



## Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 10:31 pm BST

PDB ID : 7B7D / pdb\_00007b7d  
EMDB ID : EMD-12081  
Title : Yeast 80S ribosome bound to eEF3 and A/A- and P/P-tRNAs  
Authors : Ranjan, N.; Pochopien, A.A.; Wu, C.C.; Beckert, B.; Blanchet, S.; Green, R.;  
Rodnina, M.V.; Wilson, D.N.  
Deposited on : 2020-12-10  
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

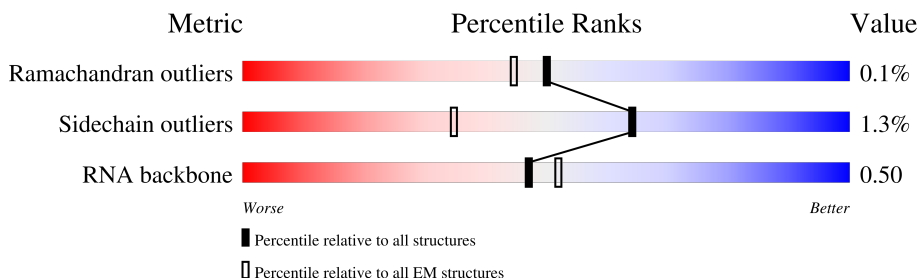
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	2	1771	
2	1	7	
3	P	206	
4	Q	232	
5	E	117	
6	R	216	
7	A	222	
8	S	258	

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Mol	Chain	Length	Quality of chain
9	B	206	
10	T	228	
11	U	184	
12	V	198	
13	W	184	
14	C	92	
15	X	142	
16	D	121	
17	Y	150	
18	Z	127	
19	F	141	
20	G	125	
21	H	145	
22	I	143	
23	J	100	
24	a	87	
25	b	129	
26	c	144	
27	d	134	
28	K	82	
29	e	97	
30	f	81	
31	M	53	
32	g	60	
33	N	73	

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Mol	Chain	Length	Quality of chain
34	O	312	
35	L	63	
36	LA	3223	
37	LB	121	
38	LC	158	
39	LD	251	
40	LE	386	
41	LF	361	
42	LG	294	
43	LH	175	
44	LI	222	
45	LJ	233	
46	LK	191	
47	LL	218	
48	LM	169	
49	LN	193	
50	LO	136	
51	LP	203	
52	LQ	197	
53	LR	183	
54	Lm	185	
55	Ln	188	
56	Lo	171	
57	Lp	159	
58	Lq	100	

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Mol	Chain	Length	Quality of chain
59	Lr	136	
60	LS	126	
61	LT	121	
62	LU	125	
63	LV	135	
64	LW	148	
65	LX	58	
66	LY	96	
67	LZ	109	
68	La	127	
69	Lb	106	
70	Lc	112	
71	Ld	119	
72	Le	99	
73	Lf	81	
74	Lg	77	
75	Lh	50	
76	Li	52	
77	Lj	25	
78	Lk	103	
79	Ll	91	
80	Sm	75	
80	Sn	75	
81	EF	1044	

## 2 Entry composition

There are 82 unique types of molecules in this entry. The entry contains 211144 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 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1771	Total	C	N	O	P	0	0
			37739	16872	6683	12413	1771		

- Molecule 2 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	7	Total	C	N	O	P	0	0
			149	67	26	49	7		

- Molecule 3 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	206	Total	C	N	O	S	0	0
			1603	1030	284	287	2		

- Molecule 4 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	226	Total	C	N	O	S	0	0
			1798	1139	330	325	4		

- Molecule 5 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	117	Total	C	N	O	S	0	0
			916	583	171	155	7		

- Molecule 6 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	216	Total	C	N	O	S	0	0
			1626	1042	287	295	2		

- Molecule 7 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	222	Total	C	N	O	S	0	0
			1729	1098	312	313	6		

- Molecule 8 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	258	Total	C	N	O	S	0	0
			2056	1308	387	358	3		

- Molecule 9 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	206	Total	C	N	O	S	0	0
			1605	1005	299	298	3		

- Molecule 10 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	T	228	Total	C	N	O	S	0	0
			1815	1138	351	323	3		

- Molecule 11 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	U	184	Total	C	N	O	S	0	0
			1473	946	263	264			

- Molecule 12 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	V	187	Total	C	N	O	S	0	0
			1476	916	295	263	2		

- Molecule 13 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	W	184	Total	C	N	O	S	0	0
			1479	935	285	258	1		

- Molecule 14 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	92	Total	C	N	O	S	0	0
			752	487	122	141	2		

- Molecule 15 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	142	Total	C	N	O	S	0	0
			1142	733	217	189	3		

- Molecule 16 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	D	121	Total	C	N	O	S	0	0
			875	551	153	169	2		

- Molecule 17 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 18 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	127	Total	C	N	O	S	0	0
			923	568	185	167	3		

- Molecule 19 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	F	141	Total	C	N	O	0	0
			1105	708	203	194		

- Molecule 20 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	G	121	Total	C	N	O	S	0	0
			948	596	179	171	2		

- Molecule 21 is a protein called 40S ribosomal protein S18-A.



Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	145	Total	C	N	O	S	0	0
			1188	741	237	208	2		

- Molecule 22 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	I	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 23 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	J	100	Total	C	N	O	S	0	0
			797	506	144	146	1		

- Molecule 24 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	87	Total	C	N	O	S	0	0
			673	415	125	131	2		

- Molecule 25 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 26 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 27 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	d	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 28 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	K	82	Total	C	N	O	0	0
			651	416	123	112		

- Molecule 29 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	97	Total	C	N	O	S	0	0
			765	473	160	127	5		

- Molecule 30 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	M	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 32 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	60	Total	C	N	O	S	0	0
			472	298	97	76	1		

- Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	N	73	Total	C	N	O	S	0	0
			556	352	105	95	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	97	ALA	LYS	conflict	UNP P05759

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	O	312	Total	C	N	O	S	0	0
			2383	1514	409	452	8		

- Molecule 35 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L	63	Total	C	N	O	S	0	0
			491	303	96	91	1		

- Molecule 36 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LA	3223	Total	C	N	O	P	0	0
			68931	30790	12416	22502	3223		

- Molecule 37 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LB	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 38 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LC	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 39 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LD	251	Total	C	N	O	S	0	0
			1899	1182	385	331	1		

- Molecule 40 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LE	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 41 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LF	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 42 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LG	294	Total	C	N	O	S	0	0
			2351	1484	410	455	2		

- Molecule 43 is a protein called 60S ribosomal protein L6-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	LH	167	Total	C	N	O	0	0
			1307	843	234	230		

- Molecule 44 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LI	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 45 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LJ	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 46 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	LK	191	Total	C	N	O	S	0	0
			1508	957	274	273	4		

- Molecule 47 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LL	218	Total	C	N	O	S	0	0
			1764	1117	334	306	7		

- Molecule 48 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	LM	169	Total	C	N	O	S	0	0
			1346	843	252	247	4		

- Molecule 49 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	LN	193	Total	C	N	O		0	0
			1543	962	315	266			

- Molecule 50 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LO	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 51 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	LP	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 52 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LQ	197	Total	C	N	O	S	197	0
			1555	1003	289	262	1		

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	LR	183	Total	C	N	O		0	0
			1416	879	284	253			

- Molecule 54 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Lm	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 55 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	Ln	188	Total	C	N	O	0	0
			1515	932	323	260		

- Molecule 56 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Lo	171	Total	C	N	O	S	0	0
			1437	925	266	243	3		

- Molecule 57 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Lp	159	Total	C	N	O	S	0	0
			1272	802	245	221	4		

- Molecule 58 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	Lq	100	Total	C	N	O	0	0
			796	516	131	149		

- Molecule 59 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Lr	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 60 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	LS	126	Total	C	N	O	S	0	0
			836	525	165	145	1		

- Molecule 61 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	LT	121	Total	C	N	O	S	0	0
			964	620	169	173	2		

- Molecule 62 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	LU	125	Total	C	N	O	0	0
			984	620	191	173		

- Molecule 63 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
63	LV	135	Total	C	N	O	0	0
			1080	701	199	180		

- Molecule 64 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	LW	148	Total	C	N	O	S	0	0
			1169	747	231	188	3		

- Molecule 65 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
65	LX	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 66 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	LY	96	Total	C	N	O	S	0	0
			737	476	123	137	1		

- Molecule 67 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	LZ	109	Total	C	N	O	S	0	0
			876	556	167	152	1		

- Molecule 68 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	La	127	Total	C	N	O	S	0	0
			1013	642	205	165	1		

- Molecule 69 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Lb	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 70 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Lc	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 71 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Ld	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 72 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Le	99	Total	C	N	O	S	0	0
			766	478	154	132	2		

- Molecule 73 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Lf	81	Total	C	N	O	S	0	0
			645	393	141	106	5		

- Molecule 74 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
74	Lg	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 75 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Lh	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 76 is a protein called Ubiquitin-60S ribosomal protein L40.



Mol	Chain	Residues	Atoms					AltConf	Trace
76	Li	52	Total	C	N	O	S	0	0
			410	254	86	65	5		

- Molecule 77 is a protein called 60S ribosomal protein L41-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Lj	25	Total	C	N	O	S	0	0
			229	139	62	27	1		

- Molecule 78 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Lk	103	Total	C	N	O	S	0	0
			824	517	167	135	5		

- Molecule 79 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Ll	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 80 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Sn	75	Total	C	N	O	P	0	0
			1606	716	297	518	75		
80	Sm	75	Total	C	N	O	P	0	0
			1605	716	297	517	75		

- Molecule 81 is a protein called Elongation factor 3A.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	EF	977	Total	C	N	O	S	Se	0	0
			7479	4729	1294	1419	32	5		

There are 5 discrepancies between the modelled and reference sequences:

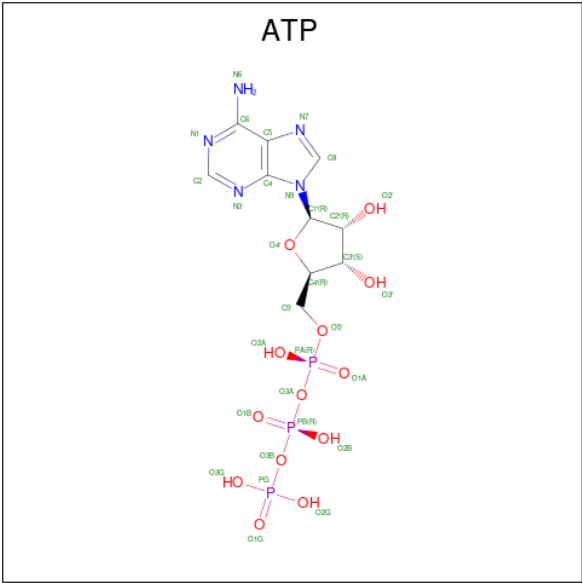
Chain	Residue	Modelled	Actual	Comment	Reference
EF	24	ASP	ASN	conflict	UNP P16521
EF	152	PHE	ILE	conflict	UNP P16521
EF	331	LEU	VAL	conflict	UNP P16521
EF	541	GLY	SER	conflict	UNP P16521

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Chain	Residue	Modelled	Actual	Comment	Reference
EF	542	SER	ALA	conflict	UNP P16521

- Molecule 82 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

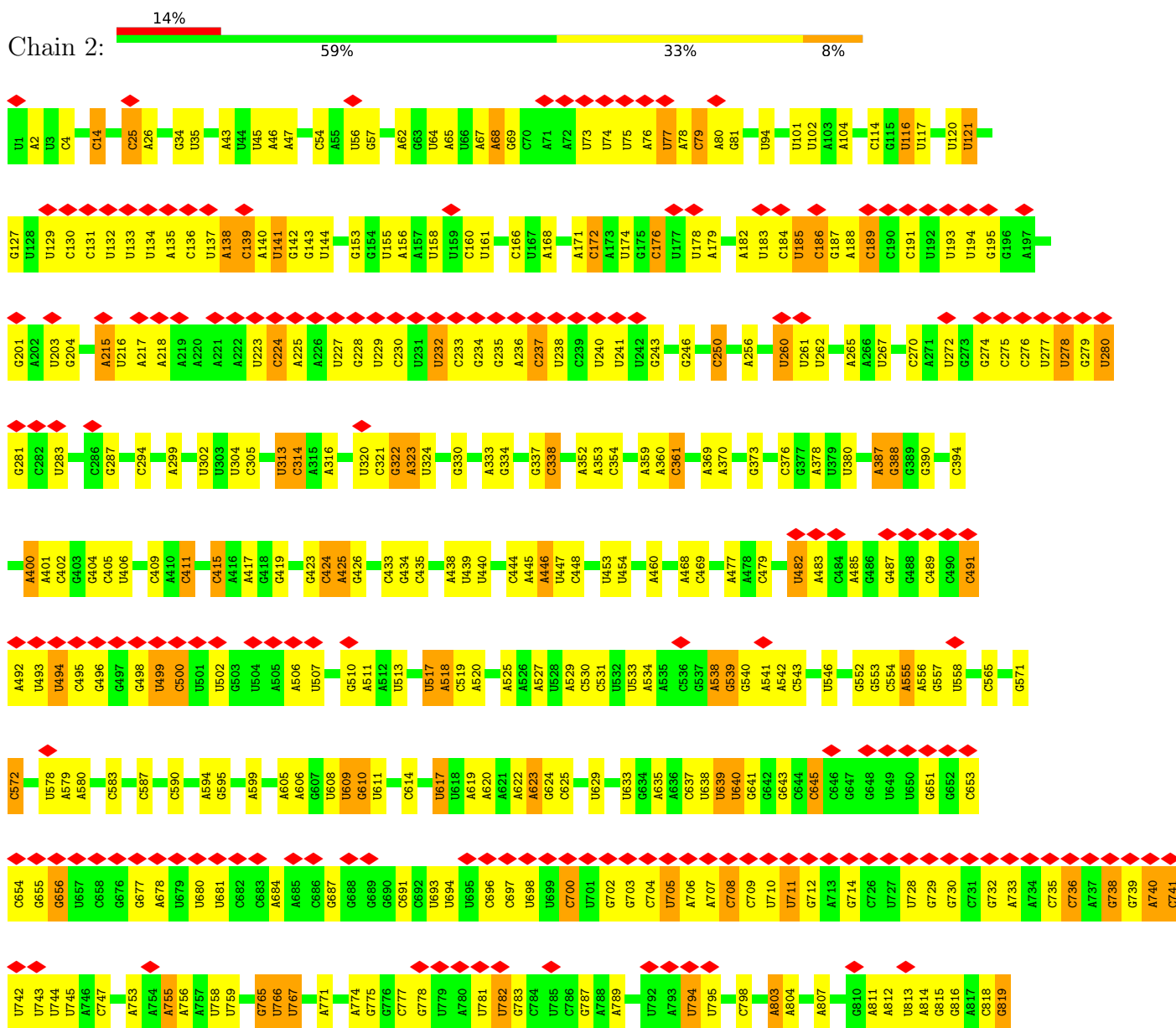


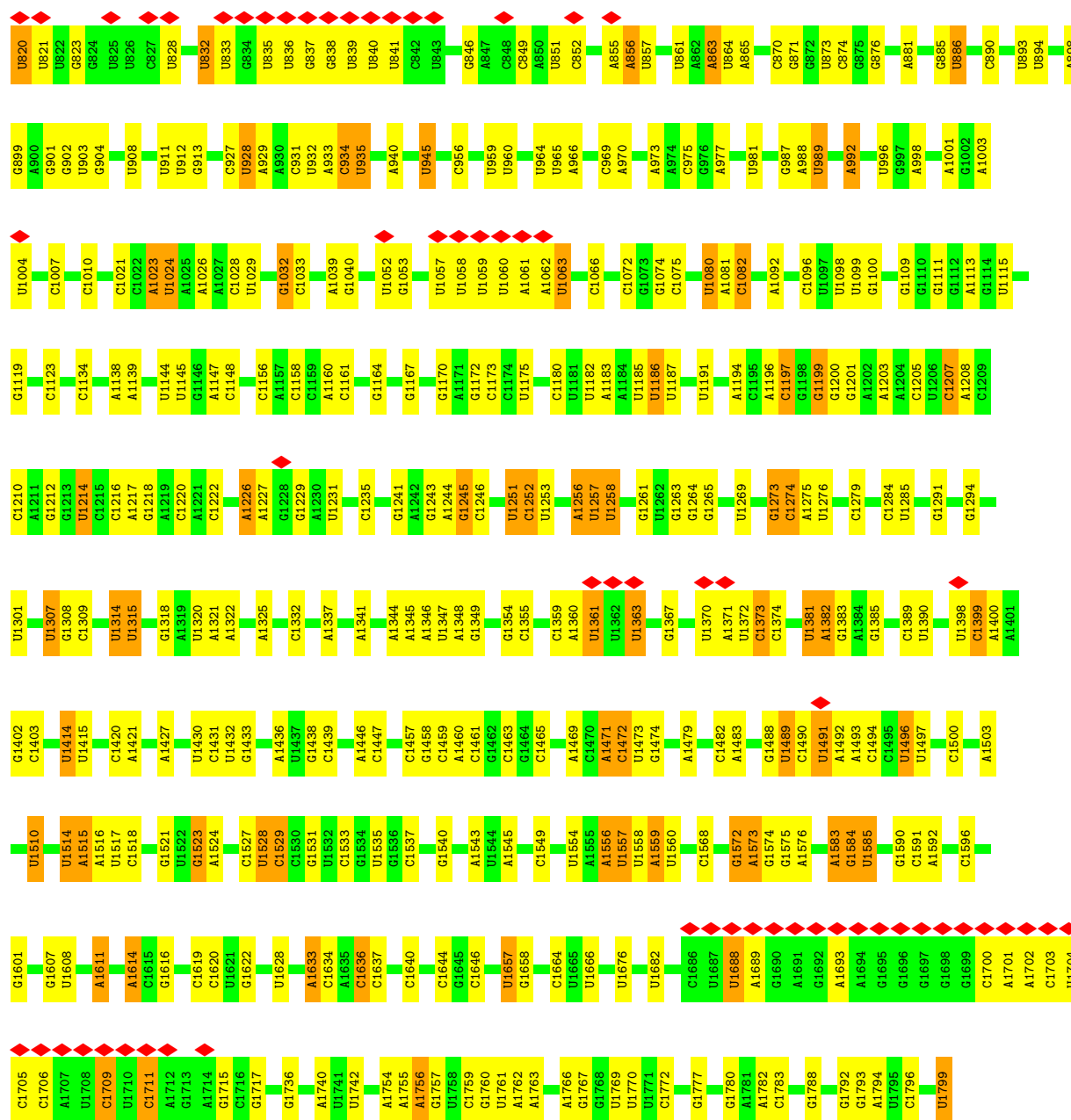
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
82	EF	1	31	10	5	13	3	0
82	EF	1	Total	C	N	O	P	0
			31	10	5	13	3	

### 3 Residue-property plots

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

#### • Molecule 1: 18S rRNA





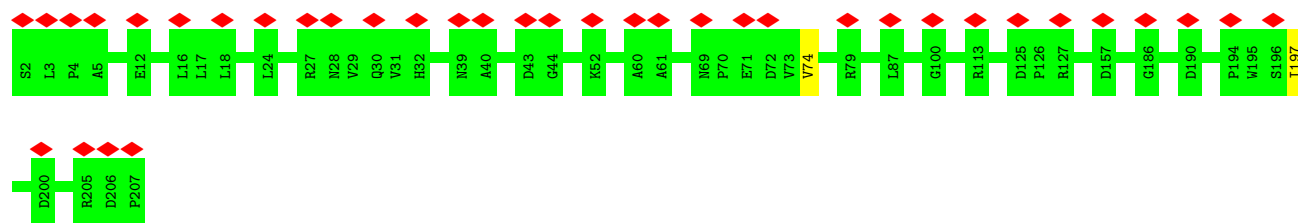
- Molecule 2: mRNA

Chain 1: 86% 14%

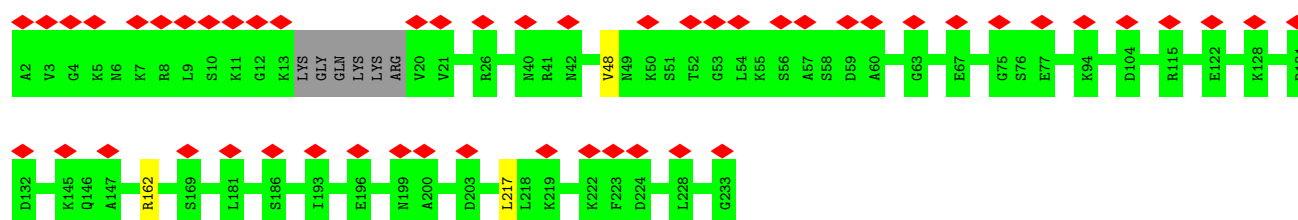


- Molecule 3: 40S ribosomal protein S0-A

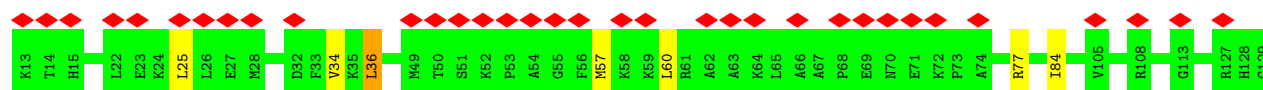
Chain P: 18% 99%



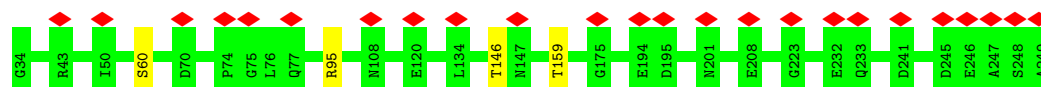
- Molecule 4: 40S ribosomal protein S1-A



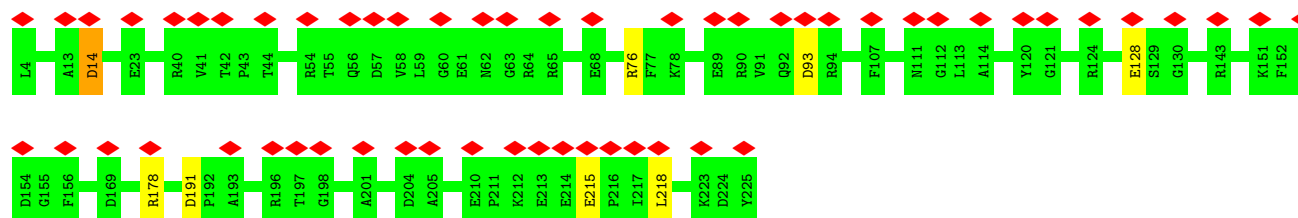
- Molecule 5: 40S ribosomal protein S15



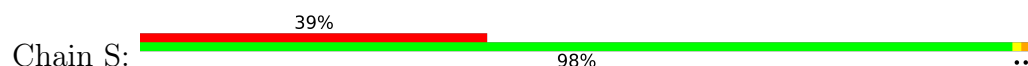
- Molecule 6: 40S ribosomal protein S2

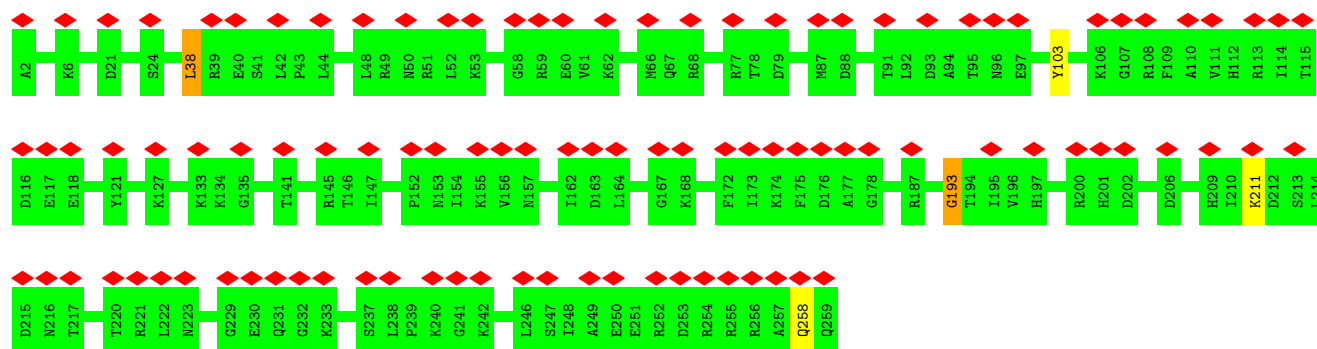


- Molecule 7: 40S ribosomal protein S3

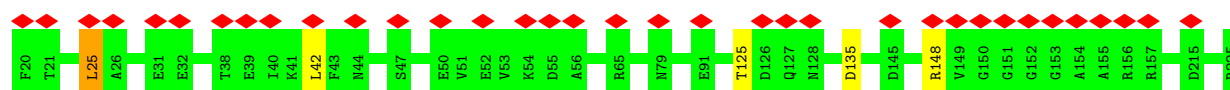


- Molecule 8: 40S ribosomal protein S4-A

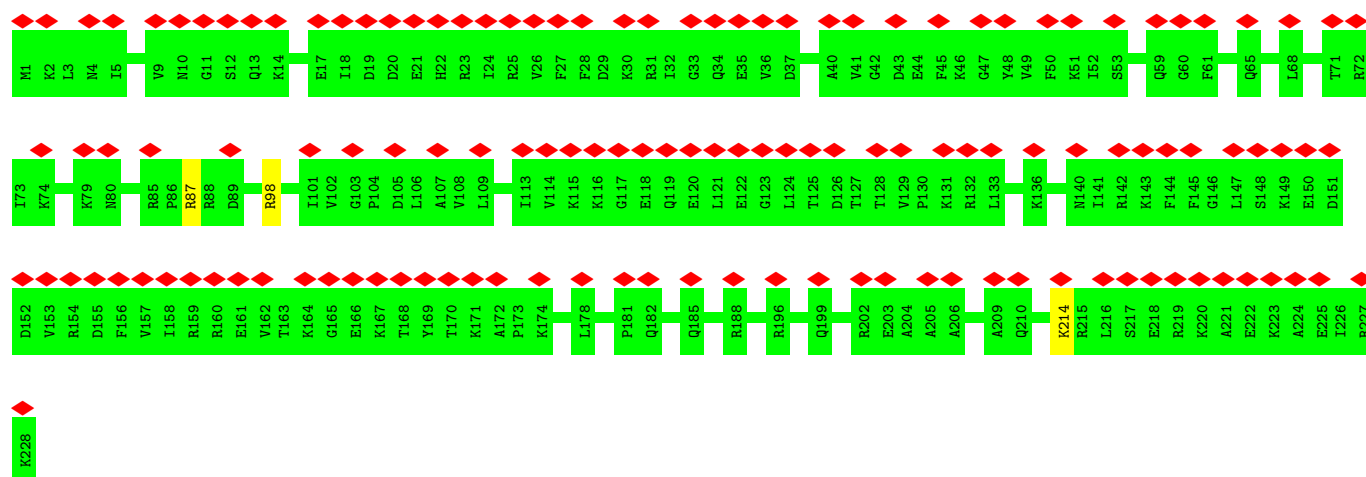




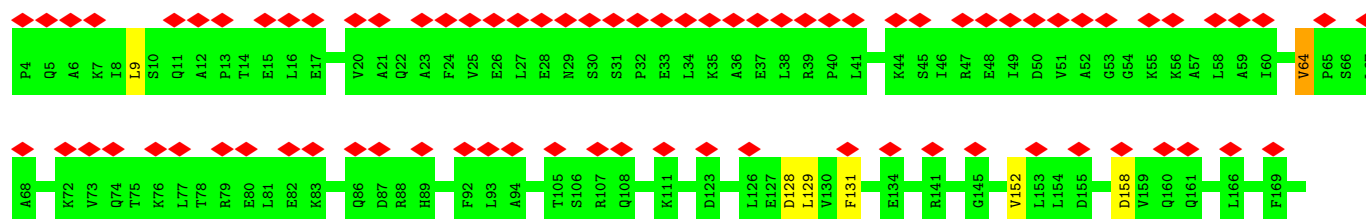
• Molecule 9: 40S ribosomal protein S5

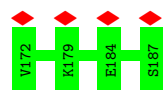


• Molecule 10: 40S ribosomal protein S6-A

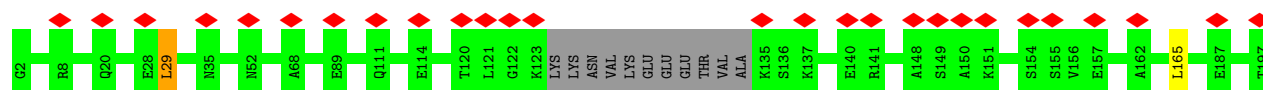


• Molecule 11: 40S ribosomal protein S7-A

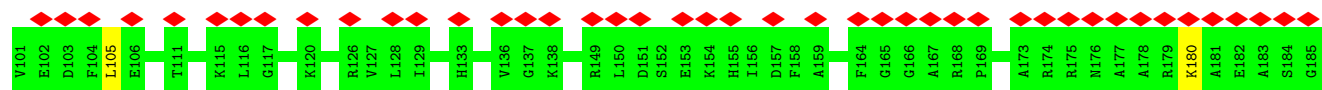
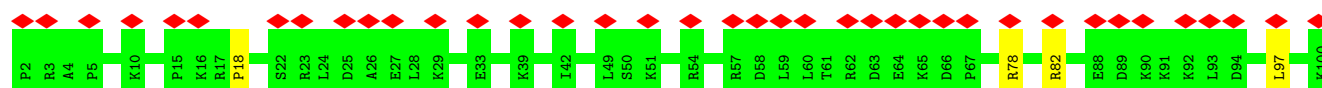




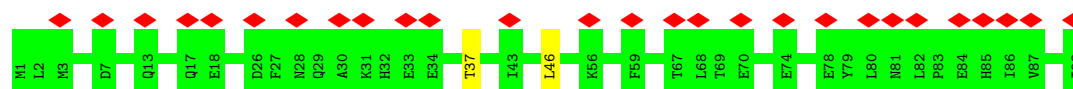
- Molecule 12: 40S ribosomal protein S8-A



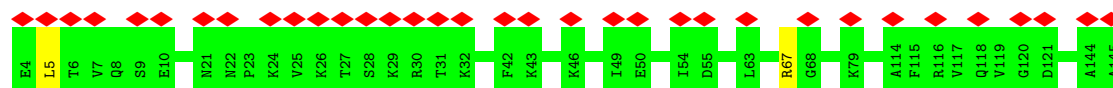
- Molecule 13: 40S ribosomal protein S9-A



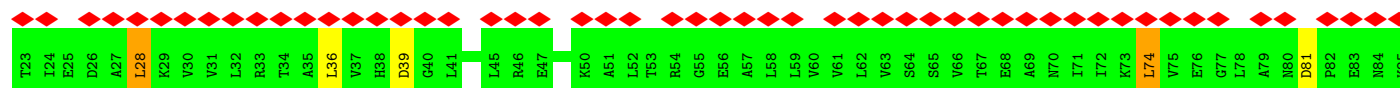
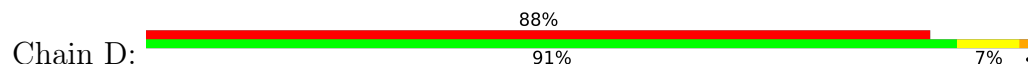
- Molecule 14: 40S ribosomal protein S10-A

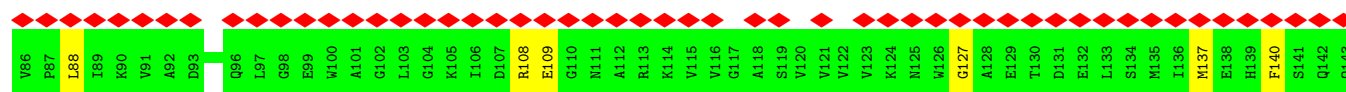


- Molecule 15: 40S ribosomal protein S11-A

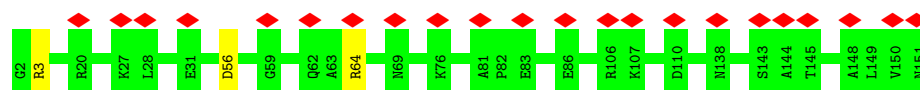


- Molecule 16: 40S ribosomal protein S12

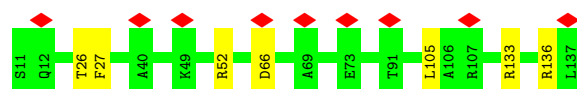




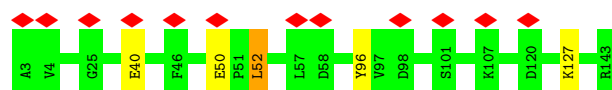
- Molecule 17: 40S ribosomal protein S13



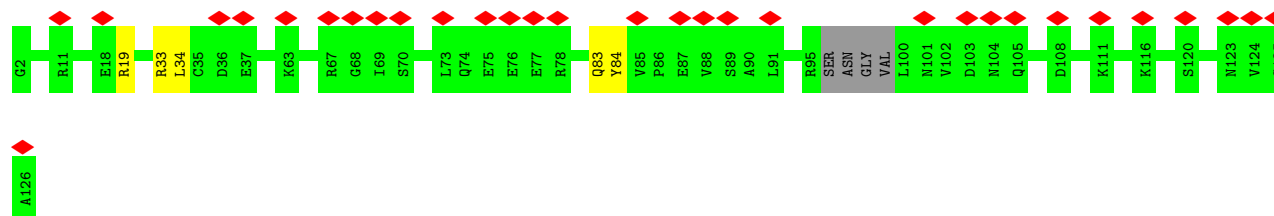
- Molecule 18: 40S ribosomal protein S14-B



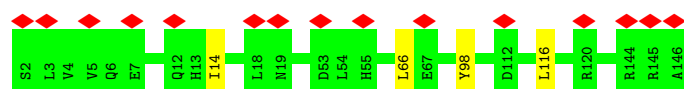
- Molecule 19: 40S ribosomal protein S16-A



- Molecule 20: 40S ribosomal protein S17-B



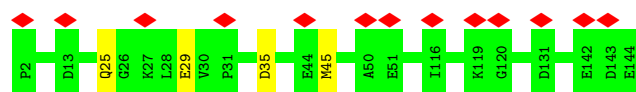
- Molecule 21: 40S ribosomal protein S18-A



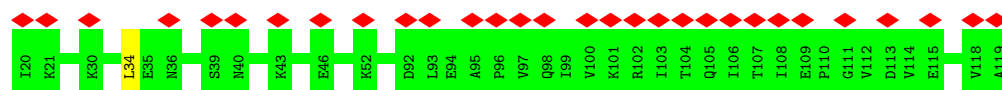
- Molecule 22: 40S ribosomal protein S19-A



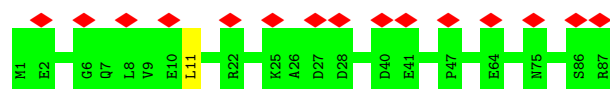




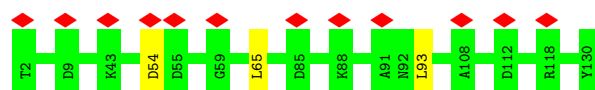
- Molecule 23: 40S ribosomal protein S20



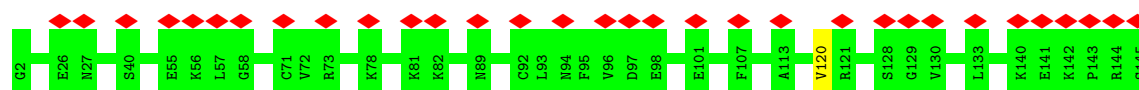
- Molecule 24: 40S ribosomal protein S21-A



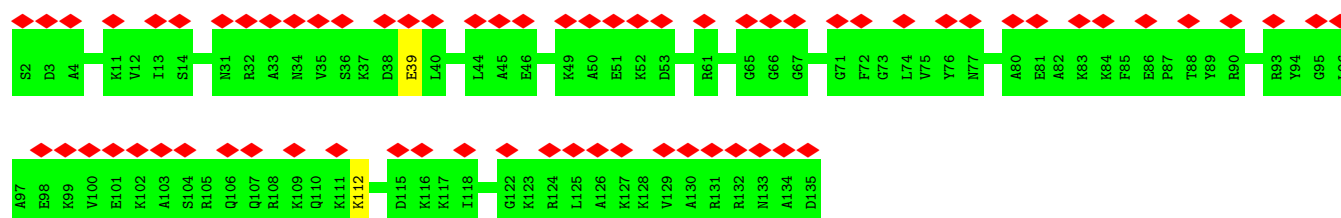
- Molecule 25: 40S ribosomal protein S22-A



- Molecule 26: 40S ribosomal protein S23-A

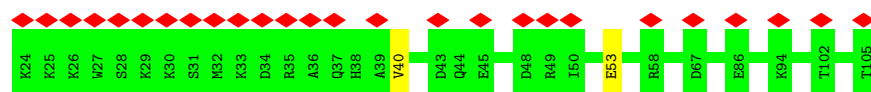


- Molecule 27: 40S ribosomal protein S24-A

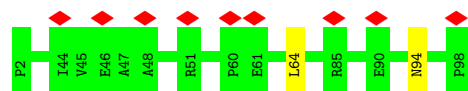


- Molecule 28: 40S ribosomal protein S25-A

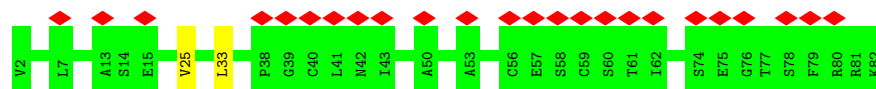




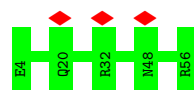
- Molecule 29: 40S ribosomal protein S26-B



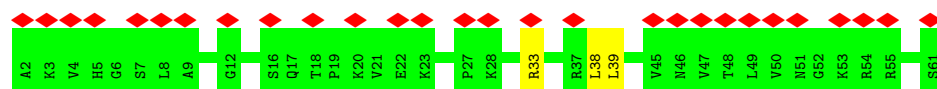
- Molecule 30: 40S ribosomal protein S27-A



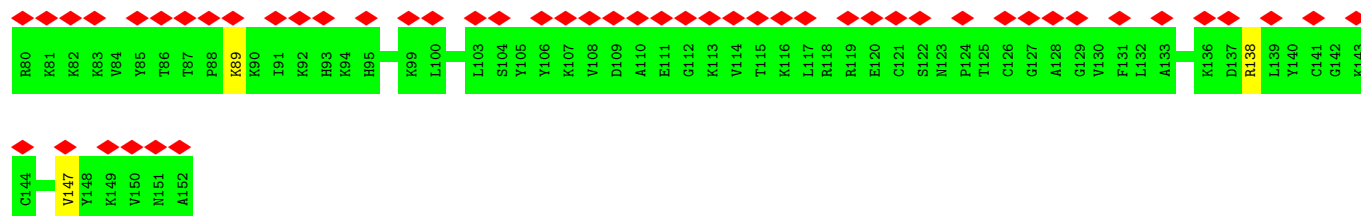
- Molecule 31: 40S ribosomal protein S29-A



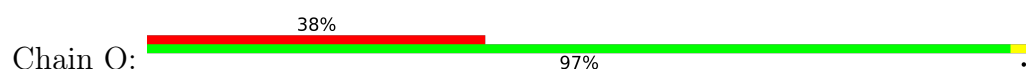
- Molecule 32: 40S ribosomal protein S30-A

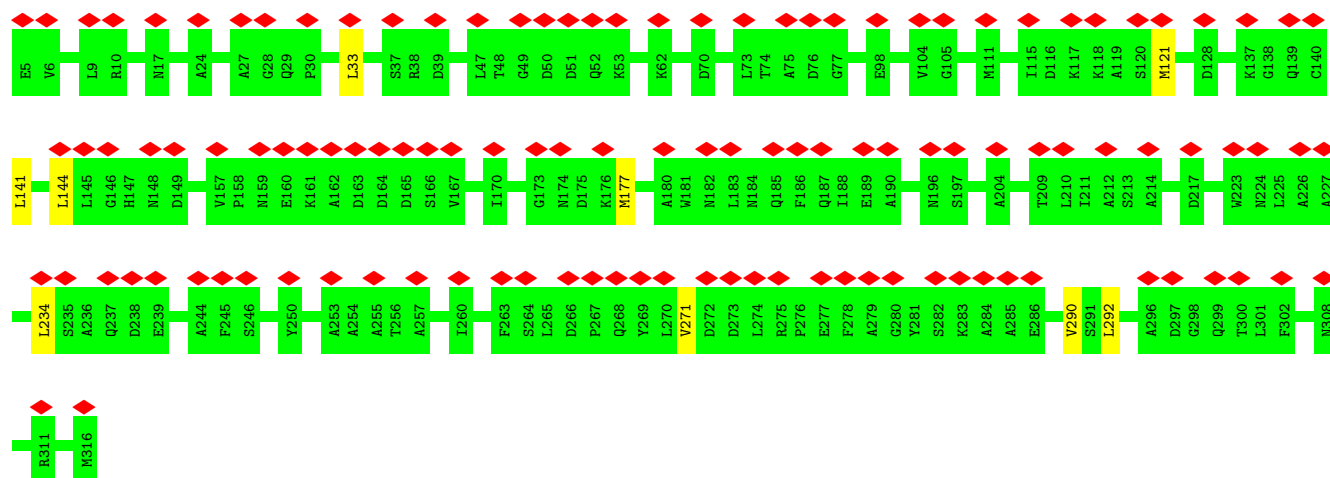


- Molecule 33: Ubiquitin-40S ribosomal protein S31

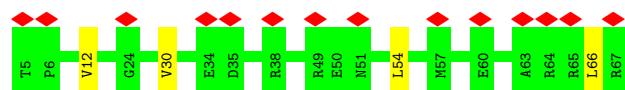


- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

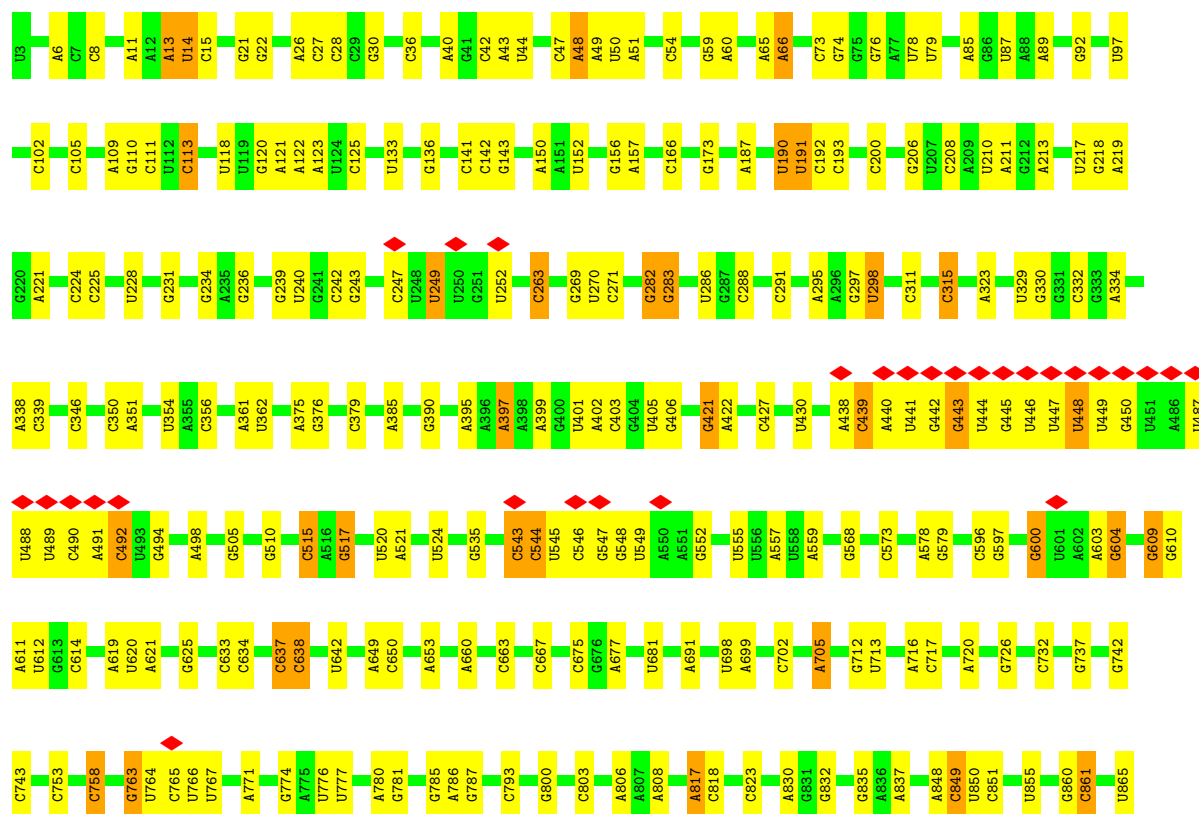




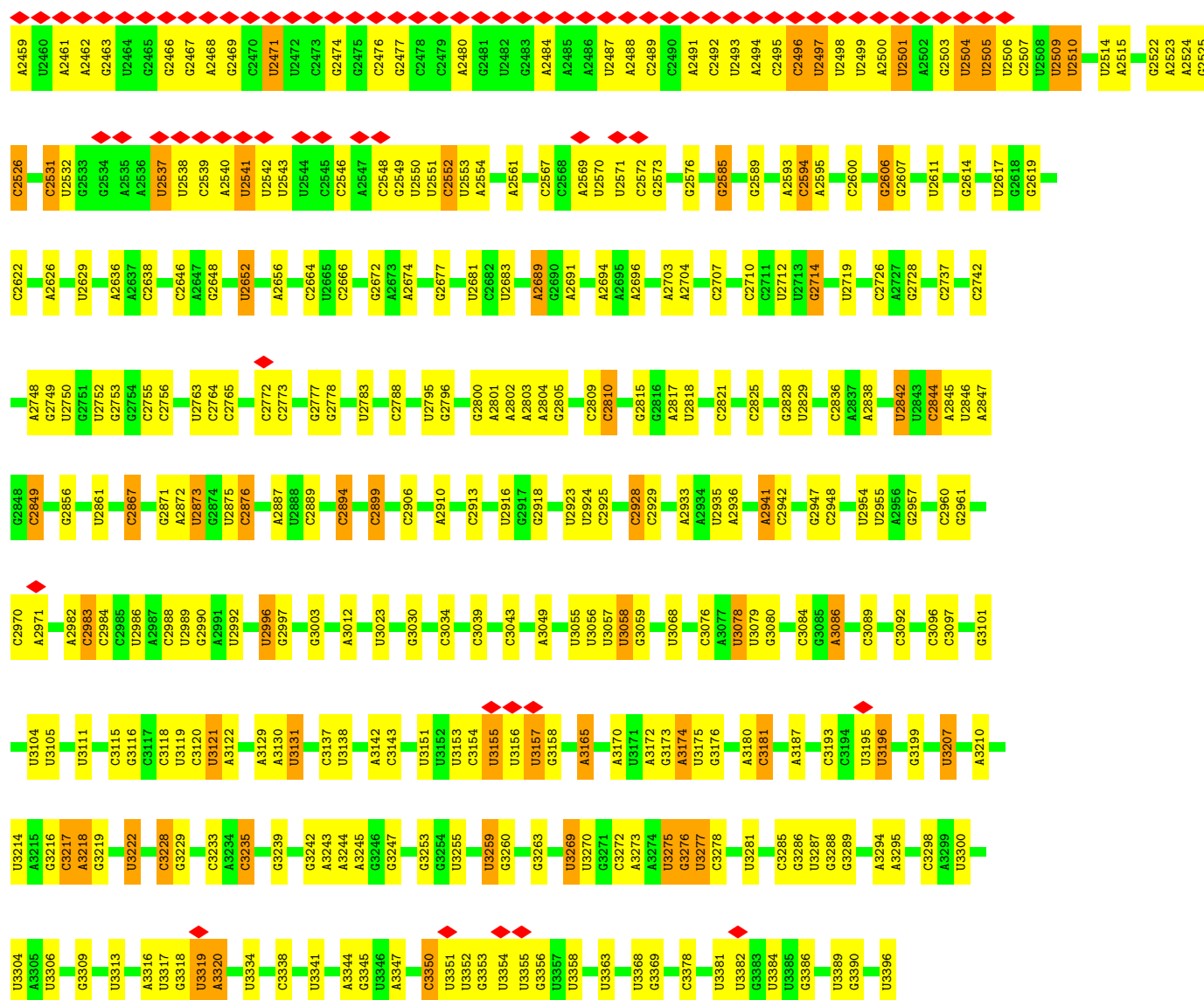
- Molecule 35: 40S ribosomal protein S28-A



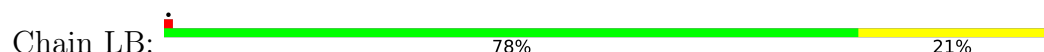
- Molecule 36: 25S rRNA



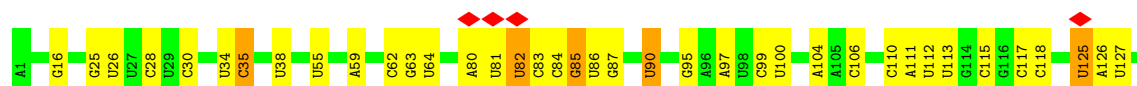


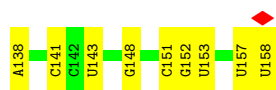


• Molecule 37: 5S rRNA



• Molecule 38: 5.8S rRNA





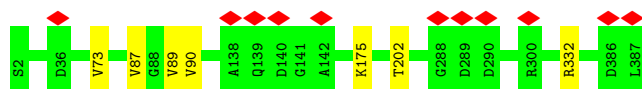
- Molecule 39: 60S ribosomal protein L2-A

Chain LD: 97%



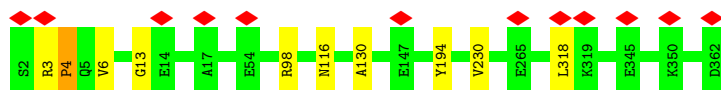
- Molecule 40: 60S ribosomal protein L3

Chain LE: 98%



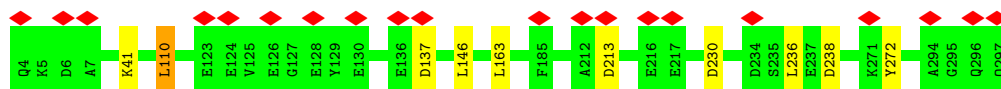
- Molecule 41: 60S ribosomal protein L4-A

Chain LF: 97%



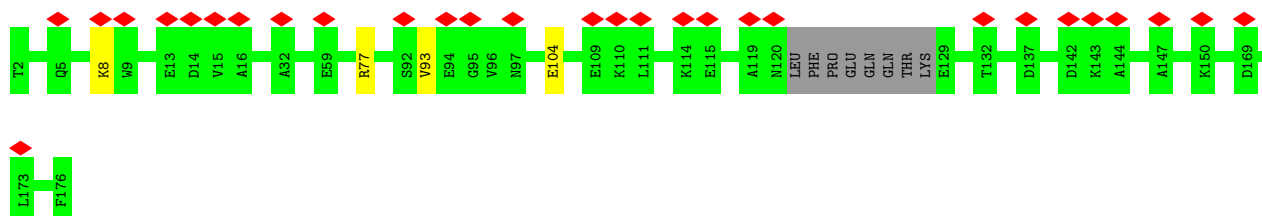
- Molecule 42: 60S ribosomal protein L5

Chain LG: 7% 97%



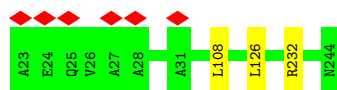
- Molecule 43: 60S ribosomal protein L6-B

Chain LH: 17% 93% 5%

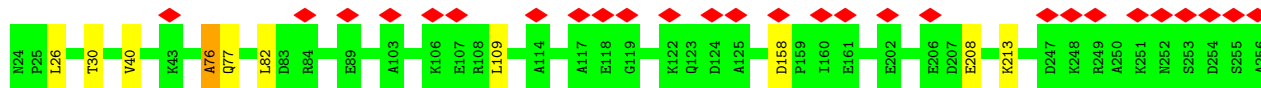


- Molecule 44: 60S ribosomal protein L7-A

Chain LI: 99%



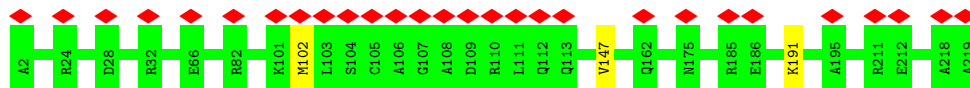
- Molecule 45: 60S ribosomal protein L8-A



- Molecule 46: 60S ribosomal protein L9-A



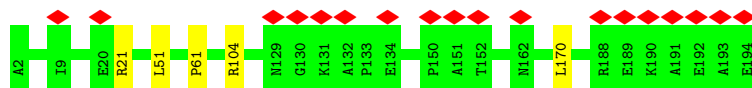
- Molecule 47: 60S ribosomal protein L10



- Molecule 48: 60S ribosomal protein L11-B



- Molecule 49: 60S ribosomal protein L13-A

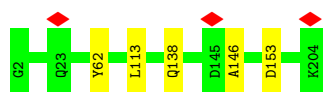


- Molecule 50: 60S ribosomal protein L14-A



- Molecule 51: 60S ribosomal protein L15-A

Chain LP:  98%



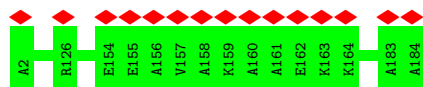
- Molecule 52: 60S ribosomal protein L16-A

Chain LQ:  99%



- Molecule 53: 60S ribosomal protein L17-A

Chain LR:  100%



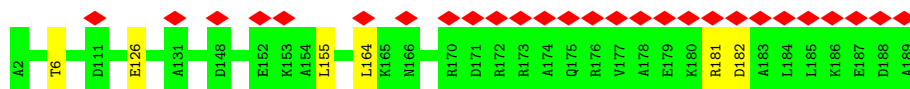
- Molecule 54: 60S ribosomal protein L18-A

Chain Lm:  95% 5%



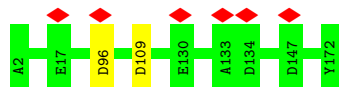
- Molecule 55: 60S ribosomal protein L19-A

Chain Ln:  97% 14%



- Molecule 56: 60S ribosomal protein L20-A

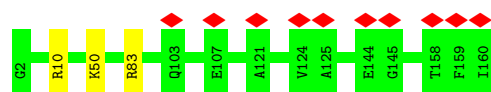
Chain Lo:  99%



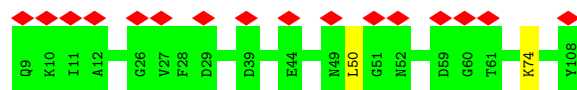
- Molecule 57: 60S ribosomal protein L21-A

Chain Lp:  98% 6%

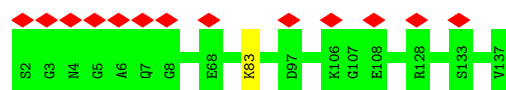




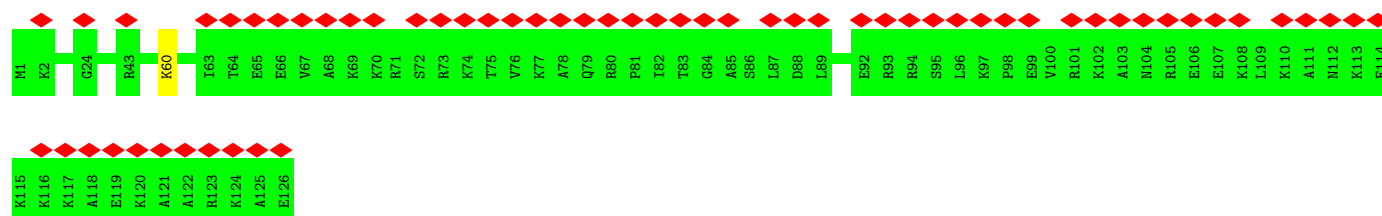
- Molecule 58: 60S ribosomal protein L22-A



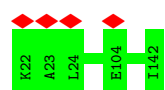
- Molecule 59: 60S ribosomal protein L23-A



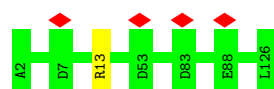
- Molecule 60: 60S ribosomal protein L24-A



- Molecule 61: 60S ribosomal protein L25

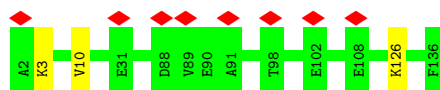


- Molecule 62: 60S ribosomal protein L26-A



- Molecule 63: 60S ribosomal protein L27-A

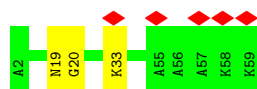




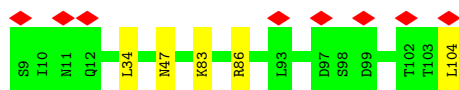
- Molecule 64: 60S ribosomal protein L28



- Molecule 65: 60S ribosomal protein L29



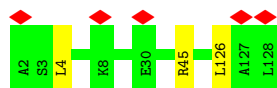
- Molecule 66: 60S ribosomal protein L30



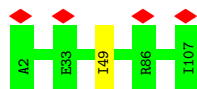
- Molecule 67: 60S ribosomal protein L31-A



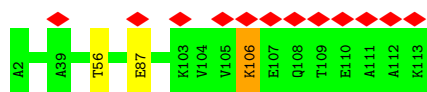
- Molecule 68: 60S ribosomal protein L32



- Molecule 69: 60S ribosomal protein L33-A



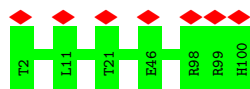
- Molecule 70: 60S ribosomal protein L34-A



- Molecule 71: 60S ribosomal protein L35-A



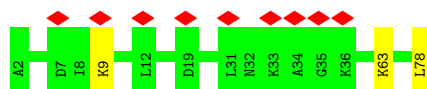
- Molecule 72: 60S ribosomal protein L36-A



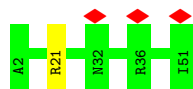
- Molecule 73: 60S ribosomal protein L37-A



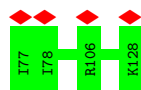
- Molecule 74: 60S ribosomal protein L38



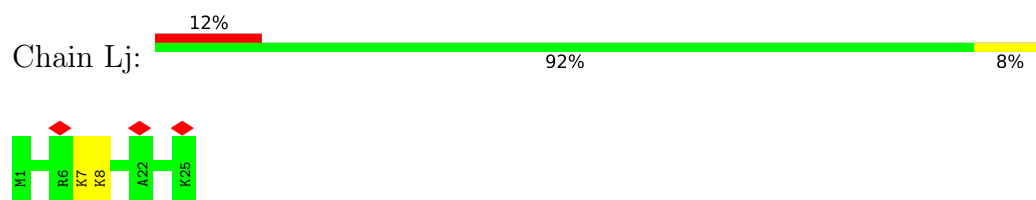
- Molecule 75: 60S ribosomal protein L39



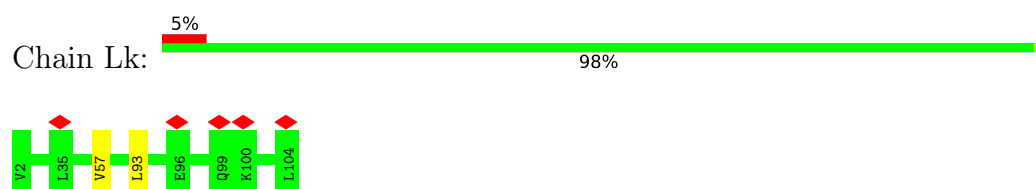
- Molecule 76: Ubiquitin-60S ribosomal protein L40



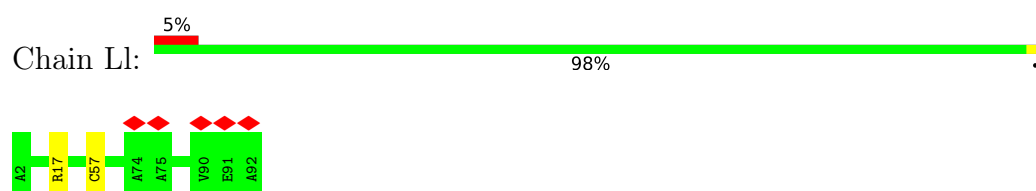
- Molecule 77: 60S ribosomal protein L41-B



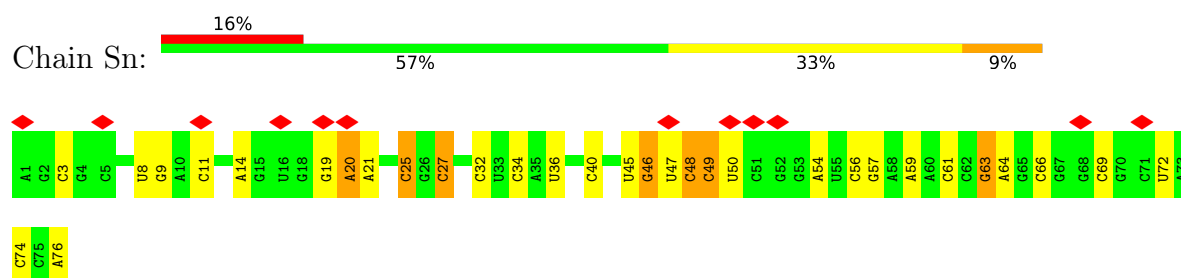
- Molecule 78: 60S ribosomal protein L42-A



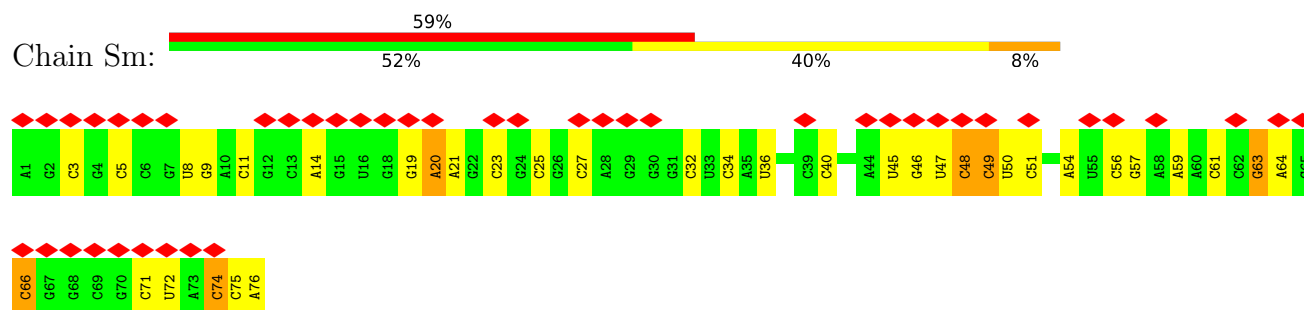
- Molecule 79: 60S ribosomal protein L43-A



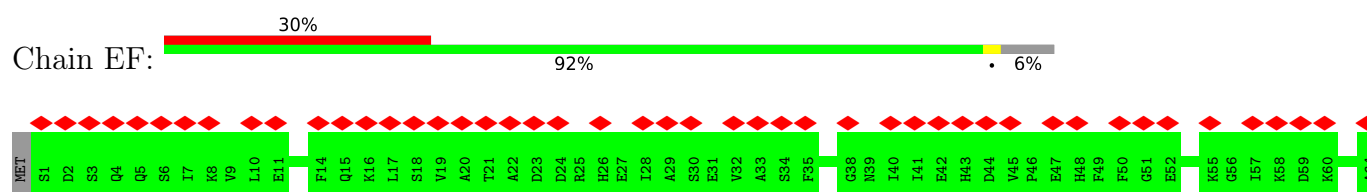
- Molecule 80: tRNA



- Molecule 80: tRNA



- Molecule 81: Elongation factor 3A





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.391	Depositor
Minimum map value	-0.234	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.04	Depositor
Map size ( $\text{\AA}$ )	455.28, 455.28, 455.28	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.084, 1.084, 1.084	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	2	0.83	1/42211 (0.0%)	1.38	575/65773 (0.9%)
2	1	0.68	0/166	1.03	0/256
3	P	0.47	1/1644 (0.1%)	0.80	1/2249 (0.0%)
4	Q	0.45	0/1823	0.90	1/2447 (0.0%)
5	E	0.54	0/936	1.02	8/1259 (0.6%)
6	R	0.51	1/1656 (0.1%)	0.84	0/2251
7	A	0.47	0/1754	0.97	5/2361 (0.2%)
8	S	0.43	0/2097	0.89	3/2823 (0.1%)
9	B	0.45	0/1625	0.86	3/2197 (0.1%)
10	T	0.39	0/1839	0.85	0/2460
11	U	0.43	0/1498	0.91	7/2019 (0.3%)
12	V	0.45	0/1501	0.85	3/2006 (0.1%)
13	W	0.41	0/1504	0.87	2/2016 (0.1%)
14	C	0.53	0/769	0.90	1/1039 (0.1%)
15	X	0.48	0/1168	0.80	1/1575 (0.1%)
16	D	0.47	1/883 (0.1%)	1.07	7/1199 (0.6%)
17	Y	0.50	0/1215	0.85	2/1638 (0.1%)
18	Z	0.51	0/934	0.95	5/1257 (0.4%)
19	F	0.56	0/1125	0.96	4/1510 (0.3%)
20	G	0.44	0/957	0.91	4/1283 (0.3%)
21	H	0.49	0/1207	0.93	3/1623 (0.2%)
22	I	0.57	0/1130	0.95	2/1517 (0.1%)
23	J	0.53	0/807	0.89	1/1091 (0.1%)
24	a	0.47	0/682	0.85	1/921 (0.1%)
25	b	0.48	0/1038	0.87	2/1395 (0.1%)
26	c	0.48	0/1139	0.87	0/1518
27	d	0.42	0/1087	0.88	1/1449 (0.1%)
28	K	0.46	0/661	0.96	1/888 (0.1%)
29	e	0.50	0/778	0.87	0/1042
30	f	0.41	0/620	0.90	1/838 (0.1%)
31	M	0.54	0/452	0.88	0/600
32	g	0.42	0/480	0.92	1/639 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	N	0.40	0/567	0.92	0/764
34	O	0.43	0/2436	0.91	5/3318 (0.2%)
35	L	0.56	1/493 (0.2%)	1.21	2/663 (0.3%)
36	LA	1.06	8/77157 (0.0%)	1.32	878/120295 (0.7%)
37	LB	0.97	0/2883	1.28	23/4491 (0.5%)
38	LC	1.01	0/3746	1.26	31/5832 (0.5%)
39	LD	0.64	1/1933 (0.1%)	0.87	3/2598 (0.1%)
40	LE	0.58	1/3146 (0.0%)	0.82	1/4228 (0.0%)
41	LF	0.55	1/2800 (0.0%)	0.81	1/3790 (0.0%)
42	LG	0.57	0/2400	0.91	12/3239 (0.4%)
43	LH	0.48	0/1329	0.87	1/1794 (0.1%)
44	LI	0.58	1/1821 (0.1%)	0.77	1/2451 (0.0%)
45	LJ	0.56	1/1836 (0.1%)	0.84	4/2481 (0.2%)
46	LK	0.56	0/1529	0.93	4/2060 (0.2%)
47	LL	0.55	0/1801	0.83	1/2416 (0.0%)
48	LM	0.53	0/1367	0.90	4/1834 (0.2%)
49	LN	0.55	0/1568	0.80	2/2106 (0.1%)
50	LO	0.48	0/1068	0.82	1/1438 (0.1%)
51	LP	0.67	0/1757	0.83	1/2354 (0.0%)
52	LQ	0.54	0/1585	0.78	1/2128 (0.0%)
53	LR	0.56	0/1439	0.79	0/1938
54	Lm	0.56	0/1465	0.88	4/1965 (0.2%)
55	Ln	0.53	0/1532	0.83	4/2043 (0.2%)
56	Lo	0.56	0/1473	0.80	1/1980 (0.1%)
57	Lp	0.60	0/1296	0.83	0/1739
58	Lq	0.52	0/812	0.81	1/1099 (0.1%)
59	Lr	0.55	0/1018	0.86	1/1369 (0.1%)
60	LS	0.44	0/850	0.70	0/1152
61	LT	0.59	0/979	0.81	0/1321
62	LU	0.50	0/995	0.76	0/1329
63	LV	0.54	1/1106 (0.1%)	0.78	0/1485
64	LW	0.59	0/1200	0.81	1/1607 (0.1%)
65	LX	0.48	0/473	0.71	0/629
66	LY	0.52	0/745	0.79	2/1001 (0.2%)
67	LZ	0.55	0/890	0.81	0/1196
68	La	0.50	0/1034	0.78	1/1385 (0.1%)
69	Lb	0.62	0/868	0.88	1/1168 (0.1%)
70	Lc	0.63	0/890	0.85	1/1189 (0.1%)
71	Ld	0.47	0/978	0.75	1/1301 (0.1%)
72	Le	0.46	0/772	0.76	0/1026
73	Lf	0.68	0/660	0.93	1/875 (0.1%)
74	Lg	0.50	0/618	0.86	1/826 (0.1%)
75	Lh	0.57	0/443	0.93	0/588



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	Li	0.55	0/416	0.82	0/553
77	Lj	0.48	0/230	0.75	0/296
78	Lk	0.58	0/836	0.84	1/1104 (0.1%)
79	Ll	0.66	0/701	0.72	0/934
80	Sm	0.58	0/1795	1.43	32/2797 (1.1%)
80	Sn	0.70	0/1796	1.52	35/2799 (1.3%)
81	EF	0.37	0/7610	0.66	7/10311 (0.1%)
All	All	0.81	19/226528 (0.0%)	1.17	1716/332424 (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
8	S	0	1
9	B	0	2
11	U	0	1
16	D	0	1
19	F	0	1
25	b	0	1
33	N	0	1
36	LA	0	1
41	LF	0	3
44	LI	0	1
45	LJ	0	3
54	Lm	0	1
64	LW	0	2
65	LX	0	2
66	LY	0	1
67	LZ	0	1
71	Ld	0	1
81	EF	0	6
All	All	0	30

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	60	SER	C-N	-6.79	1.18	1.34
45	LJ	40	VAL	C-N	-6.67	1.18	1.34
35	L	12	VAL	CB-CG1	-6.55	1.39	1.52
36	LA	1263	A	N9-C4	6.33	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1471	A	N9-C4	-6.24	1.34	1.37
63	LV	10	VAL	CB-CG1	-6.18	1.39	1.52
40	LE	73	VAL	CB-CG1	-5.80	1.40	1.52
39	LD	149	ARG	C-N	-5.58	1.21	1.34
36	LA	1330	A	N9-C4	-5.56	1.34	1.37
36	LA	361	A	N9-C4	-5.51	1.34	1.37
36	LA	361	A	N7-C5	-5.47	1.35	1.39
36	LA	1103	A	N9-C4	5.40	1.41	1.37
41	LF	230	VAL	CB-CG2	-5.34	1.41	1.52
36	LA	2714	G	N9-C4	-5.33	1.33	1.38
36	LA	66	A	N9-C4	-5.32	1.34	1.37
36	LA	860	G	C2-N3	-5.26	1.28	1.32
3	P	197	ILE	C-N	-5.25	1.22	1.34
44	LI	108	LEU	CA-CB	-5.16	1.41	1.53
16	D	81	ASP	C-N	5.09	1.44	1.34

All (1716) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	LA	3217	C	C2-N1-C1'	12.76	132.83	118.80
80	Sn	48	C	C6-N1-C2	-12.56	115.28	120.30
80	Sn	49	C	C6-N1-C2	-12.37	115.35	120.30
1	2	934	C	C2-N1-C1'	12.16	132.18	118.80
80	Sm	49	C	C6-N1-C2	-12.03	115.49	120.30
36	LA	837	A	O5'-P-OP2	-12.01	94.89	105.70
36	LA	2928	C	C6-N1-C2	-11.88	115.55	120.30
36	LA	3217	C	N1-C2-O2	11.85	126.01	118.90
7	A	218	LEU	CA-CB-CG	11.43	141.58	115.30
36	LA	1273	A	C8-N9-C4	-11.40	101.24	105.80
35	L	54	LEU	CA-CB-CG	11.18	141.01	115.30
35	L	66	LEU	CA-CB-CG	11.01	140.62	115.30
80	Sn	49	C	C5-C6-N1	10.92	126.46	121.00
1	2	555	A	N7-C8-N9	10.89	119.25	113.80
36	LA	14	U	O5'-P-OP2	-10.80	95.98	105.70
36	LA	1283	C	N1-C2-O2	10.76	125.35	118.90
1	2	1032	G	O5'-P-OP2	-10.72	96.05	105.70
36	LA	2928	C	C5-C6-N1	10.71	126.36	121.00
80	Sm	48	C	C6-N1-C2	-10.63	116.05	120.30
1	2	186	C	C2-N1-C1'	10.62	130.49	118.80
1	2	555	A	C8-N9-C4	-10.38	101.65	105.80
7	A	14	ASP	CB-CG-OD1	10.36	127.62	118.30
36	LA	1283	C	N3-C2-O2	-10.35	114.65	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	Sn	48	C	N1-C2-O2	10.33	125.10	118.90
36	LA	2846	U	N3-C2-O2	-10.15	115.09	122.20
80	Sn	48	C	N3-C2-O2	-10.12	114.82	121.90
36	LA	2366	C	C6-N1-C2	-10.12	116.25	120.30
1	2	874	C	C6-N1-C2	-10.00	116.30	120.30
1	2	1257	U	N3-C2-O2	-9.87	115.29	122.20
36	LA	922	U	C2-N1-C1'	9.87	129.55	117.70
1	2	934	C	N1-C2-O2	9.83	124.80	118.90
36	LA	3306	U	N3-C2-O2	-9.83	115.32	122.20
37	LB	34	C	C6-N1-C2	-9.81	116.38	120.30
36	LA	596	C	C6-N1-C2	-9.74	116.40	120.30
1	2	1258	U	N3-C2-O2	-9.70	115.41	122.20
1	2	1389	C	C2-N1-C1'	9.58	129.34	118.80
1	2	934	C	C6-N1-C1'	-9.52	109.38	120.80
36	LA	3344	A	O4'-C1'-N9	9.43	115.75	108.20
36	LA	3275	U	OP1-P-O3'	9.42	125.92	105.20
46	LK	107	ASP	CB-CG-OD1	9.41	126.77	118.30
80	Sm	49	C	C5-C6-N1	9.40	125.70	121.00
36	LA	3181	C	C2-N1-C1'	9.38	129.12	118.80
36	LA	3317	U	N1-C2-O2	9.36	129.35	122.80
1	2	965	U	N1-C2-O2	9.35	129.34	122.80
36	LA	3217	C	C6-N1-C1'	-9.34	109.60	120.80
80	Sm	48	C	N1-C2-O2	9.31	124.49	118.90
36	LA	2531	C	C6-N1-C2	-9.25	116.60	120.30
54	Lm	66	ARG	NE-CZ-NH2	-9.25	115.68	120.30
36	LA	3278	C	N3-C2-O2	-9.24	115.43	121.90
80	Sm	48	C	N3-C2-O2	-9.24	115.44	121.90
1	2	861	U	C2-N1-C1'	9.22	128.77	117.70
7	A	93	ASP	CB-CG-OD1	9.20	126.58	118.30
36	LA	15	C	C6-N1-C2	-9.11	116.66	120.30
1	2	1258	U	N1-C2-O2	9.10	129.17	122.80
1	2	1560	U	N3-C2-O2	-9.09	115.84	122.20
36	LA	2263	C	C5-C6-N1	9.08	125.54	121.00
38	LC	64	U	N3-C2-O2	-9.08	115.85	122.20
1	2	1082	C	C6-N1-C2	-9.07	116.67	120.30
36	LA	1279	C	C6-N1-C2	-9.07	116.67	120.30
36	LA	3317	U	N3-C2-O2	-9.04	115.87	122.20
1	2	590	C	C6-N1-C2	-9.03	116.69	120.30
36	LA	2526	C	C5-C6-N1	9.03	125.51	121.00
36	LA	282	G	C8-N9-C4	-9.02	102.79	106.40
38	LC	127	U	N1-C2-O2	9.02	129.11	122.80
1	2	116	U	N3-C2-O2	-8.98	115.92	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	I	35	ASP	CB-CG-OD1	8.97	126.37	118.30
36	LA	544	C	N3-C2-O2	-8.96	115.63	121.90
36	LA	2446	U	C5-C6-N1	8.96	127.18	122.70
7	A	191	ASP	CB-CG-OD1	8.95	126.35	118.30
1	2	1389	C	N1-C2-O2	8.89	124.24	118.90
1	2	965	U	C2-N1-C1'	8.88	128.35	117.70
1	2	1585	U	N1-C2-O2	8.88	129.01	122.80
36	LA	2617	U	N3-C2-O2	-8.87	116.00	122.20
1	2	1235	C	C6-N1-C2	-8.84	116.77	120.30
5	E	36	LEU	CA-CB-CG	8.80	135.55	115.30
1	2	1527	C	C2-N1-C1'	8.77	128.44	118.80
1	2	1585	U	C2-N3-C4	8.75	132.25	127.00
37	LB	39	C	N3-C2-O2	-8.75	115.78	121.90
48	LM	168	ASP	CB-CG-OD1	8.70	126.13	118.30
36	LA	2359	C	C5-C6-N1	8.68	125.34	121.00
38	LC	127	U	N3-C2-O2	-8.68	116.12	122.20
37	LB	34	C	C5-C6-N1	8.67	125.34	121.00
46	LK	76	ASP	CB-CG-OD1	8.66	126.10	118.30
36	LA	609	G	O5'-P-OP2	-8.64	97.92	105.70
36	LA	3120	C	C6-N1-C2	-8.64	116.84	120.30
36	LA	1496	C	C6-N1-C2	-8.64	116.84	120.30
36	LA	2146	C	C6-N1-C2	-8.64	116.84	120.30
1	2	1161	C	C5-C6-N1	8.64	125.32	121.00
36	LA	1854	C	C6-N1-C2	-8.63	116.85	120.30
36	LA	2112	U	P-O3'-C3'	8.63	130.06	119.70
36	LA	1614	C	C6-N1-C2	-8.63	116.85	120.30
1	2	1082	C	C2-N1-C1'	8.60	128.26	118.80
36	LA	2366	C	C5-C6-N1	8.60	125.30	121.00
42	LG	230	ASP	CB-CG-OD1	8.60	126.04	118.30
36	LA	2772	C	C2-N1-C1'	8.56	128.22	118.80
1	2	583	C	C2-N1-C1'	8.54	128.20	118.80
1	2	283	U	N3-C2-O2	-8.52	116.23	122.20
36	LA	2541	U	P-O3'-C3'	8.52	129.92	119.70
36	LA	1499	C	C6-N1-C2	-8.49	116.90	120.30
36	LA	1227	C	N1-C2-O2	8.49	124.00	118.90
1	2	160	C	N1-C2-O2	8.48	123.99	118.90
16	D	36	LEU	CA-CB-CG	8.47	134.78	115.30
36	LA	927	C	C6-N1-C2	-8.46	116.92	120.30
1	2	500	C	N3-C2-O2	-8.44	115.99	121.90
36	LA	1269	U	C2-N1-C1'	8.43	127.82	117.70
27	d	39	GLU	CA-CB-CG	8.42	131.92	113.40
36	LA	3181	C	N1-C2-O2	8.41	123.95	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	186	C	N1-C2-O2	8.41	123.95	118.90
1	2	1145	U	C2-N1-C1'	8.37	127.74	117.70
1	2	645	C	C6-N1-C2	-8.36	116.95	120.30
1	2	959	U	N3-C2-O2	-8.35	116.35	122.20
36	LA	1907	C	N1-C2-O2	8.35	123.91	118.90
36	LA	2836	C	N3-C2-O2	-8.35	116.06	121.90
1	2	992	A	O4'-C1'-N9	8.33	114.86	108.20
37	LB	39	C	N1-C2-O2	8.32	123.89	118.90
36	LA	2531	C	N1-C2-O2	8.32	123.89	118.90
36	LA	2537	U	P-O3'-C3'	8.31	129.67	119.70
1	2	538	A	O5'-P-OP2	-8.29	98.23	105.70
36	LA	1349	G	N3-C4-C5	-8.29	124.45	128.60
1	2	1458	G	C4-N9-C1'	8.29	137.27	126.50
36	LA	2434	U	C2-N1-C1'	8.28	127.64	117.70
36	LA	1269	U	N1-C2-O2	8.27	128.59	122.80
80	Sn	48	C	C5-C6-N1	8.27	125.14	121.00
1	2	656	G	C4-N9-C1'	8.26	137.24	126.50
1	2	1560	U	C2-N1-C1'	8.26	127.61	117.70
37	LB	68	C	C6-N1-C2	-8.26	117.00	120.30
36	LA	1496	C	C5-C6-N1	8.25	125.13	121.00
36	LA	1788	C	C6-N1-C2	-8.25	117.00	120.30
36	LA	2133	U	N3-C2-O2	-8.25	116.42	122.20
1	2	322	G	P-O3'-C3'	8.24	129.59	119.70
8	S	38	LEU	CA-CB-CG	8.23	134.23	115.30
36	LA	2277	C	C6-N1-C2	-8.22	117.01	120.30
1	2	1463	C	C6-N1-C2	-8.22	117.01	120.30
1	2	927	C	C6-N1-C2	-8.21	117.02	120.30
36	LA	2552	C	N1-C2-O2	8.21	123.82	118.90
36	LA	3278	C	N1-C2-O2	8.18	123.81	118.90
36	LA	3217	C	N3-C2-O2	-8.17	116.18	121.90
36	LA	225	C	C6-N1-C2	-8.16	117.03	120.30
36	LA	1269	U	N3-C2-O2	-8.16	116.49	122.20
36	LA	2163	C	C6-N1-C2	-8.15	117.04	120.30
1	2	992	A	C4-N9-C1'	8.14	140.96	126.30
1	2	1742	U	C5-C6-N1	8.14	126.77	122.70
36	LA	1604	G	N3-C4-N9	8.14	130.89	126.00
1	2	965	U	N3-C2-O2	-8.13	116.51	122.20
36	LA	1872	C	N1-C2-O2	8.12	123.77	118.90
36	LA	2531	C	C5-C6-N1	8.11	125.05	121.00
1	2	553	G	N3-C4-N9	-8.09	121.14	126.00
1	2	886	U	C5-C6-N1	8.09	126.75	122.70
36	LA	1907	C	N3-C2-O2	-8.08	116.24	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	LA	1155	C	C5-C6-N1	8.07	125.04	121.00
1	2	583	C	C6-N1-C2	-8.07	117.07	120.30
36	LA	2836	C	C2-N1-C1'	8.07	127.68	118.80
36	LA	2434	U	N3-C2-O2	-8.06	116.56	122.20
36	LA	3196	U	C2-N1-C1'	8.06	127.37	117.70
36	LA	1349	G	C4-N9-C1'	8.03	136.94	126.50
36	LA	3217	C	C5-C6-N1	8.03	125.01	121.00
36	LA	3306	U	C2-N1-C1'	8.03	127.33	117.70
36	LA	717	C	O5'-P-OP2	-8.02	98.48	105.70
20	G	84	TYR	CB-CG-CD2	8.02	125.81	121.00
36	LA	1716	U	P-O3'-C3'	8.02	129.32	119.70
36	LA	1263	A	C2-N3-C4	8.00	114.60	110.60
36	LA	2666	C	C6-N1-C2	-8.00	117.10	120.30
36	LA	1496	C	C2-N1-C1'	8.00	127.60	118.80
42	LG	238	ASP	CB-CG-OD1	7.99	125.49	118.30
1	2	424	C	C5-C6-N1	7.97	124.99	121.00
36	LA	1349	G	N3-C4-N9	7.96	130.78	126.00
36	LA	1579	C	N3-C2-O2	-7.94	116.34	121.90
38	LC	127	U	C2-N1-C1'	7.93	127.22	117.70
42	LG	272	TYR	CB-CG-CD1	-7.93	116.24	121.00
36	LA	2873	U	N3-C2-O2	-7.90	116.67	122.20
36	LA	2101	C	P-O3'-C3'	7.89	129.17	119.70
36	LA	2664	C	C6-N1-C2	-7.88	117.15	120.30
36	LA	969	C	C6-N1-C2	-7.88	117.15	120.30
80	Sn	56	C	C6-N1-C2	-7.88	117.15	120.30
36	LA	3214	U	C2-N1-C1'	7.87	127.14	117.70
1	2	1161	C	C6-N1-C2	-7.87	117.15	120.30
36	LA	890	C	C6-N1-C2	-7.86	117.16	120.30
1	2	1257	U	N1-C2-O2	7.85	128.30	122.80
36	LA	977	C	C6-N1-C2	-7.84	117.16	120.30
36	LA	2285	C	C6-N1-C2	-7.84	117.17	120.30
1	2	572	C	N3-C2-O2	-7.83	116.42	121.90
80	Sn	63	G	OP1-P-O3'	7.83	122.42	105.20
1	2	1182	U	C2-N1-C1'	7.82	127.08	117.70
38	LC	64	U	N1-C2-O2	7.82	128.27	122.80
1	2	959	U	C2-N1-C1'	7.82	127.08	117.70
1	2	1332	C	C6-N1-C2	-7.79	117.18	120.30
80	Sn	69	C	C6-N1-C2	-7.79	117.19	120.30
36	LA	758	C	C6-N1-C2	-7.78	117.19	120.30
36	LA	492	C	C6-N1-C2	-7.77	117.19	120.30
36	LA	2422	C	C6-N1-C2	-7.76	117.20	120.30
36	LA	36	C	N3-C2-O2	-7.75	116.47	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	LA	2277	C	C5-C6-N1	7.74	124.87	121.00
1	2	1458	G	N3-C4-C5	-7.74	124.73	128.60
36	LA	2652	U	N3-C2-O2	-7.74	116.78	122.20
36	LA	1495	U	C4-C5-C6	7.73	124.34	119.70
20	G	84	TYR	CB-CG-CD1	-7.71	116.38	121.00
1	2	1560	U	N1-C2-O2	7.69	128.18	122.80
1	2	992	A	N7-C8-N9	7.69	117.64	113.80
36	LA	36	C	N1-C2-O2	7.68	123.51	118.90
36	LA	2285	C	C5-C6-N1	7.68	124.84	121.00
1	2	354	C	C6-N1-C2	-7.67	117.23	120.30
36	LA	977	C	C5-C6-N1	7.67	124.83	121.00
36	LA	332	C	C6-N1-C2	-7.66	117.24	120.30
1	2	639	U	P-O3'-C3'	7.66	128.89	119.70
36	LA	2815	G	N1-C6-O6	-7.65	115.31	119.90
36	LA	2531	C	C2-N1-C1'	7.65	127.21	118.80
1	2	849	C	C6-N1-C2	-7.64	117.25	120.30
36	LA	15	C	C5-C6-N1	7.63	124.82	121.00
11	U	131	PHE	CB-CG-CD2	7.63	126.14	120.80
1	2	945	U	C5-C6-N1	7.62	126.51	122.70
1	2	1374	C	C6-N1-C2	-7.62	117.25	120.30
36	LA	2389	C	C6-N1-C2	-7.62	117.25	120.30
38	LC	28	C	C6-N1-C2	-7.62	117.25	120.30
36	LA	1279	C	C5-C6-N1	7.60	124.80	121.00
1	2	1527	C	N1-C2-O2	7.60	123.46	118.90
36	LA	78	U	N3-C2-O2	-7.60	116.88	122.20
1	2	1463	C	C5-C6-N1	7.59	124.79	121.00
36	LA	515	C	C6-N1-C2	-7.58	117.27	120.30
36	LA	609	G	N3-C4-N9	7.58	130.55	126.00
36	LA	2505	U	N3-C2-O2	-7.57	116.90	122.20
37	LB	44	C	C6-N1-C2	-7.57	117.27	120.30
36	LA	3120	C	C5-C6-N1	7.56	124.78	121.00
36	LA	2263	C	C6-N1-C2	-7.55	117.28	120.30
36	LA	515	C	C5-C6-N1	7.55	124.78	121.00
36	LA	3344	A	N7-C8-N9	7.54	117.57	113.80
1	2	1256	A	P-O3'-C3'	7.53	128.73	119.70
11	U	131	PHE	CB-CG-CD1	-7.53	115.53	120.80
36	LA	492	C	N1-C2-O2	7.52	123.41	118.90
36	LA	1756	C	C5-C6-N1	7.52	124.76	121.00
36	LA	2098	C	C6-N1-C2	-7.51	117.29	120.30
1	2	186	C	C6-N1-C1'	-7.51	111.79	120.80
36	LA	1815	U	P-O3'-C3'	7.50	128.70	119.70
36	LA	3120	C	O5'-P-OP2	-7.50	98.95	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1705	C	C6-N1-C2	-7.50	117.30	120.30
80	Sn	46	G	C8-N9-C4	-7.50	103.40	106.40
36	LA	3218	A	OP2-P-O3'	7.48	121.66	105.20
36	LA	927	C	C5-C6-N1	7.47	124.74	121.00
36	LA	3317	U	C2-N1-C1'	7.47	126.67	117.70
1	2	400	A	P-O3'-C3'	7.47	128.66	119.70
1	2	166	C	N1-C2-O2	7.46	123.38	118.90
36	LA	2849	C	C6-N1-C2	-7.45	117.32	120.30
1	2	934	C	N3-C2-O2	-7.43	116.70	121.90
36	LA	2983	C	C6-N1-C2	-7.42	117.33	120.30
36	LA	379	C	C6-N1-C2	-7.42	117.33	120.30
1	2	959	U	N1-C2-O2	7.42	127.99	122.80
1	2	1705	C	C5-C6-N1	7.41	124.70	121.00
1	2	1528	U	O5'-P-OP2	-7.41	99.03	105.70
36	LA	1563	C	C6-N1-C2	-7.41	117.34	120.30
5	E	60	LEU	CB-CG-CD1	-7.40	98.41	111.00
1	2	969	C	C6-N1-C2	-7.40	117.34	120.30
36	LA	544	C	C6-N1-C2	-7.40	117.34	120.30
36	LA	2359	C	C6-N1-C2	-7.39	117.34	120.30
38	LC	110	C	N1-C2-O2	7.39	123.33	118.90
54	Lm	66	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	2	189	C	C6-N1-C2	-7.38	117.35	120.30
80	Sn	69	C	C5-C6-N1	7.38	124.69	121.00
1	2	1382	A	P-O3'-C3'	7.38	128.55	119.70
1	2	1633	A	P-O3'-C3'	7.38	128.55	119.70
36	LA	2873	U	C2-N1-C1'	7.37	126.55	117.70
36	LA	1604	G	C4-N9-C1'	7.37	136.08	126.50
1	2	819	G	P-O3'-C3'	7.36	128.53	119.70
1	2	215	A	P-O3'-C3'	7.35	128.52	119.70
36	LA	2495	C	N1-C2-O2	7.35	123.31	118.90
36	LA	439	C	N3-C2-O2	-7.35	116.76	121.90
36	LA	3078	U	OP2-P-O3'	7.34	121.35	105.20
36	LA	524	U	N1-C2-O2	7.34	127.94	122.80
1	2	629	U	N3-C2-O2	-7.33	117.07	122.20
1	2	1611	A	O4'-C1'-N9	7.33	114.06	108.20
36	LA	1608	C	N1-C2-O2	7.33	123.30	118.90
36	LA	3217	C	C6-N1-C2	-7.33	117.37	120.30
1	2	969	C	C5-C6-N1	7.32	124.66	121.00
36	LA	2496	C	N1-C2-O2	7.32	123.29	118.90
80	Sn	50	U	O5'-P-OP2	-7.32	99.12	105.70
36	LA	263	C	C6-N1-C2	-7.31	117.38	120.30
36	LA	2133	U	N1-C2-O2	7.31	127.91	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	LA	1869	C	C5-C6-N1	7.30	124.65	121.00
1	2	262	U	N1-C2-O2	7.30	127.91	122.80
1	2	1023	A	OP2-P-O3'	7.30	121.25	105.20
1	2	1257	U	C2-N1-C1'	7.30	126.45	117.70
36	LA	663	C	C6-N1-C2	-7.30	117.38	120.30
45	LJ	109	LEU	CA-CB-CG	7.30	132.08	115.30
1	2	1273	G	P-O3'-C3'	7.29	128.45	119.70
36	LA	3058	U	C2-N1-C1'	7.29	126.44	117.70
36	LA	2237	C	N3-C2-O2	-7.28	116.80	121.90
36	LA	2407	C	C6-N1-C2	-7.28	117.39	120.30
36	LA	2846	U	N1-C2-O2	7.28	127.89	122.80
36	LA	3344	A	C5-N7-C8	-7.28	100.26	103.90
36	LA	2526	C	C6-N1-C2	-7.26	117.39	120.30
36	LA	3278	C	C2-N1-C1'	7.26	126.79	118.80
36	LA	1437	C	C6-N1-C2	-7.26	117.39	120.30
36	LA	439	C	N1-C2-O2	7.26	123.25	118.90
80	Sm	48	C	C5-C6-N1	7.26	124.63	121.00
1	2	453	U	N3-C2-O2	-7.25	117.12	122.20
1	2	354	C	C5-C6-N1	7.25	124.62	121.00
1	2	1644	C	C6-N1-C2	-7.25	117.40	120.30
1	2	656	G	N3-C4-C5	-7.25	124.98	128.60
1	2	798	C	C6-N1-C2	-7.25	117.40	120.30
1	2	637	C	C6-N1-C2	-7.24	117.40	120.30
1	2	992	A	C8-N9-C1'	-7.24	114.67	127.70
36	LA	2664	C	C5-C6-N1	7.24	124.62	121.00
38	LC	35	C	C6-N1-C2	-7.24	117.40	120.30
1	2	1309	C	C6-N1-C2	-7.23	117.41	120.30
36	LA	2846	U	C2-N1-C1'	7.22	126.36	117.70
36	LA	818	C	C6-N1-C2	-7.21	117.42	120.30
36	LA	1556	C	C2-N1-C1'	7.21	126.73	118.80
80	Sm	63	G	OP1-P-O3'	7.21	121.06	105.20
1	2	738	G	P-O3'-C3'	7.20	128.34	119.70
36	LA	2585	G	N3-C4-C5	-7.20	125.00	128.60
1	2	555	A	P-O3'-C3'	7.20	128.34	119.70
1	2	1258	U	C2-N1-C1'	7.20	126.34	117.70
1	2	1799	U	C2-N1-C1'	7.20	126.34	117.70
36	LA	1263	A	N1-C6-N6	-7.19	114.29	118.60
36	LA	1499	C	C5-C6-N1	7.18	124.59	121.00
1	2	14	C	C6-N1-C2	-7.17	117.43	120.30
36	LA	142	C	C6-N1-C2	-7.17	117.43	120.30
36	LA	2594	C	N1-C2-O2	7.17	123.20	118.90
36	LA	982	C	N1-C2-O2	7.17	123.20	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	77	U	P-O3'-C3'	7.16	128.30	119.70
36	LA	1716	U	OP1-P-O3'	7.16	120.94	105.20
1	2	1523	G	C4-N9-C1'	7.15	135.80	126.50
1	2	1024	U	C5-C6-N1	7.14	126.27	122.70
13	W	105	LEU	CB-CG-CD1	7.14	123.14	111.00
36	LA	803	C	C6-N1-C2	-7.13	117.45	120.30
16	D	39	ASP	CB-CG-OD1	7.13	124.72	118.30
1	2	1098	U	O5'-P-OP1	-7.13	99.28	105.70
37	LB	58	C	C6-N1-C2	-7.12	117.45	120.30
36	LA	1437	C	C2-N1-C1'	7.11	126.62	118.80
1	2	224	C	P-O3'-C3'	7.10	128.22	119.70
80	Sn	40	C	C6-N1-C2	-7.10	117.46	120.30
1	2	415	C	C5-C6-N1	7.09	124.55	121.00
1	2	911	U	N3-C2-O2	-7.09	117.24	122.20
36	LA	1103	A	C2-N3-C4	7.09	114.14	110.60
1	2	453	U	C5-C6-N1	7.08	126.24	122.70
36	LA	505	G	O5'-P-OP1	-7.08	99.33	105.70
38	LC	117	C	C6-N1-C2	-7.08	117.47	120.30
36	LA	1208	U	N1-C2-O2	7.06	127.75	122.80
1	2	160	C	C2-N1-C1'	7.06	126.57	118.80
36	LA	1582	C	OP1-P-O3'	7.06	120.74	105.20
80	Sm	49	C	N1-C2-O2	7.06	123.14	118.90
1	2	989	U	N1-C2-O2	7.06	127.74	122.80
36	LA	1227	C	C6-N1-C2	-7.06	117.48	120.30
36	LA	2434	U	N1-C2-O2	7.06	127.74	122.80
36	LA	3181	C	N3-C2-O2	-7.06	116.96	121.90
1	2	278	U	P-O3'-C3'	7.05	128.16	119.70
36	LA	50	U	N1-C2-O2	7.05	127.74	122.80
36	LA	1614	C	C5-C6-N1	7.05	124.53	121.00
1	2	553	G	N9-C4-C5	7.05	108.22	105.40
34	O	292	LEU	CA-CB-CG	7.05	131.52	115.30
36	LA	3277	U	N3-C2-O2	-7.05	117.26	122.20
36	LA	793	C	C6-N1-C2	-7.05	117.48	120.30
36	LA	1495	U	N1-C2-N3	7.05	119.13	114.90
1	2	160	C	N3-C2-O2	-7.04	116.97	121.90
36	LA	1273	A	N7-C8-N9	7.04	117.32	113.80
1	2	608	U	C2-N1-C1'	7.03	126.13	117.70
1	2	1235	C	N3-C2-O2	-7.02	116.99	121.90
21	H	66	LEU	CA-CB-CG	7.01	131.43	115.30
36	LA	2405	C	C6-N1-C2	-7.00	117.50	120.30
1	2	903	U	N3-C2-O2	-7.00	117.30	122.20
1	2	1007	C	C6-N1-C2	-7.00	117.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	LA	663	C	C5-C6-N1	7.00	124.50	121.00
36	LA	1608	C	C2-N1-C1'	7.00	126.49	118.80
36	LA	444	U	N3-C2-O2	-6.99	117.31	122.20
81	EF	869	LEU	CA-CB-CG	6.99	131.38	115.30
34	O	177	MET	CA-CB-CG	6.99	125.17	113.30
36	LA	922	U	N1-C2-O2	6.99	127.69	122.80
1	2	1145	U	N3-C2-O2	-6.98	117.31	122.20
1	2	79	C	C6-N1-C2	-6.98	117.51	120.30
1	2	935	U	N3-C2-O2	-6.98	117.31	122.20
1	2	992	A	C8-N9-C4	-6.98	103.01	105.80
80	Sm	49	C	N3-C2-O2	-6.97	117.02	121.90
1	2	121	U	N3-C2-O2	-6.97	117.32	122.20
36	LA	2772	C	N1-C2-O2	6.97	123.08	118.90
36	LA	2189	U	N1-C2-O2	6.97	127.68	122.80
36	LA	1756	C	C6-N1-C2	-6.97	117.51	120.30
80	Sn	74	C	C5-C6-N1	6.96	124.48	121.00
36	LA	2894	C	C6-N1-C2	-6.96	117.52	120.30
45	LJ	82	LEU	CA-CB-CG	6.95	131.29	115.30
1	2	639	U	N3-C2-O2	-6.95	117.33	122.20
36	LA	1222	G	O4'-C1'-N9	6.95	113.76	108.20
37	LB	26	C	C6-N1-C2	-6.95	117.52	120.30
1	2	1620	C	C6-N1-C2	-6.95	117.52	120.30
36	LA	3043	C	C6-N1-C2	-6.94	117.52	120.30
36	LA	1582	C	P-O3'-C3'	6.94	128.02	119.70
36	LA	1872	C	N3-C2-O2	-6.93	117.05	121.90
36	LA	982	C	C2-N1-C1'	6.92	126.42	118.80
36	LA	2836	C	N1-C2-O2	6.92	123.06	118.90
1	2	623	A	O4'-C1'-N9	6.92	113.74	108.20
36	LA	225	C	C5-C6-N1	6.91	124.45	121.00
36	LA	3358	U	N3-C2-O2	-6.91	117.36	122.20
36	LA	969	C	N3-C2-O2	-6.91	117.06	121.90
1	2	1279	C	C6-N1-C2	-6.89	117.54	120.30
36	LA	2849	C	C5-C6-N1	6.89	124.45	121.00
36	LA	283	G	N3-C4-C5	-6.89	125.15	128.60
1	2	415	C	C6-N1-C2	-6.89	117.55	120.30
36	LA	2505	U	N1-C2-O2	6.88	127.62	122.80
19	F	96	TYR	CB-CG-CD1	-6.88	116.87	121.00
36	LA	1644	C	C6-N1-C2	-6.88	117.55	120.30
36	LA	1706	C	C6-N1-C2	-6.88	117.55	120.30
36	LA	2495	C	C6-N1-C2	-6.88	117.55	120.30
36	LA	3350	C	P-O3'-C3'	6.88	127.95	119.70
19	F	50	GLU	CA-CB-CG	6.87	128.52	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	LA	2258	U	C5-C6-N1	6.87	126.14	122.70
5	E	60	LEU	CA-CB-CG	6.87	131.09	115.30
36	LA	444	U	N1-C2-O2	6.87	127.61	122.80
1	2	975	C	C6-N1-C2	-6.86	117.56	120.30
1	2	314	C	C6-N1-C2	-6.86	117.56	120.30
1	2	1497	U	N3-C2-O2	-6.85	117.40	122.20
1	2	989	U	N3-C2-O2	-6.85	117.41	122.20
1	2	1620	C	N1-C2-O2	6.85	123.01	118.90
36	LA	2764	C	C6-N1-C2	-6.85	117.56	120.30
36	LA	2983	C	N3-C2-O2	-6.85	117.11	121.90
36	LA	1283	C	C2-N1-C1'	6.84	126.33	118.80
36	LA	763	G	P-O3'-C3'	6.84	127.91	119.70
36	LA	1355	A	OP2-P-O3'	6.84	120.25	105.20
36	LA	444	U	C5-C6-N1	6.84	126.12	122.70
1	2	908	U	N3-C2-O2	-6.83	117.42	122.20
36	LA	2913	C	C6-N1-C2	-6.83	117.57	120.30
36	LA	1227	C	C5-C6-N1	6.83	124.41	121.00
39	LD	191	LEU	CA-CB-CG	-6.83	99.59	115.30
36	LA	3131	U	C2-N1-C1'	6.83	125.89	117.70
1	2	499	U	O4'-C1'-N1	6.82	113.66	108.20
36	LA	713	U	N3-C2-O2	-6.82	117.43	122.20
36	LA	3181	C	C6-N1-C1'	-6.82	112.62	120.80
36	LA	922	U	C6-N1-C1'	-6.81	111.66	121.20
36	LA	2552	C	N3-C2-O2	-6.80	117.14	121.90
16	D	74	LEU	CA-CB-CG	6.80	130.93	115.30
36	LA	2541	U	C2-N1-C1'	6.80	125.86	117.70
36	LA	1032	C	C6-N1-C2	-6.79	117.58	120.30
1	2	1203	A	C8-N9-C4	-6.79	103.08	105.80
1	2	590	C	C5-C6-N1	6.79	124.39	121.00
1	2	139	C	P-O3'-C3'	6.79	127.84	119.70
1	2	782	U	C5-C6-N1	6.79	126.09	122.70
36	LA	1155	C	N1-C2-O2	6.79	122.97	118.90
36	LA	3057	U	N3-C2-O2	-6.79	117.45	122.20
36	LA	982	C	C6-N1-C2	-6.78	117.59	120.30
80	Sm	32	C	C5-C6-N1	6.78	124.39	121.00
1	2	517	U	N1-C2-O2	6.77	127.54	122.80
36	LA	881	C	C6-N1-C2	-6.77	117.59	120.30
54	Lm	41	ASP	CB-CG-OD1	6.77	124.39	118.30
1	2	453	U	C6-N1-C2	-6.76	116.94	121.00
36	LA	886	C	C6-N1-C2	-6.76	117.59	120.30
1	2	1115	U	N1-C2-O2	6.76	127.53	122.80
36	LA	3306	U	N1-C2-O2	6.76	127.53	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1201	G	OP1-P-O3'	6.75	120.05	105.20
36	LA	2496	C	C2-N1-C1'	6.75	126.22	118.80
1	2	1458	G	N3-C4-N9	6.74	130.05	126.00
36	LA	1869	C	C6-N1-C2	-6.74	117.60	120.30
1	2	185	U	N3-C2-O2	-6.74	117.48	122.20
1	2	394	C	C5-C6-N1	6.74	124.37	121.00
9	B	25	LEU	CA-CB-CG	6.73	130.79	115.30
14	C	46	LEU	CA-CB-CG	-6.73	99.82	115.30
1	2	183	U	C5-C6-N1	6.73	126.07	122.70
37	LB	78	U	C5-C6-N1	6.73	126.06	122.70
36	LA	397	A	O4'-C1'-N9	-6.72	102.82	108.20
36	LA	3195	U	N1-C2-O2	6.72	127.51	122.80
1	2	1186	U	O5'-P-OP2	-6.71	99.66	105.70
1	2	1314	U	OP2-P-O3'	6.71	119.97	105.20
80	Sm	71	C	C6-N1-C2	-6.71	117.62	120.30
1	2	1274	C	P-O3'-C3'	6.71	127.75	119.70
36	LA	1604	G	C8-N9-C1'	-6.71	118.28	127.00
1	2	614	C	C5-C6-N1	6.70	124.35	121.00
1	2	640	U	P-O3'-C3'	6.70	127.74	119.70
21	H	14	ILE	CG1-CB-CG2	-6.70	96.66	111.40
36	LA	2531	C	N3-C2-O2	-6.70	117.21	121.90
38	LC	55	U	C5-C6-N1	6.70	126.05	122.70
36	LA	13	A	OP2-P-O3'	6.69	119.92	105.20
1	2	530	C	N1-C2-O2	6.69	122.91	118.90
1	2	625	C	C6-N1-C2	-6.69	117.62	120.30
42	LG	110	LEU	CB-CG-CD1	6.69	122.37	111.00
1	2	629	U	N1-C2-O2	6.69	127.48	122.80
36	LA	803	C	C5-C6-N1	6.68	124.34	121.00
36	LA	3089	C	C6-N1-C2	-6.68	117.63	120.30
1	2	1414	U	N1-C2-O2	6.68	127.48	122.80
1	2	1381	U	C2-N1-C1'	6.68	125.71	117.70
1	2	1389	C	C6-N1-C1'	-6.67	112.79	120.80
1	2	1573	A	P-O3'-C3'	6.67	127.70	119.70
1	2	405	C	C6-N1-C2	-6.67	117.63	120.30
36	LA	2446	U	C6-N1-C2	-6.67	117.00	121.00
36	LA	2495	C	N3-C2-O2	-6.67	117.23	121.90
36	LA	2756	C	C6-N1-C2	-6.67	117.63	120.30
36	LA	2389	C	C5-C6-N1	6.67	124.33	121.00
36	LA	1263	A	C8-N9-C4	-6.67	103.13	105.80
1	2	1799	U	N1-C2-O2	6.66	127.46	122.80
1	2	1523	G	C8-N9-C1'	-6.66	118.34	127.00
1	2	1148	C	C6-N1-C2	-6.66	117.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1489	U	C2-N1-C1'	6.66	125.69	117.70
1	2	1273	G	OP2-P-O3'	6.65	119.84	105.20
1	2	1527	C	C5-C6-N1	6.65	124.33	121.00
36	LA	2600	C	C5-C6-N1	6.65	124.33	121.00
1	2	479	C	C6-N1-C2	-6.65	117.64	120.30
36	LA	543	C	N3-C2-O2	-6.65	117.25	121.90
36	LA	1660	C	C5-C6-N1	6.65	124.32	121.00
36	LA	2137	U	C2-N1-C1'	6.64	125.67	117.70
1	2	864	U	N3-C2-O2	-6.64	117.55	122.20
1	2	1633	A	OP2-P-O3'	6.64	119.81	105.20
11	U	158	ASP	CB-CG-OD1	6.64	124.28	118.30
36	LA	1608	C	C5-C6-N1	6.64	124.32	121.00
51	LP	113	LEU	CA-CB-CG	6.64	130.57	115.30
1	2	1497	U	N1-C2-O2	6.63	127.44	122.80
1	2	433	C	C6-N1-C2	-6.63	117.65	120.30
36	LA	311	C	C6-N1-C2	-6.63	117.65	120.30
36	LA	2960	C	C6-N1-C2	-6.62	117.65	120.30
19	F	52	LEU	CA-CB-CG	6.61	130.50	115.30
36	LA	1788	C	C5-C6-N1	6.61	124.31	121.00
1	2	849	C	C5-C6-N1	6.61	124.30	121.00
52	LQ	84[A]	LEU	CB-CG-CD1	-6.61	99.77	111.00
36	LA	444	U	C6-N1-C2	-6.61	117.04	121.00
36	LA	1349	G	C8-N9-C1'	-6.61	118.41	127.00
36	LA	2281	A	O4'-C1'-N9	6.61	113.48	108.20
1	2	1389	C	C5-C6-N1	6.60	124.30	121.00
42	LG	163	LEU	CB-CG-CD2	-6.60	99.78	111.00
1	2	965	U	C6-N1-C1'	-6.60	111.96	121.20
1	2	1251	U	P-O3'-C3'	6.60	127.62	119.70
36	LA	42	C	C5-C6-N1	6.60	124.30	121.00
36	LA	3214	U	N3-C2-O2	-6.59	117.59	122.20
1	2	911	U	N1-C2-O2	6.59	127.41	122.80
5	E	25	LEU	CA-CB-CG	6.58	130.44	115.30
36	LA	2112	U	OP2-P-O3'	6.57	119.66	105.20
36	LA	379	C	C5-C6-N1	6.57	124.28	121.00
1	2	494	U	C2-N1-C1'	6.57	125.58	117.70
1	2	1063	U	N1-C2-O2	6.57	127.40	122.80
36	LA	2495	C	C2-N1-C1'	6.57	126.02	118.80
36	LA	2422	C	C5-C6-N1	6.56	124.28	121.00
36	LA	2737	C	C6-N1-C2	-6.56	117.67	120.30
36	LA	3155	U	N3-C2-O2	-6.56	117.61	122.20
36	LA	2842	U	N1-C2-O2	6.56	127.39	122.80
1	2	186	C	C6-N1-C2	-6.56	117.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	Sn	46	G	O4'-C1'-N9	6.55	113.44	108.20
36	LA	1854	C	C5-C6-N1	6.55	124.28	121.00
1	2	1584	G	P-O3'-C3'	6.54	127.55	119.70
36	LA	87	U	C2-N1-C1'	6.54	125.55	117.70
36	LA	2132	C	N3-C2-O2	-6.54	117.32	121.90
80	Sn	3	C	C6-N1-C2	-6.54	117.68	120.30
1	2	874	C	C5-C6-N1	6.54	124.27	121.00
36	LA	3195	U	C2-N1-C1'	6.54	125.55	117.70
36	LA	2550	U	N3-C2-O2	-6.53	117.63	122.20
36	LA	3034	C	N1-C2-O2	6.53	122.82	118.90
36	LA	931	C	C6-N1-C2	-6.53	117.69	120.30
36	LA	1684	U	N3-C2-O2	-6.53	117.63	122.20
36	LA	118	U	N3-C2-O2	-6.53	117.63	122.20
36	LA	3058	U	N1-C2-O2	6.52	127.37	122.80
36	LA	2504	U	P-O3'-C3'	6.52	127.53	119.70
36	LA	1819	U	C2-N1-C1'	6.52	125.52	117.70
16	D	88	LEU	CA-CB-CG	6.51	130.28	115.30
36	LA	1155	C	C2-N1-C1'	6.51	125.96	118.80
36	LA	524	U	N3-C2-O2	-6.51	117.64	122.20
36	LA	675	C	C6-N1-C2	-6.50	117.70	120.30
36	LA	2553	U	C2-N1-C1'	6.50	125.50	117.70
1	2	1145	U	C6-N1-C1'	-6.50	112.10	121.20
36	LA	283	G	N3-C4-N9	6.50	129.90	126.00
36	LA	2151	C	C6-N1-C2	-6.50	117.70	120.30
1	2	141	U	P-O3'-C3'	6.49	127.48	119.70
1	2	294	C	C6-N1-C2	-6.49	117.70	120.30
36	LA	609	G	OP2-P-O3'	6.49	119.47	105.20
80	Sn	34	C	N1-C2-O2	6.48	122.79	118.90
36	LA	1276	U	C6-N1-C2	-6.48	117.11	121.00
36	LA	2189	U	N3-C2-O2	-6.48	117.67	122.20
80	Sn	72	U	N1-C2-O2	6.48	127.33	122.80
36	LA	1556	C	C6-N1-C2	-6.48	117.71	120.30
36	LA	1562	C	P-O3'-C3'	6.48	127.47	119.70
1	2	794	U	N3-C2-O2	-6.47	117.67	122.20
36	LA	1579	C	N1-C2-O2	6.47	122.78	118.90
1	2	1620	C	C2-N1-C1'	6.47	125.92	118.80
36	LA	954	U	N3-C2-O2	-6.47	117.67	122.20
1	2	1180	C	C6-N1-C2	-6.47	117.71	120.30
36	LA	2992	U	N3-C2-O2	-6.46	117.68	122.20
1	2	572	C	C6-N1-C2	-6.46	117.72	120.30
36	LA	979	U	N3-C2-O2	-6.46	117.68	122.20
36	LA	2763	U	N3-C2-O2	-6.46	117.68	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	553	G	C8-N9-C1'	6.46	135.40	127.00
1	2	184	C	C6-N1-C2	-6.46	117.72	120.30
1	2	538	A	O4'-C1'-N9	-6.46	103.03	108.20
1	2	1458	G	C8-N9-C1'	-6.46	118.60	127.00
36	LA	957	C	C5-C6-N1	6.46	124.23	121.00
36	LA	1660	C	C6-N1-C2	-6.46	117.72	120.30
1	2	1220	C	C6-N1-C2	-6.46	117.72	120.30
37	LB	98	C	C5-C6-N1	6.46	124.23	121.00
36	LA	3155	U	N1-C2-O2	6.45	127.32	122.80
36	LA	2842	U	N3-C2-O2	-6.45	117.69	122.20
38	LC	151	C	C6-N1-C2	-6.45	117.72	120.30
36	LA	3218	A	P-O3'-C3'	6.45	127.44	119.70
36	LA	2100	A	O4'-C1'-N9	6.44	113.36	108.20
36	LA	3235	C	C2-N1-C1'	6.44	125.89	118.80
1	2	500	C	N1-C2-O2	6.44	122.76	118.90
1	2	262	U	C2-N1-C1'	6.44	125.42	117.70
1	2	283	U	N1-C2-O2	6.43	127.30	122.80
36	LA	1146	C	C6-N1-C2	-6.43	117.73	120.30
42	LG	236	LEU	CA-CB-CG	6.43	130.09	115.30
1	2	1010	C	C5-C6-N1	6.43	124.21	121.00
1	2	614	C	C6-N1-C2	-6.42	117.73	120.30
1	2	656	G	C8-N9-C1'	-6.42	118.65	127.00
80	Sm	32	C	C6-N1-C2	-6.42	117.73	120.30
81	EF	418	PRO	N-CA-CB	6.42	111.00	103.30
38	LC	141	C	C6-N1-C2	-6.41	117.73	120.30
36	LA	2146	C	C5-C6-N1	6.41	124.21	121.00
36	LA	2867	C	C6-N1-C2	-6.41	117.74	120.30
36	LA	966	U	C5-C6-N1	6.41	125.90	122.70
36	LA	2622	C	N1-C2-O2	6.40	122.74	118.90
1	2	185	U	N1-C2-O2	6.40	127.28	122.80
36	LA	1540	U	N3-C2-O2	-6.40	117.72	122.20
1	2	1010	C	C6-N1-C2	-6.40	117.74	120.30
1	2	139	C	OP2-P-O3'	6.39	119.27	105.20
1	2	1754	A	O4'-C1'-N9	-6.39	103.09	108.20
80	Sm	40	C	N3-C2-O2	-6.39	117.43	121.90
18	Z	66	ASP	CB-CG-OD1	6.39	124.05	118.30
1	2	120	U	C2-N1-C1'	6.39	125.36	117.70
80	Sn	25	C	C6-N1-C2	-6.38	117.75	120.30
1	2	517	U	N3-C2-O2	-6.38	117.73	122.20
1	2	555	A	C4-N9-C1'	6.38	137.79	126.30
19	F	96	TYR	CB-CG-CD2	6.38	124.83	121.00
1	2	645	C	C5-C6-N1	6.38	124.19	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	LB	58	C	C5-C6-N1	6.38	124.19	121.00
1	2	1556	A	P-O3'-C3'	6.37	127.35	119.70
1	2	1066	C	C6-N1-C2	-6.37	117.75	120.30
36	LA	1820	U	P-O3'-C3'	6.37	127.34	119.70
36	LA	2714	G	N3-C4-C5	6.37	131.78	128.60
36	LA	2765	C	C6-N1-C2	-6.36	117.75	120.30
68	La	4	LEU	CA-CB-CG	6.36	129.94	115.30
1	2	186	C	N3-C2-O2	-6.36	117.45	121.90
8	S	193	GLY	N-CA-C	6.36	129.00	113.10
36	LA	354	U	N1-C2-O2	6.36	127.25	122.80
36	LA	3097	C	C5-C6-N1	6.36	124.18	121.00
36	LA	2132	C	N1-C2-O2	6.36	122.71	118.90
1	2	1527	C	C6-N1-C2	-6.36	117.76	120.30
36	LA	2763	U	N1-C2-O2	6.35	127.25	122.80
1	2	313	U	P-O3'-C3'	6.35	127.32	119.70
1	2	705	U	P-O3'-C3'	6.35	127.32	119.70
1	2	1756	A	P-O3'-C3'	6.35	127.32	119.70
36	LA	573	C	C6-N1-C2	-6.35	117.76	120.30
36	LA	2773	C	C6-N1-C2	-6.35	117.76	120.30
1	2	1585	U	C5-C6-N1	6.35	125.87	122.70
38	LC	30	C	C6-N1-C2	-6.34	117.77	120.30
36	LA	543	C	N1-C2-O2	6.33	122.70	118.90
1	2	387	A	P-O3'-C3'	6.33	127.30	119.70
1	2	1307	U	N3-C2-O2	-6.33	117.77	122.20
36	LA	2256	A	O5'-P-OP2	-6.33	100.00	105.70
80	Sn	32	C	N1-C2-O2	6.33	122.70	118.90
1	2	1033	C	C6-N1-C2	-6.33	117.77	120.30
36	LA	3300	U	N3-C2-O2	-6.33	117.77	122.20
1	2	758	U	N1-C2-O2	6.33	127.23	122.80
36	LA	3277	U	C2-N1-C1'	6.33	125.29	117.70
1	2	1799	U	N3-C2-O2	-6.32	117.77	122.20
36	LA	1556	C	N3-C2-O2	-6.32	117.47	121.90
36	LA	3111	U	C5-C6-N1	6.32	125.86	122.70
1	2	1389	C	C6-N1-C2	-6.32	117.77	120.30
36	LA	271	C	N3-C2-O2	-6.32	117.48	121.90
36	LA	2585	G	N3-C4-N9	6.32	129.79	126.00
36	LA	1583	A	O5'-P-OP1	-6.32	100.02	105.70
1	2	755	A	P-O3'-C3'	6.32	127.28	119.70
36	LA	1155	C	C6-N1-C2	-6.32	117.77	120.30
38	LC	100	U	N1-C2-O2	6.31	127.22	122.80
42	LG	272	TYR	CB-CG-CD2	6.31	124.78	121.00
36	LA	2795	U	O5'-P-OP2	-6.30	100.03	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	656	G	N3-C4-N9	6.30	129.78	126.00
1	2	928	U	P-O3'-C3'	6.30	127.26	119.70
36	LA	969	C	N1-C2-O2	6.30	122.68	118.90
36	LA	1525	G	C4-N9-C1'	6.30	134.69	126.50
1	2	1596	C	N3-C2-O2	-6.29	117.50	121.90
36	LA	1496	C	N1-C2-O2	6.29	122.68	118.90
36	LA	2378	C	C2-N1-C1'	6.29	125.72	118.80
1	2	1439	C	C6-N1-C2	-6.29	117.78	120.30
36	LA	1355	A	P-O3'-C3'	6.29	127.25	119.70
36	LA	1722	U	N3-C2-O2	-6.29	117.80	122.20
37	LB	39	C	C6-N1-C2	-6.29	117.78	120.30
1	2	1557	U	P-O3'-C3'	6.29	127.25	119.70
36	LA	1115	G	O5'-P-OP1	-6.28	100.05	105.70
1	2	394	C	C6-N1-C2	-6.28	117.79	120.30
1	2	1657	U	C2-N1-C1'	6.28	125.24	117.70
36	LA	2899	C	C2-N1-C1'	6.28	125.71	118.80
38	LC	26	U	C5-C6-N1	6.28	125.84	122.70
36	LA	1448	U	C2-N1-C1'	6.28	125.23	117.70
36	LA	1604	G	C6-C5-N7	-6.28	126.63	130.40
1	2	583	C	C5-C6-N1	6.28	124.14	121.00
1	2	1082	C	N3-C2-O2	-6.27	117.51	121.90
36	LA	743	C	C6-N1-C2	-6.27	117.79	120.30
1	2	765	G	O4'-C1'-N9	6.27	113.21	108.20
36	LA	2137	U	O4'-C1'-N1	6.27	113.21	108.20
1	2	1389	C	N3-C2-O2	-6.27	117.51	121.90
1	2	803	A	P-O3'-C3'	6.26	127.22	119.70
36	LA	861	C	C5-C6-N1	6.26	124.13	121.00
36	LA	1097	G	P-O3'-C3'	6.26	127.22	119.70
1	2	1585	U	N3-C2-O2	-6.26	117.82	122.20
36	LA	963	G	C6-C5-N7	-6.26	126.65	130.40
1	2	1620	C	N3-C2-O2	-6.25	117.53	121.90
1	2	736	C	N1-C2-O2	6.24	122.64	118.90
36	LA	191	U	O5'-P-OP2	-6.24	100.08	105.70
36	LA	1685	C	C6-N1-C2	-6.24	117.80	120.30
36	LA	1951	C	C6-N1-C2	-6.24	117.81	120.30
1	2	583	C	N1-C2-O2	6.24	122.64	118.90
80	Sm	56	C	N1-C2-O2	6.23	122.64	118.90
1	2	552	G	N3-C4-N9	6.23	129.74	126.00
36	LA	1516	C	C6-N1-C2	-6.23	117.81	120.30
36	LA	1858	A	O4'-C1'-N9	6.23	113.18	108.20
36	LA	3259	U	C5-C6-N1	6.22	125.81	122.70
36	LA	492	C	N3-C2-O2	-6.22	117.55	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	469	C	C6-N1-C2	-6.22	117.81	120.30
1	2	736	C	N3-C2-O2	-6.22	117.55	121.90
36	LA	3222	U	C5-C6-N1	6.22	125.81	122.70
36	LA	915	A	C4-N9-C1'	6.21	137.49	126.30
36	LA	1580	A	O4'-C1'-N9	6.21	113.17	108.20
36	LA	2444	C	N1-C2-O2	6.21	122.63	118.90
36	LA	3269	U	P-O3'-C3'	6.21	127.15	119.70
1	2	453	U	C2-N1-C1'	6.21	125.15	117.70
80	Sm	5	C	N1-C2-O2	6.21	122.62	118.90
36	LA	3084	C	C6-N1-C2	-6.21	117.82	120.30
1	2	185	U	C6-N1-C2	-6.20	117.28	121.00
36	LA	2984	C	C5-C6-N1	6.20	124.10	121.00
1	2	767	U	N3-C2-O2	-6.20	117.86	122.20
1	2	794	U	N1-C2-O2	6.20	127.14	122.80
1	2	861	U	C6-N1-C1'	-6.20	112.52	121.20
16	D	28	LEU	CA-CB-CG	6.20	129.56	115.30
36	LA	3217	C	C2-N3-C4	6.20	123.00	119.90
80	Sm	3	C	C6-N1-C2	-6.20	117.82	120.30
1	2	1207	C	P-O3'-C3'	6.20	127.14	119.70
1	2	262	U	N3-C2-O2	-6.19	117.86	122.20
36	LA	1227	C	N3-C2-O2	-6.19	117.56	121.90
56	Lo	109	ASP	CB-CG-OD1	6.19	123.87	118.30
36	LA	1878	G	C4-N9-C1'	6.18	134.54	126.50
1	2	1145	U	N1-C2-O2	6.18	127.13	122.80
18	Z	27	PHE	CB-CG-CD1	6.18	125.12	120.80
1	2	1596	C	C2-N1-C1'	6.18	125.60	118.80
36	LA	544	C	N1-C2-O2	6.18	122.61	118.90
36	LA	3214	U	N1-C2-O2	6.17	127.12	122.80
1	2	185	U	C5-C6-N1	6.17	125.78	122.70
1	2	405	C	C5-C6-N1	6.17	124.08	121.00
36	LA	2594	C	C2-N1-C1'	6.17	125.59	118.80
36	LA	288	C	C6-N1-C2	-6.17	117.83	120.30
80	Sm	40	C	N1-C2-O2	6.17	122.60	118.90
1	2	767	U	C2-N1-C1'	6.16	125.09	117.70
36	LA	702	C	C6-N1-C2	-6.16	117.84	120.30
1	2	864	U	N1-C2-O2	6.16	127.11	122.80
1	2	1172	G	N7-C8-N9	6.16	116.18	113.10
37	LB	100	C	C6-N1-C2	-6.16	117.84	120.30
1	2	499	U	C6-N1-C2	-6.15	117.31	121.00
36	LA	1208	U	N3-C2-O2	-6.15	117.89	122.20
36	LA	2638	C	N1-C2-O2	6.15	122.59	118.90
36	LA	2322	C	C6-N1-C2	-6.14	117.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	LA	1578	C	C5-C6-N1	6.14	124.07	121.00
37	LB	78	U	C2-N1-C1'	6.14	125.07	117.70
36	LA	297	G	O4'-C1'-N9	6.13	113.11	108.20
36	LA	911	C	C6-N1-C2	-6.13	117.85	120.30
1	2	1568	C	C6-N1-C2	-6.13	117.85	120.30
36	LA	1835	A	C6-N1-C2	6.13	122.28	118.60
80	Sn	72	U	N3-C2-O2	-6.12	117.92	122.20
1	2	1494	C	C6-N1-C2	-6.12	117.85	120.30
36	LA	2237	C	N1-C2-O2	6.12	122.57	118.90
36	LA	2773	C	C5-C6-N1	6.12	124.06	121.00
36	LA	1307	G	P-O3'-C3'	6.12	127.04	119.70
1	2	267	U	N3-C2-O2	-6.12	117.92	122.20
36	LA	1604	G	C4-C5-N7	6.12	113.25	110.80
55	Ln	155	LEU	CA-CB-CG	6.12	129.37	115.30
1	2	453	U	N1-C2-O2	6.11	127.08	122.80
1	2	1458	G	C8-N9-C4	-6.11	103.96	106.40
36	LA	1901	A	C8-N9-C4	-6.11	103.36	105.80
36	LA	271	C	N1-C2-O2	6.10	122.56	118.90
36	LA	818	C	C5-C6-N1	6.10	124.05	121.00
36	LA	36	C	C6-N1-C2	-6.10	117.86	120.30
36	LA	427	C	C6-N1-C2	-6.10	117.86	120.30
36	LA	3309	G	N3-C4-N9	6.10	129.66	126.00
1	2	1115	U	N3-C2-O2	-6.10	117.93	122.20
36	LA	118	U	C2-N1-C1'	6.10	125.02	117.70
36	LA	1604	G	N3-C4-C5	-6.10	125.55	128.60
36	LA	152	U	O5'-P-OP2	-6.09	100.22	105.70
36	LA	2551	U	C2-N1-C1'	6.09	125.01	117.70
80	Sn	72	U	C2-N1-C1'	6.09	125.01	117.70
1	2	766	U	C2-N1-C1'	6.09	125.00	117.70
1	2	553	G	N1-C6-O6	-6.09	116.25	119.90
36	LA	3096	C	C6-N1-C2	-6.09	117.86	120.30
1	2	184	C	C5-C6-N1	6.08	124.04	121.00
1	2	323	A	C8-N9-C4	-6.08	103.37	105.80
38	LC	35	C	C5-C6-N1	6.08	124.04	121.00
1	2	553	G	C4-C5-N7	-6.08	108.37	110.80
36	LA	1283	C	C6-N1-C2	-6.08	117.87	120.30
80	Sn	34	C	N3-C2-O2	-6.08	117.64	121.90
1	2	388	G	O5'-P-OP1	-6.08	100.23	105.70
25	b	93	LEU	CA-CB-CG	6.08	129.27	115.30
36	LA	2683	U	N3-C2-O2	-6.08	117.95	122.20
47	LL	102	MET	CG-SD-CE	6.07	109.92	100.20
36	LA	50	U	N3-C2-O2	-6.07	117.95	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	LA	2257	C	O5'-P-OP2	-6.07	100.24	105.70
36	LA	2137	U	C5-C6-N1	6.07	125.73	122.70
1	2	992	A	C5-N7-C8	-6.07	100.87	103.90
1	2	1024	U	C6-N1-C2	-6.07	117.36	121.00
1	2	1528	U	N3-C2-O2	-6.07	117.95	122.20
1	2	1500	C	C6-N1-C2	-6.06	117.87	120.30
1	2	1075	C	C6-N1-C2	-6.06	117.88	120.30
1	2	1596	C	C6-N1-C2	-6.06	117.88	120.30
36	LA	105	C	C6-N1-C2	-6.06	117.88	120.30
36	LA	922	U	N3-C2-O2	-6.06	117.96	122.20
36	LA	2783	U	N3-C2-O2	-6.06	117.96	122.20
36	LA	614	C	C6-N1-C2	-6.05	117.88	120.30
1	2	820	U	N3-C2-O2	-6.05	117.97	122.20
36	LA	1698	C	C6-N1-C2	-6.05	117.88	120.30
36	LA	224	C	C6-N1-C2	-6.04	117.88	120.30
36	LA	3320	A	O5'-P-OP1	-6.04	100.26	105.70
36	LA	2983	C	C2-N1-C1'	6.03	125.43	118.80
36	LA	2114	C	C6-N1-C2	-6.03	117.89	120.30
36	LA	2836	C	C6-N1-C2	-6.03	117.89	120.30
36	LA	2941	A	O5'-P-OP1	-6.03	100.27	105.70
1	2	1363	U	C5-C6-N1	6.02	125.71	122.70
36	LA	705	A	O4'-C1'-N9	-6.02	103.38	108.20
69	Lb	49	ILE	CG1-CB-CG2	-6.02	98.15	111.40
1	2	400	A	OP2-P-O3'	6.02	118.44	105.20
42	LG	137	ASP	CB-CG-OD1	6.01	123.71	118.30
1	2	820	U	N1-C2-O2	6.01	127.01	122.80
36	LA	354	U	C2-N1-C1'	6.01	124.91	117.70
36	LA	3338	C	C6-N1-C2	-6.01	117.90	120.30
36	LA	2714	G	N3-C4-N9	-6.01	122.40	126.00
1	2	1173	C	C6-N1-C2	-6.00	117.90	120.30
36	LA	443	G	N9-C1'-C2'	-5.99	105.41	112.00
36	LA	282	G	P-O3'-C3'	5.99	126.89	119.70
1	2	302	U	N3-C2-O2	-5.99	118.01	122.20
1	2	1274	C	OP2-P-O3'	5.99	118.37	105.20
36	LA	2509	U	P-O3'-C3'	5.99	126.88	119.70
1	2	172	C	C2-N1-C1'	5.98	125.38	118.80
1	2	482	U	N3-C2-O2	-5.98	118.01	122.20
36	LA	332	C	C5-C6-N1	5.98	123.99	121.00
12	V	165	LEU	CA-CB-CG	5.98	129.06	115.30
1	2	758	U	N3-C2-O2	-5.98	118.01	122.20
36	LA	1896	A	C2-N3-C4	5.98	113.59	110.60
38	LC	115	C	C6-N1-C2	-5.98	117.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1363	U	N1-C2-O2	5.98	126.98	122.80
38	LC	100	U	C2-N1-C1'	5.98	124.87	117.70
36	LA	1556	C	N1-C2-O2	5.97	122.48	118.90
1	2	424	C	C4-C5-C6	-5.97	114.41	117.40
30	f	33	LEU	CA-CB-CG	5.97	129.04	115.30
37	LB	52	G	P-O3'-C3'	5.97	126.87	119.70
1	2	1664	C	C6-N1-C2	-5.97	117.91	120.30
1	2	1414	U	N3-C2-O2	-5.97	118.02	122.20
1	2	1657	U	N1-C2-O2	5.96	126.97	122.80
1	2	552	G	C4-N9-C1'	5.96	134.24	126.50
1	2	553	G	C4-N9-C1'	-5.96	118.76	126.50
36	LA	2788	C	C6-N1-C2	-5.96	117.92	120.30
8	S	103	TYR	CB-CG-CD2	-5.95	117.43	121.00
37	LB	26	C	C5-C6-N1	5.95	123.98	121.00
36	LA	1333	C	C5-C6-N1	5.95	123.98	121.00
1	2	1214	U	C2-N1-C1'	5.95	124.84	117.70
36	LA	2664	C	C2-N1-C1'	5.95	125.35	118.80
36	LA	3058	U	N3-C2-O2	-5.95	118.03	122.20
36	LA	3153	U	N3-C2-O2	-5.95	118.04	122.20
4	Q	217	LEU	CA-CB-CG	5.94	128.97	115.30
36	LA	911	C	C5-C6-N1	5.94	123.97	121.00
36	LA	1923	C	C6-N1-C2	-5.93	117.93	120.30
1	2	120	U	N3-C2-O2	-5.92	118.06	122.20
36	LA	1275	C	C6-N1-C2	-5.92	117.93	120.30
46	LK	112	ILE	CG1-CB-CG2	-5.92	98.38	111.40
1	2	121	U	C2-N1-C1'	5.92	124.80	117.70
36	LA	125	C	C6-N1-C2	-5.92	117.93	120.30
23	J	34	LEU	CB-CG-CD2	-5.92	100.94	111.00
1	2	1123	C	C5-C6-N1	5.91	123.96	121.00
1	2	1461	C	C5-C6-N1	5.91	123.96	121.00
36	LA	1235	U	N3-C4-O4	-5.91	115.26	119.40
36	LA	2451	G	P-O3'-C3'	5.91	126.79	119.70
1	2	1245	G	P-O3'-C3'	5.91	126.79	119.70
36	LA	609	G	C4-C5-N7	5.91	113.16	110.80
1	2	587	C	C6-N1-C2	-5.91	117.94	120.30
1	2	935	U	N1-C2-O2	5.91	126.93	122.80
1	2	1381	U	C5-C6-N1	5.91	125.65	122.70
36	LA	3363	U	N3-C2-O2	-5.91	118.07	122.20
81	EF	415	PRO	N-CA-CB	5.90	110.39	103.30
36	LA	224	C	O5'-P-OP1	-5.90	100.39	105.70
36	LA	1835	A	N1-C2-N3	-5.90	126.35	129.30
36	LA	2772	C	C6-N1-C1'	-5.90	113.72	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	LA	1446	A	O5'-P-OP1	-5.90	100.39	105.70
1	2	1614	A	O4'-C1'-N9	5.90	112.92	108.20
36	LA	979	U	N1-C2-O2	5.90	126.93	122.80
36	LA	2274	U	N1-C2-O2	5.90	126.93	122.80
36	LA	1832	C	C6-N1-C2	-5.90	117.94	120.30
36	LA	2176	U	N1-C2-O2	5.89	126.92	122.80
1	2	1072	C	C6-N1-C2	-5.89	117.94	120.30
36	LA	2242	A	C8-N9-C4	-5.89	103.44	105.80
36	LA	1771	C	C6-N1-C2	-5.89	117.94	120.30
36	LA	2132	C	C6-N1-C2	-5.88	117.95	120.30
1	2	1527	C	C6-N1-C1'	-5.88	113.75	120.80
36	LA	3076	C	C6-N1-C2	-5.88	117.95	120.30
1	2	803	A	OP2-P-O3'	5.87	118.12	105.20
36	LA	2206	G	N3-C4-C5	-5.87	125.66	128.60
22	I	45	MET	CA-CB-CG	5.87	123.28	113.30
36	LA	2611	U	C6-N1-C2	-5.87	117.48	121.00
1	2	1465	C	C5-C6-N1	5.87	123.93	121.00
36	LA	270	U	N3-C2-O2	-5.87	118.09	122.20
36	LA	311	C	C5-C6-N1	5.87	123.93	121.00
36	LA	1276	U	N3-C2-O2	-5.86	118.10	122.20
1	2	1640	C	C6-N1-C2	-5.86	117.96	120.30
36	LA	1644	C	C5-C6-N1	5.86	123.93	121.00
1	2	101	U	N1-C2-O2	5.86	126.90	122.80
36	LA	2585	G	C4-N9-C1'	5.86	134.12	126.50
36	LA	2552	C	C2-N1-C1'	5.86	125.24	118.80
36	LA	2828	G	N3-C4-C5	-5.86	125.67	128.60
36	LA	217	U	OP1-P-O3'	5.85	118.07	105.20
1	2	1182	U	N1-C2-O2	5.84	126.89	122.80
1	2	1471	A	C5'-C4'-C3'	-5.84	106.65	116.00
36	LA	1495	U	C5-C6-N1	-5.84	119.78	122.70
1	2	176	C	C5-C6-N1	5.84	123.92	121.00
36	LA	1276	U	C5-C6-N1	5.84	125.62	122.70
36	LA	2279	A	C2-N3-C4	5.84	113.52	110.60
36	LA	1581	C	C6-N1-C2	-5.84	117.97	120.30
1	2	143	G	O5'-P-OP2	-5.83	100.45	105.70
36	LA	1278	A	C8-N9-C4	-5.83	103.47	105.80
80	Sm	74	C	O3'-P-O5'	5.83	115.08	104.00
36	LA	637	C	OP1-P-O3'	5.82	118.01	105.20
1	2	711	U	P-O3'-C3'	5.82	126.69	119.70
36	LA	406	G	N1-C6-O6	-5.82	116.41	119.90
1	2	530	C	N3-C2-O2	-5.82	117.83	121.90
1	2	1438	G	N3-C4-C5	-5.82	125.69	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1363	U	C2-N1-C1'	5.81	124.68	117.70
1	2	1461	C	C6-N1-C2	-5.81	117.97	120.30
36	LA	653	A	O5'-P-OP2	-5.81	100.47	105.70
45	LJ	76	ALA	N-CA-CB	5.81	118.23	110.10
36	LA	2617	U	N1-C2-O2	5.80	126.86	122.80
36	LA	2420	C	C5-C6-N1	5.80	123.90	121.00
36	LA	2988	C	C5-C6-N1	5.80	123.90	121.00
36	LA	113	C	C6-N1-C2	-5.80	117.98	120.30
38	LC	110	C	N3-C2-O2	-5.80	117.84	121.90
1	2	1527	C	N3-C2-O2	-5.80	117.84	121.90
36	LA	1822	C	C6-N1-C2	-5.80	117.98	120.30
36	LA	2541	U	C6-N1-C1'	-5.80	113.09	121.20
1	2	1253	U	C5-C6-N1	5.79	125.60	122.70
36	LA	421	G	C4-N9-C1'	5.79	134.03	126.50
1	2	552	G	N3-C4-C5	-5.79	125.70	128.60
36	LA	430	U	N1-C2-O2	5.79	126.85	122.80
36	LA	3153	U	N1-C2-O2	5.79	126.85	122.80
1	2	740	A	N7-C8-N9	5.79	116.69	113.80
1	2	1082	C	O4'-C1'-N1	5.79	112.83	108.20
36	LA	2750	U	C6-N1-C2	-5.78	117.53	121.00
36	LA	2350	C	C6-N1-C2	-5.78	117.99	120.30
80	Sm	56	C	N3-C2-O2	-5.78	117.85	121.90
1	2	886	U	C2-N1-C1'	5.78	124.64	117.70
1	2	1688	U	C2-N1-C1'	5.78	124.64	117.70
36	LA	405	U	O5'-P-OP1	-5.78	100.50	105.70
37	LB	105	C	N1-C2-O2	5.78	122.37	118.90
36	LA	315	C	C6-N1-C2	-5.77	117.99	120.30
1	2	1583	A	O4'-C1'-N9	5.77	112.81	108.20
36	LA	2444	C	N3-C2-O2	-5.76	117.87	121.90
1	2	25	C	N1-C2-O2	5.76	122.36	118.90
1	2	518	A	P-O3'-C3'	5.76	126.61	119.70
1	2	553	G	C6-C5-N7	5.76	133.85	130.40
36	LA	549	U	C5-C6-N1	5.76	125.58	122.70
1	2	1458	G	N7-C8-N9	5.76	115.98	113.10
36	LA	2756	C	C5-C6-N1	5.76	123.88	121.00
36	LA	1128	U	C5-C6-N1	5.76	125.58	122.70
1	2	250	C	C5-C6-N1	5.75	123.88	121.00
36	LA	634	C	C6-N1-C2	-5.75	118.00	120.30
36	LA	835	G	O4'-C1'-N9	5.75	112.80	108.20
36	LA	957	C	C6-N1-C2	-5.75	118.00	120.30
36	LA	2646	C	C6-N1-C2	-5.75	118.00	120.30
36	LA	3196	U	O4'-C1'-N1	5.75	112.80	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	LN	170	LEU	CB-CG-CD2	-5.75	101.22	111.00
48	LM	117	ASP	CB-CG-OD1	5.75	123.47	118.30
1	2	1175	U	C5-C6-N1	5.75	125.57	122.70
1	2	322	G	OP2-P-O3'	5.74	117.84	105.20
1	2	931	C	OP1-P-O3'	5.74	117.83	105.20
36	LA	2638	C	C6-N1-C2	-5.74	118.00	120.30
1	2	1688	U	N1-C2-O2	5.74	126.82	122.80
1	2	656	G	C8-N9-C4	-5.74	104.11	106.40
36	LA	637	C	P-O3'-C3'	5.74	126.59	119.70
36	LA	2825	C	C6-N1-C2	-5.74	118.00	120.30
80	Sm	72	U	N1-C2-O2	5.74	126.82	122.80
36	LA	3298	C	C6-N1-C2	-5.74	118.01	120.30
36	LA	27	C	N1-C2-O2	5.73	122.34	118.90
1	2	54	C	C6-N1-C2	-5.73	118.01	120.30
1	2	1709	C	N1-C2-O2	5.73	122.34	118.90
36	LA	87	U	N1-C2-O2	5.73	126.81	122.80
1	2	121	U	C6-N1-C2	-5.73	117.56	121.00
36	LA	3174	A	O4'-C1'-N9	5.73	112.78	108.20
1	2	1231	U	C5-C6-N1	5.73	125.56	122.70
1	2	1066	C	C2-N1-C1'	5.73	125.10	118.80
36	LA	2290	C	C6-N1-C2	-5.73	118.01	120.30
36	LA	702	C	C5-C6-N1	5.72	123.86	121.00
36	LA	2101	C	C6-N1-C2	-5.72	118.01	120.30
36	LA	2889	C	C5-C6-N1	5.72	123.86	121.00
1	2	934	C	C5-C6-N1	5.72	123.86	121.00
36	LA	1307	G	OP2-P-O3'	5.72	117.78	105.20
36	LA	638	C	O5'-P-OP2	-5.72	100.56	105.70
36	LA	1333	C	C6-N1-C2	-5.72	118.01	120.30
1	2	121	U	N1-C2-O2	5.71	126.80	122.80
1	2	1706	C	N3-C2-O2	-5.71	117.90	121.90
36	LA	2929	C	C6-N1-C2	-5.71	118.02	120.30
70	Lc	106	LYS	CA-CB-CG	5.71	125.97	113.40
1	2	747	C	C2-N1-C1'	5.71	125.08	118.80
36	LA	3269	U	C2-N1-C1'	5.71	124.55	117.70
36	LA	2325	G	O5'-P-OP2	-5.71	100.56	105.70
36	LA	2906	C	C6-N1-C2	-5.71	118.02	120.30
1	2	908	U	N1-C2-O2	5.70	126.79	122.80
36	LA	633	C	C6-N1-C2	-5.70	118.02	120.30
36	LA	2411	U	N3-C2-O2	-5.70	118.21	122.20
36	LA	3344	A	C8-N9-C4	-5.70	103.52	105.80
1	2	1274	C	N1-C2-O2	5.70	122.32	118.90
1	2	1688	U	N3-C2-O2	-5.70	118.21	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1777	G	N3-C4-N9	5.70	129.42	126.00
36	LA	2873	U	N1-C2-O2	5.70	126.79	122.80
9	B	148	ARG	CA-CB-CG	5.70	125.93	113.40
36	LA	2388	U	N3-C2-O2	-5.70	118.21	122.20
38	LC	85	G	P-O3'-C3'	5.69	126.53	119.70
38	LC	100	U	N3-C2-O2	-5.69	118.21	122.20
1	2	609	U	P-O3'-C3'	5.69	126.53	119.70
1	2	1399	C	C6-N1-C2	-5.69	118.02	120.30
1	2	1763	A	O5'-P-OP2	-5.69	100.58	105.70
36	LA	141	C	C6-N1-C2	-5.69	118.02	120.30
36	LA	208	C	C6-N1-C2	-5.69	118.02	120.30
36	LA	849	C	P-O3'-C3'	5.69	126.52	119.70
36	LA	1941	C	C6-N1-C2	-5.69	118.03	120.30
80	Sn	50	U	C5-C6-N1	5.69	125.54	122.70
1	2	864	U	C2-N1-C1'	5.68	124.52	117.70
1	2	890	C	C6-N1-C2	-5.68	118.03	120.30
1	2	94	U	C6-N1-C2	-5.68	117.59	121.00
1	2	338	C	C6-N1-C2	-5.68	118.03	120.30
36	LA	28	C	C6-N1-C2	-5.68	118.03	120.30
36	LA	1103	A	N3-C4-N9	5.68	131.94	127.40
1	2	1636	C	P-O3'-C3'	5.68	126.52	119.70
12	V	29	LEU	CB-CG-CD2	5.68	120.65	111.00
36	LA	886	C	C5-C6-N1	5.68	123.84	121.00
36	LA	1271	A	P-O3'-C3'	5.68	126.52	119.70
36	LA	2279	A	N1-C6-N6	-5.68	115.19	118.60
36	LA	2101	C	OP1-P-O3'	5.68	117.69	105.20
1	2	1666	U	N1-C2-O2	5.67	126.77	122.80
36	LA	3165	A	N7-C8-N9	5.67	116.64	113.80
1	2	1549	C	C6-N1-C2	-5.67	118.03	120.30
1	2	116	U	N1-C2-O2	5.66	126.77	122.80
1	2	411	C	C6-N1-C2	-5.66	118.03	120.30
1	2	531	C	N3-C2-O2	-5.66	117.94	121.90
1	2	553	G	C5-C6-O6	5.66	132.00	128.60
1	2	1706	C	N1-C2-O2	5.66	122.30	118.90
36	LA	27	C	N3-C2-O2	-5.66	117.94	121.90
36	LA	375	A	OP1-P-O3'	5.66	117.66	105.20
1	2	120	U	N1-C2-O2	5.66	126.76	122.80
36	LA	1901	A	N7-C8-N9	5.66	116.63	113.80
36	LA	2550	U	C2-N1-C1'	5.66	124.49	117.70
36	LA	800	G	N3-C4-C5	-5.66	125.77	128.60
80	Sm	66	C	O4'-C1'-N1	5.66	112.72	108.20
36	LA	860	G	N3-C2-N2	-5.65	115.94	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	74	VAL	CA-CB-CG1	5.65	119.38	110.90
36	LA	922	U	C5-C6-N1	5.65	125.53	122.70
1	2	1205	C	C5-C6-N1	5.65	123.83	121.00
36	LA	2894	C	C5-C6-N1	5.65	123.83	121.00
32	g	39	LEU	CB-CG-CD1	5.65	120.60	111.00
36	LA	873	C	P-O3'-C3'	5.65	126.48	119.70
36	LA	881	C	C2-N1-C1'	5.64	125.01	118.80
36	LA	1238	C	C6-N1-C2	-5.64	118.04	120.30
36	LA	2181	C	C6-N1-C2	-5.64	118.04	120.30
36	LA	2505	U	O4'-C1'-N1	5.64	112.71	108.20
36	LA	1832	C	C5-C6-N1	5.64	123.82	121.00
74	Lg	78	LEU	CA-CB-CG	5.64	128.27	115.30
36	LA	2913	C	C5-C6-N1	5.64	123.82	121.00
36	LA	1064	A	OP2-P-O3'	5.64	117.60	105.20
36	LA	2274	U	C2-N1-C1'	5.64	124.46	117.70
41	LF	4	PRO	C-N-CA	5.64	135.79	121.70
20	G	33	ARG	NE-CZ-NH2	-5.63	117.48	120.30
36	LA	1579	C	C6-N1-C2	-5.63	118.05	120.30
48	LM	108	GLU	CA-CB-CG	5.63	125.80	113.40
1	2	1533	C	N3-C2-O2	-5.63	117.96	121.90
34	O	234	LEU	CA-CB-CG	5.63	128.25	115.30
36	LA	3214	U	O4'-C1'-N1	5.63	112.70	108.20
1	2	1199	G	C2-N3-C4	5.63	114.72	111.90
36	LA	982	C	C5-C6-N1	5.63	123.81	121.00
36	LA	1368	U	C2-N1-C1'	5.63	124.45	117.70
1	2	795	U	N1-C2-O2	5.63	126.74	122.80
36	LA	1762	C	C6-N1-C2	-5.63	118.05	120.30
37	LB	44	C	N3-C2-O2	-5.62	117.96	121.90
1	2	1332	C	C2-N1-C1'	5.62	124.99	118.80
36	LA	142	C	N1-C2-O2	5.62	122.28	118.90
1	2	275	C	C5-C6-N1	5.62	123.81	121.00
25	b	65	LEU	CA-CB-CG	5.62	128.23	115.30
36	LA	955	U	N3-C2-O2	-5.62	118.27	122.20
36	LA	1103	A	N3-C4-C5	-5.62	122.86	126.80
36	LA	2712	U	C2-N1-C1'	5.62	124.44	117.70
80	Sm	72	U	N3-C2-O2	-5.62	118.27	122.20
1	2	305	C	C6-N1-C2	-5.62	118.05	120.30
36	LA	2681	U	C5-C6-N1	5.62	125.51	122.70
36	LA	2707	C	C6-N1-C2	-5.62	118.05	120.30
36	LA	1126	G	C6-C5-N7	-5.61	127.03	130.40
36	LA	1219	C	N1-C2-O2	5.61	122.27	118.90
36	LA	2772	C	N3-C2-O2	-5.61	117.97	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	LK	140	VAL	CA-CB-CG2	5.61	119.32	110.90
36	LA	2401	A	O5'-P-OP2	-5.61	100.65	105.70
1	2	861	U	C5-C6-N1	5.61	125.50	122.70
1	2	1216	C	N3-C2-O2	-5.61	117.97	121.90
36	LA	356	C	C5-C6-N1	5.61	123.80	121.00
36	LA	1296	C	C5-C6-N1	5.61	123.80	121.00
1	2	1361	U	N3-C2-O2	-5.61	118.28	122.20
36	LA	2710	C	C6-N1-C2	-5.60	118.06	120.30
36	LA	1156	C	C6-N1-C2	-5.60	118.06	120.30
80	Sm	5	C	N3-C2-O2	-5.60	117.98	121.90
1	2	280	U	P-O3'-C3'	5.59	126.41	119.70
36	LA	3196	U	C6-N1-C1'	-5.59	113.37	121.20
1	2	14	C	C5-C6-N1	5.59	123.80	121.00
36	LA	2772	C	C6-N1-C2	-5.59	118.06	120.30
36	LA	2340	U	C5-C6-N1	5.59	125.49	122.70
1	2	1226	A	P-O3'-C3'	5.59	126.40	119.70
1	2	1347	U	N1-C2-O2	5.59	126.71	122.80
11	U	128	ASP	CB-CG-OD1	5.58	123.33	118.30
36	LA	3269	U	N1-C2-O2	5.58	126.71	122.80
18	Z	52	ARG	CB-CA-C	-5.58	99.24	110.40
36	LA	2331	C	C6-N1-C2	-5.58	118.07	120.30
1	2	555	A	C5-N7-C8	-5.58	101.11	103.90
1	2	1503	A	O4'-C1'-N9	5.58	112.66	108.20
50	LO	65	LEU	CB-CG-CD1	5.58	120.48	111.00
80	Sn	49	C	N1-C2-O2	5.58	122.25	118.90
36	LA	3039	C	C6-N1-C2	-5.58	118.07	120.30
36	LA	2710	C	C5-C6-N1	5.57	123.79	121.00
1	2	64	U	N3-C2-O2	-5.57	118.30	122.20
1	2	1472	C	C6-N1-C2	-5.57	118.07	120.30
1	2	1628	U	C5-C6-N1	5.57	125.49	122.70
1	2	499	U	C5-C6-N1	5.57	125.48	122.70
36	LA	2986	U	C5-C6-N1	5.57	125.48	122.70
37	LB	68	C	C5-C6-N1	5.56	123.78	121.00
36	LA	3309	G	N3-C4-C5	-5.56	125.82	128.60
1	2	1216	C	N1-C2-O2	5.56	122.24	118.90
36	LA	1759	C	C6-N1-C2	-5.56	118.08	120.30
1	2	1611	A	C2-N3-C4	-5.56	107.82	110.60
36	LA	3228	C	OP2-P-O3'	5.56	117.43	105.20
36	LA	1448	U	C5-C6-N1	5.55	125.48	122.70
36	LA	492	C	C5-C6-N1	5.55	123.78	121.00
36	LA	2297	U	N1-C2-N3	5.55	118.23	114.90
36	LA	3155	U	C2-N1-C1'	5.55	124.36	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	O	141	LEU	CA-CB-CG	5.55	128.07	115.30
36	LA	54	C	C6-N1-C2	-5.55	118.08	120.30
39	LD	219	ILE	CG1-CB-CG2	-5.55	99.19	111.40
36	LA	2689	A	C8-N9-C4	-5.55	103.58	105.80
36	LA	1898	G	O4'-C1'-N9	5.55	112.64	108.20
1	2	1355	C	C6-N1-C2	-5.54	118.08	120.30
36	LA	2267	C	C6-N1-C2	-5.54	118.08	120.30
36	LA	288	C	C5-C6-N1	5.54	123.77	121.00
36	LA	1722	U	N1-C2-O2	5.54	126.68	122.80
44	LI	126	LEU	CA-CB-CG	5.54	128.05	115.30
36	LA	3181	C	C6-N1-C2	-5.54	118.08	120.30
36	LA	2256	A	O4'-C1'-N9	5.54	112.63	108.20
80	Sn	25	C	N1-C2-O2	5.54	122.22	118.90
36	LA	102	C	C6-N1-C2	-5.54	118.08	120.30
36	LA	1273	A	C8-N9-C1'	-5.54	117.73	127.70
36	LA	142	C	C5-C6-N1	5.54	123.77	121.00
36	LA	2606	G	N3-C4-C5	-5.54	125.83	128.60
81	EF	692	LEU	CA-CB-CG	5.54	128.03	115.30
1	2	1251	U	C6-N1-C2	-5.53	117.68	121.00
36	LA	2405	C	C5-C6-N1	5.53	123.77	121.00
38	LC	143	U	C5-C6-N1	5.53	125.47	122.70
7	A	14	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	2	1515	A	C8-N9-C4	-5.53	103.59	105.80
36	LA	2331	C	C5-C6-N1	5.53	123.77	121.00
1	2	1007	C	C5-C6-N1	5.53	123.77	121.00
18	Z	105	LEU	CA-CB-CG	5.53	128.02	115.30
1	2	610	G	C4-N9-C1'	5.53	133.69	126.50
36	LA	2961	G	C8-N9-C4	-5.53	104.19	106.40
36	LA	1183	C	C5-C6-N1	5.53	123.76	121.00
36	LA	1820	U	OP2-P-O3'	5.53	117.36	105.20
36	LA	3097	C	C6-N1-C2	-5.53	118.09	120.30
1	2	1284	C	C2-N1-C1'	5.52	124.88	118.80
1	2	1210	C	C6-N1-C2	-5.52	118.09	120.30
1	2	1420	C	C6-N1-C2	-5.52	118.09	120.30
36	LA	1190	A	C4-N9-C1'	5.52	136.24	126.30
1	2	740	A	C8-N9-C4	-5.52	103.59	105.80
1	2	1199	G	N3-C4-C5	-5.52	125.84	128.60
36	LA	1759	C	C5-C6-N1	5.52	123.76	121.00
36	LA	548	G	O4'-C1'-N9	5.52	112.61	108.20
36	LA	753	C	C6-N1-C2	-5.52	118.09	120.30
1	2	700	C	C6-N1-C2	-5.51	118.09	120.30
36	LA	8	C	C6-N1-C2	-5.51	118.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	LG	110	LEU	CA-CB-CG	5.51	127.98	115.30
36	LA	3363	U	N1-C2-O2	5.51	126.66	122.80
1	2	1646	C	N1-C2-O2	5.51	122.21	118.90
36	LA	915	A	C8-N9-C1'	-5.51	117.78	127.70
36	LA	2828	G	N3-C4-N9	5.51	129.31	126.00
1	2	863	A	C8-N9-C4	-5.51	103.60	105.80
36	LA	2257	C	C2-N1-C1'	5.51	124.86	118.80
36	LA	2652	U	N1-C2-O2	5.51	126.66	122.80
37	LB	116	C	C6-N1-C2	-5.51	118.10	120.30
58	Lq	50	LEU	CA-CB-CG	5.51	127.97	115.30
80	Sn	27	C	C6-N1-C2	-5.51	118.10	120.30
55	Ln	182	ASP	CB-CG-OD1	5.50	123.25	118.30
36	LA	982	C	N3-C2-O2	-5.50	118.05	121.90
36	LA	1265	U	N1-C2-O2	5.50	126.65	122.80
36	LA	1844	C	C6-N1-C2	-5.50	118.10	120.30
1	2	708	C	C6-N1-C2	-5.50	118.10	120.30
1	2	1082	C	C6-N1-C1'	-5.50	114.20	120.80
36	LA	2420	C	C6-N1-C2	-5.50	118.10	120.30
36	LA	2996	U	C2-N1-C1'	5.50	124.30	117.70
36	LA	2617	U	C5-C4-O4	5.50	129.20	125.90
1	2	691	C	C6-N1-C2	-5.50	118.10	120.30
1	2	160	C	C6-N1-C2	-5.49	118.10	120.30
17	Y	56	ASP	CB-CG-OD1	5.49	123.24	118.30
1	2	856	A	P-O3'-C3'	5.49	126.29	119.70
1	2	1201	G	N3-C4-N9	-5.49	122.71	126.00
37	LB	33	U	C2-N1-C1'	-5.49	111.11	117.70
36	LA	1907	C	C6-N1-C2	-5.49	118.10	120.30
36	LA	793	C	C5-C6-N1	5.49	123.74	121.00
36	LA	1227	C	C2-N1-C1'	5.49	124.83	118.80
36	LA	2689	A	C4-N9-C1'	5.48	136.17	126.30
1	2	893	U	N3-C2-O2	-5.48	118.36	122.20
36	LA	3228	C	P-O3'-C3'	5.48	126.28	119.70
36	LA	3277	U	N1-C2-O2	5.48	126.64	122.80
1	2	237	C	N3-C2-O2	-5.48	118.06	121.90
36	LA	2110	G	O4'-C1'-N9	5.48	112.58	108.20
36	LA	2622	C	N3-C2-O2	-5.48	118.07	121.90
36	LA	1263	A	N3-C4-C5	-5.48	122.97	126.80
36	LA	3275	U	N1-C2-O2	5.48	126.63	122.80
1	2	885	G	C8-N9-C4	-5.47	104.21	106.40
36	LA	889	U	C5-C6-N1	5.47	125.44	122.70
36	LA	1633	C	C5-C6-N1	5.47	123.73	121.00
36	LA	1605	A	O4'-C1'-N9	5.47	112.57	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	LA	3269	U	OP2-P-O3'	5.47	117.23	105.20
36	LA	3285	C	C6-N1-C2	-5.47	118.11	120.30
1	2	981	U	N3-C2-O2	-5.46	118.38	122.20
36	LA	448	U	C5-C6-N1	5.46	125.43	122.70
36	LA	1780	G	C4-N9-C1'	5.46	133.60	126.50
36	LA	1842	A	O4'-C1'-N9	-5.46	103.83	108.20
1	2	835	U	C5-C6-N1	5.46	125.43	122.70
1	2	101	U	N3-C2-O2	-5.46	118.38	122.20
36	LA	47	C	C6-N1-C2	-5.45	118.12	120.30
36	LA	875	G	N3-C4-N9	5.45	129.27	126.00
36	LA	955	U	N1-C2-O2	5.45	126.62	122.80
1	2	425	A	OP2-P-O3'	5.45	117.19	105.20
1	2	1596	C	N1-C2-O2	5.45	122.17	118.90
36	LA	3350	C	O4'-C1'-N1	5.45	112.56	108.20
1	2	361	C	C6-N1-C2	-5.45	118.12	120.30
1	2	35	U	N3-C2-O2	-5.44	118.39	122.20
1	2	166	C	N3-C2-O2	-5.44	118.09	121.90
1	2	184	C	C2-N1-C1'	5.44	124.79	118.80
1	2	250	C	C6-N1-C2	-5.44	118.12	120.30
1	2	1307	U	N1-C2-O2	5.44	126.61	122.80
36	LA	2257	C	N1-C2-O2	5.44	122.17	118.90
36	LA	192	C	C6-N1-C2	-5.44	118.12	120.30
36	LA	3233	C	C6-N1-C2	-5.44	118.12	120.30
36	LA	1470	U	N3-C2-O2	-5.44	118.39	122.20
36	LA	1609	C	C6-N1-C2	-5.44	118.12	120.30
1	2	304	U	N3-C2-O2	-5.43	118.40	122.20
18	Z	27	PHE	CB-CG-CD2	-5.43	117.00	120.80
36	LA	985	U	N3-C2-O2	-5.43	118.39	122.20
1	2	477	A	O5'-P-OP1	-5.43	100.81	105.70
1	2	1205	C	C2-N1-C1'	5.43	124.78	118.80
36	LA	1665	C	C5-C6-N1	5.43	123.72	121.00
36	LA	3298	C	C5-C6-N1	5.43	123.72	121.00
36	LA	1907	C	C2-N1-C1'	5.43	124.77	118.80
9	B	135	ASP	CB-CG-OD1	5.43	123.19	118.30
36	LA	2961	G	N7-C8-N9	5.43	115.81	113.10
36	LA	600	G	C6-C5-N7	-5.43	127.14	130.40
1	2	599	A	O5'-P-OP1	5.42	117.21	110.70
36	LA	492	C	C2-N1-C1'	5.42	124.77	118.80
36	LA	3105	U	N3-C2-O2	-5.42	118.40	122.20
1	2	1003	A	O4'-C1'-N9	5.42	112.54	108.20
1	2	1308	G	C4-N9-C1'	5.42	133.55	126.50
36	LA	881	C	C5-C6-N1	5.42	123.71	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	LA	2622	C	C6-N1-C2	-5.42	118.13	120.30
1	2	469	C	C5-C6-N1	5.42	123.71	121.00
1	2	186	C	C5-C6-N1	5.42	123.71	121.00
1	2	446	A	C4-N9-C1'	5.42	136.05	126.30
36	LA	3214	U	C6-N1-C1'	-5.42	113.62	121.20
80	Sn	3	C	C5-C6-N1	5.42	123.71	121.00
1	2	1688	U	C5-C6-N1	5.42	125.41	122.70
36	LA	698	U	C5-C6-N1	5.42	125.41	122.70
36	LA	855	U	C2-N1-C1'	5.41	124.20	117.70
1	2	609	U	OP2-P-O3'	5.41	117.11	105.20
36	LA	228	U	C6-N1-C2	-5.41	117.75	121.00
36	LA	191	U	C5-C6-N1	5.41	125.41	122.70
54	Lm	89	ASP	CB-CG-OD1	5.41	123.17	118.30
55	Ln	181	ARG	CA-CB-CG	5.41	125.30	113.40
1	2	871	G	N3-C4-C5	-5.41	125.90	128.60
36	LA	3057	U	N1-C2-O2	5.41	126.58	122.80
42	LG	213	ASP	CB-CG-OD1	5.41	123.17	118.30
1	2	1182	U	N3-C2-O2	-5.41	118.42	122.20
36	LA	1843	C	C6-N1-C2	-5.41	118.14	120.30
36	LA	2501	U	N1-C2-O2	5.41	126.58	122.80
36	LA	3068	U	OP1-P-O3'	5.41	117.09	105.20
1	2	1491	U	C2-N1-C1'	5.40	124.18	117.70
36	LA	2356	A	C5-N7-C8	-5.40	101.20	103.90
1	2	1403	C	C6-N1-C2	-5.40	118.14	120.30
17	Y	3	ARG	CB-CG-CD	5.40	125.64	111.60
36	LA	2407	C	C5-C6-N1	5.40	123.70	121.00
1	2	1620	C	C5-C6-N1	5.40	123.70	121.00
36	LA	823	C	C5-C6-N1	5.40	123.70	121.00
36	LA	1224	C	C6-N1-C2	-5.40	118.14	120.30
80	Sn	32	C	N3-C2-O2	-5.40	118.12	121.90
36	LA	282	G	N7-C8-N9	5.40	115.80	113.10
36	LA	1446	A	O4'-C1'-N9	-5.40	103.88	108.20
36	LA	247	C	C6-N1-C2	-5.39	118.14	120.30
36	LA	3193	C	C6-N1-C2	-5.39	118.14	120.30
1	2	1359	C	C5-C6-N1	5.39	123.69	121.00
1	2	1706	C	C6-N1-C2	-5.39	118.14	120.30
36	LA	2619	G	C6-C5-N7	-5.39	127.17	130.40
28	K	53	GLU	CA-CB-CG	5.39	125.26	113.40
36	LA	1578	C	C6-N1-C2	-5.39	118.14	120.30
38	LC	115	C	C5-C6-N1	5.39	123.69	121.00
43	LH	77	ARG	N-CA-CB	5.39	120.30	110.60
80	Sm	50	U	O5'-P-OP2	-5.39	100.85	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	LA	596	C	N3-C2-O2	-5.39	118.13	121.90
36	LA	2356	A	C4-C5-N7	5.39	113.39	110.70
36	LA	3253	G	O4'-C1'-N9	5.39	112.51	108.20
1	2	1491	U	N1-C2-O2	5.38	126.57	122.80
36	LA	2970	C	C6-N1-C1'	5.38	127.26	120.80
42	LG	146	LEU	CB-CG-CD1	-5.38	101.85	111.00
1	2	741	C	C6-N1-C2	-5.38	118.15	120.30
1	2	1261	G	N3-C4-C5	-5.38	125.91	128.60
1	2	1320	U	N3-C2-O2	-5.38	118.44	122.20
36	LA	2712	U	N1-C2-O2	5.38	126.56	122.80
36	LA	2405	C	C2-N1-C1'	5.37	124.71	118.80
36	LA	2810	C	C6-N1-C2	-5.37	118.15	120.30
36	LA	1581	C	N1-C2-O2	5.37	122.12	118.90
80	Sm	34	C	N3-C2-O2	-5.37	118.14	121.90
1	2	409	C	C6-N1-C2	-5.37	118.15	120.30
1	2	1182	U	C6-N1-C1'	-5.37	113.69	121.20
36	LA	193	C	C6-N1-C2	-5.37	118.15	120.30
36	LA	427	C	C5-C6-N1	5.37	123.68	121.00
36	LA	2726	C	C2-N1-C1'	5.37	124.70	118.80
36	LA	2846	U	C6-N1-C2	-5.37	117.78	121.00
36	LA	800	G	C8-N9-C4	-5.36	104.25	106.40
1	2	747	C	N1-C2-O2	5.36	122.12	118.90
1	2	533	U	C5-C6-N1	5.36	125.38	122.70
1	2	1510	U	C5-C6-N1	5.36	125.38	122.70
36	LA	1278	A	O4'-C1'-N9	5.36	112.49	108.20
36	LA	1562	C	C3'-C2'-C1'	5.36	105.79	101.50
36	LA	609	G	C5-C6-O6	-5.36	125.39	128.60
36	LA	1920	U	OP2-P-O3'	5.36	116.99	105.20
49	LN	51	LEU	CA-CB-CG	5.36	127.62	115.30
1	2	1528	U	C2-N1-C1'	5.36	124.13	117.70
36	LA	3089	C	C5-C6-N1	5.36	123.68	121.00
1	2	1308	G	C8-N9-C1'	-5.35	120.04	127.00
1	2	1657	U	N3-C2-O2	-5.35	118.45	122.20
1	2	956	C	C6-N1-C2	-5.35	118.16	120.30
36	LA	3138	U	O5'-P-OP2	-5.35	100.88	105.70
1	2	1535	U	C2-N1-C1'	5.35	124.12	117.70
36	LA	315	C	C2-N1-C1'	5.35	124.69	118.80
37	LB	98	C	C6-N1-C2	-5.35	118.16	120.30
1	2	323	A	C2-N3-C4	5.35	113.27	110.60
36	LA	2836	C	C6-N1-C1'	-5.35	114.38	120.80
36	LA	732	C	C6-N1-C2	-5.34	118.16	120.30
66	LY	104	LEU	CA-CB-CG	5.34	127.59	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	861	U	N1-C2-O2	5.34	126.54	122.80
5	E	57	MET	CB-CG-SD	5.34	128.43	112.40
1	2	260	U	C6-N1-C2	-5.34	117.80	121.00
1	2	546	U	O4'-C1'-N1	5.34	112.47	108.20
36	LA	1657	C	C6-N1-C2	-5.34	118.16	120.30
36	LA	3195	U	N3-C2-O2	-5.34	118.46	122.20
80	Sm	20	A	C8-N9-C4	-5.34	103.66	105.80
36	LA	1943	C	C6-N1-C2	-5.34	118.17	120.30
36	LA	1859	A	C8-N9-C4	-5.34	103.67	105.80
36	LA	2476	C	C6-N1-C2	-5.34	118.17	120.30
36	LA	2773	C	C2-N1-C1'	5.33	124.67	118.80
1	2	433	C	C5-C6-N1	5.33	123.67	121.00
36	LA	421	G	C8-N9-C1'	-5.33	120.07	127.00
36	LA	1269	U	C6-N1-C1'	-5.33	113.74	121.20
36	LA	1843	C	N1-C2-O2	5.33	122.10	118.90
36	LA	2765	C	C5-C6-N1	5.33	123.67	121.00
36	LA	3306	U	O4'-C1'-N1	5.33	112.46	108.20
36	LA	1172	G	C8-N9-C4	-5.33	104.27	106.40
1	2	1235	C	C2-N1-C1'	5.33	124.66	118.80
36	LA	2594	C	C5-C6-N1	5.32	123.66	121.00
1	2	494	U	N1-C2-O2	5.32	126.53	122.80
36	LA	915	A	N7-C8-N9	5.32	116.46	113.80
36	LA	3034	C	C6-N1-C2	-5.32	118.17	120.30
36	LA	517	G	N3-C4-N9	5.32	129.19	126.00
36	LA	1741	A	O4'-C1'-N9	5.32	112.45	108.20
36	LA	3121	U	O5'-P-OP1	-5.31	100.92	105.70
36	LA	2712	U	N3-C2-O2	-5.31	118.48	122.20
36	LA	1851	G	C6-C5-N7	-5.31	127.22	130.40
36	LA	2726	C	N3-C2-O2	-5.31	118.19	121.90
1	2	530	C	C2-N1-C1'	5.30	124.64	118.80
36	LA	2594	C	N3-C2-O2	-5.30	118.19	121.90
36	LA	3278	C	C6-N1-C1'	-5.30	114.44	120.80
36	LA	2497	U	C5'-C4'-O4'	-5.30	102.74	109.10
80	Sm	56	C	C6-N1-C2	-5.30	118.18	120.30
36	LA	2274	U	N3-C2-O2	-5.30	118.49	122.20
1	2	1646	C	N3-C2-O2	-5.30	118.19	121.90
36	LA	2194	G	C4-N9-C1'	5.30	133.39	126.50
36	LA	1604	G	C2-N3-C4	5.30	114.55	111.90
1	2	185	U	C2-N1-C1'	5.29	124.05	117.70
1	2	387	A	OP2-P-O3'	5.29	116.84	105.20
36	LA	1296	C	C6-N1-C2	-5.29	118.18	120.30
36	LA	614	C	C5-C6-N1	5.29	123.65	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	LA	79	U	C5-C6-N1	5.29	125.34	122.70
36	LA	609	G	N9-C4-C5	-5.29	103.28	105.40
36	LA	1386	A	O5'-P-OP2	-5.29	100.94	105.70
38	LC	127	U	C5-C6-N1	5.29	125.34	122.70
1	2	633	U	N3-C2-O2	-5.29	118.50	122.20
36	LA	283	G	C4-N9-C1'	5.29	133.38	126.50
36	LA	800	G	C4-N9-C1'	5.29	133.38	126.50
36	LA	1339	C	C6-N1-C2	-5.29	118.18	120.30
36	LA	2714	G	C2-N3-C4	-5.28	109.26	111.90
36	LA	2925	C	C6-N1-C2	-5.28	118.19	120.30
36	LA	959	C	P-O3'-C3'	5.28	126.03	119.70
36	LA	2501	U	N3-C2-O2	-5.28	118.50	122.20
36	LA	1943	C	C5-C6-N1	5.28	123.64	121.00
36	LA	3275	U	P-O3'-C3'	5.28	126.03	119.70
1	2	1491	U	N3-C2-O2	-5.28	118.51	122.20
36	LA	517	G	N3-C4-C5	-5.28	125.96	128.60
36	LA	1766	G	N3-C4-N9	5.28	129.16	126.00
80	Sm	72	U	C5'-C4'-C3'	5.28	124.44	116.00
36	LA	1230	G	N3-C4-N9	5.27	129.16	126.00
36	LA	1581	C	C5-C6-N1	5.27	123.64	121.00
36	LA	3384	U	C5-C6-N1	5.27	125.34	122.70
80	Sm	75	C	C6-N1-C2	-5.27	118.19	120.30
36	LA	1433	A	O4'-C1'-N9	-5.27	103.98	108.20
36	LA	2619	G	C4-N9-C1'	5.27	133.35	126.50
1	2	1759	C	C6-N1-C2	-5.27	118.19	120.30
1	2	172	C	C6-N1-C2	-5.27	118.19	120.30
1	2	1080	U	C2-N1-C1'	5.27	124.02	117.70
36	LA	2187	G	N1-C6-O6	-5.27	116.74	119.90
1	2	1279	C	C5-C6-N1	5.26	123.63	121.00
36	LA	1501	U	C5-C6-N1	5.26	125.33	122.70
36	LA	439	C	C6-N1-C2	-5.26	118.19	120.30
1	2	189	C	C5-C6-N1	5.26	123.63	121.00
1	2	894	U	N3-C2-O2	-5.26	118.52	122.20
36	LA	1751	G	C4-N9-C1'	-5.26	119.66	126.50
1	2	1214	U	C5-C6-N1	5.26	125.33	122.70
36	LA	861	C	C6-N1-C2	-5.26	118.20	120.30
1	2	539	G	P-O3'-C3'	5.25	126.00	119.70
1	2	828	U	N3-C2-O2	-5.25	118.52	122.20
1	2	1572	G	O4'-C1'-N9	5.25	112.40	108.20
36	LA	1023	C	C5-C6-N1	5.25	123.63	121.00
36	LA	2551	U	C6-N1-C2	-5.25	117.85	121.00
1	2	1510	U	N3-C2-O2	-5.25	118.52	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	G	34	LEU	CA-CB-CG	5.25	127.38	115.30
36	LA	1183	C	C6-N1-C2	-5.25	118.20	120.30
1	2	1585	U	C6-N1-C2	-5.25	117.85	121.00
36	LA	3255	U	C5-C6-N1	5.25	125.33	122.70
80	Sn	74	C	C6-N1-C2	-5.25	118.20	120.30
36	LA	298	U	N1-C2-O2	5.25	126.47	122.80
36	LA	439	C	P-O3'-C3'	5.25	126.00	119.70
36	LA	2274	U	C5-C6-N1	5.25	125.32	122.70
1	2	25	C	N3-C2-O2	-5.24	118.23	121.90
36	LA	2983	C	O4'-C1'-N1	5.24	112.39	108.20
73	Lf	72	ARG	CG-CD-NE	5.24	122.81	111.80
1	2	54	C	C5-C6-N1	5.24	123.62	121.00
1	2	1535	U	N3-C2-O2	-5.24	118.53	122.20
1	2	1172	G	C8-N9-C4	-5.24	104.30	106.40
1	2	1291	G	C4-N9-C1'	5.24	133.31	126.50
1	2	1556	A	OP2-P-O3'	5.24	116.72	105.20
36	LA	3350	C	C6-N1-C2	-5.24	118.20	120.30
1	2	759	U	N3-C2-O2	-5.24	118.53	122.20
36	LA	2209	U	N1-C2-O2	5.24	126.46	122.80
36	LA	2982	A	C4-C5-N7	5.24	113.32	110.70
36	LA	193	C	C5-C6-N1	5.23	123.62	121.00
1	2	1214	U	N1-C2-O2	5.23	126.46	122.80
36	LA	2844	C	C6-N1-C2	-5.23	118.21	120.30
36	LA	3137	C	C6-N1-C2	-5.23	118.21	120.30
36	LA	3196	U	C5-C6-N1	5.23	125.31	122.70
42	LG	41	LYS	CA-CB-CG	5.23	124.91	113.40
45	LJ	26	LEU	CA-CB-CG	5.23	127.33	115.30
36	LA	291	C	C5-C6-N1	5.23	123.61	121.00
36	LA	3049	A	C2-N3-C4	5.23	113.22	110.60
1	2	838	G	P-O3'-C3'	5.23	125.97	119.70
5	E	77	ARG	CG-CD-NE	5.23	122.77	111.80
1	2	777	C	C6-N1-C2	-5.22	118.21	120.30
36	LA	2434	U	C6-N1-C1'	-5.22	113.89	121.20
1	2	795	U	C2-N1-C1'	5.22	123.97	117.70
1	2	795	U	C5-C6-N1	5.22	125.31	122.70
80	Sn	20	A	OP2-P-O3'	5.22	116.69	105.20
36	LA	1876	U	C5-C6-N1	5.22	125.31	122.70
1	2	587	C	C5-C6-N1	5.22	123.61	121.00
37	LB	33	U	C6-N1-C1'	5.22	128.50	121.20
1	2	1222	C	C6-N1-C2	-5.22	118.21	120.30
1	2	68	A	P-O3'-C3'	5.21	125.96	119.70
1	2	1471	A	OP1-P-O3'	5.21	116.67	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	LM	167	TYR	CB-CG-CD1	-5.21	117.87	121.00
1	2	681	U	O5'-P-OP2	-5.21	101.01	105.70
36	LA	1764	U	P-O3'-C3'	5.21	125.95	119.70
36	LA	3157	U	P-O3'-C3'	5.21	125.96	119.70
1	2	1063	U	N3-C2-O2	-5.21	118.55	122.20
1	2	1559	A	O5'-P-OP2	-5.21	101.01	105.70
36	LA	1870	C	C6-N1-C2	-5.21	118.22	120.30
66	LY	34	LEU	CA-CB-CG	5.21	127.28	115.30
1	2	552	G	C8-N9-C1'	-5.21	120.23	127.00
36	LA	1086	C	C6-N1-C2	-5.21	118.22	120.30
36	LA	1873	U	N1-C2-O2	5.21	126.44	122.80
36	LA	3121	U	OP1-P-O3'	5.21	116.66	105.20
36	LA	1238	C	N1-C2-O2	5.21	122.02	118.90
36	LA	1093	A	O4'-C1'-N9	-5.20	104.04	108.20
36	LA	1819	U	N3-C2-O2	-5.20	118.56	122.20
38	LC	125	U	O4'-C1'-N1	5.20	112.36	108.20
1	2	440	U	N1-C2-N3	5.20	118.02	114.90
36	LA	1358	C	C6-N1-C2	-5.20	118.22	120.30
36	LA	1822	C	C5-C6-N1	5.20	123.60	121.00
36	LA	2829	U	C5-C6-N1	5.20	125.30	122.70
1	2	1235	C	C5-C6-N1	5.20	123.60	121.00
36	LA	713	U	C6-N1-C2	-5.20	117.88	121.00
36	LA	1228	C	N1-C2-O2	5.20	122.02	118.90
36	LA	2809	C	C5-C6-N1	5.20	123.60	121.00
36	LA	2207	A	C5-C6-N6	-5.20	119.54	123.70
1	2	304	U	N1-C2-O2	5.20	126.44	122.80
36	LA	893	C	C6-N1-C2	-5.20	118.22	120.30
36	LA	2889	C	C6-N1-C2	-5.20	118.22	120.30
38	LC	90	U	C5-C6-N1	5.20	125.30	122.70
36	LA	1230	G	C6-C5-N7	-5.19	127.28	130.40
36	LA	1878	G	C8-N9-C1'	-5.19	120.25	127.00
36	LA	3023	U	N1-C2-O2	5.19	126.44	122.80
36	LA	3023	U	N3-C2-O2	-5.19	118.56	122.20
39	LD	5	ILE	CG1-CB-CG2	-5.19	99.97	111.40
1	2	1252	C	C6-N1-C2	-5.19	118.22	120.30
1	2	1560	U	C6-N1-C1'	-5.19	113.93	121.20
36	LA	604	G	C4-C5-N7	5.19	112.88	110.80
36	LA	1275	C	N3-C2-O2	-5.19	118.27	121.90
36	LA	3207	U	O4'-C1'-N1	5.19	112.35	108.20
36	LA	2924	U	N3-C2-O2	-5.19	118.57	122.20
1	2	1197	C	C6-N1-C2	-5.19	118.22	120.30
36	LA	2510	U	O4'-C1'-N1	5.19	112.35	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	EF	967	ASP	CB-CG-OD1	5.19	122.97	118.30
1	2	446	A	C8-N9-C1'	-5.19	118.36	127.70
1	2	1591	C	C6-N1-C2	-5.19	118.22	120.30
36	LA	354	U	C5-C6-N1	5.19	125.29	122.70
36	LA	2551	U	N3-C2-O2	-5.19	118.57	122.20
36	LA	2742	C	C6-N1-C2	-5.19	118.22	120.30
80	Sm	63	G	P-O3'-C3'	5.19	125.92	119.70
1	2	928	U	OP2-P-O3'	5.18	116.61	105.20
36	LA	102	C	C5-C6-N1	5.18	123.59	121.00
1	2	121	U	C5-C6-N1	5.18	125.29	122.70
1	2	1144	U	C5-C6-N1	5.18	125.29	122.70
1	2	1465	C	C6-N1-C2	-5.18	118.23	120.30
36	LA	125	C	C5-C6-N1	5.18	123.59	121.00
36	LA	2207	A	N9-C4-C5	-5.18	103.73	105.80
1	2	1023	A	P-O3'-C3'	5.18	125.92	119.70
36	LA	1665	C	C6-N1-C2	-5.18	118.23	120.30
1	2	138	A	C2-N3-C4	5.18	113.19	110.60
36	LA	1273	A	C4-N9-C1'	5.18	135.62	126.30
1	2	1514	U	C2-N1-C1'	5.18	123.91	117.70
11	U	64	VAL	CA-CB-CG1	5.18	118.67	110.90
1	2	553	G	OP1-P-O3'	5.17	116.58	105.20
1	2	1711	C	C6-N1-C2	-5.17	118.23	120.30
1	2	735	C	N3-C2-O2	-5.17	118.28	121.90
36	LA	1023	C	C6-N1-C2	-5.17	118.23	120.30
1	2	1119	G	N3-C4-N9	5.17	129.10	126.00
13	W	97	LEU	CA-CB-CG	5.17	127.19	115.30
36	LA	1146	C	C5-C6-N1	5.17	123.58	121.00
36	LA	2815	G	C5-C6-O6	5.17	131.70	128.60
36	LA	2899	C	O4'-C1'-N1	5.17	112.33	108.20
1	2	1436	A	C8-N9-C4	-5.16	103.74	105.80
36	LA	2567	C	C2-N1-C1'	5.16	124.48	118.80
24	a	11	LEU	CB-CG-CD1	5.16	119.77	111.00
36	LA	3269	U	N3-C2-O2	-5.16	118.59	122.20
1	2	530	C	C6-N1-C2	-5.16	118.24	120.30
1	2	1528	U	N1-C2-O2	5.16	126.41	122.80
16	D	140	PHE	CB-CG-CD1	-5.16	117.19	120.80
36	LA	142	C	N3-C2-O2	-5.16	118.29	121.90
36	LA	1064	A	P-O3'-C3'	5.15	125.89	119.70
80	Sn	25	C	C5-C6-N1	5.15	123.58	121.00
36	LA	1609	C	C5-C6-N1	5.15	123.58	121.00
1	2	1307	U	C2-N1-C1'	5.15	123.88	117.70
1	2	1399	C	C6-N1-C1'	5.15	126.98	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	U	9	LEU	CA-CB-CG	5.15	127.14	115.30
36	LA	2989	U	N3-C2-O2	-5.15	118.60	122.20
36	LA	15	C	N3-C2-O2	-5.15	118.30	121.90
36	LA	2541	U	N1-C2-O2	5.15	126.40	122.80
36	LA	3317	U	C5-C6-N1	5.14	125.27	122.70
1	2	283	U	C2-N1-C1'	5.14	123.87	117.70
36	LA	2876	C	C5-C6-N1	5.14	123.57	121.00
36	LA	1168	U	N3-C2-O2	-5.14	118.60	122.20
36	LA	2452	G	P-O5'-C5'	5.14	129.12	120.90
1	2	1021	C	C6-N1-C2	-5.14	118.25	120.30
11	U	129	LEU	CA-CB-CG	5.14	127.12	115.30
36	LA	1597	C	C6-N1-C2	-5.14	118.25	120.30
36	LA	1889	G	C4-N9-C1'	5.13	133.18	126.50
1	2	625	C	C5-C6-N1	5.13	123.57	121.00
1	2	1381	U	C6-N1-C1'	-5.13	114.01	121.20
12	V	29	LEU	CA-CB-CG	5.13	127.10	115.30
36	LA	249	U	O5'-P-OP2	-5.13	101.08	105.70
36	LA	2434	U	C6-N1-C2	-5.13	117.92	121.00
1	2	881	A	N9-C4-C5	-5.13	103.75	105.80
5	E	84	ILE	CG1-CB-CG2	-5.13	100.11	111.40
40	LE	87	VAL	CG1-CB-CG2	-5.13	102.69	110.90
1	2	935	U	O5'-P-OP2	-5.13	101.08	105.70
36	LA	963	G	N3-C4-N9	5.13	129.08	126.00
36	LA	2227	C	C6-N1-C2	-5.13	118.25	120.30
34	O	33	LEU	CA-CB-CG	5.13	127.09	115.30
36	LA	87	U	C5-C6-N1	5.13	125.26	122.70
36	LA	1126	G	C4-C5-N7	5.13	112.85	110.80
36	LA	1879	A	C8-N9-C4	-5.13	103.75	105.80
1	2	491	C	C6-N1-C2	-5.12	118.25	120.30
1	2	965	U	OP1-P-O3'	5.12	116.47	105.20
36	LA	855	U	N1-C2-O2	5.12	126.39	122.80
36	LA	1235	U	C5-C4-O4	5.12	128.97	125.90
1	2	1082	C	N1-C2-O2	5.12	121.97	118.90
36	LA	2948	C	C6-N1-C2	-5.12	118.25	120.30
36	LA	2600	C	C6-N1-C2	-5.12	118.25	120.30
36	LA	2638	C	C5-C6-N1	5.12	123.56	121.00
36	LA	1805	C	C6-N1-C2	-5.12	118.25	120.30
36	LA	3277	U	O4'-C1'-N1	5.12	112.29	108.20
36	LA	1228	C	C6-N1-C2	-5.12	118.25	120.30
36	LA	1395	G	N3-C4-C5	-5.12	126.04	128.60
1	2	605	A	OP1-P-O3'	5.11	116.45	105.20
36	LA	2961	G	C4-N9-C1'	5.11	133.15	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	LA	1706	C	C5-C6-N1	5.11	123.56	121.00
36	LA	1879	A	O4'-C1'-N9	5.11	112.29	108.20
38	LC	118	C	C6-N1-C2	-5.11	118.26	120.30
36	LA	604	G	C5-C6-O6	-5.11	125.53	128.60
36	LA	2414	G	N3-C4-N9	5.11	129.07	126.00
1	2	617	U	C2-N1-C1'	5.11	123.83	117.70
36	LA	190	U	OP2-P-O3'	5.11	116.44	105.20
36	LA	2906	C	C5-C6-N1	5.11	123.55	121.00
36	LA	3131	U	N3-C2-O2	-5.11	118.62	122.20
1	2	176	C	C4-C5-C6	-5.11	114.85	117.40
80	Sn	49	C	C2-N3-C4	5.11	122.45	119.90
36	LA	3058	U	C6-N1-C1'	-5.10	114.06	121.20
38	LC	28	C	C5-C6-N1	5.10	123.55	121.00
80	Sm	23	C	C6-N1-C2	-5.10	118.26	120.30
36	LA	2567	C	C6-N1-C2	-5.10	118.26	120.30
36	LA	242	C	N1-C2-O2	5.09	121.96	118.90
1	2	1148	C	C5-C6-N1	5.09	123.55	121.00
36	LA	97	U	N3-C2-O2	-5.09	118.64	122.20
1	2	832	U	OP2-P-O3'	5.09	116.39	105.20
36	LA	1540	U	N1-C2-O2	5.09	126.36	122.80
36	LA	2378	C	N1-C2-O2	5.09	121.95	118.90
36	LA	2726	C	C6-N1-C2	-5.09	118.27	120.30
38	LC	153	U	N3-C2-O2	-5.09	118.64	122.20
1	2	1274	C	N3-C2-O2	-5.08	118.34	121.90
36	LA	1403	C	C6-N1-C2	-5.08	118.27	120.30
1	2	555	A	C4-C5-C6	5.08	119.54	117.00
1	2	583	C	C6-N1-C1'	-5.08	114.70	120.80
36	LA	1901	A	C4-N9-C1'	5.08	135.44	126.30
36	LA	2362	C	C5-C6-N1	5.08	123.54	121.00
1	2	1205	C	C6-N1-C2	-5.08	118.27	120.30
36	LA	916	G	P-O3'-C3'	5.08	125.80	119.70
36	LA	1279	C	N3-C4-N4	5.08	121.56	118.00
1	2	376	C	C6-N1-C2	-5.08	118.27	120.30
36	LA	42	C	C6-N1-C2	-5.08	118.27	120.30
36	LA	362	U	N3-C2-O2	-5.08	118.65	122.20
36	LA	817	A	C2-N3-C4	5.08	113.14	110.60
36	LA	1190	A	C8-N9-C1'	-5.08	118.56	127.70
36	LA	1751	G	C8-N9-C1'	5.08	133.60	127.00
36	LA	2146	C	C2-N1-C1'	5.08	124.39	118.80
36	LA	2619	G	C8-N9-C1'	-5.08	120.40	127.00
1	2	1024	U	O4'-C1'-N1	5.08	112.26	108.20
1	2	1772	C	C6-N1-C2	-5.08	118.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1496	U	N1-C2-O2	5.07	126.35	122.80
36	LA	1764	U	OP1-P-O3'	5.07	116.36	105.20
1	2	870	C	C6-N1-C2	-5.07	118.27	120.30
36	LA	2184	U	C5-C6-N1	5.07	125.23	122.70
80	Sn	32	C	C6-N1-C2	-5.07	118.27	120.30
1	2	415	C	C2-N1-C1'	5.07	124.38	118.80
1	2	1147	A	N7-C8-N9	5.07	116.33	113.80
1	2	1704	U	N3-C2-O2	-5.07	118.65	122.20
36	LA	439	C	OP1-P-O3'	5.07	116.35	105.20
36	LA	1096	U	O4'-C1'-N1	-5.07	104.15	108.20
36	LA	1126	G	N9-C4-C5	-5.07	103.37	105.40
80	Sm	51	C	C6-N1-C2	-5.06	118.27	120.30
1	2	975	C	C5-C6-N1	5.06	123.53	121.00
1	2	117	U	C5-C6-N1	5.06	125.23	122.70
36	LA	354	U	N3-C2-O2	-5.06	118.66	122.20
36	LA	600	G	C4-C5-N7	5.06	112.82	110.80
1	2	1274	C	C2-N1-C1'	5.06	124.36	118.80
36	LA	283	G	C2-N3-C4	5.06	114.43	111.90
38	LC	151	C	C5-C6-N1	5.06	123.53	121.00
1	2	166	C	C6-N1-C2	-5.06	118.28	120.30
36	LA	3276	G	O5'-P-OP1	-5.06	101.15	105.70
64	LW	78	LEU	CA-CB-CG	5.05	126.92	115.30
1	2	1119	G	N3-C4-C5	-5.05	126.08	128.60
1	2	1514	U	C6-N1-C1'	-5.05	114.13	121.20
36	LA	609	G	N3-C4-C5	-5.05	126.08	128.60
36	LA	2553	U	C6-N1-C1'	-5.05	114.13	121.20
16	D	137	MET	CA-CB-CG	5.05	121.88	113.30
36	LA	2252	A	N7-C8-N9	5.05	116.32	113.80
36	LA	2867	C	C5-C6-N1	5.05	123.52	121.00
1	2	102	U	C5-C6-N1	5.05	125.22	122.70
36	LA	2471	U	N1-C2-O2	5.05	126.33	122.80
1	2	237	C	OP2-P-O3'	5.04	116.30	105.20
1	2	583	C	N3-C2-O2	-5.04	118.37	121.90
36	LA	3319	U	OP1-P-O3'	5.04	116.30	105.20
1	2	747	C	C6-N1-C2	-5.04	118.28	120.30
1	2	1235	C	N1-C2-O2	5.04	121.93	118.90
1	2	1666	U	N3-C2-O2	-5.04	118.67	122.20
36	LA	1819	U	N1-C2-O2	5.04	126.33	122.80
36	LA	2108	C	C6-N1-C2	-5.04	118.28	120.30
36	LA	2252	A	C8-N9-C4	-5.04	103.78	105.80
80	Sn	49	C	C2-N1-C1'	5.04	124.35	118.80
1	2	1761	U	N3-C2-O2	-5.04	118.67	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1554	U	N1-C2-O2	5.04	126.33	122.80
36	LA	2496	C	C6-N1-C1'	-5.04	114.75	120.80
55	Ln	126	GLU	CA-CB-CG	5.04	124.48	113.40
1	2	934	C	C6-N1-C2	-5.04	118.28	120.30
1	2	1529	C	C6-N1-C2	-5.04	118.28	120.30
36	LA	1894	U	N1-C2-N3	5.04	117.92	114.90
36	LA	2689	A	N7-C8-N9	5.04	116.32	113.80
59	Lr	83	LYS	CB-CG-CD	5.04	124.69	111.60
81	EF	508	LEU	CA-CB-CG	5.04	126.88	115.30
1	2	1438	G	N3-C4-N9	5.03	129.02	126.00
36	LA	1175	C	C6-N1-C2	-5.03	118.29	120.30
36	LA	2585	G	C2-N3-C4	5.03	114.42	111.90
1	2	229	U	N3-C2-O2	-5.03	118.68	122.20
1	2	1134	C	C6-N1-C2	-5.03	118.29	120.30
1	2	1373	C	N1-C2-O2	5.03	121.92	118.90
36	LA	600	G	C5-C6-O6	-5.03	125.58	128.60
1	2	176	C	C6-N1-C2	-5.03	118.29	120.30
1	2	959	U	C6-N1-C2	-5.03	117.98	121.00
5	E	34	VAL	CA-CB-CG1	5.03	118.44	110.90
36	LA	600	G	N1-C6-O6	5.03	122.92	119.90
36	LA	15	C	N1-C2-O2	5.03	121.92	118.90
36	LA	1368	U	C5-C6-N1	5.03	125.21	122.70
36	LA	2118	C	C5-C6-N1	5.03	123.51	121.00
1	2	144	U	C5-C4-O4	-5.02	122.89	125.90
78	Lk	93	LEU	CA-CB-CG	5.02	126.86	115.30
36	LA	123	A	C5-C6-N1	5.02	120.21	117.70
36	LA	885	U	N3-C2-O2	-5.02	118.69	122.20
36	LA	283	G	OP1-P-O3'	5.02	116.25	105.20
36	LA	548	G	N1-C2-N2	-5.02	111.68	116.20
36	LA	1508	C	N1-C2-O2	5.02	121.91	118.90
38	LC	82	U	OP1-P-O3'	5.02	116.24	105.20
1	2	232	U	O4'-C1'-N1	5.02	112.22	108.20
1	2	1315	U	N1-C2-O2	5.02	126.31	122.80
36	LA	2372	A	O4'-C1'-N9	-5.02	104.19	108.20
36	LA	2496	C	N3-C2-O2	-5.02	118.39	121.90
1	2	735	C	N1-C2-O2	5.01	121.91	118.90
36	LA	1239	C	N1-C2-O2	5.01	121.91	118.90
36	LA	1857	C	C5-C6-N1	5.01	123.51	121.00
36	LA	1889	G	C8-N9-C1'	-5.01	120.48	127.00
36	LA	2209	U	C2-N1-C1'	5.01	123.72	117.70
1	2	1608	U	N3-C2-O2	-5.01	118.69	122.20
15	X	5	LEU	CA-CB-CG	5.01	126.83	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	LA	609	G	C2-N3-C4	5.01	114.41	111.90
36	LA	48	A	O5'-P-OP2	-5.01	101.19	105.70
81	EF	331	LEU	CA-CB-CG	5.01	126.82	115.30
21	H	116	LEU	CB-CG-CD1	5.01	119.52	111.00
36	LA	787	G	O5'-P-OP1	-5.01	101.19	105.70
71	Ld	33	VAL	CA-CB-CG1	5.01	118.42	110.90
1	2	1474	G	C8-N9-C4	-5.01	104.40	106.40
36	LA	2505	U	P-O3'-C3'	5.01	125.71	119.70
36	LA	3086	A	N7-C8-N9	5.01	116.30	113.80
36	LA	1751	G	N3-C4-N9	-5.01	123.00	126.00
1	2	424	C	C6-N1-C2	-5.00	118.30	120.30
1	2	445	A	C2-N3-C4	5.00	113.10	110.60
1	2	1347	U	C2-N1-C1'	5.00	123.70	117.70

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	B	125	THR	Peptide
9	B	42	LEU	Peptide
16	D	108	ARG	Peptide
81	EF	465	GLY	Peptide
81	EF	663	LYS	Peptide
81	EF	760	GLN	Peptide
81	EF	78	ASN	Peptide
81	EF	80	SER	Peptide
81	EF	955	THR	Peptide
19	F	40	GLU	Peptide
36	LA	1273	A	Sidechain
41	LF	13	GLY	Peptide
41	LF	3	ARG	Peptide
41	LF	318	LEU	Peptide
44	LI	232	ARG	Peptide
45	LJ	30	THR	Peptide
45	LJ	76	ALA	Peptide
45	LJ	77	GLN	Peptide
64	LW	115	LYS	Peptide
64	LW	14	HIS	Peptide
65	LX	19	ASN	Peptide
65	LX	20	GLY	Peptide
66	LY	47	ASN	Peptide
67	LZ	7	VAL	Peptide

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Mol	Chain	Res	Type	Group
71	Ld	83	LYS	Peptide
54	Lm	161	LYS	Peptide
33	N	147	VAL	Peptide
8	S	193	GLY	Peptide
11	U	64	VAL	Peptide
25	b	54	ASP	Peptide

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	204/206 (99%)	182 (89%)	22 (11%)	0	100	100
4	Q	222/232 (96%)	196 (88%)	26 (12%)	0	100	100
5	E	115/117 (98%)	100 (87%)	15 (13%)	0	100	100
6	R	214/216 (99%)	188 (88%)	26 (12%)	0	100	100
7	A	220/222 (99%)	209 (95%)	11 (5%)	0	100	100
8	S	256/258 (99%)	229 (90%)	27 (10%)	0	100	100
9	B	204/206 (99%)	188 (92%)	16 (8%)	0	100	100
10	T	226/228 (99%)	212 (94%)	14 (6%)	0	100	100
11	U	182/184 (99%)	162 (89%)	20 (11%)	0	100	100
12	V	183/198 (92%)	168 (92%)	15 (8%)	0	100	100
13	W	182/184 (99%)	165 (91%)	16 (9%)	1 (0%)	25	56
14	C	90/92 (98%)	79 (88%)	11 (12%)	0	100	100
15	X	140/142 (99%)	124 (89%)	16 (11%)	0	100	100
16	D	119/121 (98%)	90 (76%)	27 (23%)	2 (2%)	7	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Y	148/150 (99%)	134 (90%)	14 (10%)	0	100	100
18	Z	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
19	F	139/141 (99%)	127 (91%)	12 (9%)	0	100	100
20	G	117/125 (94%)	112 (96%)	5 (4%)	0	100	100
21	H	143/145 (99%)	130 (91%)	13 (9%)	0	100	100
22	I	141/143 (99%)	129 (92%)	10 (7%)	2 (1%)	9	34
23	J	98/100 (98%)	89 (91%)	9 (9%)	0	100	100
24	a	85/87 (98%)	71 (84%)	14 (16%)	0	100	100
25	b	127/129 (98%)	113 (89%)	14 (11%)	0	100	100
26	c	142/144 (99%)	125 (88%)	17 (12%)	0	100	100
27	d	132/134 (98%)	124 (94%)	8 (6%)	0	100	100
28	K	80/82 (98%)	70 (88%)	10 (12%)	0	100	100
29	e	95/97 (98%)	86 (90%)	9 (10%)	0	100	100
30	f	79/81 (98%)	70 (89%)	9 (11%)	0	100	100
31	M	51/53 (96%)	50 (98%)	1 (2%)	0	100	100
32	g	58/60 (97%)	49 (84%)	9 (16%)	0	100	100
33	N	71/73 (97%)	51 (72%)	20 (28%)	0	100	100
34	O	310/312 (99%)	269 (87%)	41 (13%)	0	100	100
35	L	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
39	LD	249/251 (99%)	222 (89%)	27 (11%)	0	100	100
40	LE	384/386 (100%)	357 (93%)	27 (7%)	0	100	100
41	LF	359/361 (99%)	324 (90%)	33 (9%)	2 (1%)	22	53
42	LG	292/294 (99%)	266 (91%)	26 (9%)	0	100	100
43	LH	163/175 (93%)	146 (90%)	17 (10%)	0	100	100
44	LI	220/222 (99%)	206 (94%)	14 (6%)	0	100	100
45	LJ	231/233 (99%)	210 (91%)	21 (9%)	0	100	100
46	LK	189/191 (99%)	172 (91%)	17 (9%)	0	100	100
47	LL	216/218 (99%)	190 (88%)	26 (12%)	0	100	100
48	LM	167/169 (99%)	153 (92%)	14 (8%)	0	100	100
49	LN	191/193 (99%)	171 (90%)	19 (10%)	1 (0%)	25	56
50	LO	134/136 (98%)	120 (90%)	13 (10%)	1 (1%)	19	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	LP	201/203 (99%)	181 (90%)	19 (10%)	1 (0%)	25	56
52	LQ	195/197 (99%)	187 (96%)	8 (4%)	0	100	100
53	LR	181/183 (99%)	168 (93%)	13 (7%)	0	100	100
54	Lm	183/185 (99%)	168 (92%)	15 (8%)	0	100	100
55	Ln	186/188 (99%)	180 (97%)	6 (3%)	0	100	100
56	Lo	169/171 (99%)	155 (92%)	14 (8%)	0	100	100
57	Lp	157/159 (99%)	143 (91%)	14 (9%)	0	100	100
58	Lq	98/100 (98%)	92 (94%)	6 (6%)	0	100	100
59	Lr	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
60	LS	124/126 (98%)	109 (88%)	15 (12%)	0	100	100
61	LT	119/121 (98%)	111 (93%)	8 (7%)	0	100	100
62	LU	123/125 (98%)	117 (95%)	6 (5%)	0	100	100
63	LV	133/135 (98%)	117 (88%)	16 (12%)	0	100	100
64	LW	146/148 (99%)	127 (87%)	19 (13%)	0	100	100
65	LX	56/58 (97%)	48 (86%)	8 (14%)	0	100	100
66	LY	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
67	LZ	107/109 (98%)	92 (86%)	15 (14%)	0	100	100
68	La	125/127 (98%)	115 (92%)	10 (8%)	0	100	100
69	Lb	104/106 (98%)	98 (94%)	6 (6%)	0	100	100
70	Lc	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
71	Ld	117/119 (98%)	109 (93%)	8 (7%)	0	100	100
72	Le	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
73	Lf	79/81 (98%)	70 (89%)	9 (11%)	0	100	100
74	Lg	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
75	Lh	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
76	Li	50/52 (96%)	44 (88%)	6 (12%)	0	100	100
77	Lj	23/25 (92%)	23 (100%)	0	0	100	100
78	Lk	101/103 (98%)	94 (93%)	7 (7%)	0	100	100
79	Ll	89/91 (98%)	87 (98%)	2 (2%)	0	100	100
81	EF	975/1044 (93%)	857 (88%)	117 (12%)	1 (0%)	48	76
All	All	11953/12207 (98%)	10821 (90%)	1121 (9%)	11 (0%)	50	76

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
81	EF	418	PRO
16	D	109	GLU
22	I	25	GLN
22	I	29	GLU
41	LF	4	PRO
41	LF	130	ALA
50	LO	135	LEU
51	LP	146	ALA
49	LN	61	PRO
16	D	127	GLY
13	W	18	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	
3	P	170/173 (98%)	170 (100%)	0	100	100
4	Q	200/205 (98%)	198 (99%)	2 (1%)	73	84
5	E	95/98 (97%)	94 (99%)	1 (1%)	70	82
6	R	175/175 (100%)	172 (98%)	3 (2%)	56	74
7	A	182/182 (100%)	177 (97%)	5 (3%)	40	65
8	S	220/220 (100%)	217 (99%)	3 (1%)	62	78
9	B	172/173 (99%)	171 (99%)	1 (1%)	84	90
10	T	189/195 (97%)	186 (98%)	3 (2%)	58	76
11	U	163/165 (99%)	162 (99%)	1 (1%)	84	90
12	V	148/159 (93%)	147 (99%)	1 (1%)	81	88
13	W	156/157 (99%)	153 (98%)	3 (2%)	52	72
14	C	77/85 (91%)	76 (99%)	1 (1%)	65	79
15	X	126/127 (99%)	125 (99%)	1 (1%)	79	87
16	D	88/98 (90%)	86 (98%)	2 (2%)	45	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Y	127/127 (100%)	126 (99%)	1 (1%)	79	87
18	Z	90/96 (94%)	87 (97%)	3 (3%)	33	60
19	F	117/117 (100%)	115 (98%)	2 (2%)	56	74
20	G	101/113 (89%)	99 (98%)	2 (2%)	50	71
21	H	127/128 (99%)	126 (99%)	1 (1%)	79	87
22	I	115/115 (100%)	115 (100%)	0	100	100
23	J	93/93 (100%)	93 (100%)	0	100	100
24	a	71/74 (96%)	71 (100%)	0	100	100
25	b	110/110 (100%)	110 (100%)	0	100	100
26	c	119/119 (100%)	118 (99%)	1 (1%)	79	87
27	d	112/112 (100%)	111 (99%)	1 (1%)	75	85
28	K	67/73 (92%)	66 (98%)	1 (2%)	60	77
29	e	82/83 (99%)	80 (98%)	2 (2%)	44	68
30	f	70/70 (100%)	69 (99%)	1 (1%)	62	78
31	M	47/47 (100%)	47 (100%)	0	100	100
32	g	50/51 (98%)	48 (96%)	2 (4%)	27	55
33	N	56/63 (89%)	54 (96%)	2 (4%)	30	57
34	O	250/257 (97%)	246 (98%)	4 (2%)	58	76
35	L	55/56 (98%)	54 (98%)	1 (2%)	54	74
39	LD	190/193 (98%)	186 (98%)	4 (2%)	48	70
40	LE	321/322 (100%)	316 (98%)	5 (2%)	58	76
41	LF	288/288 (100%)	284 (99%)	4 (1%)	62	78
42	LG	241/243 (99%)	240 (100%)	1 (0%)	89	93
43	LH	139/154 (90%)	136 (98%)	3 (2%)	47	69
44	LI	186/186 (100%)	186 (100%)	0	100	100
45	LJ	187/191 (98%)	184 (98%)	3 (2%)	58	76
46	LK	168/171 (98%)	164 (98%)	4 (2%)	44	68
47	LL	185/185 (100%)	183 (99%)	2 (1%)	70	82
48	LM	145/147 (99%)	145 (100%)	0	100	100
49	LN	154/154 (100%)	152 (99%)	2 (1%)	65	79
50	LO	107/107 (100%)	105 (98%)	2 (2%)	52	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	LP	175/175 (100%)	172 (98%)	3 (2%)	56	74
52	LQ	160/160 (100%)	159 (99%)	1 (1%)	84	90
53	LR	138/145 (95%)	138 (100%)	0	100	100
54	Lm	150/150 (100%)	145 (97%)	5 (3%)	33	60
55	Ln	152/153 (99%)	150 (99%)	2 (1%)	65	79
56	Lo	155/155 (100%)	154 (99%)	1 (1%)	84	90
57	Lp	135/136 (99%)	132 (98%)	3 (2%)	47	69
58	Lq	87/87 (100%)	86 (99%)	1 (1%)	70	82
59	Lr	104/104 (100%)	104 (100%)	0	100	100
60	LS	56/108 (52%)	55 (98%)	1 (2%)	54	74
61	LT	104/105 (99%)	104 (100%)	0	100	100
62	LU	108/108 (100%)	107 (99%)	1 (1%)	75	85
63	LV	112/115 (97%)	110 (98%)	2 (2%)	54	74
64	LW	117/118 (99%)	116 (99%)	1 (1%)	75	85
65	LX	46/46 (100%)	45 (98%)	1 (2%)	47	69
66	LY	81/81 (100%)	79 (98%)	2 (2%)	42	67
67	LZ	92/96 (96%)	90 (98%)	2 (2%)	47	69
68	La	107/109 (98%)	105 (98%)	2 (2%)	52	72
69	Lb	90/90 (100%)	90 (100%)	0	100	100
70	Lc	95/95 (100%)	92 (97%)	3 (3%)	34	61
71	Ld	104/104 (100%)	101 (97%)	3 (3%)	37	63
72	Le	80/81 (99%)	80 (100%)	0	100	100
73	Lf	67/67 (100%)	66 (98%)	1 (2%)	60	77
74	Lg	68/68 (100%)	66 (97%)	2 (3%)	37	63
75	Lh	45/45 (100%)	44 (98%)	1 (2%)	47	69
76	Li	45/47 (96%)	45 (100%)	0	100	100
77	Lj	22/23 (96%)	20 (91%)	2 (9%)	7	27
78	Lk	87/88 (99%)	86 (99%)	1 (1%)	70	82
79	Ll	71/71 (100%)	69 (97%)	2 (3%)	38	64
81	EF	789/885 (89%)	782 (99%)	7 (1%)	75	85
All	All	9973/10272 (97%)	9842 (99%)	131 (1%)	64	79

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	Q	48	VAL
4	Q	162	ARG
5	E	36	LEU
6	R	95	ARG
6	R	146	THR
6	R	159	THR
7	A	14	ASP
7	A	76	ARG
7	A	128	GLU
7	A	178	ARG
7	A	215	GLU
8	S	38	LEU
8	S	211	LYS
8	S	258	GLN
9	B	25	LEU
10	T	87	ARG
10	T	98	ARG
10	T	214	LYS
11	U	152	VAL
12	V	29	LEU
13	W	78	ARG
13	W	82	ARG
13	W	180	LYS
14	C	37	THR
15	X	67	ARG
16	D	28	LEU
16	D	74	LEU
17	Y	64	ARG
18	Z	26	THR
18	Z	133	ARG
18	Z	136	ARG
19	F	52	LEU
19	F	127	LYS
20	G	19	ARG
20	G	83	GLN
21	H	98	TYR
26	c	120	VAL
27	d	112	LYS
28	K	40	VAL
29	e	64	LEU
29	e	94	ASN
30	f	25	VAL

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Mol	Chain	Res	Type
32	g	33	ARG
32	g	38	LEU
33	N	89	LYS
33	N	138	ARG
34	O	121	MET
34	O	144	LEU
34	O	271	VAL
34	O	290	VAL
35	L	30	VAL
39	LD	92	LYS
39	LD	163	ARG
39	LD	193	ARG
39	LD	242	ARG
40	LE	89	VAL
40	LE	90	VAL
40	LE	175	LYS
40	LE	202	THR
40	LE	332	ARG
41	LF	6	VAL
41	LF	98	ARG
41	LF	116	ASN
41	LF	194	TYR
42	LG	110	LEU
43	LH	8	LYS
43	LH	93	VAL
43	LH	104	GLU
45	LJ	158	ASP
45	LJ	208	GLU
45	LJ	213	LYS
46	LK	47	LYS
46	LK	68	LEU
46	LK	88	TYR
46	LK	124	ARG
47	LL	147	VAL
47	LL	191	LYS
49	LN	21	ARG
49	LN	104	ARG
50	LO	78	THR
50	LO	117	ARG
51	LP	62	TYR
51	LP	138	GLN
51	LP	153	ASP

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Mol	Chain	Res	Type
52	LQ	125[A]	ARG
54	Lm	12	ARG
54	Lm	31	LYS
54	Lm	147	ARG
54	Lm	159	LYS
54	Lm	176	ARG
55	Ln	6	THR
55	Ln	164	LEU
56	Lo	96	ASP
57	Lp	10	ARG
57	Lp	50	LYS
57	Lp	83	ARG
58	Lq	74	LYS
60	LS	60	LYS
62	LU	13	ARG
63	LV	3	LYS
63	LV	126	LYS
64	LW	77	LYS
65	LX	33	LYS
66	LY	83	LYS
66	LY	86	ARG
67	LZ	9	THR
67	LZ	107	VAL
68	La	45	ARG
68	La	126	LEU
70	Lc	56	THR
70	Lc	87	GLU
70	Lc	106	LYS
71	Ld	33	VAL
71	Ld	59	ASN
71	Ld	90	ARG
73	Lf	45	ARG
74	Lg	9	LYS
74	Lg	63	LYS
75	Lh	21	ARG
77	Lj	7	LYS
77	Lj	8	LYS
78	Lk	57	VAL
79	Ll	17	ARG
79	Ll	57	CYS
81	EF	257	ARG
81	EF	407	ARG

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Mol	Chain	Res	Type
81	EF	457	ARG
81	EF	464	ASN
81	EF	604	ASN
81	EF	611	ASN
81	EF	976	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
3	P	23	HIS
8	S	258	GLN
9	B	63	GLN
9	B	104	ASN
10	T	182	GLN
11	U	86	GLN
14	C	9	ASN
15	X	14	GLN
15	X	81	HIS
17	Y	58	HIS
17	Y	105	ASN
17	Y	123	HIS
19	F	83	GLN
22	I	12	GLN
22	I	101	ASN
24	a	29	HIS
27	d	22	GLN
27	d	29	HIS
29	e	94	ASN
33	N	123	ASN
34	O	16	HIS
34	O	198	ASN
34	O	308	ASN
35	L	27	GLN
35	L	43	ASN
39	LD	47	GLN
39	LD	132	ASN
40	LE	273	HIS
40	LE	319	ASN
41	LF	48	GLN
41	LF	110	ASN
41	LF	296	GLN
43	LH	102	ASN

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Mol	Chain	Res	Type
44	LI	93	ASN
44	LI	172	ASN
45	LJ	59	GLN
45	LJ	192	GLN
46	LK	51	GLN
46	LK	58	HIS
46	LK	125	ASN
47	LL	23	ASN
51	LP	11	GLN
51	LP	117	ASN
53	LR	97	ASN
55	Ln	166	ASN
56	Lo	142	GLN
63	LV	40	HIS
65	LX	43	HIS
68	La	104	ASN
75	Lh	43	ASN
78	Lk	82	GLN
81	EF	97	ASN
81	EF	100	ASN
81	EF	255	ASN
81	EF	296	ASN
81	EF	395	HIS
81	EF	464	ASN
81	EF	486	GLN
81	EF	496	HIS
81	EF	577	ASN
81	EF	611	ASN
81	EF	727	HIS
81	EF	729	ASN
81	EF	976	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1768/1771 (99%)	534 (30%)	54 (3%)
2	1	6/7 (85%)	1 (16%)	0
36	LA	3220/3223 (99%)	751 (23%)	42 (1%)
37	LB	120/121 (99%)	15 (12%)	1 (0%)
38	LC	157/158 (99%)	32 (20%)	3 (1%)
80	Sm	74/75 (98%)	24 (32%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
80	Sn	74/75 (98%)	23 (31%)	0
All	All	5419/5430 (99%)	1380 (25%)	100 (1%)

All (1380) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	14	C
1	2	25	C
1	2	26	A
1	2	34	G
1	2	43	A
1	2	45	U
1	2	46	A
1	2	47	A
1	2	56	U
1	2	57	G
1	2	62	A
1	2	65	A
1	2	67	A
1	2	68	A
1	2	69	G
1	2	73	U
1	2	74	U
1	2	75	U
1	2	76	A
1	2	78	A
1	2	79	C
1	2	80	A
1	2	81	G
1	2	104	A
1	2	114	C
1	2	116	U
1	2	121	U
1	2	127	G
1	2	129	U
1	2	130	C
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U

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Mol	Chain	Res	Type
1	2	135	A
1	2	136	C
1	2	137	U
1	2	138	A
1	2	140	A
1	2	141	U
1	2	142	G
1	2	153	G
1	2	155	U
1	2	156	A
1	2	158	U
1	2	161	U
1	2	168	A
1	2	171	A
1	2	172	C
1	2	174	U
1	2	176	C
1	2	178	U
1	2	179	A
1	2	182	A
1	2	185	U
1	2	186	C
1	2	187	G
1	2	188	A
1	2	189	C
1	2	191	C
1	2	193	U
1	2	194	U
1	2	195	G
1	2	201	G
1	2	203	U
1	2	204	G
1	2	216	U
1	2	217	A
1	2	218	A
1	2	223	U
1	2	224	C
1	2	225	A
1	2	227	U
1	2	228	G
1	2	230	C
1	2	232	U

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Mol	Chain	Res	Type
1	2	233	C
1	2	234	G
1	2	235	G
1	2	236	A
1	2	238	U
1	2	240	U
1	2	241	U
1	2	243	G
1	2	246	G
1	2	250	C
1	2	256	A
1	2	260	U
1	2	261	U
1	2	265	A
1	2	270	C
1	2	272	U
1	2	274	G
1	2	276	C
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	287	G
1	2	299	A
1	2	313	U
1	2	314	C
1	2	316	A
1	2	320	U
1	2	321	C
1	2	322	G
1	2	323	A
1	2	324	U
1	2	330	G
1	2	333	A
1	2	334	G
1	2	337	G
1	2	338	C
1	2	352	A
1	2	353	A
1	2	359	A
1	2	360	A

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Mol	Chain	Res	Type
1	2	361	C
1	2	369	A
1	2	370	A
1	2	373	G
1	2	378	A
1	2	380	U
1	2	388	G
1	2	390	G
1	2	400	A
1	2	401	A
1	2	402	C
1	2	404	G
1	2	406	U
1	2	411	C
1	2	415	C
1	2	417	A
1	2	419	G
1	2	423	G
1	2	424	C
1	2	425	A
1	2	426	G
1	2	434	G
1	2	435	C
1	2	438	A
1	2	439	U
1	2	444	C
1	2	446	A
1	2	448	C
1	2	454	U
1	2	460	A
1	2	468	A
1	2	482	U
1	2	483	A
1	2	485	A
1	2	487	G
1	2	489	C
1	2	491	C
1	2	492	A
1	2	493	U
1	2	494	U
1	2	495	C
1	2	496	G

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Mol	Chain	Res	Type
1	2	498	G
1	2	499	U
1	2	500	C
1	2	502	U
1	2	506	A
1	2	507	U
1	2	510	G
1	2	511	A
1	2	513	U
1	2	517	U
1	2	518	A
1	2	519	C
1	2	520	A
1	2	525	A
1	2	527	A
1	2	529	A
1	2	534	A
1	2	538	A
1	2	539	G
1	2	540	G
1	2	541	A
1	2	542	A
1	2	543	C
1	2	554	C
1	2	555	A
1	2	556	A
1	2	557	G
1	2	558	U
1	2	565	C
1	2	571	G
1	2	572	C
1	2	578	U
1	2	579	A
1	2	580	A
1	2	594	A
1	2	595	G
1	2	606	A
1	2	609	U
1	2	610	G
1	2	611	U
1	2	617	U
1	2	619	A

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Mol	Chain	Res	Type
1	2	620	A
1	2	622	A
1	2	623	A
1	2	624	G
1	2	635	A
1	2	638	U
1	2	639	U
1	2	640	U
1	2	641	G
1	2	643	G
1	2	645	C
1	2	651	G
1	2	653	C
1	2	654	C
1	2	655	G
1	2	656	G
1	2	677	G
1	2	678	A
1	2	680	U
1	2	684	A
1	2	687	G
1	2	693	U
1	2	694	U
1	2	696	C
1	2	697	C
1	2	698	U
1	2	700	C
1	2	702	G
1	2	703	G
1	2	704	C
1	2	705	U
1	2	706	A
1	2	707	A
1	2	708	C
1	2	709	C
1	2	710	U
1	2	711	U
1	2	712	G
1	2	714	G
1	2	728	U
1	2	729	G
1	2	730	G

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Mol	Chain	Res	Type
1	2	732	G
1	2	733	A
1	2	736	C
1	2	738	G
1	2	739	G
1	2	741	C
1	2	742	U
1	2	743	U
1	2	744	U
1	2	745	U
1	2	753	A
1	2	755	A
1	2	756	A
1	2	765	G
1	2	766	U
1	2	767	U
1	2	771	A
1	2	774	A
1	2	775	G
1	2	778	G
1	2	781	U
1	2	782	U
1	2	783	G
1	2	787	G
1	2	789	A
1	2	794	U
1	2	804	A
1	2	807	A
1	2	811	A
1	2	812	A
1	2	813	U
1	2	814	A
1	2	815	G
1	2	816	G
1	2	818	C
1	2	819	G
1	2	820	U
1	2	821	U
1	2	823	G
1	2	832	U
1	2	833	U
1	2	836	U

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Mol	Chain	Res	Type
1	2	837	G
1	2	839	U
1	2	840	U
1	2	841	U
1	2	846	G
1	2	851	U
1	2	852	C
1	2	855	A
1	2	856	A
1	2	857	U
1	2	863	A
1	2	865	A
1	2	873	U
1	2	876	G
1	2	886	U
1	2	898	A
1	2	899	G
1	2	901	G
1	2	902	G
1	2	904	G
1	2	912	U
1	2	913	G
1	2	929	A
1	2	932	U
1	2	933	A
1	2	934	C
1	2	935	U
1	2	940	A
1	2	945	U
1	2	960	U
1	2	964	U
1	2	966	A
1	2	970	A
1	2	973	A
1	2	977	A
1	2	988	A
1	2	989	U
1	2	992	A
1	2	996	U
1	2	998	A
1	2	1001	A
1	2	1004	U

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Mol	Chain	Res	Type
1	2	1024	U
1	2	1026	A
1	2	1028	C
1	2	1029	U
1	2	1032	G
1	2	1039	A
1	2	1040	G
1	2	1052	U
1	2	1053	G
1	2	1057	U
1	2	1058	U
1	2	1059	U
1	2	1060	U
1	2	1061	A
1	2	1062	A
1	2	1063	U
1	2	1074	G
1	2	1080	U
1	2	1081	A
1	2	1082	C
1	2	1092	A
1	2	1096	C
1	2	1099	U
1	2	1100	G
1	2	1109	G
1	2	1111	G
1	2	1113	A
1	2	1138	A
1	2	1139	A
1	2	1156	C
1	2	1158	C
1	2	1160	A
1	2	1164	G
1	2	1167	G
1	2	1170	G
1	2	1183	A
1	2	1185	U
1	2	1186	U
1	2	1187	U
1	2	1191	U
1	2	1194	A
1	2	1196	A

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Mol	Chain	Res	Type
1	2	1197	C
1	2	1199	G
1	2	1200	G
1	2	1208	A
1	2	1212	G
1	2	1214	U
1	2	1217	A
1	2	1218	G
1	2	1227	A
1	2	1229	G
1	2	1241	G
1	2	1243	G
1	2	1244	A
1	2	1245	G
1	2	1246	C
1	2	1252	C
1	2	1256	A
1	2	1257	U
1	2	1258	U
1	2	1263	G
1	2	1264	G
1	2	1265	G
1	2	1269	U
1	2	1273	G
1	2	1274	C
1	2	1275	A
1	2	1276	U
1	2	1285	U
1	2	1294	G
1	2	1301	U
1	2	1307	U
1	2	1314	U
1	2	1315	U
1	2	1318	G
1	2	1321	A
1	2	1322	A
1	2	1325	A
1	2	1337	A
1	2	1341	A
1	2	1344	A
1	2	1345	A
1	2	1346	A

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Mol	Chain	Res	Type
1	2	1348	A
1	2	1349	G
1	2	1354	G
1	2	1360	A
1	2	1361	U
1	2	1363	U
1	2	1367	G
1	2	1370	U
1	2	1371	A
1	2	1372	U
1	2	1373	C
1	2	1381	U
1	2	1382	A
1	2	1383	G
1	2	1385	G
1	2	1390	U
1	2	1398	U
1	2	1399	C
1	2	1400	A
1	2	1402	G
1	2	1414	U
1	2	1415	U
1	2	1421	A
1	2	1427	A
1	2	1431	C
1	2	1432	U
1	2	1433	G
1	2	1446	A
1	2	1447	C
1	2	1457	C
1	2	1459	C
1	2	1460	A
1	2	1469	A
1	2	1471	A
1	2	1472	C
1	2	1473	U
1	2	1479	A
1	2	1482	C
1	2	1483	A
1	2	1488	G
1	2	1489	U
1	2	1490	C

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Mol	Chain	Res	Type
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1496	U
1	2	1510	U
1	2	1514	U
1	2	1515	A
1	2	1516	A
1	2	1517	U
1	2	1518	C
1	2	1521	G
1	2	1523	G
1	2	1524	A
1	2	1528	U
1	2	1529	C
1	2	1531	G
1	2	1537	C
1	2	1540	G
1	2	1543	A
1	2	1545	A
1	2	1556	A
1	2	1557	U
1	2	1558	U
1	2	1559	A
1	2	1572	G
1	2	1573	A
1	2	1574	G
1	2	1575	G
1	2	1576	A
1	2	1583	A
1	2	1584	G
1	2	1585	U
1	2	1590	G
1	2	1592	A
1	2	1601	G
1	2	1607	G
1	2	1611	A
1	2	1614	A
1	2	1616	G
1	2	1619	C
1	2	1622	G
1	2	1634	C

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Mol	Chain	Res	Type
1	2	1637	C
1	2	1657	U
1	2	1658	G
1	2	1676	U
1	2	1682	U
1	2	1688	U
1	2	1689	A
1	2	1693	A
1	2	1700	C
1	2	1701	A
1	2	1702	A
1	2	1703	C
1	2	1709	C
1	2	1711	C
1	2	1715	G
1	2	1717	G
1	2	1736	G
1	2	1740	A
1	2	1755	A
1	2	1756	A
1	2	1757	G
1	2	1760	G
1	2	1762	A
1	2	1766	A
1	2	1767	G
1	2	1769	U
1	2	1770	U
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1788	G
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1796	C
1	2	1799	U
2	1	4	A
36	LA	6	A
36	LA	11	A
36	LA	14	U
36	LA	21	G
36	LA	22	G

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Mol	Chain	Res	Type
36	LA	26	A
36	LA	30	G
36	LA	40	A
36	LA	43	A
36	LA	44	U
36	LA	48	A
36	LA	49	A
36	LA	51	A
36	LA	59	G
36	LA	60	A
36	LA	65	A
36	LA	66	A
36	LA	73	C
36	LA	74	G
36	LA	76	G
36	LA	85	A
36	LA	89	A
36	LA	92	G
36	LA	109	A
36	LA	110	G
36	LA	111	C
36	LA	113	C
36	LA	120	G
36	LA	121	A
36	LA	122	A
36	LA	133	U
36	LA	136	G
36	LA	143	G
36	LA	150	A
36	LA	156	G
36	LA	157	A
36	LA	166	C
36	LA	173	G
36	LA	187	A
36	LA	190	U
36	LA	191	U
36	LA	200	C
36	LA	206	G
36	LA	210	U
36	LA	211	A
36	LA	213	A
36	LA	218	G

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Mol	Chain	Res	Type
36	LA	219	A
36	LA	221	A
36	LA	231	G
36	LA	234	G
36	LA	236	G
36	LA	239	G
36	LA	240	U
36	LA	243	G
36	LA	249	U
36	LA	252	U
36	LA	263	C
36	LA	269	G
36	LA	282	G
36	LA	283	G
36	LA	286	U
36	LA	295	A
36	LA	298	U
36	LA	315	C
36	LA	323	A
36	LA	329	U
36	LA	330	G
36	LA	334	A
36	LA	338	A
36	LA	339	C
36	LA	346	C
36	LA	350	C
36	LA	351	A
36	LA	376	G
36	LA	385	A
36	LA	390	G
36	LA	395	A
36	LA	397	A
36	LA	399	A
36	LA	401	U
36	LA	402	A
36	LA	403	C
36	LA	421	G
36	LA	422	A
36	LA	438	A
36	LA	440	A
36	LA	441	U
36	LA	442	G

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Mol	Chain	Res	Type
36	LA	443	G
36	LA	445	G
36	LA	446	U
36	LA	447	U
36	LA	448	U
36	LA	449	U
36	LA	450	G
36	LA	487	U
36	LA	488	U
36	LA	489	U
36	LA	490	C
36	LA	491	A
36	LA	492	C
36	LA	494	G
36	LA	498	A
36	LA	510	G
36	LA	515	C
36	LA	517	G
36	LA	520	U
36	LA	521	A
36	LA	535	G
36	LA	543	C
36	LA	544	C
36	LA	545	U
36	LA	546	C
36	LA	547	G
36	LA	552	G
36	LA	555	U
36	LA	557	A
36	LA	559	A
36	LA	568	G
36	LA	578	A
36	LA	579	G
36	LA	597	G
36	LA	600	G
36	LA	603	A
36	LA	604	G
36	LA	609	G
36	LA	610	G
36	LA	611	A
36	LA	612	U
36	LA	619	A

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Mol	Chain	Res	Type
36	LA	620	U
36	LA	621	A
36	LA	625	G
36	LA	637	C
36	LA	638	C
36	LA	642	U
36	LA	649	A
36	LA	650	C
36	LA	660	A
36	LA	667	C
36	LA	677	A
36	LA	681	U
36	LA	691	A
36	LA	699	A
36	LA	705	A
36	LA	712	G
36	LA	716	A
36	LA	720	A
36	LA	726	G
36	LA	737	G
36	LA	742	G
36	LA	758	C
36	LA	763	G
36	LA	764	U
36	LA	765	C
36	LA	766	U
36	LA	767	U
36	LA	771	A
36	LA	774	G
36	LA	776	U
36	LA	777	U
36	LA	780	A
36	LA	781	G
36	LA	785	G
36	LA	786	A
36	LA	806	A
36	LA	808	A
36	LA	817	A
36	LA	830	A
36	LA	832	G
36	LA	848	A
36	LA	849	C

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Mol	Chain	Res	Type
36	LA	850	U
36	LA	851	C
36	LA	861	C
36	LA	865	U
36	LA	868	C
36	LA	871	U
36	LA	874	U
36	LA	879	U
36	LA	894	G
36	LA	895	A
36	LA	896	A
36	LA	899	U
36	LA	906	A
36	LA	907	G
36	LA	908	G
36	LA	914	A
36	LA	916	G
36	LA	917	A
36	LA	921	A
36	LA	923	C
36	LA	932	U
36	LA	934	G
36	LA	937	G
36	LA	944	C
36	LA	959	C
36	LA	960	U
36	LA	971	G
36	LA	974	G
36	LA	981	U
36	LA	982	C
36	LA	991	G
36	LA	1002	A
36	LA	1015	U
36	LA	1018	G
36	LA	1020	G
36	LA	1021	G
36	LA	1024	G
36	LA	1028	U
36	LA	1029	G
36	LA	1040	A
36	LA	1041	U
36	LA	1045	C

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Mol	Chain	Res	Type
36	LA	1047	A
36	LA	1049	C
36	LA	1064	A
36	LA	1065	A
36	LA	1072	G
36	LA	1081	U
36	LA	1093	A
36	LA	1094	U
36	LA	1095	U
36	LA	1096	U
36	LA	1097	G
36	LA	1098	A
36	LA	1103	A
36	LA	1104	G
36	LA	1117	G
36	LA	1118	C
36	LA	1128	U
36	LA	1131	G
36	LA	1144	U
36	LA	1145	G
36	LA	1148	G
36	LA	1153	A
36	LA	1158	A
36	LA	1159	A
36	LA	1177	G
36	LA	1178	G
36	LA	1180	A
36	LA	1181	U
36	LA	1182	A
36	LA	1190	A
36	LA	1192	C
36	LA	1193	A
36	LA	1196	C
36	LA	1197	A
36	LA	1201	C
36	LA	1202	A
36	LA	1206	G
36	LA	1208	U
36	LA	1217	A
36	LA	1218	U
36	LA	1222	G
36	LA	1223	A

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Mol	Chain	Res	Type
36	LA	1227	C
36	LA	1229	G
36	LA	1234	G
36	LA	1236	G
36	LA	1237	G
36	LA	1238	C
36	LA	1239	C
36	LA	1240	A
36	LA	1241	U
36	LA	1242	G
36	LA	1243	G
36	LA	1244	A
36	LA	1245	A
36	LA	1246	G
36	LA	1248	C
36	LA	1251	A
36	LA	1253	U
36	LA	1258	U
36	LA	1262	G
36	LA	1263	A
36	LA	1264	G
36	LA	1266	G
36	LA	1267	U
36	LA	1269	U
36	LA	1270	A
36	LA	1271	A
36	LA	1272	C
36	LA	1278	A
36	LA	1279	C
36	LA	1280	C
36	LA	1282	G
36	LA	1285	G
36	LA	1286	A
36	LA	1287	A
36	LA	1295	G
36	LA	1307	G
36	LA	1308	A
36	LA	1309	U
36	LA	1313	G
36	LA	1316	C
36	LA	1318	A
36	LA	1325	U

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Mol	Chain	Res	Type
36	LA	1330	A
36	LA	1345	G
36	LA	1348	U
36	LA	1349	G
36	LA	1351	U
36	LA	1352	A
36	LA	1353	U
36	LA	1354	G
36	LA	1355	A
36	LA	1356	U
36	LA	1357	G
36	LA	1386	A
36	LA	1392	G
36	LA	1399	A
36	LA	1400	G
36	LA	1418	A
36	LA	1419	A
36	LA	1421	G
36	LA	1429	G
36	LA	1430	U
36	LA	1431	G
36	LA	1434	G
36	LA	1437	C
36	LA	1442	U
36	LA	1443	G
36	LA	1446	A
36	LA	1450	G
36	LA	1455	U
36	LA	1481	A
36	LA	1482	A
36	LA	1483	G
36	LA	1484	U
36	LA	1487	G
36	LA	1488	G
36	LA	1503	A
36	LA	1508	C
36	LA	1523	U
36	LA	1528	G
36	LA	1533	U
36	LA	1536	G
36	LA	1542	G
36	LA	1549	U

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Mol	Chain	Res	Type
36	LA	1555	U
36	LA	1556	C
36	LA	1557	A
36	LA	1559	A
36	LA	1560	G
36	LA	1562	C
36	LA	1563	C
36	LA	1565	G
36	LA	1566	A
36	LA	1567	U
36	LA	1568	U
36	LA	1569	U
36	LA	1572	U
36	LA	1573	G
36	LA	1574	C
36	LA	1575	A
36	LA	1576	G
36	LA	1580	A
36	LA	1581	C
36	LA	1582	C
36	LA	1583	A
36	LA	1587	A
36	LA	1588	A
36	LA	1589	A
36	LA	1590	G
36	LA	1602	A
36	LA	1605	A
36	LA	1607	U
36	LA	1621	A
36	LA	1629	U
36	LA	1632	A
36	LA	1639	C
36	LA	1642	A
36	LA	1643	A
36	LA	1645	U
36	LA	1658	G
36	LA	1677	G
36	LA	1683	A
36	LA	1687	U
36	LA	1688	U
36	LA	1696	A
36	LA	1704	A

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Mol	Chain	Res	Type
36	LA	1705	U
36	LA	1715	A
36	LA	1716	U
36	LA	1717	U
36	LA	1722	U
36	LA	1724	U
36	LA	1725	C
36	LA	1750	A
36	LA	1751	G
36	LA	1756	C
36	LA	1760	A
36	LA	1765	U
36	LA	1766	G
36	LA	1770	G
36	LA	1775	G
36	LA	1780	G
36	LA	1788	C
36	LA	1796	G
36	LA	1797	A
36	LA	1812	G
36	LA	1814	A
36	LA	1816	A
36	LA	1817	G
36	LA	1819	U
36	LA	1820	U
36	LA	1821	U
36	LA	1822	C
36	LA	1835	A
36	LA	1839	A
36	LA	1840	U
36	LA	1841	A
36	LA	1842	A
36	LA	1846	C
36	LA	1849	C
36	LA	1850	A
36	LA	1866	C
36	LA	1867	A
36	LA	1874	A
36	LA	1880	U
36	LA	1881	A
36	LA	1893	A
36	LA	1897	G

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Mol	Chain	Res	Type
36	LA	1906	G
36	LA	1908	A
36	LA	1930	A
36	LA	1935	G
36	LA	1943	C
36	LA	1951	C
36	LA	1952	G
36	LA	1953	G
36	LA	1954	G
36	LA	2101	C
36	LA	2102	U
36	LA	2111	G
36	LA	2113	A
36	LA	2121	G
36	LA	2122	G
36	LA	2131	A
36	LA	2139	A
36	LA	2149	A
36	LA	2158	A
36	LA	2169	G
36	LA	2170	U
36	LA	2187	G
36	LA	2188	A
36	LA	2201	G
36	LA	2205	U
36	LA	2206	G
36	LA	2207	A
36	LA	2209	U
36	LA	2223	A
36	LA	2228	A
36	LA	2244	A
36	LA	2249	G
36	LA	2250	G
36	LA	2252	A
36	LA	2256	A
36	LA	2257	C
36	LA	2262	A
36	LA	2272	G
36	LA	2273	G
36	LA	2274	U
36	LA	2279	A
36	LA	2280	A

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Mol	Chain	Res	Type
36	LA	2281	A
36	LA	2282	U
36	LA	2284	C
36	LA	2285	C
36	LA	2288	G
36	LA	2299	A
36	LA	2306	C
36	LA	2307	G
36	LA	2308	C
36	LA	2309	A
36	LA	2310	U
36	LA	2313	A
36	LA	2314	U
36	LA	2315	G
36	LA	2335	G
36	LA	2336	U
36	LA	2347	U
36	LA	2364	G
36	LA	2372	A
36	LA	2373	A
36	LA	2374	C
36	LA	2375	G
36	LA	2385	G
36	LA	2388	U
36	LA	2393	G
36	LA	2394	G
36	LA	2397	A
36	LA	2402	A
36	LA	2403	G
36	LA	2404	A
36	LA	2411	U
36	LA	2412	G
36	LA	2419	A
36	LA	2422	C
36	LA	2434	U
36	LA	2435	G
36	LA	2437	G
36	LA	2438	A
36	LA	2439	A
36	LA	2440	G
36	LA	2452	G
36	LA	2453	U

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Mol	Chain	Res	Type
36	LA	2454	G
36	LA	2455	U
36	LA	2456	A
36	LA	2457	G
36	LA	2458	A
36	LA	2459	A
36	LA	2461	A
36	LA	2462	A
36	LA	2463	G
36	LA	2466	G
36	LA	2467	G
36	LA	2468	A
36	LA	2469	G
36	LA	2471	U
36	LA	2474	G
36	LA	2477	G
36	LA	2480	A
36	LA	2484	A
36	LA	2487	U
36	LA	2488	A
36	LA	2489	C
36	LA	2491	A
36	LA	2492	C
36	LA	2493	U
36	LA	2494	A
36	LA	2496	C
36	LA	2497	U
36	LA	2498	U
36	LA	2499	U
36	LA	2500	A
36	LA	2501	U
36	LA	2503	G
36	LA	2505	U
36	LA	2506	U
36	LA	2507	C
36	LA	2510	U
36	LA	2514	U
36	LA	2515	A
36	LA	2522	G
36	LA	2523	A
36	LA	2524	A
36	LA	2525	G

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Mol	Chain	Res	Type
36	LA	2526	C
36	LA	2531	C
36	LA	2532	U
36	LA	2537	U
36	LA	2538	U
36	LA	2539	C
36	LA	2540	A
36	LA	2541	U
36	LA	2542	U
36	LA	2543	U
36	LA	2546	C
36	LA	2548	C
36	LA	2549	G
36	LA	2552	C
36	LA	2554	A
36	LA	2561	A
36	LA	2569	A
36	LA	2570	U
36	LA	2571	U
36	LA	2572	C
36	LA	2573	G
36	LA	2576	G
36	LA	2585	G
36	LA	2589	G
36	LA	2593	A
36	LA	2594	C
36	LA	2595	A
36	LA	2606	G
36	LA	2607	G
36	LA	2614	G
36	LA	2626	A
36	LA	2629	U
36	LA	2636	A
36	LA	2648	G
36	LA	2652	U
36	LA	2656	A
36	LA	2672	G
36	LA	2674	A
36	LA	2677	G
36	LA	2689	A
36	LA	2691	A
36	LA	2694	A

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Mol	Chain	Res	Type
36	LA	2696	A
36	LA	2703	A
36	LA	2704	A
36	LA	2714	G
36	LA	2719	U
36	LA	2728	G
36	LA	2748	A
36	LA	2749	G
36	LA	2752	U
36	LA	2753	G
36	LA	2755	C
36	LA	2777	G
36	LA	2778	G
36	LA	2796	G
36	LA	2800	G
36	LA	2801	A
36	LA	2802	A
36	LA	2803	A
36	LA	2804	A
36	LA	2805	G
36	LA	2810	C
36	LA	2817	A
36	LA	2818	U
36	LA	2821	C
36	LA	2838	A
36	LA	2842	U
36	LA	2844	C
36	LA	2845	A
36	LA	2847	A
36	LA	2849	C
36	LA	2856	G
36	LA	2861	U
36	LA	2867	C
36	LA	2871	G
36	LA	2872	A
36	LA	2873	U
36	LA	2875	U
36	LA	2876	C
36	LA	2887	A
36	LA	2894	C
36	LA	2899	C
36	LA	2910	A

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Mol	Chain	Res	Type
36	LA	2916	U
36	LA	2918	G
36	LA	2923	U
36	LA	2928	C
36	LA	2933	A
36	LA	2935	U
36	LA	2936	A
36	LA	2941	A
36	LA	2942	C
36	LA	2947	G
36	LA	2954	U
36	LA	2955	U
36	LA	2957	G
36	LA	2971	A
36	LA	2983	C
36	LA	2990	G
36	LA	2996	U
36	LA	2997	G
36	LA	3003	G
36	LA	3012	A
36	LA	3030	G
36	LA	3055	U
36	LA	3056	U
36	LA	3058	U
36	LA	3059	G
36	LA	3078	U
36	LA	3079	U
36	LA	3080	G
36	LA	3086	A
36	LA	3092	C
36	LA	3101	G
36	LA	3104	U
36	LA	3115	C
36	LA	3116	G
36	LA	3118	C
36	LA	3119	U
36	LA	3122	A
36	LA	3129	A
36	LA	3130	A
36	LA	3131	U
36	LA	3142	A
36	LA	3143	C

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Mol	Chain	Res	Type
36	LA	3151	U
36	LA	3154	C
36	LA	3155	U
36	LA	3156	U
36	LA	3157	U
36	LA	3158	G
36	LA	3165	A
36	LA	3170	A
36	LA	3172	A
36	LA	3173	G
36	LA	3174	A
36	LA	3175	U
36	LA	3176	G
36	LA	3180	A
36	LA	3181	C
36	LA	3187	A
36	LA	3196	U
36	LA	3199	G
36	LA	3207	U
36	LA	3210	A
36	LA	3216	G
36	LA	3217	C
36	LA	3218	A
36	LA	3219	G
36	LA	3222	U
36	LA	3229	G
36	LA	3235	C
36	LA	3239	G
36	LA	3242	G
36	LA	3243	A
36	LA	3244	A
36	LA	3245	A
36	LA	3247	G
36	LA	3259	U
36	LA	3260	G
36	LA	3263	G
36	LA	3269	U
36	LA	3270	U
36	LA	3272	C
36	LA	3273	A
36	LA	3276	G
36	LA	3277	U

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Mol	Chain	Res	Type
36	LA	3281	U
36	LA	3286	G
36	LA	3287	U
36	LA	3288	G
36	LA	3289	G
36	LA	3294	A
36	LA	3295	A
36	LA	3304	U
36	LA	3313	U
36	LA	3316	A
36	LA	3318	G
36	LA	3319	U
36	LA	3320	A
36	LA	3334	U
36	LA	3341	U
36	LA	3345	G
36	LA	3347	A
36	LA	3351	U
36	LA	3352	U
36	LA	3353	G
36	LA	3354	U
36	LA	3355	U
36	LA	3356	G
36	LA	3368	U
36	LA	3369	G
36	LA	3378	C
36	LA	3381	U
36	LA	3382	U
36	LA	3386	G
36	LA	3389	U
36	LA	3390	G
36	LA	3396	U
37	LB	7	G
37	LB	10	C
37	LB	17	A
37	LB	22	A
37	LB	35	C
37	LB	52	G
37	LB	53	U
37	LB	54	U
37	LB	65	G
37	LB	74	C

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Mol	Chain	Res	Type
37	LB	76	A
37	LB	99	G
37	LB	102	A
37	LB	112	G
37	LB	121	U
38	LC	16	G
38	LC	25	G
38	LC	34	U
38	LC	35	C
38	LC	38	U
38	LC	59	A
38	LC	62	C
38	LC	63	G
38	LC	80	A
38	LC	81	U
38	LC	82	U
38	LC	83	C
38	LC	84	C
38	LC	85	G
38	LC	86	U
38	LC	87	G
38	LC	90	U
38	LC	95	G
38	LC	97	A
38	LC	99	C
38	LC	104	A
38	LC	106	C
38	LC	111	A
38	LC	112	U
38	LC	113	U
38	LC	125	U
38	LC	126	A
38	LC	138	A
38	LC	148	G
38	LC	152	G
38	LC	157	U
38	LC	158	U
80	Sn	8	U
80	Sn	9	G
80	Sn	11	C
80	Sn	14	A
80	Sn	19	G

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Mol	Chain	Res	Type
80	Sn	20	A
80	Sn	21	A
80	Sn	25	C
80	Sn	27	C
80	Sn	36	U
80	Sn	45	U
80	Sn	46	G
80	Sn	47	U
80	Sn	48	C
80	Sn	49	C
80	Sn	54	A
80	Sn	57	G
80	Sn	59	A
80	Sn	61	C
80	Sn	63	G
80	Sn	64	A
80	Sn	66	C
80	Sn	76	A
80	Sm	8	U
80	Sm	9	G
80	Sm	11	C
80	Sm	14	A
80	Sm	19	G
80	Sm	20	A
80	Sm	21	A
80	Sm	25	C
80	Sm	27	C
80	Sm	36	U
80	Sm	45	U
80	Sm	46	G
80	Sm	47	U
80	Sm	48	C
80	Sm	49	C
80	Sm	54	A
80	Sm	57	G
80	Sm	59	A
80	Sm	61	C
80	Sm	63	G
80	Sm	64	A
80	Sm	66	C
80	Sm	74	C
80	Sm	76	A

All (100) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	68	A
1	2	77	U
1	2	139	C
1	2	141	U
1	2	215	A
1	2	224	C
1	2	237	C
1	2	278	U
1	2	280	U
1	2	313	U
1	2	322	G
1	2	352	A
1	2	387	A
1	2	400	A
1	2	447	U
1	2	518	A
1	2	539	G
1	2	541	A
1	2	555	A
1	2	609	U
1	2	639	U
1	2	640	U
1	2	705	U
1	2	711	U
1	2	740	A
1	2	755	A
1	2	803	A
1	2	819	G
1	2	912	U
1	2	928	U
1	2	987	G
1	2	1023	A
1	2	1207	C
1	2	1226	A
1	2	1245	G
1	2	1251	U
1	2	1256	A
1	2	1273	G
1	2	1274	C
1	2	1314	U
1	2	1344	A
1	2	1348	A

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Mol	Chain	Res	Type
1	2	1382	A
1	2	1399	C
1	2	1430	U
1	2	1471	A
1	2	1556	A
1	2	1557	U
1	2	1573	A
1	2	1584	G
1	2	1633	A
1	2	1636	C
1	2	1700	C
1	2	1755	A
36	LA	13	A
36	LA	282	G
36	LA	439	C
36	LA	637	C
36	LA	763	G
36	LA	849	C
36	LA	873	C
36	LA	896	A
36	LA	916	G
36	LA	993	G
36	LA	1064	A
36	LA	1097	G
36	LA	1271	A
36	LA	1307	G
36	LA	1355	A
36	LA	1562	C
36	LA	1572	U
36	LA	1582	C
36	LA	1716	U
36	LA	1815	U
36	LA	1820	U
36	LA	2101	C
36	LA	2112	U
36	LA	2227	C
36	LA	2256	A
36	LA	2500	A
36	LA	2504	U
36	LA	2505	U
36	LA	2509	U
36	LA	2525	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
36	LA	2537	U
36	LA	2538	U
36	LA	2541	U
36	LA	3055	U
36	LA	3078	U
36	LA	3121	U
36	LA	3218	A
36	LA	3228	C
36	LA	3269	U
36	LA	3275	U
36	LA	3319	U
36	LA	3350	C
37	LB	52	G
38	LC	82	U
38	LC	85	G
38	LC	125	U

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
82	ATP	EF	1101	81	26,33,33	0.92	1 (3%)	31,52,52	1.67	6 (19%)
82	ATP	EF	1102	81	26,33,33	0.90	1 (3%)	31,52,52	1.45	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	ATP	EF	1101	81	-	3/18/38/38	0/3/3/3
82	ATP	EF	1102	81	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	EF	1101	ATP	C5-C4	2.21	1.46	1.40
82	EF	1102	ATP	C5-C4	2.08	1.46	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	EF	1101	ATP	PB-O3B-PG	-4.33	117.97	132.83
82	EF	1101	ATP	C3'-C2'-C1'	3.71	106.56	100.98
82	EF	1101	ATP	PA-O3A-PB	-3.21	121.82	132.83
82	EF	1101	ATP	N3-C2-N1	-3.13	123.78	128.68
82	EF	1102	ATP	N3-C2-N1	-3.05	123.91	128.68
82	EF	1102	ATP	C4-C5-N7	-2.89	106.38	109.40
82	EF	1102	ATP	PB-O3B-PG	-2.67	123.67	132.83
82	EF	1101	ATP	C4-C5-N7	-2.58	106.71	109.40
82	EF	1102	ATP	PA-O3A-PB	-2.51	124.22	132.83
82	EF	1101	ATP	O2A-PA-O1A	2.11	122.65	112.24

There are no chirality outliers.

All (3) torsion outliers are listed below:

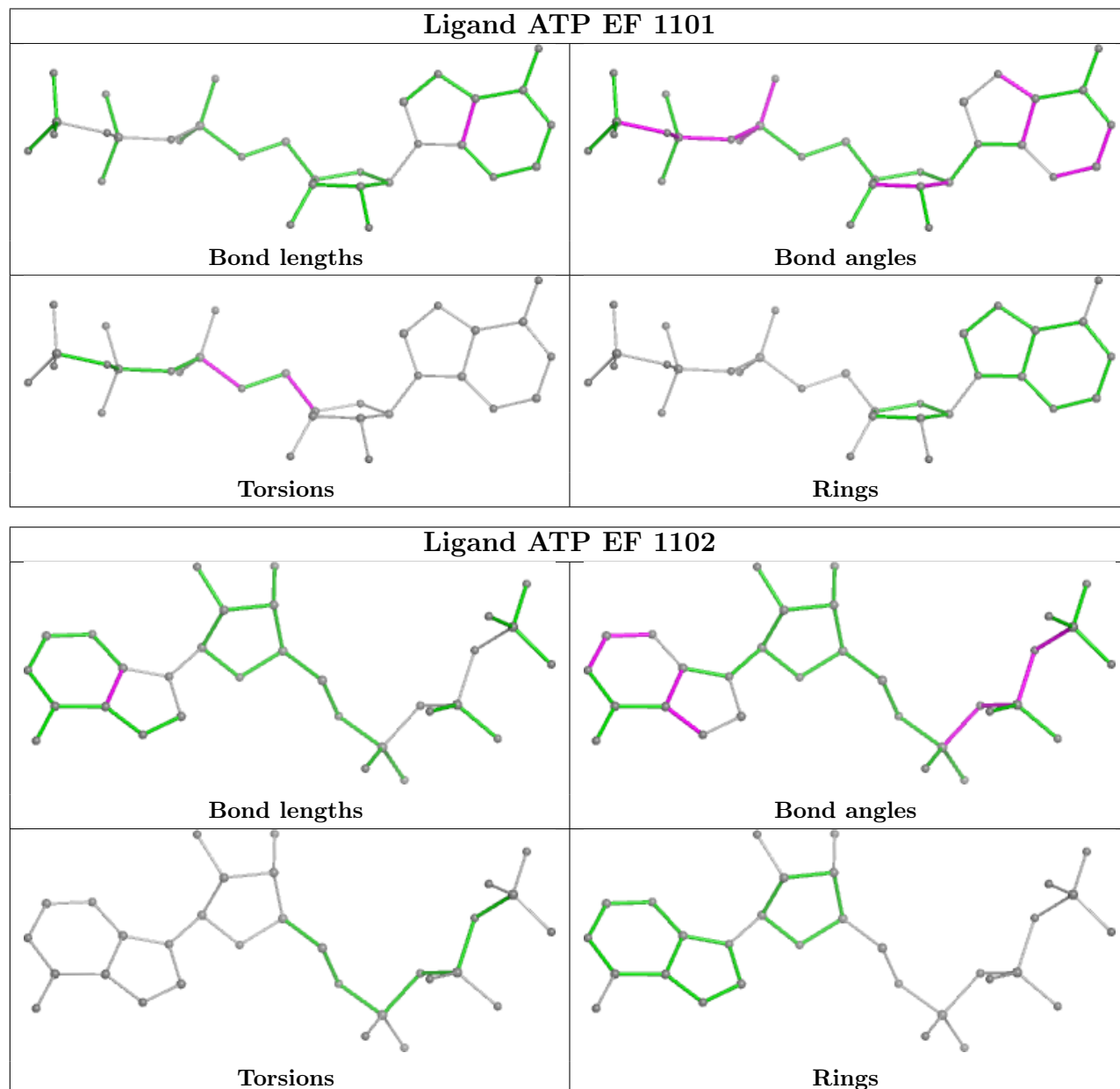
Mol	Chain	Res	Type	Atoms
82	EF	1101	ATP	C5'-O5'-PA-O2A
82	EF	1101	ATP	C5'-O5'-PA-O3A
82	EF	1101	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
36	LA	2
1	2	2
6	R	1
45	LJ	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	LA	1955:U	O3'	2093:A	P	27.27
1	2	658:C	O3'	676:G	P	15.54
1	LA	451:U	O3'	486:A	P	11.17
1	2	714:G	O3'	726:C	P	10.44
1	R	60:SER	C	61:LEU	N	1.18
1	LJ	40:VAL	C	41:GLN	N	1.18

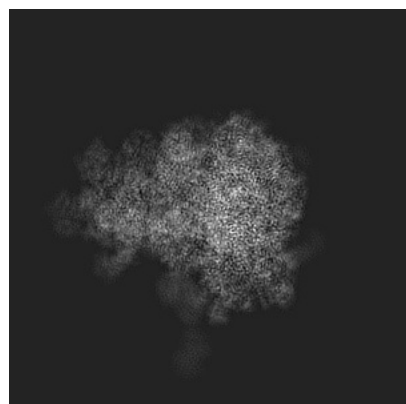
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12081. These allow visual inspection of the internal detail of the map and identification of artifacts.

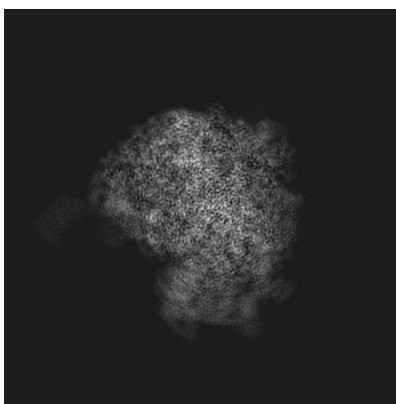
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

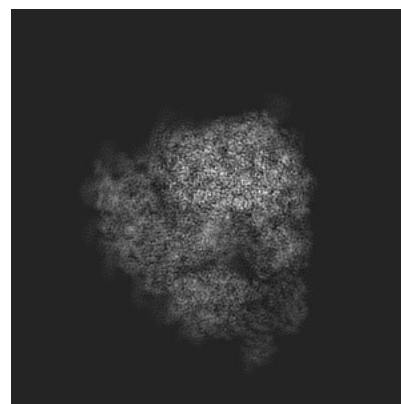
#### 6.1.1 Primary map



X

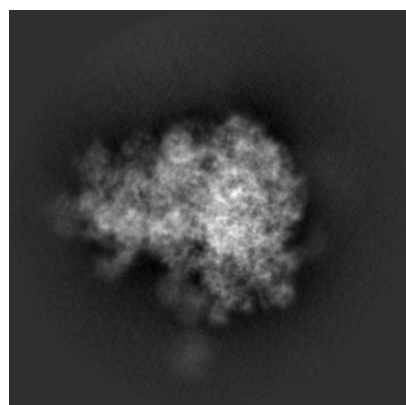


Y

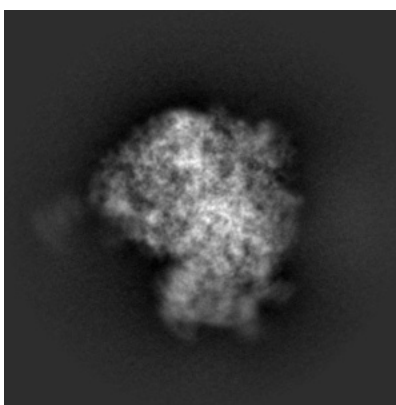


Z

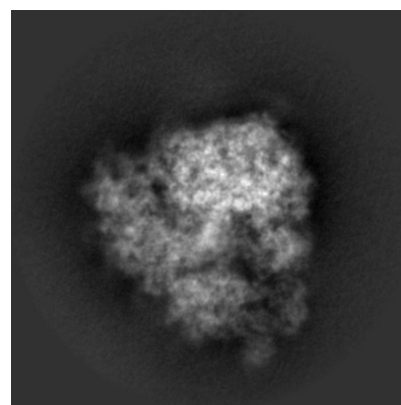
#### 6.1.2 Raw map



X



Y

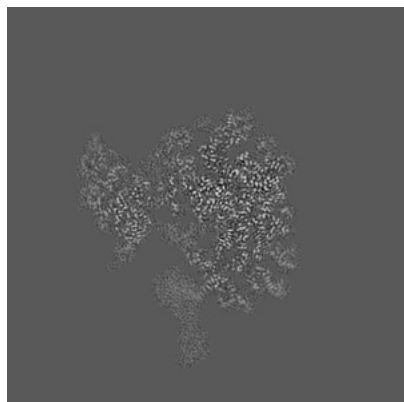


Z

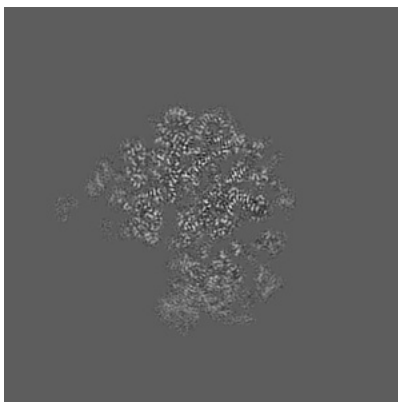
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

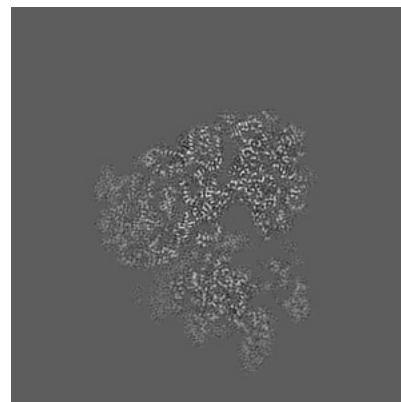
### 6.2.1 Primary map



X Index: 210

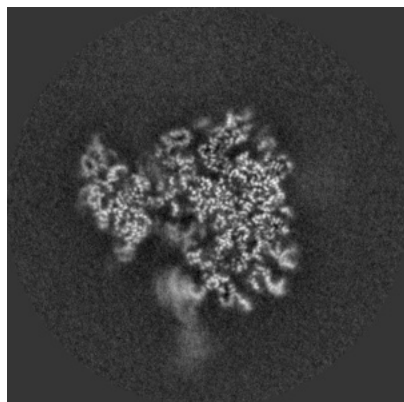


Y Index: 210

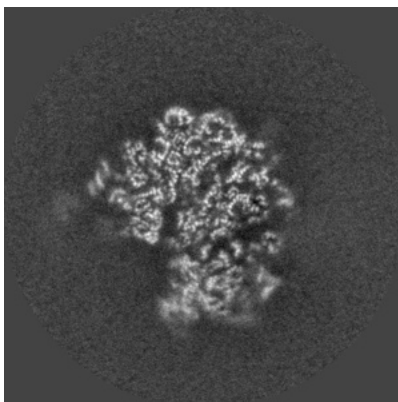


Z Index: 210

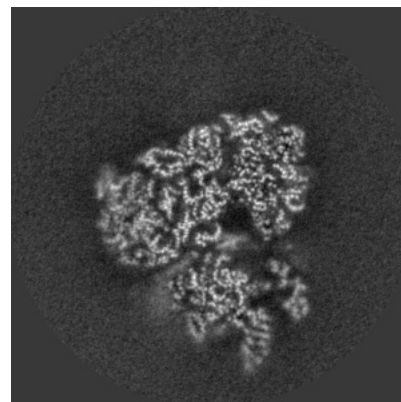
### 6.2.2 Raw map



X Index: 210



Y Index: 210

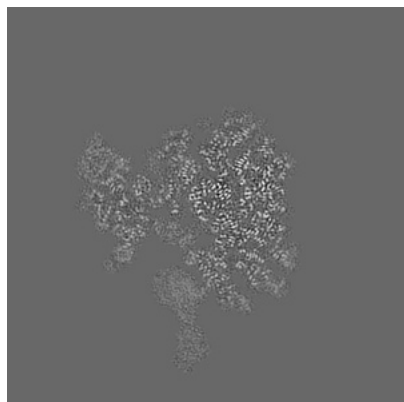


Z Index: 210

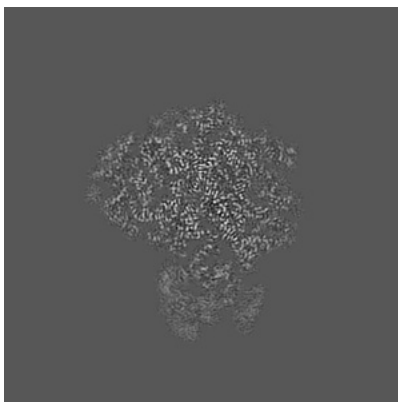
The images above show central slices of the map in three orthogonal directions.

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

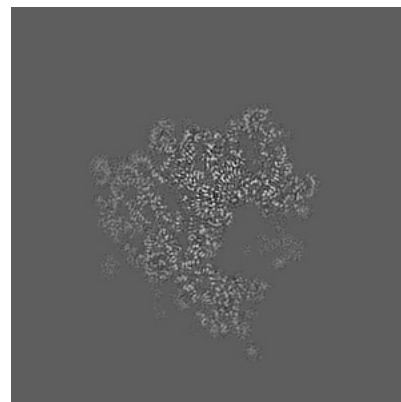
### 6.3.1 Primary map



X Index: 207

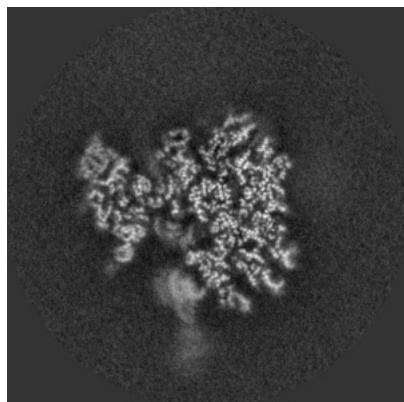


Y Index: 228

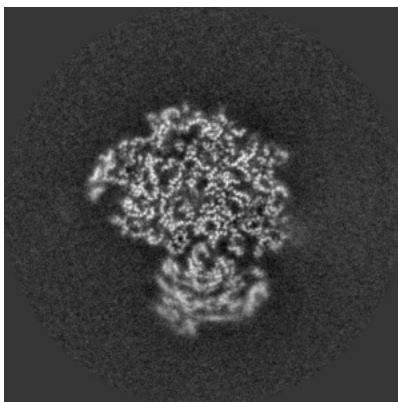


Z Index: 228

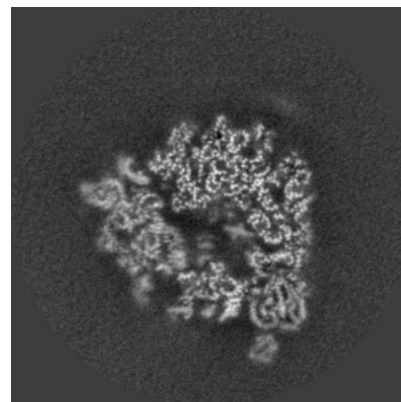
### 6.3.2 Raw map



X Index: 207



Y Index: 219



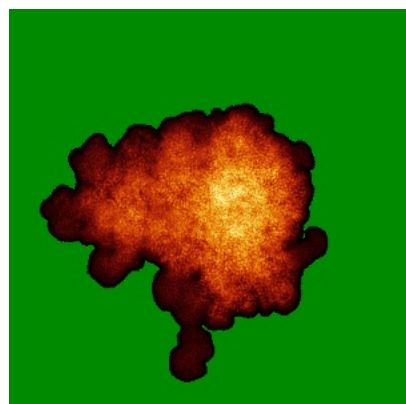
Z Index: 192

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

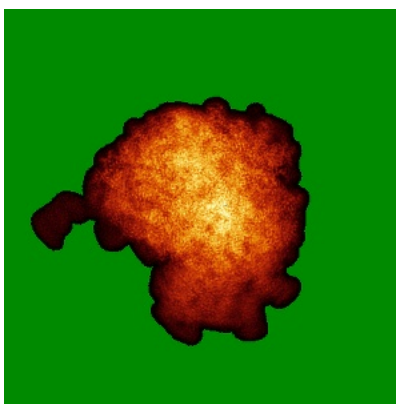


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

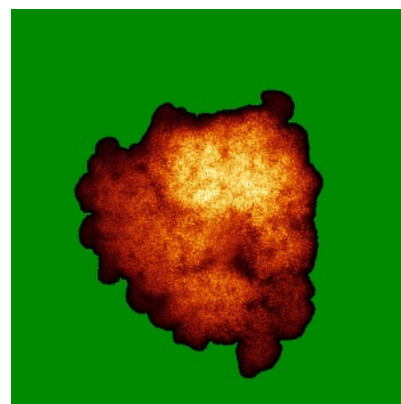
### 6.4.1 Primary map



X

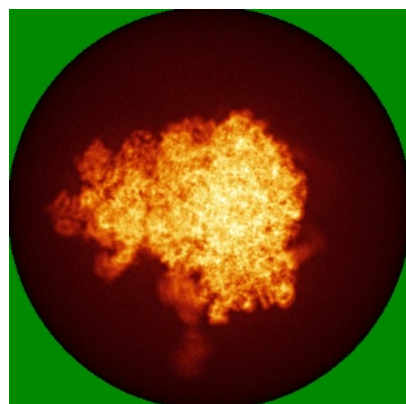


Y

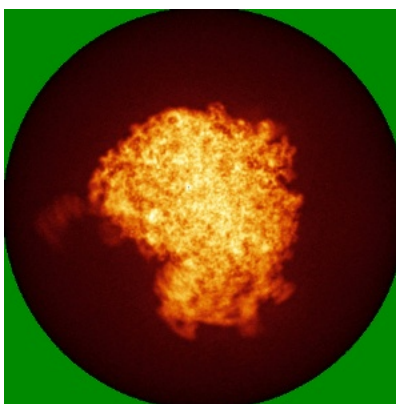


Z

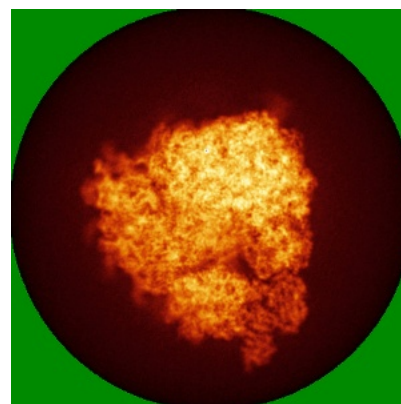
### 6.4.2 Raw map



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.

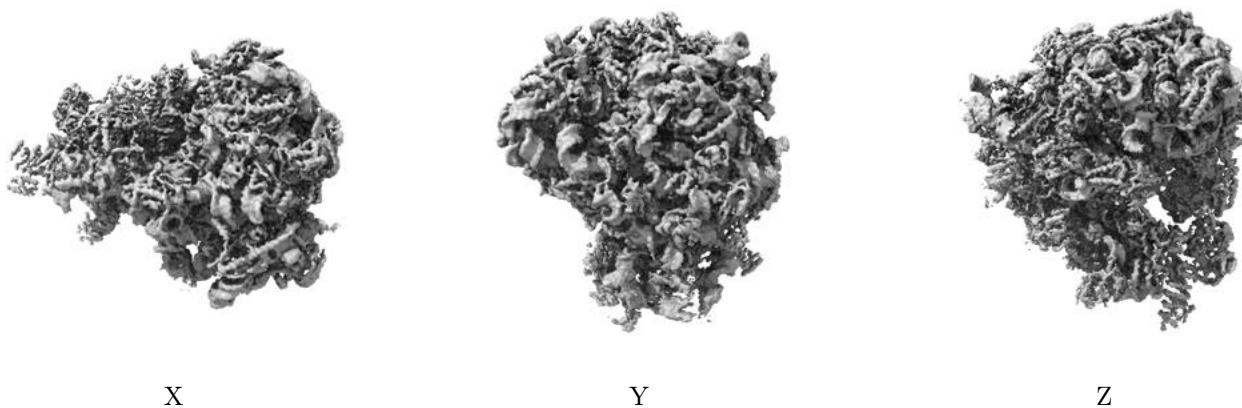
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

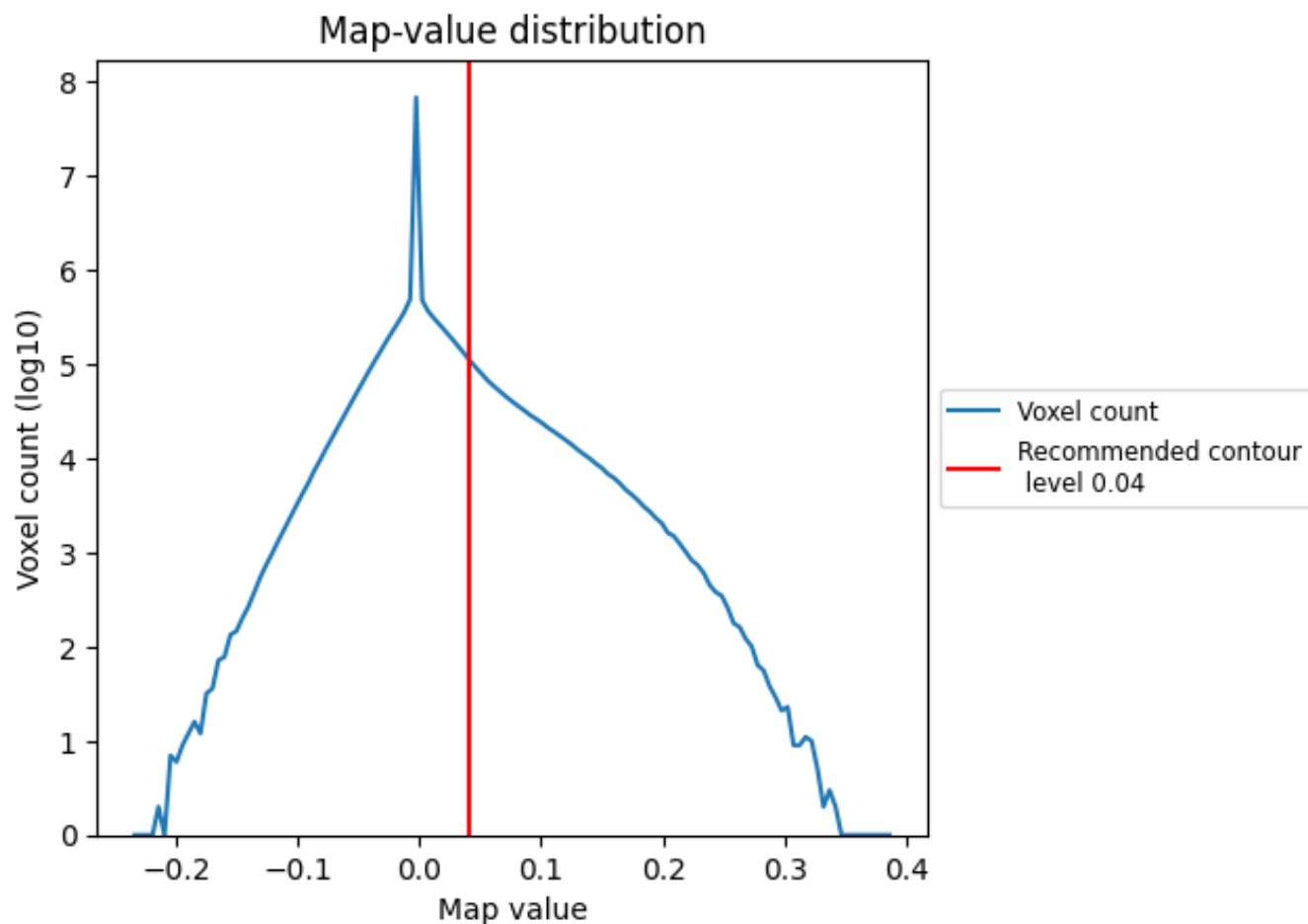
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

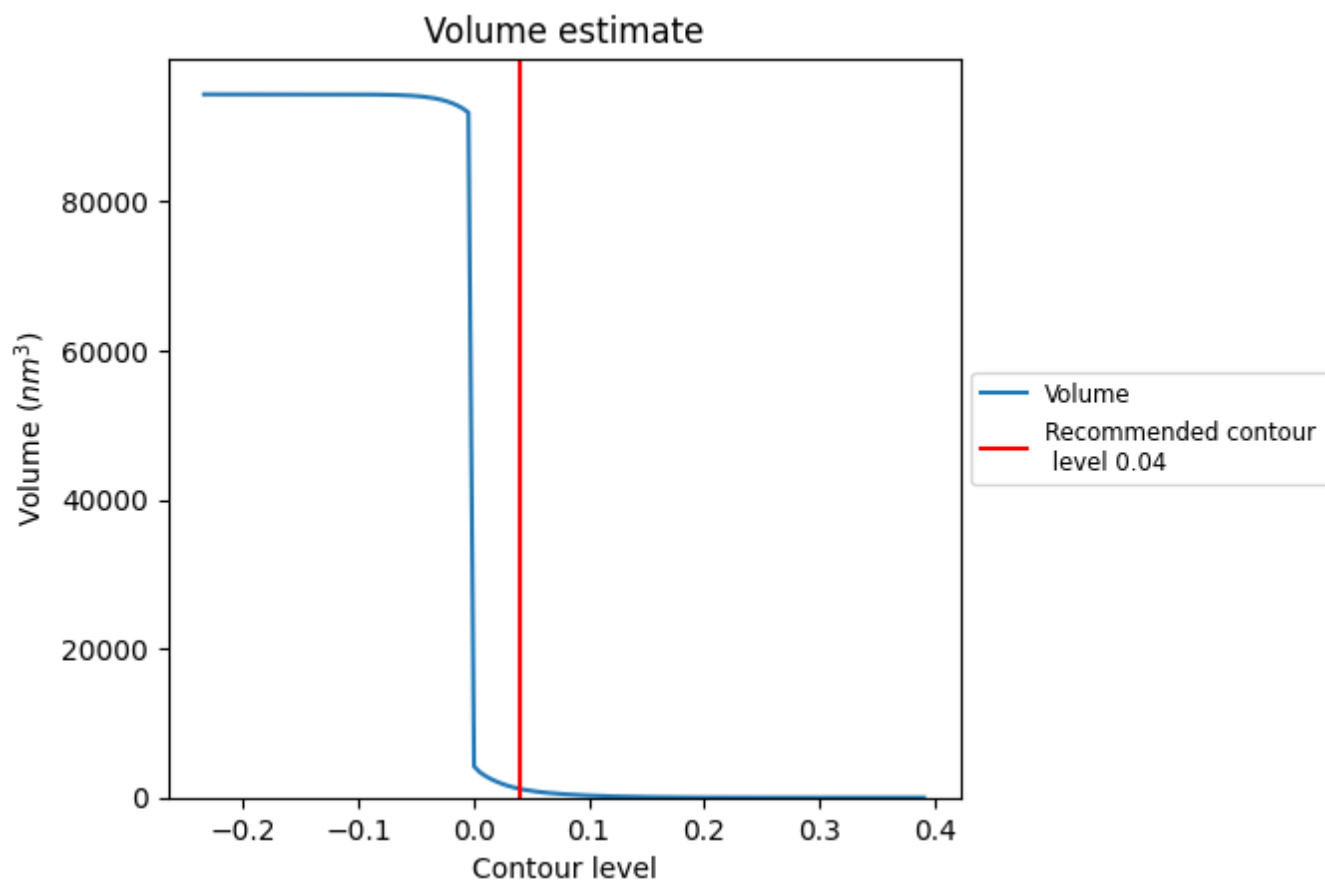
This section contains the results of statistical analysis of the map.

### 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.

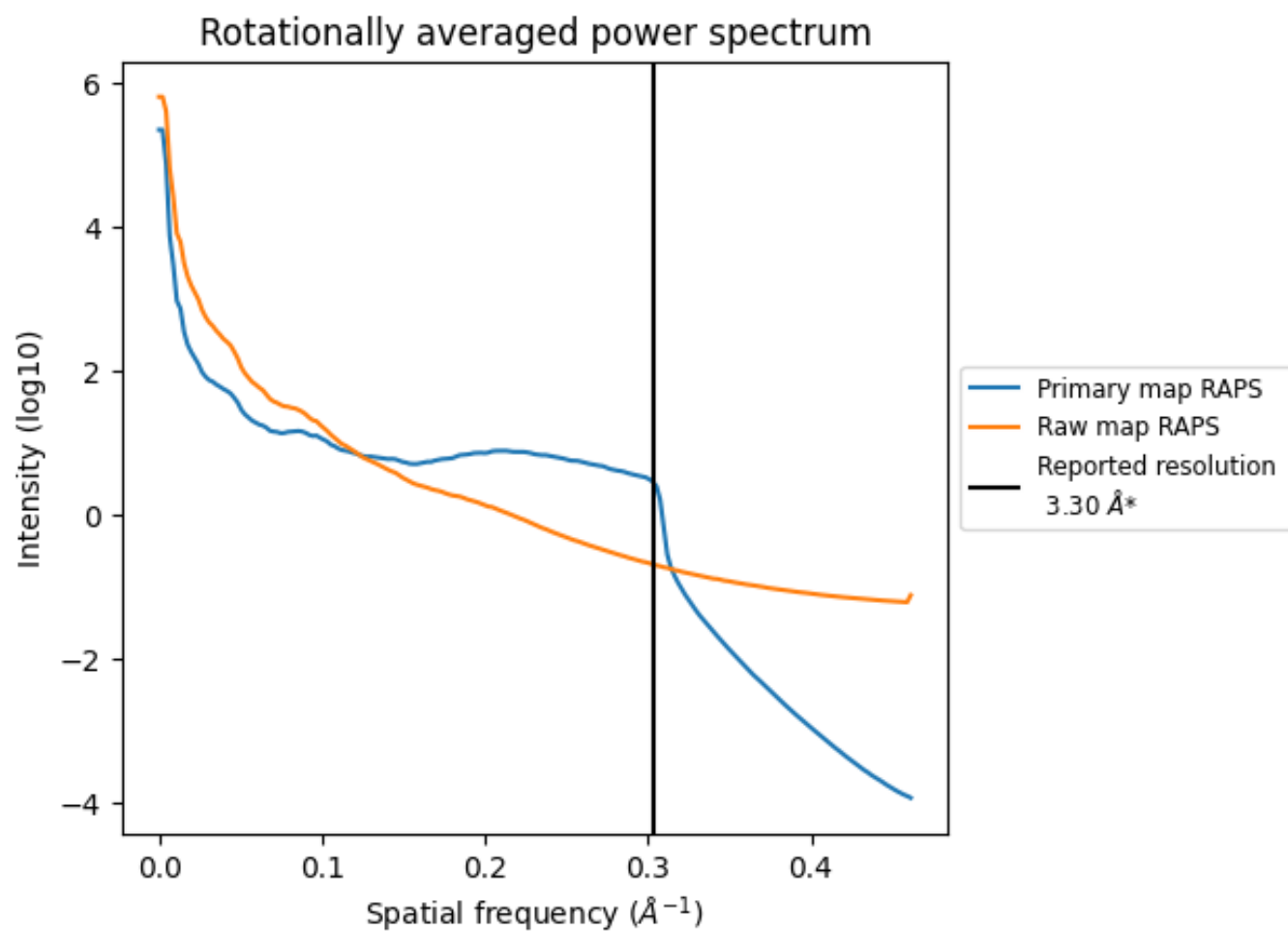
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1176 nm<sup>3</sup>; this corresponds to an approximate mass of 1062 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 ⓘ

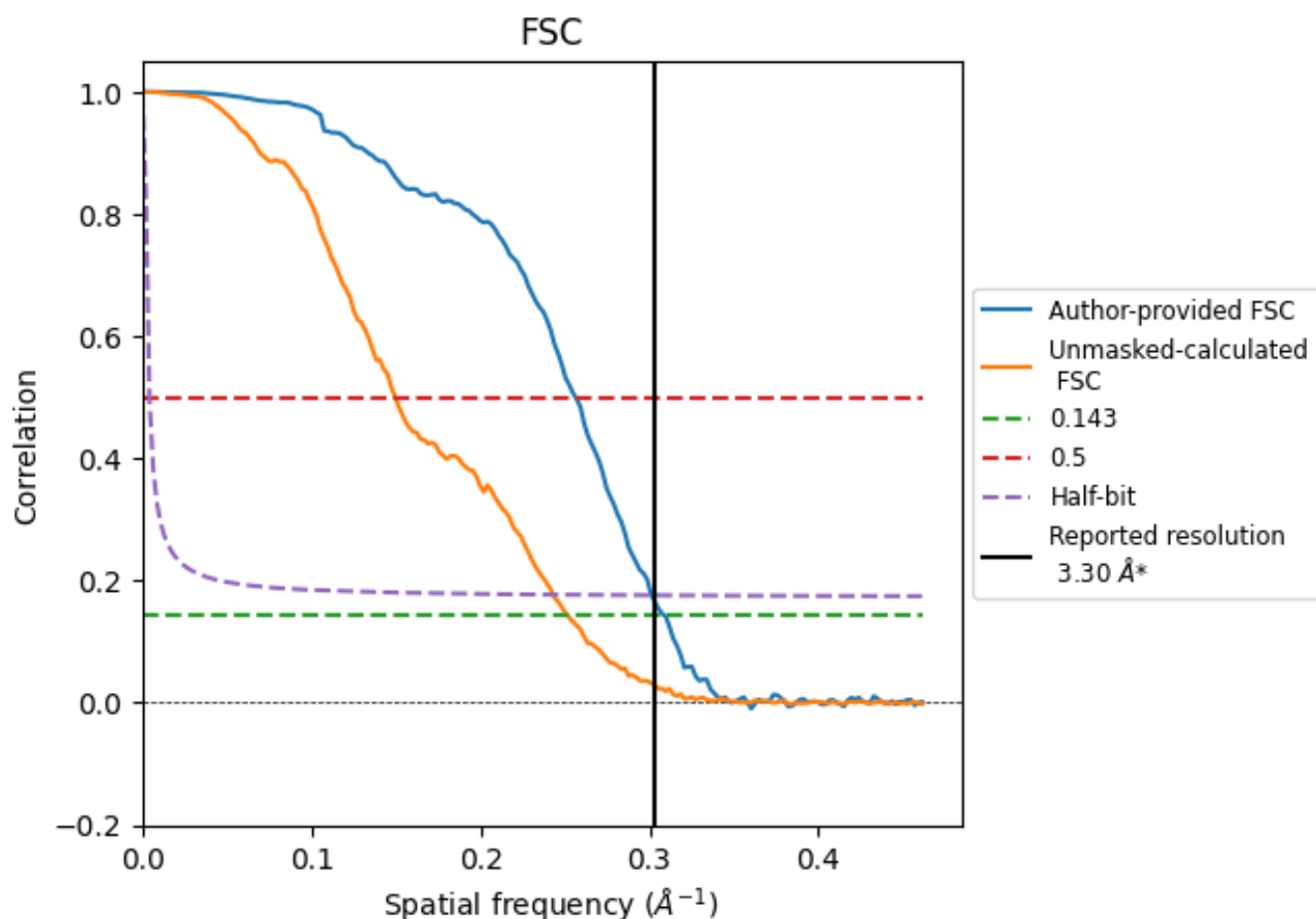


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

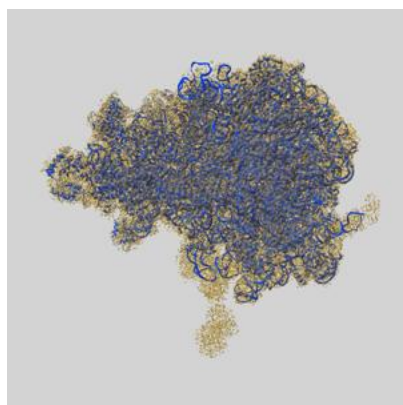
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.24	3.90	3.32
Unmasked-calculated*	3.98	6.68	4.12

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 3.3 by more than 10 %

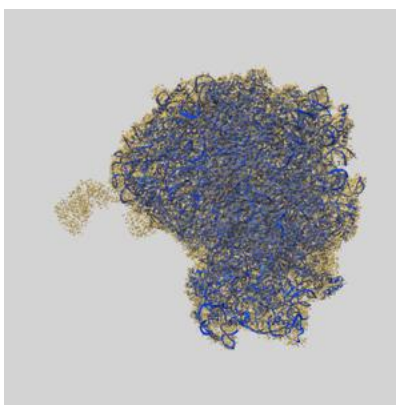
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12081 and PDB model 7B7D. Per-residue inclusion information can be found in [section 3](#) on [page 19](#).

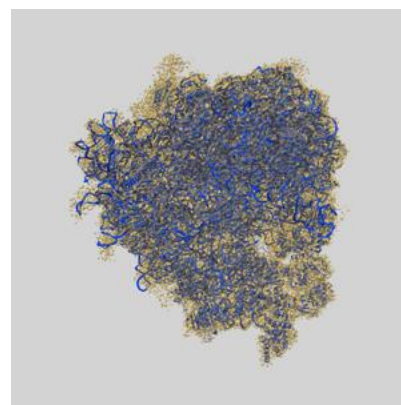
### 9.1 Map-model overlay [i](#)



X



Y

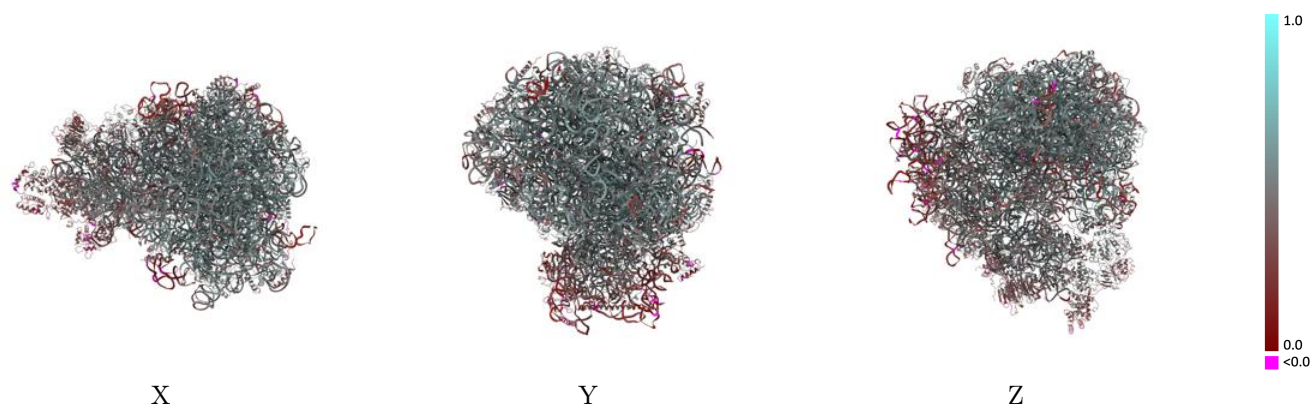


Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

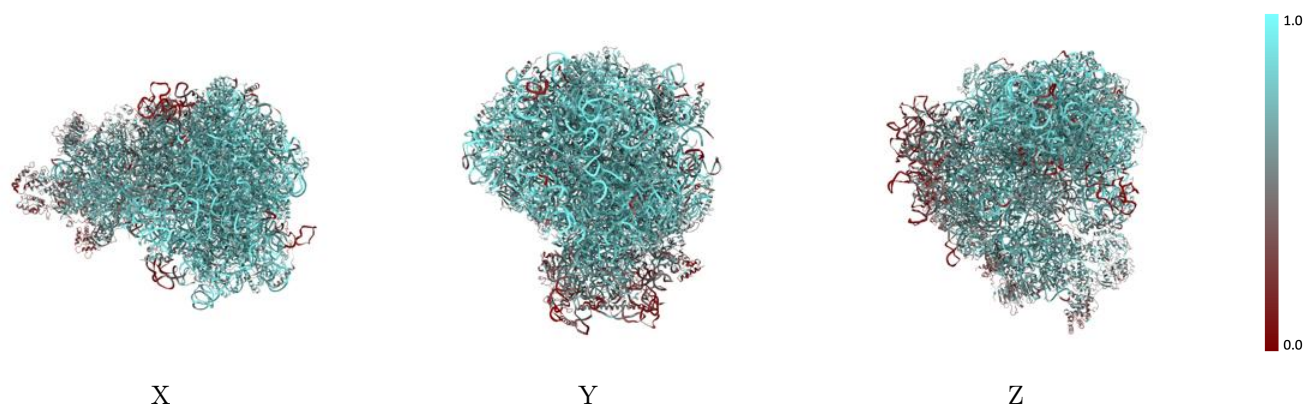


## 9.2 Q-score mapped to coordinate model [i](#)



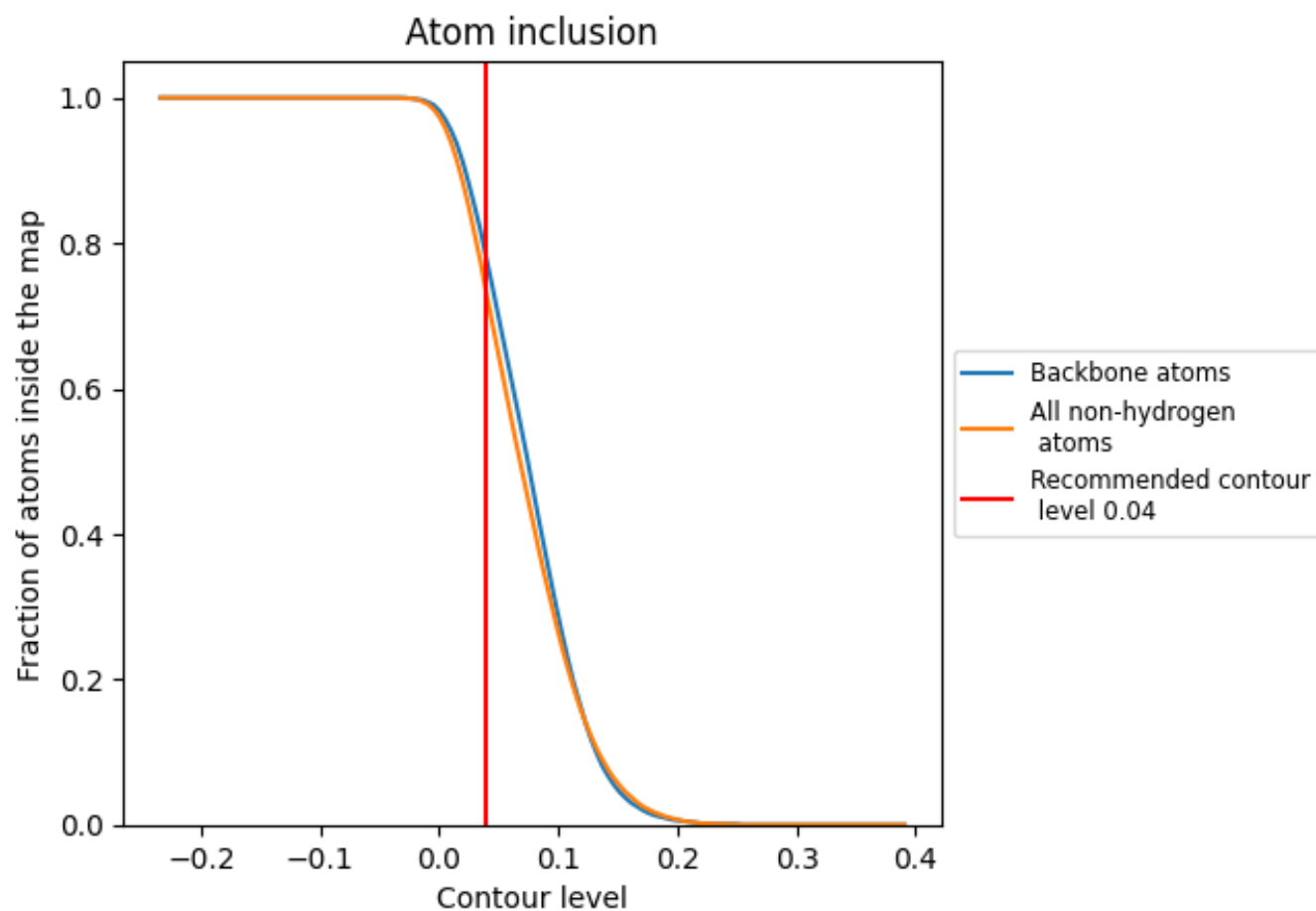
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 73% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7290	 0.4640
1	 0.7920	 0.5060
2	 0.7210	 0.4320
A	 0.5500	 0.3880
B	 0.6250	 0.4200
C	 0.5240	 0.3600
D	 0.1780	 0.1740
E	 0.5960	 0.3720
EF	 0.5300	 0.3800
F	 0.6830	 0.4600
G	 0.5620	 0.3970
H	 0.6630	 0.4310
I	 0.6900	 0.4610
J	 0.5550	 0.3880
K	 0.5510	 0.3510
L	 0.5730	 0.3960
LA	 0.8460	 0.5110
LB	 0.9010	 0.5280
LC	 0.8830	 0.5340
LD	 0.8060	 0.5400
LE	 0.7770	 0.5110
LF	 0.7670	 0.5080
LG	 0.7200	 0.4630
LH	 0.6570	 0.4420
LI	 0.7670	 0.5060
LJ	 0.6720	 0.4510
LK	 0.7140	 0.4790
LL	 0.6820	 0.4670
LM	 0.7090	 0.4590
LN	 0.7380	 0.5010
LO	 0.7240	 0.4810
LP	 0.8140	 0.5480
LQ	 0.7650	 0.5150
LR	 0.7690	 0.5070
LS	 0.5130	 0.3850















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Chain	Atom inclusion	Q-score
LT	 0.7530	 0.5070
LU	 0.7470	 0.5030
LV	 0.7140	 0.4740
LW	 0.7950	 0.5280
LX	 0.7210	 0.4960
LY	 0.6730	 0.4670
LZ	 0.7210	 0.4880
La	 0.7690	 0.5240
Lb	 0.7980	 0.5420
Lc	 0.7230	 0.5140
Ld	 0.7210	 0.4930
Le	 0.6820	 0.4630
Lf	 0.8400	 0.5520
Lg	 0.6330	 0.4260
Lh	 0.7660	 0.5160
Li	 0.7200	 0.4920
Lj	 0.6680	 0.4970
Lk	 0.7580	 0.5130
Ll	 0.7400	 0.5190
Lm	 0.7630	 0.5190
Ln	 0.7010	 0.4730
Lo	 0.7500	 0.5100
Lp	 0.7480	 0.5080
Lq	 0.6610	 0.4310
Lr	 0.7100	 0.4990
M	 0.7560	 0.4810
N	 0.2840	 0.2210
O	 0.4890	 0.3320
P	 0.6060	 0.4190
Q	 0.5690	 0.4120
R	 0.6370	 0.4490
S	 0.4670	 0.3650
Sm	 0.3710	 0.3140
Sn	 0.5750	 0.3680
T	 0.3780	 0.2810
U	 0.4310	 0.3330
V	 0.6210	 0.4270
W	 0.4410	 0.3450
X	 0.5830	 0.4370
Y	 0.6330	 0.4370
Z	 0.6660	 0.4590
a	 0.6100	 0.4220

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Chain	Atom inclusion	Q-score
b	 0.6780	 0.4810
c	 0.5630	 0.4070
d	 0.4090	 0.3280
e	 0.7120	 0.4760
f	 0.5490	 0.3830
g	 0.4100	 0.2890