/1849 (0.5%)
14	L	0.71	2/1734 (0.1%)	1.12	16/2318 (0.7%)
15	M	0.76	2/1152 (0.2%)	1.11	5/1539 (0.3%)
16	N	0.84	4/1746 (0.2%)	1.33	23/2338 (1.0%)
17	O	0.72	3/1684 (0.2%)	1.11	12/2251 (0.5%)
18	P	0.74	2/1268 (0.2%)	1.10	9/1701 (0.5%)
19	Q	0.69	0/1530	1.35	31/2041 (1.5%)
20	R	0.79	3/1524 (0.2%)	1.27	20/2013 (1.0%)
21	S	0.95	8/1493 (0.5%)	1.30	20/2002 (1.0%)
22	T	0.67	1/1326 (0.1%)	1.04	7/1770 (0.4%)
23	U	0.63	1/822 (0.1%)	1.03	3/1103 (0.3%)
24	V	0.89	4/993 (0.4%)	1.11	7/1332 (0.5%)
25	W	0.72	0/541	1.23	5/720 (0.7%)
26	X	0.64	0/993	1.09	10/1334 (0.7%)
27	Y	0.72	0/1132	1.24	20/1504 (1.3%)
28	Z	0.63	0/1130	1.11	9/1507 (0.6%)
29	a	0.93	6/1192 (0.5%)	1.37	16/1591 (1.0%)
30	b	0.88	2/620 (0.3%)	1.17	5/819 (0.6%)
31	c	0.70	0/742	1.14	5/996 (0.5%)
32	d	0.84	3/903 (0.3%)	1.37	16/1216 (1.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	0.90	3/1071 (0.3%)	1.23	14/1429 (1.0%)
34	f	1.02	2/895 (0.2%)	1.34	17/1198 (1.4%)
35	g	0.65	0/916	1.08	5/1220 (0.4%)
36	h	0.63	0/1023	1.21	13/1350 (1.0%)
37	i	0.63	0/843	1.19	8/1115 (0.7%)
38	j	0.97	1/721 (0.1%)	1.43	11/953 (1.2%)
39	k	0.59	0/575	0.98	1/761 (0.1%)
40	l	0.68	0/454	1.07	3/599 (0.5%)
41	m	0.57	0/435	1.02	3/575 (0.5%)
42	n	0.49	0/223	1.02	0/284
43	o	0.64	0/864	1.27	9/1140 (0.8%)
44	p	0.64	1/718 (0.1%)	1.00	3/953 (0.3%)
45	r	0.68	0/1017	1.12	8/1365 (0.6%)
46	z	0.46	0/1768	0.73	0/2368
47	1	0.59	2/2969 (0.1%)	0.72	3/4014 (0.1%)
48	2	0.46	0/504	0.62	0/673
50	S2	0.68	37/41243 (0.1%)	1.12	315/64257 (0.5%)
51	SA	0.94	4/1679 (0.2%)	1.06	6/2283 (0.3%)
52	SB	1.42	7/1752 (0.4%)	1.63	20/2347 (0.9%)
53	SC	0.98	8/1726 (0.5%)	1.09	9/2332 (0.4%)
54	SD	1.39	12/1793 (0.7%)	1.08	9/2414 (0.4%)
55	SE	0.83	8/2118 (0.4%)	0.98	8/2849 (0.3%)
56	SF	0.74	1/1531 (0.1%)	1.08	11/2059 (0.5%)
57	SG	0.97	10/1946 (0.5%)	1.03	9/2590 (0.3%)
58	SH	0.73	2/1544 (0.1%)	1.02	8/2068 (0.4%)
59	SI	0.97	8/1715 (0.5%)	1.12	10/2287 (0.4%)
60	SJ	1.07	12/1550 (0.8%)	1.28	16/2069 (0.8%)
61	SK	0.75	1/851 (0.1%)	1.00	3/1147 (0.3%)
62	SL	0.85	5/1298 (0.4%)	1.08	7/1735 (0.4%)
63	SM	2.22	2/970 (0.2%)	1.21	8/1300 (0.6%)
64	SN	0.82	4/1232 (0.3%)	1.15	10/1656 (0.6%)
65	SO	1.18	7/1029 (0.7%)	1.38	11/1380 (0.8%)
66	SP	1.52	6/816 (0.7%)	1.29	8/1084 (0.7%)
67	SQ	0.72	2/1142 (0.2%)	1.01	8/1528 (0.5%)
68	SR	0.82	5/1060 (0.5%)	1.08	5/1421 (0.4%)
69	SS	0.66	1/1157 (0.1%)	1.18	13/1548 (0.8%)
70	ST	0.67	2/1119 (0.2%)	1.08	7/1499 (0.5%)
71	SU	0.94	4/828 (0.5%)	0.96	1/1112 (0.1%)
72	SV	0.73	0/631	0.97	0/844
73	SW	1.06	7/1051 (0.7%)	1.22	5/1406 (0.4%)
74	SX	0.95	6/1118 (0.5%)	1.10	11/1493 (0.7%)
75	SY	1.64	5/1040 (0.5%)	1.11	9/1382 (0.7%)
76	SZ	0.56	0/604	0.87	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
77	Sa	0.81	1/794 (0.1%)	1.20	4/1065 (0.4%)
78	Sb	0.59	0/665	0.90	0/891
79	Sc	0.68	0/508	1.13	4/680 (0.6%)
80	Sd	0.79	0/445	1.12	1/589 (0.2%)
81	Se	0.72	1/458 (0.2%)	1.17	5/602 (0.8%)
82	Sf	1.08	6/593 (1.0%)	1.57	12/786 (1.5%)
83	Sg	0.80	11/2493 (0.4%)	0.89	8/3394 (0.2%)
84	S4	0.23	0/219	0.63	0/337
85	S5	1.22	1/1762 (0.1%)	0.80	2/2739 (0.1%)
86	S6	0.31	1/1812 (0.1%)	1.00	5/2823 (0.2%)
All	All	0.77	357/238566 (0.1%)	1.13	1895/350392 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	5	1	157
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	5
13	J	0	2
14	L	0	5
15	M	0	4
16	N	0	10
17	O	0	3
18	P	0	1
19	Q	0	5
20	R	0	6
21	S	0	11
22	T	0	2
23	U	0	2
24	V	0	3

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
77	Sa	0	1
78	Sb	0	1
80	Sd	0	2
82	Sf	0	4
All	All	2	455

All (357) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	2037	C	O3'-P	-68.26	0.79	1.61
63	SM	58	GLU	CD-OE1	64.53	1.96	1.25
85	S5	47	U	O3'-P	-49.36	1.01	1.61
52	SB	145	LYS	C-N	-44.69	0.31	1.34
54	SD	216	GLU	CD-OE1	43.79	1.73	1.25
50	S2	1373	C	O3'-P	43.08	2.12	1.61
1	5	1823	G	O3'-P	41.45	2.10	1.61
75	SY	86	GLU	CD-OE2	39.68	1.69	1.25
1	5	4116	C	O3'-P	-34.82	1.19	1.61
1	5	1566	C	O3'-P	34.59	2.02	1.61
66	SP	21	ASP	CG-OD1	30.90	1.96	1.25
75	SY	86	GLU	CG-CD	22.59	1.85	1.51
57	SG	205	GLU	CD-OE1	21.13	1.48	1.25
47	1	272	TYR	C-N	20.43	1.81	1.34
65	SO	130	GLU	CD-OE1	17.44	1.44	1.25
73	SW	117	ARG	NE-CZ	16.49	1.54	1.33
10	G	109	GLU	CD-OE2	16.12	1.43	1.25
11	H	66	GLU	CD-OE1	15.82	1.43	1.25
60	SJ	59	GLU	CG-CD	15.75	1.75	1.51
34	f	6	TRP	CB-CG	-15.75	1.22	1.50
52	SB	221	PRO	C-N	14.76	1.68	1.34
55	SE	251	GLU	CD-OE1	14.43	1.41	1.25
51	SA	118	GLU	CG-CD	13.78	1.72	1.51
57	SG	205	GLU	CD-OE2	13.49	1.40	1.25
30	b	16	TRP	CB-CG	-13.48	1.25	1.50
60	SJ	34	GLU	CG-CD	13.18	1.71	1.51
65	SO	130	GLU	CD-OE2	12.85	1.39	1.25
66	SP	31	GLU	CD-OE2	12.79	1.39	1.25
51	SA	151	ASP	CB-CG	12.73	1.78	1.51
66	SP	31	GLU	CD-OE1	12.56	1.39	1.25
65	SO	104	ARG	CZ-NH1	12.22	1.49	1.33
51	SA	118	GLU	CD-OE2	12.18	1.39	1.25
71	SU	33	GLU	CD-OE1	12.14	1.39	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	R	95	TRP	CB-CG	-12.08	1.28	1.50
24	V	97	TYR	CB-CG	-11.79	1.33	1.51
58	SH	132	ASP	CG-OD2	11.76	1.52	1.25
59	SI	111	GLN	CD-NE2	11.66	1.62	1.32
59	SI	188	TYR	CE1-CZ	11.57	1.53	1.38
53	SC	90	GLU	CD-OE1	11.29	1.38	1.25
74	SX	58	GLU	CD-OE1	11.18	1.38	1.25
52	SB	198	GLU	CG-CD	11.05	1.68	1.51
55	SE	250	GLU	CD-OE2	10.91	1.37	1.25
75	SY	118	ARG	CZ-NH1	10.64	1.46	1.33
50	S2	1433	C	O3'-P	10.61	1.73	1.61
83	Sg	107	ASP	CB-CG	10.38	1.73	1.51
59	SI	188	TYR	CG-CD1	10.32	1.52	1.39
83	Sg	60	ARG	CZ-NH1	10.25	1.46	1.33
33	e	35	TRP	CB-CG	-10.23	1.31	1.50
74	SX	39	ASN	CG-ND2	10.20	1.58	1.32
65	SO	130	GLU	CG-CD	10.04	1.67	1.51
75	SY	80	ASP	CB-CG	9.97	1.72	1.51
59	SI	188	TYR	CG-CD2	9.83	1.51	1.39
10	G	54	PHE	CB-CG	-9.82	1.34	1.51
71	SU	90	ASP	CB-CG	9.80	1.72	1.51
54	SD	38	GLU	CD-OE2	9.75	1.36	1.25
74	SX	88	ASP	CG-OD2	9.58	1.47	1.25
50	S2	619	A	O3'-P	-9.47	1.49	1.61
59	SI	99	ASN	CG-OD1	9.46	1.44	1.24
54	SD	162	ASP	CG-OD1	9.44	1.47	1.25
53	SC	220	ASP	CG-OD2	9.40	1.47	1.25
71	SU	113	GLU	CD-OE2	9.38	1.35	1.25
62	SL	100	ASN	CB-CG	9.35	1.72	1.51
16	N	192	TRP	CB-CG	-9.35	1.33	1.50
53	SC	90	GLU	CG-CD	9.35	1.66	1.51
66	SP	21	ASP	CB-CG	9.25	1.71	1.51
68	SR	87	GLU	CD-OE1	9.12	1.35	1.25
53	SC	121	ARG	CZ-NH1	9.08	1.44	1.33
15	M	6	PHE	CB-CG	-9.00	1.36	1.51
56	SF	130	ARG	CZ-NH1	8.87	1.44	1.33
5	B	215	GLU	CD-OE1	8.85	1.35	1.25
50	S2	1291	A	O3'-P	8.82	1.71	1.61
60	SJ	64	ASP	CG-OD2	8.78	1.45	1.25
86	S6	56	C	O3'-P	-8.71	1.50	1.61
24	V	97	TYR	CA-CB	8.61	1.72	1.53
55	SE	250	GLU	CD-OE1	8.54	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	SD	216	GLU	CD-OE2	8.49	1.34	1.25
8	E	278	TYR	CA-CB	8.49	1.72	1.53
57	SG	208	GLU	CG-CD	8.48	1.64	1.51
59	SI	188	TYR	CE2-CZ	8.35	1.49	1.38
29	a	109	TYR	CA-CB	8.35	1.72	1.53
1	5	4547	C	O3'-P	8.32	1.71	1.61
50	S2	1292	C	O3'-P	8.28	1.71	1.61
62	SL	31	GLU	CD-OE1	8.25	1.34	1.25
60	SJ	158	ASP	CG-OD2	8.25	1.44	1.25
82	Sf	120	GLU	CG-CD	8.25	1.64	1.51
54	SD	38	GLU	CG-CD	8.13	1.64	1.51
21	S	81	TRP	CA-CB	8.07	1.71	1.53
21	S	10	TYR	CB-CG	-8.07	1.39	1.51
1	5	3652	A	O3'-P	8.03	1.70	1.61
1	5	45	U	O3'-P	-7.97	1.51	1.61
54	SD	135	GLU	CD-OE1	7.92	1.34	1.25
8	E	278	TYR	CB-CG	-7.90	1.39	1.51
20	R	132	PHE	CB-CG	-7.87	1.38	1.51
67	SQ	85	ARG	CZ-NH1	7.86	1.43	1.33
50	S2	1309	C	O3'-P	7.84	1.70	1.61
54	SD	23	GLU	CD-OE2	7.82	1.34	1.25
29	a	84	GLU	CD-OE1	7.76	1.34	1.25
57	SG	204	GLU	CD-OE1	7.76	1.34	1.25
60	SJ	38	ARG	CZ-NH1	7.76	1.43	1.33
54	SD	216	GLU	CG-CD	7.72	1.63	1.51
29	a	109	TYR	CB-CG	-7.64	1.40	1.51
54	SD	162	ASP	CG-OD2	7.55	1.42	1.25
60	SJ	104	ASP	CG-OD2	7.50	1.42	1.25
50	S2	1142	G	O3'-P	7.48	1.70	1.61
34	f	6	TRP	CA-CB	7.37	1.70	1.53
55	SE	104	ASP	CG-OD2	7.33	1.42	1.25
1	5	4566	U	O3'-P	-7.33	1.52	1.61
57	SG	35	GLU	CD-OE1	7.32	1.33	1.25
77	Sa	22	ARG	CZ-NH1	7.22	1.42	1.33
60	SJ	158	ASP	CG-OD1	7.14	1.41	1.25
47	1	273	ARG	C-N	7.14	1.46	1.33
1	5	2510	G	O3'-P	-7.13	1.52	1.61
68	SR	87	GLU	CD-OE2	7.10	1.33	1.25
57	SG	20	ASP	CG-OD2	7.07	1.41	1.25
51	SA	33	GLN	CD-NE2	7.07	1.50	1.32
1	5	2361	G	O3'-P	7.03	1.69	1.61
54	SD	135	GLU	CG-CD	7.03	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	SP	27	ASP	CG-OD2	7.03	1.41	1.25
6	C	267	TRP	CB-CG	-6.99	1.37	1.50
1	5	1851	G	O3'-P	-6.97	1.52	1.61
5	B	119	TYR	CB-CG	-6.97	1.41	1.51
1	5	1849	U	O3'-P	-6.91	1.52	1.61
21	S	81	TRP	CB-CG	-6.90	1.37	1.50
50	S2	1839	U	O3'-P	6.86	1.69	1.61
13	J	14	GLU	CD-OE1	6.85	1.33	1.25
1	5	1364	U	O3'-P	6.82	1.69	1.61
73	SW	87	GLU	CD-OE1	6.82	1.33	1.25
50	S2	1290	G	O3'-P	6.79	1.69	1.61
29	a	128	PHE	CB-CG	-6.78	1.39	1.51
1	5	4693	C	O3'-P	6.78	1.69	1.61
38	j	49	TRP	CB-CG	-6.77	1.38	1.50
22	T	13	TYR	CB-CG	-6.75	1.41	1.51
73	SW	51	GLU	CD-OE1	6.73	1.33	1.25
74	SX	88	ASP	CG-OD1	6.72	1.40	1.25
50	S2	1079	C	O3'-P	-6.71	1.53	1.61
1	5	514	U	O3'-P	6.70	1.69	1.61
60	SJ	103	GLU	CD-OE2	6.70	1.33	1.25
62	SL	13	GLN	CD-NE2	6.70	1.49	1.32
83	Sg	83	TRP	CB-CG	-6.69	1.38	1.50
55	SE	104	ASP	CG-OD1	6.69	1.40	1.25
1	5	2692	U	O3'-P	-6.68	1.53	1.61
32	d	25	TYR	CB-CG	-6.68	1.41	1.51
5	B	274	TYR	CA-CB	6.67	1.68	1.53
53	SC	220	ASP	CG-OD1	6.64	1.40	1.25
1	5	3692	A	O3'-P	6.62	1.69	1.61
1	5	2053	C	O3'-P	-6.62	1.53	1.61
71	SU	33	GLU	CG-CD	6.61	1.61	1.51
1	5	964	A	O3'-P	6.58	1.69	1.61
68	SR	37	GLU	CG-CD	6.57	1.61	1.51
12	I	171	TRP	CB-CG	-6.56	1.38	1.50
21	S	33	PHE	CB-CG	-6.55	1.40	1.51
1	5	1522	G	O3'-P	6.54	1.69	1.61
1	5	4375	C	O3'-P	-6.51	1.53	1.61
83	Sg	187	ASN	CG-OD1	6.51	1.38	1.24
2	7	90	A	O3'-P	-6.51	1.53	1.61
1	5	1912	G	O3'-P	-6.49	1.53	1.61
74	SX	39	ASN	CG-OD1	6.46	1.38	1.24
6	C	111	TRP	CB-CG	-6.44	1.38	1.50
82	Sf	146	LEU	CA-CB	6.44	1.68	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	2442	G	O3'-P	-6.43	1.53	1.61
50	S2	646	G	O3'-P	6.41	1.68	1.61
50	S2	1858	G	O3'-P	6.41	1.68	1.61
70	ST	32	GLU	CD-OE1	6.40	1.32	1.25
10	G	54	PHE	CA-CB	6.40	1.68	1.53
14	L	17	ASP	CG-OD2	6.37	1.40	1.25
62	SL	89	ARG	CZ-NH1	6.37	1.41	1.33
17	O	194	GLU	CD-OE1	6.36	1.32	1.25
70	ST	32	GLU	CD-OE2	6.35	1.32	1.25
1	5	1669	A	O3'-P	-6.35	1.53	1.61
7	D	213	GLU	CG-CD	6.30	1.61	1.51
8	E	101	ARG	CZ-NH2	6.30	1.41	1.33
58	SH	177	TYR	CB-CG	-6.26	1.42	1.51
83	Sg	36	ARG	CZ-NH1	6.25	1.41	1.33
1	5	207	G	O3'-P	-6.23	1.53	1.61
64	SN	13	GLN	CD-NE2	6.23	1.48	1.32
21	S	10	TYR	CA-CB	6.22	1.67	1.53
1	5	171	U	O3'-P	-6.21	1.53	1.61
17	O	106	ASP	CG-OD2	6.19	1.39	1.25
50	S2	9	U	O3'-P	6.14	1.68	1.61
11	H	61	TRP	CB-CG	-6.14	1.39	1.50
9	F	120	PHE	CB-CG	-6.12	1.41	1.51
1	5	2589	C	O3'-P	6.10	1.68	1.61
50	S2	1139	C	O3'-P	-6.10	1.53	1.61
1	5	1591	U	O3'-P	-6.10	1.53	1.61
1	5	3901	A	O3'-P	-6.09	1.53	1.61
83	Sg	4	GLN	CD-OE1	6.09	1.37	1.24
59	SI	99	ASN	CG-ND2	6.08	1.48	1.32
60	SJ	48	PHE	CB-CG	-6.08	1.41	1.51
1	5	1756	U	C4-O4	-6.06	1.18	1.23
7	D	44	TYR	CA-CB	6.05	1.67	1.53
1	5	4464	A	O3'-P	6.01	1.68	1.61
65	SO	104	ARG	NE-CZ	6.00	1.40	1.33
73	SW	115	GLU	CD-OE2	6.00	1.32	1.25
1	5	1636	U	O3'-P	-5.99	1.53	1.61
50	S2	1838	U	O3'-P	5.98	1.68	1.61
64	SN	128	TYR	CG-CD2	-5.97	1.31	1.39
55	SE	251	GLU	CD-OE2	5.96	1.32	1.25
50	S2	922	A	O3'-P	-5.96	1.53	1.61
61	SK	34	GLU	CD-OE1	5.96	1.32	1.25
23	U	99	TRP	CB-CG	-5.94	1.39	1.50
50	S2	1055	A	O3'-P	-5.92	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	SB	157	GLN	CG-CD	5.92	1.64	1.51
82	Sf	150	PHE	CB-CG	5.91	1.61	1.51
32	d	73	TRP	CB-CG	-5.91	1.39	1.50
1	5	2811	G	O3'-P	5.89	1.68	1.61
1	5	1395	U	O3'-P	-5.89	1.54	1.61
18	P	139	TYR	CB-CG	-5.88	1.42	1.51
30	b	16	TRP	CA-CB	5.88	1.66	1.53
54	SD	103	GLU	CD-OE1	5.88	1.32	1.25
21	S	152	PHE	CB-CG	-5.87	1.41	1.51
1	5	2520	C	O3'-P	-5.87	1.54	1.61
55	SE	121	TYR	CB-CG	-5.87	1.42	1.51
65	SO	147	ARG	CG-CD	5.86	1.66	1.51
1	5	1357	C	O3'-P	5.85	1.68	1.61
53	SC	236	PHE	CA-CB	5.85	1.66	1.53
54	SD	38	GLU	CD-OE1	5.84	1.32	1.25
82	Sf	120	GLU	CD-OE1	-5.84	1.19	1.25
83	Sg	145	GLU	CG-CD	5.83	1.60	1.51
5	B	119	TYR	CA-CB	5.83	1.66	1.53
60	SJ	48	PHE	CA-CB	5.81	1.66	1.53
5	B	274	TYR	CB-CG	-5.80	1.43	1.51
52	SB	89	GLU	CD-OE2	5.80	1.32	1.25
50	S2	1190	A	O3'-P	-5.80	1.54	1.61
1	5	3635	A	O3'-P	5.79	1.68	1.61
50	S2	798	A	O3'-P	5.78	1.68	1.61
53	SC	236	PHE	CB-CG	-5.76	1.41	1.51
18	P	139	TYR	CA-CB	5.76	1.66	1.53
50	S2	397	G	O3'-P	-5.75	1.54	1.61
65	SO	25	GLU	CG-CD	5.75	1.60	1.51
67	SQ	29	ASN	CG-ND2	5.74	1.47	1.32
44	p	18	TYR	CB-CG	-5.72	1.43	1.51
1	5	2394	G	O3'-P	-5.72	1.54	1.61
68	SR	82	ASP	CG-OD1	5.70	1.38	1.25
50	S2	1798	C	O3'-P	-5.70	1.54	1.61
1	5	2055	G	O3'-P	5.70	1.68	1.61
1	5	90	G	O3'-P	-5.69	1.54	1.61
1	5	2325	C	O3'-P	5.69	1.68	1.61
1	5	32	G	O3'-P	-5.68	1.54	1.61
1	5	1627	G	O3'-P	5.68	1.68	1.61
5	B	235	TRP	CG-CD1	-5.68	1.28	1.36
1	5	147	A	O3'-P	-5.67	1.54	1.61
24	V	97	TYR	CD2-CE2	-5.67	1.30	1.39
1	5	2649	G	O3'-P	-5.67	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	d	25	TYR	CA-CB	5.65	1.66	1.53
64	SN	83	ASP	CB-CG	5.64	1.63	1.51
1	5	4239	A	O3'-P	5.64	1.68	1.61
14	L	173	GLU	CD-OE2	5.64	1.31	1.25
52	SB	198	GLU	CD-OE2	5.62	1.31	1.25
50	S2	1851	A	O3'-P	-5.61	1.54	1.61
57	SG	142	ARG	CZ-NH1	5.60	1.40	1.33
50	S2	657	U	O3'-P	-5.60	1.54	1.61
1	5	2051	C	O3'-P	5.58	1.67	1.61
50	S2	92	A	O3'-P	5.58	1.67	1.61
16	N	119	TYR	CB-CG	-5.57	1.43	1.51
73	SW	115	GLU	CD-OE1	5.57	1.31	1.25
1	5	2535	G	O3'-P	-5.56	1.54	1.61
73	SW	80	ASP	CB-CG	5.54	1.63	1.51
1	5	332	C	O3'-P	-5.53	1.54	1.61
10	G	109	GLU	CG-CD	5.53	1.60	1.51
74	SX	58	GLU	CD-OE2	5.53	1.31	1.25
1	5	53	C	O3'-P	5.52	1.67	1.61
1	5	5001	U	O3'-P	-5.52	1.54	1.61
53	SC	241	PHE	CB-CG	-5.51	1.42	1.51
1	5	4326	G	O3'-P	-5.49	1.54	1.61
50	S2	640	A	O3'-P	-5.49	1.54	1.61
50	S2	1687	C	O3'-P	5.49	1.67	1.61
29	a	79	TRP	CB-CG	-5.47	1.40	1.50
57	SG	204	GLU	CG-CD	5.46	1.60	1.51
66	SP	27	ASP	CG-OD1	5.45	1.37	1.25
1	5	1282	G	O3'-P	-5.44	1.54	1.61
1	5	3875	G	O3'-P	5.44	1.67	1.61
64	SN	83	ASP	CG-OD1	5.43	1.37	1.25
82	Sf	151	ASN	CA-C	5.42	1.67	1.52
3	8	64	U	O3'-P	5.42	1.67	1.61
21	S	29	ARG	CG-CD	5.41	1.65	1.51
1	5	1381	U	O3'-P	-5.41	1.54	1.61
1	5	4276	G	O3'-P	5.40	1.67	1.61
50	S2	848	U	N3-C4	5.39	1.43	1.38
15	M	6	PHE	CA-CB	5.39	1.65	1.53
57	SG	17	GLU	CD-OE2	5.39	1.31	1.25
50	S2	1843	G	O3'-P	-5.39	1.54	1.61
62	SL	3	ASP	CB-CG	5.38	1.63	1.51
68	SR	104	GLU	CD-OE2	5.38	1.31	1.25
52	SB	205	TYR	CE2-CZ	5.37	1.45	1.38
81	Se	23	GLU	CG-CD	5.37	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	O	106	ASP	CG-OD1	5.36	1.37	1.25
1	5	89	C	O3'-P	-5.36	1.54	1.61
33	e	74	PHE	CB-CG	-5.35	1.42	1.51
1	5	4977	A	O3'-P	-5.31	1.54	1.61
50	S2	357	C	O3'-P	5.29	1.67	1.61
1	5	372	A	O3'-P	-5.28	1.54	1.61
1	5	4548	A	O5'-C5'	5.28	1.52	1.44
1	5	2043	A	O3'-P	-5.27	1.54	1.61
24	V	98	PHE	CB-CG	-5.26	1.42	1.51
4	A	40	TYR	CA-CB	5.26	1.65	1.53
4	A	211	PHE	CA-CB	5.26	1.65	1.53
60	SJ	104	ASP	CG-OD1	5.26	1.37	1.25
83	Sg	3	GLU	CD-OE2	5.25	1.31	1.25
1	5	2297	G	O3'-P	-5.24	1.54	1.61
8	E	250	ASP	CG-OD2	5.24	1.37	1.25
1	5	4237	C	O3'-P	-5.24	1.54	1.61
59	SI	27	TYR	CB-CG	-5.24	1.43	1.51
1	5	2037	C	C2-O2	-5.24	1.19	1.24
11	H	66	GLU	CD-OE2	5.23	1.31	1.25
1	5	4275	G	O3'-P	5.22	1.67	1.61
1	5	937	U	O3'-P	-5.21	1.54	1.61
83	Sg	285	GLN	CD-NE2	5.21	1.45	1.32
1	5	2368	A	O3'-P	-5.21	1.54	1.61
20	R	132	PHE	CA-CB	5.21	1.65	1.53
69	SS	130	ARG	CZ-NH1	5.20	1.39	1.33
1	5	1917	A	O3'-P	-5.20	1.54	1.61
5	B	137	TRP	CB-CG	-5.20	1.40	1.50
8	E	97	ASN	CG-ND2	5.20	1.45	1.32
1	5	1457	G	O3'-P	-5.19	1.54	1.61
50	S2	1293	A	O3'-P	5.18	1.67	1.61
1	5	943	A	O3'-P	-5.17	1.54	1.61
3	8	80	A	O3'-P	5.17	1.67	1.61
83	Sg	116	ASP	CG-OD1	5.16	1.37	1.25
5	B	257	TRP	CE3-CZ3	-5.15	1.29	1.38
75	SY	80	ASP	CG-OD2	5.15	1.37	1.25
1	5	1283	G	O3'-P	-5.15	1.54	1.61
1	5	381	U	O3'-P	-5.14	1.54	1.61
50	S2	999	G	O3'-P	5.14	1.67	1.61
4	A	209	HIS	CA-CB	5.13	1.65	1.53
16	N	130	PHE	CB-CG	-5.13	1.42	1.51
1	5	1682	A	C6-N6	-5.13	1.29	1.33
1	5	2406	G	O3'-P	5.12	1.67	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	N	120	TRP	CE3-CZ3	-5.12	1.29	1.38
55	SE	251	GLU	CG-CD	5.12	1.59	1.51
9	F	228	HIS	CA-CB	5.11	1.65	1.53
1	5	4489	G	O3'-P	5.09	1.67	1.61
1	5	97	G	O3'-P	5.09	1.67	1.61
1	5	4206	C	O3'-P	-5.09	1.55	1.61
50	S2	672	A	O3'-P	-5.08	1.55	1.61
63	SM	58	GLU	CD-OE2	5.08	1.31	1.25
83	Sg	60	ARG	NE-CZ	5.08	1.39	1.33
1	5	2054	U	O3'-P	-5.07	1.55	1.61
1	5	1883	G	O3'-P	-5.07	1.55	1.61
1	5	4334	U	O3'-P	-5.07	1.55	1.61
50	S2	1039	C	O3'-P	5.06	1.67	1.61
1	5	2324	C	O3'-P	5.06	1.67	1.61
21	S	152	PHE	CG-CD2	-5.06	1.31	1.38
50	S2	1168	G	O3'-P	-5.05	1.55	1.61
6	C	102	PHE	CG-CD2	-5.04	1.31	1.38
50	S2	957	A	O3'-P	-5.04	1.55	1.61
50	S2	1552	G	O3'-P	5.04	1.67	1.61
1	5	4751	G	O3'-P	-5.04	1.55	1.61
82	Sf	149	CYS	N-CA	5.04	1.56	1.46
60	SJ	108	ARG	CZ-NH1	5.04	1.39	1.33
50	S2	427	U	O5'-C5'	5.03	1.52	1.44
6	C	35	ASP	CG-OD1	5.03	1.36	1.25
29	a	79	TRP	CA-CB	5.03	1.65	1.53
1	5	2667	C	O3'-P	-5.02	1.55	1.61
57	SG	152	ASP	CG-OD2	5.02	1.36	1.25
33	e	35	TRP	CG-CD1	-5.02	1.29	1.36
3	8	73	U	O3'-P	5.01	1.67	1.61
73	SW	49	GLU	CD-OE1	5.00	1.31	1.25

All (1895) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	SB	145	LYS	CA-C-N	-33.88	42.66	117.20
1	5	4116	C	P-O3'-C3'	33.09	159.40	119.70
52	SB	145	LYS	O-C-N	-27.76	78.29	122.70
1	5	4116	C	O3'-P-O5'	-27.74	51.30	104.00
86	S6	55	U	OP2-P-O3'	27.36	165.39	105.20
86	S6	55	U	OP1-P-O3'	-23.88	52.66	105.20
47	1	432	SER	O-C-N	-20.67	89.63	122.70
73	SW	117	ARG	NE-CZ-NH2	-20.64	109.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	SB	221	PRO	O-C-N	20.46	155.44	122.70
66	SP	21	ASP	CB-CG-OD1	-19.20	101.02	118.30
52	SB	145	LYS	C-N-CA	-18.08	76.50	121.70
1	5	1566	C	O3'-P-O5'	-16.79	72.11	104.00
82	Sf	146	LEU	CA-CB-CG	16.61	153.51	115.30
3	8	60	G	N9-C1'-C2'	16.16	135.01	114.00
65	SO	146	ARG	NE-CZ-NH1	15.18	127.89	120.30
1	5	3942	A	O3'-P-O5'	14.89	132.29	104.00
77	Sa	28	ARG	NE-CZ-NH1	14.80	127.70	120.30
52	SB	221	PRO	C-N-CA	-14.72	84.91	121.70
50	S2	1109	C	O4'-C1'-N1	14.29	119.64	108.20
52	SB	221	PRO	CA-C-N	-14.18	86.00	117.20
38	j	11	ARG	NE-CZ-NH2	-13.88	113.36	120.30
65	SO	104	ARG	NE-CZ-NH2	-13.35	113.63	120.30
85	S5	48	C	O5'-P-OP1	13.26	126.61	110.70
50	S2	1434	C	O5'-P-OP1	-12.96	94.04	105.70
1	5	3942	A	OP2-P-O3'	-12.86	76.90	105.20
19	Q	37	ARG	NE-CZ-NH2	12.80	126.70	120.30
1	5	92	C	N1-C1'-C2'	-12.63	97.58	114.00
50	S2	1433	C	O5'-P-OP2	-12.40	94.54	105.70
50	S2	1838	U	O4'-C1'-N1	-12.40	98.28	108.20
50	S2	1109	C	N1-C1'-C2'	12.33	130.03	114.00
12	I	139	ARG	CG-CD-NE	12.29	137.61	111.80
65	SO	146	ARG	NE-CZ-NH2	-12.27	114.17	120.30
50	S2	1838	U	N1-C1'-C2'	12.01	129.62	114.00
50	S2	1373	C	O3'-P-O5'	-11.99	81.22	104.00
1	5	1214	C	N1-C1'-C2'	11.92	129.50	114.00
1	5	1	C	N1-C1'-C2'	11.83	129.38	114.00
4	A	3	ARG	NE-CZ-NH1	11.77	126.18	120.30
1	5	4501	U	O3'-P-O5'	-11.70	81.78	104.00
66	SP	21	ASP	CB-CG-OD2	11.38	128.54	118.30
32	d	44	ARG	NE-CZ-NH1	11.30	125.95	120.30
7	D	265	ARG	NE-CZ-NH1	11.27	125.94	120.30
59	SI	49	ARG	NE-CZ-NH1	11.22	125.91	120.30
75	SY	80	ASP	CB-CG-OD2	-11.20	108.22	118.30
1	5	4693	C	O4'-C1'-N1	-11.15	99.28	108.20
20	R	132	PHE	CB-CA-C	11.12	132.65	110.40
62	SL	89	ARG	NE-CZ-NH2	-11.12	114.74	120.30
1	5	4275	G	N9-C1'-C2'	-11.09	99.59	114.00
36	h	93	ARG	NE-CZ-NH1	11.06	125.83	120.30
1	5	4373	G	N9-C1'-C2'	11.06	128.37	114.00
29	a	61	TYR	CA-CB-CG	10.98	134.27	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2361	G	N9-C1'-C2'	-10.94	99.77	114.00
50	S2	1293	A	N9-C1'-C2'	10.93	128.21	114.00
1	5	4871	C	N1-C1'-C2'	10.91	128.19	114.00
1	5	1938	C	N1-C1'-C2'	10.87	128.14	114.00
20	R	108	ARG	NE-CZ-NH1	10.86	125.73	120.30
1	5	151	G	N9-C1'-C2'	-10.78	99.98	114.00
29	a	132	ARG	NE-CZ-NH1	10.76	125.68	120.30
15	M	6	PHE	CB-CG-CD2	-10.73	113.29	120.80
16	N	192	TRP	CA-CB-CG	10.64	133.91	113.70
27	Y	87	ARG	NE-CZ-NH2	10.60	125.60	120.30
16	N	131	GLU	CA-CB-CG	10.55	136.61	113.40
54	SD	216	GLU	CG-CD-OE1	-10.55	97.20	118.30
50	S2	642	U	C4'-C3'-O3'	10.54	134.08	113.00
37	i	85	ARG	NE-CZ-NH1	10.54	125.57	120.30
56	SF	130	ARG	NE-CZ-NH2	-10.53	115.03	120.30
50	S2	848	U	N1-C1'-C2'	10.53	127.69	114.00
1	5	4528	G	C2'-C3'-O3'	10.52	132.64	109.50
77	Sa	28	ARG	NE-CZ-NH2	-10.51	115.05	120.30
1	5	2513	A	N9-C1'-C2'	10.49	127.64	114.00
50	S2	642	U	N1-C1'-C2'	-10.45	100.42	114.00
1	5	4163	U	C4'-C3'-O3'	10.44	133.88	113.00
50	S2	1114	U	N1-C1'-C2'	10.41	127.53	114.00
3	8	34	U	C4'-C3'-O3'	-10.37	87.63	109.40
1	5	1211	G	C2'-C3'-O3'	10.35	132.27	109.50
75	SY	118	ARG	NE-CZ-NH2	-10.35	115.13	120.30
50	S2	24	C	C2'-C3'-O3'	10.26	132.08	109.50
60	SJ	38	ARG	NE-CZ-NH2	-10.26	115.17	120.30
67	SQ	85	ARG	NE-CZ-NH2	-10.23	115.19	120.30
29	a	109	TYR	CA-CB-CG	-10.22	93.97	113.40
63	SM	58	GLU	OE1-CD-OE2	10.22	135.57	123.30
1	5	62	A	N9-C1'-C2'	10.21	127.27	114.00
1	5	1329	G	C2'-C3'-O3'	10.18	131.91	109.50
75	SY	86	GLU	CG-CD-OE2	-10.13	98.05	118.30
43	o	78	ARG	NE-CZ-NH2	10.12	125.36	120.30
1	5	2586	G	N9-C1'-C2'	10.11	127.14	114.00
1	5	1890	G	N9-C1'-C2'	-10.09	100.89	114.00
1	5	4518	A	O5'-P-OP2	-10.07	96.63	105.70
1	5	2436	U	N1-C1'-C2'	10.07	127.09	114.00
50	S2	645	C	N1-C1'-C2'	-10.06	100.92	114.00
10	G	54	PHE	CB-CG-CD1	-10.06	113.76	120.80
1	5	664	G	O4'-C1'-N9	10.04	116.23	108.20
68	SR	28	PHE	O-C-N	-10.04	106.63	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1358	G	C4'-C3'-O3'	10.03	133.07	113.00
50	S2	92	A	N9-C1'-C2'	10.03	127.04	114.00
1	5	2389	A	C2'-C3'-O3'	9.99	131.47	109.50
32	d	25	TYR	CA-CB-CG	-9.99	94.42	113.40
1	5	1887	G	N9-C1'-C2'	-9.98	101.02	112.00
51	SA	117	ARG	CG-CD-NE	9.97	132.74	111.80
8	E	278	TYR	CA-CB-CG	-9.95	94.49	113.40
11	H	54	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	5	1974	U	N1-C1'-C2'	9.94	126.92	114.00
1	5	1992	U	N1-C1'-C2'	9.88	126.84	114.00
1	5	1379	C	O4'-C1'-N1	9.87	116.09	108.20
77	Sa	22	ARG	NE-CZ-NH2	-9.82	115.39	120.30
50	S2	428	U	N1-C1'-C2'	9.81	126.76	114.00
20	R	132	PHE	CB-CG-CD1	-9.81	113.93	120.80
1	5	2666	U	N1-C1'-C2'	-9.78	101.24	112.00
3	8	14	U	N1-C1'-C2'	9.75	126.67	114.00
1	5	4693	C	N1-C1'-C2'	9.74	126.67	114.00
25	W	44	ARG	NE-CZ-NH1	9.74	125.17	120.30
60	SJ	131	ARG	NE-CZ-NH2	-9.73	115.43	120.30
8	E	278	TYR	CB-CA-C	9.70	129.80	110.40
53	SC	121	ARG	NE-CZ-NH2	-9.70	115.45	120.30
1	5	2394	G	N9-C1'-C2'	-9.70	101.33	112.00
1	5	4750	G	N9-C1'-C2'	-9.69	101.34	112.00
34	f	36	ARG	NE-CZ-NH1	9.69	125.14	120.30
29	a	128	PHE	CB-CG-CD1	-9.68	114.02	120.80
50	S2	1063	C	N1-C1'-C2'	-9.68	101.36	112.00
1	5	1398	A	N9-C1'-C2'	9.67	126.57	114.00
50	S2	367	U	N1-C1'-C2'	-9.67	101.36	112.00
1	5	4464	A	O4'-C1'-N9	-9.66	100.47	108.20
50	S2	291	G	C4'-C3'-O3'	-9.66	89.11	109.40
1	5	2046	G	O4'-C1'-N9	9.65	115.92	108.20
69	SS	124	ARG	NE-CZ-NH1	9.65	125.13	120.30
28	Z	36	ARG	NE-CZ-NH1	9.65	125.12	120.30
81	Se	13	ARG	NE-CZ-NH1	9.65	125.12	120.30
29	a	61	TYR	CB-CG-CD2	-9.62	115.23	121.00
50	S2	28	U	O5'-P-OP1	-9.61	97.05	105.70
1	5	4162	C	N1-C1'-C2'	9.58	126.45	114.00
1	5	4677	U	N1-C1'-C2'	-9.57	101.48	112.00
1	5	514	U	N1-C1'-C2'	-9.55	101.49	112.00
65	SO	104	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	5	1501	C	O4'-C1'-N1	9.53	115.83	108.20
14	L	34	ARG	NE-CZ-NH1	9.53	125.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	5040	U	N1-C1'-C2'	9.53	126.39	114.00
58	SH	177	TYR	CB-CG-CD2	-9.50	115.30	121.00
50	S2	747	U	C2'-C3'-O3'	9.50	130.40	109.50
1	5	172	C	O4'-C1'-N1	9.49	115.79	108.20
1	5	1501	C	N1-C1'-C2'	9.47	126.31	114.00
86	S6	55	U	O3'-P-O5'	-9.44	86.06	104.00
11	H	31	ARG	NE-CZ-NH1	9.44	125.02	120.30
38	j	66	HIS	N-CA-CB	9.44	127.59	110.60
1	5	315	G	O4'-C1'-N9	9.43	115.74	108.20
17	O	178	ARG	NE-CZ-NH1	9.42	125.01	120.30
20	R	95	TRP	N-CA-CB	9.41	127.54	110.60
1	5	294	G	O4'-C1'-N9	9.40	115.72	108.20
1	5	2438	A	N9-C1'-C2'	-9.40	101.66	112.00
1	5	42	A	O4'-C1'-N9	9.39	115.71	108.20
7	D	54	ARG	CG-CD-NE	-9.39	92.09	111.80
50	S2	447	A	O4'-C1'-N9	9.36	115.69	108.20
53	SC	200	ARG	NE-CZ-NH2	9.36	124.98	120.30
65	SO	147	ARG	CA-CB-CG	9.35	133.97	113.40
61	SK	2	LEU	CA-CB-CG	9.34	136.78	115.30
54	SD	67	ARG	NE-CZ-NH1	9.32	124.96	120.30
12	I	171	TRP	CA-CB-CG	-9.32	95.99	113.70
13	J	32	ARG	NE-CZ-NH2	-9.32	115.64	120.30
56	SF	130	ARG	NE-CZ-NH1	9.31	124.96	120.30
63	SM	33	ARG	NE-CZ-NH1	9.31	124.96	120.30
50	S2	1433	C	C4'-C3'-O3'	9.31	131.62	113.00
1	5	4280	A	N9-C1'-C2'	-9.31	101.76	112.00
1	5	1534	A	N9-C1'-C2'	9.23	126.00	114.00
1	5	5059	C	C2'-C3'-O3'	9.22	129.79	109.50
1	5	280	G	O4'-C1'-N9	9.21	115.56	108.20
27	Y	27	ARG	NE-CZ-NH2	9.20	124.90	120.30
50	S2	631	U	N1-C1'-C2'	9.18	125.93	114.00
16	N	49	ARG	NE-CZ-NH1	9.15	124.88	120.30
70	ST	53	PHE	CB-CG-CD2	-9.15	114.39	120.80
1	5	2406	G	N9-C1'-C2'	-9.15	101.94	112.00
1	5	4228	G	N9-C1'-C2'	-9.14	101.95	112.00
79	Sc	31	ARG	NE-CZ-NH1	9.13	124.87	120.30
1	5	4116	C	OP2-P-O3'	9.12	125.27	105.20
1	5	2553	A	N9-C1'-C2'	9.12	125.86	114.00
50	S2	1552	G	C2'-C3'-O3'	9.09	129.51	109.50
1	5	1474	C	C2'-C3'-O3'	9.09	129.50	109.50
1	5	1685	G	N9-C1'-C2'	9.09	125.82	114.00
1	5	2658	G	N9-C1'-C2'	-9.08	102.01	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Q	91	ARG	NE-CZ-NH2	9.06	124.83	120.30
5	B	100	ARG	NE-CZ-NH2	-9.06	115.77	120.30
50	S2	1578	U	N1-C1'-C2'	9.06	125.77	114.00
6	C	78	ARG	NE-CZ-NH1	9.02	124.81	120.30
29	a	79	TRP	CA-CB-CG	-9.02	96.57	113.70
86	S6	55	U	P-O3'-C3'	-9.00	108.90	119.70
24	V	97	TYR	CB-CG-CD2	-8.99	115.61	121.00
1	5	1882	U	O5'-P-OP1	-8.97	97.62	105.70
6	C	267	TRP	CA-CB-CG	8.95	130.71	113.70
27	Y	126	ARG	NE-CZ-NH1	8.95	124.77	120.30
82	Sf	146	LEU	CB-CG-CD1	8.95	126.21	111.00
32	d	85	ARG	NE-CZ-NH1	8.95	124.77	120.30
37	i	4	ARG	NE-CZ-NH1	8.95	124.77	120.30
3	8	94	G	O4'-C1'-N9	-8.91	101.07	108.20
5	B	119	TYR	CB-CG-CD1	-8.90	115.66	121.00
50	S2	833	C	C2'-C3'-O3'	8.90	129.07	109.50
1	5	125	C	C2'-C3'-O3'	8.89	129.07	109.50
1	5	4385	A	N9-C1'-C2'	-8.89	102.22	112.00
1	5	4965	U	N1-C1'-C2'	-8.89	102.22	112.00
33	e	46	ARG	NE-CZ-NH1	8.87	124.74	120.30
1	5	4911	A	O4'-C1'-N9	8.86	115.28	108.20
83	Sg	60	ARG	NE-CZ-NH2	-8.85	115.88	120.30
32	d	25	TYR	CB-CA-C	8.85	128.09	110.40
50	S2	437	G	N9-C1'-C2'	8.85	125.50	114.00
22	T	13	TYR	CB-CG-CD2	-8.84	115.70	121.00
10	G	62	ARG	NE-CZ-NH2	-8.82	115.89	120.30
70	ST	62	ARG	NE-CZ-NH2	8.81	124.71	120.30
66	SP	10	ARG	NE-CZ-NH1	8.81	124.71	120.30
1	5	1815	G	N9-C1'-C2'	8.80	125.44	114.00
73	SW	57	ARG	NE-CZ-NH1	8.79	124.70	120.30
50	S2	1088	U	N1-C1'-C2'	8.79	125.43	114.00
1	5	1356	U	C2'-C3'-O3'	8.78	128.82	109.50
1	5	977	C	C2'-C3'-O3'	8.78	128.82	109.50
50	S2	313	A	O4'-C1'-N9	8.78	115.22	108.20
1	5	1998	A	N9-C1'-C2'	8.77	125.40	114.00
17	O	135	PHE	N-CA-C	8.77	134.67	111.00
44	p	85	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	5	1534	A	O4'-C1'-N9	-8.76	101.19	108.20
8	E	119	ARG	NE-CZ-NH1	8.75	124.68	120.30
1	5	978	G	C2'-C3'-O3'	8.75	128.75	109.50
83	Sg	60	ARG	NE-CZ-NH1	8.75	124.67	120.30
1	5	1668	A	N9-C1'-C2'	8.74	125.37	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2268	A	N9-C1'-C2'	8.74	125.37	114.00
21	S	81	TRP	CB-CA-C	8.74	127.88	110.40
50	S2	3	C	N1-C1'-C2'	8.72	125.34	114.00
1	5	1359	G	C2'-C3'-O3'	8.72	128.69	109.50
1	5	2517	A	N9-C1'-C2'	8.72	125.33	114.00
50	S2	1859	A	C8-N9-C1'	-8.72	112.01	127.70
50	S2	1429	G	C2'-C3'-O3'	8.71	128.67	109.50
1	5	4976	U	O4'-C1'-N1	-8.70	101.24	108.20
19	Q	58	ARG	NE-CZ-NH1	8.69	124.64	120.30
18	P	54	GLN	CA-CB-CG	8.68	132.48	113.40
1	5	31	U	N1-C1'-C2'	8.66	125.27	114.00
82	Sf	138	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	5	2305	U	O4'-C1'-N1	-8.66	101.27	108.20
1	5	2446	C	N1-C1'-C2'	8.65	125.25	114.00
2	7	56	G	N9-C1'-C2'	8.65	125.25	114.00
21	S	81	TRP	CA-CB-CG	-8.65	97.27	113.70
6	C	311	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	5	4404	U	N1-C1'-C2'	-8.64	102.49	112.00
1	5	4234	A	N9-C1'-C2'	8.63	125.22	114.00
36	h	117	ARG	CG-CD-NE	-8.62	93.70	111.80
1	5	1637	A	N9-C1'-C2'	-8.62	102.52	112.00
43	o	31	ASP	CB-CA-C	8.61	127.63	110.40
4	A	193	ARG	CG-CD-NE	-8.60	93.75	111.80
17	O	140	ARG	NE-CZ-NH2	8.59	124.59	120.30
1	5	1980	U	O4'-C1'-N1	8.58	115.06	108.20
50	S2	110	U	C2'-C3'-O3'	8.58	128.38	109.50
52	SB	165	ARG	NE-CZ-NH2	8.58	124.59	120.30
1	5	4221	C	N1-C1'-C2'	-8.56	102.58	112.00
28	Z	121	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	5	2851	G	N9-C1'-C2'	-8.55	102.59	112.00
69	SS	95	TYR	CA-CB-CG	8.55	129.64	113.40
1	5	352	G	N9-C1'-C2'	-8.53	102.62	112.00
14	L	74	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	5	4563	U	N1-C1'-C2'	8.50	125.05	114.00
50	S2	1859	A	C4-N9-C1'	8.50	141.59	126.30
1	5	1439	C	C4'-C3'-O3'	-8.49	91.58	109.40
1	5	1296	G	O4'-C1'-N9	8.47	114.97	108.20
1	5	1733	G	N9-C1'-C2'	-8.47	102.69	112.00
26	X	73	HIS	CB-CA-C	8.47	127.33	110.40
33	e	35	TRP	CA-CB-CG	-8.46	97.62	113.70
81	Se	41	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	5	3790	U	N1-C1'-C2'	8.44	124.97	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4119	C	C2'-C3'-O3'	8.44	128.06	109.50
59	SI	197	PHE	CB-CA-C	-8.44	93.52	110.40
50	S2	798	A	C2'-C3'-O3'	8.43	128.04	109.50
4	A	67	TYR	CA-CB-CG	8.42	129.39	113.40
36	h	78	TYR	CA-CB-CG	-8.41	97.42	113.40
9	F	120	PHE	CB-CA-C	8.40	127.21	110.40
50	S2	622	C	N1-C1'-C2'	-8.40	102.76	112.00
1	5	1937	C	N1-C1'-C2'	8.39	124.91	114.00
3	8	85	U	C2'-C3'-O3'	8.39	127.96	109.50
21	S	29	ARG	CA-CB-CG	8.38	131.84	113.40
7	D	268	ARG	NE-CZ-NH1	8.37	124.48	120.30
8	E	268	ARG	NE-CZ-NH1	8.37	124.48	120.30
58	SH	177	TYR	CB-CA-C	-8.36	93.67	110.40
50	S2	421	G	N9-C1'-C2'	8.36	124.87	114.00
74	SX	67	ARG	NE-CZ-NH2	8.33	124.47	120.30
1	5	4501	U	OP2-P-O3'	8.32	123.51	105.20
43	o	48	TYR	CB-CA-C	8.32	127.04	110.40
60	SJ	127	ARG	NE-CZ-NH1	8.32	124.46	120.30
20	R	74	ARG	NE-CZ-NH1	-8.32	116.14	120.30
58	SH	177	TYR	CA-CB-CG	8.32	129.20	113.40
50	S2	1407	U	N1-C1'-C2'	8.29	124.78	114.00
1	5	292	G	N9-C1'-C2'	8.29	124.77	114.00
50	S2	294	U	N1-C1'-C2'	8.29	124.78	114.00
1	5	958	G	C2'-C3'-O3'	8.27	127.70	109.50
36	h	78	TYR	CB-CA-C	8.25	126.90	110.40
1	5	2087	C	N1-C1'-C2'	-8.25	102.93	112.00
10	G	53	ARG	NE-CZ-NH2	-8.25	116.18	120.30
3	8	70	G	N9-C1'-C2'	-8.23	102.94	112.00
21	S	29	ARG	CG-CD-NE	-8.23	94.51	111.80
43	o	57	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	5	1566	C	OP2-P-O3'	8.22	123.29	105.20
1	5	3653	A	N9-C1'-C2'	-8.21	102.96	112.00
69	SS	86	ARG	NE-CZ-NH1	-8.21	116.19	120.30
21	S	10	TYR	CA-CB-CG	-8.21	97.80	113.40
1	5	3879	G	N9-C1'-C2'	-8.21	102.97	112.00
20	R	132	PHE	N-CA-C	-8.19	88.88	111.00
50	S2	1408	U	N1-C1'-C2'	8.18	124.64	114.00
51	SA	151	ASP	CB-CG-OD2	8.18	125.67	118.30
17	O	37	ARG	NE-CZ-NH2	-8.17	116.21	120.30
50	S2	1623	A	C2'-C3'-O3'	8.17	127.48	109.50
86	S6	56	C	P-O3'-C3'	-8.17	109.89	119.70
1	5	93	G	N9-C1'-C2'	8.17	124.62	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4498	U	N1-C1'-C2'	-8.16	103.02	112.00
50	S2	594	A	N9-C1'-C2'	-8.16	103.02	112.00
67	SQ	126	ARG	NE-CZ-NH2	8.16	124.38	120.30
1	5	3938	G	N9-C1'-C2'	8.15	124.60	114.00
1	5	2797	C	N1-C1'-C2'	-8.15	103.04	112.00
34	f	4	ARG	CA-CB-CG	8.14	131.32	113.40
50	S2	381	C	N1-C1'-C2'	8.14	124.59	114.00
1	5	2465	C	N1-C1'-C2'	8.14	124.58	114.00
1	5	2553	A	O4'-C1'-N9	8.14	114.71	108.20
1	5	2246	C	C2'-C3'-O3'	8.09	127.31	109.50
1	5	3735	G	C2'-C3'-O3'	8.09	127.31	109.50
1	5	2806	A	N9-C1'-C2'	-8.09	103.10	112.00
9	F	58	HIS	CB-CA-C	-8.09	94.23	110.40
3	8	34	U	C2'-C3'-O3'	8.09	127.29	109.50
30	b	44	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	5	3773	U	C4'-C3'-O3'	8.08	129.16	113.00
4	A	193	ARG	NE-CZ-NH2	-8.08	116.26	120.30
56	SF	136	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	5	4723	A	C4-N9-C1'	8.07	140.82	126.30
1	5	3635	A	N9-C1'-C2'	-8.06	103.14	112.00
1	5	235	A	O4'-C1'-N9	8.06	114.64	108.20
3	8	94	G	C2'-C3'-O3'	8.06	127.22	109.50
1	5	1867	A	N9-C1'-C2'	8.05	124.47	114.00
7	D	44	TYR	CB-CA-C	8.05	126.51	110.40
7	D	248	ARG	NE-CZ-NH2	-8.05	116.27	120.30
16	N	139	HIS	N-CA-CB	8.05	125.10	110.60
1	5	4600	G	N9-C1'-C2'	-8.04	103.15	112.00
1	5	2683	C	C2'-C3'-O3'	8.04	127.18	109.50
1	5	3908	A	N9-C1'-C2'	8.04	124.45	114.00
34	f	85	ARG	NE-CZ-NH2	-8.04	116.28	120.30
24	V	98	PHE	CB-CG-CD1	-8.03	115.18	120.80
1	5	3905	A	C2'-C3'-O3'	8.03	127.16	109.50
67	SQ	126	ARG	NE-CZ-NH1	-8.01	116.30	120.30
65	SO	147	ARG	CG-CD-NE	-8.00	94.99	111.80
1	5	4885	U	C2'-C3'-O3'	7.99	127.08	109.50
34	f	22	ARG	NE-CZ-NH1	7.99	124.30	120.30
16	N	143	ARG	CG-CD-NE	-7.98	95.05	111.80
1	5	4497	U	N1-C1'-C2'	-7.97	103.23	112.00
47	1	432	SER	C-N-CA	-7.97	101.78	121.70
27	Y	11	ARG	NE-CZ-NH2	-7.96	116.32	120.30
5	B	62	ARG	NE-CZ-NH1	7.95	124.28	120.30
15	M	119	ARG	NE-CZ-NH2	7.95	124.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4371	G	O4'-C1'-N9	7.95	114.56	108.20
3	8	34	U	C5'-C4'-O4'	7.95	118.64	109.10
5	B	169	ARG	NE-CZ-NH1	7.95	124.27	120.30
19	Q	174	PHE	CB-CA-C	7.94	126.28	110.40
1	5	315	G	C1'-O4'-C4'	-7.93	103.55	109.90
1	5	3692	A	C2'-C3'-O3'	7.93	126.94	109.50
52	SB	146	ARG	NE-CZ-NH2	-7.92	116.34	120.30
50	S2	1292	C	C4'-C3'-O3'	7.92	128.84	113.00
12	I	119	PHE	CB-CG-CD1	7.92	126.34	120.80
17	O	110	PRO	C-N-CD	-7.91	103.19	120.60
50	S2	399	C	N1-C1'-C2'	-7.91	103.30	112.00
50	S2	968	U	N1-C1'-C2'	-7.91	103.30	112.00
1	5	2394	G	O4'-C1'-N9	7.90	114.52	108.20
1	5	4723	A	C8-N9-C1'	-7.90	113.48	127.70
50	S2	964	A	N9-C1'-C2'	7.90	124.27	114.00
1	5	4163	U	N1-C1'-C2'	-7.90	103.31	112.00
74	SX	67	ARG	NE-CZ-NH1	-7.89	116.35	120.30
18	P	3	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	5	2263	A	C5'-C4'-O4'	7.88	118.56	109.10
68	SR	82	ASP	CB-CG-OD2	-7.88	111.21	118.30
1	5	668	C	C2'-C3'-O3'	7.87	126.81	109.50
69	SS	42	HIS	CB-CA-C	-7.87	94.67	110.40
79	Sc	44	ARG	NE-CZ-NH2	7.84	124.22	120.30
1	5	1805	A	N9-C1'-C2'	7.83	124.18	114.00
50	S2	1703	C	N1-C1'-C2'	-7.82	103.40	112.00
50	S2	164	A	N9-C1'-C2'	-7.82	103.40	112.00
1	5	716	C	C2'-C3'-O3'	7.81	126.68	109.50
1	5	4501	U	P-O3'-C3'	7.81	129.07	119.70
1	5	157	U	O4'-C1'-N1	7.81	114.44	108.20
1	5	353	A	N9-C1'-C2'	-7.80	103.42	112.00
1	5	962	C	N1-C1'-C2'	7.80	124.14	114.00
3	8	64	U	N1-C1'-C2'	7.79	124.13	114.00
22	T	13	TYR	N-CA-CB	-7.79	96.59	110.60
1	5	4463	U	N1-C1'-C2'	-7.78	103.44	112.00
1	5	964	A	C4'-C3'-O3'	7.77	128.54	113.00
1	5	2263	A	O4'-C1'-N9	-7.74	102.01	108.20
7	D	198	HIS	CB-CA-C	7.72	125.85	110.40
1	5	43	U	N1-C1'-C2'	-7.72	103.51	112.00
1	5	5066	U	N1-C1'-C2'	7.71	124.03	114.00
53	SC	241	PHE	N-CA-CB	7.71	124.48	110.60
9	F	168	ARG	CG-CD-NE	-7.69	95.66	111.80
1	5	4282	A	N9-C1'-C2'	7.68	123.98	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1522	G	N9-C1'-C2'	-7.67	103.56	112.00
1	5	4194	U	N1-C1'-C2'	-7.67	103.57	112.00
29	a	128	PHE	CB-CA-C	7.67	125.73	110.40
71	SU	90	ASP	CB-CG-OD1	7.66	125.19	118.30
60	SJ	48	PHE	N-CA-CB	7.65	124.37	110.60
1	5	2790	U	N1-C1'-C2'	7.65	123.94	114.00
5	B	116	ARG	CG-CD-NE	7.65	127.86	111.80
4	A	37	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	5	4238	G	N9-C1'-C2'	-7.64	103.60	112.00
1	5	4464	A	C5'-C4'-O4'	7.64	118.26	109.10
34	f	4	ARG	CG-CD-NE	-7.64	95.76	111.80
4	A	211	PHE	CB-CA-C	7.63	125.65	110.40
1	5	292	G	O4'-C1'-N9	-7.62	102.10	108.20
50	S2	1395	C	C2'-C3'-O3'	7.62	126.25	109.50
73	SW	117	ARG	NH1-CZ-NH2	7.61	127.78	119.40
1	5	53	C	C2'-C3'-O3'	7.61	126.24	109.50
1	5	294	G	C1'-O4'-C4'	-7.61	103.81	109.90
3	8	94	G	C5'-C4'-O4'	7.60	118.22	109.10
50	S2	1701	C	N1-C1'-C2'	7.60	123.89	114.00
1	5	158	A	N9-C1'-C2'	-7.60	103.64	112.00
7	D	210	TYR	CA-CB-CG	-7.60	98.96	113.40
64	SN	83	ASP	CB-CG-OD2	-7.60	111.46	118.30
68	SR	28	PHE	C-N-CA	7.60	140.69	121.70
1	5	1575	A	N9-C1'-C2'	7.59	123.87	114.00
50	S2	349	A	C2'-C3'-O3'	7.59	126.21	109.50
53	SC	236	PHE	N-CA-CB	7.59	124.26	110.60
64	SN	113	PHE	CB-CA-C	-7.58	95.24	110.40
1	5	4548	A	O4'-C1'-N9	-7.57	102.14	108.20
1	5	4045	G	N9-C1'-C2'	-7.57	103.68	112.00
3	8	38	U	O4'-C1'-N1	7.57	114.25	108.20
36	h	119	PHE	CB-CA-C	-7.57	95.27	110.40
1	5	4583	C	N1-C1'-C2'	-7.56	103.68	112.00
50	S2	1664	A	C2'-C3'-O3'	7.56	126.14	109.50
1	5	354	U	N1-C1'-C2'	-7.55	103.69	112.00
1	5	1377	G	C2'-C3'-O3'	7.55	126.12	109.50
1	5	1881	C	N1-C1'-C2'	7.55	123.82	114.00
1	5	1916	G	N9-C1'-C2'	7.55	123.81	114.00
50	S2	1114	U	O4'-C1'-N1	7.55	114.24	108.20
1	5	4737	G	N9-C1'-C2'	7.54	123.80	114.00
12	I	4	ARG	CG-CD-NE	-7.54	95.98	111.80
1	5	1724	G	O4'-C4'-C3'	-7.53	96.47	104.00
1	5	4911	A	C1'-O4'-C4'	-7.53	103.88	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1382	G	N9-C1'-C2'	7.53	123.78	114.00
6	C	222	ARG	NE-CZ-NH1	7.53	124.06	120.30
8	E	179	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	5	5046	U	C2'-C3'-O3'	7.51	126.03	109.50
3	8	104	A	O4'-C1'-N9	-7.51	102.19	108.20
12	I	171	TRP	N-CA-CB	7.51	124.11	110.60
9	F	228	HIS	N-CA-CB	7.50	124.10	110.60
50	S2	9	U	N1-C1'-C2'	-7.50	103.75	112.00
29	a	79	TRP	CB-CA-C	7.50	125.40	110.40
50	S2	732	U	C2'-C3'-O3'	7.49	125.97	109.50
9	F	36	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	5	3868	G	N9-C1'-C2'	-7.48	103.77	112.00
50	S2	1142	G	N9-C1'-C2'	-7.47	103.78	112.00
50	S2	1542	C	N1-C1'-C2'	7.47	123.71	114.00
1	5	2588	C	C4'-C3'-O3'	7.47	127.94	113.00
37	i	28	ARG	CG-CD-NE	-7.47	96.12	111.80
1	5	2092	G	N9-C1'-C2'	7.46	123.70	114.00
5	B	117	ARG	NE-CZ-NH2	-7.46	116.57	120.30
16	N	131	GLU	CB-CG-CD	-7.46	94.07	114.20
1	5	4212	A	N9-C1'-C2'	7.45	123.69	114.00
19	Q	34	PHE	N-CA-CB	7.45	124.01	110.60
50	S2	1	U	C5'-C4'-O4'	7.45	118.04	109.10
1	5	157	U	N1-C1'-C2'	-7.45	103.81	112.00
1	5	1521	C	N1-C1'-C2'	-7.45	103.81	112.00
7	D	35	ARG	NE-CZ-NH1	7.45	124.02	120.30
3	8	73	U	N1-C1'-C2'	-7.44	103.81	112.00
59	SI	113	TYR	CA-CB-CG	7.44	127.54	113.40
1	5	1378	C	N1-C1'-C2'	7.44	123.67	114.00
1	5	4322	G	N9-C1'-C2'	-7.44	103.81	112.00
1	5	4535	A	C2'-C3'-O3'	7.44	125.87	109.50
74	SX	88	ASP	CB-CG-OD2	-7.44	111.60	118.30
82	Sf	143	LYS	CD-CE-NZ	7.44	128.81	111.70
50	S2	1113	A	N9-C1'-C2'	7.44	123.67	114.00
50	S2	1606	G	N9-C1'-C2'	-7.43	103.82	112.00
29	a	34	ASN	CB-CA-C	7.43	125.26	110.40
50	S2	384	U	N1-C1'-C2'	-7.43	103.83	112.00
50	S2	427	U	N1-C1'-C2'	7.43	123.66	114.00
1	5	2046	G	C1'-O4'-C4'	-7.43	103.96	109.90
1	5	4120	U	N1-C1'-C2'	-7.42	103.83	112.00
83	Sg	125	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	5	4693	C	C5'-C4'-O4'	7.41	117.99	109.10
16	N	180	PHE	CB-CA-C	7.40	125.20	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	3871	A	N9-C1'-C2'	7.40	123.62	114.00
52	SB	136	ARG	NE-CZ-NH2	7.40	124.00	120.30
82	Sf	116	ARG	NE-CZ-NH1	7.39	123.99	120.30
1	5	1445	U	C2'-C3'-O3'	7.39	125.75	109.50
50	S2	1659	U	N1-C1'-C2'	-7.39	103.88	112.00
1	5	2124	G	C2'-C3'-O3'	7.38	125.74	109.50
1	5	1266	G	C2'-C3'-O3'	7.38	125.74	109.50
1	5	1440	U	C2'-C3'-O3'	7.38	125.74	109.50
4	A	189	TYR	CA-CB-CG	7.38	127.42	113.40
1	5	4981	G	N9-C1'-C2'	-7.38	103.89	112.00
60	SJ	69	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	5	4464	A	N9-C1'-C2'	7.37	123.59	114.00
7	D	223	PHE	CB-CG-CD2	-7.37	115.64	120.80
1	5	394	G	N9-C1'-C2'	-7.37	103.89	112.00
69	SS	86	ARG	CG-CD-NE	-7.36	96.33	111.80
50	S2	1249	C	N1-C1'-C2'	-7.36	103.90	112.00
7	D	210	TYR	N-CA-CB	7.36	123.84	110.60
1	5	4531	U	N1-C1'-C2'	7.35	123.56	114.00
1	5	4251	A	N9-C1'-C2'	7.35	123.56	114.00
1	5	3843	C	N1-C1'-C2'	7.34	123.55	114.00
1	5	979	C	C2'-C3'-O3'	7.34	125.65	109.50
1	5	5061	A	C2'-C3'-O3'	7.34	125.65	109.50
4	A	242	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	5	1370	G	N9-C1'-C2'	7.34	123.54	114.00
1	5	2769	U	N1-C1'-C2'	-7.33	103.94	112.00
1	5	3938	G	O4'-C1'-N9	-7.33	102.34	108.20
1	5	147	A	N9-C1'-C2'	7.33	123.52	114.00
1	5	55	G	N9-C1'-C2'	-7.32	103.95	112.00
1	5	974	C	C2'-C3'-O3'	7.32	125.61	109.50
1	5	450	G	N9-C1'-C2'	-7.32	103.95	112.00
50	S2	1623	A	N9-C1'-C2'	-7.32	103.95	112.00
10	G	235	ARG	NE-CZ-NH1	7.32	123.96	120.30
50	S2	1115	U	N1-C1'-C2'	7.32	123.51	114.00
1	5	1601	A	N9-C1'-C2'	-7.31	103.96	112.00
1	5	1379	C	C1'-O4'-C4'	-7.31	104.06	109.90
50	S2	1486	A	N9-C1'-C2'	-7.30	103.97	112.00
1	5	486	C	C2'-C3'-O3'	7.30	125.55	109.50
1	5	406	C	C2'-C3'-O3'	7.29	125.54	109.50
1	5	97	G	N9-C1'-C2'	-7.29	103.99	112.00
1	5	2280	G	N9-C1'-C2'	7.28	123.47	114.00
52	SB	82	ARG	CG-CD-NE	-7.28	96.52	111.80
1	5	4519	C	N1-C1'-C2'	-7.27	104.00	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4084	G	C2'-C3'-O3'	7.26	125.48	109.50
58	SH	99	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	5	2848	G	N9-C1'-C2'	-7.25	104.02	112.00
1	5	2796	G	N9-C1'-C2'	7.25	123.42	114.00
1	5	1481	C	C2'-C3'-O3'	7.24	125.44	109.50
1	5	4966	A	N9-C1'-C2'	7.24	123.41	114.00
26	X	48	ARG	NE-CZ-NH1	7.23	123.92	120.30
60	SJ	115	PHE	CB-CG-CD2	-7.23	115.74	120.80
1	5	100	C	N1-C1'-C2'	-7.22	104.06	112.00
29	a	109	TYR	CB-CA-C	7.20	124.81	110.40
1	5	4279	A	N9-C1'-C2'	-7.20	104.08	112.00
1	5	664	G	C1'-O4'-C4'	-7.20	104.14	109.90
1	5	2511	A	C4'-C3'-O3'	-7.19	94.30	109.40
38	j	71	TYR	CA-CB-CG	7.19	127.06	113.40
1	5	2812	A	N9-C1'-C2'	7.18	123.34	114.00
50	S2	1339	U	N1-C1'-C2'	-7.18	104.10	112.00
54	SD	216	GLU	CG-CD-OE2	7.18	132.66	118.30
1	5	4750	G	C1'-O4'-C4'	-7.18	104.16	109.90
1	5	1534	A	C5'-C4'-O4'	7.18	117.71	109.10
50	S2	1419	C	N1-C1'-C2'	-7.17	104.11	112.00
1	5	1359	G	C4'-C3'-O3'	-7.17	94.34	109.40
50	S2	24	C	N1-C1'-C2'	-7.17	104.11	112.00
6	C	41	HIS	N-CA-CB	7.16	123.50	110.60
50	S2	798	A	N9-C1'-C2'	-7.16	104.12	112.00
60	SJ	115	PHE	CB-CG-CD1	7.16	125.81	120.80
3	8	34	U	O4'-C1'-N1	-7.16	102.47	108.20
50	S2	402	C	N1-C1'-C2'	-7.15	104.13	112.00
1	5	4750	G	O4'-C1'-N9	7.14	113.92	108.20
21	S	28	TYR	CB-CG-CD1	7.14	125.29	121.00
55	SE	104	ASP	CB-CG-OD2	-7.14	111.88	118.30
14	L	82	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	5	1946	G	N9-C1'-C2'	-7.13	104.15	112.00
38	j	11	ARG	NE-CZ-NH1	7.13	123.87	120.30
50	S2	1404	U	C4'-C3'-O3'	-7.13	94.42	109.40
50	S2	1645	C	N1-C1'-C2'	7.13	123.27	114.00
36	h	89	ARG	NE-CZ-NH1	7.13	123.86	120.30
37	i	39	PHE	N-CA-CB	7.12	123.42	110.60
1	5	350	C	N1-C1'-C2'	7.12	123.25	114.00
1	5	383	A	C1'-C2'-O2'	-7.12	89.24	110.60
32	d	73	TRP	N-CA-CB	-7.12	97.79	110.60
1	5	1500	A	C4'-C3'-O3'	7.12	127.23	113.00
74	SX	20	HIS	CB-CA-C	7.11	124.62	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	29	G	N9-C1'-C2'	7.11	123.24	114.00
1	5	4519	C	O4'-C1'-N1	7.11	113.89	108.20
29	a	62	HIS	N-CA-CB	7.11	123.39	110.60
9	F	194	HIS	CB-CA-C	-7.10	96.19	110.40
36	h	51	ARG	NE-CZ-NH1	7.10	123.85	120.30
26	X	48	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	5	2038	U	N1-C1'-C2'	7.10	123.22	114.00
1	5	291	U	N1-C1'-C2'	7.09	123.22	114.00
3	8	38	U	C1'-O4'-C4'	-7.09	104.23	109.90
1	5	4589	A	O4'-C1'-N9	-7.08	102.53	108.20
1	5	2046	G	C2'-C3'-O3'	7.08	125.09	109.50
1	5	2324	C	C2'-C3'-O3'	7.08	125.08	109.50
3	8	94	G	N9-C1'-C2'	7.08	123.20	114.00
38	j	27	TYR	CA-CB-CG	-7.08	99.95	113.40
1	5	1355	G	N9-C1'-C2'	7.07	123.19	114.00
1	5	4341	C	N1-C1'-C2'	-7.07	104.22	112.00
56	SF	122	ARG	NE-CZ-NH1	7.07	123.83	120.30
8	E	219	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	5	30	C	N1-C1'-C2'	7.06	123.18	114.00
4	A	3	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	5	4464	A	C2'-C3'-O3'	7.06	125.02	109.50
33	e	74	PHE	CB-CG-CD1	-7.05	115.86	120.80
50	S2	863	U	N1-C1'-C2'	7.05	123.17	114.00
1	5	1625	G	N9-C1'-C2'	7.05	123.17	114.00
1	5	1479	G	N9-C1'-C2'	7.05	123.16	114.00
11	H	156	ASN	N-CA-CB	7.05	123.29	110.60
1	5	157	U	C1'-O4'-C4'	-7.05	104.26	109.90
54	SD	67	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	5	514	U	C2'-C3'-O3'	7.04	124.99	109.50
50	S2	821	G	O4'-C1'-N9	-7.04	102.57	108.20
52	SB	205	TYR	CA-CB-CG	-7.04	100.03	113.40
1	5	1455	G	C2'-C3'-O3'	7.04	124.98	109.50
67	SQ	85	ARG	CG-CD-NE	-7.04	97.02	111.80
81	Se	13	ARG	NE-CZ-NH2	-7.03	116.79	120.30
13	J	64	ARG	NE-CZ-NH2	7.02	123.81	120.30
1	5	669	C	O4'-C1'-N1	7.02	113.82	108.20
1	5	4500	U	O5'-P-OP1	-7.02	99.38	105.70
1	5	4510	A	O4'-C1'-N9	-7.01	102.59	108.20
1	5	1552	G	N9-C1'-C2'	-7.01	104.29	112.00
1	5	3817	A	N9-C1'-C2'	7.01	123.11	114.00
50	S2	384	U	C2'-C3'-O3'	7.01	124.92	109.50
1	5	2695	A	C2'-C3'-O3'	7.01	124.92	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	O	49	ARG	NE-CZ-NH1	7.00	123.80	120.30
25	W	8	PHE	CB-CG-CD1	7.00	125.70	120.80
1	5	235	A	N9-C1'-C2'	-6.99	104.31	112.00
50	S2	1157	G	N9-C1'-C2'	-6.99	104.31	112.00
1	5	1676	C	C1'-C2'-O2'	-6.99	89.63	110.60
32	d	25	TYR	CB-CG-CD1	-6.99	116.81	121.00
6	C	35	ASP	CB-CG-OD1	6.99	124.59	118.30
50	S2	104	A	C2'-C3'-O3'	6.98	124.87	113.70
43	o	48	TYR	CA-CB-CG	-6.98	100.14	113.40
50	S2	427	U	O4'-C1'-N1	-6.98	102.62	108.20
1	5	2851	G	C2'-C3'-O3'	6.97	124.86	113.70
50	S2	1839	U	C2-N1-C1'	6.97	126.07	117.70
1	5	42	A	C1'-O4'-C4'	-6.97	104.32	109.90
9	F	197	TYR	CB-CA-C	-6.97	96.47	110.40
60	SJ	138	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	5	209	U	O4'-C1'-N1	6.96	113.77	108.20
50	S2	448	A	N9-C1'-C2'	-6.96	104.35	112.00
1	5	4265	U	N1-C1'-C2'	6.95	123.04	114.00
1	5	4270	C	N1-C1'-C2'	-6.95	104.35	112.00
50	S2	1022	U	O4'-C1'-N1	6.95	113.76	108.20
1	5	332	C	N1-C1'-C2'	6.95	123.03	114.00
13	J	32	ARG	NE-CZ-NH1	6.94	123.77	120.30
5	B	100	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	5	4531	U	O4'-C1'-N1	-6.93	102.65	108.20
20	R	88	ARG	NE-CZ-NH1	6.93	123.77	120.30
24	V	97	TYR	N-CA-C	-6.93	92.29	111.00
50	S2	617	G	N9-C1'-C2'	-6.93	104.38	112.00
1	5	2589	C	C2'-C3'-O3'	6.93	124.78	113.70
13	J	146	ARG	CG-CD-NE	-6.93	97.25	111.80
1	5	4589	A	N9-C1'-C2'	6.93	123.00	114.00
59	SI	197	PHE	CB-CG-CD2	-6.92	115.95	120.80
1	5	54	G	N9-C1'-C2'	-6.91	104.40	112.00
1	5	1832	C	C2'-C3'-O3'	6.90	124.74	113.70
50	S2	923	G	C2'-C3'-O3'	6.90	124.74	113.70
68	SR	28	PHE	CA-C-N	6.90	132.38	117.20
36	h	93	ARG	NE-CZ-NH2	-6.90	116.85	120.30
10	G	49	ARG	NE-CZ-NH2	-6.90	116.85	120.30
50	S2	1143	A	O5'-P-OP1	-6.89	99.50	105.70
50	S2	674	C	O5'-P-OP2	-6.89	99.50	105.70
50	S2	55	U	N1-C1'-C2'	6.88	122.95	114.00
11	H	156	ASN	N-CA-C	-6.88	92.42	111.00
1	5	1319	U	N1-C1'-C2'	-6.88	104.44	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	S2	1247	C	N1-C1'-C2'	6.88	122.94	114.00
1	5	964	A	O4'-C1'-C2'	-6.87	98.93	105.80
1	5	943	A	N9-C1'-C2'	-6.87	104.44	112.00
50	S2	1373	C	OP1-P-O3'	6.87	120.31	105.20
1	5	1815	G	O4'-C1'-N9	6.87	113.69	108.20
1	5	454	U	C2'-C3'-O3'	6.86	124.68	113.70
1	5	5001	U	N1-C1'-C2'	6.86	122.92	114.00
19	Q	37	ARG	NE-CZ-NH1	-6.86	116.87	120.30
50	S2	77	A	N9-C1'-C2'	-6.86	104.45	112.00
5	B	274	TYR	CA-CB-CG	-6.85	100.38	113.40
50	S2	104	A	N9-C1'-C2'	-6.84	104.47	112.00
1	5	226	G	N9-C1'-C2'	-6.84	104.47	112.00
50	S2	992	A	N9-C1'-C2'	-6.84	104.47	112.00
34	f	4	ARG	N-CA-CB	6.83	122.90	110.60
34	f	85	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	5	1631	A	O4'-C1'-N9	-6.83	102.73	108.20
50	S2	1039	C	C2'-C3'-O3'	6.83	124.63	113.70
1	5	4518	A	O5'-P-OP1	6.83	118.90	110.70
1	5	5047	C	O5'-P-OP2	-6.83	99.55	105.70
64	SN	18	TYR	N-CA-CB	6.83	122.89	110.60
9	F	168	ARG	NE-CZ-NH2	-6.83	116.89	120.30
9	F	219	ARG	NE-CZ-NH1	6.83	123.71	120.30
16	N	49	ARG	NE-CZ-NH2	-6.82	116.89	120.30
50	S2	182	C	C2'-C3'-O3'	6.82	124.62	113.70
3	8	64	U	C2'-C3'-O3'	6.82	124.61	113.70
20	R	74	ARG	NE-CZ-NH2	6.82	123.71	120.30
63	SM	127	TYR	CA-CB-CG	6.81	126.33	113.40
24	V	97	TYR	CA-CB-CG	-6.80	100.47	113.40
28	Z	65	ARG	CG-CD-NE	-6.80	97.52	111.80
1	5	3625	G	C2'-C3'-O3'	6.79	124.56	113.70
10	G	73	ARG	NE-CZ-NH1	6.79	123.69	120.30
50	S2	73	C	O4'-C1'-N1	6.79	113.63	108.20
10	G	54	PHE	CB-CG-CD2	-6.78	116.05	120.80
11	H	125	ARG	NE-CZ-NH1	6.78	123.69	120.30
19	Q	75	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	5	2271	C	N1-C1'-C2'	6.77	122.80	114.00
2	7	72	U	C2'-C3'-O3'	6.77	124.53	113.70
1	5	1	C	O4'-C1'-N1	6.76	113.61	108.20
1	5	3611	A	N9-C1'-C2'	6.76	122.79	114.00
13	J	99	PHE	CB-CA-C	6.76	123.91	110.40
50	S2	1198	G	C2'-C3'-O3'	6.76	124.51	113.70
50	S2	1838	U	O4'-C4'-C3'	-6.76	97.24	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	3901	A	O4'-C1'-N9	-6.75	102.80	108.20
50	S2	61	A	C4'-C3'-O3'	-6.75	95.23	109.40
1	5	2395	A	N9-C1'-C2'	-6.74	104.58	112.00
8	E	101	ARG	NE-CZ-NH1	-6.74	116.93	120.30
19	Q	33	ARG	CG-CD-NE	-6.74	97.64	111.80
50	S2	596	U	N1-C1'-C2'	6.74	122.77	114.00
1	5	1292	C	C2'-C3'-O3'	6.74	124.48	113.70
1	5	84	A	O4'-C1'-N9	-6.74	102.81	108.20
1	5	3875	G	N9-C1'-C2'	-6.74	104.59	112.00
1	5	2319	C	N1-C1'-C2'	6.73	122.75	114.00
8	E	278	TYR	N-CA-C	-6.72	92.84	111.00
50	S2	1433	C	C5'-C4'-C3'	6.72	126.75	116.00
1	5	1364	U	C2'-C3'-O3'	6.72	124.45	113.70
28	Z	38	TYR	CB-CA-C	6.72	123.83	110.40
50	S2	983	A	C4-N9-C1'	6.71	138.39	126.30
50	S2	983	A	C8-N9-C1'	-6.71	115.61	127.70
1	5	2675	G	N9-C1'-C2'	-6.71	104.62	112.00
50	S2	1114	U	C1'-O4'-C4'	-6.71	104.53	109.90
50	S2	1663	A	O4'-C1'-N9	6.71	113.57	108.20
19	Q	15	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	5	1631	A	N9-C1'-C2'	6.70	122.71	114.00
1	5	2305	U	N1-C1'-C2'	6.70	122.71	114.00
1	5	2827	G	O4'-C1'-N9	-6.69	102.84	108.20
1	5	3882	C	N1-C1'-C2'	6.69	122.70	114.00
32	d	73	TRP	CA-CB-CG	6.69	126.41	113.70
50	S2	824	C	N1-C1'-C2'	6.69	122.69	114.00
60	SJ	108	ARG	NE-CZ-NH2	-6.69	116.96	120.30
53	SC	200	ARG	NE-CZ-NH1	-6.68	116.96	120.30
1	5	4280	A	C2'-C3'-O3'	6.68	124.39	113.70
32	d	87	ARG	N-CA-C	-6.67	92.98	111.00
1	5	4197	G	N9-C1'-C2'	-6.67	104.66	112.00
18	P	42	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	5	4936	G	N9-C1'-C2'	-6.67	104.67	112.00
1	5	4230	C	O5'-P-OP1	-6.66	99.70	105.70
1	5	58	G	N9-C1'-C2'	6.66	122.65	114.00
8	E	179	ARG	NE-CZ-NH2	-6.66	116.97	120.30
50	S2	532	C	C2'-C3'-O3'	6.65	124.35	113.70
50	S2	1838	U	C5'-C4'-O4'	6.65	117.08	109.10
1	5	4325	A	N9-C1'-C2'	6.65	122.65	114.00
50	S2	313	A	C1'-O4'-C4'	-6.65	104.58	109.90
50	S2	1667	U	N1-C1'-C2'	6.65	122.64	114.00
58	SH	116	ARG	NE-CZ-NH2	-6.65	116.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	SM	33	ARG	CG-CD-NE	6.65	125.76	111.80
50	S2	918	U	N1-C1'-C2'	6.64	122.64	114.00
1	5	3790	U	O4'-C1'-N1	-6.64	102.89	108.20
30	b	7	HIS	CB-CA-C	-6.64	97.13	110.40
50	S2	1452	A	N9-C1'-C2'	6.64	122.63	114.00
75	SY	76	TYR	CA-CB-CG	-6.63	100.80	113.40
50	S2	620	G	O5'-P-OP1	6.63	118.66	110.70
50	S2	415	A	C4-N9-C1'	-6.63	114.37	126.30
3	8	1	C	C5'-C4'-O4'	6.62	117.05	109.10
34	f	109	ARG	NE-CZ-NH1	6.62	123.61	120.30
63	SM	33	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	5	314	G	N9-C1'-C2'	-6.61	104.73	112.00
1	5	5022	U	C2'-C3'-O3'	6.61	124.28	113.70
50	S2	1401	A	C2'-C3'-O3'	6.61	124.28	113.70
1	5	4518	A	C2'-C3'-O3'	-6.61	94.95	109.50
3	8	81	C	C1'-O4'-C4'	-6.61	104.61	109.90
1	5	3883	U	N1-C1'-C2'	6.61	122.59	114.00
1	5	4693	C	C2'-C3'-O3'	6.60	124.25	113.70
1	5	2782	U	C4'-C3'-O3'	6.59	126.18	113.00
5	B	26	ARG	CG-CD-NE	-6.58	97.98	111.80
50	S2	1394	G	C2'-C3'-O3'	6.58	124.23	113.70
1	5	336	A	O4'-C1'-N9	6.58	113.46	108.20
50	S2	415	A	C8-N9-C1'	6.58	139.54	127.70
1	5	927	G	C2'-C3'-O3'	6.57	124.21	113.70
50	S2	631	U	O4'-C1'-N1	-6.57	102.95	108.20
50	S2	1434	C	N1-C1'-C2'	6.56	122.53	114.00
1	5	514	U	C5'-C4'-O4'	6.56	116.97	109.10
1	5	1650	A	O4'-C1'-N9	-6.56	102.95	108.20
1	5	187	U	C2'-C3'-O3'	6.55	124.18	113.70
1	5	432	U	N1-C1'-C2'	-6.55	104.79	112.00
50	S2	160	U	C2'-C3'-O3'	6.55	124.18	113.70
1	5	4227	U	C2'-C3'-O3'	6.55	124.18	113.70
16	N	150	TRP	CA-CB-CG	6.55	126.14	113.70
27	Y	81	TYR	CA-CB-CG	-6.55	100.95	113.40
1	5	505	G	C2'-C3'-O3'	6.55	124.17	113.70
32	d	85	ARG	NE-CZ-NH2	-6.55	117.03	120.30
35	g	14	ASN	N-CA-CB	6.54	122.38	110.60
54	SD	162	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	5	1215	C	O5'-P-OP2	-6.54	99.81	105.70
1	5	1930	U	N1-C1'-C2'	6.54	122.50	114.00
1	5	4338	G	N9-C1'-C2'	-6.54	104.81	112.00
38	j	27	TYR	CB-CG-CD1	-6.54	117.08	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	SA	9	GLN	CA-CB-CG	6.53	127.77	113.40
1	5	964	A	N9-C1'-C2'	-6.53	104.82	112.00
59	SI	55	TYR	CA-CB-CG	-6.53	101.00	113.40
63	SM	26	LEU	CB-CG-CD2	6.53	122.10	111.00
1	5	384	A	N9-C1'-C2'	6.53	122.48	114.00
1	5	5043	A	N9-C1'-C2'	6.52	122.48	114.00
1	5	2075	G	C2'-C3'-O3'	6.52	124.13	113.70
1	5	4336	A	N9-C1'-C2'	-6.52	104.83	112.00
50	S2	499	G	C2'-C3'-O3'	6.51	124.12	113.70
1	5	3827	G	N9-C1'-C2'	-6.51	104.84	112.00
70	ST	62	ARG	NE-CZ-NH1	-6.51	117.04	120.30
18	P	25	HIS	CB-CA-C	6.51	123.42	110.40
1	5	1379	C	N1-C1'-C2'	6.51	122.46	114.00
50	S2	149	A	N9-C1'-C2'	6.51	122.46	114.00
15	M	109	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	5	1887	G	C2'-C3'-O3'	6.50	124.10	113.70
50	S2	1830	U	N1-C1'-C2'	-6.50	104.85	112.00
9	F	209	PHE	N-CA-CB	6.50	122.30	110.60
18	P	23	ARG	NE-CZ-NH1	6.50	123.55	120.30
65	SO	147	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	5	209	U	C4'-C3'-O3'	6.49	125.98	113.00
50	S2	1838	U	C2-N1-C1'	-6.49	109.91	117.70
1	5	2118	G	C4'-C3'-O3'	6.48	125.96	113.00
1	5	136	C	N1-C1'-C2'	-6.48	104.88	112.00
50	S2	1272	C	O5'-P-OP1	-6.48	99.87	105.70
1	5	1671	U	O4'-C1'-C2'	-6.47	99.33	105.80
50	S2	1850	A	N9-C1'-C2'	6.47	122.42	114.00
1	5	98	A	N9-C1'-C2'	-6.47	104.88	112.00
50	S2	1291	A	P-O3'-C3'	6.47	127.47	119.70
1	5	119	G	O4'-C4'-C3'	-6.47	97.53	104.00
1	5	307	A	N9-C1'-C2'	6.47	122.41	114.00
1	5	1573	G	N9-C1'-C2'	6.47	122.41	114.00
1	5	4199	C	C4'-C3'-O3'	6.47	125.93	113.00
64	SN	64	ARG	NE-CZ-NH2	-6.47	117.07	120.30
17	O	37	ARG	NE-CZ-NH1	6.46	123.53	120.30
74	SX	27	TYR	CA-CB-CG	6.46	125.68	113.40
50	S2	427	U	C5'-C4'-O4'	6.46	116.85	109.10
1	5	2665	U	C2'-C3'-O3'	6.45	124.02	113.70
50	S2	1860	A	N9-C1'-C2'	-6.45	104.91	112.00
64	SN	18	TYR	CA-CB-CG	-6.45	101.15	113.40
19	Q	181	ARG	CA-CB-CG	6.44	127.58	113.40
1	5	2546	G	C4'-C3'-O3'	6.44	125.88	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4127	A	O4'-C1'-N9	6.44	113.35	108.20
3	8	64	U	C5'-C4'-O4'	6.44	116.83	109.10
1	5	1572	U	N1-C1'-C2'	6.43	122.37	114.00
50	S2	1116	C	O5'-P-OP1	-6.43	99.91	105.70
51	SA	186	ARG	NE-CZ-NH1	6.43	123.52	120.30
3	8	35	C	N1-C1'-C2'	6.43	122.36	114.00
1	5	946	C	O4'-C1'-N1	6.43	113.34	108.20
1	5	4911	A	O5'-P-OP2	-6.43	99.91	105.70
45	r	31	ASN	N-CA-CB	6.43	122.17	110.60
79	Sc	44	ARG	CG-CD-NE	6.43	125.30	111.80
3	8	86	U	O4'-C1'-C2'	-6.42	99.38	105.80
6	C	143	ARG	NE-CZ-NH2	-6.42	117.09	120.30
50	S2	427	U	P-O5'-C5'	6.42	131.17	120.90
1	5	1853	G	N9-C1'-C2'	-6.41	104.94	112.00
1	5	4976	U	N1-C1'-C2'	6.41	122.33	114.00
1	5	4076	G	N9-C1'-C2'	-6.41	104.95	112.00
22	T	13	TYR	CA-CB-CG	6.41	125.57	113.40
9	F	168	ARG	CB-CG-CD	6.40	128.24	111.60
1	5	336	A	C1'-O4'-C4'	-6.40	104.78	109.90
1	5	4534	G	N9-C1'-C2'	-6.40	104.96	112.00
10	G	223	ARG	NE-CZ-NH1	6.40	123.50	120.30
47	1	432	SER	CA-C-N	-6.40	103.13	117.20
1	5	1241	C	C2'-C3'-O3'	6.40	123.93	113.70
1	5	1980	U	C1'-O4'-C4'	-6.40	104.78	109.90
1	5	2581	A	N9-C1'-C2'	6.40	122.31	114.00
4	A	63	PHE	CB-CG-CD1	6.39	125.28	120.80
50	S2	848	U	C2-N1-C1'	6.39	125.37	117.70
7	D	223	PHE	CB-CG-CD1	6.39	125.27	120.80
50	S2	1851	A	N9-C1'-C2'	6.39	122.30	114.00
1	5	1642	A	C4'-C3'-O3'	-6.39	95.99	109.40
27	Y	81	TYR	CB-CA-C	6.39	123.17	110.40
50	S2	1059	G	N9-C1'-C2'	6.39	122.30	114.00
1	5	1724	G	C4'-C3'-O3'	-6.38	95.99	109.40
57	SG	88	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	5	2649	G	N9-C1'-C2'	6.37	122.28	114.00
50	S2	1082	A	N9-C1'-C2'	6.37	122.28	114.00
65	SO	147	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	5	4519	C	C2'-C3'-O3'	6.37	123.89	113.70
50	S2	654	A	N9-C1'-C2'	-6.37	104.99	112.00
69	SS	14	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	5	2088	A	C2'-C3'-O3'	6.36	123.88	113.70
1	5	2554	U	C2'-C3'-O3'	6.36	123.87	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	S2	1249	C	C2'-C3'-O3'	6.36	123.87	113.70
1	5	1615	C	C2'-C3'-O3'	6.35	123.86	113.70
67	SQ	138	ARG	NE-CZ-NH1	6.34	123.47	120.30
50	S2	91	A	N9-C1'-C2'	-6.34	105.02	112.00
50	S2	1109	C	C1'-O4'-C4'	-6.34	104.83	109.90
1	5	84	A	N9-C1'-C2'	6.34	122.24	114.00
50	S2	1584	G	N9-C1'-C2'	6.34	122.24	114.00
1	5	294	G	N9-C1'-C2'	6.33	122.24	114.00
27	Y	78	TYR	CB-CA-C	6.33	123.07	110.40
74	SX	9	THR	N-CA-C	-6.33	93.91	111.00
10	G	235	ARG	CG-CD-NE	6.33	125.09	111.80
56	SF	146	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	5	1272	C	O4'-C1'-N1	6.33	113.26	108.20
9	F	136	ARG	NE-CZ-NH2	-6.32	117.14	120.30
29	a	109	TYR	CB-CG-CD2	-6.32	117.21	121.00
1	5	1672	U	C2-N1-C1'	6.32	125.28	117.70
1	5	3671	G	N9-C1'-C2'	6.32	122.21	114.00
50	S2	960	U	C2'-C3'-O3'	6.32	123.81	113.70
50	S2	1292	C	P-O5'-C5'	6.32	131.01	120.90
1	5	3901	A	C5'-C4'-O4'	6.31	116.67	109.10
1	5	2511	A	O4'-C1'-N9	-6.31	103.15	108.20
1	5	2874	U	O4'-C1'-N1	-6.31	103.15	108.20
50	S2	1597	C	N1-C1'-C2'	6.30	122.20	114.00
9	F	36	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	5	1724	G	N9-C1'-C2'	6.30	122.19	114.00
3	8	104	A	N9-C1'-C2'	6.30	122.19	114.00
1	5	3648	A	O4'-C1'-N9	6.30	113.24	108.20
1	5	4519	C	O4'-C4'-C3'	-6.30	97.70	104.00
4	A	37	ARG	NE-CZ-NH1	6.30	123.45	120.30
18	P	139	TYR	CA-CB-CG	-6.29	101.44	113.40
1	5	3653	A	O5'-P-OP1	-6.29	100.04	105.70
1	5	2511	A	C2'-C3'-O3'	6.29	123.76	113.70
50	S2	1194	A	N9-C1'-C2'	-6.29	105.09	112.00
50	S2	1669	G	N9-C1'-C2'	6.28	122.17	114.00
7	D	145	TYR	CB-CA-C	6.28	122.96	110.40
16	N	96	ARG	NE-CZ-NH1	-6.27	117.16	120.30
50	S2	1420	G	O5'-P-OP2	-6.27	100.06	105.70
7	D	35	ARG	CG-CD-NE	6.27	124.96	111.80
7	D	30	TYR	CB-CA-C	6.27	122.93	110.40
56	SF	165	ASN	N-CA-CB	6.26	121.88	110.60
1	5	417	G	O4'-C1'-N9	6.26	113.21	108.20
1	5	2827	G	N9-C1'-C2'	6.26	122.14	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	3880	G	N9-C1'-C2'	6.26	122.14	114.00
82	Sf	148	TYR	CA-CB-CG	6.26	125.30	113.40
12	I	34	PHE	CB-CG-CD1	-6.26	116.42	120.80
3	8	62	A	C8-N9-C1'	6.25	138.96	127.70
7	D	293	ARG	NE-CZ-NH1	6.25	123.43	120.30
21	S	83	ARG	CG-CD-NE	6.25	124.93	111.80
50	S2	1519	U	N1-C1'-C2'	6.25	122.13	114.00
50	S2	1855	G	O5'-P-OP2	-6.25	100.07	105.70
1	5	4519	C	C4'-C3'-C2'	-6.25	96.35	102.60
50	S2	841	G	O4'-C1'-C2'	-6.25	99.55	105.80
1	5	2403	A	N9-C1'-C2'	6.24	122.12	114.00
25	W	8	PHE	CB-CG-CD2	-6.24	116.43	120.80
62	SL	89	ARG	NE-CZ-NH1	6.24	123.42	120.30
50	S2	475	C	O5'-P-OP1	-6.24	100.08	105.70
50	S2	1453	C	O4'-C1'-N1	6.24	113.19	108.20
1	5	1282	G	O5'-P-OP1	-6.24	100.08	105.70
14	L	192	PHE	N-CA-CB	6.24	121.83	110.60
50	S2	41	G	N9-C1'-C2'	-6.24	105.14	112.00
83	Sg	140	TYR	CA-CB-CG	-6.24	101.55	113.40
1	5	1279	A	C2'-C3'-O3'	6.24	123.68	113.70
1	5	1961	G	C2'-C3'-O3'	6.24	123.68	113.70
1	5	2673	G	O4'-C1'-C2'	-6.24	99.56	105.80
33	e	5	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	5	99	A	N9-C1'-C2'	-6.23	105.14	112.00
1	5	4718	G	N9-C1'-C2'	-6.23	105.15	112.00
50	S2	1022	U	C1'-O4'-C4'	-6.23	104.92	109.90
77	Sa	10	ARG	CG-CD-NE	-6.23	98.73	111.80
50	S2	66	G	N9-C1'-C2'	-6.22	105.15	112.00
20	R	107	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	5	4677	U	C3'-C2'-C1'	6.22	106.48	101.50
50	S2	1	U	C5'-C4'-C3'	6.22	125.95	116.00
3	8	81	C	O4'-C1'-N1	6.22	113.17	108.20
25	W	55	TYR	CB-CG-CD1	6.22	124.73	121.00
1	5	2082	G	N9-C1'-C2'	6.21	122.08	114.00
1	5	3791	C	O4'-C1'-N1	-6.21	103.23	108.20
1	5	4548	A	P-O5'-C5'	6.21	130.84	120.90
14	L	82	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	5	220	C	C2'-C3'-O3'	6.21	123.64	113.70
27	Y	15	ARG	NE-CZ-NH1	-6.21	117.19	120.30
36	h	89	ARG	CG-CD-NE	6.21	124.84	111.80
50	S2	1857	G	N9-C1'-C2'	-6.21	105.17	112.00
29	a	61	TYR	CB-CG-CD1	6.21	124.73	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	S2	980	A	C2'-C3'-O3'	6.21	123.64	113.70
38	j	11	ARG	CG-CD-NE	-6.21	98.77	111.80
31	c	90	ARG	CA-CB-CG	6.20	127.05	113.40
1	5	219	G	O5'-P-OP2	-6.20	100.12	105.70
50	S2	963	A	N9-C1'-C2'	6.20	122.06	114.00
50	S2	1668	U	N1-C1'-C2'	6.20	122.06	114.00
34	f	19	ARG	NE-CZ-NH2	-6.20	117.20	120.30
7	D	44	TYR	CA-CB-CG	-6.19	101.63	113.40
19	Q	33	ARG	NE-CZ-NH2	-6.19	117.20	120.30
50	S2	1223	A	N9-C1'-C2'	-6.19	105.19	112.00
1	5	1934	A	N9-C1'-C2'	-6.19	105.19	112.00
1	5	2666	U	C4'-C3'-C2'	-6.19	96.41	102.60
1	5	747	A	C2'-C3'-O3'	6.18	123.59	113.70
6	C	35	ASP	CB-CG-OD2	-6.18	112.73	118.30
10	G	54	PHE	CB-CA-C	6.18	122.77	110.40
50	S2	1617	G	N9-C1'-C2'	-6.18	105.20	112.00
1	5	5056	A	N9-C1'-C2'	6.18	122.04	114.00
1	5	5006	U	N1-C1'-C2'	-6.18	105.20	112.00
63	SM	127	TYR	CB-CG-CD1	6.18	124.71	121.00
5	B	137	TRP	CA-CB-CG	-6.18	101.97	113.70
61	SK	8	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	5	514	U	C4'-C3'-C2'	-6.17	96.42	102.60
6	C	80	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	5	4579	U	C2-N1-C1'	6.17	125.11	117.70
1	5	962	C	C4'-C3'-O3'	-6.17	96.44	109.40
52	SB	165	ARG	NE-CZ-NH1	-6.17	117.22	120.30
1	5	4560	C	O4'-C1'-N1	-6.17	103.27	108.20
19	Q	4	ASP	CB-CA-C	6.17	122.73	110.40
9	F	168	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	5	1379	C	C5'-C4'-O4'	6.16	116.50	109.10
82	Sf	146	LEU	N-CA-CB	6.16	122.73	110.40
50	S2	1839	U	C6-N1-C1'	-6.16	112.58	121.20
1	5	2470	C	O4'-C1'-C2'	-6.16	99.64	105.80
32	d	87	ARG	CA-CB-CG	6.16	126.94	113.40
50	S2	1123	C	O5'-P-OP1	-6.16	100.16	105.70
9	F	239	GLU	CA-CB-CG	6.15	126.94	113.40
35	g	90	ARG	CG-CD-NE	-6.15	98.88	111.80
1	5	3727	A	N9-C1'-C2'	6.15	122.00	114.00
1	5	2854	G	C2'-C3'-O3'	6.15	123.54	113.70
1	5	4451	G	N9-C1'-C2'	6.15	121.99	114.00
1	5	4976	U	C5'-C4'-O4'	6.15	116.48	109.10
20	R	9	ARG	NE-CZ-NH1	6.15	123.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4239	A	C2'-C3'-O3'	6.14	123.53	113.70
1	5	4880	C	N1-C1'-C2'	6.14	121.98	114.00
11	H	31	ARG	NE-CZ-NH2	-6.14	117.23	120.30
9	F	98	ARG	NE-CZ-NH2	-6.14	117.23	120.30
66	SP	44	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	5	409	G	N9-C1'-C2'	-6.14	105.25	112.00
1	5	2854	G	N9-C1'-C2'	-6.14	105.25	112.00
50	S2	1545	A	N9-C1'-C2'	6.13	121.97	114.00
1	5	1379	C	P-O5'-C5'	6.13	130.71	120.90
1	5	2107	C	C2'-C3'-O3'	6.13	123.51	113.70
50	S2	1603	G	O4'-C1'-N9	-6.13	103.30	108.20
31	c	39	ARG	CG-CD-NE	-6.13	98.93	111.80
50	S2	1735	A	N9-C1'-C2'	6.13	121.97	114.00
17	O	117	ARG	NE-CZ-NH1	6.13	123.36	120.30
50	S2	19	A	C2'-C3'-O3'	6.13	123.50	113.70
56	SF	164	ARG	CG-CD-NE	-6.13	98.94	111.80
29	a	132	ARG	NE-CZ-NH2	-6.12	117.24	120.30
6	C	311	ARG	NE-CZ-NH1	6.12	123.36	120.30
66	SP	42	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	5	1649	U	N1-C1'-C2'	6.12	121.95	114.00
50	S2	1021	U	N1-C1'-C2'	6.12	121.95	114.00
1	5	219	G	O4'-C1'-C2'	-6.11	99.69	105.80
19	Q	58	ARG	NE-CZ-NH2	-6.11	117.24	120.30
81	Se	41	ARG	CG-CD-NE	6.11	124.63	111.80
5	B	102	PHE	CB-CA-C	-6.11	98.19	110.40
8	E	59	TYR	N-CA-C	-6.11	94.51	111.00
8	E	157	ARG	NE-CZ-NH1	-6.11	117.25	120.30
50	S2	531	A	C2'-C3'-O3'	6.10	123.46	113.70
1	5	4948	C	C2'-C3'-O3'	6.10	123.46	113.70
3	8	62	A	C4-N9-C1'	-6.10	115.33	126.30
3	8	66	A	N9-C1'-C2'	6.10	121.93	114.00
7	D	145	TYR	CA-CB-CG	-6.09	101.82	113.40
67	SQ	62	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	5	1488	G	C2'-C3'-O3'	6.09	123.44	113.70
1	5	1614	C	C2'-C3'-O3'	6.09	123.44	113.70
50	S2	313	A	N9-C1'-C2'	6.08	121.91	114.00
38	j	39	TYR	CB-CA-C	-6.08	98.24	110.40
32	d	87	ARG	CG-CD-NE	-6.08	99.04	111.80
50	S2	1552	G	N9-C1'-C2'	-6.08	105.32	112.00
70	ST	53	PHE	CB-CG-CD1	6.08	125.05	120.80
45	r	45	HIS	CB-CA-C	-6.07	98.26	110.40
1	5	1214	C	O4'-C1'-N1	-6.07	103.34	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	5040	U	C4'-C3'-O3'	-6.07	96.65	109.40
64	SN	128	TYR	CB-CG-CD1	6.07	124.64	121.00
43	o	78	ARG	NE-CZ-NH1	-6.07	117.27	120.30
50	S2	943	U	C2-N1-C1'	6.07	124.98	117.70
14	L	36	ARG	NE-CZ-NH1	6.06	123.33	120.30
19	Q	181	ARG	CG-CD-NE	-6.06	99.07	111.80
1	5	235	A	C1'-O4'-C4'	-6.06	105.05	109.90
1	5	4871	C	O4'-C1'-N1	-6.06	103.35	108.20
6	C	78	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	5	4876	U	N1-C1'-C2'	6.06	121.88	114.00
60	SJ	20	PHE	CB-CG-CD1	6.06	125.04	120.80
1	5	3843	C	O4'-C1'-N1	-6.05	103.36	108.20
3	8	64	U	C2-N1-C1'	6.05	124.96	117.70
50	S2	1419	C	C2'-C3'-O3'	6.05	123.38	113.70
20	R	108	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	5	4731	G	O4'-C1'-N9	6.05	113.04	108.20
1	5	4049	U	O4'-C1'-N1	6.04	113.04	108.20
19	Q	166	TYR	CB-CG-CD1	6.04	124.63	121.00
50	S2	959	G	C2'-C3'-O3'	6.04	123.37	113.70
4	A	83	HIS	N-CA-C	-6.04	94.69	111.00
50	S2	9	U	C2'-C3'-O3'	6.04	123.36	113.70
1	5	4270	C	C2'-C3'-O3'	6.04	123.36	113.70
1	5	4694	G	O5'-P-OP1	-6.04	100.27	105.70
16	N	71	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	5	4519	C	C1'-O4'-C4'	-6.03	105.07	109.90
1	5	3738	G	N9-C1'-C2'	-6.03	105.37	112.00
1	5	2119	C	O4'-C1'-N1	6.03	113.02	108.20
1	5	4599	A	N9-C1'-C2'	6.03	121.83	114.00
1	5	1210	C	N1-C1'-C2'	6.03	121.83	114.00
50	S2	1588	A	N9-C1'-C2'	6.02	121.83	114.00
1	5	67	C	N1-C1'-C2'	-6.02	105.38	112.00
1	5	1658	G	N9-C1'-C2'	6.02	121.83	114.00
25	W	57	ARG	NE-CZ-NH1	6.02	123.31	120.30
50	S2	1433	C	C4'-C3'-C2'	-6.02	96.58	102.60
1	5	4986	G	N9-C1'-C2'	6.01	121.82	114.00
6	C	312	ARG	CG-CD-NE	-6.01	99.17	111.80
34	f	36	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	5	3739	C	O4'-C1'-C2'	-6.01	99.79	105.80
31	c	56	ARG	NE-CZ-NH1	6.01	123.31	120.30
50	S2	398	A	N9-C1'-C2'	-6.01	105.39	112.00
2	7	58	A	N9-C1'-C2'	-6.01	105.39	112.00
1	5	52	G	C2'-C3'-O3'	6.00	123.30	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	h	84	ARG	CG-CD-NE	-6.00	99.20	111.80
3	8	13	G	N9-C1'-C2'	6.00	121.80	114.00
1	5	2744	A	N9-C1'-C2'	6.00	121.80	114.00
18	P	127	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	5	1697	G	O5'-P-OP2	6.00	117.89	110.70
50	S2	1858	G	C2'-C3'-O3'	6.00	123.29	113.70
50	S2	1433	C	O4'-C4'-C3'	-5.99	98.01	104.00
1	5	1523	A	O5'-P-OP1	-5.98	100.31	105.70
45	r	103	ARG	NE-CZ-NH1	5.98	123.29	120.30
57	SG	191	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	5	3913	G	C2'-C3'-O3'	5.98	123.27	113.70
50	S2	73	C	N1-C1'-C2'	5.98	121.77	114.00
50	S2	855	G	N9-C1'-C2'	-5.98	105.42	112.00
2	7	58	A	C2'-C3'-O3'	5.97	123.26	113.70
50	S2	400	C	N1-C1'-C2'	-5.97	105.43	112.00
52	SB	82	ARG	NE-CZ-NH1	-5.97	117.31	120.30
50	S2	1084	A	N9-C1'-C2'	-5.97	105.43	112.00
7	D	265	ARG	NE-CZ-NH2	-5.97	117.32	120.30
50	S2	918	U	C1'-O4'-C4'	-5.97	105.13	109.90
7	D	54	ARG	CB-CG-CD	5.96	127.10	111.60
27	Y	126	ARG	NE-CZ-NH2	-5.96	117.32	120.30
52	SB	107	ARG	NE-CZ-NH1	5.96	123.28	120.30
5	B	258	HIS	N-CA-C	5.96	127.09	111.00
37	i	85	ARG	NE-CZ-NH2	-5.96	117.32	120.30
50	S2	795	A	N9-C1'-C2'	5.96	121.75	114.00
50	S2	1420	G	C2'-C3'-O3'	5.96	123.23	113.70
1	5	4291	G	N9-C1'-C2'	5.95	121.74	114.00
1	5	4979	A	N9-C1'-C2'	5.95	121.74	114.00
29	a	65	ARG	CG-CD-NE	-5.95	99.30	111.80
50	S2	1114	U	C2'-C3'-O3'	5.95	123.22	113.70
50	S2	1857	G	C2'-C3'-O3'	5.95	123.22	113.70
50	S2	1416	C	C2'-C3'-O3'	5.95	123.22	113.70
1	5	2307	A	N9-C1'-C2'	5.95	121.73	114.00
1	5	2323	C	N1-C1'-C2'	-5.95	105.46	112.00
64	SN	55	ARG	CG-CD-NE	5.94	124.28	111.80
1	5	1398	A	O5'-P-OP2	-5.94	100.35	105.70
1	5	1992	U	O4'-C1'-N1	5.94	112.95	108.20
1	5	2373	C	N1-C1'-C2'	5.94	121.72	114.00
50	S2	417	C	C2'-C3'-O3'	5.94	123.20	113.70
1	5	4670	C	O4'-C1'-N1	-5.94	103.45	108.20
15	M	6	PHE	CB-CA-C	5.94	122.27	110.40
1	5	231	U	C4'-C3'-O3'	-5.93	96.94	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	T	57	TYR	CA-CB-CG	5.93	124.68	113.40
33	e	46	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	5	4473	A	C4-N9-C1'	5.93	136.98	126.30
1	5	53	C	N1-C1'-C2'	-5.93	105.47	112.00
14	L	82	ARG	CG-CD-NE	-5.93	99.35	111.80
1	5	669	C	C1'-O4'-C4'	-5.93	105.16	109.90
15	M	90	ARG	CG-CD-NE	-5.92	99.36	111.80
1	5	1495	G	N9-C1'-C2'	5.92	121.70	114.00
1	5	1894	C	N1-C1'-C2'	5.92	121.70	114.00
31	c	56	ARG	CD-NE-CZ	5.92	131.89	123.60
50	S2	993	G	C5'-C4'-O4'	5.92	116.20	109.10
1	5	936	C	C4'-C3'-O3'	5.92	124.83	113.00
50	S2	1309	C	C4'-C3'-O3'	5.91	124.83	113.00
50	S2	474	G	C2'-C3'-O3'	5.91	123.16	113.70
1	5	2322	G	C2'-C3'-O3'	5.91	123.15	113.70
1	5	2515	G	N9-C1'-C2'	-5.91	105.50	112.00
6	C	102	PHE	N-CA-CB	5.91	121.23	110.60
50	S2	482	G	N9-C1'-C2'	-5.91	105.50	112.00
1	5	4479	A	N9-C1'-C2'	-5.91	105.50	112.00
1	5	1930	U	O4'-C1'-N1	-5.91	103.47	108.20
62	SL	92	TYR	CA-CB-CG	5.91	124.62	113.40
1	5	4510	A	N9-C1'-C2'	5.90	121.67	114.00
60	SJ	45	ARG	NE-CZ-NH2	-5.90	117.35	120.30
33	e	20	PHE	CB-CG-CD1	-5.90	116.67	120.80
1	5	4449	A	N9-C1'-C2'	-5.90	105.51	112.00
1	5	2070	U	N1-C1'-C2'	5.90	121.67	114.00
1	5	40	G	N9-C1'-C2'	5.89	121.66	114.00
1	5	4215	C	O4'-C1'-C2'	-5.89	99.91	105.80
32	d	78	ARG	NE-CZ-NH1	5.89	123.25	120.30
50	S2	65	C	O4'-C1'-N1	5.89	112.91	108.20
50	S2	446	G	C2'-C3'-O3'	5.89	123.13	113.70
85	S5	47	U	OP1-P-O3'	-5.89	92.24	105.20
50	S2	1273	C	N1-C1'-C2'	-5.89	105.53	112.00
1	5	3774	A	N9-C1'-C2'	5.88	121.65	114.00
62	SL	62	PHE	CB-CA-C	5.88	122.17	110.40
50	S2	365	C	N1-C1'-C2'	-5.88	105.53	112.00
1	5	2642	A	N9-C1'-C2'	-5.88	105.53	112.00
50	S2	1868	U	N1-C1'-C2'	5.88	121.64	114.00
43	o	40	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	5	1324	A	N9-C1'-C2'	5.87	121.64	114.00
50	S2	26	U	C2'-C3'-O3'	5.87	123.09	113.70
57	SG	213	LEU	CA-CB-CG	5.87	128.80	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	SX	17	ARG	CG-CD-NE	-5.87	99.47	111.80
1	5	2305	U	O4'-C4'-C3'	-5.87	98.13	104.00
1	5	1487	G	C2'-C3'-O3'	5.86	123.08	113.70
21	S	84	TYR	CB-CG-CD1	5.86	124.52	121.00
54	SD	67	ARG	CG-CD-NE	5.86	124.11	111.80
1	5	33	A	N9-C1'-C2'	5.86	121.62	114.00
1	5	4481	U	C5'-C4'-O4'	5.86	116.13	109.10
60	SJ	48	PHE	CB-CG-CD1	-5.86	116.70	120.80
1	5	934	C	O4'-C1'-N1	-5.86	103.52	108.20
1	5	4763	U	O4'-C1'-N1	5.86	112.89	108.20
8	E	275	ASN	N-CA-CB	5.86	121.14	110.60
73	SW	3	ARG	CG-CD-NE	-5.86	99.50	111.80
14	L	34	ARG	NE-CZ-NH2	-5.86	117.37	120.30
50	S2	30	C	N1-C1'-C2'	5.86	121.61	114.00
1	5	4074	C	N1-C1'-C2'	5.85	121.61	114.00
1	5	4201	G	N9-C1'-C2'	5.85	121.61	114.00
50	S2	1313	A	N9-C1'-C2'	5.85	121.61	114.00
11	H	54	ARG	NE-CZ-NH2	-5.85	117.37	120.30
50	S2	848	U	C2-N3-C4	-5.85	123.49	127.00
1	5	2305	U	C5'-C4'-O4'	5.85	116.12	109.10
50	S2	1367	U	C2'-C3'-O3'	5.85	123.06	113.70
50	S2	1477	U	C2'-C3'-O3'	5.85	123.06	113.70
1	5	2268	A	O4'-C1'-N9	-5.84	103.53	108.20
1	5	4199	C	O4'-C1'-C2'	-5.84	99.96	105.80
3	8	81	C	C5'-C4'-C3'	5.84	125.35	116.00
52	SB	67	PHE	N-CA-CB	-5.84	100.10	110.60
1	5	2586	G	O4'-C1'-N9	5.83	112.87	108.20
50	S2	441	C	C4'-C3'-O3'	-5.83	97.15	109.40
50	S2	92	A	O4'-C1'-N9	-5.83	103.53	108.20
75	SY	76	TYR	CB-CG-CD1	-5.83	117.50	121.00
27	Y	121	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	5	72	C	C1'-O4'-C4'	-5.83	105.24	109.90
1	5	657	C	C2'-C3'-O3'	5.83	123.02	113.70
60	SJ	108	ARG	NE-CZ-NH1	5.83	123.21	120.30
33	e	60	TYR	CB-CA-C	5.82	122.04	110.40
50	S2	1658	G	N9-C1'-C2'	-5.82	105.60	112.00
50	S2	548	C	C2'-C3'-O3'	5.82	123.01	113.70
1	5	4548	A	C5'-C4'-O4'	5.81	116.08	109.10
4	A	147	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	5	920	C	C5'-C4'-O4'	5.81	116.08	109.10
1	5	1650	A	C4-N9-C1'	-5.81	115.84	126.30
50	S2	454	U	N1-C1'-C2'	5.81	121.55	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4481	U	N1-C1'-C2'	5.80	121.55	114.00
55	SE	121	TYR	CA-CB-CG	-5.80	102.37	113.40
1	5	2448	G	N9-C1'-C2'	5.80	121.54	114.00
6	C	350	ARG	NE-CZ-NH2	-5.80	117.40	120.30
50	S2	563	G	N9-C1'-C2'	-5.80	105.62	112.00
12	I	94	PHE	CB-CG-CD2	-5.79	116.74	120.80
53	SC	241	PHE	CB-CG-CD2	-5.79	116.75	120.80
59	SI	112	TRP	CA-CB-CG	5.79	124.71	113.70
12	I	119	PHE	CB-CG-CD2	-5.79	116.75	120.80
1	5	85	G	N9-C1'-C2'	-5.79	105.63	112.00
1	5	2119	C	C1'-O4'-C4'	-5.79	105.27	109.90
50	S2	621	C	N1-C1'-C2'	-5.79	105.63	112.00
52	SB	133	TYR	CA-CB-CG	5.79	124.40	113.40
67	SQ	71	ARG	NE-CZ-NH1	5.79	123.19	120.30
50	S2	918	U	O4'-C1'-N1	5.79	112.83	108.20
34	f	6	TRP	N-CA-C	-5.79	95.38	111.00
1	5	2553	A	C1'-O4'-C4'	-5.78	105.27	109.90
44	p	14	TYR	CB-CA-C	5.78	121.96	110.40
1	5	1341	U	N1-C1'-C2'	5.78	121.51	114.00
50	S2	649	U	O5'-P-OP1	-5.78	100.50	105.70
5	B	117	ARG	CG-CD-NE	-5.77	99.68	111.80
1	5	197	A	N9-C1'-C2'	5.77	121.50	114.00
8	E	268	ARG	NE-CZ-NH2	-5.77	117.41	120.30
50	S2	848	U	C6-N1-C1'	-5.77	113.12	121.20
52	SB	205	TYR	CB-CG-CD1	-5.77	117.54	121.00
3	8	34	U	C3'-C2'-C1'	5.77	106.12	101.50
1	5	1815	G	C1'-O4'-C4'	-5.77	105.29	109.90
16	N	30	TYR	N-CA-CB	-5.77	100.22	110.60
80	Sd	40	ARG	NE-CZ-NH1	5.77	123.18	120.30
50	S2	855	G	C2'-C3'-O3'	5.76	122.92	113.70
1	5	4473	A	C8-N9-C1'	-5.76	117.33	127.70
1	5	4463	U	O4'-C1'-N1	5.76	112.81	108.20
50	S2	662	G	N9-C1'-C2'	5.76	121.49	114.00
58	SH	189	PHE	CB-CA-C	5.76	121.92	110.40
3	8	115	G	C2'-C3'-O3'	5.76	122.91	113.70
21	S	97	TYR	CA-CB-CG	-5.76	102.46	113.40
4	A	63	PHE	CB-CG-CD2	-5.75	116.77	120.80
50	S2	1832	A	O5'-P-OP2	-5.75	100.52	105.70
50	S2	495	U	C1'-C2'-O2'	-5.75	93.35	110.60
1	5	1285	U	O4'-C1'-N1	5.75	112.80	108.20
1	5	2769	U	O4'-C1'-N1	5.75	112.80	108.20
69	SS	86	ARG	NE-CZ-NH2	5.75	123.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2807	A	C2'-C3'-O3'	5.75	122.90	113.70
1	5	1398	A	O4'-C1'-N9	5.75	112.80	108.20
3	8	79	G	N9-C1'-C2'	5.74	121.47	114.00
50	S2	594	A	C8-N9-C1'	-5.74	117.36	127.70
55	SE	18	TRP	CB-CA-C	5.74	121.89	110.40
1	5	292	G	C4-N9-C1'	-5.74	119.04	126.50
1	5	1506	G	N9-C1'-C2'	-5.73	105.69	112.00
19	Q	32	TYR	CA-CB-CG	5.73	124.29	113.40
74	SX	17	ARG	NE-CZ-NH1	-5.73	117.43	120.30
3	8	135	C	N1-C1'-C2'	5.73	121.45	114.00
69	SS	130	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	5	3686	G	N9-C1'-C2'	-5.73	105.70	112.00
1	5	4125	C	C4'-C3'-O3'	-5.73	97.37	109.40
1	5	88	A	N9-C1'-C2'	5.72	121.44	114.00
1	5	3691	G	N9-C1'-C2'	5.72	121.44	114.00
1	5	236	G	N9-C1'-C2'	5.72	121.44	114.00
1	5	1398	A	O5'-P-OP1	5.72	117.56	110.70
27	Y	18	HIS	N-CA-CB	5.72	120.89	110.60
36	h	119	PHE	CB-CG-CD2	-5.72	116.80	120.80
50	S2	662	G	O4'-C1'-N9	-5.72	103.62	108.20
1	5	4385	A	C2'-C3'-O3'	-5.72	96.92	109.50
75	SY	63	HIS	N-CA-CB	5.72	120.89	110.60
1	5	1264	C	C2'-C3'-O3'	5.71	122.84	113.70
4	A	34	PHE	N-CA-CB	5.71	120.89	110.60
1	5	111	C	N1-C1'-C2'	-5.71	105.72	112.00
9	F	100	ILE	CG1-CB-CG2	5.71	123.96	111.40
6	C	200	ARG	NE-CZ-NH2	-5.71	117.45	120.30
55	SE	99	PHE	CB-CG-CD1	5.71	124.80	120.80
69	SS	82	TRP	CA-CB-CG	5.71	124.55	113.70
1	5	2282	A	N9-C1'-C2'	5.70	121.41	114.00
1	5	2360	A	N9-C1'-C2'	5.70	121.41	114.00
1	5	2405	G	N9-C1'-C2'	-5.70	105.73	112.00
1	5	85	G	O4'-C1'-C2'	-5.70	100.10	105.80
9	F	136	ARG	CG-CD-NE	-5.70	99.83	111.80
21	S	10	TYR	CB-CG-CD1	-5.70	117.58	121.00
1	5	1438	U	C2'-C3'-O3'	5.69	122.81	113.70
1	5	2118	G	O4'-C4'-C3'	-5.69	98.31	104.00
19	Q	68	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	5	84	A	C4-N9-C1'	-5.69	116.06	126.30
50	S2	146	G	N9-C1'-C2'	-5.69	105.74	112.00
50	S2	1842	C	N1-C1'-C2'	5.68	121.39	114.00
83	Sg	83	TRP	CA-CB-CG	-5.68	102.90	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	101	ARG	NE-CZ-NH2	5.68	123.14	120.30
20	R	97	ARG	CG-CD-NE	-5.68	99.87	111.80
1	5	2643	G	C2'-C3'-O3'	5.68	122.79	113.70
57	SG	156	TYR	CA-CB-CG	-5.68	102.61	113.40
1	5	100	C	C5'-C4'-O4'	5.68	115.92	109.10
1	5	1696	C	C2'-C3'-O3'	5.68	122.79	113.70
50	S2	504	G	N9-C1'-C2'	5.67	121.38	114.00
1	5	1281	G	C5'-C4'-O4'	5.67	115.91	109.10
1	5	1849	U	O5'-P-OP1	5.67	117.50	110.70
30	b	17	HIS	CB-CA-C	-5.67	99.06	110.40
26	X	137	TYR	CB-CG-CD1	5.67	124.40	121.00
50	S2	369	C	N1-C1'-C2'	5.67	121.37	114.00
4	A	37	ARG	CG-CD-NE	-5.67	99.90	111.80
50	S2	1291	A	C3'-C2'-C1'	5.67	106.03	101.50
2	7	7	G	C5'-C4'-O4'	5.66	115.90	109.10
27	Y	61	HIS	N-CA-CB	5.66	120.79	110.60
1	5	1494	U	N1-C1'-C2'	5.66	121.36	114.00
5	B	169	ARG	NE-CZ-NH2	-5.66	117.47	120.30
19	Q	32	TYR	CB-CG-CD2	-5.66	117.61	121.00
55	SE	99	PHE	CB-CG-CD2	-5.66	116.84	120.80
58	SH	116	ARG	NE-CZ-NH1	5.66	123.13	120.30
7	D	35	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	5	1639	U	N1-C1'-C2'	5.65	121.35	114.00
33	e	75	ARG	CG-CD-NE	-5.65	99.93	111.80
1	5	85	G	O4'-C1'-N9	5.65	112.72	108.20
1	5	3776	G	N9-C1'-C2'	-5.65	105.79	112.00
38	j	27	TYR	N-CA-CB	5.65	120.77	110.60
62	SL	89	ARG	CG-CD-NE	-5.65	99.94	111.80
65	SO	121	ARG	NE-CZ-NH1	5.65	123.12	120.30
75	SY	61	ARG	CG-CD-NE	-5.64	99.95	111.80
1	5	514	U	C4'-C3'-O3'	5.64	124.28	113.00
50	S2	1546	G	N9-C1'-C2'	5.64	121.33	114.00
50	S2	382	C	N1-C1'-C2'	5.64	121.33	114.00
1	5	2665	U	N1-C1'-C2'	-5.64	105.80	112.00
5	B	246	ARG	NE-CZ-NH1	5.64	123.12	120.30
60	SJ	150	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	5	1642	A	P-O3'-C3'	5.63	126.46	119.70
1	5	370	U	N1-C1'-C2'	5.63	121.32	114.00
8	E	278	TYR	CB-CG-CD1	-5.63	117.62	121.00
11	H	180	TYR	CA-CB-CG	5.63	124.10	113.40
50	S2	746	C	C2'-C3'-O3'	5.63	122.71	113.70
1	5	4966	A	C8-N9-C1'	-5.63	117.57	127.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4114	C	N1-C1'-C2'	5.63	121.32	114.00
21	S	94	TYR	CA-CB-CG	-5.63	102.71	113.40
1	5	490	C	N1-C1'-C2'	5.63	121.31	114.00
1	5	1539	G	C2'-C3'-O3'	5.63	122.70	113.70
1	5	1876	U	C2'-C3'-O3'	5.63	122.70	113.70
1	5	5062	G	P-O5'-C5'	5.63	129.90	120.90
19	Q	176	ARG	CG-CD-NE	-5.63	99.98	111.80
50	S2	60	A	C1'-C2'-O2'	-5.63	93.72	110.60
50	S2	1243	U	C2'-C3'-O3'	5.63	122.70	113.70
1	5	703	G	C1'-O4'-C4'	-5.62	105.40	109.90
1	5	4753	U	C2'-C3'-O3'	5.62	122.70	113.70
5	B	169	ARG	CG-CD-NE	5.62	123.61	111.80
20	R	110	ARG	NE-CZ-NH1	5.62	123.11	120.30
50	S2	943	U	C5'-C4'-O4'	5.62	115.84	109.10
1	5	2383	C	N1-C1'-C2'	5.62	121.30	114.00
1	5	3773	U	N1-C1'-C2'	-5.62	105.82	112.00
50	S2	1395	C	O4'-C1'-C2'	-5.62	100.18	105.80
3	8	39	G	N9-C1'-C2'	-5.61	105.83	112.00
6	C	311	ARG	CG-CD-NE	-5.61	100.01	111.80
38	j	66	HIS	CA-CB-CG	-5.61	104.06	113.60
28	Z	121	ARG	NE-CZ-NH2	-5.61	117.50	120.30
50	S2	1085	C	N1-C1'-C2'	5.61	121.29	114.00
52	SB	196	ASP	CB-CG-OD1	5.61	123.35	118.30
14	L	7	GLY	N-CA-C	-5.60	99.09	113.10
55	SE	51	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	5	1295	C	N1-C1'-C2'	5.60	121.28	114.00
1	5	2686	G	N9-C1'-C2'	-5.60	105.84	112.00
69	SS	124	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	5	1521	C	C2'-C3'-O3'	5.60	122.66	113.70
1	5	2088	A	N9-C1'-C2'	-5.60	105.84	112.00
1	5	2857	A	C1'-C2'-O2'	-5.59	93.82	110.60
7	D	210	TYR	CB-CG-CD1	-5.59	117.64	121.00
40	l	12	PHE	CB-CG-CD2	-5.59	116.88	120.80
50	S2	26	U	O4'-C1'-C2'	-5.59	100.21	105.80
50	S2	1376	A	C2'-C3'-O3'	5.59	122.65	113.70
1	5	2487	G	C2'-C3'-O3'	5.59	122.65	113.70
45	r	21	ASN	CB-CA-C	5.59	121.58	110.40
1	5	2077	C	N1-C1'-C2'	-5.59	105.85	112.00
10	G	57	TRP	CA-CB-CG	-5.58	103.10	113.70
50	S2	649	U	N1-C1'-C2'	5.58	121.26	114.00
1	5	3663	A	O4'-C1'-N9	-5.58	103.74	108.20
1	5	118	C	C2'-C3'-O3'	5.58	122.62	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	I	213	HIS	CB-CA-C	5.58	121.56	110.40
19	Q	178	ARG	CG-CD-NE	-5.58	100.09	111.80
50	S2	821	G	O4'-C4'-C3'	-5.58	98.42	104.00
1	5	1614	C	N1-C1'-C2'	-5.58	105.87	112.00
11	H	115	ARG	CG-CD-NE	-5.58	100.09	111.80
14	L	6	ASN	N-CA-CB	5.58	120.64	110.60
54	SD	65	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	5	4950	U	N1-C1'-C2'	5.57	121.25	114.00
56	SF	204	ARG	NE-CZ-NH1	5.57	123.09	120.30
81	Se	38	TYR	CA-CB-CG	5.57	123.99	113.40
1	5	4767	C	C2'-C3'-O3'	5.57	122.61	113.70
1	5	3773	U	C4'-C3'-C2'	-5.57	97.03	102.60
1	5	1632	A	O4'-C1'-N9	5.57	112.65	108.20
1	5	1932	A	N9-C1'-C2'	5.57	121.24	114.00
57	SG	191	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	5	2360	A	O4'-C1'-N9	-5.56	103.75	108.20
1	5	4723	A	C5'-C4'-O4'	5.56	115.78	109.10
14	L	163	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	5	2474	G	C2'-C3'-O3'	5.56	122.60	113.70
1	5	1534	A	P-O5'-C5'	5.56	129.80	120.90
2	7	75	G	O4'-C1'-N9	5.56	112.65	108.20
65	SO	128	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	5	1672	U	C6-N1-C1'	-5.56	113.42	121.20
35	g	9	ARG	CG-CD-NE	-5.56	100.13	111.80
1	5	977	C	C4'-C3'-C2'	-5.55	97.05	102.60
1	5	4693	C	O4'-C4'-C3'	-5.55	98.45	104.00
28	Z	28	ASN	N-CA-C	-5.55	96.00	111.00
50	S2	642	U	O5'-P-OP2	-5.55	100.70	105.70
4	A	211	PHE	CB-CG-CD2	-5.55	116.91	120.80
16	N	182	HIS	N-CA-CB	5.55	120.59	110.60
1	5	1734	G	N9-C1'-C2'	-5.55	105.89	112.00
50	S2	457	C	N1-C1'-C2'	-5.55	105.90	112.00
1	5	1827	C	N1-C1'-C2'	5.55	121.21	114.00
50	S2	661	U	N1-C1'-C2'	-5.54	105.90	112.00
23	U	101	ARG	NE-CZ-NH1	5.54	123.07	120.30
50	S2	844	U	C1'-O4'-C4'	-5.54	105.47	109.90
1	5	687	U	N1-C1'-C2'	-5.54	105.91	112.00
66	SP	47	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	5	3735	G	C4'-C3'-O3'	-5.53	97.79	109.40
10	G	235	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	5	1501	C	C1'-O4'-C4'	-5.53	105.48	109.90
1	5	4076	G	C1'-O4'-C4'	-5.53	105.48	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1359	G	N9-C1'-C2'	5.53	121.18	114.00
9	F	98	ARG	NE-CZ-NH1	5.53	123.06	120.30
13	J	54	ARG	NE-CZ-NH1	5.53	123.06	120.30
52	SB	198	GLU	OE1-CD-OE2	-5.53	116.67	123.30
1	5	4326	G	N9-C1'-C2'	5.52	121.18	114.00
50	S2	1292	C	O4'-C4'-C3'	-5.52	98.48	104.00
1	5	4944	C	N1-C1'-C2'	5.52	121.18	114.00
9	F	72	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	5	1626	G	N9-C1'-C2'	-5.52	105.93	112.00
1	5	1631	A	C5'-C4'-O4'	5.52	115.72	109.10
1	5	2754	G	N9-C1'-C2'	-5.52	105.93	112.00
1	5	956	A	N9-C1'-C2'	-5.52	105.93	112.00
23	U	90	TYR	CB-CA-C	-5.52	99.36	110.40
1	5	1398	A	C2'-C3'-O3'	5.52	122.53	113.70
1	5	2385	U	N1-C1'-C2'	5.51	121.17	114.00
1	5	2396	A	N9-C1'-C2'	5.51	121.17	114.00
19	Q	184	ARG	CB-CG-CD	5.51	125.94	111.60
1	5	2398	U	C2'-C3'-O3'	5.51	122.52	113.70
1	5	2468	U	C4'-C3'-O3'	5.51	124.03	113.00
29	a	61	TYR	N-CA-C	-5.51	96.11	111.00
33	e	35	TRP	CB-CG-CD1	-5.51	119.83	127.00
19	Q	104	ARG	NE-CZ-NH1	5.51	123.06	120.30
44	p	18	TYR	CA-CB-CG	5.51	123.87	113.40
45	r	45	HIS	N-CA-CB	-5.51	100.68	110.60
50	S2	839	C	N1-C1'-C2'	5.51	121.16	114.00
1	5	1282	G	O5'-P-OP2	5.51	117.31	110.70
69	SS	11	HIS	CB-CA-C	5.51	121.42	110.40
1	5	3886	G	N9-C1'-C2'	-5.50	105.94	112.00
50	S2	868	G	N9-C1'-C2'	-5.50	105.94	112.00
1	5	3906	A	N9-C1'-C2'	-5.50	105.95	112.00
21	S	152	PHE	CB-CG-CD2	-5.50	116.95	120.80
50	S2	924	G	N9-C1'-C2'	-5.50	105.95	112.00
1	5	2450	G	N9-C1'-C2'	-5.50	105.95	112.00
1	5	4731	G	N9-C1'-C2'	5.50	121.14	114.00
1	5	4978	G	N9-C1'-C2'	5.50	121.15	114.00
1	5	4076	G	O4'-C1'-N9	5.49	112.59	108.20
1	5	3667	C	C2'-C3'-O3'	5.49	122.48	113.70
1	5	4497	U	P-O3'-C3'	5.49	126.28	119.70
1	5	4909	A	C1'-O4'-C4'	-5.48	105.52	109.90
43	o	26	TYR	CB-CG-CD1	5.48	124.29	121.00
1	5	398	A	N9-C1'-C2'	5.48	121.12	114.00
1	5	977	C	C5'-C4'-O4'	5.48	115.68	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	e	36	ARG	NE-CZ-NH1	-5.48	117.56	120.30
50	S2	447	A	C1'-O4'-C4'	-5.48	105.52	109.90
1	5	3912	U	C1'-C2'-O2'	-5.48	94.16	110.60
31	c	78	ASN	N-CA-CB	5.48	120.46	110.60
1	5	2583	C	C2'-C3'-O3'	5.48	122.46	113.70
1	5	2056	G	N9-C1'-C2'	-5.47	105.98	112.00
8	E	153	HIS	N-CA-CB	-5.47	100.75	110.60
1	5	421	C	C2'-C3'-O3'	5.47	122.46	113.70
1	5	3905	A	N9-C1'-C2'	-5.47	105.98	112.00
50	S2	393	U	O4'-C1'-N1	5.47	112.58	108.20
1	5	2673	G	C1'-O4'-C4'	-5.47	105.52	109.90
1	5	2858	A	N9-C1'-C2'	5.47	121.11	114.00
1	5	4975	G	O4'-C1'-N9	5.47	112.57	108.20
8	E	278	TYR	CB-CG-CD2	-5.47	117.72	121.00
50	S2	31	U	N1-C1'-C2'	5.47	121.11	114.00
40	l	45	ARG	CB-CG-CD	5.46	125.81	111.60
1	5	3634	G	C2'-C3'-O3'	5.46	122.44	113.70
50	S2	1315	U	C2'-C3'-O3'	5.46	122.44	113.70
1	5	1724	G	C8-N9-C1'	-5.46	119.91	127.00
1	5	3898	G	C2'-C3'-O3'	5.46	122.43	113.70
1	5	2852	U	O4'-C1'-C2'	-5.45	100.35	105.80
16	N	114	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	5	3875	G	C2'-C3'-O3'	5.45	122.42	113.70
10	G	49	ARG	CG-CD-NE	-5.45	100.35	111.80
50	S2	604	A	C2'-C3'-O3'	5.45	122.42	113.70
66	SP	81	ARG	NE-CZ-NH1	5.45	123.03	120.30
53	SC	97	PHE	CB-CG-CD2	-5.45	116.99	120.80
1	5	693	C	C2'-C3'-O3'	5.45	122.41	113.70
1	5	4873	G	N9-C1'-C2'	5.45	121.08	114.00
50	S2	1419	C	O5'-P-OP2	-5.45	100.80	105.70
1	5	2325	C	O4'-C1'-C2'	-5.44	100.36	105.80
4	A	16	PHE	CB-CA-C	5.44	121.28	110.40
34	f	6	TRP	CB-CA-C	5.44	121.28	110.40
50	S2	381	C	C3'-C2'-C1'	5.44	105.85	101.50
19	Q	26	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	5	1211	G	N9-C1'-C2'	-5.43	106.03	112.00
62	SL	100	ASN	N-CA-C	5.43	125.67	111.00
1	5	2268	A	C2'-C3'-O3'	5.43	122.39	113.70
7	D	66	TYR	CB-CG-CD1	5.43	124.26	121.00
26	X	117	TYR	CB-CA-C	5.43	121.26	110.40
33	e	43	ASN	CB-CA-C	5.43	121.26	110.40
1	5	372	A	N9-C1'-C2'	5.43	121.06	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2054	U	C1'-O4'-C4'	-5.43	105.56	109.90
1	5	4909	A	O4'-C1'-N9	5.42	112.54	108.20
20	R	108	ARG	CD-NE-CZ	5.42	131.19	123.60
64	SN	64	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	5	210	C	N1-C1'-C2'	5.42	121.05	114.00
13	J	32	ARG	CG-CD-NE	-5.42	100.42	111.80
1	5	280	G	C1'-O4'-C4'	-5.42	105.57	109.90
1	5	3648	A	C1'-O4'-C4'	-5.42	105.57	109.90
32	d	44	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	5	1975	G	O4'-C1'-N9	-5.41	103.87	108.20
1	5	4713	G	C2'-C3'-O3'	5.41	122.36	113.70
50	S2	1432	U	N1-C1'-C2'	5.41	121.04	114.00
1	5	4481	U	C2-N1-C1'	5.41	124.19	117.70
21	S	171	ARG	CG-CD-NE	5.41	123.16	111.80
60	SJ	64	ASP	CB-CG-OD1	-5.41	113.43	118.30
1	5	1852	U	N1-C1'-C2'	-5.41	106.05	112.00
1	5	2117	G	O4'-C4'-C3'	-5.41	98.59	104.00
5	B	119	TYR	CB-CA-C	5.41	121.22	110.40
8	E	129	PHE	CB-CG-CD1	5.41	124.58	120.80
1	5	4579	U	C6-N1-C1'	-5.41	113.63	121.20
30	b	6	ASN	CB-CA-C	5.41	121.21	110.40
1	5	2272	C	C1'-C2'-O2'	-5.40	94.39	110.60
1	5	4280	A	C4'-C3'-C2'	-5.40	97.20	102.60
1	5	1365	C	C4'-C3'-O3'	5.40	123.81	113.00
1	5	3625	G	C4'-C3'-O3'	-5.40	98.06	109.40
1	5	4915	G	C2'-C3'-O3'	5.40	122.34	113.70
21	S	28	TYR	CA-CB-CG	5.40	123.66	113.40
50	S2	578	C	C2'-C3'-O3'	5.40	122.34	113.70
50	S2	619	A	C3'-C2'-C1'	-5.40	97.18	101.50
1	5	293	G	C2'-C3'-O3'	5.40	122.34	113.70
3	8	68	G	N9-C1'-C2'	5.40	121.02	114.00
19	Q	75	ARG	NE-CZ-NH2	-5.40	117.60	120.30
50	S2	1643	U	C1'-C2'-O2'	-5.39	94.42	110.60
1	5	1588	U	N1-C1'-C2'	5.39	121.01	114.00
50	S2	1557	C	N1-C1'-C2'	-5.39	106.07	112.00
1	5	2014	C	C2'-C3'-O3'	5.39	122.32	113.70
37	i	26	HIS	N-CA-CB	5.39	120.30	110.60
75	SY	20	ARG	NE-CZ-NH2	5.39	122.99	120.30
74	SX	17	ARG	NE-CZ-NH2	5.39	122.99	120.30
1	5	4975	G	N9-C1'-C2'	-5.39	106.08	112.00
45	r	103	ARG	NE-CZ-NH2	-5.39	117.61	120.30
50	S2	1662	U	N1-C1'-C2'	-5.39	106.07	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1464	C	N1-C1'-C2'	-5.38	106.08	112.00
18	P	42	ARG	CG-CD-NE	5.38	123.11	111.80
50	S2	579	C	N1-C1'-C2'	-5.38	106.08	112.00
1	5	3626	G	N9-C1'-C2'	-5.38	106.08	112.00
50	S2	444	G	O4'-C1'-C2'	-5.38	100.42	105.80
4	A	19	HIS	N-CA-CB	-5.38	100.92	110.60
18	P	30	ARG	NE-CZ-NH2	-5.38	117.61	120.30
36	h	70	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	5	1667	G	C2'-C3'-O3'	5.38	122.30	113.70
1	5	4745	G	N9-C1'-C2'	5.38	120.99	114.00
24	V	14	PHE	CB-CG-CD2	-5.38	117.04	120.80
1	5	82	U	N1-C1'-C2'	-5.37	106.09	112.00
8	E	236	TYR	CA-CB-CG	-5.37	103.20	113.40
21	S	81	TRP	N-CA-C	-5.37	96.51	111.00
41	m	106	ARG	NE-CZ-NH1	5.37	122.98	120.30
33	e	47	ARG	NE-CZ-NH2	-5.37	117.62	120.30
50	S2	1666	C	N1-C1'-C2'	5.36	120.97	114.00
1	5	911	U	C2'-C3'-O3'	5.36	122.28	113.70
50	S2	426	A	C4'-C3'-O3'	5.36	123.71	113.00
2	7	59	G	N9-C1'-C2'	-5.36	106.11	112.00
19	Q	174	PHE	CB-CG-CD1	-5.36	117.05	120.80
65	SO	117	ARG	NE-CZ-NH1	-5.36	117.62	120.30
12	I	139	ARG	CB-CG-CD	-5.35	97.68	111.60
19	Q	168	ARG	NE-CZ-NH1	5.35	122.98	120.30
27	Y	45	ARG	NE-CZ-NH1	5.35	122.98	120.30
50	S2	1136	U	N1-C1'-C2'	5.35	120.96	114.00
50	S2	553	U	N1-C1'-C2'	5.35	120.95	114.00
50	S2	1292	C	C5'-C4'-C3'	5.35	124.56	116.00
37	i	29	ARG	NE-CZ-NH1	5.35	122.97	120.30
82	Sf	148	TYR	C-N-CA	5.35	135.07	121.70
1	5	703	G	N9-C1'-C2'	-5.34	106.12	112.00
50	S2	646	G	N9-C1'-C2'	-5.34	106.12	112.00
7	D	20	PHE	CB-CA-C	5.34	121.08	110.40
16	N	192	TRP	N-CA-CB	-5.34	100.98	110.60
50	S2	1415	C	N1-C1'-C2'	5.34	120.94	114.00
1	5	4228	G	O4'-C1'-N9	5.34	112.47	108.20
1	5	215	C	C4'-C3'-O3'	-5.34	98.19	109.40
26	X	79	PHE	CB-CG-CD1	5.34	124.54	120.80
50	S2	1034	A	N9-C1'-C2'	5.34	120.94	114.00
8	E	212	TYR	CA-CB-CG	5.33	123.54	113.40
20	R	60	ARG	NE-CZ-NH1	5.33	122.97	120.30
24	V	97	TYR	CB-CA-C	5.33	121.07	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	T	140	PHE	CB-CA-C	-5.33	99.73	110.40
70	ST	83	GLN	CA-CB-CG	5.33	125.13	113.40
1	5	1632	A	N9-C1'-C2'	-5.33	106.14	112.00
68	SR	33	ARG	CG-CD-NE	-5.33	100.60	111.80
5	B	62	ARG	NE-CZ-NH2	-5.33	117.64	120.30
50	S2	56	G	N9-C1'-C2'	5.33	120.93	114.00
1	5	3590	G	C2'-C3'-O3'	5.32	122.22	113.70
1	5	4883	C	O4'-C1'-N1	5.32	112.45	108.20
11	H	115	ARG	CA-CB-CG	5.32	125.10	113.40
1	5	1390	G	N9-C1'-C2'	-5.32	106.15	112.00
1	5	3753	G	C2'-C3'-O3'	5.32	122.20	113.70
5	B	117	ARG	NE-CZ-NH1	5.32	122.96	120.30
50	S2	438	G	N9-C1'-C2'	5.32	120.91	114.00
59	SI	49	ARG	NE-CZ-NH2	-5.32	117.64	120.30
3	8	34	U	C2-N1-C1'	-5.31	111.33	117.70
1	5	212	A	N9-C1'-C2'	5.31	120.91	114.00
16	N	143	ARG	NE-CZ-NH2	-5.31	117.64	120.30
17	O	128	ARG	NE-CZ-NH2	5.31	122.96	120.30
63	SM	26	LEU	CA-CB-CG	5.31	127.51	115.30
79	Sc	44	ARG	CD-NE-CZ	5.31	131.03	123.60
1	5	1272	C	O4'-C1'-C2'	-5.30	100.50	105.80
51	SA	39	TYR	CA-CB-CG	5.30	123.48	113.40
1	5	1961	G	C4'-C3'-C2'	-5.30	97.30	102.60
33	e	36	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	5	3726	A	N9-C1'-C2'	5.30	120.89	114.00
70	ST	67	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	5	194	C	N1-C1'-C2'	-5.30	106.17	112.00
9	F	136	ARG	CA-CB-CG	5.29	125.03	113.40
40	l	45	ARG	CG-CD-NE	-5.29	100.69	111.80
1	5	2817	C	C2'-C3'-O3'	5.29	122.16	113.70
1	5	2056	G	P-O5'-C5'	-5.29	112.44	120.90
1	5	4302	U	N1-C1'-C2'	-5.28	106.19	112.00
61	SK	43	LEU	CA-CB-CG	5.28	127.45	115.30
1	5	4528	G	O4'-C1'-C2'	-5.28	100.52	105.80
9	F	228	HIS	CA-CB-CG	-5.28	104.62	113.60
16	N	192	TRP	CB-CG-CD1	-5.28	120.14	127.00
50	S2	943	U	C6-N1-C1'	-5.28	113.81	121.20
62	SL	17	PHE	N-CA-CB	5.28	120.10	110.60
50	S2	114	G	N9-C1'-C2'	-5.28	106.20	112.00
50	S2	1567	G	C1'-O4'-C4'	-5.28	105.68	109.90
1	5	4497	U	C2'-C3'-O3'	5.27	122.14	113.70
1	5	416	U	N1-C1'-C2'	5.27	120.86	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	3666	C	N1-C1'-C2'	-5.27	106.20	112.00
37	i	39	PHE	CB-CG-CD1	-5.27	117.11	120.80
50	S2	800	U	O4'-C4'-C3'	-5.27	98.73	104.00
57	SG	74	ARG	NE-CZ-NH1	5.27	122.94	120.30
75	SY	86	GLU	CB-CG-CD	-5.27	99.96	114.20
19	Q	75	ARG	CG-CD-NE	5.27	122.87	111.80
1	5	3692	A	N9-C1'-C2'	-5.27	106.20	112.00
1	5	2348	G	O4'-C1'-N9	-5.27	103.98	108.20
1	5	3739	C	C2'-C3'-O3'	5.27	122.13	113.70
26	X	129	ARG	NE-CZ-NH2	5.27	122.93	120.30
36	h	72	PHE	CB-CG-CD2	-5.27	117.11	120.80
1	5	1390	G	C2'-C3'-O3'	5.27	122.12	113.70
83	Sg	15	ASN	CB-CA-C	5.26	120.92	110.40
50	S2	983	A	C5'-C4'-O4'	5.26	115.41	109.10
1	5	1886	G	N9-C1'-C2'	-5.25	106.22	112.00
57	SG	198	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	5	1211	G	C4'-C3'-C2'	-5.25	97.35	102.60
6	C	110	ARG	NE-CZ-NH1	5.25	122.93	120.30
53	SC	236	PHE	CB-CG-CD1	-5.25	117.12	120.80
64	SN	55	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	5	2263	A	C2'-C3'-O3'	5.25	122.10	113.70
26	X	137	TYR	CA-CB-CG	5.25	123.38	113.40
41	m	97	ARG	NE-CZ-NH2	5.25	122.92	120.30
45	r	77	TYR	CB-CG-CD2	-5.25	117.85	121.00
50	S2	1097	G	C2'-C3'-O3'	5.25	122.09	113.70
1	5	2467	U	N1-C1'-C2'	-5.25	106.23	112.00
1	5	4736	C	N1-C1'-C2'	5.24	120.81	114.00
17	O	178	ARG	NE-CZ-NH2	-5.24	117.68	120.30
24	V	128	LEU	CA-CB-CG	5.24	127.36	115.30
50	S2	368	U	C2'-C3'-O3'	5.24	122.09	113.70
5	B	119	TYR	CA-CB-CG	-5.24	103.45	113.40
9	F	136	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	5	63	G	N9-C1'-C2'	5.24	120.81	114.00
1	5	1484	G	O4'-C4'-C3'	-5.24	98.77	104.00
26	X	137	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	5	1	C	C3'-C2'-C1'	-5.23	97.31	101.50
70	ST	53	PHE	N-CA-CB	-5.23	101.18	110.60
27	Y	87	ARG	CD-NE-CZ	5.23	130.93	123.60
34	f	19	ARG	CG-CD-NE	-5.23	100.81	111.80
1	5	2262	G	N9-C1'-C2'	5.23	120.80	114.00
1	5	4463	U	O4'-C1'-C2'	-5.23	100.57	105.80
50	S2	1167	G	N9-C1'-C2'	5.23	120.80	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	SB	67	PHE	CB-CG-CD2	-5.23	117.14	120.80
4	A	89	TYR	CB-CA-C	5.23	120.86	110.40
50	S2	65	C	C2'-C3'-O3'	5.23	122.06	113.70
1	5	2597	G	N9-C1'-C2'	5.22	120.79	114.00
5	B	246	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	5	931	C	N1-C1'-C2'	5.22	120.79	114.00
50	S2	1093	A	C5'-C4'-O4'	5.22	115.37	109.10
13	J	147	ARG	NE-CZ-NH1	5.22	122.91	120.30
5	B	25	HIS	CB-CA-C	5.22	120.83	110.40
34	f	19	ARG	CA-CB-CG	5.22	124.88	113.40
50	S2	1292	C	C5'-C4'-O4'	5.22	115.36	109.10
59	SI	188	TYR	CB-CG-CD1	-5.22	117.87	121.00
1	5	2443	G	N9-C1'-C2'	5.21	120.78	114.00
1	5	4966	A	C4-N9-C1'	5.21	135.69	126.30
50	S2	501	C	O4'-C1'-C2'	-5.21	100.58	105.80
50	S2	1542	C	C1'-C2'-O2'	-5.21	94.96	110.60
1	5	2753	G	C2'-C3'-O3'	5.21	122.04	113.70
1	5	1394	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	216	C	C2'-C3'-O3'	5.21	122.03	113.70
50	S2	1243	U	O5'-P-OP2	-5.21	101.01	105.70
1	5	2529	A	O4'-C1'-N9	5.21	112.36	108.20
1	5	267	G	C2'-C3'-O3'	5.21	122.03	113.70
16	N	65	ARG	NE-CZ-NH2	5.21	122.90	120.30
5	B	274	TYR	CB-CG-CD1	-5.20	117.88	121.00
30	b	45	PHE	CB-CG-CD1	-5.20	117.16	120.80
41	m	97	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	5	2310	C	C2'-C3'-O3'	5.20	122.02	113.70
34	f	51	TYR	CA-CB-CG	5.20	123.28	113.40
35	g	14	ASN	N-CA-C	-5.20	96.96	111.00
12	I	98	ARG	NE-CZ-NH2	5.20	122.90	120.30
56	SF	188	TYR	CA-CB-CG	-5.20	103.53	113.40
57	SG	156	TYR	CB-CA-C	5.20	120.79	110.40
1	5	2325	C	C2'-C3'-O3'	5.19	122.00	113.70
9	F	58	HIS	N-CA-CB	5.19	119.94	110.60
69	SS	95	TYR	CB-CG-CD2	-5.19	117.89	121.00
50	S2	594	A	C4'-C3'-O3'	5.19	123.37	113.00
1	5	664	G	C4'-C3'-O3'	5.18	123.37	113.00
1	5	2044	U	C3'-C2'-C1'	5.18	105.65	101.50
69	SS	124	ARG	CG-CD-NE	5.18	122.69	111.80
50	S2	919	A	C2'-C3'-O3'	-5.18	98.10	109.50
1	5	4041	C	N1-C1'-C2'	-5.18	106.30	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	S	77	ASN	CB-CA-C	5.18	120.76	110.40
34	f	102	ARG	NE-CZ-NH1	5.18	122.89	120.30
50	S2	672	A	C3'-C2'-C1'	-5.18	97.36	101.50
50	S2	1663	A	C1'-O4'-C4'	-5.18	105.76	109.90
1	5	4165	C	C2'-C3'-O3'	5.18	121.98	113.70
1	5	172	C	O4'-C1'-C2'	-5.18	100.62	105.80
1	5	2075	G	N9-C1'-C2'	-5.18	106.31	112.00
50	S2	1578	U	O4'-C1'-N1	-5.18	104.06	108.20
1	5	1698	C	O5'-P-OP1	-5.17	101.04	105.70
1	5	2256	C	N1-C1'-C2'	5.17	120.73	114.00
14	L	198	ARG	NE-CZ-NH2	-5.17	117.71	120.30
50	S2	1394	G	O4'-C1'-C2'	-5.17	100.62	105.80
60	SJ	175	ARG	NE-CZ-NH1	5.17	122.89	120.30
7	D	268	ARG	CG-CD-NE	5.17	122.66	111.80
1	5	703	G	O4'-C1'-N9	5.17	112.34	108.20
2	7	6	C	C2'-C3'-O3'	5.17	121.97	113.70
1	5	2879	A	N9-C1'-C2'	5.17	120.72	114.00
20	R	108	ARG	CG-CD-NE	5.17	122.66	111.80
20	R	124	TYR	CA-CB-CG	5.17	123.22	113.40
1	5	961	G	C4'-C3'-O3'	5.17	123.33	113.00
9	F	72	ARG	NE-CZ-NH1	5.17	122.88	120.30
32	d	24	GLU	CA-CB-CG	5.17	124.77	113.40
38	j	76	HIS	CB-CA-C	5.17	120.73	110.40
59	SI	188	TYR	CD1-CG-CD2	5.17	123.58	117.90
1	5	658	C	C2'-C3'-O3'	5.16	121.96	113.70
1	5	4328	G	N9-C1'-C2'	-5.16	106.32	112.00
14	L	99	ASP	CB-CG-OD1	-5.16	113.65	118.30
74	SX	5	ARG	NE-CZ-NH2	5.16	122.88	120.30
16	N	63	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	5	272	U	N1-C1'-C2'	5.16	120.71	114.00
1	5	1642	A	C5'-C4'-O4'	5.16	115.29	109.10
1	5	4436	U	N1-C1'-C2'	-5.16	106.32	112.00
50	S2	1579	A	C2'-C3'-O3'	5.16	121.96	113.70
64	SN	55	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	5	1850	A	N9-C1'-C2'	5.16	120.70	114.00
13	J	147	ARG	NE-CZ-NH2	-5.16	117.72	120.30
19	Q	68	ARG	CG-CD-NE	-5.16	100.97	111.80
21	S	29	ARG	CB-CA-C	5.16	120.71	110.40
1	5	405	U	C2'-C3'-O3'	5.15	121.95	113.70
1	5	1577	G	N9-C1'-C2'	-5.15	106.33	112.00
1	5	2323	C	C2'-C3'-O3'	5.15	121.94	113.70
1	5	2538	U	O5'-P-OP1	-5.15	101.06	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4543	G	N9-C1'-C2'	5.15	120.70	114.00
2	7	65	G	C2'-C3'-O3'	5.15	121.94	113.70
82	Sf	138	ARG	CD-NE-CZ	5.15	130.81	123.60
3	8	1	C	C5'-C4'-C3'	5.15	124.24	116.00
34	f	6	TRP	CA-CB-CG	-5.15	103.92	113.70
16	N	130	PHE	CB-CA-C	5.14	120.69	110.40
1	5	268	G	C2'-C3'-O3'	5.14	121.93	113.70
16	N	59	TYR	CA-CB-CG	5.14	123.17	113.40
28	Z	36	ARG	NE-CZ-NH2	-5.14	117.73	120.30
27	Y	87	ARG	NE-CZ-NH1	-5.14	117.73	120.30
6	C	143	ARG	NE-CZ-NH1	5.14	122.87	120.30
35	g	4	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	5	4163	U	C4'-C3'-C2'	-5.14	97.46	102.60
1	5	1615	C	N1-C1'-C2'	-5.14	106.35	112.00
9	F	197	TYR	N-CA-CB	5.14	119.84	110.60
3	8	46	G	N9-C1'-C2'	5.13	120.67	114.00
50	S2	797	C	O4'-C1'-C2'	-5.13	100.67	105.80
50	S2	1150	A	N9-C1'-C2'	5.13	120.67	114.00
1	5	107	G	N9-C1'-C2'	-5.13	106.35	112.00
1	5	2785	C	N1-C1'-C2'	5.13	120.67	114.00
7	D	130	TYR	CA-CB-CG	-5.13	103.66	113.40
19	Q	38	ARG	NE-CZ-NH2	-5.13	117.74	120.30
33	e	47	ARG	N-CA-C	-5.13	97.15	111.00
50	S2	1603	G	N9-C1'-C2'	5.13	120.67	114.00
50	S2	996	A	C4-N9-C1'	-5.13	117.07	126.30
17	O	140	ARG	NE-CZ-NH1	-5.12	117.74	120.30
21	S	10	TYR	CB-CA-C	5.12	120.65	110.40
3	8	125	C	O4'-C1'-N1	-5.12	104.10	108.20
27	Y	126	ARG	CD-NE-CZ	5.12	130.77	123.60
50	S2	72	C	O4'-C1'-N1	5.12	112.30	108.20
1	5	4276	G	N9-C1'-C2'	-5.12	106.37	112.00
66	SP	10	ARG	NE-CZ-NH2	-5.12	117.74	120.30
14	L	99	ASP	N-CA-C	-5.11	97.19	111.00
21	S	28	TYR	CB-CG-CD2	-5.11	117.93	121.00
7	D	248	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	5	3870	C	N1-C1'-C2'	5.10	120.64	114.00
1	5	3880	G	C1'-C2'-O2'	-5.10	95.29	110.60
57	SG	205	GLU	OE1-CD-OE2	5.10	129.42	123.30
82	Sf	138	ARG	CG-CD-NE	5.10	122.51	111.80
1	5	2117	G	C1'-O4'-C4'	-5.10	105.82	109.90
1	5	3667	C	N1-C1'-C2'	-5.10	106.39	112.00
50	S2	1368	U	N1-C1'-C2'	-5.10	106.39	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	SA	9	GLN	CB-CG-CD	-5.10	98.34	111.60
1	5	1887	G	C4'-C3'-C2'	-5.10	97.50	102.60
3	8	104	A	P-O5'-C5'	5.10	129.06	120.90
5	B	161	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	5	4975	G	C1'-O4'-C4'	-5.09	105.82	109.90
17	O	117	ARG	NE-CZ-NH2	-5.09	117.75	120.30
28	Z	36	ARG	CG-CD-NE	5.09	122.50	111.80
45	r	77	TYR	N-CA-CB	-5.09	101.43	110.60
50	S2	102	A	C2'-C3'-O3'	5.09	121.85	113.70
50	S2	1567	G	N9-C1'-C2'	5.09	120.62	114.00
1	5	4670	C	P-O5'-C5'	5.09	129.04	120.90
1	5	218	A	N9-C1'-C2'	-5.09	106.40	112.00
1	5	3666	C	C2'-C3'-O3'	5.09	121.84	113.70
4	A	209	HIS	CA-CB-CG	-5.09	104.95	113.60
32	d	85	ARG	CG-CD-NE	5.09	122.48	111.80
50	S2	141	A	C2'-C3'-O3'	5.08	121.84	113.70
1	5	1268	G	N9-C1'-C2'	5.08	120.61	114.00
32	d	87	ARG	N-CA-CB	5.08	119.75	110.60
1	5	1398	A	C3'-C2'-C1'	-5.08	97.44	101.50
20	R	9	ARG	CG-CD-NE	5.08	122.47	111.80
27	Y	87	ARG	CG-CD-NE	5.08	122.47	111.80
1	5	1358	G	O4'-C1'-C2'	-5.08	100.72	105.80
1	5	1361	G	C2'-C3'-O3'	5.08	121.82	113.70
55	SE	30	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	5	297	U	N1-C1'-C2'	-5.07	106.42	112.00
1	5	648	G	C2'-C3'-O3'	5.07	121.82	113.70
23	U	46	ARG	NE-CZ-NH1	5.07	122.84	120.30
50	S2	853	C	C2'-C3'-O3'	5.07	121.82	113.70
1	5	352	G	C3'-C2'-C1'	5.07	105.56	101.50
1	5	2614	C	N1-C1'-C2'	-5.07	106.42	112.00
1	5	4498	U	C1'-C2'-O2'	5.07	125.81	110.60
13	J	170	HIS	CB-CA-C	5.07	120.54	110.40
16	N	143	ARG	CB-CG-CD	5.07	124.78	111.60
19	Q	33	ARG	CB-CG-CD	5.07	124.78	111.60
1	5	2361	G	P-O3'-C3'	5.07	125.78	119.70
20	R	117	ARG	CB-CA-C	5.07	120.54	110.40
39	k	16	ARG	NE-CZ-NH1	5.07	122.83	120.30
50	S2	73	C	O4'-C1'-C2'	-5.07	100.73	105.80
83	Sg	125	ARG	CG-CD-NE	-5.07	101.16	111.80
1	5	1359	G	O4'-C4'-C3'	-5.07	98.94	104.00
83	Sg	36	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	5	4936	G	C4'-C3'-O3'	5.06	123.12	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	3804	G	N9-C1'-C2'	-5.06	106.44	112.00
1	5	3863	C	N1-C1'-C2'	5.06	120.58	114.00
1	5	4404	U	C3'-C2'-C1'	5.06	105.55	101.50
1	5	2054	U	N1-C1'-C2'	5.06	120.57	114.00
1	5	1216	C	C2'-C3'-O3'	5.05	121.79	113.70
1	5	3627	G	C2'-C3'-O3'	5.05	121.79	113.70
56	SF	136	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	5	336	A	N9-C1'-C2'	-5.05	106.44	112.00
1	5	1067	G	C2'-C3'-O3'	5.05	121.78	113.70
1	5	20	U	N1-C1'-C2'	-5.05	106.44	112.00
5	B	257	TRP	N-CA-CB	5.05	119.69	110.60
27	Y	126	ARG	CG-CD-NE	5.05	122.40	111.80
82	Sf	150	PHE	CB-CG-CD1	5.05	124.33	120.80
22	T	8	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	5	88	A	C1'-C2'-O2'	-5.04	95.47	110.60
1	5	1672	U	N1-C1'-C2'	5.04	120.56	114.00
1	5	1963	C	C2'-C3'-O3'	5.04	121.77	113.70
1	5	2787	A	N9-C1'-C2'	-5.04	106.45	112.00
59	SI	28	GLU	N-CA-C	-5.04	97.38	111.00
1	5	4398	C	C2'-C3'-O3'	5.04	121.77	113.70
14	L	121	ARG	NE-CZ-NH1	5.04	122.82	120.30
27	Y	74	TYR	N-CA-CB	5.04	119.67	110.60
1	5	1896	A	N9-C1'-C2'	-5.04	106.46	112.00
1	5	1947	U	C4'-C3'-O3'	5.04	123.08	113.00
14	L	103	ARG	CA-CB-CG	5.04	124.49	113.40
22	T	19	PHE	CB-CA-C	-5.04	100.33	110.40
50	S2	410	G	O5'-P-OP1	-5.04	101.17	105.70
50	S2	524	U	C2'-C3'-O3'	5.04	121.76	113.70
1	5	2459	G	N9-C1'-C2'	-5.04	106.46	112.00
1	5	2533	C	N1-C1'-C2'	5.04	120.55	114.00
50	S2	798	A	C4'-C3'-C2'	-5.04	97.56	102.60
50	S2	1080	A	O4'-C1'-N9	5.03	112.23	108.20
73	SW	57	ARG	CG-CD-NE	5.03	122.37	111.80
1	5	1895	G	N9-C1'-C2'	5.03	120.54	114.00
1	5	1953	U	N1-C1'-C2'	5.03	120.54	114.00
50	S2	967	C	N1-C1'-C2'	-5.03	106.47	112.00
1	5	54	G	C2'-C3'-O3'	5.03	121.74	113.70
1	5	4270	C	C5'-C4'-O4'	5.03	115.13	109.10
53	SC	223	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	5	1281	G	C3'-C2'-C1'	5.03	105.52	101.50
1	5	2264	C	C2'-C3'-O3'	5.03	121.74	113.70
28	Z	51	ARG	NE-CZ-NH1	5.02	122.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	o	78	ARG	CD-NE-CZ	5.02	130.63	123.60
1	5	1272	C	C5'-C4'-O4'	5.02	115.12	109.10
1	5	1365	C	N1-C1'-C2'	5.02	120.53	114.00
54	SD	67	ARG	CD-NE-CZ	5.02	130.63	123.60
1	5	74	G	N9-C1'-C2'	5.02	120.53	114.00
26	X	56	ARG	CG-CD-NE	-5.02	101.26	111.80
56	SF	122	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	5	1440	U	C4'-C3'-C2'	-5.02	97.58	102.60
1	5	3908	A	C3'-C2'-C1'	-5.02	97.48	101.50
1	5	5011	A	C2'-C3'-O3'	5.02	121.73	113.70
20	R	103	ARG	NE-CZ-NH1	5.02	122.81	120.30
82	Sf	146	LEU	N-CA-C	-5.02	97.45	111.00
50	S2	385	G	N9-C1'-C2'	5.01	120.52	114.00
54	SD	65	ARG	NE-CZ-NH2	-5.01	117.79	120.30
74	SX	20	HIS	CA-CB-CG	-5.01	105.08	113.60
1	5	2827	G	O4'-C4'-C3'	-5.01	98.99	104.00
1	5	4454	G	C2'-C3'-O3'	5.01	121.72	113.70
12	I	181	PHE	CB-CG-CD1	5.01	124.31	120.80
16	N	6	TYR	CA-CB-CG	-5.01	103.88	113.40
58	SH	99	ARG	CG-CD-NE	5.01	122.33	111.80
1	5	1479	G	C1'-C2'-O2'	-5.01	95.57	110.60
1	5	1864	G	C2'-C3'-O3'	5.01	121.72	113.70
9	F	83	PHE	N-CA-CB	-5.01	101.58	110.60
55	SE	11	ARG	NE-CZ-NH2	5.01	122.81	120.30
67	SQ	138	ARG	CG-CD-NE	5.01	122.32	111.80
1	5	4473	A	C2'-C3'-O3'	5.01	121.71	113.70
27	Y	45	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	5	2116	C	C2'-C3'-O3'	5.01	121.71	113.70
5	B	122	TRP	CA-CB-CG	5.01	123.21	113.70
7	D	119	TYR	CB-CA-C	5.01	120.41	110.40
50	S2	1407	U	C2-N1-C1'	5.01	123.71	117.70
1	5	4224	A	N9-C1'-C2'	-5.00	106.50	112.00
12	I	162	ARG	NE-CZ-NH1	-5.00	117.80	120.30
50	S2	28	U	C4'-C3'-O3'	5.00	123.01	113.00
1	5	1591	U	N1-C1'-C2'	5.00	120.50	114.00
19	Q	33	ARG	N-CA-CB	5.00	119.61	110.60
21	S	9	GLU	CA-CB-CG	5.00	124.41	113.40
50	S2	1622	U	O4'-C1'-N1	-5.00	104.20	108.20
1	5	2275	G	C2'-C3'-O3'	5.00	121.70	113.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	5	1992	U	C1'
50	S2	1109	C	C1'

All (455) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
47	1	273	ARG	Mainchain
47	1	405	ARG	Sidechain
47	1	432	SER	Mainchain
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	1539	G	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	2037	C	Sidechain
1	5	2046	G	Sidechain
1	5	2056	G	Sidechain
1	5	2077	C	Sidechain
1	5	2082	G	Sidechain

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Mol	Chain	Res	Type	Group
1	5	2087	C	Sidechain
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	2511	A	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

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Mol	Chain	Res	Type	Group
1	5	352	G	Sidechain
1	5	354	U	Sidechain
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	4239	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	4463	U	Sidechain
1	5	4464	A	Sidechain
1	5	4497	U	Sidechain

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Mol	Chain	Res	Type	Group
1	5	4498	U	Sidechain
1	5	4510	A	Sidechain
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

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Mol	Chain	Res	Type	Group
3	8	14	U	Sidechain
3	8	34	U	Sidechain
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

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Mol	Chain	Res	Type	Group
8	E	102	VAL	Peptide
8	E	103	VAL	Peptide
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	Peptide,Sidechain
11	H	50	LYS	Peptide
12	I	113	THR	Peptide
12	I	139	ARG	Sidechain
12	I	158	LYS	Peptide
12	I	77	VAL	Peptide
12	I	93	PRO	Peptide
13	J	87	LEU	Peptide
13	J	99	PHE	Sidechain
14	L	146	LEU	Peptide
14	L	147	ALA	Peptide
14	L	192	PHE	Sidechain
14	L	62	PRO	Peptide
14	L	66	TYR	Peptide
15	M	6	PHE	Sidechain
15	M	65	PRO	Peptide
15	M	79	LYS	Peptide
15	M	94	LYS	Peptide
16	N	119	TYR	Sidechain
16	N	130	PHE	Sidechain
16	N	131	GLU	Sidechain
16	N	138	PHE	Peptide

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Mol	Chain	Res	Type	Group
16	N	139	HIS	Sidechain
16	N	180	PHE	Sidechain
16	N	184	ILE	Peptide
16	N	202	ARG	Peptide
16	N	37	HIS	Sidechain
16	N	90	ASN	Peptide
17	O	110	PRO	Peptide
17	O	117	ARG	Peptide
17	O	135	PHE	Sidechain
18	P	139	TYR	Sidechain
19	Q	161	SER	Peptide
19	Q	162	HIS	Peptide
19	Q	174	PHE	Sidechain
19	Q	32	TYR	Peptide
19	Q	34	PHE	Sidechain
20	R	118	HIS	Sidechain
20	R	132	PHE	Sidechain
20	R	174	GLU	Peptide
20	R	19	LYS	Peptide
20	R	57	VAL	Peptide
20	R	94	THR	Peptide
21	S	10	TYR	Sidechain
21	S	145	PHE	Peptide,Sidechain
21	S	152	PHE	Peptide
21	S	154	LEU	Peptide
21	S	159	LEU	Peptide
21	S	164	LYS	Peptide
21	S	32	ILE	Peptide
21	S	33	PHE	Peptide
21	S	68	PHE	Peptide
21	S	90	THR	Peptide
50	S2	1034	A	Sidechain
50	S2	104	A	Sidechain
50	S2	1045	U	Sidechain
50	S2	1063	C	Sidechain
50	S2	1085	C	Sidechain
50	S2	1088	U	Sidechain
50	S2	1109	C	Sidechain
50	S2	114	G	Sidechain
50	S2	1142	G	Sidechain
50	S2	1150	A	Sidechain
50	S2	1167	G	Sidechain

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Mol	Chain	Res	Type	Group
50	S2	1181	A	Sidechain
50	S2	1249	C	Sidechain
50	S2	1283	C	Sidechain
50	S2	1315	U	Sidechain
50	S2	1565	C	Sidechain
50	S2	1578	U	Sidechain
50	S2	1603	G	Sidechain
50	S2	1606	G	Sidechain
50	S2	1623	A	Sidechain
50	S2	1659	U	Sidechain
50	S2	1663	A	Sidechain
50	S2	1703	C	Sidechain
50	S2	1838	U	Sidechain
50	S2	1849	G	Sidechain
50	S2	1850	A	Sidechain
50	S2	1851	A	Sidechain
50	S2	1860	A	Sidechain
50	S2	294	U	Sidechain
50	S2	30	C	Sidechain
50	S2	313	A	Sidechain
50	S2	367	U	Sidechain
50	S2	381	C	Sidechain
50	S2	384	U	Sidechain
50	S2	399	C	Sidechain
50	S2	421	G	Sidechain
50	S2	423	U	Sidechain
50	S2	426	A	Sidechain
50	S2	427	U	Sidechain
50	S2	428	U	Sidechain
50	S2	437	G	Sidechain
50	S2	444	G	Sidechain
50	S2	447	A	Sidechain
50	S2	482	G	Sidechain
50	S2	601	G	Sidechain
50	S2	617	G	Sidechain
50	S2	631	U	Sidechain
50	S2	642	U	Sidechain
50	S2	645	C	Sidechain
50	S2	646	G	Sidechain
50	S2	661	U	Sidechain
50	S2	662	G	Sidechain
50	S2	685	A	Sidechain

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Mol	Chain	Res	Type	Group
50	S2	821	G	Sidechain
50	S2	848	U	Sidechain
50	S2	849	A	Sidechain
50	S2	918	U	Sidechain
50	S2	92	A	Sidechain
50	S2	957	A	Sidechain
50	S2	958	G	Sidechain
50	S2	964	A	Sidechain
50	S2	999	G	Sidechain
51	SA	103	PHE	Sidechain
51	SA	131	HIS	Peptide
52	SB	141	GLY	Peptide
52	SB	145	LYS	Mainchain
52	SB	40	ASN	Peptide
52	SB	66	VAL	Peptide
52	SB	76	ASN	Peptide
53	SC	168	GLY	Peptide
53	SC	236	PHE	Sidechain
53	SC	241	PHE	Sidechain
53	SC	60	TRP	Peptide
54	SD	196	GLY	Peptide
54	SD	203	PRO	Peptide
55	SE	17	HIS	Peptide
55	SE	205	PHE	Peptide
56	SF	43	GLU	Peptide
58	SH	108	SER	Peptide
59	SI	149	TYR	Peptide
59	SI	153	LYS	Peptide
59	SI	155	ASN	Peptide
59	SI	26	LYS	Peptide
59	SI	65	PHE	Peptide
59	SI	99	ASN	Sidechain
60	SJ	165	TYR	Peptide
60	SJ	48	PHE	Sidechain
61	SK	29	MET	Peptide
62	SL	147	LYS	Peptide
62	SL	15	THR	Peptide
62	SL	151	THR	Peptide
62	SL	62	PHE	Sidechain
63	SM	32	ALA	Peptide
64	SN	113	PHE	Peptide
65	SO	147	ARG	Sidechain

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Mol	Chain	Res	Type	Group
66	SP	11	THR	Peptide
67	SQ	43	GLU	Peptide
68	SR	108	LEU	Peptide
68	SR	125	GLY	Peptide
71	SU	71	GLY	Peptide
72	SV	32	ILE	Peptide
72	SV	48	GLY	Peptide
73	SW	54	ASP	Peptide
73	SW	76	SER	Peptide
74	SX	16	HIS	Sidechain
74	SX	20	HIS	Sidechain
75	SY	86	GLU	Sidechain
76	SZ	108	ILE	Peptide
77	Sa	17	HIS	Sidechain
78	Sb	81	ARG	Peptide
80	Sd	10	HIS	Peptide
80	Sd	8	TRP	Peptide
82	Sf	132	MET	Peptide
82	Sf	135	HIS	Peptide
82	Sf	138	ARG	Peptide
82	Sf	139	HIS	Peptide
22	T	140	PHE	Sidechain
22	T	142	ARG	Peptide
23	U	110	TYR	Peptide
23	U	55	ASN	Peptide
24	V	108	ASN	Peptide
24	V	97	TYR	Sidechain
24	V	98	PHE	Sidechain
25	W	27	LYS	Peptide
26	X	73	HIS	Sidechain
27	Y	18	HIS	Sidechain
27	Y	61	HIS	Sidechain
27	Y	62	TYR	Peptide
27	Y	81	TYR	Sidechain
29	a	109	TYR	Sidechain
29	a	128	PHE	Sidechain
29	a	34	ASN	Sidechain
29	a	39	HIS	Peptide
29	a	60	HIS	Sidechain
29	a	61	TYR	Peptide,Sidechain
29	a	62	HIS	Sidechain
29	a	91	ALA	Peptide

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Mol	Chain	Res	Type	Group
30	b	6	ASN	Sidechain
31	c	77	ASN	Peptide
31	c	78	ASN	Sidechain
32	d	103	TYR	Peptide
32	d	108	TYR	Peptide
32	d	25	TYR	Sidechain
32	d	72	VAL	Peptide
33	e	20	PHE	Sidechain
33	e	3	ALA	Peptide
33	e	74	PHE	Sidechain
33	e	76	LYS	Peptide
34	f	100	ARG	Peptide
34	f	53	ALA	Peptide
35	g	6	THR	Peptide
36	h	121	VAL	Peptide
36	h	78	TYR	Sidechain
36	h	97	LYS	Peptide
37	i	26	HIS	Sidechain
37	i	39	PHE	Sidechain
37	i	49	GLY	Peptide
38	j	46	LYS	Peptide
38	j	48	ASN	Peptide
38	j	66	HIS	Sidechain
38	j	8	PHE	Sidechain
39	k	28	ASN	Peptide
43	o	31	ASP	Peptide,Sidechain
43	o	43	ARG	Peptide
43	o	47	GLY	Peptide
43	o	48	TYR	Sidechain
43	o	76	ASN	Peptide
44	p	17	ARG	Peptide
45	r	30	ASN	Peptide
45	r	31	ASN	Sidechain
45	r	45	HIS	Sidechain
45	r	70	GLN	Peptide
45	r	76	SER	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	2	23
5	B	392/394 (100%)	319 (81%)	40 (10%)	33 (8%)	0	10
6	C	365/367 (100%)	304 (83%)	45 (12%)	16 (4%)	2	21
7	D	290/297 (98%)	235 (81%)	33 (11%)	22 (8%)	1	13
8	E	232/236 (98%)	150 (65%)	51 (22%)	31 (13%)	0	3
9	F	223/225 (99%)	190 (85%)	23 (10%)	10 (4%)	2	20
10	G	239/266 (90%)	200 (84%)	32 (13%)	7 (3%)	3	27
11	H	188/192 (98%)	164 (87%)	20 (11%)	4 (2%)	5	33
12	I	211/213 (99%)	168 (80%)	30 (14%)	13 (6%)	1	16
13	J	168/178 (94%)	136 (81%)	24 (14%)	8 (5%)	2	19
14	L	208/211 (99%)	171 (82%)	26 (12%)	11 (5%)	1	18
15	M	136/213 (64%)	118 (87%)	16 (12%)	2 (2%)	8	39
16	N	201/204 (98%)	172 (86%)	23 (11%)	6 (3%)	3	27
17	O	199/201 (99%)	182 (92%)	14 (7%)	3 (2%)	8	39
18	P	151/153 (99%)	140 (93%)	9 (6%)	2 (1%)	10	41
19	Q	185/188 (98%)	160 (86%)	20 (11%)	5 (3%)	4	29
20	R	178/196 (91%)	153 (86%)	21 (12%)	4 (2%)	5	32
21	S	173/224 (77%)	146 (84%)	24 (14%)	3 (2%)	7	36
22	T	157/160 (98%)	128 (82%)	26 (17%)	3 (2%)	6	34
23	U	97/128 (76%)	74 (76%)	21 (22%)	2 (2%)	5	33
24	V	129/140 (92%)	112 (87%)	14 (11%)	3 (2%)	5	31
25	W	61/157 (39%)	57 (93%)	3 (5%)	1 (2%)	8	37
26	X	117/156 (75%)	108 (92%)	7 (6%)	2 (2%)	7	36
27	Y	132/145 (91%)	112 (85%)	14 (11%)	6 (4%)	2	20
28	Z	133/136 (98%)	113 (85%)	15 (11%)	5 (4%)	2	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	a	145/148 (98%)	111 (77%)	26 (18%)	8 (6%)	1	18
30	b	73/160 (46%)	58 (80%)	11 (15%)	4 (6%)	1	18
31	c	92/115 (80%)	78 (85%)	10 (11%)	4 (4%)	2	21
32	d	105/125 (84%)	85 (81%)	16 (15%)	4 (4%)	2	23
33	e	126/135 (93%)	110 (87%)	15 (12%)	1 (1%)	16	51
34	f	107/110 (97%)	95 (89%)	7 (6%)	5 (5%)	2	20
35	g	112/117 (96%)	103 (92%)	7 (6%)	2 (2%)	7	35
36	h	120/123 (98%)	103 (86%)	14 (12%)	3 (2%)	4	30
37	i	100/105 (95%)	91 (91%)	7 (7%)	2 (2%)	6	33
38	j	84/86 (98%)	67 (80%)	13 (16%)	4 (5%)	2	19
39	k	67/70 (96%)	55 (82%)	7 (10%)	5 (8%)	1	13
40	l	48/51 (94%)	42 (88%)	4 (8%)	2 (4%)	2	21
41	m	50/128 (39%)	44 (88%)	6 (12%)	0	100	100
42	n	21/25 (84%)	21 (100%)	0	0	100	100
43	o	102/106 (96%)	85 (83%)	11 (11%)	6 (6%)	1	16
44	p	89/91 (98%)	79 (89%)	9 (10%)	1 (1%)	12	45
45	r	123/125 (98%)	97 (79%)	20 (16%)	6 (5%)	2	19
46	z	213/217 (98%)	166 (78%)	29 (14%)	18 (8%)	0	10
47	1	363/393 (92%)	312 (86%)	36 (10%)	15 (4%)	2	22
48	2	60/68 (88%)	49 (82%)	7 (12%)	4 (7%)	1	15
51	SA	206/295 (70%)	176 (85%)	24 (12%)	6 (3%)	3	27
52	SB	209/264 (79%)	168 (80%)	26 (12%)	15 (7%)	1	14
53	SC	216/218 (99%)	188 (87%)	20 (9%)	8 (4%)	2	23
54	SD	225/243 (93%)	170 (76%)	44 (20%)	11 (5%)	2	19
55	SE	260/263 (99%)	202 (78%)	41 (16%)	17 (6%)	1	15
56	SF	189/204 (93%)	160 (85%)	19 (10%)	10 (5%)	1	18
57	SG	235/249 (94%)	194 (83%)	35 (15%)	6 (3%)	4	29
58	SH	187/194 (96%)	143 (76%)	29 (16%)	15 (8%)	1	12
59	SI	204/208 (98%)	176 (86%)	21 (10%)	7 (3%)	3	25
60	SJ	183/194 (94%)	145 (79%)	24 (13%)	14 (8%)	1	12
61	SK	96/165 (58%)	60 (62%)	26 (27%)	10 (10%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	SL	154/158 (98%)	124 (80%)	23 (15%)	7 (4%)	2	20
63	SM	122/124 (98%)	77 (63%)	25 (20%)	20 (16%)	0	3
64	SN	148/151 (98%)	115 (78%)	28 (19%)	5 (3%)	3	25
65	SO	134/151 (89%)	102 (76%)	18 (13%)	14 (10%)	0	7
66	SP	94/145 (65%)	65 (69%)	18 (19%)	11 (12%)	0	5
67	SQ	139/146 (95%)	112 (81%)	21 (15%)	6 (4%)	2	21
68	SR	127/135 (94%)	95 (75%)	22 (17%)	10 (8%)	1	12
69	SS	135/152 (89%)	104 (77%)	23 (17%)	8 (6%)	1	16
70	ST	139/145 (96%)	116 (84%)	17 (12%)	6 (4%)	2	21
71	SU	102/119 (86%)	80 (78%)	18 (18%)	4 (4%)	2	22
72	SV	80/83 (96%)	63 (79%)	10 (12%)	7 (9%)	0	10
73	SW	127/130 (98%)	112 (88%)	11 (9%)	4 (3%)	3	26
74	SX	139/143 (97%)	115 (83%)	19 (14%)	5 (4%)	3	24
75	SY	124/132 (94%)	92 (74%)	23 (18%)	9 (7%)	1	13
76	SZ	73/125 (58%)	54 (74%)	13 (18%)	6 (8%)	1	11
77	Sa	96/115 (84%)	71 (74%)	17 (18%)	8 (8%)	0	11
78	Sb	81/84 (96%)	61 (75%)	15 (18%)	5 (6%)	1	16
79	Sc	62/69 (90%)	46 (74%)	16 (26%)	0	100	100
80	Sd	50/56 (89%)	38 (76%)	9 (18%)	3 (6%)	1	16
81	Se	55/133 (41%)	40 (73%)	14 (26%)	1 (2%)	7	35
82	Sf	69/156 (44%)	39 (56%)	21 (30%)	9 (13%)	0	4
83	Sg	311/317 (98%)	250 (80%)	45 (14%)	16 (5%)	1	18
All	All	11778/13201 (89%)	9619 (82%)	1571 (13%)	588 (5%)	3	19

All (588) 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	47	LEU
5	B	108	GLU
5	B	109	HIS

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Mol	Chain	Res	Type
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
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	L	62	PRO
14	L	64	VAL
14	L	67	HIS
14	L	82	ARG
14	L	83	VAL

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Mol	Chain	Res	Type
14	L	134	PRO
15	M	7	VAL
16	N	30	TYR
16	N	89	VAL
17	O	5	GLN
17	O	111	PRO
19	Q	177	ALA
20	R	36	ASN
21	S	146	HIS
21	S	165	PRO
24	V	14	PHE
24	V	99	GLU
26	X	131	ASP
29	a	76	ASP
29	a	92	LYS
29	a	96	GLY
30	b	7	HIS
30	b	12	GLN
34	f	4	ARG
35	g	7	TYR
36	h	119	PHE
37	i	64	SER
39	k	23	VAL
39	k	59	SER
40	l	22	PRO
43	o	90	HIS
43	o	94	GLY
45	r	34	ALA
45	r	45	HIS
45	r	107	ARG
46	z	19	HIS
46	z	26	ARG
46	z	60	ARG
46	z	81	ASP
46	z	199	GLN
46	z	209	THR
47	1	201	VAL
47	1	287	SER
47	1	406	GLU
47	1	445	THR
51	SA	3	GLY
52	SB	57	ILE

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Mol	Chain	Res	Type
52	SB	179	ASN
52	SB	191	ASP
53	SC	253	PRO
53	SC	254	ASP
54	SD	54	ARG
54	SD	202	LYS
54	SD	223	ILE
55	SE	12	VAL
55	SE	95	THR
55	SE	101	LEU
55	SE	196	THR
56	SF	34	SER
56	SF	37	ASP
58	SH	16	PRO
58	SH	17	ASP
58	SH	18	GLU
58	SH	66	VAL
58	SH	116	ARG
58	SH	170	VAL
58	SH	190	PRO
59	SI	155	ASN
60	SJ	3	VAL
60	SJ	69	ARG
60	SJ	70	ARG
60	SJ	119	LEU
60	SJ	121	LYS
60	SJ	159	PHE
61	SK	30	PRO
61	SK	58	VAL
62	SL	19	ASN
62	SL	100	ASN
63	SM	15	ASN
63	SM	77	ILE
63	SM	91	LEU
63	SM	96	ARG
63	SM	102	LYS
63	SM	114	TYR
64	SN	143	SER
65	SO	56	VAL
65	SO	65	ASP
65	SO	140	THR
66	SP	14	LYS

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Mol	Chain	Res	Type
66	SP	38	SER
67	SQ	48	GLN
67	SQ	77	HIS
68	SR	70	SER
68	SR	88	VAL
69	SS	12	ILE
69	SS	90	VAL
69	SS	118	ARG
70	ST	29	LYS
71	SU	50	VAL
71	SU	107	GLU
72	SV	41	LYS
72	SV	65	SER
73	SW	77	PRO
73	SW	107	SER
74	SX	34	THR
74	SX	129	SER
76	SZ	113	THR
82	Sf	89	LYS
82	Sf	98	VAL
82	Sf	137	ASP
83	Sg	96	THR
83	Sg	142	VAL
83	Sg	182	CYS
83	Sg	282	GLU
4	A	110	GLY
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

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Mol	Chain	Res	Type
8	E	61	ARG
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	210	ARG
13	J	26	VAL
13	J	88	LYS
13	J	169	LYS
14	L	143	GLU
15	M	87	ALA
16	N	79	ALA
18	P	41	ILE
19	Q	178	ARG
20	R	39	GLN
22	T	18	PRO
22	T	44	GLY
22	T	55	LYS
26	X	86	ALA
27	Y	6	PHE
28	Z	91	LEU
29	a	60	HIS
29	a	62	HIS
29	a	97	ALA
31	c	32	LYS
31	c	80	GLU
31	c	81	LEU
32	d	93	ASN
33	e	34	ASN
36	h	122	LYS
39	k	61	PRO
43	o	33	LEU
43	o	98	LYS
45	r	123	PRO
46	z	200	ASN
47	1	174	GLY
47	1	211	GLY

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Mol	Chain	Res	Type
47	1	238	ASN
47	1	239	LEU
47	1	432	SER
48	2	8	VAL
48	2	66	VAL
51	SA	110	ASN
51	SA	187	GLY
52	SB	83	LYS
52	SB	108	ASP
52	SB	152	LYS
52	SB	204	ILE
52	SB	223	PHE
53	SC	134	ASN
53	SC	255	LEU
54	SD	219	PRO
55	SE	76	VAL
55	SE	98	ASN
55	SE	109	PHE
56	SF	21	GLY
56	SF	121	PRO
57	SG	99	GLY
58	SH	160	LYS
59	SI	126	GLY
59	SI	137	LEU
59	SI	138	ASN
60	SJ	5	ARG
60	SJ	118	GLY
62	SL	3	ASP
63	SM	35	ILE
63	SM	48	HIS
63	SM	79	VAL
64	SN	38	TYR
65	SO	32	HIS
65	SO	33	ILE
65	SO	64	ALA
65	SO	105	THR
65	SO	129	ILE
65	SO	146	ARG
66	SP	12	PHE
67	SQ	32	ILE
67	SQ	35	ASN
68	SR	72	LYS

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Mol	Chain	Res	Type
68	SR	93	GLN
68	SR	95	ILE
68	SR	110	ASP
68	SR	123	THR
69	SS	7	GLU
69	SS	133	GLY
70	ST	28	LEU
70	ST	34	VAL
70	ST	39	LEU
70	ST	49	ASP
73	SW	45	GLY
74	SX	99	GLU
75	SY	60	PHE
75	SY	84	LYS
75	SY	118	ARG
75	SY	120	THR
76	SZ	42	ASP
76	SZ	102	LYS
76	SZ	104	ARG
76	SZ	108	ILE
77	Sa	5	ARG
77	Sa	8	ASN
77	Sa	25	ASN
78	Sb	6	ASP
78	Sb	59	CYS
82	Sf	112	GLY
83	Sg	97	THR
83	Sg	139	LYS
83	Sg	141	THR
83	Sg	161	SER
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	92	VAL

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Mol	Chain	Res	Type
8	E	95	ASP
8	E	104	LYS
8	E	153	HIS
8	E	206	LYS
8	E	218	LEU
8	E	255	ARG
9	F	105	PRO
12	I	94	PHE
12	I	106	ALA
13	J	124	GLY
14	L	172	GLU
18	P	54	GLN
19	Q	52	PHE
19	Q	146	ARG
20	R	130	ASN
21	S	153	PRO
23	U	38	ASN
27	Y	11	ARG
27	Y	18	HIS
28	Z	8	GLY
28	Z	33	THR
29	a	93	ASN
32	d	38	PHE
34	f	80	ASN
34	f	107	PRO
40	l	47	THR
43	o	49	GLY
46	z	154	THR
46	z	196	LYS
46	z	212	LYS
47	1	28	PHE
47	1	288	ASN
48	2	64	ILE
51	SA	105	PRO
52	SB	43	ASN
53	SC	264	SER
54	SD	178	ARG
54	SD	179	GLN
55	SE	24	THR
55	SE	163	ASP
55	SE	171	ASP
56	SF	163	PHE

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Mol	Chain	Res	Type
58	SH	107	LYS
58	SH	110	THR
59	SI	143	LYS
61	SK	63	ALA
61	SK	92	ALA
62	SL	28	THR
63	SM	65	VAL
63	SM	95	ASP
63	SM	103	VAL
63	SM	116	LYS
63	SM	117	GLU
65	SO	128	ARG
66	SP	50	ARG
66	SP	73	PRO
66	SP	74	GLU
66	SP	87	PRO
68	SR	127	ASN
69	SS	92	ASP
70	ST	128	GLN
72	SV	3	ASN
73	SW	30	CYS
74	SX	114	ASP
75	SY	104	ARG
76	SZ	80	ARG
77	Sa	61	ALA
77	Sa	62	TYR
77	Sa	97	PRO
80	Sd	7	TYR
82	Sf	83	LYS
82	Sf	99	LYS
82	Sf	100	LEU
83	Sg	65	PHE
83	Sg	144	ASP
83	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

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Mol	Chain	Res	Type
6	C	49	ARG
7	D	20	PHE
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
16	N	182	HIS
19	Q	55	ARG
20	R	131	VAL
23	U	98	ASP
24	V	110	GLY
25	W	43	LYS
29	a	98	ALA
30	b	10	HIS
32	d	58	GLY
32	d	102	LEU
34	f	5	LEU
39	k	29	LYS
43	o	8	ARG
46	z	71	GLN
51	SA	188	THR
52	SB	77	ASP
52	SB	146	ARG
54	SD	218	LEU
55	SE	132	GLY
56	SF	131	ALA
56	SF	132	GLY
56	SF	143	PRO
57	SG	146	ASN
57	SG	152	ASP
58	SH	35	ASP
58	SH	57	ARG
58	SH	111	LYS
60	SJ	39	ASN

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Mol	Chain	Res	Type
60	SJ	92	MET
60	SJ	120	ALA
60	SJ	125	HIS
61	SK	3	MET
62	SL	8	ARG
63	SM	36	ARG
63	SM	76	LEU
63	SM	119	GLN
66	SP	8	LYS
66	SP	75	VAL
67	SQ	116	ASP
72	SV	10	ASP
75	SY	30	PRO
75	SY	34	THR
77	Sa	35	ALA
78	Sb	75	GLU
80	Sd	8	TRP
82	Sf	87	THR
83	Sg	37	ASP
83	Sg	160	SER
83	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
13	J	32	ARG
16	N	40	PRO
16	N	55	ALA
27	Y	85	VAL
28	Z	124	THR
30	b	21	ILE
31	c	77	ASN

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Mol	Chain	Res	Type
34	f	106	TYR
35	g	84	ALA
38	j	5	THR
38	j	38	GLY
46	z	153	SER
46	z	175	THR
46	z	198	TRP
48	2	27	LYS
52	SB	22	VAL
52	SB	76	ASN
52	SB	93	GLY
53	SC	181	PRO
53	SC	189	GLY
54	SD	199	GLY
54	SD	214	LYS
55	SE	38	LEU
56	SF	68	ILE
57	SG	20	ASP
57	SG	59	GLN
58	SH	100	ILE
58	SH	159	ASP
61	SK	39	ASN
61	SK	65	ARG
61	SK	67	PHE
61	SK	69	TRP
62	SL	147	LYS
63	SM	81	ASP
64	SN	58	HIS
64	SN	138	ASN
65	SO	39	ASP
65	SO	149	ARG
67	SQ	43	GLU
69	SS	82	TRP
71	SU	118	ASP
72	SV	42	VAL
72	SV	45	ARG
77	Sa	72	HIS
80	Sd	10	HIS
82	Sf	138	ARG
5	B	17	LEU
5	B	112	ASP
5	B	144	ALA

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Mol	Chain	Res	Type
6	C	198	ASN
8	E	40	CYS
8	E	100	THR
12	I	110	ARG
13	J	27	GLY
14	L	169	ILE
17	O	110	PRO
27	Y	63	LYS
27	Y	79	VAL
28	Z	4	PHE
38	j	9	GLY
38	j	75	ARG
44	p	4	ARG
45	r	103	ARG
47	1	199	THR
47	1	237	GLN
47	1	353	SER
51	SA	43	SER
55	SE	30	ARG
55	SE	35	PRO
59	SI	131	PRO
61	SK	41	PRO
62	SL	69	ARG
66	SP	27	ASP
66	SP	49	LEU
68	SR	121	GLN
69	SS	117	ILE
72	SV	81	LYS
74	SX	104	GLY
78	Sb	48	SER
5	B	110	ILE
5	B	259	PRO
7	D	114	GLY
39	k	63	GLY
46	z	83	PRO
53	SC	171	GLY
54	SD	222	PRO
56	SF	166	ILE
75	SY	95	GLY
83	Sg	190	GLY
14	L	100	PRO
46	z	87	ILE

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Mol	Chain	Res	Type
55	SE	15	PRO
57	SG	161	PRO
64	SN	37	ILE
75	SY	67	GLY
81	Se	54	GLY
7	D	261	VAL
12	I	47	PRO
46	z	58	THR
47	1	179	ILE
54	SD	194	PRO
55	SE	131	VAL
60	SJ	8	VAL
60	SJ	169	ARG
63	SM	94	ILE
68	SR	86	PRO
71	SU	52	GLY
78	Sb	58	GLY
83	Sg	163	PRO
5	B	321	VAL
8	E	90	LYS
9	F	100	ILE
10	G	58	PRO
14	L	28	GLN
36	h	38	GLY
37	i	63	VAL
45	r	44	ILE
52	SB	114	VAL
55	SE	90	ILE
63	SM	104	VAL
65	SO	24	GLY
65	SO	53	ILE
6	C	6	PRO
9	F	199	VAL
46	z	211	GLY
59	SI	20	PRO

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	187/199 (94%)	139 (74%)	48 (26%)	0	3
5	B	335/335 (100%)	265 (79%)	70 (21%)	1	5
6	C	305/305 (100%)	239 (78%)	66 (22%)	1	5
7	D	246/250 (98%)	178 (72%)	68 (28%)	0	2
8	E	209/209 (100%)	157 (75%)	52 (25%)	0	3
9	F	194/194 (100%)	145 (75%)	49 (25%)	0	3
10	G	206/226 (91%)	158 (77%)	48 (23%)	0	4
11	H	169/171 (99%)	125 (74%)	44 (26%)	0	3
12	I	180/180 (100%)	136 (76%)	44 (24%)	0	4
13	J	143/149 (96%)	115 (80%)	28 (20%)	1	7
14	L	176/177 (99%)	135 (77%)	41 (23%)	0	4
15	M	116/160 (72%)	95 (82%)	21 (18%)	1	9
16	N	171/172 (99%)	129 (75%)	42 (25%)	0	3
17	O	172/172 (100%)	146 (85%)	26 (15%)	2	14
18	P	134/134 (100%)	112 (84%)	22 (16%)	2	12
19	Q	163/164 (99%)	132 (81%)	31 (19%)	1	7
20	R	159/175 (91%)	120 (76%)	39 (24%)	0	3
21	S	156/192 (81%)	121 (78%)	35 (22%)	1	5
22	T	139/140 (99%)	112 (81%)	27 (19%)	1	7
23	U	89/114 (78%)	67 (75%)	22 (25%)	0	3
24	V	101/107 (94%)	77 (76%)	24 (24%)	0	4
25	W	55/126 (44%)	42 (76%)	13 (24%)	0	4
26	X	107/133 (80%)	89 (83%)	18 (17%)	1	11
27	Y	124/135 (92%)	96 (77%)	28 (23%)	1	5
28	Z	117/118 (99%)	93 (80%)	24 (20%)	1	6
29	a	119/120 (99%)	102 (86%)	17 (14%)	2	16
30	b	63/123 (51%)	45 (71%)	18 (29%)	0	2
31	c	79/97 (81%)	60 (76%)	19 (24%)	0	4
32	d	98/110 (89%)	66 (67%)	32 (33%)	0	1
33	e	114/121 (94%)	89 (78%)	25 (22%)	1	5
34	f	88/89 (99%)	73 (83%)	15 (17%)	1	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	g	98/100 (98%)	79 (81%)	19 (19%)	1	7
36	h	109/110 (99%)	92 (84%)	17 (16%)	2	13
37	i	86/89 (97%)	71 (83%)	15 (17%)	1	10
38	j	73/73 (100%)	60 (82%)	13 (18%)	1	10
39	k	64/65 (98%)	52 (81%)	12 (19%)	1	8
40	l	47/48 (98%)	39 (83%)	8 (17%)	1	11
41	m	48/116 (41%)	36 (75%)	12 (25%)	0	3
42	n	22/24 (92%)	17 (77%)	5 (23%)	0	4
43	o	92/94 (98%)	70 (76%)	22 (24%)	0	4
44	p	74/74 (100%)	61 (82%)	13 (18%)	1	10
45	r	109/109 (100%)	85 (78%)	24 (22%)	1	5
46	z	195/196 (100%)	169 (87%)	26 (13%)	3	18
47	1	316/331 (96%)	300 (95%)	16 (5%)	20	45
48	2	53/59 (90%)	49 (92%)	4 (8%)	11	34
51	SA	174/245 (71%)	141 (81%)	33 (19%)	1	7
52	SB	194/231 (84%)	164 (84%)	30 (16%)	2	13
53	SC	184/184 (100%)	148 (80%)	36 (20%)	1	7
54	SD	190/202 (94%)	163 (86%)	27 (14%)	2	16
55	SE	224/225 (100%)	180 (80%)	44 (20%)	1	7
56	SF	161/170 (95%)	129 (80%)	32 (20%)	1	6
57	SG	207/218 (95%)	171 (83%)	36 (17%)	1	10
58	SH	169/174 (97%)	149 (88%)	20 (12%)	4	20
59	SI	178/180 (99%)	148 (83%)	30 (17%)	1	11
60	SJ	161/168 (96%)	128 (80%)	33 (20%)	1	6
61	SK	89/136 (65%)	68 (76%)	21 (24%)	0	4
62	SL	140/142 (99%)	118 (84%)	22 (16%)	2	13
63	SM	104/104 (100%)	76 (73%)	28 (27%)	0	3
64	SN	130/131 (99%)	101 (78%)	29 (22%)	1	5
65	SO	106/119 (89%)	83 (78%)	23 (22%)	1	5
66	SP	88/130 (68%)	73 (83%)	15 (17%)	1	11
67	SQ	117/121 (97%)	100 (86%)	17 (14%)	2	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	SR	117/121 (97%)	102 (87%)	15 (13%)	3	18
69	SS	119/132 (90%)	97 (82%)	22 (18%)	1	8
70	ST	112/115 (97%)	89 (80%)	23 (20%)	1	6
71	SU	94/107 (88%)	84 (89%)	10 (11%)	5	22
72	SV	66/67 (98%)	53 (80%)	13 (20%)	1	7
73	SW	112/113 (99%)	93 (83%)	19 (17%)	1	11
74	SX	113/115 (98%)	98 (87%)	15 (13%)	3	18
75	SY	108/114 (95%)	86 (80%)	22 (20%)	1	6
76	SZ	66/103 (64%)	54 (82%)	12 (18%)	1	9
77	Sa	85/98 (87%)	70 (82%)	15 (18%)	1	10
78	Sb	75/76 (99%)	64 (85%)	11 (15%)	2	15
79	Sc	57/62 (92%)	43 (75%)	14 (25%)	0	3
80	Sd	45/48 (94%)	35 (78%)	10 (22%)	1	5
81	Se	46/105 (44%)	35 (76%)	11 (24%)	0	4
82	Sf	64/140 (46%)	45 (70%)	19 (30%)	0	2
83	Sg	272/275 (99%)	242 (89%)	30 (11%)	5	21
All	All	10267/11256 (91%)	8268 (80%)	1999 (20%)	3	7

All (1999) 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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
8	E	115	GLU
8	E	119	ARG
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
12	I	128	ARG
12	I	143	GLN
12	I	146	GLU
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
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	L	5	ARG
14	L	10	LEU

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Mol	Chain	Res	Type
14	L	13	HIS
14	L	19	GLN
14	L	28	GLN
14	L	31	ARG
14	L	34	ARG
14	L	36	ARG
14	L	39	ARG
14	L	45	ARG
14	L	49	ARG
14	L	56	ARG
14	L	65	ARG
14	L	66	TYR
14	L	67	HIS
14	L	74	ARG
14	L	79	GLU
14	L	82	ARG
14	L	92	ARG
14	L	99	ASP
14	L	101	ARG
14	L	103	ARG
14	L	111	GLN
14	L	113	ASN
14	L	115	GLN
14	L	119	GLU
14	L	123	LYS
14	L	127	PHE
14	L	129	ARG
14	L	130	LYS
14	L	146	LEU
14	L	158	ARG
14	L	162	LYS
14	L	163	ARG
14	L	165	LYS
14	L	172	GLU
14	L	176	PHE
14	L	186	ARG
14	L	195	ARG
14	L	201	GLU
14	L	205	GLN
15	M	8	GLU
15	M	11	ARG
15	M	17	PHE

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Mol	Chain	Res	Type
15	M	29	ASP
15	M	32	ASP
15	M	33	GLN
15	M	34	ASN
15	M	38	VAL
15	M	47	ARG
15	M	56	GLN
15	M	57	LEU
15	M	59	ASP
15	M	61	ILE
15	M	66	HIS
15	M	70	GLN
15	M	79	LYS
15	M	89	THR
15	M	90	ARG
15	M	91	TRP
15	M	98	ARG
15	M	119	ARG
16	N	4	TYR
16	N	9	GLU
16	N	11	TRP
16	N	26	ARG
16	N	29	GLN
16	N	49	ARG
16	N	50	ARG
16	N	53	TYR
16	N	54	LYS
16	N	59	TYR
16	N	63	ARG
16	N	67	ARG
16	N	71	ARG
16	N	72	LYS
16	N	80	THR
16	N	86	HIS
16	N	87	HIS
16	N	91	GLN
16	N	92	LEU
16	N	104	GLU
16	N	108	ARG
16	N	119	TYR
16	N	123	GLU
16	N	126	THR

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Mol	Chain	Res	Type
16	N	127	TYR
16	N	131	GLU
16	N	136	ASP
16	N	138	PHE
16	N	139	HIS
16	N	147	ASP
16	N	150	TRP
16	N	162	ARG
16	N	169	ARG
16	N	174	LEU
16	N	178	HIS
16	N	182	HIS
16	N	189	ARG
16	N	192	TRP
16	N	195	ARG
16	N	196	ASN
16	N	199	GLN
16	N	203	TYR
17	O	5	GLN
17	O	42	ASN
17	O	46	ASN
17	O	49	ARG
17	O	57	PHE
17	O	59	ARG
17	O	60	LYS
17	O	61	ARG
17	O	62	MET
17	O	74	ARG
17	O	78	ARG
17	O	82	ARG
17	O	85	ARG
17	O	110	PRO
17	O	113	ASP
17	O	140	ARG
17	O	160	ARG
17	O	167	HIS
17	O	173	GLN
17	O	178	ARG
17	O	184	ASN
17	O	187	LYS
17	O	188	LYS
17	O	191	ARG

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Mol	Chain	Res	Type
17	O	192	PHE
17	O	194	GLU
18	P	3	ARG
18	P	9	GLU
18	P	10	ASN
18	P	13	LYS
18	P	18	ARG
18	P	23	ARG
18	P	24	VAL
18	P	28	ASN
18	P	30	ARG
18	P	40	HIS
18	P	42	ARG
18	P	61	ARG
18	P	69	ARG
18	P	70	CYS
18	P	78	TRP
18	P	90	PHE
18	P	91	LEU
18	P	110	ASP
18	P	128	ARG
18	P	133	HIS
18	P	135	ARG
18	P	154	GLU
19	Q	5	ILE
19	Q	9	LYS
19	Q	14	ARG
19	Q	15	ARG
19	Q	16	LYS
19	Q	32	TYR
19	Q	37	ARG
19	Q	44	ASN
19	Q	54	SER
19	Q	58	ARG
19	Q	61	LEU
19	Q	65	ARG
19	Q	68	ARG
19	Q	72	LEU
19	Q	75	ARG
19	Q	79	THR
19	Q	85	THR
19	Q	89	ASP

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Mol	Chain	Res	Type
19	Q	91	ARG
19	Q	93	GLN
19	Q	97	LYS
19	Q	108	ARG
19	Q	110	ARG
19	Q	112	ARG
19	Q	119	LYS
19	Q	146	ARG
19	Q	150	ARG
19	Q	166	TYR
19	Q	173	LYS
19	Q	180	ARG
19	Q	181	ARG
20	R	5	ARG
20	R	6	LEU
20	R	9	ARG
20	R	23	TRP
20	R	30	ASN
20	R	39	GLN
20	R	40	GLN
20	R	47	ASP
20	R	50	ILE
20	R	58	HIS
20	R	60	ARG
20	R	74	ARG
20	R	81	ARG
20	R	86	ASN
20	R	89	MET
20	R	99	MET
20	R	104	ARG
20	R	105	LEU
20	R	107	ARG
20	R	108	ARG
20	R	109	TYR
20	R	113	LYS
20	R	114	LYS
20	R	117	ARG
20	R	118	HIS
20	R	120	TYR
20	R	124	TYR
20	R	131	VAL
20	R	133	LYS

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Mol	Chain	Res	Type
20	R	136	ARG
20	R	138	LEU
20	R	141	HIS
20	R	163	ARG
20	R	168	GLU
20	R	172	ARG
20	R	175	GLU
20	R	177	LEU
20	R	178	GLN
20	R	180	LYS
21	S	2	LYS
21	S	15	ARG
21	S	28	TYR
21	S	29	ARG
21	S	37	HIS
21	S	44	PHE
21	S	47	PHE
21	S	48	VAL
21	S	53	LYS
21	S	57	SER
21	S	64	CYS
21	S	68	PHE
21	S	70	LYS
21	S	82	LEU
21	S	83	ARG
21	S	84	TYR
21	S	86	SER
21	S	90	THR
21	S	95	ARG
21	S	99	ASP
21	S	100	LEU
21	S	101	THR
21	S	127	MET
21	S	128	LYS
21	S	138	ARG
21	S	146	HIS
21	S	147	ASP
21	S	150	ILE
21	S	151	LYS
21	S	156	HIS
21	S	157	ARG
21	S	159	LEU

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Mol	Chain	Res	Type
21	S	162	GLN
21	S	168	THR
21	S	171	ARG
22	T	5	LYS
22	T	7	LYS
22	T	9	ARG
22	T	13	TYR
22	T	19	PHE
22	T	30	TYR
22	T	32	ARG
22	T	33	ILE
22	T	35	LYS
22	T	36	LYS
22	T	38	ASP
22	T	41	ASP
22	T	54	HIS
22	T	60	LYS
22	T	70	HIS
22	T	76	VAL
22	T	88	ARG
22	T	102	ARG
22	T	103	ASP
22	T	107	LYS
22	T	113	ASP
22	T	118	GLU
22	T	121	GLU
22	T	139	HIS
22	T	142	ARG
22	T	144	ASN
22	T	152	GLU
23	U	21	PHE
23	U	23	LEU
23	U	27	HIS
23	U	33	ILE
23	U	38	ASN
23	U	39	PHE
23	U	40	GLU
23	U	42	PHE
23	U	46	ARG
23	U	50	ASN
23	U	52	LYS
23	U	62	THR

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Mol	Chain	Res	Type
23	U	64	GLU
23	U	65	ARG
23	U	67	LYS
23	U	69	LYS
23	U	82	TYR
23	U	89	LYS
23	U	90	TYR
23	U	98	ASP
23	U	101	ARG
23	U	113	ARG
24	V	13	LYS
24	V	14	PHE
24	V	15	ARG
24	V	18	LEU
24	V	27	ASN
24	V	30	ASP
24	V	36	ASN
24	V	46	LYS
24	V	48	ARG
24	V	50	ASN
24	V	51	ARG
24	V	59	ASP
24	V	60	MET
24	V	73	ARG
24	V	77	HIS
24	V	84	GLN
24	V	91	LYS
24	V	98	PHE
24	V	100	ASP
24	V	107	ASN
24	V	109	LYS
24	V	111	GLU
24	V	123	LYS
24	V	128	LEU
25	W	3	VAL
25	W	4	GLU
25	W	8	PHE
25	W	12	LYS
25	W	17	HIS
25	W	25	ASP
25	W	33	ASN
25	W	44	ARG

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Mol	Chain	Res	Type
25	W	50	ASN
25	W	55	TYR
25	W	56	ARG
25	W	57	ARG
25	W	59	HIS
26	X	39	LYS
26	X	45	THR
26	X	48	ARG
26	X	60	TYR
26	X	62	ARG
26	X	72	ASP
26	X	79	PHE
26	X	84	GLU
26	X	94	ASN
26	X	117	TYR
26	X	120	ASP
26	X	129	ARG
26	X	133	GLU
26	X	137	TYR
26	X	139	ARG
26	X	144	TYR
26	X	148	ASP
26	X	151	ASN
27	Y	2	LYS
27	Y	4	ASN
27	Y	11	ARG
27	Y	15	ARG
27	Y	17	ARG
27	Y	18	HIS
27	Y	19	PHE
27	Y	27	ARG
27	Y	36	LYS
27	Y	45	ARG
27	Y	49	ILE
27	Y	50	ARG
27	Y	53	ASP
27	Y	56	GLN
27	Y	59	ARG
27	Y	62	TYR
27	Y	65	GLN
27	Y	72	GLN
27	Y	82	ILE

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Mol	Chain	Res	Type
27	Y	83	GLU
27	Y	84	ARG
27	Y	87	ARG
27	Y	91	ASN
27	Y	112	ASP
27	Y	114	ASP
27	Y	115	ARG
27	Y	126	ARG
27	Y	127	GLN
28	Z	4	PHE
28	Z	17	ARG
28	Z	21	ARG
28	Z	27	LYS
28	Z	30	ASP
28	Z	36	ARG
28	Z	38	TYR
28	Z	54	THR
28	Z	57	MET
28	Z	60	LYS
28	Z	64	LYS
28	Z	76	ASN
28	Z	78	ASN
28	Z	88	ASP
28	Z	92	ASP
28	Z	93	LYS
28	Z	98	LYS
28	Z	102	ARG
28	Z	108	ARG
28	Z	109	LYS
28	Z	112	ARG
28	Z	121	ARG
28	Z	122	TYR
28	Z	136	PHE
29	a	7	LYS
29	a	10	LYS
29	a	14	HIS
29	a	19	HIS
29	a	21	ARG
29	a	40	HIS
29	a	41	HIS
29	a	46	ASP
29	a	49	HIS

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Mol	Chain	Res	Type
29	a	52	TYR
29	a	59	ARG
29	a	61	TYR
29	a	63	LEU
29	a	77	LYS
29	a	84	GLU
29	a	105	ARG
29	a	132	ARG
30	b	6	ASN
30	b	7	HIS
30	b	12	GLN
30	b	16	TRP
30	b	18	ARG
30	b	19	ASN
30	b	22	LYS
30	b	23	LYS
30	b	25	ARG
30	b	27	GLN
30	b	28	ARG
30	b	30	GLU
30	b	39	PHE
30	b	43	MET
30	b	44	ARG
30	b	51	LYS
30	b	55	LYS
30	b	65	MET
31	c	18	LEU
31	c	27	TYR
31	c	31	TYR
31	c	37	MET
31	c	39	ARG
31	c	42	LYS
31	c	44	LYS
31	c	52	CYS
31	c	55	LEU
31	c	56	ARG
31	c	59	GLU
31	c	66	LEU
31	c	72	HIS
31	c	73	HIS
31	c	74	TYR
31	c	77	ASN

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Mol	Chain	Res	Type
31	c	78	ASN
31	c	81	LEU
31	c	88	TYR
32	d	18	ASN
32	d	19	GLU
32	d	23	ARG
32	d	26	THR
32	d	28	ASN
32	d	31	LYS
32	d	32	ARG
32	d	38	PHE
32	d	39	LYS
32	d	44	ARG
32	d	67	ARG
32	d	73	TRP
32	d	78	ARG
32	d	79	ASN
32	d	83	ARG
32	d	85	ARG
32	d	86	VAL
32	d	87	ARG
32	d	91	LYS
32	d	93	ASN
32	d	94	GLU
32	d	95	ASP
32	d	101	LYS
32	d	103	TYR
32	d	108	TYR
32	d	109	VAL
32	d	116	ASN
32	d	117	LEU
32	d	118	GLN
32	d	119	THR
32	d	121	ASN
32	d	123	ASP
33	e	11	LYS
33	e	16	ARG
33	e	21	ILE
33	e	26	ASP
33	e	36	ARG
33	e	42	ASP
33	e	43	ASN

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Mol	Chain	Res	Type
33	e	46	ARG
33	e	49	PHE
33	e	52	GLN
33	e	57	ASN
33	e	64	LYS
33	e	68	HIS
33	e	77	PHE
33	e	78	LEU
33	e	85	LEU
33	e	92	ASN
33	e	95	TYR
33	e	106	LYS
33	e	107	ASN
33	e	108	ARG
33	e	113	GLU
33	e	124	ASN
33	e	126	ASN
33	e	128	ARG
34	f	4	ARG
34	f	5	LEU
34	f	7	SER
34	f	14	TYR
34	f	16	ARG
34	f	19	ARG
34	f	22	ARG
34	f	24	HIS
34	f	36	ARG
34	f	49	TYR
34	f	51	TYR
34	f	52	LYS
34	f	71	TRP
34	f	101	ILE
34	f	109	ARG
35	g	3	GLN
35	g	4	ARG
35	g	5	LEU
35	g	12	SER
35	g	14	ASN
35	g	29	ARG
35	g	32	TYR
35	g	52	ARG
35	g	54	ARG

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Mol	Chain	Res	Type
35	g	57	ARG
35	g	60	ARG
35	g	66	ARG
35	g	75	SER
35	g	81	SER
35	g	88	ARG
35	g	93	ARG
35	g	95	PHE
35	g	114	GLN
35	g	115	LYS
36	h	8	ASP
36	h	10	ARG
36	h	15	GLU
36	h	23	ASP
36	h	28	LEU
36	h	48	ARG
36	h	51	ARG
36	h	67	GLU
36	h	68	ASN
36	h	72	PHE
36	h	73	TYR
36	h	89	ARG
36	h	93	ARG
36	h	97	LYS
36	h	100	GLU
36	h	119	PHE
36	h	122	LYS
37	i	3	LEU
37	i	4	ARG
37	i	12	ASN
37	i	20	ASN
37	i	27	SER
37	i	30	ARG
37	i	33	LEU
37	i	42	ASP
37	i	46	GLU
37	i	50	PHE
37	i	54	GLU
37	i	68	ARG
37	i	85	ARG
37	i	88	GLU
37	i	103	LYS

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Mol	Chain	Res	Type
38	j	10	LYS
38	j	25	LYS
38	j	27	TYR
38	j	39	TYR
38	j	45	ARG
38	j	47	TYR
38	j	48	ASN
38	j	55	ARG
38	j	56	ARG
38	j	57	ASN
38	j	71	TYR
38	j	79	ARG
38	j	80	GLU
39	k	14	THR
39	k	19	ASP
39	k	21	LYS
39	k	27	LYS
39	k	30	ASP
39	k	35	LYS
39	k	37	ARG
39	k	51	GLU
39	k	54	GLU
39	k	56	LEU
39	k	60	LEU
39	k	70	LYS
40	l	11	ARG
40	l	12	PHE
40	l	16	LYS
40	l	17	GLN
40	l	21	ARG
40	l	36	ARG
40	l	46	ARG
40	l	49	LEU
41	m	79	GLU
41	m	84	GLN
41	m	87	GLN
41	m	89	TYR
41	m	90	ASN
41	m	96	CYS
41	m	97	ARG
41	m	104	HIS
41	m	106	ARG

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Mol	Chain	Res	Type
41	m	109	ASN
41	m	111	ARG
41	m	119	ASN
42	n	8	LYS
42	n	9	ARG
42	n	18	ARG
42	n	20	MET
42	n	21	ARG
43	o	6	LYS
43	o	11	PHE
43	o	24	THR
43	o	26	TYR
43	o	33	LEU
43	o	36	GLN
43	o	42	ASP
43	o	45	GLN
43	o	48	TYR
43	o	57	ARG
43	o	58	LYS
43	o	59	LYS
43	o	61	LYS
43	o	64	LYS
43	o	69	ARG
43	o	76	ASN
43	o	78	ARG
43	o	79	SER
43	o	81	ARG
43	o	82	MET
43	o	99	ARG
43	o	102	GLN
44	p	3	LYS
44	p	4	ARG
44	p	16	THR
44	p	30	GLU
44	p	34	HIS
44	p	48	LYS
44	p	49	ARG
44	p	69	TRP
44	p	71	TYR
44	p	84	ARG
44	p	85	ARG
44	p	87	LYS

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Mol	Chain	Res	Type
44	p	92	GLN
45	r	7	TRP
45	r	11	ARG
45	r	13	CYS
45	r	15	SER
45	r	16	PHE
45	r	18	ILE
45	r	26	SER
45	r	28	GLU
45	r	30	ASN
45	r	33	LYS
45	r	35	ARG
45	r	39	ARG
45	r	46	HIS
45	r	64	ILE
45	r	66	ARG
45	r	67	ARG
45	r	71	ARG
45	r	73	PRO
45	r	83	ASN
45	r	102	TYR
45	r	106	LEU
45	r	107	ARG
45	r	112	ARG
45	r	115	SER
46	z	28	PHE
46	z	29	LEU
46	z	41	TYR
46	z	42	ASP
46	z	58	THR
46	z	91	LYS
46	z	93	LEU
46	z	99	LEU
46	z	101	LYS
46	z	107	TYR
46	z	108	ASP
46	z	111	LEU
46	z	130	LYS
46	z	143	ASN
46	z	147	LYS
46	z	150	GLU
46	z	154	THR

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Mol	Chain	Res	Type
46	z	156	LYS
46	z	159	MET
46	z	160	LYS
46	z	163	LEU
46	z	174	MET
46	z	196	LYS
46	z	197	ASN
46	z	202	ARG
46	z	212	LYS
47	1	25	LYS
47	1	149	LEU
47	1	201	VAL
47	1	205	ARG
47	1	207	MET
47	1	226	LYS
47	1	235	TYR
47	1	239	LEU
47	1	243	MET
47	1	273	ARG
47	1	355	LEU
47	1	368	MET
47	1	395	LYS
47	1	412	GLU
47	1	415	ARG
47	1	457	TYR
48	2	8	VAL
48	2	21	LEU
48	2	24	ARG
48	2	32	GLU
51	SA	8	LEU
51	SA	32	PHE
51	SA	39	TYR
51	SA	44	ASP
51	SA	53	ARG
51	SA	58	LEU
51	SA	60	LEU
51	SA	73	ASP
51	SA	79	SER
51	SA	81	ASN
51	SA	89	LYS
51	SA	90	PHE
51	SA	99	ILE

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Mol	Chain	Res	Type
51	SA	102	ARG
51	SA	105	PRO
51	SA	111	GLN
51	SA	116	PHE
51	SA	128	ARG
51	SA	130	ASP
51	SA	140	VAL
51	SA	141	ASN
51	SA	151	ASP
51	SA	158	ASP
51	SA	169	HIS
51	SA	177	MET
51	SA	178	LEU
51	SA	180	ARG
51	SA	181	GLU
51	SA	186	ARG
51	SA	195	TRP
51	SA	198	MET
51	SA	203	PHE
51	SA	206	ASP
52	SB	27	LYS
52	SB	31	TYR
52	SB	48	LEU
52	SB	51	ARG
52	SB	52	THR
52	SB	56	LYS
52	SB	60	ASP
52	SB	67	PHE
52	SB	76	ASN
52	SB	77	ASP
52	SB	81	PHE
52	SB	99	ASN
52	SB	105	LEU
52	SB	107	ARG
52	SB	119	THR
52	SB	133	TYR
52	SB	136	ARG
52	SB	142	PHE
52	SB	146	ARG
52	SB	148	ASN
52	SB	150	ILE
52	SB	155	TYR

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Mol	Chain	Res	Type
52	SB	158	HIS
52	SB	162	ARG
52	SB	180	ASP
52	SB	181	LEU
52	SB	191	ASP
52	SB	196	ASP
52	SB	205	TYR
52	SB	208	HIS
53	SC	60	TRP
53	SC	61	MET
53	SC	65	LYS
53	SC	71	LYS
53	SC	72	ASP
53	SC	78	LEU
53	SC	79	GLU
53	SC	92	GLU
53	SC	97	PHE
53	SC	101	SER
53	SC	104	ASP
53	SC	110	MET
53	SC	114	LYS
53	SC	115	GLN
53	SC	120	GLN
53	SC	121	ARG
53	SC	134	ASN
53	SC	137	VAL
53	SC	142	LYS
53	SC	152	ARG
53	SC	167	ARG
53	SC	169	TYR
53	SC	200	ARG
53	SC	215	MET
53	SC	221	ASP
53	SC	227	ARG
53	SC	235	ASN
53	SC	236	PHE
53	SC	242	ASP
53	SC	245	SER
53	SC	250	TYR
53	SC	253	PRO
53	SC	255	LEU
53	SC	262	THR

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Mol	Chain	Res	Type
53	SC	272	HIS
53	SC	275	LYS
54	SD	6	SER
54	SD	9	ARG
54	SD	22	ASN
54	SD	23	GLU
54	SD	24	PHE
54	SD	32	ASP
54	SD	53	THR
54	SD	67	ARG
54	SD	76	ARG
54	SD	87	TYR
54	SD	94	ARG
54	SD	103	GLU
54	SD	107	TYR
54	SD	129	SER
54	SD	135	GLU
54	SD	152	PHE
54	SD	154	ASP
54	SD	158	ILE
54	SD	167	TYR
54	SD	169	ASP
54	SD	177	LEU
54	SD	178	ARG
54	SD	206	ASP
54	SD	212	GLU
54	SD	216	GLU
54	SD	218	LEU
54	SD	225	GLU
55	SE	3	ARG
55	SE	8	HIS
55	SE	9	LEU
55	SE	11	ARG
55	SE	15	PRO
55	SE	18	TRP
55	SE	21	ASP
55	SE	30	ARG
55	SE	39	ARG
55	SE	49	ARG
55	SE	51	ARG
55	SE	54	TYR
55	SE	66	MET

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Mol	Chain	Res	Type
55	SE	67	GLN
55	SE	73	ASP
55	SE	93	ASP
55	SE	95	THR
55	SE	98	ASN
55	SE	99	PHE
55	SE	106	LYS
55	SE	117	GLU
55	SE	118	GLU
55	SE	121	TYR
55	SE	127	ARG
55	SE	130	PHE
55	SE	155	LYS
55	SE	158	ASP
55	SE	164	LEU
55	SE	165	GLU
55	SE	179	ASN
55	SE	180	LEU
55	SE	191	ARG
55	SE	198	ARG
55	SE	205	PHE
55	SE	206	ASP
55	SE	220	THR
55	SE	224	ASN
55	SE	226	PHE
55	SE	240	ARG
55	SE	242	LYS
55	SE	253	ASP
55	SE	255	ARG
55	SE	259	LYS
55	SE	260	GLN
56	SF	23	TRP
56	SF	29	GLN
56	SF	38	TYR
56	SF	42	LYS
56	SF	49	LEU
56	SF	63	LYS
56	SF	65	GLN
56	SF	79	HIS
56	SF	82	ASN
56	SF	83	ASN
56	SF	88	MET

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Mol	Chain	Res	Type
56	SF	95	HIS
56	SF	106	GLU
56	SF	109	LEU
56	SF	110	GLN
56	SF	118	ASN
56	SF	122	ARG
56	SF	123	GLU
56	SF	124	ASP
56	SF	130	ARG
56	SF	136	ARG
56	SF	137	GLN
56	SF	140	ASP
56	SF	145	ARG
56	SF	171	GLU
56	SF	172	CYS
56	SF	176	GLU
56	SF	186	ASN
56	SF	190	ILE
56	SF	194	ASP
56	SF	195	GLU
56	SF	198	ARG
57	SG	12	CYS
57	SG	20	ASP
57	SG	21	GLU
57	SG	30	LYS
57	SG	31	ARG
57	SG	32	MET
57	SG	56	ASN
57	SG	58	LYS
57	SG	59	GLN
57	SG	64	LYS
57	SG	70	HIS
57	SG	74	ARG
57	SG	76	LEU
57	SG	87	ARG
57	SG	88	ARG
57	SG	110	ASN
57	SG	120	ASP
57	SG	121	ILE
57	SG	126	ASP
57	SG	132	ARG
57	SG	136	LYS

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Mol	Chain	Res	Type
57	SG	140	ARG
57	SG	143	LYS
57	SG	152	ASP
57	SG	159	ARG
57	SG	162	LEU
57	SG	164	LYS
57	SG	165	GLU
57	SG	170	ARG
57	SG	191	ARG
57	SG	196	LYS
57	SG	198	ARG
57	SG	213	LEU
57	SG	225	GLN
57	SG	227	GLN
57	SG	236	SER
58	SH	16	PRO
58	SH	23	ILE
58	SH	33	ASN
58	SH	35	ASP
58	SH	36	LEU
58	SH	40	LEU
58	SH	57	ARG
58	SH	74	LYS
58	SH	81	ARG
58	SH	83	LEU
58	SH	87	PHE
58	SH	99	ARG
58	SH	135	PHE
58	SH	151	SER
58	SH	159	ASP
58	SH	162	GLN
58	SH	165	ASN
58	SH	166	VAL
58	SH	184	ASP
58	SH	186	ASN
59	SI	6	ASP
59	SI	8	TRP
59	SI	12	ARG
59	SI	21	TYR
59	SI	22	HIS
59	SI	27	TYR
59	SI	47	ARG

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Mol	Chain	Res	Type
59	SI	49	ARG
59	SI	52	ASN
59	SI	58	LEU
59	SI	67	TRP
59	SI	70	GLU
59	SI	73	THR
59	SI	74	ARG
59	SI	83	TYR
59	SI	87	ASN
59	SI	105	ASP
59	SI	106	SER
59	SI	110	ARG
59	SI	112	TRP
59	SI	123	ARG
59	SI	140	LYS
59	SI	149	TYR
59	SI	155	ASN
59	SI	178	ARG
59	SI	191	GLU
59	SI	196	GLU
59	SI	197	PHE
59	SI	203	LYS
59	SI	206	LYS
60	SJ	5	ARG
60	SJ	9	CYS
60	SJ	10	ARG
60	SJ	17	ARG
60	SJ	18	ARG
60	SJ	20	PHE
60	SJ	26	ASP
60	SJ	29	LEU
60	SJ	39	ASN
60	SJ	67	ASP
60	SJ	69	ARG
60	SJ	79	ARG
60	SJ	93	LYS
60	SJ	101	LYS
60	SJ	104	ASP
60	SJ	108	ARG
60	SJ	109	ARG
60	SJ	110	LEU
60	SJ	115	PHE

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Mol	Chain	Res	Type
60	SJ	116	LYS
60	SJ	123	ILE
60	SJ	124	HIS
60	SJ	127	ARG
60	SJ	131	ARG
60	SJ	138	ARG
60	SJ	139	LYS
60	SJ	147	PHE
60	SJ	150	ARG
60	SJ	152	ASP
60	SJ	159	PHE
60	SJ	162	ARG
60	SJ	165	TYR
60	SJ	169	ARG
61	SK	1	MET
61	SK	2	LEU
61	SK	5	LYS
61	SK	8	ARG
61	SK	13	GLU
61	SK	16	PHE
61	SK	32	HIS
61	SK	37	ASP
61	SK	39	ASN
61	SK	40	VAL
61	SK	43	LEU
61	SK	46	MET
61	SK	61	GLN
61	SK	65	ARG
61	SK	66	HIS
61	SK	74	GLU
61	SK	80	ARG
61	SK	81	ASP
61	SK	84	HIS
61	SK	89	ILE
61	SK	95	ARG
62	SL	8	ARG
62	SL	16	ILE
62	SL	20	LYS
62	SL	22	ARG
62	SL	27	GLU
62	SL	35	ARG
62	SL	39	ASN

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Mol	Chain	Res	Type
62	SL	40	ILE
62	SL	65	ASN
62	SL	69	ARG
62	SL	92	TYR
62	SL	97	ARG
62	SL	103	GLU
62	SL	108	ASN
62	SL	113	LEU
62	SL	116	CYS
62	SL	117	PHE
62	SL	121	GLN
62	SL	124	ASP
62	SL	147	LYS
62	SL	155	PHE
62	SL	156	GLN
63	SM	12	MET
63	SM	13	ASP
63	SM	18	LEU
63	SM	26	LEU
63	SM	29	ASP
63	SM	31	LEU
63	SM	33	ARG
63	SM	36	ARG
63	SM	45	ARG
63	SM	48	HIS
63	SM	52	GLN
63	SM	57	ASP
63	SM	73	GLN
63	SM	75	ASN
63	SM	76	LEU
63	SM	77	ILE
63	SM	83	LYS
63	SM	88	TRP
63	SM	91	LEU
63	SM	95	ASP
63	SM	96	ARG
63	SM	99	ASN
63	SM	101	ARG
63	SM	102	LYS
63	SM	104	VAL
63	SM	113	ASP
63	SM	114	TYR

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Mol	Chain	Res	Type
63	SM	127	TYR
64	SN	3	ARG
64	SN	25	TRP
64	SN	27	LYS
64	SN	31	ASP
64	SN	38	TYR
64	SN	55	ARG
64	SN	56	ASP
64	SN	58	HIS
64	SN	62	GLN
64	SN	64	ARG
64	SN	69	ASN
64	SN	76	LYS
64	SN	83	ASP
64	SN	84	LEU
64	SN	86	GLU
64	SN	87	ASP
64	SN	89	TYR
64	SN	99	ARG
64	SN	101	HIS
64	SN	104	ARG
64	SN	105	ASN
64	SN	113	PHE
64	SN	121	ARG
64	SN	125	LEU
64	SN	127	ARG
64	SN	128	TYR
64	SN	132	LYS
64	SN	133	ARG
64	SN	144	SER
65	SO	17	LEU
65	SO	34	PHE
65	SO	39	ASP
65	SO	41	PHE
65	SO	43	HIS
65	SO	51	GLU
65	SO	52	THR
65	SO	63	LYS
65	SO	65	ASP
65	SO	80	ASP
65	SO	84	ARG
65	SO	86	LYS

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Mol	Chain	Res	Type
65	SO	94	HIS
65	SO	103	ASN
65	SO	106	LYS
65	SO	116	LEU
65	SO	117	ARG
65	SO	121	ARG
65	SO	128	ARG
65	SO	130	GLU
65	SO	146	ARG
65	SO	147	ARG
65	SO	150	ARG
66	SP	5	GLU
66	SP	7	LYS
66	SP	10	ARG
66	SP	12	PHE
66	SP	15	PHE
66	SP	40	ARG
66	SP	41	GLN
66	SP	42	ARG
66	SP	43	ARG
66	SP	44	ARG
66	SP	50	ARG
66	SP	51	ARG
66	SP	52	LYS
66	SP	79	HIS
66	SP	86	LEU
67	SQ	15	ARG
67	SQ	26	LYS
67	SQ	35	ASN
67	SQ	41	MET
67	SQ	45	ARG
67	SQ	62	ARG
67	SQ	73	LYS
67	SQ	85	ARG
67	SQ	90	LYS
67	SQ	99	TYR
67	SQ	114	GLN
67	SQ	123	ASP
67	SQ	126	ARG
67	SQ	128	GLU
67	SQ	138	ARG
67	SQ	140	ARG

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Mol	Chain	Res	Type
67	SQ	145	TYR
68	SR	3	ARG
68	SR	18	GLU
68	SR	31	ASN
68	SR	37	GLU
68	SR	56	HIS
68	SR	78	ARG
68	SR	79	GLU
68	SR	83	ASN
68	SR	87	GLU
68	SR	91	LEU
68	SR	93	GLN
68	SR	109	LEU
68	SR	118	GLN
68	SR	120	THR
68	SR	121	GLN
69	SS	8	LYS
69	SS	10	GLN
69	SS	14	ARG
69	SS	23	ARG
69	SS	28	PHE
69	SS	34	LYS
69	SS	39	ARG
69	SS	63	GLU
69	SS	78	LYS
69	SS	82	TRP
69	SS	85	ASN
69	SS	86	ARG
69	SS	87	GLN
69	SS	92	ASP
69	SS	95	TYR
69	SS	108	ARG
69	SS	118	ARG
69	SS	124	ARG
69	SS	125	HIS
69	SS	134	GLN
69	SS	135	HIS
69	SS	142	ARG
70	ST	11	GLN
70	ST	13	GLU
70	ST	16	ARG
70	ST	21	PHE

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Mol	Chain	Res	Type
70	ST	28	LEU
70	ST	33	TRP
70	ST	35	ASP
70	ST	42	HIS
70	ST	53	PHE
70	ST	62	ARG
70	ST	63	HIS
70	ST	74	SER
70	ST	79	TYR
70	ST	82	ARG
70	ST	83	GLN
70	ST	84	ARG
70	ST	92	PHE
70	ST	94	ARG
70	ST	97	LYS
70	ST	118	ASP
70	ST	121	ARG
70	ST	128	GLN
70	ST	129	ARG
71	SU	19	ARG
71	SU	47	ASN
71	SU	48	LEU
71	SU	49	LYS
71	SU	51	LYS
71	SU	55	ARG
71	SU	56	MET
71	SU	77	TRP
71	SU	87	ARG
71	SU	111	GLU
72	SV	1	MET
72	SV	2	GLN
72	SV	4	ASP
72	SV	11	LEU
72	SV	18	SER
72	SV	21	ASN
72	SV	39	VAL
72	SV	45	ARG
72	SV	47	ASN
72	SV	49	GLN
72	SV	50	PHE
72	SV	81	LYS
72	SV	82	ASN

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Mol	Chain	Res	Type
73	SW	2	VAL
73	SW	3	ARG
73	SW	12	LYS
73	SW	24	GLN
73	SW	28	ARG
73	SW	36	ARG
73	SW	37	PHE
73	SW	52	ILE
73	SW	56	HIS
73	SW	57	ARG
73	SW	70	ASN
73	SW	78	ARG
73	SW	80	ASP
73	SW	85	ASP
73	SW	90	GLN
73	SW	91	ASN
73	SW	98	GLN
73	SW	104	LEU
73	SW	105	THR
74	SX	5	ARG
74	SX	17	ARG
74	SX	19	ASP
74	SX	32	LEU
74	SX	45	SER
74	SX	46	HIS
74	SX	61	GLN
74	SX	67	ARG
74	SX	87	ASN
74	SX	88	ASP
74	SX	105	PHE
74	SX	107	ARG
74	SX	114	ASP
74	SX	131	LEU
74	SX	135	LYS
75	SY	3	ASP
75	SY	16	ARG
75	SY	17	LEU
75	SY	19	GLN
75	SY	20	ARG
75	SY	23	MET
75	SY	29	HIS
75	SY	47	MET

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Mol	Chain	Res	Type
75	SY	54	VAL
75	SY	61	ARG
75	SY	63	HIS
75	SY	64	PHE
75	SY	69	THR
75	SY	80	ASP
75	SY	93	ARG
75	SY	96	LEU
75	SY	98	GLU
75	SY	99	LYS
75	SY	101	LYS
75	SY	107	ARG
75	SY	111	LYS
75	SY	118	ARG
76	SZ	44	LEU
76	SZ	45	ASN
76	SZ	49	LEU
76	SZ	64	ASN
76	SZ	69	THR
76	SZ	85	ARG
76	SZ	94	LYS
76	SZ	97	ILE
76	SZ	104	ARG
76	SZ	109	TYR
76	SZ	110	THR
76	SZ	114	LYS
77	Sa	3	LYS
77	Sa	4	LYS
77	Sa	28	ARG
77	Sa	41	ILE
77	Sa	43	ASN
77	Sa	51	ARG
77	Sa	52	ASP
77	Sa	62	TYR
77	Sa	72	HIS
77	Sa	85	ARG
77	Sa	86	ASN
77	Sa	87	ARG
77	Sa	92	ARG
77	Sa	94	ASP
77	Sa	95	ARG
78	Sb	14	GLU

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Mol	Chain	Res	Type
78	Sb	17	ARG
78	Sb	26	GLN
78	Sb	34	ASP
78	Sb	37	CYS
78	Sb	47	PHE
78	Sb	59	CYS
78	Sb	72	ARG
78	Sb	78	SER
78	Sb	83	GLN
78	Sb	84	HIS
79	Sc	5	ARG
79	Sc	7	GLN
79	Sc	13	ARG
79	Sc	21	THR
79	Sc	26	GLN
79	Sc	31	ARG
79	Sc	33	GLU
79	Sc	34	PHE
79	Sc	40	ARG
79	Sc	44	ARG
79	Sc	51	ARG
79	Sc	54	ASP
79	Sc	60	GLU
79	Sc	67	ARG
80	Sd	6	PHE
80	Sd	8	TRP
80	Sd	10	HIS
80	Sd	12	ARG
80	Sd	19	ARG
80	Sd	26	ASN
80	Sd	30	LEU
80	Sd	32	ARG
80	Sd	43	PHE
80	Sd	56	ASP
81	Se	13	ARG
81	Se	15	GLN
81	Se	18	LYS
81	Se	26	LYS
81	Se	28	LYS
81	Se	31	ARG
81	Se	34	ARG
81	Se	35	ARG

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Mol	Chain	Res	Type
81	Se	40	ARG
81	Se	41	ARG
81	Se	52	LYS
82	Sf	87	THR
82	Sf	89	LYS
82	Sf	95	ARG
82	Sf	98	VAL
82	Sf	106	TYR
82	Sf	116	ARG
82	Sf	119	ARG
82	Sf	126	CYS
82	Sf	131	PHE
82	Sf	136	PHE
82	Sf	138	ARG
82	Sf	139	HIS
82	Sf	140	TYR
82	Sf	141	CYS
82	Sf	146	LEU
82	Sf	148	TYR
82	Sf	149	CYS
82	Sf	150	PHE
82	Sf	152	LYS
83	Sg	8	ARG
83	Sg	15	ASN
83	Sg	17	TRP
83	Sg	20	GLN
83	Sg	24	THR
83	Sg	44	LYS
83	Sg	47	ARG
83	Sg	49	GLU
83	Sg	60	ARG
83	Sg	65	PHE
83	Sg	74	ASP
83	Sg	84	ASP
83	Sg	99	ARG
83	Sg	100	ARG
83	Sg	107	ASP
83	Sg	118	ARG
83	Sg	133	ASN
83	Sg	140	TYR
83	Sg	143	GLN
83	Sg	167	SER

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Mol	Chain	Res	Type
83	Sg	194	TYR
83	Sg	226	HIS
83	Sg	229	THR
83	Sg	234	ASP
83	Sg	249	CYS
83	Sg	268	ASP
83	Sg	282	GLU
83	Sg	294	ASP
83	Sg	297	THR
83	Sg	306	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (278) 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	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

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Mol	Chain	Res	Type
7	D	45	ASN
7	D	94	ASN
7	D	111	ASN
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	42	ASN
11	H	63	ASN
11	H	106	GLN
12	I	59	GLN
12	I	100	ASN
12	I	144	ASN

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Mol	Chain	Res	Type
12	I	163	GLN
12	I	213	HIS
13	J	155	HIS
14	L	6	ASN
14	L	28	GLN
14	L	104	ASN
14	L	113	ASN
14	L	159	ASN
15	M	33	GLN
15	M	34	ASN
15	M	48	GLN
15	M	66	HIS
16	N	8	GLN
16	N	90	ASN
16	N	178	HIS
16	N	181	HIS
16	N	182	HIS
16	N	196	ASN
16	N	201	HIS
17	O	65	ASN
17	O	96	GLN
17	O	173	GLN
18	P	25	HIS
18	P	28	ASN
18	P	54	GLN
18	P	64	ASN
18	P	72	GLN
18	P	80	GLN
18	P	97	ASN
18	P	133	HIS
18	P	145	HIS
19	Q	7	HIS
19	Q	40	ASN
19	Q	57	ASN
20	R	36	ASN
20	R	66	ASN
20	R	75	HIS
20	R	118	HIS
20	R	143	HIS
21	S	37	HIS
21	S	91	HIS
21	S	92	ASN

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Mol	Chain	Res	Type
21	S	122	HIS
21	S	125	GLN
21	S	163	HIS
22	T	58	HIS
22	T	70	HIS
22	T	139	HIS
23	U	55	ASN
24	V	36	ASN
25	W	17	HIS
25	W	59	HIS
26	X	93	ASN
26	X	111	GLN
27	Y	24	HIS
27	Y	56	GLN
27	Y	72	GLN
27	Y	86	GLN
27	Y	100	HIS
27	Y	127	GLN
28	Z	79	HIS
29	a	41	HIS
29	a	62	HIS
29	a	66	ASN
29	a	67	GLN
30	b	6	ASN
30	b	7	HIS
30	b	12	GLN
30	b	19	ASN
30	b	27	GLN
30	b	42	ASN
31	c	19	GLN
31	c	40	GLN
31	c	73	HIS
31	c	77	ASN
32	d	30	HIS
32	d	93	ASN
32	d	100	ASN
33	e	24	GLN
33	e	43	ASN
33	e	126	ASN
34	f	21	GLN
34	f	24	HIS
34	f	55	ASN

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Mol	Chain	Res	Type
34	f	80	ASN
35	g	18	ASN
35	g	110	GLN
36	h	68	ASN
36	h	98	HIS
38	j	16	HIS
38	j	48	ASN
40	l	19	GLN
40	l	25	GLN
41	m	84	GLN
41	m	87	GLN
41	m	109	ASN
43	o	21	HIS
43	o	25	GLN
43	o	45	GLN
43	o	76	ASN
43	o	90	HIS
45	r	6	GLN
45	r	12	ASN
45	r	21	ASN
45	r	31	ASN
45	r	36	ASN
45	r	41	ASN
45	r	70	GLN
45	r	83	ASN
46	z	44	GLN
46	z	119	GLN
46	z	141	ASN
46	z	200	ASN
47	1	127	GLN
47	1	218	HIS
47	1	241	ASN
47	1	244	ASN
51	SA	24	HIS
51	SA	33	GLN
51	SA	84	GLN
51	SA	110	ASN
51	SA	113	GLN
51	SA	141	ASN
51	SA	169	HIS
52	SB	99	ASN
52	SB	101	HIS

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Mol	Chain	Res	Type
52	SB	118	GLN
52	SB	124	HIS
52	SB	148	ASN
53	SC	115	GLN
53	SC	120	GLN
53	SC	134	ASN
53	SC	272	HIS
54	SD	4	GLN
54	SD	22	ASN
54	SD	179	GLN
55	SE	36	HIS
55	SE	138	HIS
55	SE	161	GLN
56	SF	29	GLN
56	SF	65	GLN
56	SF	82	ASN
56	SF	95	HIS
56	SF	137	GLN
56	SF	186	ASN
56	SF	203	ASN
57	SG	59	GLN
57	SG	65	GLN
57	SG	110	ASN
59	SI	9	HIS
59	SI	44	HIS
59	SI	155	ASN
59	SI	165	GLN
60	SJ	111	GLN
60	SJ	177	ASN
61	SK	28	HIS
61	SK	39	ASN
62	SL	19	ASN
62	SL	106	HIS
62	SL	141	ASN
62	SL	156	GLN
63	SM	19	GLN
63	SM	48	HIS
63	SM	99	ASN
64	SN	5	HIS
64	SN	69	ASN
65	SO	38	ASN
66	SP	41	GLN

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Mol	Chain	Res	Type
66	SP	46	ASN
67	SQ	48	GLN
67	SQ	114	GLN
67	SQ	142	GLN
68	SR	83	ASN
69	SS	10	GLN
69	SS	42	HIS
69	SS	120	HIS
69	SS	125	HIS
69	SS	135	HIS
70	ST	51	ASN
70	ST	63	HIS
71	SU	47	ASN
72	SV	29	HIS
72	SV	47	ASN
72	SV	49	GLN
73	SW	64	ASN
73	SW	82	GLN
73	SW	98	GLN
74	SX	20	HIS
74	SX	23	HIS
74	SX	61	GLN
74	SX	63	ASN
75	SY	85	ASN
75	SY	94	HIS
75	SY	112	ASN
76	SZ	103	HIS
77	Sa	17	HIS
77	Sa	72	HIS
78	Sb	19	HIS
79	Sc	7	GLN
79	Sc	24	GLN
79	Sc	26	GLN
80	Sd	10	HIS
80	Sd	26	ASN
80	Sd	28	HIS
82	Sf	111	ASN
83	Sg	119	GLN
83	Sg	181	ASN
83	Sg	215	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3703/3722 (99%)	1640 (44%)	636 (17%)
2	7	119/120 (99%)	31 (26%)	9 (7%)
3	8	155/156 (99%)	61 (39%)	22 (14%)
50	S2	1717/1742 (98%)	771 (44%)	273 (15%)
84	S4	9/10 (90%)	9 (100%)	0
85	S5	71/74 (95%)	47 (66%)	10 (14%)
86	S6	75/76 (98%)	53 (70%)	8 (10%)
All	All	5849/5900 (99%)	2612 (44%)	958 (16%)

All (2612) 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
1	5	48	G
1	5	49	U
1	5	50	C
1	5	51	A
1	5	54	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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
1	5	1562	G
1	5	1564	A
1	5	1566	C
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	1764	G
1	5	1765	A
1	5	1766	A
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	1947	U
1	5	1948	G
1	5	1951	G
1	5	1952	G
1	5	1956	A
1	5	1959	U
1	5	1961	G
1	5	1962	A
1	5	1964	A
1	5	1965	G
1	5	1966	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

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Mol	Chain	Res	Type
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	2023	C
1	5	2024	G
1	5	2025	A
1	5	2026	A
1	5	2033	A
1	5	2034	G
1	5	2035	C
1	5	2040	A
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

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Mol	Chain	Res	Type
1	5	2075	G
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	2456	G
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	3944	G
1	5	3945	A

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Mol	Chain	Res	Type
1	5	3951	G
1	5	3954	A
1	5	3956	G
1	5	3960	A
1	5	3961	G
1	5	3962	A
1	5	3963	A
1	5	3964	U
1	5	3965	A
1	5	3969	G
1	5	3973	G
1	5	4037	C
1	5	4038	C
1	5	4039	G
1	5	4041	C
1	5	4042	G
1	5	4043	G
1	5	4044	U
1	5	4045	G
1	5	4047	A
1	5	4048	A
1	5	4049	U
1	5	4051	C
1	5	4053	A
1	5	4069	U
1	5	4070	U
1	5	4071	U
1	5	4072	C
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	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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	4499	G
1	5	4500	U

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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
50	S2	3	C
50	S2	4	C
50	S2	9	U
50	S2	10	G
50	S2	17	C
50	S2	18	C
50	S2	20	G
50	S2	23	G
50	S2	24	C
50	S2	25	A
50	S2	27	A
50	S2	33	G
50	S2	39	A
50	S2	44	U
50	S2	45	A
50	S2	46	A
50	S2	49	C
50	S2	51	U
50	S2	53	C
50	S2	56	G
50	S2	57	U

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Mol	Chain	Res	Type
50	S2	58	C
50	S2	59	U
50	S2	60	A
50	S2	61	A
50	S2	62	G
50	S2	63	U
50	S2	64	A
50	S2	65	C
50	S2	66	G
50	S2	67	C
50	S2	68	A
50	S2	71	G
50	S2	72	C
50	S2	73	C
50	S2	74	G
50	S2	75	G
50	S2	76	U
50	S2	77	A
50	S2	78	C
50	S2	79	A
50	S2	80	G
50	S2	84	A
50	S2	88	G
50	S2	89	C
50	S2	92	A
50	S2	98	C
50	S2	99	A
50	S2	101	U
50	S2	103	A
50	S2	105	U
50	S2	111	A
50	S2	113	G
50	S2	114	G
50	S2	115	U
50	S2	116	U
50	S2	117	C
50	S2	123	G
50	S2	125	C
50	S2	127	C
50	S2	139	C
50	S2	140	C
50	S2	141	A

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Mol	Chain	Res	Type
50	S2	142	C
50	S2	143	U
50	S2	144	U
50	S2	146	G
50	S2	147	A
50	S2	148	U
50	S2	150	A
50	S2	153	G
50	S2	154	U
50	S2	155	G
50	S2	156	G
50	S2	159	A
50	S2	160	U
50	S2	161	U
50	S2	162	C
50	S2	163	U
50	S2	164	A
50	S2	165	G
50	S2	167	G
50	S2	169	U
50	S2	170	A
50	S2	173	A
50	S2	176	U
50	S2	180	G
50	S2	181	A
50	S2	182	C
50	S2	183	G
50	S2	184	G
50	S2	188	C
50	S2	189	U
50	S2	191	A
50	S2	192	C
50	S2	200	G
50	S2	202	G
50	S2	206	G
50	S2	209	A
50	S2	210	U
50	S2	211	G
50	S2	213	G
50	S2	215	G
50	S2	216	C
50	S2	217	A

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Mol	Chain	Res	Type
50	S2	290	U
50	S2	291	G
50	S2	292	A
50	S2	293	C
50	S2	295	C
50	S2	302	A
50	S2	305	U
50	S2	306	C
50	S2	307	G
50	S2	308	G
50	S2	309	G
50	S2	310	C
50	S2	311	C
50	S2	312	G
50	S2	313	A
50	S2	314	U
50	S2	316	G
50	S2	317	C
50	S2	318	A
50	S2	319	C
50	S2	321	C
50	S2	324	C
50	S2	325	C
50	S2	326	C
50	S2	328	U
50	S2	338	G
50	S2	340	C
50	S2	341	C
50	S2	342	C
50	S2	343	A
50	S2	346	C
50	S2	347	G
50	S2	350	C
50	S2	355	G
50	S2	356	C
50	S2	357	C
50	S2	360	A
50	S2	362	C
50	S2	364	A
50	S2	365	C
50	S2	367	U
50	S2	368	U

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Mol	Chain	Res	Type
50	S2	369	C
50	S2	370	G
50	S2	373	G
50	S2	377	G
50	S2	380	G
50	S2	381	C
50	S2	382	C
50	S2	384	U
50	S2	385	G
50	S2	386	C
50	S2	394	G
50	S2	398	A
50	S2	400	C
50	S2	407	G
50	S2	408	A
50	S2	409	C
50	S2	411	G
50	S2	414	A
50	S2	416	U
50	S2	417	C
50	S2	418	A
50	S2	419	G
50	S2	425	G
50	S2	426	A
50	S2	427	U
50	S2	428	U
50	S2	429	C
50	S2	435	A
50	S2	436	G
50	S2	438	G
50	S2	441	C
50	S2	444	G
50	S2	445	A
50	S2	447	A
50	S2	448	A
50	S2	449	A
50	S2	450	C
50	S2	453	C
50	S2	454	U
50	S2	455	A
50	S2	459	C
50	S2	460	A

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Mol	Chain	Res	Type
50	S2	464	A
50	S2	465	A
50	S2	466	G
50	S2	467	G
50	S2	468	A
50	S2	469	A
50	S2	471	G
50	S2	472	C
50	S2	473	A
50	S2	474	G
50	S2	476	A
50	S2	482	G
50	S2	487	U
50	S2	488	U
50	S2	489	A
50	S2	492	C
50	S2	493	A
50	S2	496	C
50	S2	500	A
50	S2	501	C
50	S2	507	G
50	S2	508	A
50	S2	516	A
50	S2	518	G
50	S2	523	A
50	S2	525	A
50	S2	528	A
50	S2	530	U
50	S2	532	C
50	S2	533	A
50	S2	534	G
50	S2	542	U
50	S2	544	G
50	S2	548	C
50	S2	549	C
50	S2	550	C
50	S2	551	U
50	S2	552	G
50	S2	554	A
50	S2	555	A
50	S2	556	U
50	S2	557	U

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Mol	Chain	Res	Type
50	S2	559	G
50	S2	560	A
50	S2	562	U
50	S2	563	G
50	S2	564	A
50	S2	568	C
50	S2	575	A
50	S2	576	A
50	S2	579	C
50	S2	580	U
50	S2	583	C
50	S2	588	G
50	S2	589	G
50	S2	590	A
50	S2	591	U
50	S2	592	C
50	S2	593	C
50	S2	595	U
50	S2	596	U
50	S2	598	G
50	S2	600	G
50	S2	601	G
50	S2	602	G
50	S2	604	A
50	S2	605	A
50	S2	607	U
50	S2	608	C
50	S2	612	U
50	S2	614	C
50	S2	616	A
50	S2	617	G
50	S2	621	C
50	S2	623	G
50	S2	626	G
50	S2	627	U
50	S2	628	A
50	S2	629	A
50	S2	630	U
50	S2	631	U
50	S2	632	C
50	S2	643	A
50	S2	644	G

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Mol	Chain	Res	Type
50	S2	646	G
50	S2	649	U
50	S2	655	A
50	S2	657	U
50	S2	660	C
50	S2	662	G
50	S2	666	U
50	S2	667	U
50	S2	668	A
50	S2	669	A
50	S2	671	A
50	S2	672	A
50	S2	673	G
50	S2	679	A
50	S2	683	G
50	S2	684	G
50	S2	687	C
50	S2	688	U
50	S2	689	U
50	S2	690	G
50	S2	693	A
50	S2	694	G
50	S2	695	C
50	S2	698	G
50	S2	731	G
50	S2	733	C
50	S2	734	C
50	S2	735	C
50	S2	736	C
50	S2	738	C
50	S2	739	C
50	S2	745	C
50	S2	747	U
50	S2	748	C
50	S2	749	U
50	S2	751	G
50	S2	752	G
50	S2	753	C
50	S2	788	G
50	S2	791	C
50	S2	797	C
50	S2	798	A

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Mol	Chain	Res	Type
50	S2	799	U
50	S2	800	U
50	S2	809	A
50	S2	810	A
50	S2	811	A
50	S2	812	A
50	S2	820	U
50	S2	821	G
50	S2	822	U
50	S2	827	A
50	S2	830	A
50	S2	833	C
50	S2	834	C
50	S2	835	C
50	S2	836	G
50	S2	837	A
50	S2	838	G
50	S2	840	C
50	S2	841	G
50	S2	842	C
50	S2	843	C
50	S2	845	G
50	S2	847	A
50	S2	848	U
50	S2	856	C
50	S2	861	A
50	S2	867	G
50	S2	868	G
50	S2	869	A
50	S2	870	A
50	S2	871	U
50	S2	872	A
50	S2	873	G
50	S2	875	A
50	S2	877	C
50	S2	878	G
50	S2	879	C
50	S2	880	G
50	S2	881	G
50	S2	887	U
50	S2	888	U
50	S2	890	U

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Mol	Chain	Res	Type
50	S2	891	G
50	S2	892	U
50	S2	897	U
50	S2	898	U
50	S2	903	A
50	S2	910	G
50	S2	913	A
50	S2	914	U
50	S2	915	G
50	S2	917	U
50	S2	918	U
50	S2	919	A
50	S2	920	A
50	S2	921	G
50	S2	930	C
50	S2	933	G
50	S2	934	G
50	S2	938	A
50	S2	943	U
50	S2	954	U
50	S2	955	A
50	S2	956	G
50	S2	957	A
50	S2	958	G
50	S2	959	G
50	S2	960	U
50	S2	961	G
50	S2	962	A
50	S2	964	A
50	S2	965	U
50	S2	966	U
50	S2	968	U
50	S2	969	U
50	S2	970	G
50	S2	971	G
50	S2	979	C
50	S2	980	A
50	S2	981	A
50	S2	990	A
50	S2	991	G
50	S2	992	A
50	S2	996	A

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Mol	Chain	Res	Type
50	S2	997	A
50	S2	999	G
50	S2	1001	A
50	S2	1002	U
50	S2	1008	A
50	S2	1017	U
50	S2	1023	A
50	S2	1033	G
50	S2	1034	A
50	S2	1035	A
50	S2	1040	G
50	S2	1041	G
50	S2	1044	G
50	S2	1045	U
50	S2	1049	A
50	S2	1050	A
50	S2	1060	A
50	S2	1062	A
50	S2	1067	C
50	S2	1070	A
50	S2	1072	U
50	S2	1073	U
50	S2	1077	A
50	S2	1078	C
50	S2	1083	A
50	S2	1084	A
50	S2	1085	C
50	S2	1087	A
50	S2	1088	U
50	S2	1089	G
50	S2	1091	C
50	S2	1096	G
50	S2	1099	G
50	S2	1100	A
50	S2	1102	G
50	S2	1109	C
50	S2	1110	G
50	S2	1111	U
50	S2	1114	U
50	S2	1115	U
50	S2	1116	C
50	S2	1117	C

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Mol	Chain	Res	Type
50	S2	1118	C
50	S2	1120	U
50	S2	1123	C
50	S2	1126	G
50	S2	1130	G
50	S2	1131	G
50	S2	1133	A
50	S2	1138	C
50	S2	1139	C
50	S2	1143	A
50	S2	1144	A
50	S2	1146	C
50	S2	1148	A
50	S2	1149	A
50	S2	1150	A
50	S2	1151	G
50	S2	1153	C
50	S2	1154	U
50	S2	1157	G
50	S2	1165	G
50	S2	1166	G
50	S2	1171	G
50	S2	1172	U
50	S2	1181	A
50	S2	1182	A
50	S2	1186	U
50	S2	1187	G
50	S2	1192	U
50	S2	1194	A
50	S2	1195	A
50	S2	1199	A
50	S2	1203	G
50	S2	1204	A
50	S2	1205	C
50	S2	1206	G
50	S2	1207	G
50	S2	1208	A
50	S2	1209	A
50	S2	1210	G
50	S2	1211	G
50	S2	1212	G
50	S2	1213	C

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Mol	Chain	Res	Type
50	S2	1214	A
50	S2	1215	C
50	S2	1216	C
50	S2	1217	A
50	S2	1221	G
50	S2	1224	G
50	S2	1234	C
50	S2	1242	U
50	S2	1243	U
50	S2	1244	U
50	S2	1247	C
50	S2	1248	U
50	S2	1250	A
50	S2	1251	A
50	S2	1253	A
50	S2	1254	C
50	S2	1256	G
50	S2	1257	G
50	S2	1258	A
50	S2	1259	A
50	S2	1264	C
50	S2	1265	A
50	S2	1266	C
50	S2	1267	C
50	S2	1268	C
50	S2	1269	G
50	S2	1271	C
50	S2	1273	C
50	S2	1274	G
50	S2	1275	G
50	S2	1276	A
50	S2	1280	G
50	S2	1282	A
50	S2	1283	C
50	S2	1284	A
50	S2	1285	G
50	S2	1286	G
50	S2	1288	U
50	S2	1289	U
50	S2	1292	C
50	S2	1293	A
50	S2	1296	U

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Mol	Chain	Res	Type
50	S2	1298	G
50	S2	1299	A
50	S2	1301	A
50	S2	1302	G
50	S2	1303	C
50	S2	1304	U
50	S2	1305	C
50	S2	1306	U
50	S2	1308	U
50	S2	1309	C
50	S2	1312	G
50	S2	1313	A
50	S2	1314	U
50	S2	1315	U
50	S2	1316	C
50	S2	1322	G
50	S2	1324	G
50	S2	1326	U
50	S2	1330	G
50	S2	1331	C
50	S2	1332	A
50	S2	1333	U
50	S2	1337	C
50	S2	1342	U
50	S2	1344	A
50	S2	1345	G
50	S2	1346	U
50	S2	1348	G
50	S2	1352	G
50	S2	1353	A
50	S2	1354	G
50	S2	1355	C
50	S2	1356	G
50	S2	1357	A
50	S2	1358	U
50	S2	1367	U
50	S2	1370	A
50	S2	1371	U
50	S2	1372	U
50	S2	1373	C
50	S2	1377	U
50	S2	1378	A

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Mol	Chain	Res	Type
50	S2	1379	A
50	S2	1380	C
50	S2	1383	A
50	S2	1384	C
50	S2	1385	G
50	S2	1386	A
50	S2	1387	G
50	S2	1394	G
50	S2	1395	C
50	S2	1396	A
50	S2	1397	U
50	S2	1401	A
50	S2	1402	A
50	S2	1403	C
50	S2	1404	U
50	S2	1405	A
50	S2	1407	U
50	S2	1410	C
50	S2	1411	G
50	S2	1412	C
50	S2	1414	A
50	S2	1417	C
50	S2	1418	C
50	S2	1419	C
50	S2	1420	G
50	S2	1424	G
50	S2	1426	U
50	S2	1430	C
50	S2	1431	G
50	S2	1432	U
50	S2	1433	C
50	S2	1434	C
50	S2	1435	C
50	S2	1437	C
50	S2	1438	A
50	S2	1441	U
50	S2	1442	U
50	S2	1449	G
50	S2	1450	G
50	S2	1452	A
50	S2	1454	A
50	S2	1455	A

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Mol	Chain	Res	Type
50	S2	1456	G
50	S2	1462	U
50	S2	1463	U
50	S2	1464	C
50	S2	1466	G
50	S2	1467	C
50	S2	1474	A
50	S2	1475	G
50	S2	1476	A
50	S2	1477	U
50	S2	1478	U
50	S2	1483	A
50	S2	1484	A
50	S2	1485	U
50	S2	1489	A
50	S2	1490	G
50	S2	1493	C
50	S2	1494	U
50	S2	1495	G
50	S2	1496	U
50	S2	1506	A
50	S2	1507	G
50	S2	1508	A
50	S2	1509	U
50	S2	1510	G
50	S2	1512	C
50	S2	1513	C
50	S2	1514	G
50	S2	1515	G
50	S2	1520	G
50	S2	1521	C
50	S2	1522	A
50	S2	1525	C
50	S2	1527	C
50	S2	1531	A
50	S2	1534	C
50	S2	1535	U
50	S2	1536	G
50	S2	1537	A
50	S2	1541	G
50	S2	1542	C
50	S2	1543	U

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Mol	Chain	Res	Type
50	S2	1544	C
50	S2	1545	A
50	S2	1546	G
50	S2	1548	G
50	S2	1550	G
50	S2	1551	U
50	S2	1552	G
50	S2	1553	C
50	S2	1554	C
50	S2	1555	U
50	S2	1556	A
50	S2	1557	C
50	S2	1558	C
50	S2	1560	U
50	S2	1567	G
50	S2	1568	C
50	S2	1570	G
50	S2	1574	C
50	S2	1578	U
50	S2	1579	A
50	S2	1580	A
50	S2	1581	C
50	S2	1585	U
50	S2	1586	U
50	S2	1587	G
50	S2	1588	A
50	S2	1589	A
50	S2	1590	C
50	S2	1593	C
50	S2	1595	U
50	S2	1596	U
50	S2	1598	G
50	S2	1599	U
50	S2	1600	G
50	S2	1601	A
50	S2	1602	U
50	S2	1604	G
50	S2	1606	G
50	S2	1609	C
50	S2	1610	G
50	S2	1621	U
50	S2	1622	U

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Mol	Chain	Res	Type
50	S2	1623	A
50	S2	1625	U
50	S2	1633	A
50	S2	1637	A
50	S2	1638	G
50	S2	1644	C
50	S2	1648	G
50	S2	1649	U
50	S2	1656	G
50	S2	1660	C
50	S2	1663	A
50	S2	1664	A
50	S2	1665	G
50	S2	1666	C
50	S2	1674	G
50	S2	1679	A
50	S2	1680	G
50	S2	1682	C
50	S2	1683	C
50	S2	1684	C
50	S2	1688	C
50	S2	1689	C
50	S2	1692	U
50	S2	1693	G
50	S2	1695	A
50	S2	1696	C
50	S2	1697	A
50	S2	1699	A
50	S2	1700	C
50	S2	1701	C
50	S2	1702	G
50	S2	1707	U
50	S2	1720	U
50	S2	1721	U
50	S2	1722	G
50	S2	1729	U
50	S2	1730	U
50	S2	1734	G
50	S2	1742	C
50	S2	1745	A
50	S2	1746	U
50	S2	1751	C

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Mol	Chain	Res	Type
50	S2	1753	C
50	S2	1783	C
50	S2	1785	C
50	S2	1786	U
50	S2	1792	G
50	S2	1793	A
50	S2	1795	G
50	S2	1797	U
50	S2	1798	C
50	S2	1804	U
50	S2	1805	G
50	S2	1816	G
50	S2	1823	A
50	S2	1824	A
50	S2	1825	A
50	S2	1826	G
50	S2	1831	A
50	S2	1834	A
50	S2	1835	A
50	S2	1836	G
50	S2	1837	G
50	S2	1838	U
50	S2	1839	U
50	S2	1841	C
50	S2	1849	G
50	S2	1850	A
50	S2	1851	A
50	S2	1852	C
50	S2	1860	A
50	S2	1861	G
50	S2	1862	G
50	S2	1863	A
50	S2	1864	U
50	S2	1865	C
50	S2	1868	U
50	S2	1869	A
84	S4	16	U
84	S4	17	U
84	S4	18	U
84	S4	19	U
84	S4	20	U
84	S4	21	U

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Mol	Chain	Res	Type
84	S4	22	U
84	S4	23	U
84	S4	24	A
85	S5	2	C
85	S5	3	C
85	S5	4	C
85	S5	6	G
85	S5	7	A
85	S5	8	U
85	S5	9	A
85	S5	13	C
85	S5	15	G
85	S5	19	G
85	S5	20	U
85	S5	21	A
85	S5	22	G
85	S5	23	A
85	S5	26	A
85	S5	27	G
85	S5	28	G
85	S5	29	G
85	S5	30	G
85	S5	31	A
85	S5	32	U
85	S5	33	U
85	S5	34	G
85	S5	35	A
85	S5	36	A
85	S5	37	A
85	S5	38	A
85	S5	39	U
85	S5	40	C
85	S5	41	C
85	S5	44	G
85	S5	46	G
85	S5	47	U
85	S5	49	C
85	S5	51	U
85	S5	57	G
85	S5	64	A
85	S5	65	G
85	S5	67	C

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Mol	Chain	Res	Type
85	S5	68	C
85	S5	70	G
85	S5	71	G
85	S5	72	C
85	S5	73	A
85	S5	74	C
85	S5	75	C
85	S5	76	A
86	S6	2	G
86	S6	3	C
86	S6	4	C
86	S6	5	C
86	S6	6	G
86	S6	7	G
86	S6	8	U
86	S6	9	A
86	S6	12	C
86	S6	13	C
86	S6	14	C
86	S6	15	G
86	S6	17	A
86	S6	18	G
86	S6	19	G
86	S6	20	U
86	S6	21	A
86	S6	22	G
86	S6	23	A
86	S6	26	A
86	S6	30	G
86	S6	33	U
86	S6	34	G
86	S6	35	A
86	S6	38	A
86	S6	42	C
86	S6	44	G
86	S6	46	G
86	S6	47	U
86	S6	48	C
86	S6	49	C
86	S6	50	U
86	S6	51	U
86	S6	52	G

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Mol	Chain	Res	Type
86	S6	53	G
86	S6	54	U
86	S6	56	C
86	S6	57	G
86	S6	58	A
86	S6	59	U
86	S6	60	U
86	S6	61	C
86	S6	62	C
86	S6	64	A
86	S6	65	G
86	S6	68	C
86	S6	69	G
86	S6	70	G
86	S6	71	G
86	S6	72	C
86	S6	73	A
86	S6	74	C
86	S6	76	A

All (958) 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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	1563	A
1	5	1564	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

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Mol	Chain	Res	Type
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
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	1945	G
1	5	1946	G
1	5	1961	G
1	5	1963	C
1	5	1974	U
1	5	1975	G

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Mol	Chain	Res	Type
1	5	1980	U
1	5	1983	A
1	5	1992	U
1	5	1998	A
1	5	2007	G
1	5	2008	U
1	5	2009	A
1	5	2014	C
1	5	2025	A
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	5	2769	U
1	5	2782	U
1	5	2786	C
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
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

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Mol	Chain	Res	Type
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
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	3942	A
1	5	3959	U
1	5	3965	A
1	5	3968	U
1	5	3972	A
1	5	4036	G
1	5	4040	C
1	5	4041	C
1	5	4058	U
1	5	4069	U
1	5	4070	U

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Mol	Chain	Res	Type
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	4116	C
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
50	S2	1	U
50	S2	2	A
50	S2	9	U
50	S2	19	A
50	S2	24	C
50	S2	50	A
50	S2	55	U
50	S2	60	A
50	S2	61	A
50	S2	65	C
50	S2	66	G
50	S2	67	C
50	S2	72	C
50	S2	73	C
50	S2	74	G
50	S2	90	G
50	S2	91	A
50	S2	98	C
50	S2	102	A
50	S2	104	A
50	S2	110	U
50	S2	113	G
50	S2	126	G
50	S2	127	C

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Mol	Chain	Res	Type
50	S2	139	C
50	S2	140	C
50	S2	141	A
50	S2	142	C
50	S2	158	A
50	S2	160	U
50	S2	163	U
50	S2	164	A
50	S2	180	G
50	S2	181	A
50	S2	182	C
50	S2	183	G
50	S2	190	G
50	S2	215	G
50	S2	291	G
50	S2	294	U
50	S2	304	C
50	S2	305	U
50	S2	312	G
50	S2	313	A
50	S2	327	G
50	S2	333	G
50	S2	340	C
50	S2	349	A
50	S2	355	G
50	S2	357	C
50	S2	360	A
50	S2	368	U
50	S2	369	C
50	S2	377	G
50	S2	381	C
50	S2	384	U
50	S2	385	G
50	S2	409	C
50	S2	421	G
50	S2	427	U
50	S2	435	A
50	S2	443	U
50	S2	444	G
50	S2	446	G
50	S2	448	A
50	S2	452	G

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Mol	Chain	Res	Type
50	S2	453	C
50	S2	458	A
50	S2	465	A
50	S2	468	A
50	S2	471	G
50	S2	473	A
50	S2	482	G
50	S2	492	C
50	S2	499	G
50	S2	515	G
50	S2	532	C
50	S2	539	C
50	S2	548	C
50	S2	550	C
50	S2	577	U
50	S2	578	C
50	S2	579	C
50	S2	601	G
50	S2	604	A
50	S2	606	G
50	S2	607	U
50	S2	613	G
50	S2	615	C
50	S2	618	C
50	S2	642	U
50	S2	646	G
50	S2	649	U
50	S2	656	G
50	S2	671	A
50	S2	687	C
50	S2	688	U
50	S2	732	U
50	S2	733	C
50	S2	746	C
50	S2	747	U
50	S2	751	G
50	S2	752	G
50	S2	797	C
50	S2	798	A
50	S2	799	U
50	S2	800	U
50	S2	810	A

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Mol	Chain	Res	Type
50	S2	815	U
50	S2	821	G
50	S2	827	A
50	S2	833	C
50	S2	841	G
50	S2	855	G
50	S2	867	G
50	S2	868	G
50	S2	869	A
50	S2	870	A
50	S2	871	U
50	S2	872	A
50	S2	918	U
50	S2	919	A
50	S2	924	G
50	S2	950	C
50	S2	956	G
50	S2	957	A
50	S2	958	G
50	S2	959	G
50	S2	960	U
50	S2	964	A
50	S2	967	C
50	S2	970	G
50	S2	980	A
50	S2	991	G
50	S2	992	A
50	S2	993	G
50	S2	999	G
50	S2	1001	A
50	S2	1016	U
50	S2	1039	C
50	S2	1050	A
50	S2	1051	G
50	S2	1083	A
50	S2	1085	C
50	S2	1087	A
50	S2	1088	U
50	S2	1093	A
50	S2	1097	G
50	S2	1098	C
50	S2	1109	C

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Mol	Chain	Res	Type
50	S2	1110	G
50	S2	1114	U
50	S2	1115	U
50	S2	1121	G
50	S2	1132	C
50	S2	1133	A
50	S2	1137	U
50	S2	1138	C
50	S2	1141	G
50	S2	1142	G
50	S2	1150	A
50	S2	1153	C
50	S2	1165	G
50	S2	1171	G
50	S2	1181	A
50	S2	1194	A
50	S2	1204	A
50	S2	1205	C
50	S2	1223	A
50	S2	1244	U
50	S2	1247	C
50	S2	1249	C
50	S2	1250	A
50	S2	1253	A
50	S2	1265	A
50	S2	1273	C
50	S2	1275	G
50	S2	1283	C
50	S2	1292	C
50	S2	1298	G
50	S2	1302	G
50	S2	1312	G
50	S2	1313	A
50	S2	1315	U
50	S2	1330	G
50	S2	1341	C
50	S2	1342	U
50	S2	1353	A
50	S2	1357	A
50	S2	1367	U
50	S2	1368	U
50	S2	1372	U

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Mol	Chain	Res	Type
50	S2	1378	A
50	S2	1393	G
50	S2	1395	C
50	S2	1396	A
50	S2	1401	A
50	S2	1404	U
50	S2	1416	C
50	S2	1417	C
50	S2	1418	C
50	S2	1419	C
50	S2	1421	A
50	S2	1429	G
50	S2	1433	C
50	S2	1434	C
50	S2	1440	C
50	S2	1441	U
50	S2	1442	U
50	S2	1446	A
50	S2	1454	A
50	S2	1462	U
50	S2	1463	U
50	S2	1474	A
50	S2	1475	G
50	S2	1477	U
50	S2	1489	A
50	S2	1493	C
50	S2	1494	U
50	S2	1506	A
50	S2	1512	C
50	S2	1521	C
50	S2	1522	A
50	S2	1534	C
50	S2	1537	A
50	S2	1540	G
50	S2	1542	C
50	S2	1543	U
50	S2	1552	G
50	S2	1555	U
50	S2	1556	A
50	S2	1557	C
50	S2	1561	A
50	S2	1568	C

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Mol	Chain	Res	Type
50	S2	1579	A
50	S2	1585	U
50	S2	1588	A
50	S2	1593	C
50	S2	1597	C
50	S2	1598	G
50	S2	1599	U
50	S2	1603	G
50	S2	1605	G
50	S2	1623	A
50	S2	1629	C
50	S2	1637	A
50	S2	1643	U
50	S2	1648	G
50	S2	1659	U
50	S2	1664	A
50	S2	1678	A
50	S2	1679	A
50	S2	1682	C
50	S2	1688	C
50	S2	1692	U
50	S2	1696	C
50	S2	1698	C
50	S2	1699	A
50	S2	1703	C
50	S2	1720	U
50	S2	1744	G
50	S2	1756	C
50	S2	1825	A
50	S2	1830	U
50	S2	1835	A
50	S2	1836	G
50	S2	1838	U
50	S2	1849	G
50	S2	1857	G
50	S2	1858	G
50	S2	1860	A
50	S2	1863	A
50	S2	1868	U
85	S5	2	C
85	S5	6	G
85	S5	9	A

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Mol	Chain	Res	Type
85	S5	18	G
85	S5	19	G
85	S5	34	G
85	S5	38	A
85	S5	43	C
85	S5	47	U
85	S5	75	C
86	S6	8	U
86	S6	34	G
86	S6	48	C
86	S6	50	U
86	S6	53	G
86	S6	57	G
86	S6	70	G
86	S6	71	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	5	18
47	1	6
50	S2	5
85	S5	4
52	SB	3
8	E	1
46	z	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	3977:C	O3'	4034:G	P	16.30
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	1	312:PHE	C	337:PRO	N	11.28
1	1	133:MET	C	148:CYS	N	10.01
1	5	1051:G	O3'	1064:G	P	9.59
1	S5	15:G	O3'	18:G	P	7.89
1	S2	739:C	O3'	744:G	P	7.74
1	S2	225:G	O3'	287:U	P	6.54
1	S5	58:A	O3'	59:U	P	4.88
1	5	4087:G	O3'	4088:C	P	4.33
1	5	1222:A	O3'	1232:G	P	3.97
1	S5	60:U	O3'	61:C	P	3.51
1	1	25:LYS	C	26:ILE	N	3.38
1	5	1699:A	O3'	1718:C	P	3.33
1	1	26:ILE	C	27:GLN	N	3.27
1	z	100:VAL	C	101:LYS	N	3.20
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	1	449:LEU	C	450:ALA	N	2.47
1	5	3939:G	O3'	3940:U	P	2.44

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	1373:C	O3'	1374:C	P	2.12
1	SB	144:LYS	C	145:LYS	N	2.05
1	5	1566:C	O3'	1567:U	P	2.02
1	1	272:TYR	C	273:ARG	N	1.81
1	SB	221:PRO	C	222:LYS	N	1.68
1	5	4116:C	O3'	4117:U	P	1.19
1	S5	47:U	O3'	48:C	P	1.01
1	5	2037:C	O3'	2038:U	P	0.79
1	SB	145:LYS	C	146:ARG	N	0.31

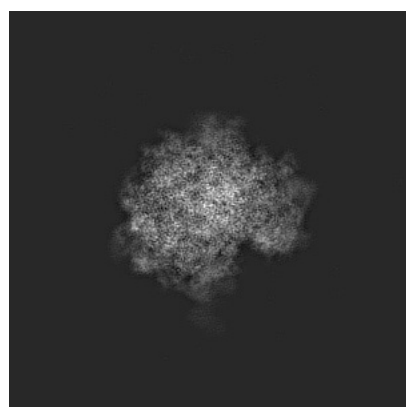
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2644. These allow visual inspection of the internal detail of the map and identification of artifacts.

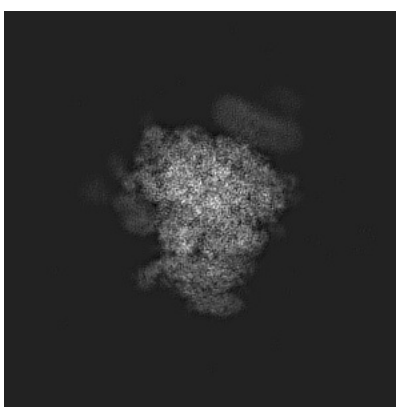
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

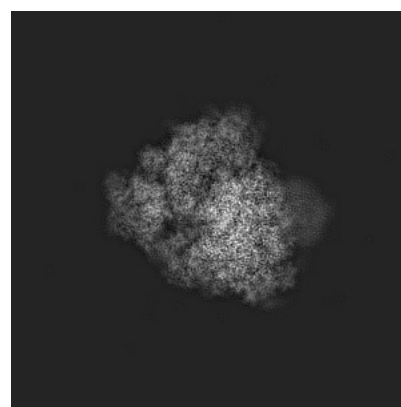
6.1.1 Primary map



X



Y

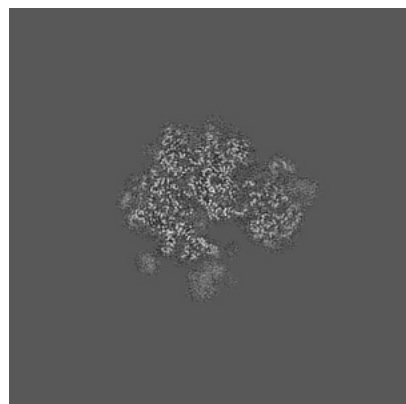


Z

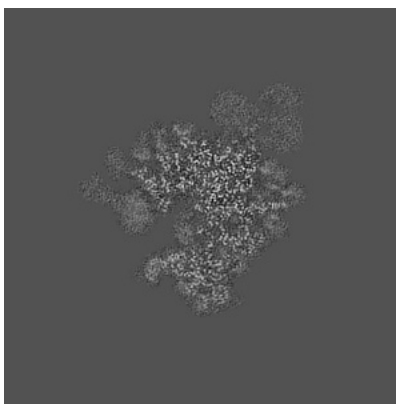
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

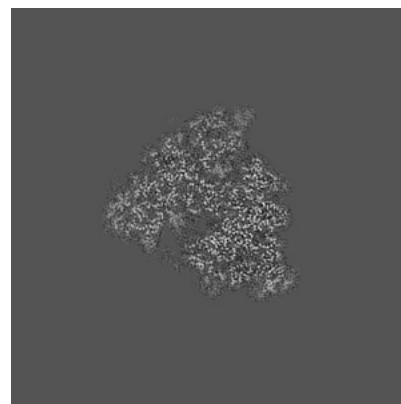
6.2.1 Primary map



X Index: 210



Y Index: 210

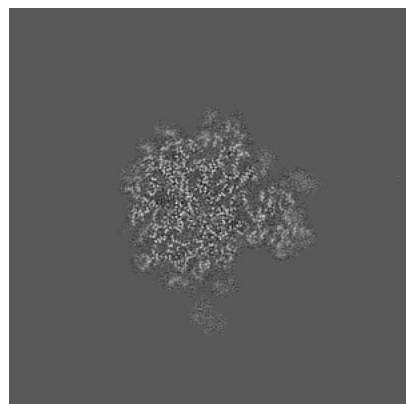


Z Index: 210

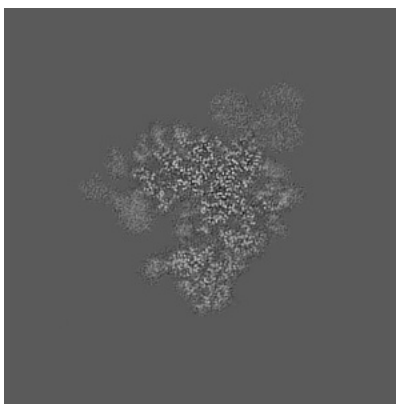
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

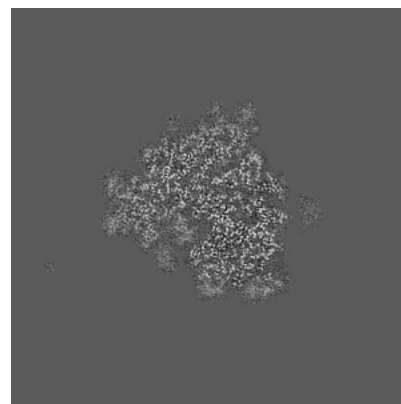
6.3.1 Primary map



X Index: 230



Y Index: 208

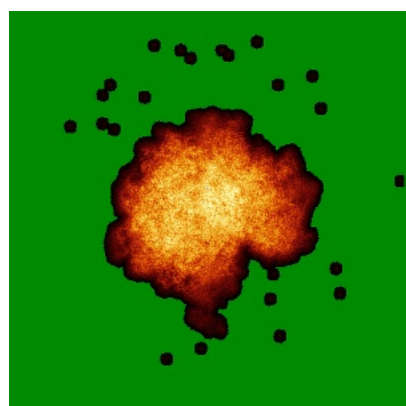


Z Index: 218

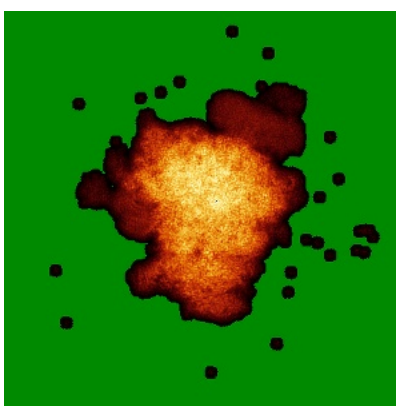
The images above show the largest variance slices of the map in three orthogonal directions.

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

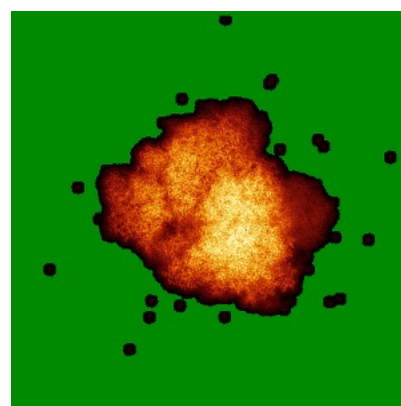
6.4.1 Primary map



X



Y

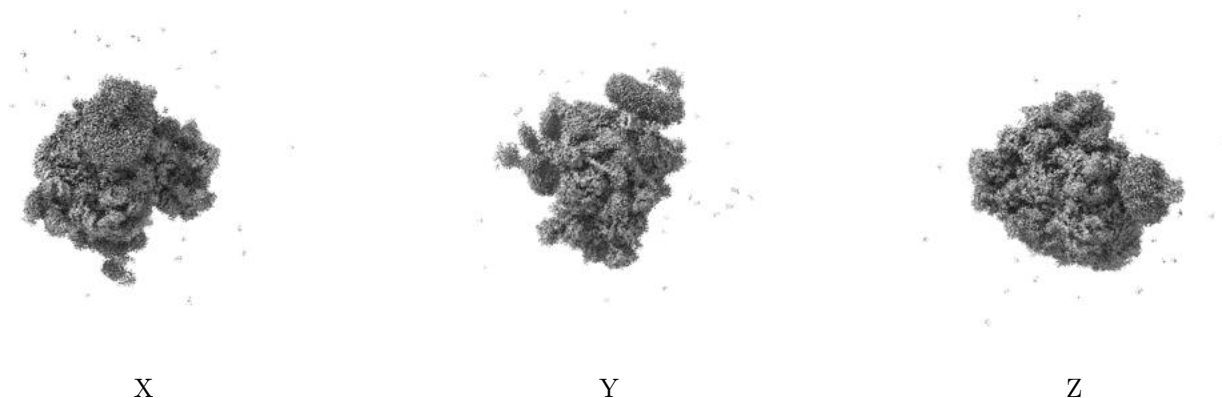


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

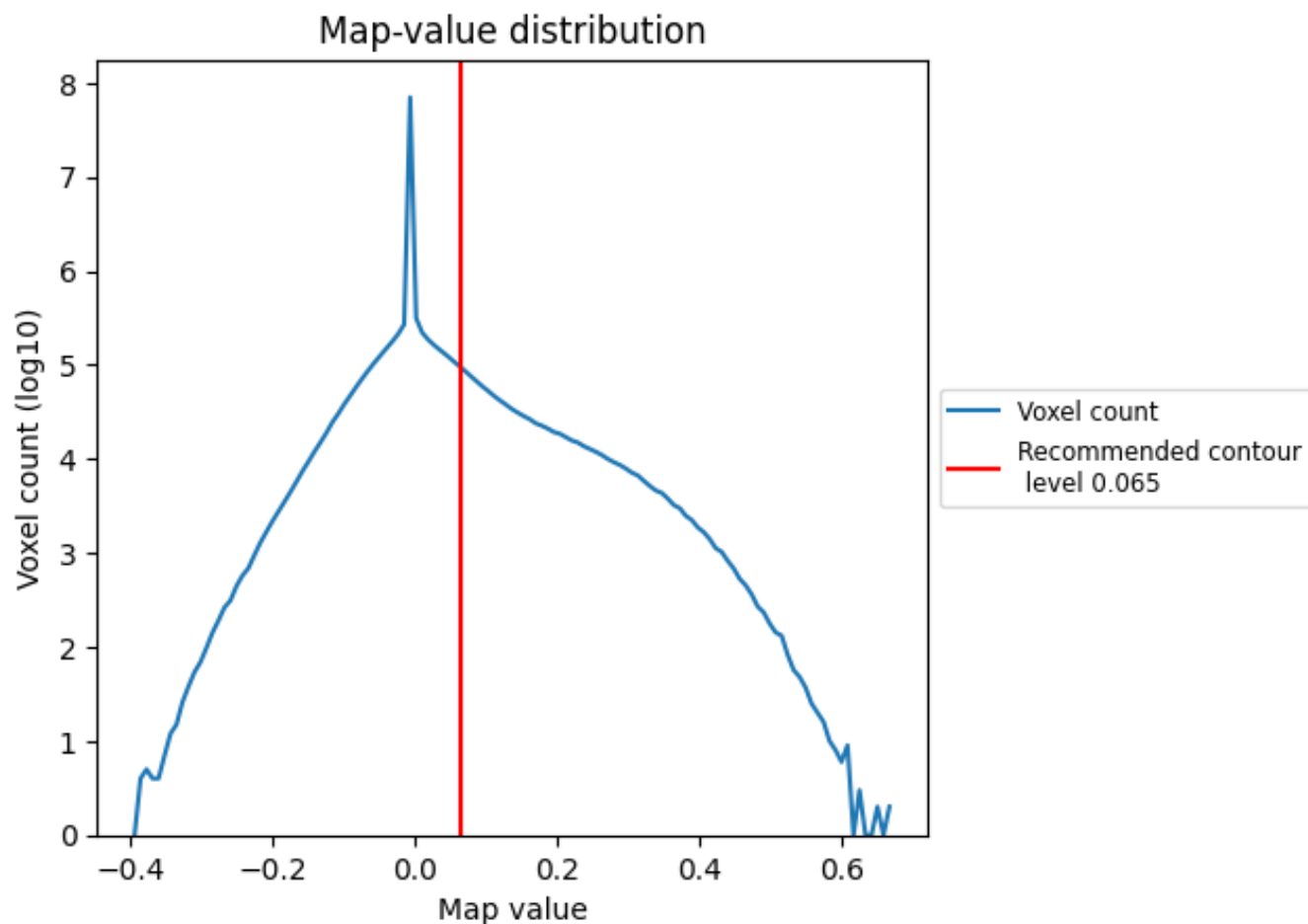
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

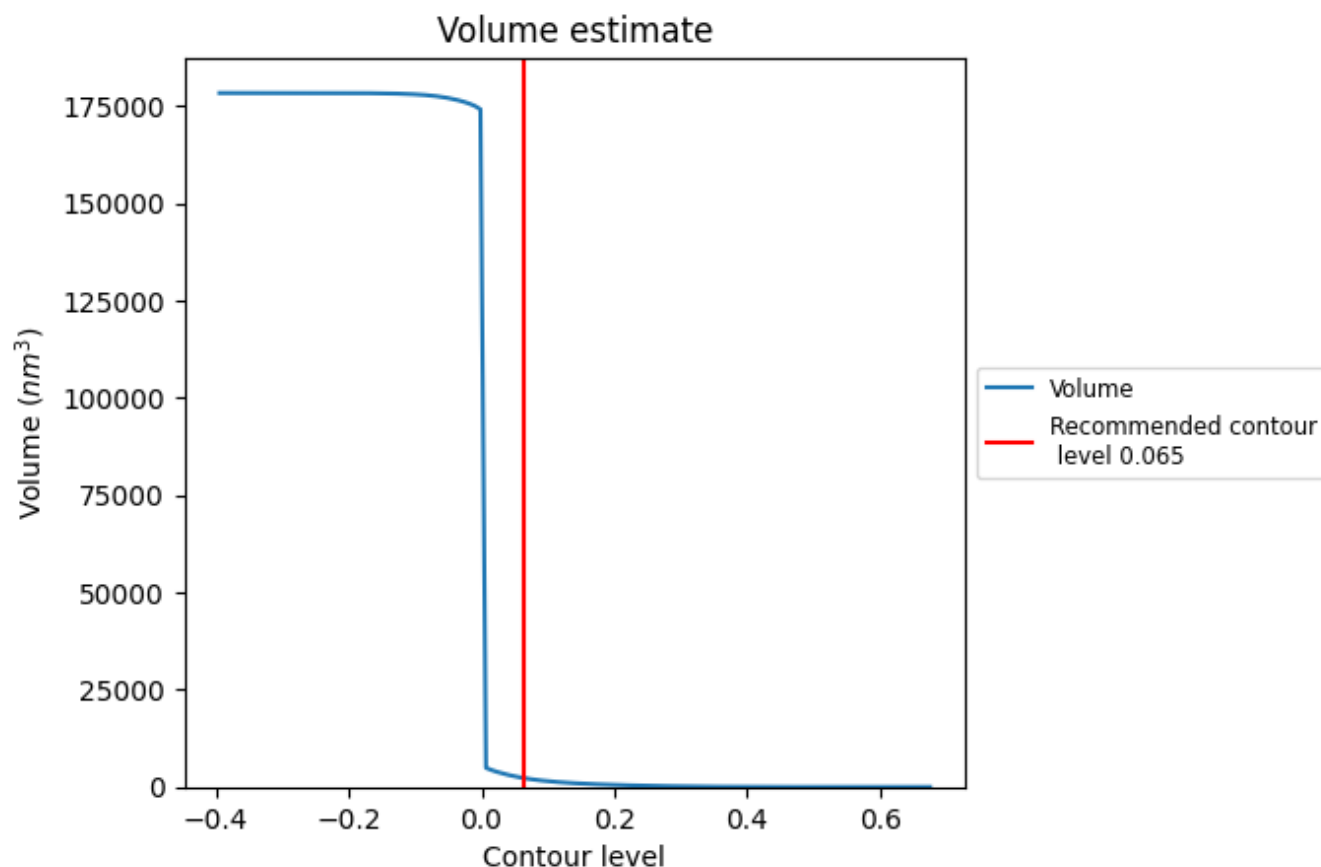
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

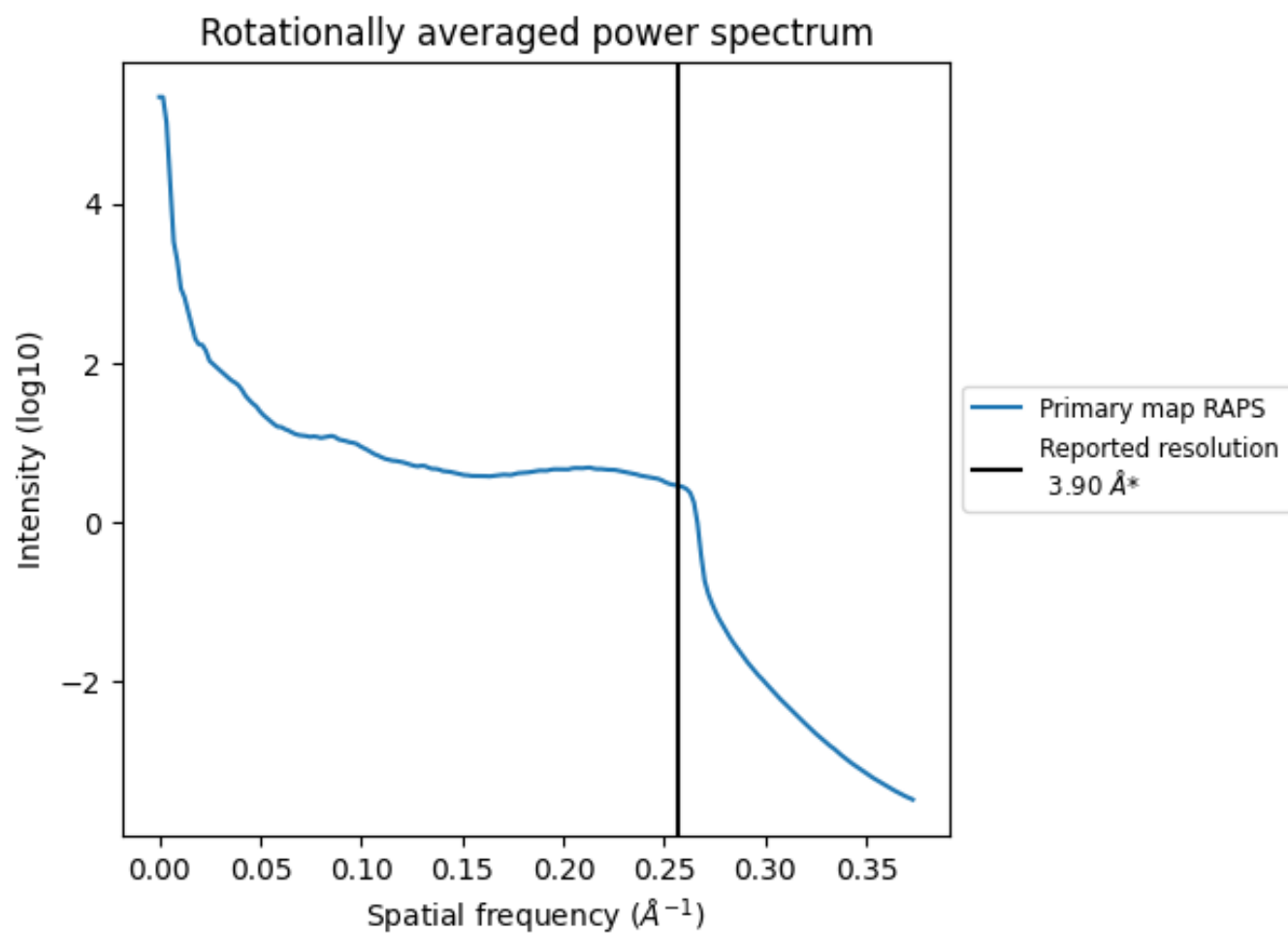
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2249 nm³; this corresponds to an approximate mass of 2032 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

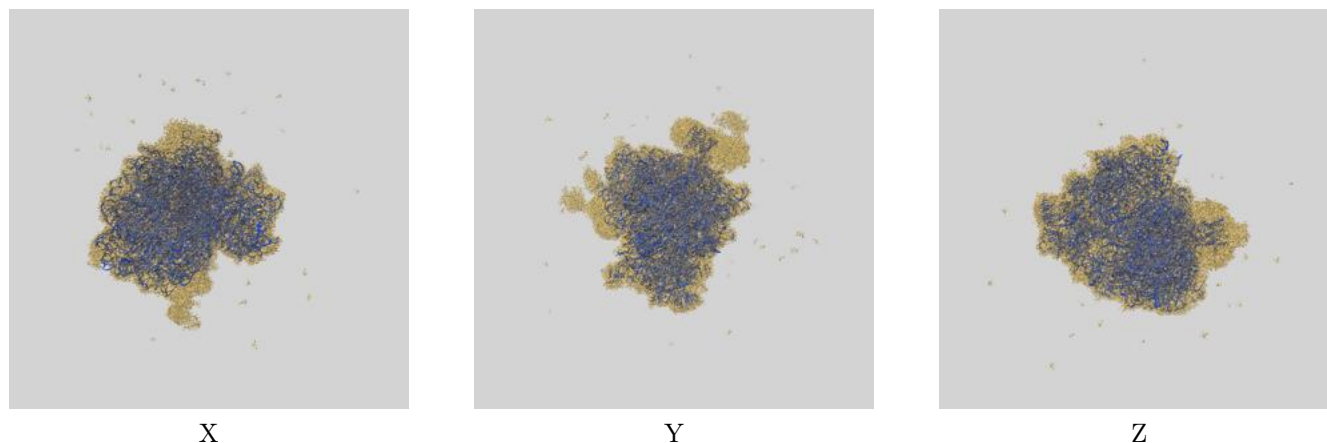
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

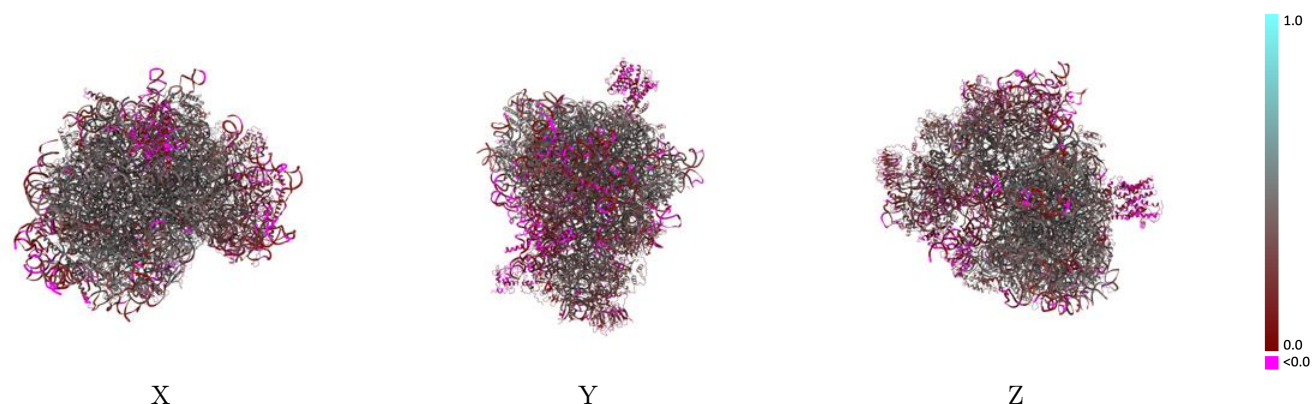
This section contains information regarding the fit between EMDB map EMD-2644 and PDB model 3J7R. Per-residue inclusion information can be found in [section 3](#) on [page 40](#).

9.1 Map-model overlay [i](#)



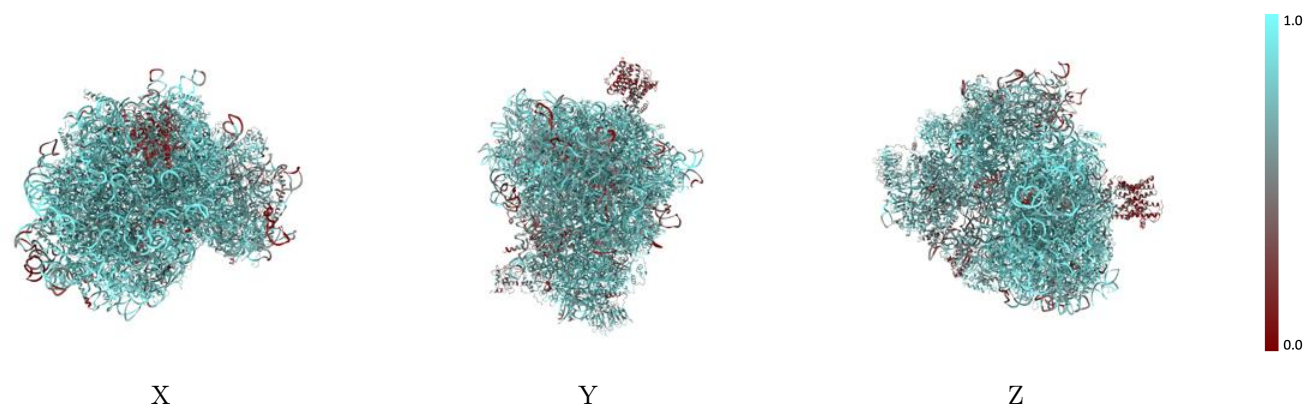
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



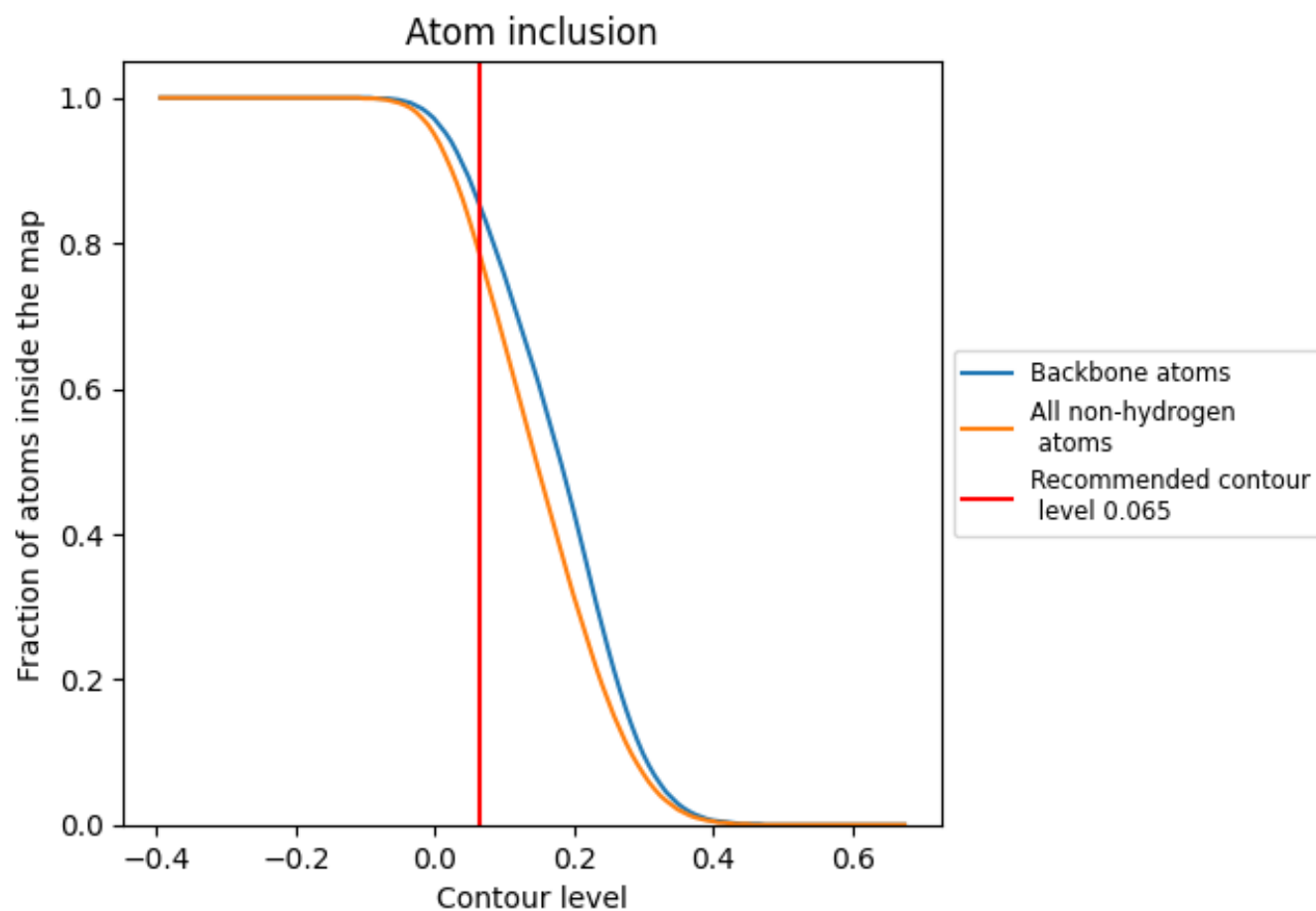
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































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

Chain	Atom inclusion	Q-score
All	 0.7830	 0.3280
1	 0.3180	 0.0870
2	 0.2760	 0.0550
3	 0.1500	 0.0260
5	 0.8370	 0.3450
7	 0.9290	 0.4110
8	 0.8700	 0.3830
A	 0.8350	 0.4610
B	 0.8450	 0.4450
C	 0.8150	 0.4310
D	 0.7970	 0.3500
E	 0.7770	 0.3780
F	 0.8250	 0.4320
G	 0.7880	 0.3800
H	 0.8220	 0.4230
I	 0.8110	 0.4170
J	 0.7150	 0.2960
L	 0.7930	 0.4020
M	 0.8490	 0.4300
N	 0.8420	 0.4500
O	 0.8380	 0.4490
P	 0.8420	 0.4540
Q	 0.8500	 0.4570
R	 0.7940	 0.3910
S	 0.8460	 0.4380
S2	 0.8050	 0.2890
S4	 0.9350	 0.4180
S5	 0.5760	 0.1580
S6	 0.7030	 0.1880
SA	 0.8010	 0.3670
SB	 0.7190	 0.2930
SC	 0.8100	 0.3880
SD	 0.7190	 0.3080
SE	 0.6020	 0.1750
SF	 0.5930	 0.1730























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Chain	Atom inclusion	Q-score
SG	 0.6640	 0.2190
SH	 0.6940	 0.2780
SI	 0.6460	 0.2250
SJ	 0.4990	 0.0670
SK	 0.6500	 0.1850
SL	 0.6460	 0.2660
SM	 0.4030	 0.0090
SN	 0.7810	 0.3620
SO	 0.6720	 0.2480
SP	 0.5760	 0.1370
SQ	 0.7480	 0.3180
SR	 0.6830	 0.2750
SS	 0.6520	 0.2000
ST	 0.7320	 0.2990
SU	 0.7010	 0.2960
SV	 0.8020	 0.3830
SW	 0.8010	 0.3940
SX	 0.7250	 0.3160
SY	 0.4960	 0.0490
SZ	 0.4730	 0.0290
Sa	 0.8010	 0.3960
Sb	 0.7230	 0.3230
Sc	 0.4320	 0.1010
Sd	 0.7740	 0.3550
Se	 0.4460	 0.1010
Sf	 0.4060	 0.0160
Sg	 0.6410	 0.1780
T	 0.8300	 0.4420
U	 0.7780	 0.3480
V	 0.7980	 0.4380
W	 0.8090	 0.4100
X	 0.7930	 0.4320
Y	 0.8000	 0.4190
Z	 0.8340	 0.4270
a	 0.8440	 0.4470
b	 0.7520	 0.3750
c	 0.8100	 0.4130
d	 0.7860	 0.4040
e	 0.8430	 0.4530
f	 0.8590	 0.4610
g	 0.8010	 0.4170
h	 0.7970	 0.4150

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Chain	Atom inclusion	Q-score
i	 0.7940	 0.3990
j	 0.8810	 0.4600
k	 0.7520	 0.3590
l	 0.8250	 0.4470
m	 0.8460	 0.4230
n	 0.7710	 0.3940
o	 0.7880	 0.4210
p	 0.8140	 0.4420
r	 0.8470	 0.4490
z	 0.3580	 0.0590