



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 07:20 AM UTC

PDB ID : 3JBN / pdb_00003jbn
EMDB ID : EMD-6456
Title : Cryo-electron microscopy reconstruction of the Plasmodium falciparum 80S ribosome bound to P-tRNA
Authors : Sun, M.; Li, W.; Blomqvist, K.; Das, S.; Hashem, Y.; Dvorin, J.D.; Frank, J.
Deposited on : 2015-09-16
Resolution : 4.70 Å(reported)
Based on initial models : 3J7A, 3J79

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

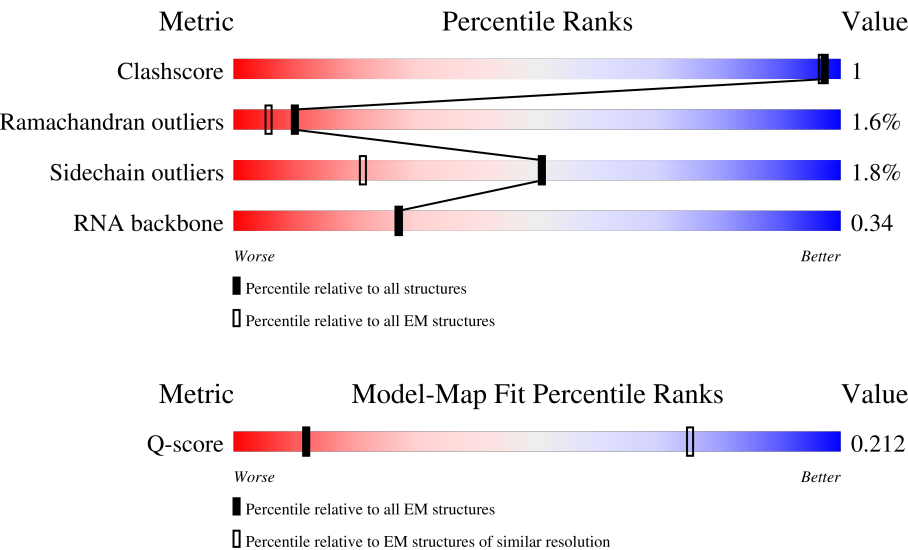
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.70 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	523 (6.20 - 7.20)

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

Mol	Chain	Length	Quality of chain
1	A	1608	14% 59% 32% 8%
2	7	76	16% 67% 25% 7%
3	D	209	16% 72% 25%

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Mol	Chain	Length	Quality of chain
4	E	185	
5	G	224	
6	I	189	
7	K	129	
8	M	138	
9	W	108	
10	R	114	
11	O	79	
12	Y	154	
13	Z	72	
14	1	120	
15	2	68	
16	3	95	
17	4	76	
18	5	65	
19	6	43	
20	B	210	
21	F	257	
22	H	214	
23	J	188	
24	L	214	
25	N	98	
26	P	127	
27	Q	144	
28	S	128	

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Mol	Chain	Length	Quality of chain
29	T	48	
30	U	149	
31	V	156	
32	X	103	
33	C	195	
34	AA	3193	
35	AC	151	
36	AB	118	
37	AL	211	
38	A1	145	
39	A2	118	
40	A4	66	
41	A6	98	
42	A7	102	
43	AN	146	
44	A8	125	
45	A9	103	
46	Aa	106	
47	Ab	105	
48	Ad	76	
49	Ae	50	
50	Af	51	
51	AP	204	
52	Ah	85	
53	Ai	95	

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Mol	Chain	Length	Quality of chain
54	AI	213	
55	AJ	244	
56	Ac	89	
57	AK	201	
58	AM	132	
59	AS	186	
60	AO	147	
61	AQ	205	
62	AR	289	
63	AW	170	
64	AY	101	
65	AT	181	
66	AZ	121	
67	A3	119	
68	A5	223	
69	AD	247	
70	AE	380	
71	AF	390	
72	AG	159	
73	AU	180	
74	AH	185	
75	AV	155	
76	Ag	37	
77	AX	97	
78	A0	62	

2 Entry composition

There are 78 unique types of molecules in this entry. The entry contains 193061 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1608	Total	C	N	O	P	0	0
			34207	15346	6106	11169	1586		

- Molecule 2 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	76	Total	C	N	O	P	0	0
			1620	723	295	527	75		

- Molecule 3 is a protein called 40S ribosomal protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	157	Total	C	N	O	S	0	0
			1229	782	225	215	7		

- Molecule 4 is a protein called 40S ribosomal protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	185	Total	C	N	O	S	0	0
			1515	962	290	261	2		

- Molecule 5 is a protein called 40S ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	224	Total	C	N	O	S	0	0
			1758	1132	307	310	9		

- Molecule 6 is a protein called 40S ribosomal protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	180	Total	C	N	O	S	0	0
			1424	893	263	258	10		

- Molecule 7 is a protein called 40S ribosomal protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	129	Total	C	N	O	S	0	0
			1037	665	189	178	5		

- Molecule 8 is a protein called 40S ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	138	Total	C	N	O	S	0	0
			1099	704	200	194	1		

- Molecule 9 is a protein called 40S ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	W	95	Total	C	N	O	S	0	0
			786	498	149	136	3		

- Molecule 10 is a protein called 40S ribosomal protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	R	98	Total	C	N	O	S	0	0
			747	474	123	146	4		

- Molecule 11 is a protein called 40S ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	79	Total	C	N	O	S	0	0
			687	450	116	119	2		

- Molecule 12 is a protein called 40S ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Y	154	Total	C	N	O	S	0	0
			1267	811	239	215	2		

- Molecule 13 is a protein called 40S ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Z	72	Total	C	N	O	S	0	0
			557	346	102	105	4		

- Molecule 14 is a protein called 40S ribosomal protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1	120	Total	C	N	O	S	0	0
			986	632	189	163	2		

- Molecule 15 is a protein called 40S ribosomal protein eS25.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	2	41	Total	C	N	O	0	0
			321	208	56	57		

- Molecule 16 is a protein called 40S ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3	95	Total	C	N	O	S	0	0
			782	478	169	129	6		

- Molecule 17 is a protein called 40S ribosomal protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	4	76	Total	C	N	O	S	0	0
			586	368	102	107	9		

- Molecule 18 is a protein called 40S ribosomal protein eS28.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	5	58	Total	C	N	O	0	0
			458	285	93	80		

- Molecule 19 is a protein called 40S ribosomal protein eS30.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	6	43	Total	C	N	O	0	0
			346	213	75	58		

- Molecule 20 is a protein called 40S ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B	210	Total	C	N	O	S	0	0
			1714	1097	301	304	12		

- Molecule 21 is a protein called 40S ribosomal protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	F	257	Total	C	N	O	S	0	0
			2062	1320	377	357	8		

- Molecule 22 is a protein called 40S ribosomal protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	H	204	Total	C	N	O	S	0	0
			1648	1045	313	284	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	158	ILE	-	insertion	UNP Q8IDR9
H	195	ASP	GLU	conflict	UNP Q8IDR9

- Molecule 23 is a protein called 40S ribosomal protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	J	188	Total	C	N	O	S	0	0
			1529	982	264	279	4		

- Molecule 24 is a protein called 40S ribosomal protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	L	171	Total	C	N	O	S	0	0
			1383	872	264	243	4		

- Molecule 25 is a protein called 40S ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	N	98	Total	C	N	O	S	0	0
			772	484	135	148	5		

- Molecule 26 is a protein called 40S ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	P	127	Total	C	N	O	S	0	0
			954	591	184	176	3		

- Molecule 27 is a protein called 40S ribosomal protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Q	144	Total	C	N	O	S	0	0
			1129	712	222	193	2		

- Molecule 28 is a protein called 40S ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	128	Total	C	N	O	S	0	0
			1047	657	205	181	4		

- Molecule 29 is a protein called 40S ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	T	48	Total	C	N	O	S	0	0
			405	252	85	64	4		

- Molecule 30 is a protein called 40S ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	U	149	Total	C	N	O	S	0	0
			1202	769	220	210	3		

- Molecule 31 is a protein called 40S ribosomal protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	V	146	Total	C	N	O	S	0	0
			1206	772	227	200	7		

- Molecule 32 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	X	96	Total	C	N	O	S	0	0
			777	497	137	139	4		

- Molecule 33 is a protein called 40S ribosomal protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	C	195	Total	C	N	O	S	0	0
			1539	990	266	274	9		

- Molecule 34 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	AA	3193	Total	C	N	O	P	0	0
			67884	30446	12054	22223	3161		

- Molecule 35 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AC	151	Total	C	N	O	P	0	0
			3215	1444	589	1034	148		

- Molecule 36 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	AB	118	Total	C	N	O	P	0	0
			2522	1128	461	816	117		

- Molecule 37 is a protein called 60S ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	AL	211	Total	C	N	O	S	0	0
			1757	1116	346	291	4		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AL	19	HIS	ARG	conflict	UNP Q8IAX6
AL	20	ARG	HIS	conflict	UNP Q8IAX6
AL	201	CYS	ARG	conflict	UNP Q8IAX6

- Molecule 38 is a protein called 60S ribosomal protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A1	140	Total	C	N	O	S	0	0
			1134	736	204	191	3		

- Molecule 39 is a protein called 60S ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	A2	104	Total	C	N	O	S	0	0
			831	529	151	148	3		

- Molecule 40 is a protein called 60S ribosomal protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	A4	66	Total	C	N	O	S	0	0
			555	347	116	90	2		

- Molecule 41 is a protein called 60S ribosomal protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	A6	98	Total	C	N	O	S	0	0
			741	462	132	140	7		

- Molecule 42 is a protein called 60S ribosomal protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	A7	96	Total	C	N	O	S	0	0
			794	508	151	130	5		

- Molecule 43 is a protein called 60S ribosomal protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	AN	146	Total	C	N	O	S	0	0
			1202	781	210	205	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AN	?	-	LYS	deletion	UNP Q8ILE8

- Molecule 44 is a protein called 60S ribosomal protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	A8	125	Total	C	N	O	S	0	0
			1037	660	206	164	7		

- Molecule 45 is a protein called 60S ribosomal protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	A9	103	Total	C	N	O	S	0	0
			845	543	163	136	3		

- Molecule 46 is a protein called 60S ribosomal protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Aa	106	Total	C	N	O	S	0	0
			859	530	184	139	6		

- Molecule 47 is a protein called 60S ribosomal protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Ab	95	Total	C	N	O	S	0	0
			757	477	150	130			

- Molecule 48 is a protein called 60S ribosomal protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Ad	72	Total	C	N	O	S	0	0
			604	395	107	100	2		

- Molecule 49 is a protein called 60S ribosomal protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Ae	43	Total	C	N	O	S	0	0
			388	243	92	52	1		

- Molecule 50 is a protein called 60S ribosomal protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Af	51	Total	C	N	O	S	0	0
			414	255	87	67	5		

- Molecule 51 is a protein called 60S ribosomal protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AP	204	Total	C	N	O	S	0	0
			1697	1075	351	267	4		

- Molecule 52 is a protein called 60S ribosomal protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Ah	85	Total	C	N	O	S	0	0
			659	417	127	108	7		

- Molecule 53 is a protein called 60S ribosomal protein eL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Ai	95	Total	C	N	O	S	0	0
			779	490	152	128	9		

- Molecule 54 is a protein called 60S ribosomal protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AI	207	Total	C	N	O	S	0	0
			1685	1096	298	286	5		

- Molecule 55 is a protein called 60S ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AJ	222	Total	C	N	O	S	0	0
			1813	1174	323	309	7		

- Molecule 56 is a protein called 60S ribosomal protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Ac	89	Total	C	N	O	S	0	0
			710	441	150	114	5		

- Molecule 57 is a protein called 60S ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AK	201	Total	C	N	O	S	0	0
			1660	1064	311	277	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AK	109	ALA	TYR	conflict	UNP Q8IJZ7

- Molecule 58 is a protein called 60S ribosomal protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AM	132	Total	C	N	O	S	0	0
			996	631	179	178	8		

- Molecule 59 is a protein called 60S ribosomal protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AS	186	Total	C	N	O	S	0	0
			1503	958	299	241	5		

- Molecule 60 is a protein called 60S ribosomal protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AO	147	Total	C	N	O	S	0	0
			1172	747	232	189	4		

- Molecule 61 is a protein called 60S ribosomal protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AQ	189	Total	C	N	O	S	0	0
			1545	984	291	262	8		

- Molecule 62 is a protein called 60S ribosomal protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AR	252	Total	C	N	O	S	0	0
			2050	1300	385	359	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AR	?	-	LYS	deletion	UNP Q8ILL3

- Molecule 63 is a protein called 60S ribosomal protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AW	170	Total	C	N	O	S	0	0
			1319	824	266	222	7		

- Molecule 64 is a protein called 60S ribosomal protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AY	101	Total	C	N	O	S	0	0
			797	502	144	145	6		

- Molecule 65 is a protein called 60S ribosomal protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AT	181	Total	C	N	O	S	0	0
			1509	952	309	244	4		

- Molecule 66 is a protein called 60S ribosomal protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AZ	121	Total	C	N	O	S	0	0
			1001	626	206	166	3		

- Molecule 67 is a protein called 60S ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	A3	119	Total	C	N	O	S	0	0
			995	635	194	164	2		

- Molecule 68 is a protein called 60S ribosomal protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	A5	223	Total	C	N	O	S	0	0
			1879	1211	357	306	5		

- Molecule 69 is a protein called 60S ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	AD	247	Total	C	N	O	S	0	0
			1867	1166	374	318	9		

- Molecule 70 is a protein called 60S ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	AE	380	Total	C	N	O	S	0	0
			3062	1948	575	522	17		

- Molecule 71 is a protein called 60S ribosomal protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	AF	390	Total	C	N	O	S	0	0
			3095	1962	594	528	11		

- Molecule 72 is a protein called 60S ribosomal protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	AG	124	Total	C	N	O	S	0	0
			1011	636	197	172	6		

- Molecule 73 is a protein called 60S ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	AU	180	Total	C	N	O	S	0	0
			1497	946	289	255	7		

- Molecule 74 is a protein called 60S ribosomal protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	AH	185	Total	C	N	O	S	0	0
			1476	950	264	256	6		

- Molecule 75 is a protein called 60S ribosomal protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	AV	155	Total	C	N	O	S	0	0
			1276	814	241	215	6		

- Molecule 76 is a protein called 60S ribosomal protein eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Ag	37	Total	C	N	O	S	0	0
			343	210	86	45	2		

- Molecule 77 is a protein called 60S ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	AX	97	Total	C	N	O	S	0	0
			825	548	135	140	2		

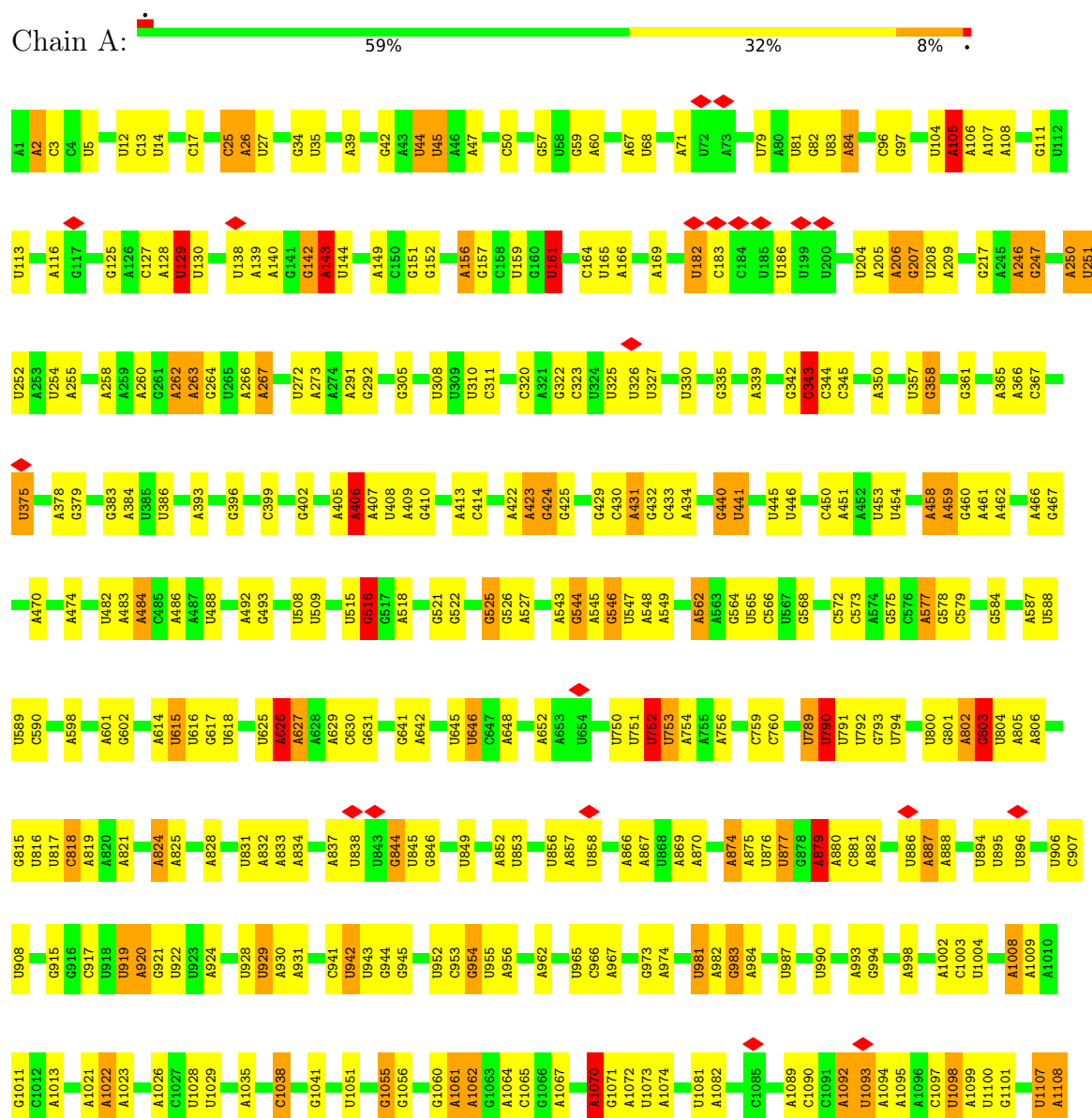
- Molecule 78 is a protein called 60S ribosomal protein eL24.

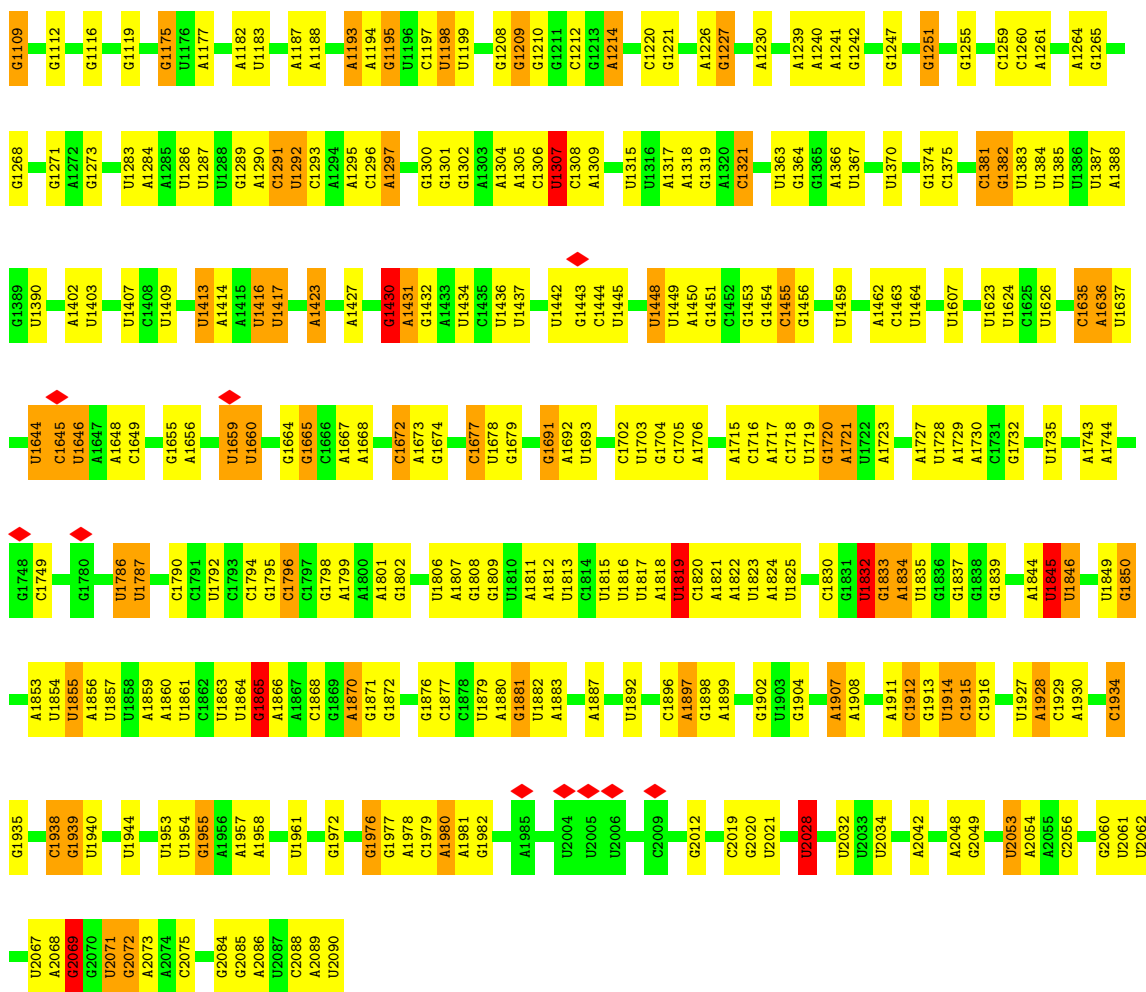
Mol	Chain	Residues	Atoms					AltConf	Trace
78	A0	62	Total	C	N	O	S	0	0
			522	336	97	88	1		

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 ribosomal RNA

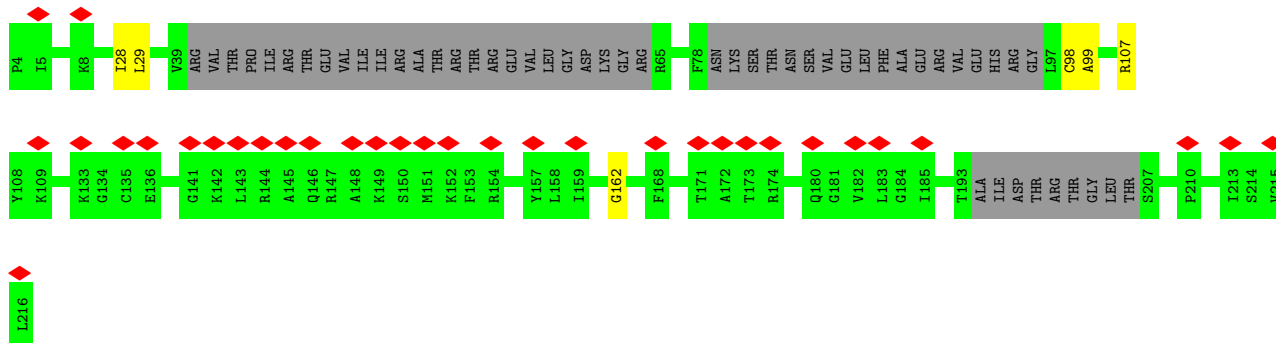




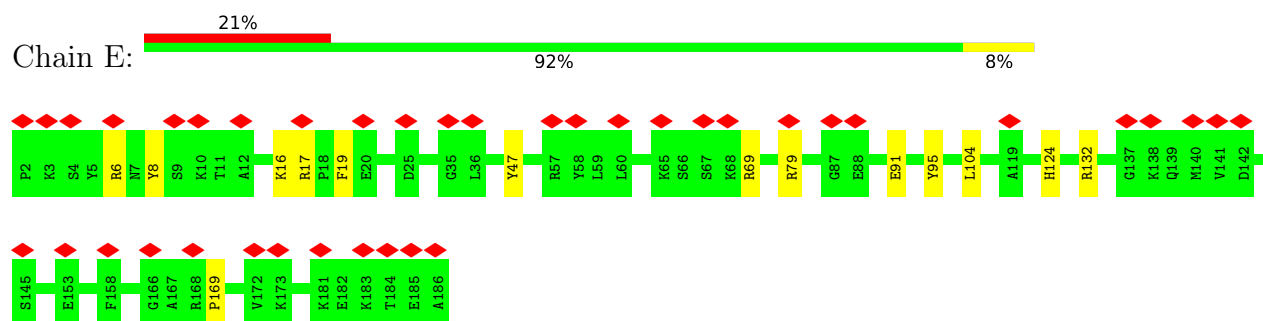
- Molecule 2: P-tRNA



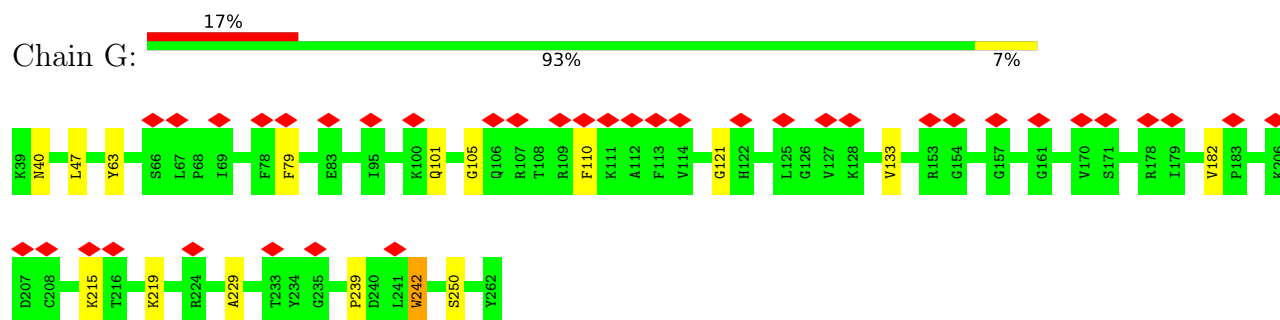
- Molecule 3: 40S ribosomal protein uS3



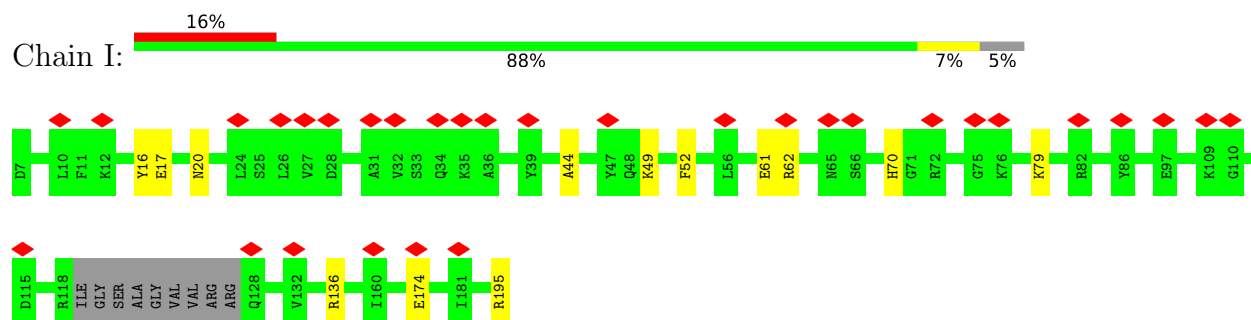
- Molecule 4: 40S ribosomal protein uS4



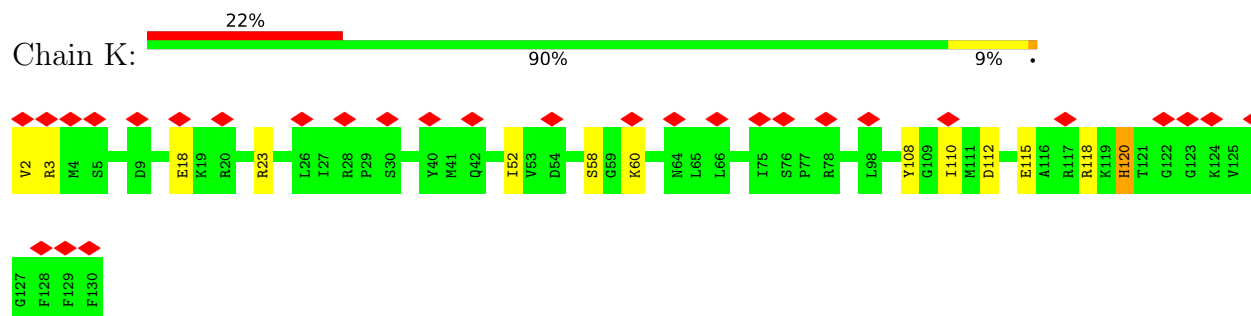
- Molecule 5: 40S ribosomal protein uS5



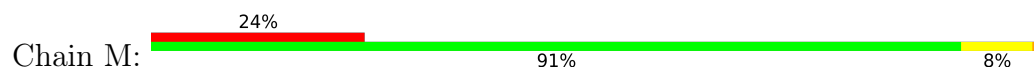
- Molecule 6: 40S ribosomal protein uS7

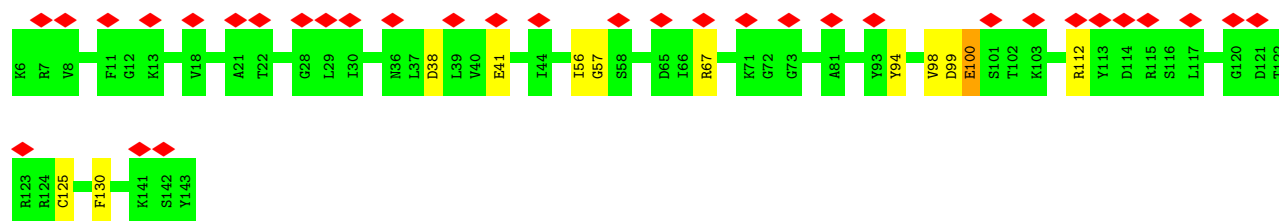


- Molecule 7: 40S ribosomal protein uS8

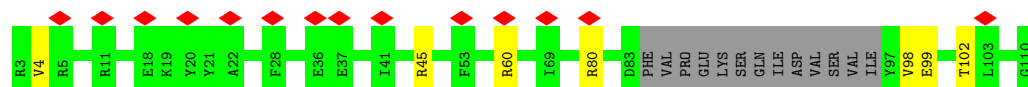
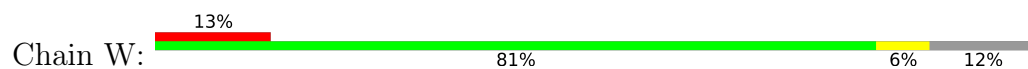


- Molecule 8: 40S ribosomal protein uS9

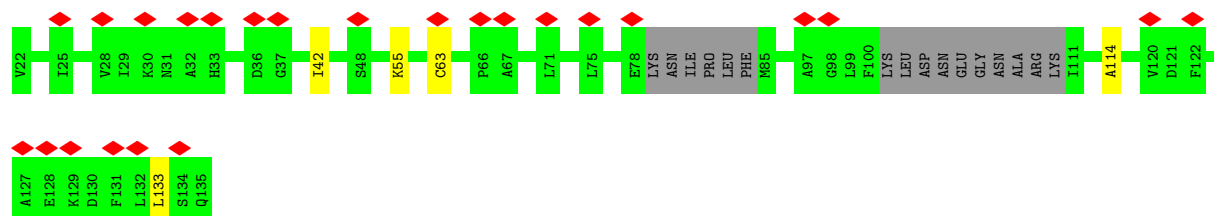
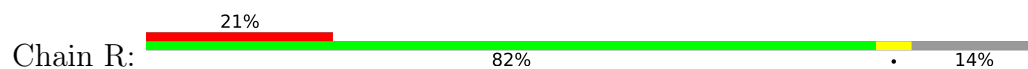




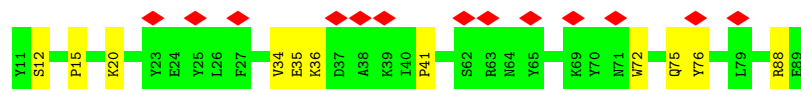
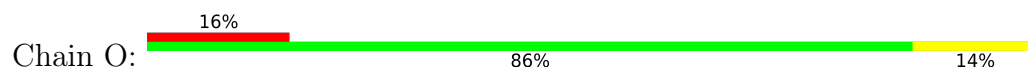
• Molecule 9: 40S ribosomal protein eS17



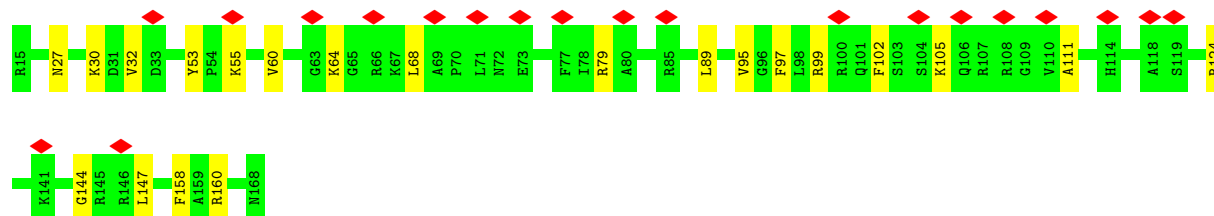
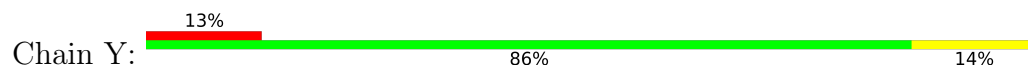
• Molecule 10: 40S ribosomal protein eS12



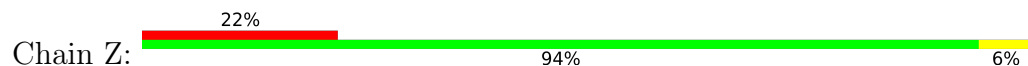
• Molecule 11: 40S ribosomal protein eS10

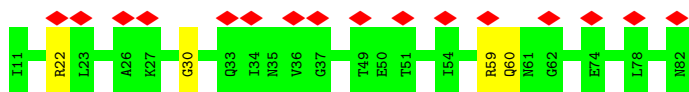


• Molecule 12: 40S ribosomal protein eS19

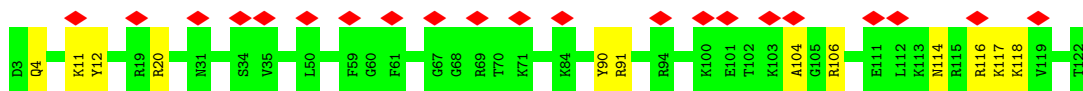
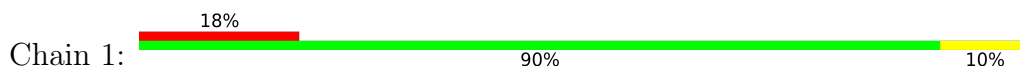


• Molecule 13: 40S ribosomal protein eS21

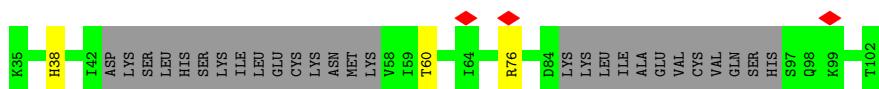




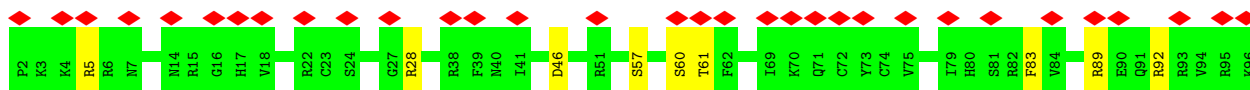
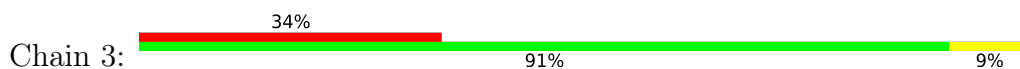
- Molecule 14: 40S ribosomal protein eS24



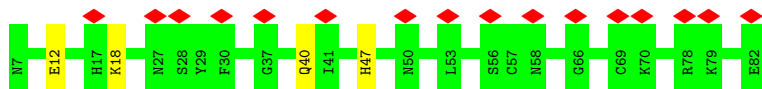
- Molecule 15: 40S ribosomal protein eS25



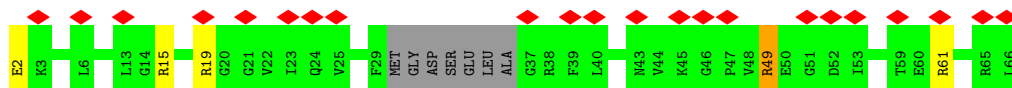
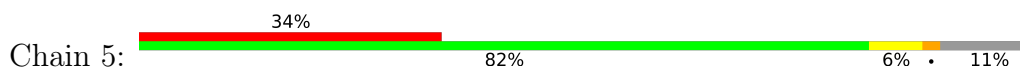
- Molecule 16: 40S ribosomal protein eS26



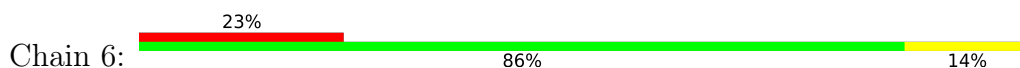
- Molecule 17: 40S ribosomal protein eS27



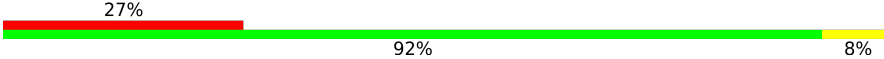
- Molecule 18: 40S ribosomal protein eS28

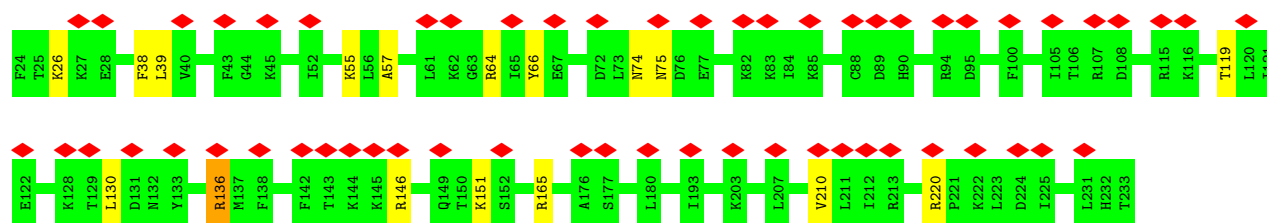


- Molecule 19: 40S ribosomal protein eS30

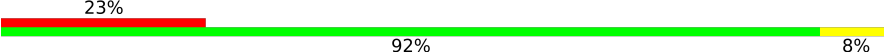


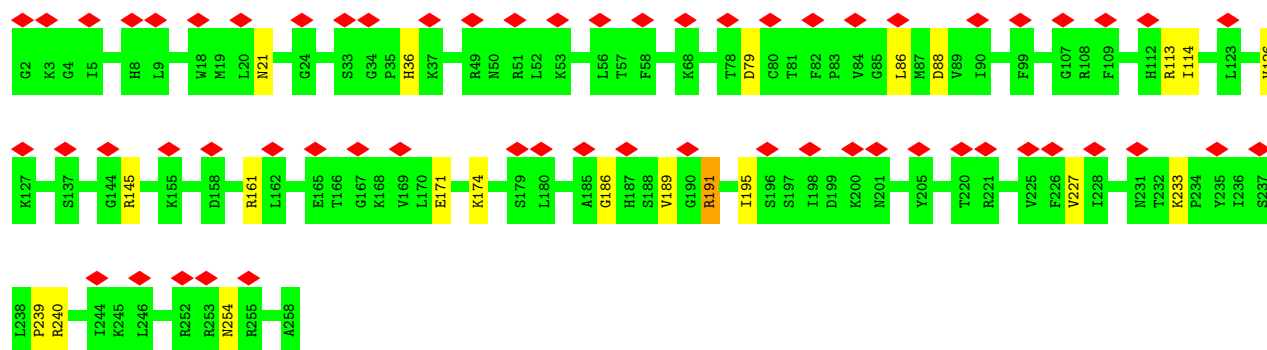
- Molecule 20: 40S ribosomal protein eS1

Chain B: 

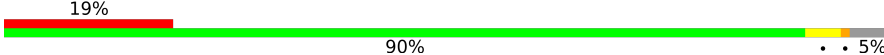


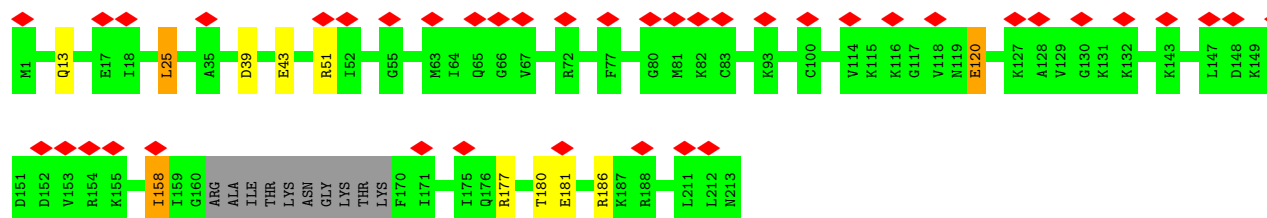
- Molecule 21: 40S ribosomal protein eS4

Chain F: 



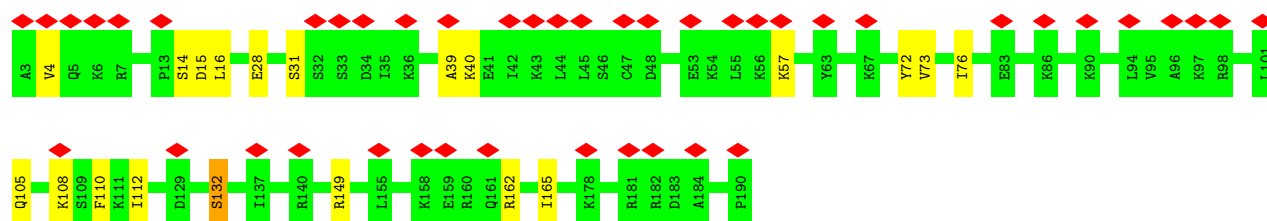
- Molecule 22: 40S ribosomal protein eS6

Chain H: 



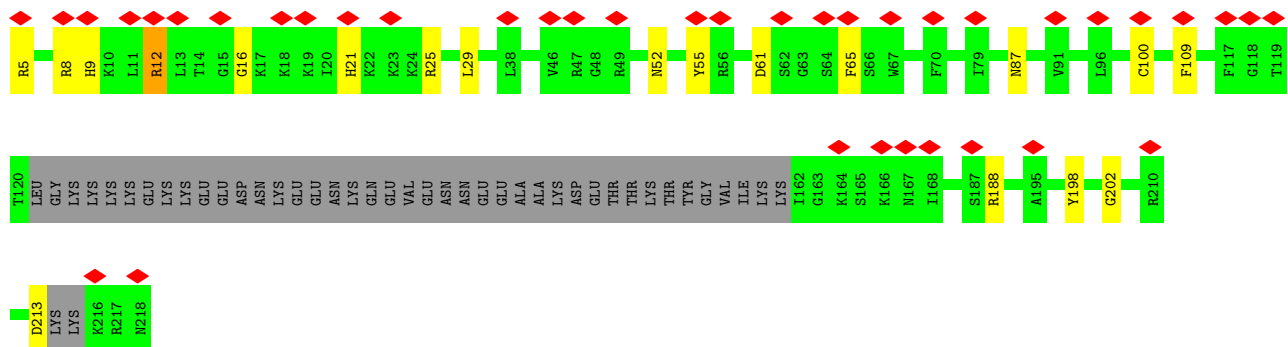
- Molecule 23: 40S ribosomal protein eS7

Chain J: 

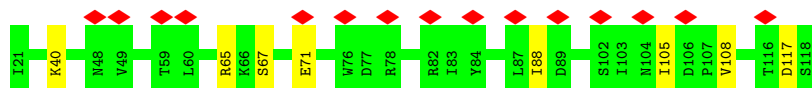
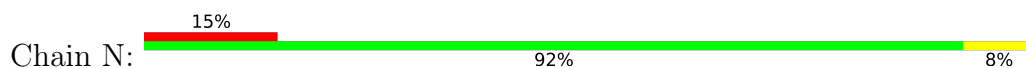


- Molecule 24: 40S ribosomal protein eS8

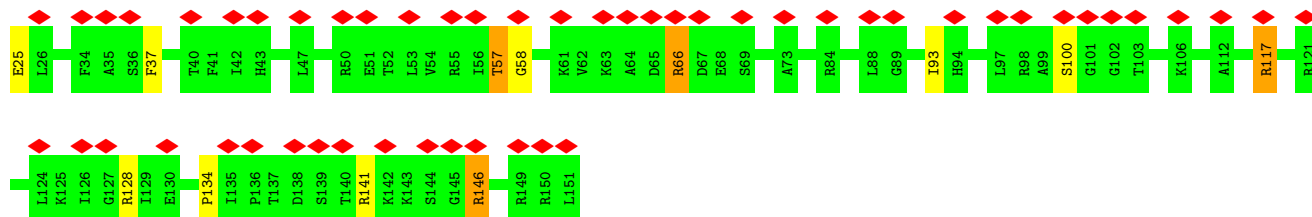
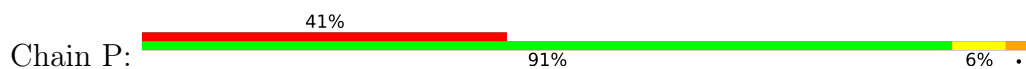
Chain L: 



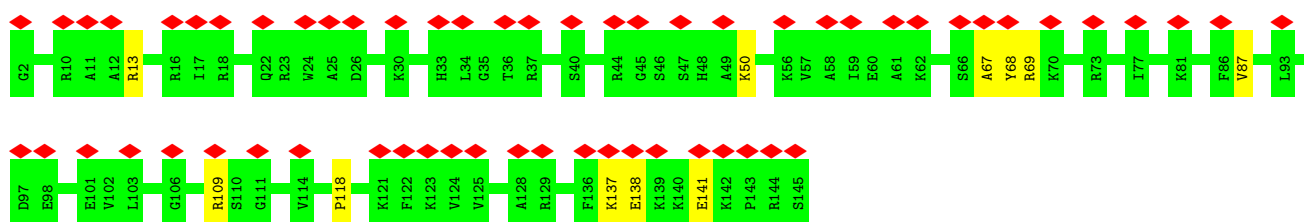
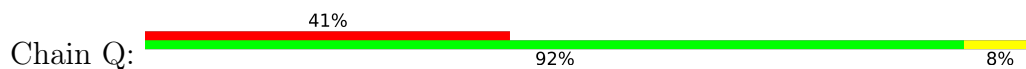
- Molecule 25: 40S ribosomal protein uS10



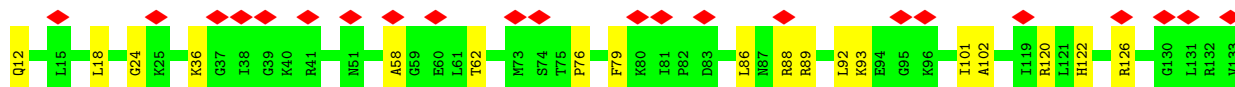
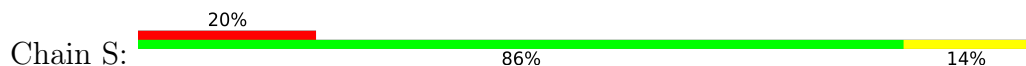
- Molecule 26: 40S ribosomal protein uS11

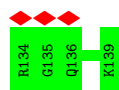


- Molecule 27: 40S ribosomal protein uS12

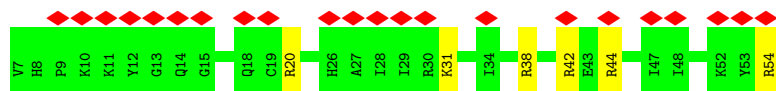
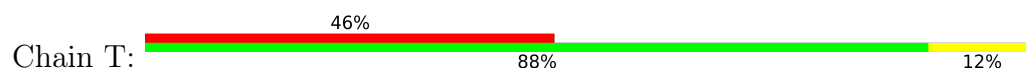


- Molecule 28: 40S ribosomal protein uS13

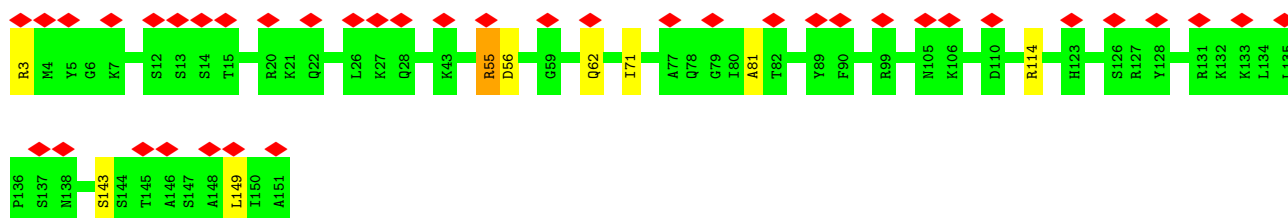




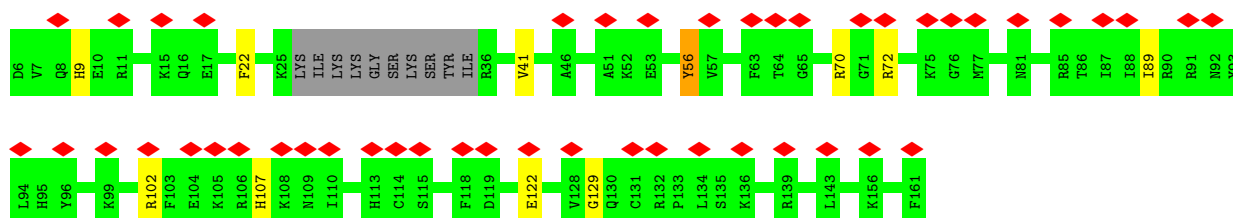
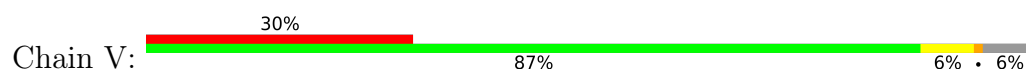
- Molecule 29: 40S ribosomal protein uS14



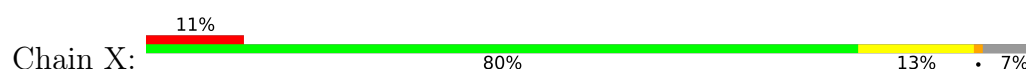
- Molecule 30: 40S ribosomal protein uS15



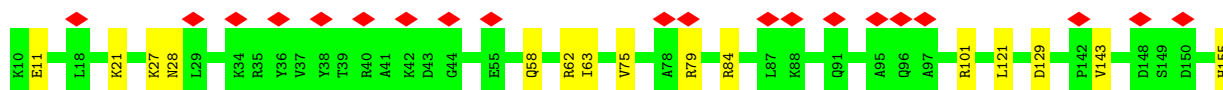
- Molecule 31: 40S ribosomal protein uS17



- Molecule 32: 40S ribosomal protein uS19



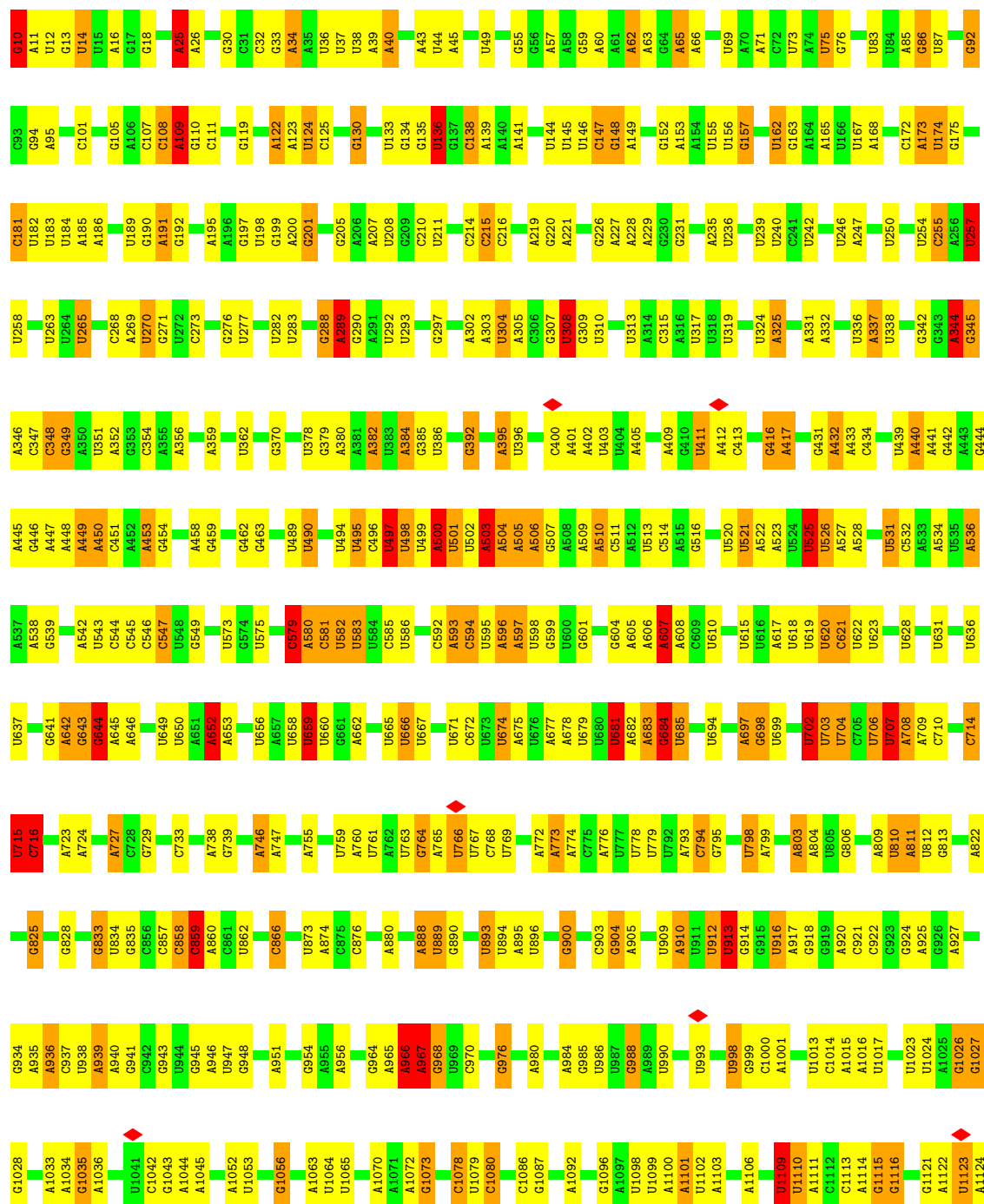
- Molecule 33: 40S ribosomal protein uS2

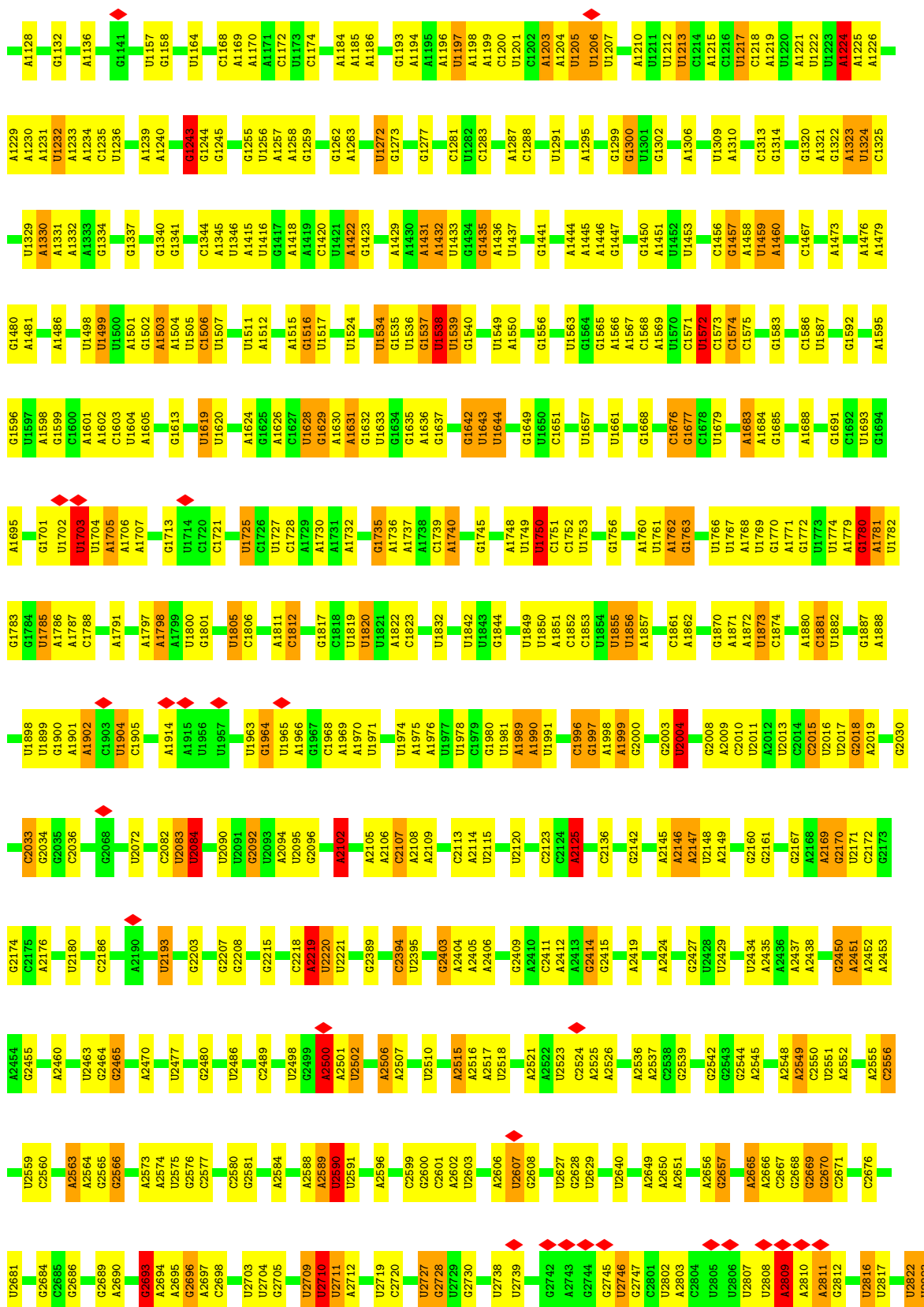


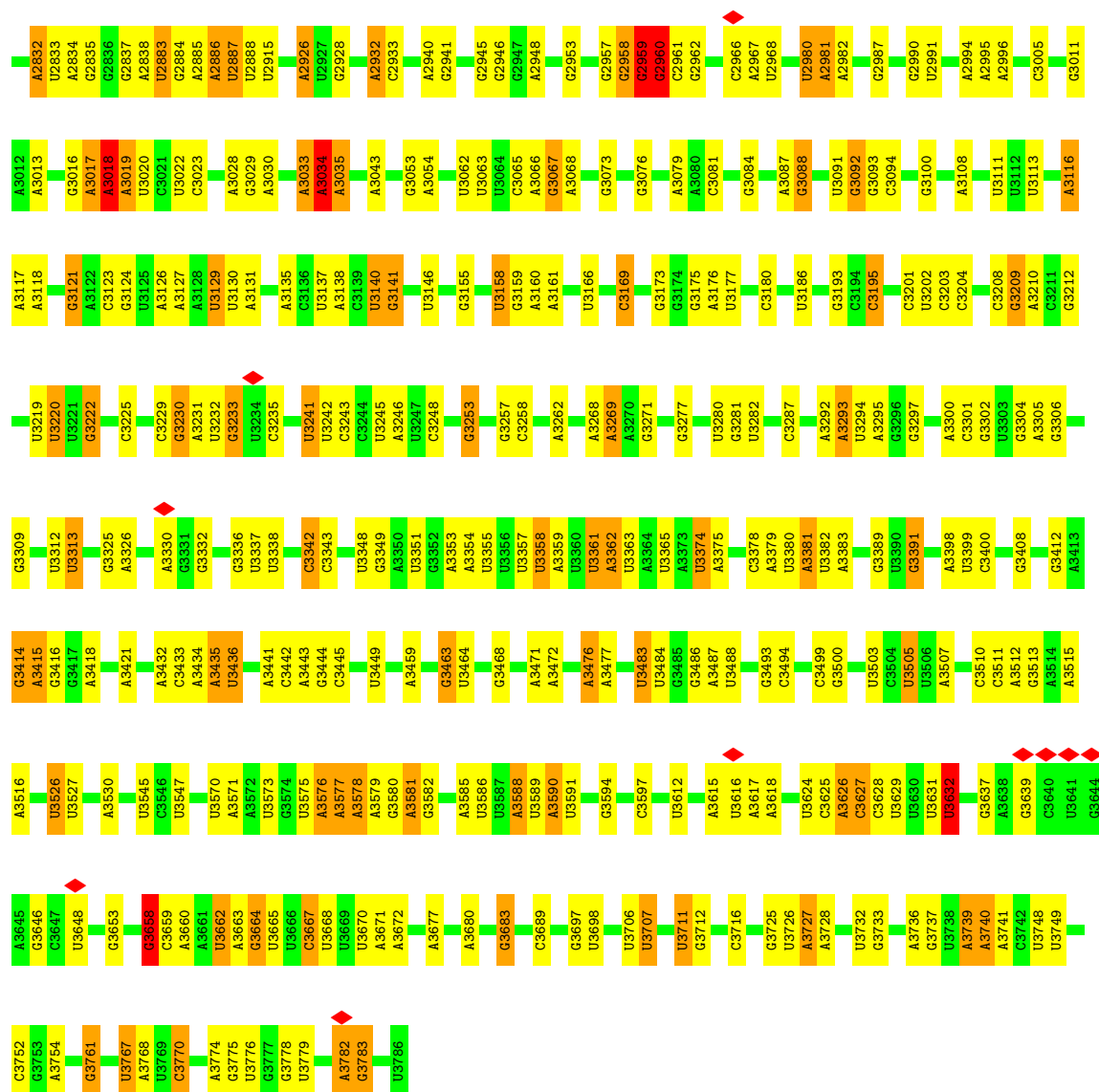


• Molecule 34: 28S ribosomal RNA

Chain AA: 57% 32% 9%

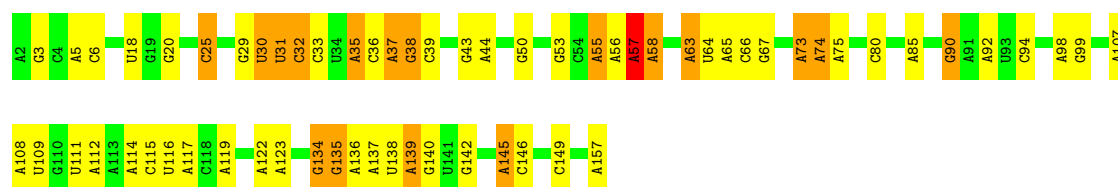






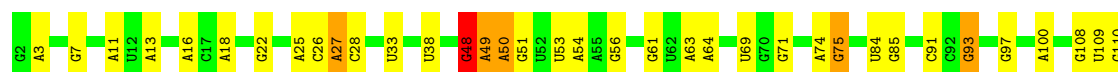
• Molecule 35: 5.8S ribosomal RNA

Chain AC: 58% 30% 11%



• Molecule 36: 5S ribosomal RNA

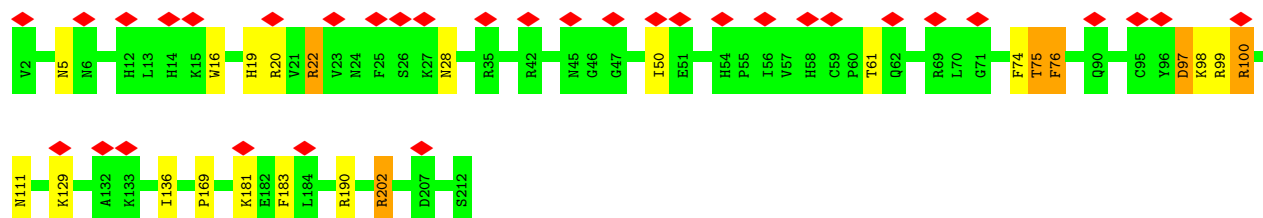
Chain AB: 69% 26%





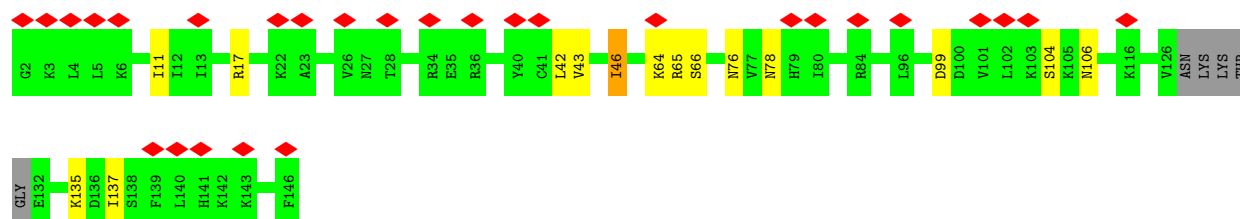
- Molecule 37: 60S ribosomal protein eL13

Chain AL:



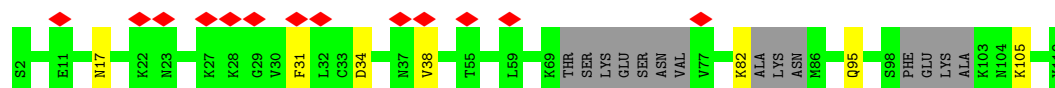
- Molecule 38: 60S ribosomal protein eL27

Chain A1:



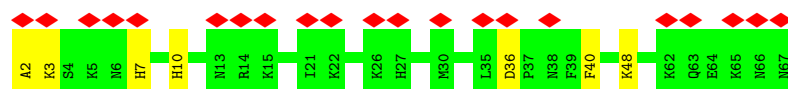
- Molecule 39: 60S ribosomal protein eL28

Chain A2:



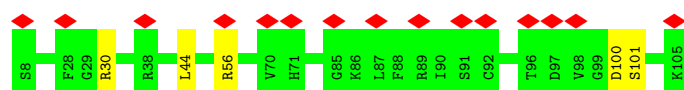
- Molecule 40: 60S ribosomal protein eL29

Chain A4:

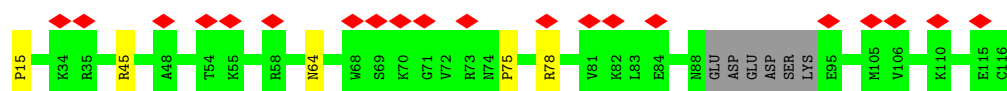
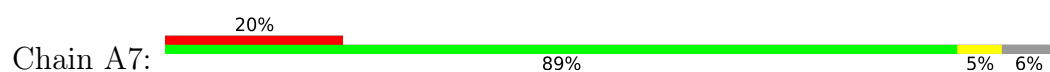


- Molecule 41: 60S ribosomal protein eL30

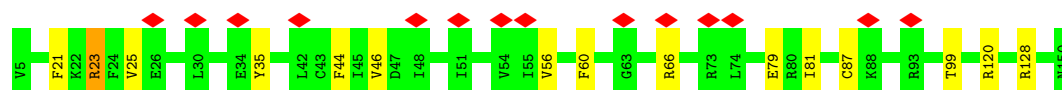
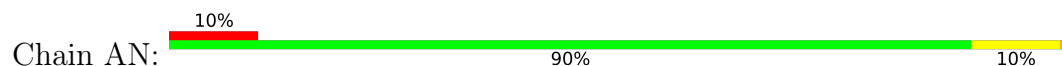
Chain A6:



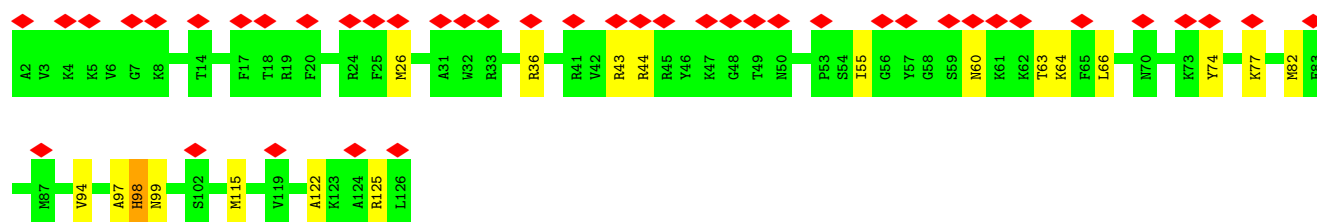
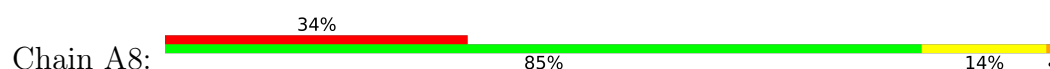
- Molecule 42: 60S ribosomal protein eL31



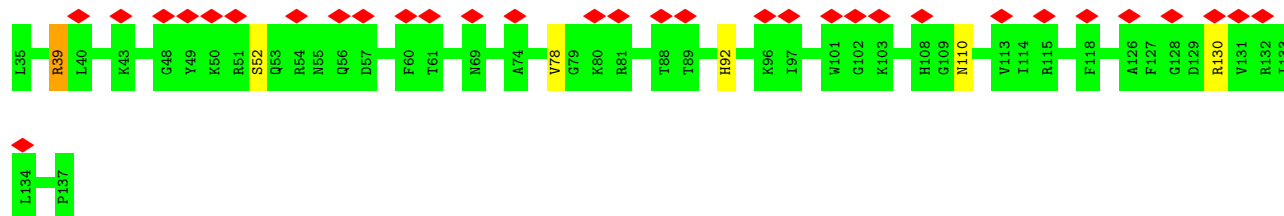
- Molecule 43: 60S ribosomal protein eL14



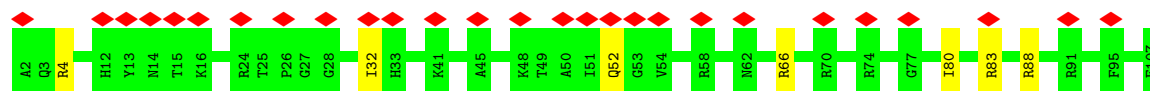
- Molecule 44: 60S ribosomal protein eL32



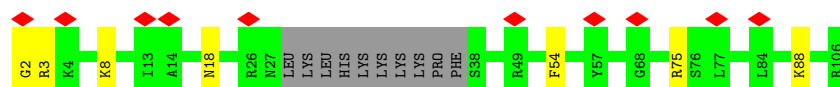
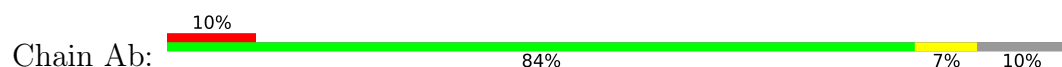
- Molecule 45: 60S ribosomal protein eL33



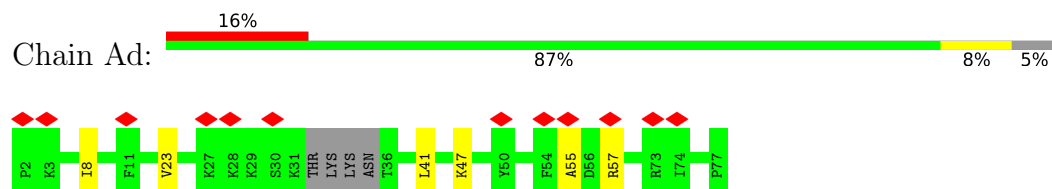
- Molecule 46: 60S ribosomal protein eL34



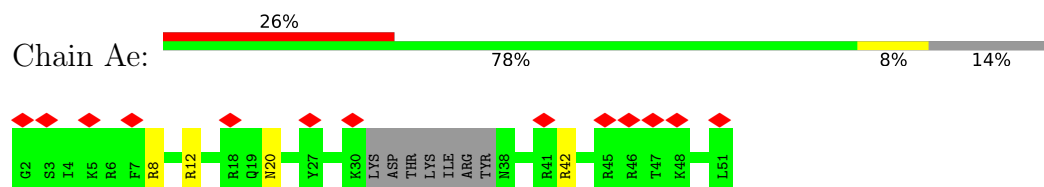
- Molecule 47: 60S ribosomal protein eL36



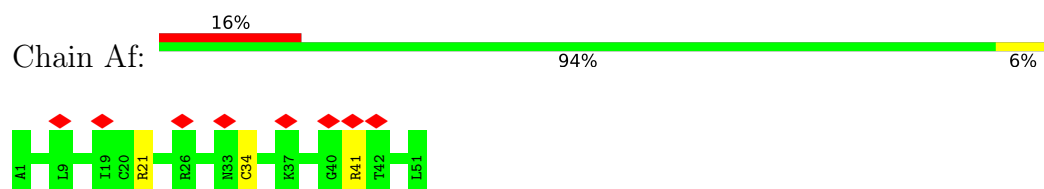
- Molecule 48: 60S ribosomal protein eL38



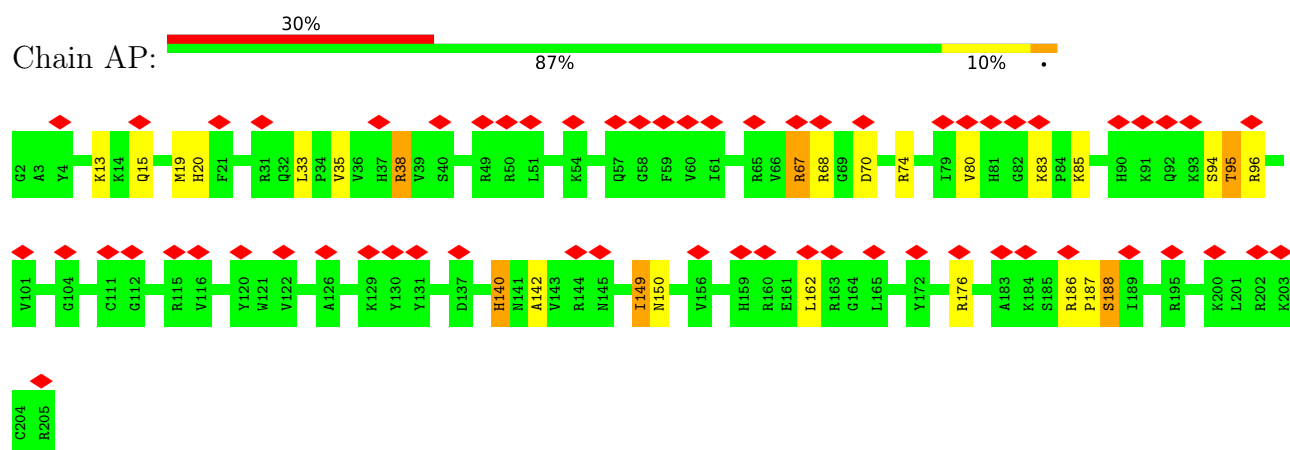
- Molecule 49: 60S ribosomal protein eL39



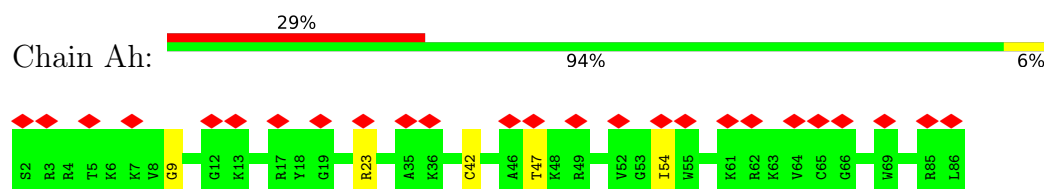
- Molecule 50: 60S ribosomal protein eL40



- Molecule 51: 60S ribosomal protein eL15

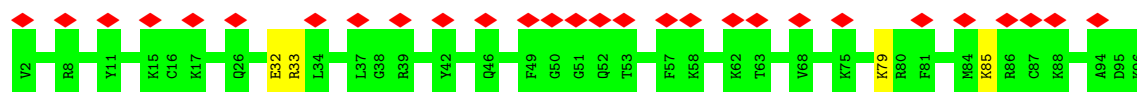


- Molecule 52: 60S ribosomal protein eL43

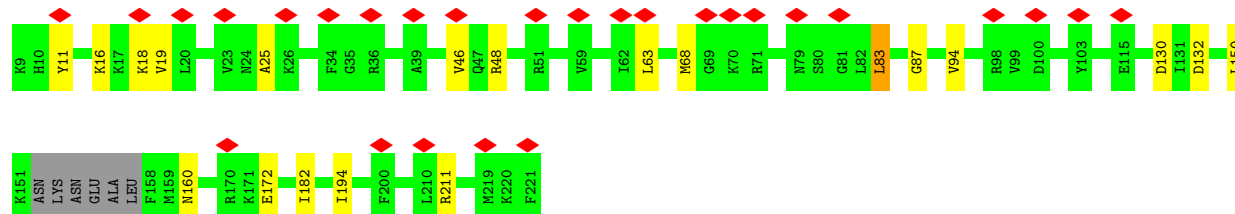
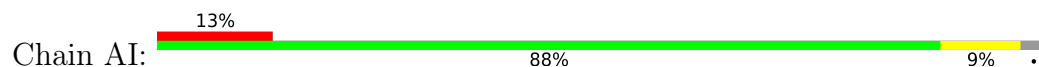


- Molecule 53: 60S ribosomal protein eL44

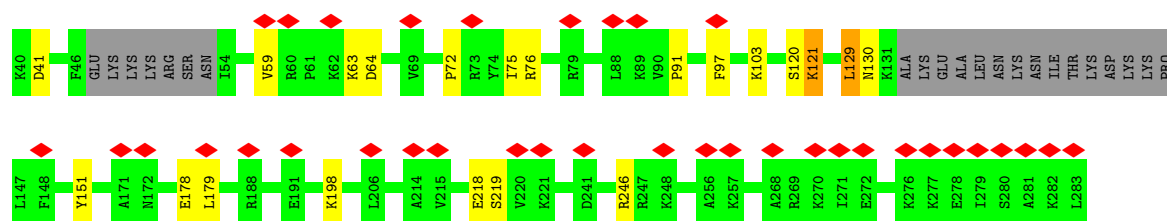
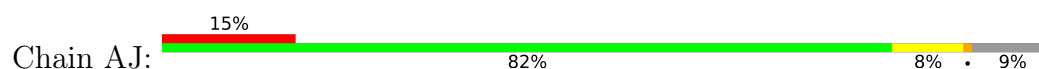




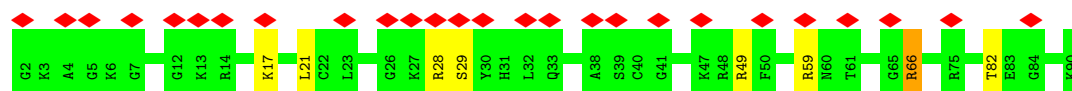
- Molecule 54: 60S ribosomal protein eL6



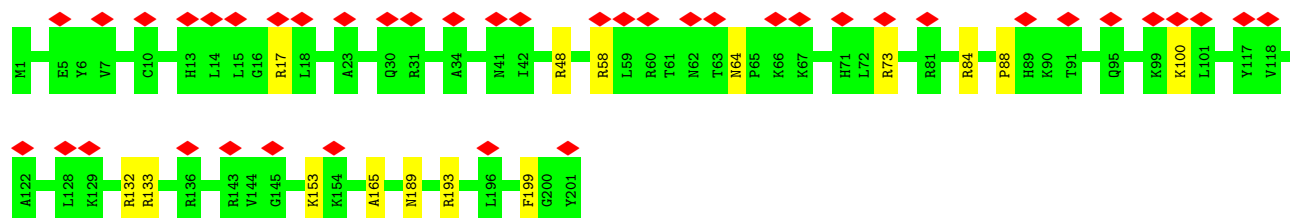
- Molecule 55: 60S ribosomal protein eL8



- Molecule 56: 60S ribosomal protein eL37

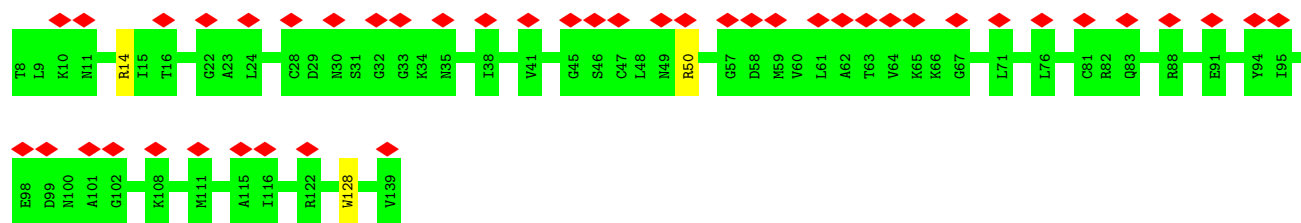


- Molecule 57: 60S ribosomal protein uL13

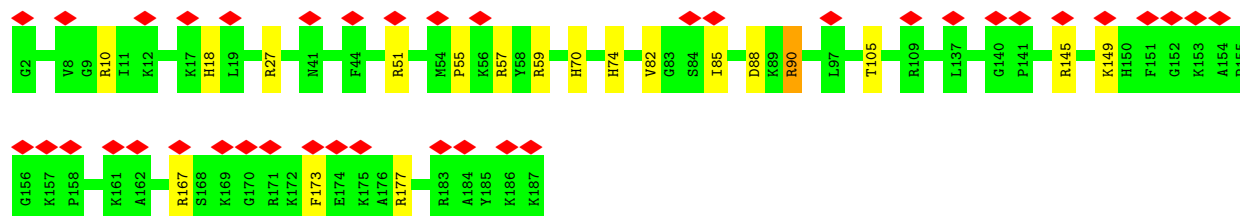
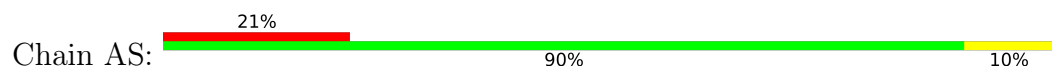


- Molecule 58: 60S ribosomal protein uL14

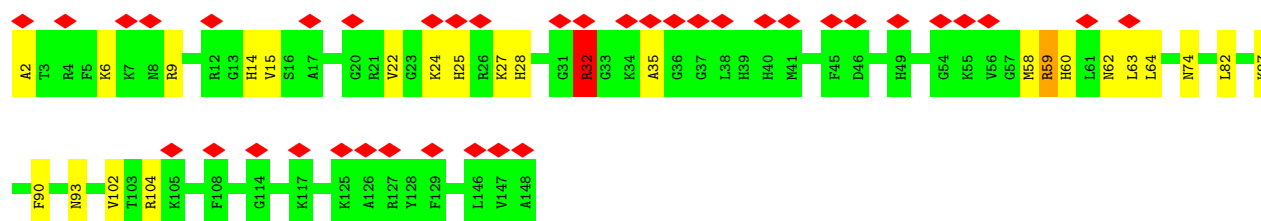
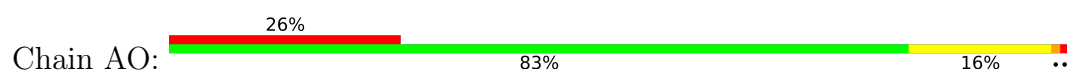




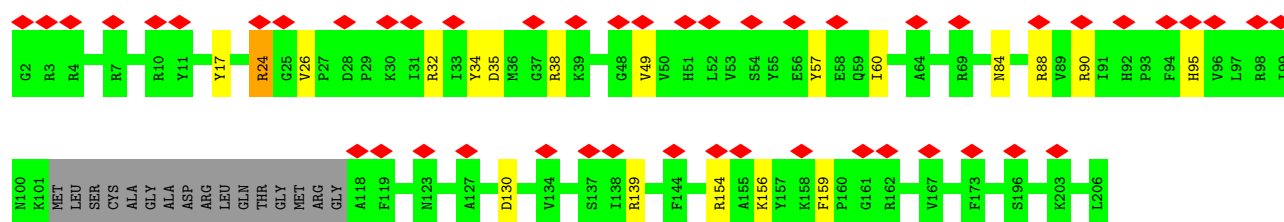
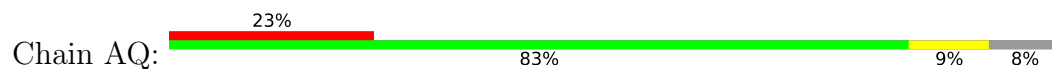
• Molecule 59: 60S ribosomal protein eL18



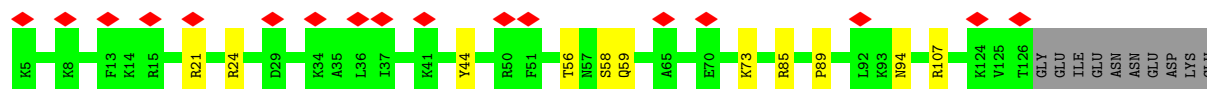
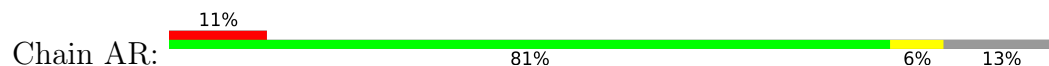
• Molecule 60: 60S ribosomal protein uL15

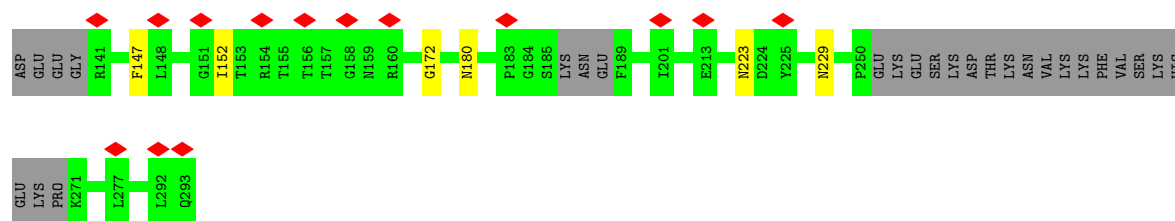


• Molecule 61: 60S ribosomal protein uL16

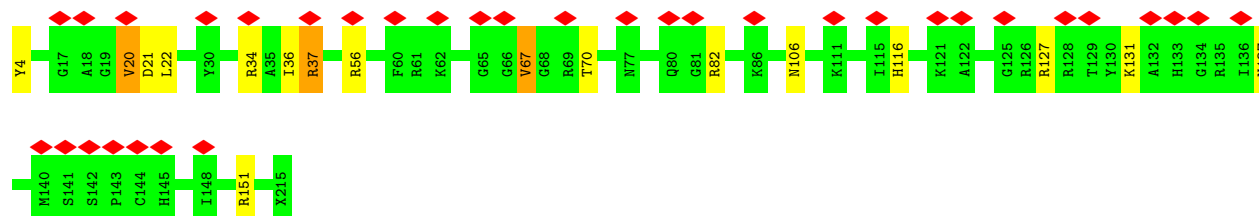


• Molecule 62: 60S ribosomal protein uL18

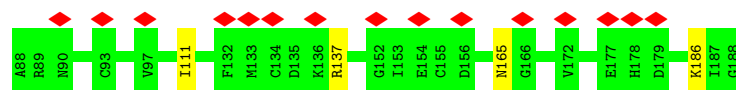




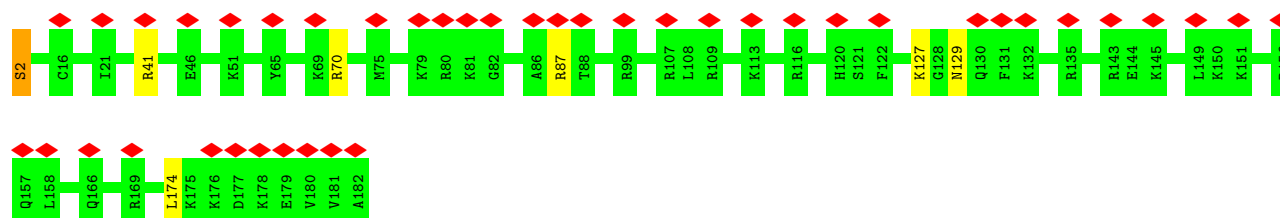
• Molecule 63: 60S ribosomal protein uL22



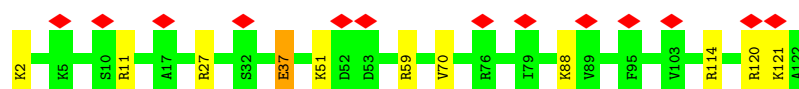
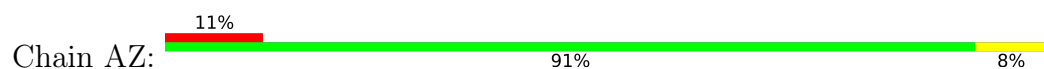
• Molecule 64: 60S ribosomal protein uL23



• Molecule 65: 60S ribosomal protein eL19

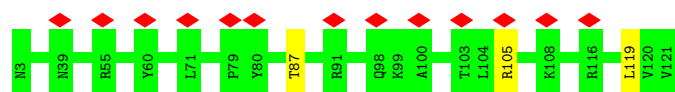


• Molecule 66: 60S ribosomal protein uL24

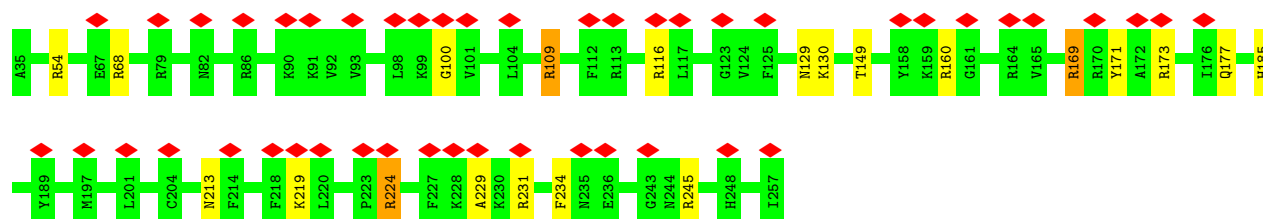


• Molecule 67: 60S ribosomal protein uL29

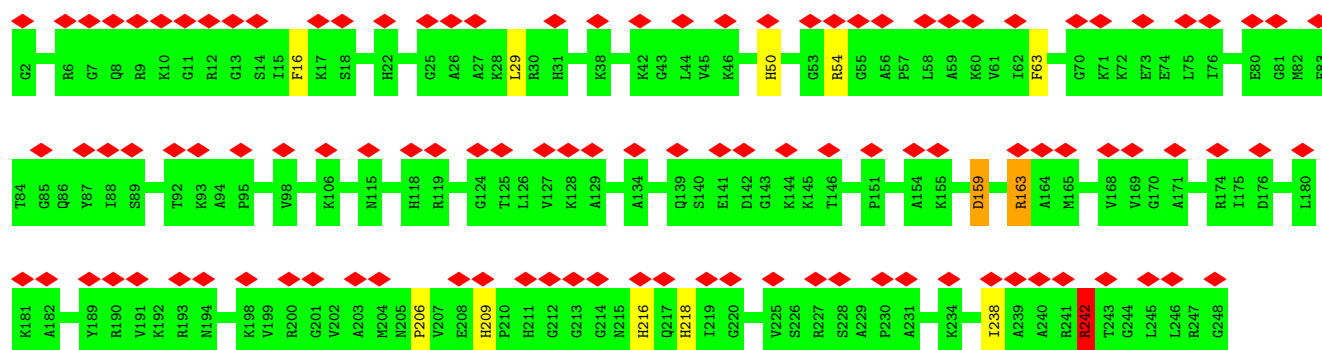




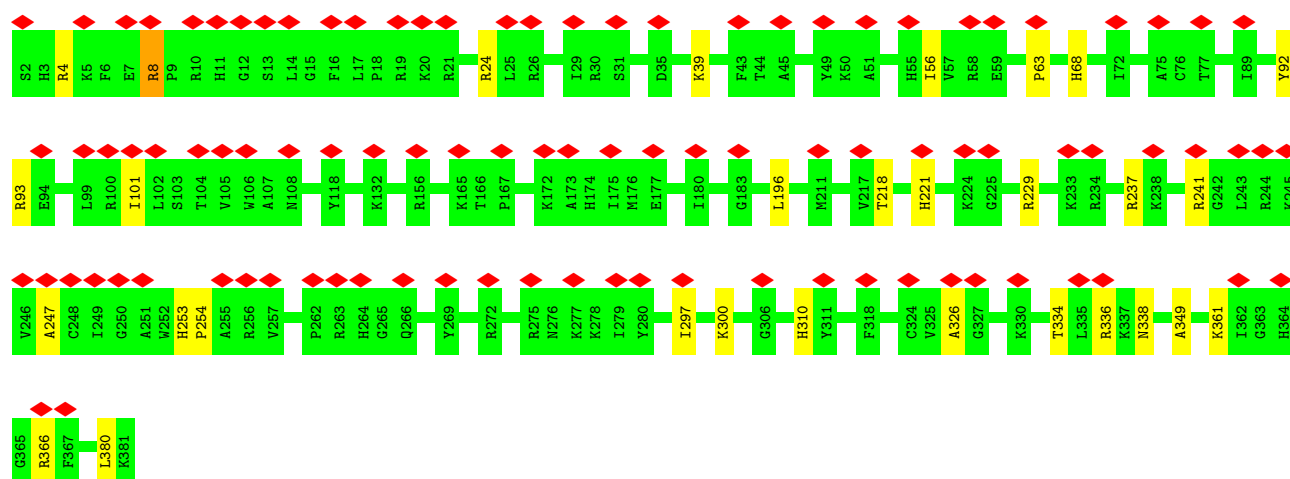
- Molecule 68: 60S ribosomal protein uL30



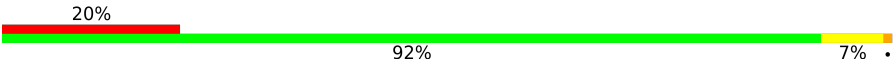
- Molecule 69: 60S ribosomal protein uL2

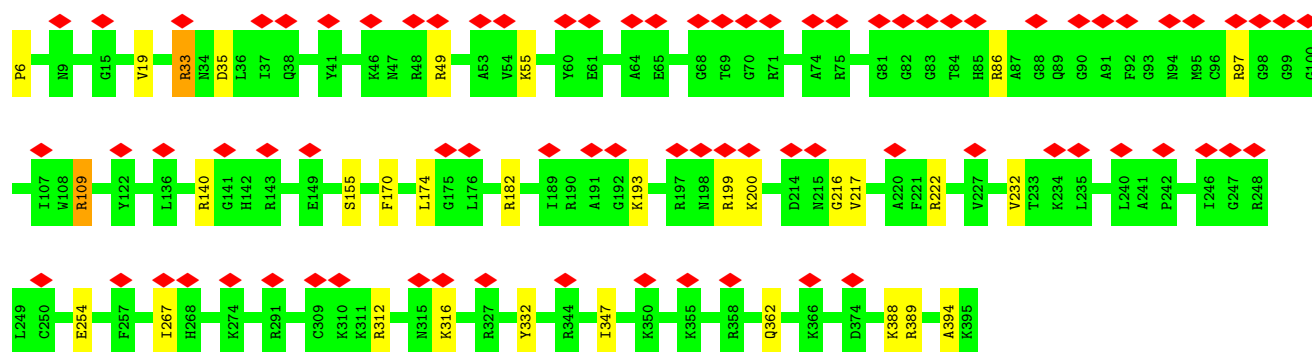


- Molecule 70: 60S ribosomal protein uL3



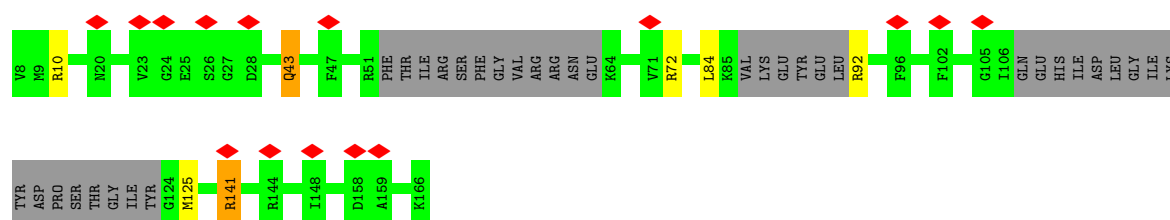
- Molecule 71: 60S ribosomal protein uL4

Chain AF: 



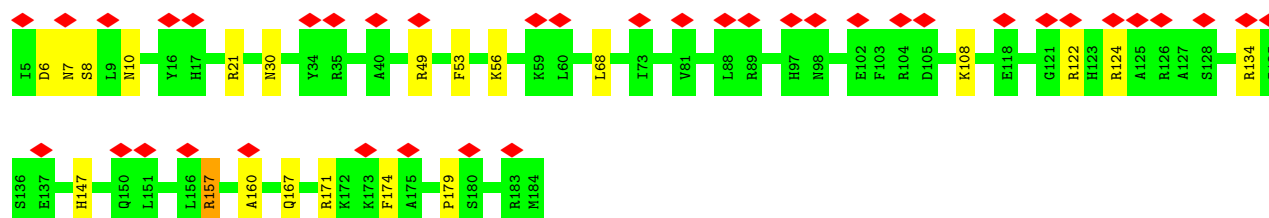
• Molecule 72: 60S ribosomal protein uL5

Chain AG: 

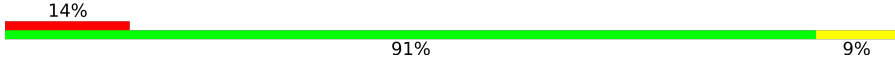


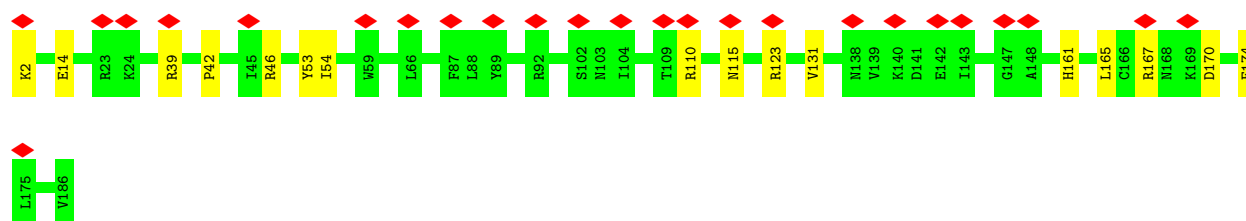
• Molecule 73: 60S ribosomal protein eL20

Chain AU: 

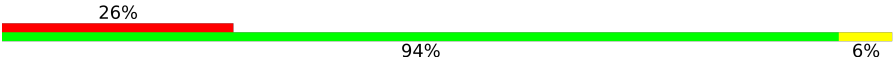


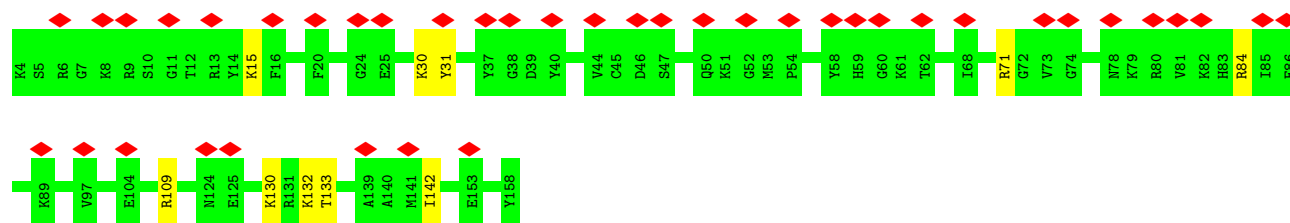
• Molecule 74: 60S ribosomal protein uL6

Chain AH: 

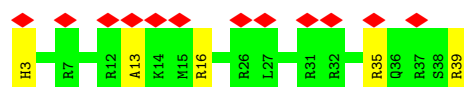
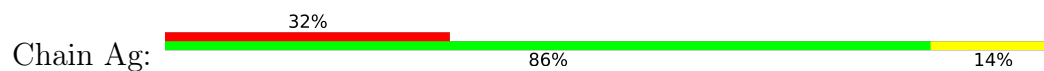


• Molecule 75: 60S ribosomal protein eL21

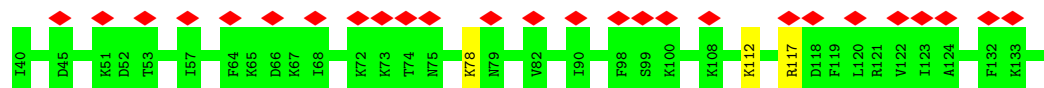
Chain AV: 



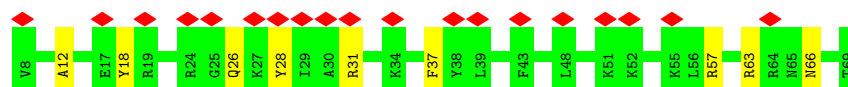
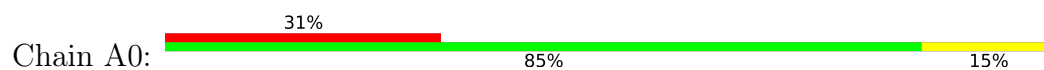
- Molecule 76: 60S ribosomal protein eL41



- Molecule 77: 60S ribosomal protein eL22



- Molecule 78: 60S ribosomal protein eL24



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	14696	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each micrograph	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	30120	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.133	Depositor
Minimum map value	-0.088	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	491.36, 491.36, 491.36	wwPDB
Map dimensions	296, 296, 296	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.66, 1.66, 1.66	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.94	0/38275	1.14	120/59596 (0.2%)
2	7	0.95	0/1810	1.19	9/2821 (0.3%)
3	D	0.89	0/1241	1.43	4/1652 (0.2%)
4	E	0.87	0/1539	1.51	3/2055 (0.1%)
5	G	0.82	0/1800	1.48	10/2429 (0.4%)
6	I	0.85	0/1443	1.56	3/1936 (0.2%)
7	K	0.86	0/1054	1.48	3/1411 (0.2%)
8	M	0.83	0/1114	1.43	4/1487 (0.3%)
9	W	0.86	0/793	1.61	8/1053 (0.8%)
10	R	0.91	0/755	1.56	5/1013 (0.5%)
11	O	0.86	0/706	1.50	2/950 (0.2%)
12	Y	0.86	0/1295	1.63	12/1742 (0.7%)
13	Z	0.84	0/565	1.48	2/758 (0.3%)
14	1	0.85	0/999	1.50	3/1321 (0.2%)
15	2	0.90	0/324	1.45	0/435
16	3	0.92	0/794	1.55	7/1055 (0.7%)
17	4	0.81	0/597	1.46	0/801
18	5	0.91	0/459	1.40	4/606 (0.7%)
19	6	0.91	0/349	1.59	2/458 (0.4%)
20	B	0.82	0/1738	1.55	8/2321 (0.3%)
21	F	0.85	0/2098	1.45	9/2819 (0.3%)
22	H	0.82	0/1665	1.46	7/2210 (0.3%)
23	J	0.81	0/1545	1.51	12/2064 (0.6%)
24	L	0.87	0/1407	1.52	10/1879 (0.5%)
25	N	0.83	0/780	1.52	4/1053 (0.4%)
26	P	0.87	0/966	1.60	10/1295 (0.8%)
27	Q	0.86	0/1149	1.51	1/1532 (0.1%)
28	S	0.87	0/1063	1.65	8/1425 (0.6%)
29	T	0.90	0/412	1.40	0/544
30	U	0.83	0/1223	1.53	5/1634 (0.3%)
31	V	0.87	0/1233	1.41	3/1645 (0.2%)
32	X	0.86	0/788	1.62	13/1050 (1.2%)
33	C	0.82	0/1570	1.51	11/2129 (0.5%)
34	AA	0.93	0/75947	1.14	279/118255 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	AC	0.94	0/3599	1.15	14/5603 (0.2%)
36	AB	0.93	0/2823	1.07	8/4400 (0.2%)
37	AL	0.85	0/1789	1.61	12/2381 (0.5%)
38	A1	0.84	0/1151	1.54	11/1531 (0.7%)
39	A2	0.83	0/840	1.47	2/1114 (0.2%)
40	A4	0.85	0/564	1.67	4/737 (0.5%)
41	A6	0.84	0/749	1.49	5/1001 (0.5%)
42	A7	0.89	0/806	1.53	1/1073 (0.1%)
43	AN	0.81	0/1218	1.54	7/1621 (0.4%)
44	A8	0.85	0/1054	1.63	13/1399 (0.9%)
45	A9	0.88	0/865	1.47	5/1160 (0.4%)
46	Aa	0.89	0/872	1.52	0/1161
47	Ab	0.88	0/763	1.52	2/1008 (0.2%)
48	Ad	0.84	0/612	1.51	1/812 (0.1%)
49	Ae	0.99	0/396	1.46	1/521 (0.2%)
50	Af	0.87	0/419	1.46	1/556 (0.2%)
51	AP	0.89	0/1735	1.58	15/2320 (0.6%)
52	Ah	0.83	0/668	1.42	0/887
53	Ai	0.82	0/789	1.36	0/1032
54	AI	0.81	0/1708	1.55	17/2274 (0.7%)
55	AJ	0.83	0/1840	1.55	10/2456 (0.4%)
56	Ac	0.88	0/723	1.55	2/951 (0.2%)
57	AK	0.83	0/1690	1.53	9/2260 (0.4%)
58	AM	0.83	0/1012	1.45	2/1363 (0.1%)
59	AS	0.86	0/1531	1.51	8/2040 (0.4%)
60	AO	0.87	0/1199	1.57	15/1597 (0.9%)
61	AQ	0.87	0/1580	1.52	10/2113 (0.5%)
62	AR	0.86	0/2079	1.54	4/2777 (0.1%)
63	AW	0.88	0/1244	1.51	7/1663 (0.4%)
64	AY	0.80	0/806	1.45	2/1074 (0.2%)
65	AT	0.85	0/1525	1.52	4/2016 (0.2%)
66	AZ	0.86	0/1013	1.49	2/1339 (0.1%)
67	A3	0.83	0/1005	1.55	1/1329 (0.1%)
68	A5	0.86	0/1917	1.53	11/2562 (0.4%)
69	AD	0.85	0/1902	1.51	12/2544 (0.5%)
70	AE	0.84	0/3130	1.50	6/4195 (0.1%)
71	AF	0.86	0/3145	1.56	9/4205 (0.2%)
72	AG	0.90	0/1021	1.59	1/1349 (0.1%)
73	AU	0.87	0/1527	1.51	7/2043 (0.3%)
74	AH	0.84	0/1501	1.50	9/2025 (0.4%)
75	AV	0.84	0/1301	1.48	2/1732 (0.1%)
76	Ag	0.98	0/348	1.67	1/448 (0.2%)
77	AX	0.81	0/842	1.44	5/1125 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
78	A0	0.84	0/534	1.57	4/711 (0.6%)
All	All	0.90	0/207331	1.30	843/303942 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	127
2	7	0	8
4	E	0	7
5	G	0	1
6	I	0	2
7	K	0	3
8	M	0	3
9	W	0	2
12	Y	0	3
14	1	0	3
15	2	0	1
16	3	0	3
18	5	0	2
19	6	0	3
20	B	1	5
21	F	0	3
22	H	0	2
23	J	0	4
24	L	0	4
25	N	0	1
26	P	0	3
27	Q	0	3
28	S	0	1
29	T	0	5
30	U	0	1
31	V	0	4
32	X	0	3
33	C	0	2
34	AA	1	304
35	AC	0	10
36	AB	0	9
37	AL	0	6
38	A1	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
40	A4	0	1
41	A6	0	1
42	A7	0	3
43	AN	0	5
44	A8	0	4
45	A9	0	2
46	Aa	0	3
47	Ab	0	1
48	Ad	0	1
49	Ae	0	2
50	Af	0	2
51	AP	0	7
52	Ah	0	1
53	Ai	0	1
54	AI	0	4
55	AJ	0	2
56	Ac	0	4
57	AK	0	7
58	AM	0	3
59	AS	0	7
60	AO	0	3
61	AQ	0	6
62	AR	0	4
63	AW	0	4
64	AY	0	1
65	AT	0	4
66	AZ	0	5
67	A3	0	1
68	A5	0	5
69	AD	0	1
70	AE	0	7
71	AF	0	10
72	AG	0	3
73	AU	0	5
75	AV	0	3
76	Ag	0	2
78	A0	0	4
All	All	2	668

There are no bond length outliers.

All (843) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AA	255	C	P-O5'-C5'	13.59	141.29	120.90
36	AB	27	A	O3'-P-O5'	-13.46	83.82	104.00
1	A	1659	U	P-O3'-C3'	12.57	139.06	120.20
1	A	981	U	P-O3'-C3'	12.15	138.43	120.20
34	AA	811	A	P-O3'-C3'	11.88	138.02	120.20
34	AA	3632	U	P-O5'-C5'	11.39	137.99	120.90
1	A	1865	G	P-O3'-C3'	10.69	136.24	120.20
1	A	1912	C	P-O3'-C3'	10.54	136.01	120.20
34	AA	257	U	P-O3'-C3'	10.42	135.84	120.20
35	AC	37	A	P-O3'-C3'	10.24	135.56	120.20
34	AA	3667	C	P-O3'-C3'	10.23	135.55	120.20
34	AA	181	C	P-O3'-C3'	10.14	135.41	120.20
1	A	1897	A	P-O3'-C3'	10.13	135.40	120.20
34	AA	3782	A	P-O5'-C5'	9.90	135.75	120.90
1	A	492	A	P-O5'-C5'	9.90	135.75	120.90
36	AB	28	C	P-O5'-C5'	9.88	135.72	120.90
34	AA	2219	A	C2'-C3'-O3'	9.83	124.24	109.50
1	A	1109	G	P-O5'-C5'	9.79	135.59	120.90
34	AA	504	A	P-O3'-C3'	9.67	134.70	120.20
34	AA	3140	U	P-O3'-C3'	9.57	134.55	120.20
35	AC	35	A	P-O3'-C3'	9.49	134.44	120.20
1	A	1321	C	C5'-C4'-C3'	-9.45	101.83	116.00
34	AA	3658	G	P-O3'-C3'	9.23	134.04	120.20
34	AA	674	U	P-O3'-C3'	9.14	133.91	120.20
34	AA	1206	U	P-O3'-C3'	9.14	133.91	120.20
34	AA	579	C	P-O3'-C3'	9.13	133.90	120.20
2	7	39	C	P-O5'-C5'	9.02	134.42	120.90
34	AA	715	U	P-O3'-C3'	8.99	133.68	120.20
34	AA	254	U	O3'-P-O5'	-8.96	90.56	104.00
34	AA	1035	G	P-O3'-C3'	8.95	133.62	120.20
34	AA	2932	A	P-O3'-C3'	8.91	133.56	120.20
1	A	844	G	P-O3'-C3'	8.89	133.53	120.20
1	A	789	U	P-O3'-C3'	8.88	133.53	120.20
34	AA	1996	C	P-O3'-C3'	8.85	133.47	120.20
1	A	1381	C	P-O3'-C3'	8.72	133.28	120.20
34	AA	596	A	P-O3'-C3'	8.62	133.13	120.20
34	AA	411	U	P-O3'-C3'	8.62	133.13	120.20
43	AN	21	PHE	CA-CB-CG	-8.50	105.30	113.80
34	AA	620	U	P-O3'-C3'	8.46	132.89	120.20
51	AP	94	SER	CA-C-N	8.44	131.59	120.28
51	AP	94	SER	C-N-CA	8.44	131.59	120.28
34	AA	1224	A	P-O3'-C3'	8.36	132.75	120.20
34	AA	2960	G	C5'-C4'-C3'	-8.36	103.45	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7	76	A	P-O5'-C5'	8.33	133.39	120.90
1	A	544	G	P-O3'-C3'	8.29	132.64	120.20
34	AA	580	A	P-O3'-C3'	8.24	132.57	120.20
34	AA	3476	A	C2'-C3'-O3'	8.22	121.83	109.50
34	AA	3043	A	C2'-C3'-O3'	8.22	121.82	109.50
34	AA	859	C	P-O3'-C3'	8.18	132.46	120.20
34	AA	3280	U	O4'-C4'-C3'	8.12	112.12	104.00
34	AA	2959	G	C5'-C4'-C3'	-8.11	103.83	116.00
34	AA	1989	A	P-O3'-C3'	8.11	132.36	120.20
34	AA	621	C	P-O3'-C3'	8.11	132.36	120.20
34	AA	2219	A	P-O3'-C3'	8.10	132.35	120.20
1	A	1659	U	C2'-C3'-O3'	8.06	121.59	109.50
34	AA	162	U	P-O3'-C3'	7.97	132.16	120.20
36	AB	28	C	C5'-C4'-C3'	7.94	127.91	116.00
1	A	1832	U	P-O3'-C3'	7.91	132.06	120.20
34	AA	1881	C	C2'-C3'-O3'	7.90	121.35	109.50
34	AA	2959	G	P-O3'-C3'	7.90	132.05	120.20
34	AA	697	A	P-O3'-C3'	7.86	132.00	120.20
65	AT	127	LYS	CA-C-N	7.86	128.87	119.99
65	AT	127	LYS	C-N-CA	7.86	128.87	119.99
1	A	1808	G	P-O5'-C5'	7.82	132.62	120.90
34	AA	581	C	P-O3'-C3'	7.82	131.93	120.20
34	AA	620	U	C2'-C3'-O3'	7.72	121.08	109.50
1	A	874	A	C2'-C3'-O3'	7.72	121.08	109.50
34	AA	500	A	P-O3'-C3'	7.71	131.76	120.20
34	AA	3067	G	O3'-P-O5'	-7.70	92.45	104.00
34	AA	3576	A	C2'-C3'-O3'	7.65	120.98	109.50
1	A	1455	C	P-O3'-C3'	7.64	131.66	120.20
74	AH	165	LEU	N-CA-C	7.61	121.01	110.35
34	AA	33	G	O3'-P-O5'	-7.60	92.59	104.00
34	AA	1574	C	P-O3'-C3'	7.59	131.59	120.20
1	A	156	A	P-O3'-C3'	7.58	131.58	120.20
1	A	1907	A	C4'-C3'-C2'	-7.57	95.03	102.60
1	A	246	A	P-O3'-C3'	7.54	131.51	120.20
34	AA	3576	A	P-O3'-C3'	7.49	131.43	120.20
1	A	423	A	P-O3'-C3'	7.48	131.42	120.20
34	AA	289	A	P-O3'-C3'	7.45	131.38	120.20
25	N	40	LYS	CA-C-N	7.44	128.20	119.94
25	N	40	LYS	C-N-CA	7.44	128.20	119.94
34	AA	811	A	C2'-C3'-O3'	7.42	120.64	109.50
34	AA	215	C	P-O3'-C3'	7.41	131.31	120.20
34	AA	1805	U	P-O3'-C3'	7.39	131.29	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	AD	206	PRO	CA-C-N	7.39	130.59	120.46
69	AD	206	PRO	C-N-CA	7.39	130.59	120.46
40	A4	40	PHE	CA-CB-CG	-7.39	106.41	113.80
34	AA	3019	A	P-O5'-C5'	7.38	131.96	120.90
54	AI	18	LYS	N-CA-C	7.38	119.32	111.28
34	AA	2394	C	P-O3'-C3'	7.34	131.20	120.20
1	A	1448	U	P-O3'-C3'	7.29	131.13	120.20
34	AA	1881	C	P-O3'-C3'	7.28	131.12	120.20
34	AA	1217	U	P-O3'-C3'	7.26	131.09	120.20
1	A	291	A	P-O3'-C3'	7.25	131.08	120.20
34	AA	308	U	C2'-C3'-O3'	7.25	120.37	109.50
34	AA	1503	A	P-O3'-C3'	7.24	131.06	120.20
1	A	874	A	P-O3'-C3'	7.24	131.05	120.20
34	AA	1435	G	P-O3'-C3'	7.23	131.05	120.20
1	A	752	U	C2'-C3'-O3'	7.23	120.34	109.50
28	S	89	ARG	N-CA-C	7.19	118.76	111.07
35	AC	145	A	P-O3'-C3'	7.19	130.98	120.20
1	A	2053	U	C2'-C3'-O3'	7.17	120.25	109.50
1	A	105	A	C2'-C3'-O3'	7.15	120.23	109.50
1	A	1064	A	O3'-P-O5'	-7.15	93.27	104.00
34	AA	146	U	C2'-C3'-O3'	7.13	120.20	109.50
34	AA	698	G	P-O3'-C3'	7.10	130.85	120.20
36	AB	27	A	C5'-C4'-C3'	7.10	126.65	116.00
34	AA	1538	U	C2'-C3'-O3'	7.09	120.13	109.50
34	AA	1568	C	P-O3'-C3'	-7.09	109.57	120.20
1	A	1300	G	P-O3'-C3'	7.08	130.82	120.20
34	AA	2816	U	P-O3'-C3'	7.08	130.82	120.20
34	AA	3577	A	C2'-C3'-O3'	7.08	120.11	109.50
1	A	1382	G	P-O5'-C5'	7.07	131.51	120.90
34	AA	2013	U	O3'-P-O5'	-7.07	93.40	104.00
1	A	251	U	C2'-C3'-O3'	7.04	120.05	109.50
34	AA	2822	U	P-O3'-C3'	7.03	130.74	120.20
34	AA	2693	G	P-O3'-C3'	7.01	130.72	120.20
34	AA	3381	A	C2'-C3'-O3'	7.00	120.01	109.50
34	AA	607	A	P-O3'-C3'	7.00	130.70	120.20
1	A	1413	U	P-O3'-C3'	6.98	130.67	120.20
34	AA	62	A	P-O3'-C3'	6.98	130.67	120.20
75	AV	84	ARG	NE-CZ-NH2	6.97	125.47	119.20
34	AA	1873	U	P-O3'-C3'	6.94	130.62	120.20
1	A	981	U	C2'-C3'-O3'	6.93	119.90	109.50
34	AA	3588	A	P-O3'-C3'	6.92	130.58	120.20
54	AI	132	ASP	CA-C-N	6.91	129.85	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	AI	132	ASP	C-N-CA	6.91	129.85	120.38
45	A9	52	SER	N-CA-C	-6.91	98.67	108.96
1	A	879	A	C2'-C3'-O3'	6.91	119.86	109.50
1	A	1976	G	P-O3'-C3'	6.89	130.54	120.20
2	7	13	C	P-O5'-C5'	6.86	131.19	120.90
1	A	25	C	P-O3'-C3'	6.85	130.48	120.20
1	A	1070	A	P-O3'-C3'	6.85	130.48	120.20
34	AA	3590	A	C2'-C3'-O3'	6.84	119.76	109.50
34	AA	521	U	C2'-C3'-O3'	6.83	119.74	109.50
1	A	1431	A	P-O3'-C3'	6.82	130.42	120.20
34	AA	3034	A	C2'-C3'-O3'	6.81	119.72	109.50
34	AA	3230	G	P-O3'-C3'	6.81	130.41	120.20
23	J	15	ASP	N-CA-C	6.80	118.70	111.28
34	AA	501	U	P-O3'-C3'	6.78	130.36	120.20
1	A	790	U	C2'-C3'-O3'	6.77	119.65	109.50
34	AA	3361	U	C2'-C3'-O3'	6.76	119.64	109.50
1	A	759	C	P-O5'-C5'	6.75	131.03	120.90
63	AW	37	ARG	N-CA-C	6.73	119.78	110.35
16	3	60	SER	CA-C-N	6.73	129.19	120.44
16	3	60	SER	C-N-CA	6.73	129.19	120.44
1	A	1980	A	C2'-C3'-O3'	6.70	119.55	109.50
34	AA	1705	A	P-O3'-C3'	6.69	130.23	120.20
1	A	250	A	P-O3'-C3'	6.68	130.22	120.20
32	X	43	ARG	NE-CZ-NH1	-6.68	114.82	121.50
2	7	4	G	C2'-C3'-O3'	6.67	119.50	109.50
34	AA	1780	G	P-O5'-C5'	6.66	130.89	120.90
34	AA	3782	A	P-O3'-C3'	6.65	130.17	120.20
24	L	29	LEU	CA-C-O	6.64	122.52	118.33
34	AA	1568	C	O3'-P-O5'	-6.63	94.05	104.00
2	7	18	G	C2'-C3'-O3'	6.61	119.42	109.50
34	AA	1904	U	P-O3'-C3'	6.60	130.10	120.20
34	AA	876	C	O3'-P-O5'	-6.59	94.11	104.00
37	AL	28	ASN	CA-CB-CG	-6.58	106.02	112.60
1	A	1292	U	P-O3'-C3'	6.58	130.07	120.20
31	V	22	PHE	CA-CB-CG	-6.58	107.22	113.80
34	AA	162	U	C2'-C3'-O3'	6.57	119.36	109.50
37	AL	22	ARG	NE-CZ-NH2	6.56	125.10	119.20
35	AC	57	A	P-O3'-C3'	6.55	130.03	120.20
43	AN	60	PHE	CA-CB-CG	-6.55	107.25	113.80
1	A	2053	U	P-O3'-C3'	6.52	129.98	120.20
1	A	752	U	P-O3'-C3'	6.51	129.96	120.20
34	AA	270	U	P-O3'-C3'	6.50	129.95	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AA	900	G	P-O5'-C5'	6.50	130.66	120.90
34	AA	1703	U	C2'-C3'-O3'	6.50	119.25	109.50
34	AA	2883	U	P-O3'-C3'	6.50	129.95	120.20
34	AA	1101	A	P-O3'-C3'	6.50	129.94	120.20
61	AQ	130	ASP	CA-C-N	6.50	129.20	120.50
61	AQ	130	ASP	C-N-CA	6.50	129.20	120.50
34	AA	1873	U	C2'-C3'-O3'	6.49	119.23	109.50
34	AA	3233	G	C5'-C4'-C3'	-6.49	106.27	116.00
1	A	818	C	P-O3'-C3'	6.48	129.92	120.20
74	AH	167	ARG	NE-CZ-NH2	6.48	125.03	119.20
71	AF	362	GLN	N-CA-C	6.46	118.86	111.11
34	AA	1217	U	C2'-C3'-O3'	6.46	119.18	109.50
34	AA	1990	A	P-O3'-C3'	6.44	129.87	120.20
34	AA	1435	G	C2'-C3'-O3'	6.44	119.17	109.50
34	AA	2959	G	O5'-C5'-C4'	6.44	121.16	111.50
45	A9	110	ASN	CA-CB-CG	-6.44	106.16	112.60
54	AI	16	LYS	N-CA-C	6.44	118.30	111.28
34	AA	650	U	P-O5'-C5'	-6.44	111.24	120.90
34	AA	3018	A	P-O3'-C3'	6.43	129.84	120.20
30	U	81	ALA	N-CA-C	6.42	119.79	110.42
1	A	790	U	P-O3'-C3'	6.41	129.82	120.20
45	A9	78	VAL	N-CA-C	6.41	117.16	110.62
30	U	71	ILE	N-CA-C	6.38	117.13	110.62
37	AL	50	ILE	CA-C-N	6.36	130.36	120.75
37	AL	50	ILE	C-N-CA	6.36	130.36	120.75
1	A	1870	A	P-O3'-C3'	6.35	129.72	120.20
34	AA	1999	A	P-O3'-C3'	6.34	129.72	120.20
6	I	52	PHE	CA-CB-CG	-6.34	107.46	113.80
34	AA	893	U	C4'-C3'-C2'	-6.33	96.27	102.60
73	AU	53	PHE	CA-CB-CG	-6.32	107.48	113.80
69	AD	163	ARG	NE-CZ-NH1	-6.32	115.18	121.50
34	AA	3494	C	P-O3'-C3'	6.32	129.67	120.20
1	A	1691	G	P-O3'-C3'	6.30	129.66	120.20
34	AA	1880	A	P-O5'-C5'	-6.30	111.45	120.90
34	AA	652	A	C2'-C3'-O3'	6.29	123.14	113.70
34	AA	3767	U	O5'-C5'-C4'	6.29	121.13	111.70
34	AA	1705	A	C2'-C3'-O3'	6.28	118.91	109.50
49	Ae	20	ASN	N-CA-C	6.27	118.64	111.11
22	H	43	GLU	CA-C-N	6.27	129.54	120.38
22	H	43	GLU	C-N-CA	6.27	129.54	120.38
34	AA	1904	U	C2'-C3'-O3'	6.27	118.91	109.50
40	A4	48	LYS	CA-C-N	6.27	126.90	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	A4	48	LYS	C-N-CA	6.27	126.90	119.94
34	AA	3280	U	C5'-C4'-O4'	6.26	119.20	109.80
12	Y	124	ARG	NE-CZ-NH2	6.26	124.83	119.20
34	AA	1027	G	P-O5'-C5'	-6.24	111.54	120.90
34	AA	3590	A	P-O3'-C3'	6.23	129.55	120.20
34	AA	1537	G	P-O5'-C5'	6.22	130.24	120.90
34	AA	1968	C	C5'-C4'-C3'	-6.22	106.66	116.00
33	C	21	LYS	CA-C-N	6.22	128.98	120.46
33	C	21	LYS	C-N-CA	6.22	128.98	120.46
34	AA	3667	C	C2'-C3'-O3'	6.22	118.83	109.50
60	AO	32	ARG	N-CA-C	6.21	118.80	110.35
1	A	250	A	C2'-C3'-O3'	6.21	118.81	109.50
45	A9	92	HIS	CA-CB-CG	-6.20	107.60	113.80
1	A	45	U	C2'-C3'-O3'	6.20	118.80	109.50
25	N	108	VAL	N-CA-C	6.20	116.98	110.72
39	A2	38	VAL	N-CA-C	6.20	116.36	110.53
1	A	1819	U	P-O5'-C5'	6.19	130.19	120.90
34	AA	432	A	P-O3'-C3'	6.19	129.48	120.20
34	AA	270	U	C2'-C3'-O3'	6.18	122.97	113.70
34	AA	2015	C	C2'-C3'-O3'	6.18	118.78	109.50
51	AP	33	LEU	N-CA-C	6.18	118.43	109.84
34	AA	1750	U	C2'-C3'-O3'	6.17	118.76	109.50
1	A	1934	C	C2'-C3'-O3'	6.17	118.75	109.50
34	AA	1904	U	C4'-C3'-C2'	-6.16	96.44	102.60
34	AA	3631	U	O3'-P-O5'	-6.15	94.77	104.00
1	A	1098	U	P-O3'-C3'	6.15	129.42	120.20
32	X	82	ASN	CA-CB-CG	-6.15	106.45	112.60
34	AA	3140	U	C2'-C3'-O3'	6.14	118.71	109.50
58	AM	128	TRP	CA-C-N	6.14	125.63	119.24
58	AM	128	TRP	C-N-CA	6.14	125.63	119.24
34	AA	2959	G	C5'-C4'-O4'	6.13	119.00	109.80
77	AX	117	ARG	CA-C-N	6.13	130.02	120.82
77	AX	117	ARG	C-N-CA	6.13	130.02	120.82
1	A	1403	U	C5'-C4'-C3'	-6.13	106.81	116.00
34	AA	1460	A	P-O5'-C5'	6.13	130.09	120.90
34	AA	1017	U	O3'-P-O5'	-6.12	94.82	104.00
34	AA	681	U	C5'-C4'-C3'	-6.11	106.83	116.00
23	J	16	LEU	CA-C-N	6.11	128.38	120.44
23	J	16	LEU	C-N-CA	6.11	128.38	120.44
78	A0	66	ASN	CA-CB-CG	-6.11	106.49	112.60
66	AZ	51	LYS	N-CA-C	6.10	118.43	111.11
24	L	65	PHE	CA-CB-CG	-6.08	107.72	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AA	3381	A	P-O3'-C3'	6.08	129.32	120.20
34	AA	579	C	C2'-C3'-O3'	6.08	118.62	109.50
69	AD	163	ARG	NE-CZ-NH2	6.07	124.67	119.20
34	AA	2095	U	P-O3'-C3'	6.07	129.31	120.20
35	AC	134	G	P-O3'-C3'	6.07	129.30	120.20
61	AQ	84	ASN	CA-CB-CG	-6.06	106.54	112.60
34	AA	998	U	C2'-C3'-O3'	6.05	118.58	109.50
22	H	39	ASP	CA-CB-CG	-6.05	106.55	112.60
28	S	88	ARG	NE-CZ-NH2	6.05	124.64	119.20
34	AA	1574	C	O4'-C1'-N1	6.05	117.57	108.50
34	AA	1431	A	C2'-C3'-O3'	6.04	118.56	109.50
35	AC	145	A	C2'-C3'-O3'	6.04	122.76	113.70
1	A	815	G	P-O5'-C5'	-6.04	111.84	120.90
12	Y	102	PHE	CA-CB-CG	-6.04	107.76	113.80
57	AK	199	PHE	CA-CB-CG	-6.04	107.77	113.80
34	AA	215	C	C2'-C3'-O3'	6.03	122.75	113.70
34	AA	3280	U	C5'-C4'-C3'	6.03	125.05	116.00
34	AA	3577	A	P-O3'-C3'	6.03	129.25	120.20
42	A7	64	ASN	CA-CB-CG	-6.03	106.57	112.60
43	AN	44	PHE	CA-CB-CG	-6.03	107.77	113.80
1	A	204	U	P-O5'-C5'	6.03	129.94	120.90
1	A	2071	U	P-O3'-C3'	6.03	129.24	120.20
34	AA	1457	G	P-O3'-C3'	6.02	129.23	120.20
1	A	1297	A	P-O5'-C5'	6.02	129.93	120.90
34	AA	1762	A	C2'-C3'-O3'	6.02	118.53	109.50
20	B	220	ARG	NE-CZ-NH2	6.02	124.61	119.20
56	Ac	21	LEU	N-CA-C	6.01	117.92	111.36
1	A	1786	U	P-O3'-C3'	6.00	129.21	120.20
34	AA	505	A	P-O3'-C3'	6.00	129.19	120.20
32	X	86	ILE	N-CA-C	-5.99	103.48	108.63
34	AA	2033	C	P-O3'-C3'	5.99	129.18	120.20
28	S	86	LEU	N-CA-C	5.97	118.88	110.23
71	AF	217	VAL	N-CA-C	5.97	116.62	110.36
5	G	79	PHE	CA-CB-CG	-5.96	107.84	113.80
34	AA	3441	A	C2'-C3'-O3'	5.96	118.44	109.50
66	AZ	121	LYS	N-CA-C	5.96	117.44	111.07
1	A	1796	C	C5'-C4'-C3'	-5.94	107.09	116.00
11	O	88	ARG	N-CA-C	5.94	117.43	111.07
57	AK	84	ARG	NE-CZ-NH2	5.94	124.55	119.20
12	Y	158	PHE	CA-CB-CG	-5.94	107.86	113.80
34	AA	3408	G	C2'-C3'-O3'	5.93	118.40	109.50
24	L	100	CYS	N-CA-C	5.93	118.41	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1198	U	C2'-C3'-O3'	5.92	118.38	109.50
55	AJ	129	LEU	N-CA-C	5.92	117.74	111.28
34	AA	3526	U	C2'-C3'-O3'	5.92	118.38	109.50
14	1	20	ARG	NE-CZ-NH2	5.92	124.53	119.20
34	AA	895	A	C5'-C4'-C3'	-5.91	107.13	116.00
19	6	13	LYS	N-CA-C	5.91	118.23	111.02
74	AH	174	PHE	CA-CB-CG	-5.91	107.89	113.80
4	E	132	ARG	NE-CZ-NH2	5.90	124.51	119.20
34	AA	2083	U	O3'-P-O5'	-5.90	95.15	104.00
34	AA	772	A	P-O5'-C5'	-5.89	112.06	120.90
54	AI	130	ASP	N-CA-C	5.89	117.70	111.28
63	AW	70	THR	CA-C-N	5.89	128.17	120.28
63	AW	70	THR	C-N-CA	5.89	128.17	120.28
2	7	7	G	P-O3'-C3'	5.89	129.03	120.20
38	A1	76	ASN	CA-CB-CG	5.87	118.47	112.60
11	O	36	LYS	N-CA-C	5.87	117.76	111.36
34	AA	384	A	P-O5'-C5'	5.87	129.70	120.90
60	AO	74	ASN	CA-CB-CG	-5.87	106.73	112.60
34	AA	2807	U	P-O5'-C5'	5.86	129.69	120.90
9	W	102	THR	CA-C-N	5.85	128.12	120.28
9	W	102	THR	C-N-CA	5.85	128.12	120.28
37	AL	100	ARG	NE-CZ-NH2	5.85	124.46	119.20
45	A9	39	ARG	N-CA-C	5.85	117.45	111.14
34	AA	337	A	C2'-C3'-O3'	5.84	118.27	109.50
36	AB	75	G	C2'-C3'-O3'	5.84	118.26	109.50
1	A	562	A	P-O3'-C3'	5.84	128.96	120.20
55	AJ	198	LYS	N-CA-C	5.84	117.44	111.14
1	A	1644	U	C2'-C3'-O3'	5.83	118.25	109.50
23	J	4	VAL	N-CA-C	5.83	116.57	110.62
34	AA	86	G	C2'-C3'-O3'	5.83	118.24	109.50
51	AP	35	VAL	N-CA-C	5.82	116.01	110.42
57	AK	189	ASN	CA-C-N	5.82	125.29	119.24
57	AK	189	ASN	C-N-CA	5.82	125.29	119.24
36	AB	50	A	P-O5'-C5'	5.82	129.62	120.90
78	A0	12	ALA	CA-C-N	5.82	128.07	120.28
78	A0	12	ALA	C-N-CA	5.82	128.07	120.28
34	AA	370	G	C5'-C4'-C3'	-5.81	107.28	116.00
55	AJ	97	PHE	CA-CB-CG	-5.81	107.99	113.80
34	AA	3435	A	P-O3'-C3'	5.81	128.91	120.20
21	F	191	ARG	NE-CZ-NH2	5.81	124.43	119.20
34	AA	2556	C	C5'-C4'-C3'	-5.81	107.29	116.00
61	AQ	57	TYR	CA-C-N	5.81	129.08	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	AQ	57	TYR	C-N-CA	5.81	129.08	120.95
1	A	1907	A	C2'-C3'-O3'	5.80	118.21	109.50
21	F	79	ASP	CA-C-N	5.80	128.63	120.28
21	F	79	ASP	C-N-CA	5.80	128.63	120.28
26	P	128	ARG	NE-CZ-NH2	5.80	124.42	119.20
2	7	11	A	P-O5'-C5'	5.80	129.60	120.90
34	AA	500	A	C2'-C3'-O3'	5.80	118.20	109.50
16	3	83	PHE	CA-CB-CG	-5.79	108.02	113.80
34	AA	2832	A	C2'-C3'-O3'	5.78	118.17	109.50
32	X	47	ARG	NE-CZ-NH2	5.78	124.40	119.20
23	J	14	SER	CA-C-N	5.78	128.03	120.28
23	J	14	SER	C-N-CA	5.78	128.03	120.28
34	AA	889	U	C2'-C3'-O3'	5.78	118.17	109.50
34	AA	810	U	C2'-C3'-O3'	5.78	118.16	109.50
34	AA	2123	C	O3'-P-O5'	-5.78	95.34	104.00
1	A	129	U	C2'-C3'-O3'	5.77	118.15	109.50
1	A	127	C	C2'-C3'-O3'	5.76	118.15	109.50
1	A	206	A	P-O3'-C3'	5.76	128.84	120.20
1	A	1462	A	P-O3'-C3'	5.76	128.84	120.20
34	AA	683	A	C4'-C3'-O3'	5.75	118.03	109.40
18	5	15	ARG	NE-CZ-NH2	5.75	124.38	119.20
32	X	43	ARG	NE-CZ-NH2	5.73	124.36	119.20
34	AA	1539	U	P-O3'-C3'	5.73	128.80	120.20
55	AJ	130	ASN	N-CA-C	5.73	117.99	111.11
43	AN	87	CYS	N-CA-C	5.72	118.53	110.23
4	E	19	PHE	CA-CB-CG	-5.72	108.08	113.80
28	S	102	ALA	N-CA-C	5.72	116.47	108.00
3	D	99	ALA	N-CA-C	5.72	117.97	111.11
37	AL	74	PHE	CA-CB-CG	-5.71	108.09	113.80
61	AQ	32	ARG	NE-CZ-NH2	5.71	124.34	119.20
24	L	87	ASN	N-CA-C	5.71	117.91	110.43
34	AA	858	C	P-O3'-C3'	5.71	128.76	120.20
18	5	61	ARG	NE-CZ-NH2	5.71	124.33	119.20
61	AQ	26	VAL	N-CA-C	5.70	115.23	108.96
1	A	1870	A	C2'-C3'-O3'	5.70	118.05	109.50
26	P	117	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	A	26	A	C2'-C3'-O3'	5.70	118.04	109.50
20	B	38	PHE	CA-CB-CG	-5.70	108.10	113.80
47	Ab	3	ARG	NE-CZ-NH2	5.69	124.33	119.20
59	AS	85	ILE	N-CA-CB	5.69	117.81	110.99
34	AA	3658	G	C4'-C3'-O3'	5.68	117.92	109.40
51	AP	67	ARG	NE-CZ-NH2	5.68	124.31	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AA	2886	A	C2'-C3'-O3'	5.68	118.02	109.50
34	AA	683	A	P-O3'-C3'	5.68	128.72	120.20
60	AO	6	LYS	N-CA-C	5.68	117.87	110.43
34	AA	138	C	P-O3'-C3'	5.68	128.72	120.20
34	AA	3711	U	C2'-C3'-O3'	5.68	118.02	109.50
20	B	136	ARG	NE-CZ-NH2	5.68	124.31	119.20
35	AC	55	A	P-O5'-C5'	-5.67	112.39	120.90
59	AS	57	ARG	NE-CZ-NH1	-5.67	115.83	121.50
34	AA	1205	U	P-O3'-C3'	5.67	128.71	120.20
74	AH	170	ASP	N-CA-C	5.67	118.69	110.42
1	A	1845	U	C5'-C4'-C3'	-5.66	107.50	116.00
34	AA	3581	A	C2'-C3'-O3'	5.66	117.99	109.50
34	AA	1123	U	C2'-C3'-O3'	5.66	117.98	109.50
34	AA	1323	A	P-O3'-C3'	5.66	128.68	120.20
34	AA	889	U	P-O3'-C3'	5.65	128.68	120.20
34	AA	2746	U	C2'-C3'-O3'	5.65	117.97	109.50
20	B	74	ASN	CA-CB-CG	-5.65	106.95	112.60
37	AL	183	PHE	N-CA-C	5.65	117.58	110.24
41	A6	101	SER	N-CA-C	5.63	118.23	110.35
47	Ab	54	PHE	CA-CB-CG	-5.63	108.17	113.80
9	W	99	GLU	CA-C-N	5.63	124.82	118.97
9	W	99	GLU	C-N-CA	5.63	124.82	118.97
34	AA	581	C	P-O5'-C5'	5.63	129.34	120.90
44	A8	98	HIS	CA-C-N	5.63	128.28	120.29
44	A8	98	HIS	C-N-CA	5.63	128.28	120.29
1	A	803	G	P-O3'-C3'	5.62	128.62	120.20
37	AL	111	ASN	CA-CB-CG	-5.62	106.98	112.60
63	AW	36	ILE	N-CA-C	5.61	115.81	110.42
24	L	109	PHE	CA-CB-CG	-5.61	108.19	113.80
34	AA	2932	A	C4'-C3'-O3'	5.61	117.81	109.40
1	A	1691	G	C2'-C3'-O3'	5.61	117.91	109.50
20	B	39	LEU	N-CA-C	5.60	117.38	111.28
1	A	753	U	C2'-C3'-O3'	5.60	117.90	109.50
34	AA	3767	U	C4'-C3'-O3'	5.60	117.80	109.40
44	A8	97	ALA	CA-C-N	5.59	128.09	120.54
44	A8	97	ALA	C-N-CA	5.59	128.09	120.54
73	AU	30	ASN	CA-CB-CG	-5.59	107.01	112.60
34	AA	2036	C	P-O5'-C5'	5.59	129.28	120.90
34	AA	184	U	P-O3'-C3'	5.59	128.58	120.20
1	A	2028	U	O3'-P-O5'	-5.58	95.63	104.00
34	AA	107	C	P-O5'-C5'	5.58	129.27	120.90
38	A1	78	ASN	CA-CB-CG	-5.58	107.02	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	P	66	ARG	NE-CZ-NH2	5.57	124.21	119.20
73	AU	167	GLN	CA-C-N	5.57	129.18	120.82
73	AU	167	GLN	C-N-CA	5.57	129.18	120.82
19	6	14	VAL	N-CA-C	5.57	116.34	110.72
44	A8	66	LEU	N-CA-C	5.57	117.92	110.35
60	AO	90	PHE	CA-CB-CG	-5.57	108.23	113.80
37	AL	5	ASN	CA-CB-CG	-5.56	107.04	112.60
34	AA	986	U	P-O5'-C5'	5.56	129.23	120.90
34	AA	1642	G	C2'-C3'-O3'	5.55	117.83	109.50
34	AA	2665	A	C2'-C3'-O3'	5.55	117.83	109.50
1	A	919	U	P-O3'-C3'	5.55	128.53	120.20
34	AA	10	G	P-O3'-C3'	5.55	128.53	120.20
1	A	1980	A	C4'-C3'-C2'	-5.54	97.06	102.60
64	AY	165	ASN	CA-CB-CG	-5.54	107.06	112.60
34	AA	650	U	C4'-C3'-C2'	-5.53	97.07	102.60
34	AA	25	A	C2'-C3'-O3'	5.53	117.80	109.50
1	A	142	G	C2'-C3'-O3'	5.53	117.79	109.50
44	A8	55	ILE	CA-C-N	5.52	127.03	120.14
44	A8	55	ILE	C-N-CA	5.52	127.03	120.14
23	J	108	LYS	N-CA-C	5.51	117.29	111.28
1	A	1677	C	C4'-C3'-C2'	5.50	108.11	102.60
36	AB	93	G	P-O5'-C5'	5.50	129.15	120.90
22	H	25	LEU	N-CA-C	5.50	121.96	109.81
34	AA	257	U	C2'-C3'-O3'	5.50	121.95	113.70
6	I	20	ASN	CA-CB-CG	-5.49	107.11	112.60
54	AI	46	VAL	N-CA-C	5.49	116.49	109.30
20	B	57	ALA	CA-C-N	5.49	127.95	120.54
20	B	57	ALA	C-N-CA	5.49	127.95	120.54
44	A8	122	ALA	N-CA-C	5.49	117.26	111.28
68	A5	129	ASN	N-CA-C	-5.49	100.97	108.38
1	A	1729	A	C5'-C4'-C3'	5.49	124.23	116.00
32	X	40	ARG	CA-C-N	5.49	127.57	120.44
32	X	40	ARG	C-N-CA	5.49	127.57	120.44
34	AA	3664	G	P-O3'-C3'	5.48	128.42	120.20
1	A	626	A	C5'-C4'-C3'	5.47	124.21	116.00
1	A	1038	C	C5'-C4'-C3'	-5.47	107.79	116.00
71	AF	394	ALA	N-CA-C	5.47	116.92	111.07
34	AA	25	A	O4'-C1'-N9	5.47	116.40	108.20
34	AA	2607	U	C2'-C3'-O3'	5.46	117.69	109.50
8	M	99	ASP	CA-C-N	5.46	127.59	120.28
8	M	99	ASP	C-N-CA	5.46	127.59	120.28
1	A	1857	U	O4'-C1'-N1	5.45	116.68	108.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AA	904	G	C2'-C3'-O3'	5.45	117.68	109.50
21	F	88	ASP	CA-CB-CG	-5.45	107.15	112.60
34	AA	1812	C	C5'-C4'-C3'	-5.45	107.03	115.20
60	AO	64	LEU	CA-C-N	5.45	128.33	120.38
60	AO	64	LEU	C-N-CA	5.45	128.33	120.38
12	Y	144	GLY	CA-C-N	5.45	128.50	120.82
12	Y	144	GLY	C-N-CA	5.45	128.50	120.82
1	A	952	U	P-O5'-C5'	5.44	129.06	120.90
1	A	207	G	C2'-C3'-O3'	5.44	117.66	109.50
34	AA	798	U	P-O3'-C3'	-5.44	112.04	120.20
51	AP	188	SER	N-CA-CB	5.44	119.68	110.49
34	AA	888	A	P-O3'-C3'	5.44	128.36	120.20
12	Y	97	PHE	CA-CB-CG	-5.43	108.37	113.80
34	AA	2470	A	C2'-C3'-O3'	5.43	117.65	109.50
1	A	516	G	C2'-C3'-O3'	5.43	117.65	109.50
74	AH	161	HIS	CB-CA-C	-5.43	102.35	110.88
12	Y	111	ALA	CA-C-N	5.43	125.73	119.92
12	Y	111	ALA	C-N-CA	5.43	125.73	119.92
34	AA	210	C	P-O3'-C3'	5.42	128.34	120.20
38	A1	66	SER	CA-C-N	5.42	129.39	121.31
38	A1	66	SER	C-N-CA	5.42	129.39	121.31
1	A	1108	A	C4'-C3'-C2'	-5.42	97.18	102.60
1	A	525	G	P-O3'-C3'	5.42	128.32	120.20
32	X	42	ARG	CA-C-N	5.41	127.47	120.44
32	X	42	ARG	C-N-CA	5.41	127.47	120.44
34	AA	2693	G	C2'-C3'-O3'	5.41	117.62	109.50
73	AU	160	ALA	N-CA-C	5.41	116.98	111.14
12	Y	95	VAL	N-CA-C	5.41	116.14	110.62
60	AO	2	ALA	CA-C-N	5.41	128.28	120.38
60	AO	2	ALA	C-N-CA	5.41	128.28	120.38
34	AA	685	U	O3'-P-O5'	-5.41	95.89	104.00
63	AW	127	ARG	NE-CZ-NH2	5.41	124.06	119.20
34	AA	65	A	P-O3'-C3'	5.40	128.31	120.20
34	AA	2812	G	P-O5'-C5'	5.40	129.00	120.90
14	1	114	ASN	N-CA-C	5.40	117.92	111.71
32	X	45	PHE	CA-CB-CG	-5.40	108.40	113.80
35	AC	139	A	C2'-C3'-O3'	5.40	117.60	109.50
16	3	61	THR	N-CA-C	5.39	116.84	111.07
5	G	133	VAL	N-CA-C	5.39	115.53	110.30
34	AA	597	A	P-O3'-C3'	5.39	128.29	120.20
5	G	40	ASN	CA-CB-CG	-5.39	107.21	112.60
34	AA	833	G	P-O5'-C5'	5.39	128.98	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AA	513	U	O3'-P-O5'	-5.39	95.92	104.00
34	AA	109	A	P-O3'-C3'	5.39	128.28	120.20
51	AP	95	THR	N-CA-C	5.39	117.15	111.28
34	AA	1856	U	P-O5'-C5'	5.38	128.98	120.90
34	AA	3129	U	C2'-C3'-O3'	5.38	117.58	109.50
27	Q	13	ARG	NE-CZ-NH2	5.38	124.05	119.20
34	AA	619	U	C2'-C3'-O3'	5.38	117.57	109.50
38	A1	99	ASP	CA-C-N	5.38	128.23	120.38
38	A1	99	ASP	C-N-CA	5.38	128.23	120.38
1	A	1291	C	P-O3'-C3'	-5.37	112.14	120.20
37	AL	97	ASP	CA-CB-CG	-5.37	107.23	112.60
61	AQ	159	PHE	CA-C-N	5.37	125.38	119.90
61	AQ	159	PHE	C-N-CA	5.37	125.38	119.90
1	A	1833	G	O3'-P-O5'	-5.37	95.94	104.00
34	AA	1735	G	P-O3'-C3'	5.36	128.24	120.20
41	A6	100	ASP	CA-C-N	5.36	129.29	121.31
41	A6	100	ASP	C-N-CA	5.36	129.29	121.31
6	I	44	ALA	N-CA-C	5.36	118.63	111.24
1	A	1672	C	C2'-C3'-O3'	5.35	117.53	109.50
1	A	1864	U	P-O5'-C5'	5.35	128.93	120.90
10	R	133	LEU	CA-C-N	5.35	127.39	120.44
10	R	133	LEU	C-N-CA	5.35	127.39	120.44
24	L	12	ARG	NE-CZ-NH2	5.35	124.01	119.20
1	A	26	A	C4'-C3'-C2'	-5.34	97.26	102.60
5	G	105	GLY	N-CA-C	5.34	119.41	112.25
54	AI	160	ASN	CA-C-N	5.34	127.44	120.28
54	AI	160	ASN	C-N-CA	5.34	127.44	120.28
34	AA	1203	A	P-O3'-C3'	5.34	128.21	120.20
1	A	83	U	C5'-C4'-C3'	5.34	124.01	116.00
4	E	124	HIS	CA-CB-CG	5.34	119.14	113.80
36	AB	91	C	C5'-C4'-C3'	-5.34	108.00	116.00
70	AE	349	ALA	N-CA-C	5.33	117.18	110.24
71	AF	388	LYS	CA-C-N	5.33	127.38	120.44
71	AF	388	LYS	C-N-CA	5.33	127.38	120.44
62	AR	180	ASN	CA-CB-CG	-5.33	107.27	112.60
9	W	98	VAL	CA-C-N	5.33	128.76	120.60
9	W	98	VAL	C-N-CA	5.33	128.76	120.60
28	S	76	PRO	CA-C-N	5.33	127.42	120.28
28	S	76	PRO	C-N-CA	5.33	127.42	120.28
34	AA	34	A	O5'-C5'-C4'	-5.33	103.51	111.50
32	X	47	ARG	NE-CZ-NH1	-5.33	116.17	121.50
43	AN	23	ARG	CA-C-N	5.33	128.79	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	AN	23	ARG	C-N-CA	5.33	128.79	120.75
23	J	73	VAL	N-CA-C	5.32	115.53	110.53
26	P	37	PHE	CA-C-N	5.32	127.94	120.28
26	P	37	PHE	C-N-CA	5.32	127.94	120.28
73	AU	21	ARG	NE-CZ-NH1	-5.32	116.18	121.50
34	AA	3711	U	P-O3'-C3'	5.32	128.18	120.20
34	AA	2746	U	P-O3'-C3'	5.32	128.18	120.20
34	AA	2590	U	C2'-C3'-O3'	5.32	117.47	109.50
34	AA	2959	G	P-O5'-C5'	-5.31	112.93	120.90
38	A1	106	ASN	CA-CB-CG	-5.31	107.29	112.60
20	B	26	LYS	N-CA-C	5.30	117.56	110.35
34	AA	773	A	C2'-C3'-O3'	5.30	117.45	109.50
73	AU	179	PRO	N-CA-C	5.30	119.56	111.34
55	AJ	76	ARG	NE-CZ-NH2	5.30	123.97	119.20
69	AD	16	PHE	CA-CB-CG	-5.30	108.50	113.80
28	S	79	PHE	CA-CB-CG	-5.30	108.50	113.80
34	AA	3169	C	C5'-C4'-C3'	-5.30	108.05	116.00
34	AA	3435	A	C4'-C3'-C2'	-5.30	97.30	102.60
34	AA	913	U	P-O5'-C5'	5.30	128.84	120.90
59	AS	55	PRO	CA-C-N	5.30	127.64	120.38
59	AS	55	PRO	C-N-CA	5.30	127.64	120.38
1	A	1413	U	C2'-C3'-O3'	5.29	121.64	113.70
16	3	5	ARG	CA-C-N	5.29	127.63	120.38
16	3	5	ARG	C-N-CA	5.29	127.63	120.38
1	A	1198	U	C1'-O4'-C4'	-5.29	104.41	109.70
12	Y	99	ARG	NE-CZ-NH2	5.29	123.96	119.20
34	AA	3414	G	P-O3'-C3'	5.29	128.14	120.20
10	R	55	LYS	CA-C-N	5.29	127.70	120.35
10	R	55	LYS	C-N-CA	5.29	127.70	120.35
75	AV	84	ARG	NE-CZ-NH1	-5.29	116.21	121.50
1	A	45	U	C1'-O4'-C4'	-5.28	104.42	109.70
7	K	120	HIS	N-CA-CB	5.28	119.41	110.49
34	AA	3526	U	C1'-O4'-C4'	-5.28	104.42	109.70
34	AA	1781	A	C5'-C4'-C3'	-5.27	108.09	116.00
60	AO	24	LYS	CA-C-N	5.27	131.61	121.54
60	AO	24	LYS	C-N-CA	5.27	131.61	121.54
37	AL	76	PHE	N-CA-C	5.27	117.71	111.33
34	AA	1026	G	O4'-C1'-C2'	-5.27	100.53	105.80
34	AA	967	A	P-O5'-C5'	5.27	128.80	120.90
34	AA	1539	U	C2'-C3'-O3'	5.27	117.40	109.50
34	AA	2693	G	P-O5'-C5'	5.27	128.80	120.90
34	AA	3195	C	O4'-C1'-N1	5.27	116.10	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AA	1205	U	C2'-C3'-O3'	5.26	117.39	109.50
38	A1	46	ILE	N-CA-CB	5.26	118.30	111.67
74	AH	110	ARG	NE-CZ-NH1	-5.25	116.25	121.50
34	AA	2465	G	P-O5'-C5'	5.25	128.77	120.90
3	D	98	CYS	CA-C-N	5.25	127.62	120.54
3	D	98	CYS	C-N-CA	5.25	127.62	120.54
34	AA	659	U	C5'-C4'-C3'	-5.25	108.13	116.00
34	AA	2807	U	C5'-C4'-C3'	5.25	123.87	116.00
1	A	2069	G	P-O5'-C5'	5.24	128.76	120.90
13	Z	59	ARG	CA-C-N	5.24	127.31	120.28
13	Z	59	ARG	C-N-CA	5.24	127.31	120.28
34	AA	525	U	P-O5'-C5'	5.24	128.76	120.90
1	A	431	A	P-O5'-C5'	5.24	128.76	120.90
1	A	1003	C	P-O3'-C3'	-5.24	112.34	120.20
35	AC	57	A	C5'-C4'-O4'	5.24	117.66	109.80
34	AA	2095	U	C4'-C3'-C2'	-5.24	97.36	102.60
35	AC	74	A	C5'-C4'-C3'	-5.24	108.14	116.00
3	D	28	ILE	N-CA-C	5.24	115.45	110.53
18	5	61	ARG	CA-C-N	5.24	128.20	120.82
18	5	61	ARG	C-N-CA	5.24	128.20	120.82
34	AA	794	C	P-O5'-C5'	5.24	128.76	120.90
34	AA	644	G	C5'-C4'-C3'	-5.24	107.35	115.20
26	P	146	ARG	NE-CZ-NH2	5.23	123.91	119.20
30	U	55	ARG	NE-CZ-NH2	5.23	123.91	119.20
68	A5	173	ARG	NE-CZ-NH1	-5.23	116.27	121.50
26	P	58	GLY	CA-C-N	5.22	126.67	120.14
26	P	58	GLY	C-N-CA	5.22	126.67	120.14
69	AD	242	ARG	NE-CZ-NH1	-5.22	116.28	121.50
34	AA	3476	A	P-O3'-C3'	5.22	128.03	120.20
1	A	1193	A	C2'-C3'-O3'	5.22	117.33	109.50
30	U	143	SER	N-CA-C	5.22	116.97	111.28
33	C	101	ARG	NE-CZ-NH2	5.22	123.90	119.20
33	C	167	LYS	CA-C-N	5.22	127.22	120.44
33	C	167	LYS	C-N-CA	5.22	127.22	120.44
34	AA	1805	U	C2'-C3'-O3'	5.22	121.53	113.70
43	AN	79	GLU	N-CA-C	5.21	117.79	110.23
59	AS	105	THR	N-CA-CB	5.21	117.70	109.83
77	AX	117	ARG	NE-CZ-NH2	5.21	123.89	119.20
38	A1	64	LYS	CA-C-N	5.21	127.22	120.44
38	A1	64	LYS	C-N-CA	5.21	127.22	120.44
5	G	250	SER	N-CA-C	5.21	116.26	109.64
8	M	125	CYS	N-CA-C	5.21	117.79	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7	7	G	C2'-C3'-O3'	5.21	117.31	109.50
61	AQ	24	ARG	NE-CZ-NH2	5.21	123.89	119.20
74	AH	123	ARG	NE-CZ-NH2	5.20	123.88	119.20
76	Ag	39	ARG	NE-CZ-NH2	5.20	123.88	119.20
34	AA	3767	U	C4'-C3'-C2'	-5.20	97.40	102.60
7	K	112	ASP	CA-C-N	5.20	127.25	120.28
7	K	112	ASP	C-N-CA	5.20	127.25	120.28
60	AO	82	LEU	CA-C-N	5.20	125.19	119.89
60	AO	82	LEU	C-N-CA	5.20	125.19	119.89
34	AA	2960	G	C5'-C4'-O4'	5.19	117.59	109.80
59	AS	145	ARG	NE-CZ-NH2	5.19	123.87	119.20
74	AH	39	ARG	NE-CZ-NH2	5.19	123.87	119.20
72	AG	84	LEU	N-CA-C	5.19	117.61	111.33
34	AA	2004	U	O4'-C1'-N1	5.19	116.28	108.50
60	AO	22	VAL	CA-C-N	5.19	125.85	119.99
60	AO	22	VAL	C-N-CA	5.19	125.85	119.99
34	AA	2500	A	P-O3'-C3'	5.19	127.98	120.20
1	A	789	U	C2'-C3'-O3'	5.18	121.48	113.70
1	A	1853	A	C2'-C3'-O3'	5.18	117.28	109.50
34	AA	453	A	C5'-C4'-C3'	5.18	123.78	116.00
71	AF	193	LYS	CA-C-N	5.18	125.85	119.99
71	AF	193	LYS	C-N-CA	5.18	125.85	119.99
34	AA	2887	U	P-O5'-C5'	5.18	128.67	120.90
39	A2	31	PHE	CA-CB-CG	-5.18	108.62	113.80
74	AH	110	ARG	NE-CZ-NH2	5.18	123.86	119.20
70	AE	253	HIS	CA-CB-CG	-5.18	108.62	113.80
78	A0	37	PHE	CA-CB-CG	-5.18	108.62	113.80
68	A5	160	ARG	NE-CZ-NH2	5.18	123.86	119.20
8	M	38	ASP	N-CA-CB	-5.18	102.25	110.22
50	Af	34	CYS	N-CA-C	5.18	119.22	113.01
22	H	51	ARG	NE-CZ-NH2	5.17	123.86	119.20
34	AA	101	C	O4'-C1'-N1	5.17	116.26	108.50
34	AA	803	A	P-O3'-C3'	5.17	127.96	120.20
34	AA	108	C	P-O5'-C5'	5.17	128.66	120.90
34	AA	702	U	O4'-C1'-N1	5.17	116.25	108.50
68	A5	130	LYS	N-CA-C	-5.16	105.81	112.68
44	A8	63	THR	CA-C-N	5.16	131.40	121.54
44	A8	63	THR	C-N-CA	5.16	131.40	121.54
70	AE	8	ARG	CA-C-N	5.16	125.17	119.90
70	AE	8	ARG	C-N-CA	5.16	125.17	119.90
77	AX	112	LYS	CA-C-N	5.16	127.15	120.44
77	AX	112	LYS	C-N-CA	5.16	127.15	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AA	2738	U	P-O3'-C3'	5.16	127.94	120.20
51	AP	83	LYS	N-CA-C	5.16	117.49	110.01
23	J	40	LYS	N-CA-C	5.16	118.67	112.38
34	AA	37	U	O3'-P-O5'	-5.16	96.27	104.00
1	A	161	U	C5'-C4'-O4'	5.15	117.53	109.80
25	N	105	ILE	N-CA-C	5.15	117.92	109.78
54	AI	172	GLU	N-CA-C	5.15	116.90	111.28
21	F	126	VAL	N-CA-CB	5.15	116.14	110.53
24	L	52	ASN	CA-CB-CG	-5.15	107.45	112.60
26	P	66	ARG	NE-CZ-NH1	-5.15	116.35	121.50
34	AA	2883	U	C2'-C3'-O3'	5.15	117.23	109.50
51	AP	140	HIS	CA-C-N	5.15	127.18	120.28
51	AP	140	HIS	C-N-CA	5.15	127.18	120.28
34	AA	382	A	C2'-C3'-O3'	5.15	117.22	109.50
68	A5	109	ARG	NE-CZ-NH2	5.15	123.83	119.20
54	AI	94	VAL	CA-C-N	5.15	125.14	119.89
54	AI	94	VAL	C-N-CA	5.15	125.14	119.89
35	AC	135	G	P-O5'-C5'	-5.14	113.18	120.90
5	G	47	LEU	CA-C-N	5.14	125.65	119.94
5	G	47	LEU	C-N-CA	5.14	125.65	119.94
33	C	129	ASP	CA-C-N	5.14	127.43	120.38
33	C	129	ASP	C-N-CA	5.14	127.43	120.38
34	AA	2125	A	O4'-C1'-N9	5.14	115.91	108.20
70	AE	218	THR	N-CA-C	5.14	117.32	110.53
34	AA	547	C	O5'-C5'-C4'	5.14	119.21	111.50
34	AA	766	U	C2'-C3'-O3'	5.14	117.21	109.50
5	G	110	PHE	CA-CB-CG	-5.14	108.66	113.80
55	AJ	103	LYS	N-CA-C	5.13	116.56	111.07
59	AS	173	PHE	CA-CB-CG	-5.13	108.67	113.80
69	AD	216	HIS	CA-CB-CG	-5.13	108.67	113.80
34	AA	1501	A	O3'-P-O5'	-5.13	96.30	104.00
44	A8	26	MET	CA-C-N	5.13	127.87	120.38
44	A8	26	MET	C-N-CA	5.13	127.87	120.38
34	AA	913	U	P-O3'-C3'	-5.13	112.50	120.20
34	AA	2146	A	C2'-C3'-O3'	5.13	117.19	109.50
62	AR	147	PHE	CA-CB-CG	-5.13	108.67	113.80
34	AA	714	C	C4'-C3'-C2'	-5.13	97.47	102.60
35	AC	56	A	P-O3'-C3'	-5.13	112.51	120.20
44	A8	98	HIS	N-CA-C	5.12	117.26	111.11
34	AA	3293	A	C5'-C4'-C3'	5.12	123.68	116.00
51	AP	187	PRO	CA-C-N	5.12	131.32	121.54
51	AP	187	PRO	C-N-CA	5.12	131.32	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	A5	234	PHE	CA-C-N	5.12	127.65	120.28
68	A5	234	PHE	C-N-CA	5.12	127.65	120.28
1	A	1430	G	P-O3'-C3'	5.12	127.88	120.20
12	Y	89	LEU	N-CA-C	5.12	116.55	111.07
30	U	55	ARG	NE-CZ-NH1	-5.12	116.38	121.50
34	AA	3158	U	C2'-C3'-O3'	5.12	117.18	109.50
34	AA	1243	G	C2'-C3'-O3'	5.12	117.17	109.50
34	AA	3740	A	C2'-C3'-O3'	5.12	117.17	109.50
37	AL	136	ILE	N-CA-C	5.12	116.52	109.46
21	F	113	ARG	N-CA-C	5.11	117.97	110.30
34	AA	1539	U	C1'-O4'-C4'	-5.11	104.59	109.70
1	A	525	G	C2'-C3'-O3'	5.11	121.36	113.70
34	AA	2727	U	O4'-C1'-N1	5.11	115.86	108.20
16	3	57	SER	N-CA-C	5.11	117.30	110.35
68	A5	245	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	A	2	A	C2'-C3'-O3'	5.11	117.16	109.50
38	A1	17	ARG	NE-CZ-NH2	5.11	123.80	119.20
63	AW	137	ASN	CA-CB-CG	-5.11	107.50	112.60
68	A5	231	ARG	NE-CZ-NH2	5.11	123.80	119.20
34	AA	337	A	P-O3'-C3'	5.10	127.86	120.20
21	F	254	ASN	CA-C-N	5.10	127.43	120.54
21	F	254	ASN	C-N-CA	5.10	127.43	120.54
56	Ac	82	THR	N-CA-CB	5.10	117.47	109.97
1	A	143	A	C4'-C3'-C2'	-5.10	97.50	102.60
22	H	180	THR	CA-C-N	5.10	127.12	120.28
22	H	180	THR	C-N-CA	5.10	127.12	120.28
34	AA	1197	U	P-O3'-C3'	5.10	127.85	120.20
1	A	1819	U	C2'-C3'-O3'	5.10	117.14	109.50
71	AF	182	ARG	NE-CZ-NH2	-5.10	114.61	119.20
69	AD	159	ASP	CA-C-N	5.09	127.11	120.28
69	AD	159	ASP	C-N-CA	5.09	127.11	120.28
34	AA	33	G	P-O3'-C3'	-5.09	112.56	120.20
48	Ad	55	ALA	N-CA-C	5.09	116.83	111.28
23	J	132	SER	N-CA-C	5.09	121.06	109.81
34	AA	65	A	O4'-C1'-C2'	5.09	110.89	105.80
34	AA	40	A	C2'-C3'-O3'	5.09	117.13	109.50
1	A	343	G	C5'-C4'-C3'	-5.09	107.57	115.20
40	A4	10	HIS	N-CA-C	5.09	117.47	110.35
69	AD	63	PHE	CA-CB-CG	-5.09	108.71	113.80
1	A	14	U	C5'-C4'-C3'	-5.08	108.38	116.00
12	Y	147	LEU	N-CA-C	5.08	117.60	110.23
23	J	110	PHE	CA-CB-CG	-5.08	108.72	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	AT	174	LEU	CA-C-N	5.08	127.09	120.28
65	AT	174	LEU	C-N-CA	5.08	127.09	120.28
69	AD	242	ARG	NE-CZ-NH2	5.08	123.78	119.20
23	J	28	GLU	N-CA-C	5.08	116.51	111.07
54	AI	182	ILE	CA-C-N	5.08	127.04	120.44
54	AI	182	ILE	C-N-CA	5.08	127.04	120.44
55	AJ	120	SER	CA-C-N	5.08	127.39	120.54
55	AJ	120	SER	C-N-CA	5.08	127.39	120.54
1	A	1092	A	C2'-C3'-O3'	5.08	117.11	109.50
34	AA	2515	A	O3'-P-O5'	-5.08	96.39	104.00
57	AK	100	LYS	N-CA-C	5.08	117.47	111.33
1	A	577	A	C4'-C3'-C2'	-5.07	97.53	102.60
34	AA	1964	G	C2'-C3'-O3'	5.07	117.11	109.50
34	AA	3018	A	O4'-C1'-N9	5.07	116.11	108.50
34	AA	893	U	C2'-C3'-O3'	5.07	117.11	109.50
33	C	11	GLU	CA-C-N	5.07	127.07	120.28
33	C	11	GLU	C-N-CA	5.07	127.07	120.28
51	AP	149	ILE	CA-C-N	5.07	131.22	121.54
51	AP	149	ILE	C-N-CA	5.07	131.22	121.54
70	AE	241	ARG	NE-CZ-NH2	5.07	123.76	119.20
34	AA	3662	U	C2'-C3'-O3'	5.07	117.10	109.50
1	A	25	C	C2'-C3'-O3'	5.07	117.10	109.50
34	AA	3361	U	P-O3'-C3'	5.06	127.80	120.20
32	X	37	PHE	CA-C-N	5.06	128.26	120.82
32	X	37	PHE	C-N-CA	5.06	128.26	120.82
10	R	114	ALA	N-CA-C	5.06	117.23	110.35
35	AC	63	A	C4'-C3'-O3'	5.06	116.99	109.40
34	AA	1262	G	P-O5'-C5'	-5.06	113.31	120.90
21	F	186	GLY	O-C-N	-5.05	118.77	122.71
1	A	983	G	C2'-C3'-O3'	5.05	117.08	109.50
14	1	91	ARG	NE-CZ-NH1	-5.05	116.45	121.50
34	AA	2693	G	O4'-C1'-C2'	5.05	110.85	105.80
34	AA	536	A	C2'-C3'-O3'	5.05	117.08	109.50
41	A6	30	ARG	N-CA-C	5.05	117.17	111.11
1	A	1093	U	O5'-C5'-C4'	5.05	119.07	111.50
1	A	1645	C	P-O3'-C3'	-5.05	112.63	120.20
54	AI	194	ILE	CA-C-N	5.04	127.04	120.28
54	AI	194	ILE	C-N-CA	5.04	127.04	120.28
67	A3	87	THR	N-CA-CB	5.04	117.45	110.04
1	A	983	G	C5'-C4'-O4'	5.04	116.66	109.10
24	L	188	ARG	CA-C-N	5.04	125.07	119.32
24	L	188	ARG	C-N-CA	5.04	125.07	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	AK	165	ALA	CA-C-N	5.04	126.99	120.44
57	AK	165	ALA	C-N-CA	5.04	126.99	120.44
59	AS	177	ARG	NE-CZ-NH1	-5.04	116.46	121.50
34	AA	3754	A	C5'-C4'-C3'	5.04	123.56	116.00
5	G	229	ALA	CA-C-N	5.04	127.03	120.28
5	G	229	ALA	C-N-CA	5.04	127.03	120.28
34	AA	580	A	C5'-C4'-C3'	5.04	123.55	116.00
35	AC	35	A	C2'-C3'-O3'	5.04	121.25	113.70
34	AA	2147	A	P-O3'-C3'	-5.03	112.65	120.20
41	A6	100	ASP	CA-CB-CG	-5.03	107.57	112.60
34	AA	1534	U	C2'-C3'-O3'	5.03	117.05	109.50
51	AP	38	ARG	NE-CZ-NH2	5.03	123.73	119.20
9	W	80	ARG	CA-C-N	5.03	127.02	120.28
9	W	80	ARG	C-N-CA	5.03	127.02	120.28
55	AJ	91	PRO	CA-C-N	5.03	125.05	119.32
55	AJ	91	PRO	C-N-CA	5.03	125.05	119.32
62	AR	94	ASN	CA-C-N	5.03	127.33	120.54
62	AR	94	ASN	C-N-CA	5.03	127.33	120.54
68	A5	213	ASN	CA-C-N	5.03	127.02	120.28
68	A5	213	ASN	C-N-CA	5.03	127.02	120.28
60	AO	93	ASN	CA-CB-CG	-5.03	107.57	112.60
34	AA	345	G	C2'-C3'-O3'	5.02	117.03	109.50
26	P	141	ARG	NE-CZ-NH2	5.02	123.72	119.20
31	V	129	GLY	CA-C-N	5.02	126.97	120.44
31	V	129	GLY	C-N-CA	5.02	126.97	120.44
34	AA	2169	A	C5'-C4'-C3'	5.02	123.53	116.00
71	AF	200	LYS	N-CA-C	5.02	116.56	111.14
54	AI	68	MET	N-CA-C	5.02	116.77	110.24
24	L	16	GLY	N-CA-C	5.02	117.85	112.33
28	S	58	ALA	N-CA-C	5.02	117.40	111.33
2	7	68	C	P-O5'-C5'	5.01	128.42	120.90
69	AD	238	ILE	N-CA-C	5.01	115.57	109.30
63	AW	127	ARG	NH1-CZ-NH2	-5.01	112.78	119.30
1	A	406	A	C2'-C3'-O3'	5.01	117.02	109.50
34	AA	1459	U	C4'-C3'-O3'	5.01	116.92	109.40
54	AI	150	LEU	N-CA-C	5.01	116.43	111.07
33	C	79	ARG	CA-C-N	5.01	124.45	119.24
33	C	79	ARG	C-N-CA	5.01	124.45	119.24
57	AK	84	ARG	CA-C-N	5.01	126.44	120.13
57	AK	84	ARG	C-N-CA	5.01	126.44	120.13
64	AY	186	LYS	N-CA-C	5.01	116.43	111.07
34	AA	2092	G	O3'-P-O5'	-5.00	96.50	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AA	2670	G	C2'-C3'-O3'	5.00	117.01	109.50
34	AA	1422	A	C2'-C3'-O3'	5.00	117.00	109.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	B	225	ILE	CB
34	AA	3018	A	C3'

All (668) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	1	106	ARG	Sidechain
14	1	12	TYR	Sidechain
14	1	90	TYR	Sidechain
15	2	76	ARG	Sidechain
16	3	28	ARG	Sidechain
16	3	46	ASP	Peptide
16	3	89	ARG	Sidechain
18	5	19	ARG	Sidechain
18	5	49	ARG	Sidechain
19	6	37	ARG	Sidechain
19	6	40	TYR	Sidechain
19	6	43	ARG	Sidechain
2	7	11	A	Sidechain
2	7	22	G	Sidechain
2	7	30	G	Sidechain
2	7	4	G	Sidechain
2	7	5	G	Sidechain
2	7	54	U	Sidechain
2	7	74	C	Sidechain
2	7	75	C	Sidechain
1	A	1008	A	Sidechain
1	A	1022	A	Sidechain
1	A	1026	A	Sidechain
1	A	1041	G	Sidechain
1	A	1055	G	Sidechain
1	A	1060	G	Sidechain
1	A	1070	A	Sidechain
1	A	1081	U	Sidechain
1	A	1107	U	Sidechain
1	A	1175	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1195	G	Sidechain
1	A	1208	G	Sidechain
1	A	1209	G	Sidechain
1	A	1220	C	Sidechain
1	A	1221	G	Sidechain
1	A	1240	A	Sidechain
1	A	1241	A	Sidechain
1	A	1242	G	Sidechain
1	A	1251	G	Sidechain
1	A	1264	A	Sidechain
1	A	1273	G	Sidechain
1	A	1283	U	Sidechain
1	A	1289	G	Sidechain
1	A	129	U	Sidechain
1	A	1290	A	Sidechain
1	A	1307	U	Sidechain
1	A	1364	G	Sidechain
1	A	1402	A	Sidechain
1	A	1407	U	Sidechain
1	A	1417	U	Sidechain
1	A	1423	A	Sidechain
1	A	143	A	Sidechain
1	A	1430	G	Sidechain
1	A	1436	U	Sidechain
1	A	1442	U	Sidechain
1	A	152	G	Sidechain
1	A	1635	C	Sidechain
1	A	1636	A	Sidechain
1	A	1637	U	Sidechain
1	A	1646	U	Sidechain
1	A	1655	G	Sidechain
1	A	166	A	Sidechain
1	A	1660	U	Sidechain
1	A	1665	G	Sidechain
1	A	1730	A	Sidechain
1	A	1794	C	Sidechain
1	A	1798	G	Sidechain
1	A	1807	A	Sidechain
1	A	1809	G	Sidechain
1	A	1819	U	Sidechain
1	A	182	U	Sidechain
1	A	1823	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1832	U	Sidechain
1	A	1834	A	Sidechain
1	A	1839	G	Sidechain
1	A	1845	U	Sidechain
1	A	1849	U	Sidechain
1	A	1850	G	Sidechain
1	A	1865	G	Sidechain
1	A	1879	U	Sidechain
1	A	1880	A	Sidechain
1	A	1881	G	Sidechain
1	A	1896	C	Sidechain
1	A	1914	U	Sidechain
1	A	1939	G	Sidechain
1	A	1940	U	Sidechain
1	A	1953	U	Sidechain
1	A	1955	G	Sidechain
1	A	1972	G	Sidechain
1	A	2028	U	Sidechain
1	A	2032	U	Sidechain
1	A	2062	U	Sidechain
1	A	2067	U	Sidechain
1	A	2069	G	Sidechain
1	A	2072	G	Sidechain
1	A	247	G	Sidechain
1	A	263	A	Sidechain
1	A	267	A	Sidechain
1	A	325	U	Sidechain
1	A	343	G	Sidechain
1	A	358	G	Sidechain
1	A	375	U	Sidechain
1	A	39	A	Sidechain
1	A	393	A	Sidechain
1	A	402	G	Sidechain
1	A	406	A	Sidechain
1	A	424	G	Sidechain
1	A	429	G	Sidechain
1	A	44	U	Sidechain
1	A	440	G	Sidechain
1	A	441	U	Sidechain
1	A	453	U	Sidechain
1	A	482	U	Sidechain
1	A	486	A	Sidechain

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Mol	Chain	Res	Type	Group
1	A	493	G	Sidechain
1	A	516	G	Sidechain
1	A	522	G	Sidechain
1	A	546	G	Sidechain
1	A	573	C	Sidechain
1	A	579	C	Sidechain
1	A	598	A	Sidechain
1	A	615	U	Sidechain
1	A	625	U	Sidechain
1	A	626	A	Sidechain
1	A	627	A	Sidechain
1	A	641	G	Sidechain
1	A	646	U	Sidechain
1	A	652	A	Sidechain
1	A	750	U	Sidechain
1	A	751	U	Sidechain
1	A	752	U	Sidechain
1	A	790	U	Sidechain
1	A	802	A	Sidechain
1	A	803	G	Sidechain
1	A	831	U	Sidechain
1	A	834	A	Sidechain
1	A	838	U	Sidechain
1	A	84	A	Sidechain
1	A	877	U	Sidechain
1	A	879	A	Sidechain
1	A	894	U	Sidechain
1	A	895	U	Sidechain
1	A	907	C	Sidechain
1	A	920	A	Sidechain
1	A	942	U	Sidechain
1	A	954	G	Sidechain
1	A	987	U	Sidechain
78	A0	28	TYR	Sidechain
78	A0	31	ARG	Sidechain
78	A0	57	ARG	Sidechain
78	A0	63	ARG	Sidechain
38	A1	65	ARG	Sidechain
67	A3	105	ARG	Sidechain
40	A4	7	HIS	Peptide
68	A5	109	ARG	Sidechain
68	A5	169	ARG	Sidechain

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Mol	Chain	Res	Type	Group
68	A5	224	ARG	Sidechain
68	A5	54	ARG	Sidechain
68	A5	68	ARG	Sidechain
41	A6	56	ARG	Sidechain
42	A7	45	ARG	Sidechain
42	A7	75	PRO	Peptide
42	A7	78	ARG	Sidechain
44	A8	125	ARG	Sidechain
44	A8	43	ARG	Sidechain
44	A8	44	ARG	Peptide
44	A8	74	TYR	Sidechain
45	A9	130	ARG	Sidechain
45	A9	39	ARG	Sidechain
34	AA	10	G	Sidechain
34	AA	1001	A	Sidechain
34	AA	1023	U	Sidechain
34	AA	1044	A	Sidechain
34	AA	1045	A	Sidechain
34	AA	1056	G	Sidechain
34	AA	1073	G	Sidechain
34	AA	1078	C	Sidechain
34	AA	109	A	Sidechain
34	AA	1096	G	Sidechain
34	AA	1103	A	Sidechain
34	AA	1109	U	Sidechain
34	AA	1110	U	Sidechain
34	AA	1115	G	Sidechain
34	AA	1116	G	Sidechain
34	AA	1157	U	Sidechain
34	AA	119	G	Sidechain
34	AA	1201	U	Sidechain
34	AA	1213	U	Sidechain
34	AA	1224	A	Sidechain
34	AA	1232	U	Sidechain
34	AA	1236	U	Sidechain
34	AA	1243	G	Sidechain
34	AA	1255	G	Sidechain
34	AA	1256	U	Sidechain
34	AA	1272	U	Sidechain
34	AA	130	G	Sidechain
34	AA	1300	G	Sidechain
34	AA	1324	U	Sidechain

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Mol	Chain	Res	Type	Group
34	AA	1330	A	Sidechain
34	AA	136	U	Sidechain
34	AA	14	U	Sidechain
34	AA	1423	G	Sidechain
34	AA	1429	A	Sidechain
34	AA	1432	A	Sidechain
34	AA	1447	G	Sidechain
34	AA	1456	C	Sidechain
34	AA	147	C	Sidechain
34	AA	148	G	Sidechain
34	AA	1499	U	Sidechain
34	AA	1502	G	Sidechain
34	AA	1516	G	Sidechain
34	AA	1517	U	Sidechain
34	AA	153	A	Sidechain
34	AA	1534	U	Sidechain
34	AA	1536	U	Sidechain
34	AA	1538	U	Sidechain
34	AA	1563	U	Sidechain
34	AA	157	G	Sidechain
34	AA	1572	U	Sidechain
34	AA	1596	G	Sidechain
34	AA	1601	A	Sidechain
34	AA	1613	G	Sidechain
34	AA	1619	U	Sidechain
34	AA	1628	U	Sidechain
34	AA	1629	G	Sidechain
34	AA	1631	A	Sidechain
34	AA	1643	U	Sidechain
34	AA	1644	U	Sidechain
34	AA	1676	C	Sidechain
34	AA	1677	G	Sidechain
34	AA	1679	U	Sidechain
34	AA	1683	A	Sidechain
34	AA	1695	A	Sidechain
34	AA	1701	G	Sidechain
34	AA	1702	U	Sidechain
34	AA	1703	U	Sidechain
34	AA	1713	G	Sidechain
34	AA	1725	U	Sidechain
34	AA	1740	A	Sidechain
34	AA	1745	G	Sidechain

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Mol	Chain	Res	Type	Group
34	AA	1749	U	Sidechain
34	AA	1750	U	Sidechain
34	AA	1763	G	Sidechain
34	AA	1772	G	Sidechain
34	AA	1780	G	Sidechain
34	AA	1785	U	Sidechain
34	AA	1811	A	Sidechain
34	AA	1820	U	Sidechain
34	AA	1844	G	Sidechain
34	AA	1849	U	Sidechain
34	AA	1851	A	Sidechain
34	AA	1853	C	Sidechain
34	AA	1855	U	Sidechain
34	AA	1870	G	Sidechain
34	AA	1901	A	Sidechain
34	AA	1902	A	Sidechain
34	AA	191	A	Sidechain
34	AA	1997	G	Sidechain
34	AA	2004	U	Sidechain
34	AA	201	G	Sidechain
34	AA	2011	U	Sidechain
34	AA	2018	G	Sidechain
34	AA	205	G	Sidechain
34	AA	2084	U	Sidechain
34	AA	2102	A	Sidechain
34	AA	2105	A	Sidechain
34	AA	2107	C	Sidechain
34	AA	2120	U	Sidechain
34	AA	2125	A	Sidechain
34	AA	2142	G	Sidechain
34	AA	2167	G	Sidechain
34	AA	2170	G	Sidechain
34	AA	2176	A	Sidechain
34	AA	2180	U	Sidechain
34	AA	2193	U	Sidechain
34	AA	2215	G	Sidechain
34	AA	2219	A	Sidechain
34	AA	2220	U	Sidechain
34	AA	240	U	Sidechain
34	AA	2403	G	Sidechain
34	AA	2412	A	Sidechain
34	AA	2414	G	Sidechain

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Mol	Chain	Res	Type	Group
34	AA	2429	U	Sidechain
34	AA	2450	G	Sidechain
34	AA	2452	A	Sidechain
34	AA	2455	G	Sidechain
34	AA	2460	A	Sidechain
34	AA	2480	G	Sidechain
34	AA	2498	U	Sidechain
34	AA	25	A	Sidechain
34	AA	2500	A	Sidechain
34	AA	2502	U	Sidechain
34	AA	2515	A	Sidechain
34	AA	2517	A	Sidechain
34	AA	2549	A	Sidechain
34	AA	2566	G	Sidechain
34	AA	257	U	Sidechain
34	AA	2577	C	Sidechain
34	AA	2589	A	Sidechain
34	AA	2590	U	Sidechain
34	AA	265	U	Sidechain
34	AA	2657	G	Sidechain
34	AA	2666	A	Sidechain
34	AA	2669	G	Sidechain
34	AA	2693	G	Sidechain
34	AA	2696	G	Sidechain
34	AA	2709	U	Sidechain
34	AA	2710	U	Sidechain
34	AA	2711	U	Sidechain
34	AA	2728	G	Sidechain
34	AA	273	C	Sidechain
34	AA	2739	U	Sidechain
34	AA	2802	U	Sidechain
34	AA	2803	A	Sidechain
34	AA	2808	U	Sidechain
34	AA	2809	A	Sidechain
34	AA	2823	U	Sidechain
34	AA	2838	A	Sidechain
34	AA	288	G	Sidechain
34	AA	2915	U	Sidechain
34	AA	2926	A	Sidechain
34	AA	2948	A	Sidechain
34	AA	2957	G	Sidechain
34	AA	2958	G	Sidechain

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Mol	Chain	Res	Type	Group
34	AA	2959	G	Sidechain
34	AA	297	G	Sidechain
34	AA	2980	U	Sidechain
34	AA	3017	A	Sidechain
34	AA	3018	A	Sidechain
34	AA	3033	A	Sidechain
34	AA	3034	A	Sidechain
34	AA	3035	A	Sidechain
34	AA	304	U	Sidechain
34	AA	3062	U	Sidechain
34	AA	3063	U	Sidechain
34	AA	3065	C	Sidechain
34	AA	3066	A	Sidechain
34	AA	308	U	Sidechain
34	AA	3084	G	Sidechain
34	AA	3121	G	Sidechain
34	AA	3141	G	Sidechain
34	AA	3166	U	Sidechain
34	AA	3186	U	Sidechain
34	AA	3195	C	Sidechain
34	AA	3203	C	Sidechain
34	AA	3209	G	Sidechain
34	AA	3210	A	Sidechain
34	AA	3220	U	Sidechain
34	AA	3222	G	Sidechain
34	AA	3233	G	Sidechain
34	AA	3241	U	Sidechain
34	AA	325	A	Sidechain
34	AA	3253	G	Sidechain
34	AA	3268	A	Sidechain
34	AA	3269	A	Sidechain
34	AA	3271	G	Sidechain
34	AA	3300	A	Sidechain
34	AA	331	A	Sidechain
34	AA	3313	U	Sidechain
34	AA	332	A	Sidechain
34	AA	3348	U	Sidechain
34	AA	3355	U	Sidechain
34	AA	3362	A	Sidechain
34	AA	3363	U	Sidechain
34	AA	3365	U	Sidechain
34	AA	3374	U	Sidechain

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Mol	Chain	Res	Type	Group
34	AA	3391	G	Sidechain
34	AA	3412	G	Sidechain
34	AA	3415	A	Sidechain
34	AA	3436	U	Sidechain
34	AA	344	A	Sidechain
34	AA	3449	U	Sidechain
34	AA	346	A	Sidechain
34	AA	3463	G	Sidechain
34	AA	348	C	Sidechain
34	AA	3483	U	Sidechain
34	AA	3484	U	Sidechain
34	AA	349	G	Sidechain
34	AA	3499	C	Sidechain
34	AA	3503	U	Sidechain
34	AA	3505	U	Sidechain
34	AA	352	A	Sidechain
34	AA	3545	U	Sidechain
34	AA	3547	U	Sidechain
34	AA	3570	U	Sidechain
34	AA	3578	A	Sidechain
34	AA	3579	A	Sidechain
34	AA	36	U	Sidechain
34	AA	3629	U	Sidechain
34	AA	3639	G	Sidechain
34	AA	3646	G	Sidechain
34	AA	3658	G	Sidechain
34	AA	3660	A	Sidechain
34	AA	3683	G	Sidechain
34	AA	3706	U	Sidechain
34	AA	3707	U	Sidechain
34	AA	3725	G	Sidechain
34	AA	3739	A	Sidechain
34	AA	3748	U	Sidechain
34	AA	3749	U	Sidechain
34	AA	3761	G	Sidechain
34	AA	3776	U	Sidechain
34	AA	3783	G	Sidechain
34	AA	379	G	Sidechain
34	AA	38	U	Sidechain
34	AA	380	A	Sidechain
34	AA	39	A	Sidechain
34	AA	403	U	Sidechain

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Mol	Chain	Res	Type	Group
34	AA	416	G	Sidechain
34	AA	417	A	Sidechain
34	AA	440	A	Sidechain
34	AA	454	G	Sidechain
34	AA	490	U	Sidechain
34	AA	497	U	Sidechain
34	AA	498	U	Sidechain
34	AA	500	A	Sidechain
34	AA	503	A	Sidechain
34	AA	520	U	Sidechain
34	AA	525	U	Sidechain
34	AA	526	U	Sidechain
34	AA	528	A	Sidechain
34	AA	531	U	Sidechain
34	AA	579	C	Sidechain
34	AA	582	U	Sidechain
34	AA	583	U	Sidechain
34	AA	607	A	Sidechain
34	AA	643	G	Sidechain
34	AA	644	G	Sidechain
34	AA	652	A	Sidechain
34	AA	656	U	Sidechain
34	AA	666	U	Sidechain
34	AA	684	G	Sidechain
34	AA	702	U	Sidechain
34	AA	703	U	Sidechain
34	AA	704	U	Sidechain
34	AA	706	U	Sidechain
34	AA	707	U	Sidechain
34	AA	708	A	Sidechain
34	AA	71	A	Sidechain
34	AA	716	C	Sidechain
34	AA	724	A	Sidechain
34	AA	733	C	Sidechain
34	AA	739	G	Sidechain
34	AA	746	A	Sidechain
34	AA	75	U	Sidechain
34	AA	759	U	Sidechain
34	AA	76	G	Sidechain
34	AA	764	G	Sidechain
34	AA	776	A	Sidechain
34	AA	795	G	Sidechain

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Mol	Chain	Res	Type	Group
34	AA	798	U	Sidechain
34	AA	825	G	Sidechain
34	AA	828	G	Sidechain
34	AA	86	G	Sidechain
34	AA	910	A	Sidechain
34	AA	912	U	Sidechain
34	AA	913	U	Sidechain
34	AA	914	G	Sidechain
34	AA	916	U	Sidechain
34	AA	92	G	Sidechain
34	AA	924	G	Sidechain
34	AA	938	U	Sidechain
34	AA	939	A	Sidechain
34	AA	94	G	Sidechain
34	AA	941	G	Sidechain
34	AA	943	G	Sidechain
34	AA	954	G	Sidechain
34	AA	964	G	Sidechain
34	AA	966	A	Sidechain
34	AA	967	A	Sidechain
34	AA	976	G	Sidechain
34	AA	985	G	Sidechain
34	AA	988	G	Sidechain
36	AB	108	G	Sidechain
36	AB	109	U	Sidechain
36	AB	11	A	Sidechain
36	AB	48	G	Sidechain
36	AB	49	A	Sidechain
36	AB	50	A	Sidechain
36	AB	56	G	Sidechain
36	AB	61	G	Sidechain
36	AB	75	G	Sidechain
35	AC	18	U	Sidechain
35	AC	20	G	Sidechain
35	AC	25	C	Sidechain
35	AC	29	G	Sidechain
35	AC	3	G	Sidechain
35	AC	30	U	Sidechain
35	AC	31	U	Sidechain
35	AC	32	C	Sidechain
35	AC	38	G	Sidechain
35	AC	90	G	Sidechain

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Mol	Chain	Res	Type	Group
69	AD	242	ARG	Sidechain
70	AE	229	ARG	Sidechain
70	AE	24	ARG	Sidechain
70	AE	336	ARG	Sidechain
70	AE	4	ARG	Sidechain
70	AE	8	ARG	Sidechain
70	AE	92	TYR	Sidechain
70	AE	93	ARG	Sidechain
71	AF	109	ARG	Sidechain
71	AF	140	ARG	Sidechain
71	AF	199	ARG	Sidechain
71	AF	312	ARG	Sidechain
71	AF	33	ARG	Sidechain
71	AF	332	TYR	Sidechain
71	AF	389	ARG	Sidechain
71	AF	49	ARG	Sidechain
71	AF	86	ARG	Sidechain
71	AF	97	ARG	Sidechain
72	AG	141	ARG	Sidechain
72	AG	72	ARG	Sidechain
72	AG	92	ARG	Sidechain
54	AI	11	TYR	Sidechain
54	AI	211	ARG	Sidechain
54	AI	48	ARG	Sidechain
54	AI	87	GLY	Peptide
55	AJ	151	TYR	Sidechain
55	AJ	246	ARG	Sidechain
57	AK	132	ARG	Sidechain
57	AK	133	ARG	Sidechain
57	AK	17	ARG	Sidechain
57	AK	193	ARG	Sidechain
57	AK	48	ARG	Sidechain
57	AK	58	ARG	Sidechain
57	AK	73	ARG	Sidechain
37	AL	100	ARG	Sidechain
37	AL	190	ARG	Sidechain
37	AL	20	ARG	Sidechain
37	AL	202	ARG	Sidechain
37	AL	22	ARG	Sidechain
37	AL	99	ARG	Sidechain
58	AM	14	ARG	Sidechain
58	AM	50	ARG	Peptide,Sidechain

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Mol	Chain	Res	Type	Group
43	AN	120	ARG	Sidechain
43	AN	128	ARG	Sidechain
43	AN	23	ARG	Sidechain
43	AN	35	TYR	Sidechain
43	AN	66	ARG	Sidechain
60	AO	104	ARG	Sidechain
60	AO	59	ARG	Sidechain
60	AO	9	ARG	Sidechain
51	AP	176	ARG	Sidechain
51	AP	186	ARG	Sidechain
51	AP	38	ARG	Sidechain
51	AP	67	ARG	Sidechain
51	AP	68	ARG	Sidechain
51	AP	74	ARG	Sidechain
51	AP	96	ARG	Sidechain
61	AQ	139	ARG	Sidechain
61	AQ	154	ARG	Sidechain
61	AQ	34	TYR	Sidechain
61	AQ	38	ARG	Sidechain
61	AQ	88	ARG	Sidechain
61	AQ	90	ARG	Sidechain
62	AR	107	ARG	Sidechain
62	AR	21	ARG	Sidechain
62	AR	24	ARG	Sidechain
62	AR	85	ARG	Sidechain
59	AS	10	ARG	Sidechain
59	AS	167	ARG	Sidechain
59	AS	27	ARG	Sidechain
59	AS	51	ARG	Sidechain
59	AS	59	ARG	Sidechain
59	AS	74	HIS	Peptide
59	AS	90	ARG	Sidechain
65	AT	2	SER	Peptide
65	AT	41	ARG	Sidechain
65	AT	70	ARG	Sidechain
65	AT	87	ARG	Sidechain
73	AU	122	ARG	Sidechain
73	AU	124	ARG	Sidechain
73	AU	157	ARG	Sidechain
73	AU	171	ARG	Sidechain
73	AU	49	ARG	Sidechain
75	AV	109	ARG	Sidechain

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Mol	Chain	Res	Type	Group
75	AV	31	TYR	Sidechain
75	AV	71	ARG	Sidechain
63	AW	151	ARG	Sidechain
63	AW	34	ARG	Sidechain
63	AW	37	ARG	Sidechain
63	AW	56	ARG	Sidechain
64	AY	137	ARG	Sidechain
66	AZ	11	ARG	Sidechain
66	AZ	114	ARG	Sidechain
66	AZ	120	ARG	Sidechain
66	AZ	27	ARG	Sidechain
66	AZ	59	ARG	Sidechain
46	Aa	4	ARG	Sidechain
46	Aa	83	ARG	Sidechain
46	Aa	88	ARG	Sidechain
47	Ab	75	ARG	Sidechain
56	Ac	28	ARG	Sidechain
56	Ac	49	ARG	Sidechain
56	Ac	59	ARG	Peptide
56	Ac	66	ARG	Sidechain
48	Ad	57	ARG	Sidechain
49	Ae	12	ARG	Sidechain
49	Ae	8	ARG	Sidechain
50	Af	21	ARG	Sidechain
50	Af	41	ARG	Sidechain
76	Ag	16	ARG	Sidechain
76	Ag	35	ARG	Sidechain
52	Ah	23	ARG	Sidechain
53	Ai	33	ARG	Sidechain
20	B	136	ARG	Sidechain
20	B	165	ARG	Sidechain
20	B	55	LYS	Peptide
20	B	64	ARG	Sidechain
20	B	66	TYR	Sidechain
33	C	62	ARG	Sidechain
33	C	84	ARG	Sidechain
4	E	17	ARG	Peptide
4	E	47	TYR	Sidechain
4	E	6	ARG	Sidechain
4	E	69	ARG	Sidechain
4	E	79	ARG	Sidechain
4	E	8	TYR	Sidechain

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Mol	Chain	Res	Type	Group
4	E	95	TYR	Sidechain
21	F	145	ARG	Sidechain
21	F	191	ARG	Sidechain
21	F	240	ARG	Sidechain
5	G	63	TYR	Sidechain
22	H	177	ARG	Sidechain
22	H	186	ARG	Sidechain
6	I	136	ARG	Sidechain
6	I	195	ARG	Sidechain
23	J	162	ARG	Sidechain
23	J	39	ALA	Peptide
23	J	72	TYR	Sidechain
23	J	76	ILE	Peptide
7	K	108	TYR	Sidechain
7	K	118	ARG	Sidechain
7	K	23	ARG	Sidechain
24	L	12	ARG	Sidechain
24	L	25	ARG	Sidechain
24	L	5	ARG	Sidechain
24	L	55	TYR	Sidechain
8	M	112	ARG	Sidechain
8	M	67	ARG	Sidechain
8	M	94	TYR	Sidechain
25	N	65	ARG	Sidechain
26	P	146	ARG	Sidechain
26	P	57	THR	Peptide
26	P	66	ARG	Sidechain
27	Q	109	ARG	Sidechain
27	Q	68	TYR	Sidechain
27	Q	69	ARG	Sidechain
28	S	126	ARG	Sidechain
29	T	20	ARG	Sidechain
29	T	38	ARG	Sidechain
29	T	42	ARG	Sidechain
29	T	44	ARG	Sidechain
29	T	54	ARG	Sidechain
30	U	114	ARG	Sidechain
31	V	102	ARG	Sidechain
31	V	56	TYR	Sidechain
31	V	70	ARG	Sidechain
31	V	72	ARG	Sidechain
9	W	45	ARG	Sidechain

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Mol	Chain	Res	Type	Group
9	W	60	ARG	Sidechain
32	X	40	ARG	Sidechain
32	X	81	ARG	Sidechain
32	X	85	ILE	Peptide
12	Y	160	ARG	Sidechain
12	Y	53	TYR	Peptide
12	Y	79	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	34207	0	17266	43	0
2	7	1620	0	827	1	0
3	D	1229	0	1311	0	0
4	E	1515	0	1605	0	0
5	G	1758	0	1811	1	0
6	I	1424	0	1471	0	0
7	K	1037	0	1099	2	0
8	M	1099	0	1183	1	0
9	W	786	0	858	0	0
10	R	747	0	754	0	0
11	O	687	0	695	0	0
12	Y	1267	0	1316	0	0
13	Z	557	0	558	2	0
14	1	986	0	1076	0	0
15	2	321	0	338	0	0
16	3	782	0	820	0	0
17	4	586	0	604	0	0
18	5	458	0	496	0	0
19	6	346	0	381	0	0
20	B	1714	0	1838	0	0
21	F	2062	0	2200	2	0
22	H	1648	0	1803	3	0
23	J	1529	0	1680	1	0
24	L	1383	0	1434	1	0
25	N	772	0	813	0	0
26	P	954	0	997	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	Q	1129	0	1196	1	0
28	S	1047	0	1101	1	0
29	T	405	0	419	0	0
30	U	1202	0	1299	1	0
31	V	1206	0	1239	1	0
32	X	777	0	832	0	0
33	C	1539	0	1600	1	0
34	AA	67884	0	34242	118	0
35	AC	3215	0	1633	4	0
36	AB	2522	0	1275	2	0
37	AL	1757	0	1888	3	0
38	A1	1134	0	1245	2	0
39	A2	831	0	887	1	0
40	A4	555	0	599	1	0
41	A6	741	0	763	0	0
42	A7	794	0	869	0	0
43	AN	1202	0	1316	1	0
44	A8	1037	0	1139	3	0
45	A9	845	0	886	0	0
46	Aa	859	0	912	0	0
47	Ab	757	0	842	1	0
48	Ad	604	0	686	2	0
49	Ae	388	0	421	0	0
50	Af	414	0	452	0	0
51	AP	1697	0	1802	2	0
52	Ah	659	0	727	1	0
53	Ai	779	0	861	0	0
54	AI	1685	0	1849	1	0
55	AJ	1813	0	1985	2	0
56	Ac	710	0	761	1	0
57	AK	1660	0	1785	0	0
58	AM	996	0	1044	0	0
59	AS	1503	0	1636	2	0
60	AO	1172	0	1230	5	0
61	AQ	1545	0	1582	1	0
62	AR	2050	0	2140	1	0
63	AW	1319	0	1303	3	0
64	AY	797	0	850	0	0
65	AT	1509	0	1682	1	0
66	AZ	1001	0	1099	2	0
67	A3	995	0	1121	0	0
68	A5	1879	0	2005	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	AD	1867	0	1964	1	0
70	AE	3062	0	3205	4	0
71	AF	3095	0	3333	3	0
72	AG	1011	0	1073	1	0
73	AU	1497	0	1556	3	0
74	AH	1476	0	1574	1	0
75	AV	1276	0	1355	1	0
76	Ag	343	0	388	1	0
77	AX	825	0	882	0	0
78	A0	522	0	539	0	0
All	All	193061	0	144306	213	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (213) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:AA:3770:C:H4'	70:AE:310:HIS:CE1	2.36	0.61
1:A:458:A:H3'	1:A:459:A:C5'	2.32	0.60
34:AA:3117:A:HO2'	47:Ab:2:GLY:N	1.99	0.60
34:AA:445:A:C2	34:AA:702:U:C4	2.91	0.59
34:AA:236:U:HO2'	66:AZ:2:LYS:N	2.01	0.58
34:AA:1080:C:HO2'	40:A4:2:ALA:N	2.02	0.57
44:A8:36:ARG:HE	60:AO:14:HIS:CE1	2.22	0.57
34:AA:123:A:H3'	34:AA:124:U:H5''	1.87	0.56
34:AA:3626:A:H3'	34:AA:3627:C:H5''	1.88	0.56
73:AU:147:HIS:HE2	74:AH:2:LYS:N	2.03	0.56
1:A:1187:A:H2'	1:A:1188:A:C8	2.42	0.55
21:F:36:HIS:CD2	21:F:86:LEU:H	2.25	0.54
34:AA:3726:U:H4'	34:AA:3727:A:H5''	1.90	0.54
34:AA:746:A:H2'	34:AA:747:A:C8	2.42	0.54
34:AA:967:A:C5	34:AA:968:G:H1'	2.43	0.53
1:A:1434:U:H3	1:A:1665:G:H22	1.56	0.53
51:AP:15:GLN:HA	51:AP:20:HIS:CE1	2.44	0.53
1:A:955:U:H2'	1:A:956:A:C8	2.46	0.51
1:A:1938:C:H2'	1:A:1939:G:C8	2.45	0.51
34:AA:173:A:H3'	34:AA:174:U:H5''	1.93	0.51
34:AA:1322:G:H2'	34:AA:1323:A:C8	2.46	0.51
34:AA:681:U:C6	34:AA:681:U:H5''	2.45	0.51
34:AA:3116:A:C6	60:AO:60:HIS:CD2	2.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:AA:2669:G:H2'	34:AA:2670:G:C8	2.46	0.51
1:A:886:U:H2'	1:A:887:A:C8	2.46	0.51
48:Ad:8:ILE:HD12	48:Ad:8:ILE:H	1.76	0.50
34:AA:912:U:H2'	34:AA:913:U:C6	2.47	0.50
1:A:1061:A:C2	1:A:1062:A:C8	3.00	0.50
66:AZ:37:GLU:CD	66:AZ:37:GLU:H	2.19	0.49
34:AA:659:U:H2'	34:AA:660:U:C6	2.47	0.49
37:AL:75:THR:HG22	37:AL:76:PHE:H	1.78	0.49
1:A:484:A:C2	1:A:518:A:C2	3.01	0.49
1:A:1720:G:H2'	1:A:1721:A:C8	2.48	0.49
34:AA:2563:A:H2'	34:AA:2564:A:C8	2.48	0.49
34:AA:506:A:H2'	34:AA:507:G:C8	2.48	0.48
34:AA:2084:U:H5''	34:AA:2084:U:H6	1.79	0.48
34:AA:440:A:H2'	34:AA:441:A:C8	2.48	0.48
70:AE:63:PRO:HA	70:AE:68:HIS:CE1	2.49	0.48
34:AA:2506:A:H2'	34:AA:2507:A:C8	2.48	0.48
34:AA:2590:U:O2	34:AA:2590:U:H2'	2.13	0.48
34:AA:2709:U:H2'	34:AA:2710:U:C6	2.49	0.47
34:AA:2981:A:H2'	34:AA:2982:A:C8	2.49	0.47
35:AC:32:C:H2'	35:AC:33:C:C6	2.49	0.47
37:AL:97:ASP:CG	37:AL:98:LYS:H	2.22	0.47
34:AA:858:C:H3'	34:AA:859:C:H5''	1.95	0.47
1:A:1022:A:H2'	1:A:1023:A:C8	2.50	0.47
1:A:1307:U:H2'	1:A:1308:C:C5	2.48	0.47
34:AA:95:A:H4'	60:AO:35:ALA:HA	1.96	0.47
34:AA:858:C:C5	34:AA:859:C:C6	3.03	0.47
34:AA:2961:C:C5	34:AA:2962:G:C8	3.02	0.47
1:A:413:A:H2'	1:A:414:C:C6	2.49	0.47
7:K:18:GLU:CD	13:Z:22:ARG:HH22	2.22	0.47
34:AA:348:C:C4	34:AA:349:G:C6	3.03	0.47
35:AC:57:A:H2'	35:AC:58:A:C8	2.50	0.47
34:AA:593:A:H4'	34:AA:594:C:H5'	1.96	0.46
34:AA:3433:C:H5'	70:AE:326:ALA:HA	1.97	0.46
60:AO:28:HIS:CE1	60:AO:32:ARG:NH1	2.83	0.46
34:AA:1727:U:H2'	34:AA:1728:C:C6	2.50	0.46
34:AA:3054:A:C2	34:AA:3092:G:C6	3.04	0.46
73:AU:68:LEU:HD13	75:AV:142:ILE:HD13	1.97	0.46
34:AA:122:A:C5	34:AA:155:U:C5	3.03	0.46
34:AA:525:U:H2'	34:AA:526:U:C6	2.50	0.46
34:AA:2657:G:H22	34:AA:2689:G:H1'	1.80	0.46
34:AA:715:U:H2'	34:AA:716:C:C5	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:AA:1620:U:HO2'	65:AT:2:SER:N	2.14	0.46
34:AA:3511:C:H2'	34:AA:3512:A:C8	2.51	0.46
31:V:122:GLU:CD	31:V:122:GLU:H	2.23	0.46
34:AA:344:A:H2'	34:AA:345:G:C8	2.51	0.46
34:AA:445:A:C2	34:AA:446:G:C4	3.03	0.46
34:AA:909:U:H2'	34:AA:910:A:C8	2.51	0.46
34:AA:288:G:H2'	34:AA:289:A:C8	2.50	0.45
34:AA:2940:A:H2'	34:AA:2941:G:C8	2.51	0.45
63:AW:20:VAL:HG13	63:AW:21:ASP:H	1.82	0.45
1:A:458:A:H3'	1:A:459:A:H5''	1.99	0.45
1:A:1214:A:HO2'	76:Ag:3:HIS:N	2.15	0.45
35:AC:30:U:H2'	35:AC:31:U:C6	2.52	0.45
34:AA:1819:U:H2'	34:AA:1820:U:C6	2.52	0.45
70:AE:101:ILE:H	70:AE:101:ILE:HD12	1.81	0.45
13:Z:60:GLN:HA	33:C:155:HIS:CE1	2.52	0.45
34:AA:516:G:H5''	71:AF:316:LYS:HA	1.99	0.45
34:AA:1511:U:H2'	34:AA:1512:A:C8	2.51	0.45
34:AA:2650:A:H2'	34:AA:2651:A:C8	2.52	0.45
1:A:1859:A:H2'	1:A:1860:A:C8	2.51	0.45
8:M:100:GLU:CD	8:M:100:GLU:H	2.23	0.45
34:AA:1822:A:C2	34:AA:2004:U:C4	3.05	0.45
34:AA:1974:U:H2'	34:AA:1975:A:C8	2.52	0.45
38:A1:137:ILE:HD12	38:A1:137:ILE:H	1.82	0.45
34:AA:965:A:C6	34:AA:966:A:H1'	2.52	0.45
39:A2:105:LYS:H	39:A2:105:LYS:HD2	1.82	0.45
1:A:149:A:C2	1:A:161:U:C4	3.06	0.44
2:7:24:U:H2'	2:7:25:C:C6	2.52	0.44
59:AS:88:ASP:CG	59:AS:90:ARG:HH21	2.25	0.44
1:A:943:U:H2'	1:A:944:G:C8	2.52	0.44
1:A:1743:A:C2	1:A:1787:U:C5	3.05	0.44
34:AA:1785:U:C5	34:AA:1786:A:C5	3.05	0.44
36:AB:49:A:C5'	62:AR:223:ASN:HD22	2.31	0.44
34:AA:921:C:H2'	34:AA:922:C:C6	2.52	0.44
34:AA:2450:G:H4'	34:AA:2451:A:H5'	1.99	0.44
34:AA:3632:U:H3	34:AA:3653:G:H1	1.66	0.44
34:AA:1506:C:H2'	34:AA:1507:U:C6	2.52	0.44
34:AA:1739:C:H2'	34:AA:1740:A:C8	2.53	0.44
1:A:262:A:C5	1:A:263:A:H1'	2.52	0.44
22:H:120:GLU:H	22:H:120:GLU:CD	2.25	0.44
34:AA:606:A:H2'	34:AA:607:A:C8	2.53	0.44
34:AA:2500:A:C4	34:AA:2502:U:C5	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:AA:510:A:H2'	34:AA:511:C:C6	2.52	0.44
34:AA:3242:U:H2'	34:AA:3243:C:C6	2.53	0.44
72:AG:43:GLN:CD	72:AG:43:GLN:H	2.25	0.44
34:AA:3357:U:H4'	34:AA:3358:U:H5''	1.99	0.44
1:A:105:A:C8	1:A:366:A:C6	3.05	0.44
1:A:1876:G:H2'	1:A:1877:C:C6	2.52	0.44
34:AA:1100:A:C4	68:A5:185:HIS:CE1	3.06	0.44
34:AA:1467:C:H5'	44:A8:60:ASN:HA	2.00	0.44
55:AJ:178:GLU:H	55:AJ:178:GLU:CD	2.25	0.43
1:A:929:U:C5	1:A:930:A:C2	3.06	0.43
61:AQ:17:TYR:H	61:AQ:95:HIS:CD2	2.36	0.43
34:AA:497:U:C6	34:AA:497:U:H5''	2.53	0.43
35:AC:73:A:C6	35:AC:74:A:H1'	2.53	0.43
71:AF:170:PHE:CZ	71:AF:174:LEU:HD11	2.54	0.43
34:AA:916:U:H2'	34:AA:917:A:C8	2.52	0.43
34:AA:1644:U:C4	34:AA:2102:A:N1	2.86	0.43
34:AA:1822:A:C2	34:AA:1823:C:C2	3.07	0.43
34:AA:2809:A:C2	34:AA:2811:A:C4	3.06	0.43
1:A:1957:A:H2'	1:A:1958:A:C8	2.54	0.43
34:AA:1212:U:H2'	34:AA:1213:U:C6	2.53	0.43
44:A8:98:HIS:CG	44:A8:99:ASN:N	2.86	0.43
34:AA:1184:A:H2'	34:AA:1185:A:C8	2.54	0.43
34:AA:1572:U:C5	34:AA:1573:C:C5	3.06	0.43
34:AA:3241:U:H2'	34:AA:3242:U:C6	2.54	0.43
34:AA:136:U:C4	34:AA:141:A:C2	3.07	0.43
34:AA:1861:C:H2'	34:AA:1862:A:C8	2.54	0.43
1:A:993:A:H2'	1:A:994:G:C8	2.53	0.43
22:H:181:GLU:CD	22:H:181:GLU:H	2.27	0.43
1:A:12:U:H2'	1:A:13:C:C6	2.53	0.43
34:AA:642:A:C5	34:AA:684:G:C8	3.07	0.42
34:AA:1628:U:C5	34:AA:1629:G:C5	3.07	0.42
54:AI:83:LEU:HD13	54:AI:83:LEU:H	1.84	0.42
1:A:802:A:C5	1:A:803:G:C5	3.07	0.42
34:AA:1064:U:H2'	34:AA:1065:U:C6	2.54	0.42
34:AA:3325:G:H2'	34:AA:3326:A:C8	2.54	0.42
5:G:239:PRO:HA	5:G:242:TRP:CD2	2.54	0.42
34:AA:936:A:C6	56:Ac:17:LYS:HA	2.55	0.42
34:AA:939:A:H2'	34:AA:940:A:C8	2.54	0.42
34:AA:2207:G:C6	34:AA:2208:G:C5	3.08	0.42
30:U:55:ARG:HH11	30:U:56:ASP:CG	2.27	0.42
34:AA:3399:U:H2'	34:AA:3400:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:AL:16:TRP:CZ2	37:AL:19:HIS:CD2	3.08	0.42
1:A:1855:U:C2	28:S:122:HIS:CE1	3.08	0.42
34:AA:2083:U:H2'	34:AA:2084:U:C6	2.54	0.42
71:AF:33:ARG:HH22	71:AF:35:ASP:CG	2.28	0.42
38:A1:11:ILE:C	38:A1:11:ILE:HD12	2.45	0.42
34:AA:282:U:H2'	34:AA:283:U:C6	2.54	0.42
63:AW:67:VAL:HG23	63:AW:82:ARG:HG3	2.01	0.42
34:AA:1302:G:C6	34:AA:1446:A:C2	3.07	0.42
34:AA:3022:U:H2'	34:AA:3023:C:C6	2.54	0.42
34:AA:3486:G:H2'	34:AA:3487:A:C8	2.54	0.42
1:A:1928:A:C5	1:A:2056:C:H4'	2.54	0.42
34:AA:1109:U:H2'	34:AA:1110:U:C6	2.55	0.42
1:A:104:U:H1'	24:L:21:HIS:CE1	2.55	0.41
1:A:1390:U:C5	1:A:1416:U:C4	3.08	0.41
63:AW:4:TYR:N	63:AW:116:HIS:HE2	2.17	0.41
1:A:1226:A:C5	1:A:1227:G:H1'	2.55	0.41
1:A:2068:A:H2'	1:A:2069:G:C8	2.55	0.41
22:H:158:ILE:H	22:H:158:ILE:HD12	1.84	0.41
34:AA:709:A:H2'	34:AA:710:C:C6	2.56	0.41
34:AA:1683:A:H2'	34:AA:1684:A:C8	2.54	0.41
34:AA:1786:A:H2'	34:AA:1787:A:C8	2.55	0.41
34:AA:2525:A:H2'	34:AA:2526:A:C8	2.55	0.41
34:AA:3637:G:H1	34:AA:3648:U:H3	1.66	0.41
55:AJ:121:LYS:H	55:AJ:121:LYS:HD3	1.85	0.41
1:A:1914:U:H2'	1:A:1915:C:C6	2.55	0.41
34:AA:449:A:H2'	34:AA:450:A:C5'	2.51	0.41
34:AA:1515:A:C6	34:AA:1516:G:C6	3.09	0.41
34:AA:1752:C:H2'	34:AA:1753:U:C6	2.54	0.41
1:A:754:A:H62	23:J:105:GLN:CD	2.28	0.41
34:AA:449:A:H2'	34:AA:450:A:H5'	2.03	0.41
34:AA:453:A:C4	34:AA:503:A:C2	3.09	0.41
34:AA:723:A:C8	34:AA:727:A:C6	3.09	0.41
34:AA:1257:A:H2'	34:AA:1258:A:C8	2.55	0.41
34:AA:392:G:N2	34:AA:395:A:C8	2.89	0.41
34:AA:2008:G:H2'	34:AA:2009:A:C8	2.56	0.41
1:A:824:A:C2	1:A:825:A:C8	3.09	0.41
1:A:1815:U:H2'	1:A:1816:U:C5	2.56	0.41
34:AA:1331:A:H2'	34:AA:1332:A:C8	2.55	0.41
1:A:1008:A:H2'	1:A:1009:A:C8	2.56	0.41
1:A:441:U:H5''	27:Q:50:LYS:HG3	2.02	0.41
1:A:1845:U:H2'	1:A:1846:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:AA:445:A:N1	34:AA:702:U:C4	2.89	0.41
34:AA:706:U:H2'	34:AA:707:U:C6	2.56	0.41
34:AA:947:U:H2'	34:AA:948:G:C8	2.55	0.41
34:AA:1598:A:C2	34:AA:2649:A:C4	3.09	0.41
34:AA:2719:U:H2'	34:AA:2720:C:C6	2.56	0.41
34:AA:2960:G:H2'	34:AA:2961:C:C6	2.55	0.41
34:AA:3087:A:C5	34:AA:3088:G:H1'	2.55	0.41
36:AB:48:G:C6	36:AB:49:A:C6	3.09	0.41
43:AN:81:ILE:HG12	43:AN:99:THR:HG21	2.01	0.41
34:AA:715:U:H2'	34:AA:716:C:C6	2.56	0.41
34:AA:2559:U:H2'	34:AA:2560:C:C6	2.56	0.40
48:Ad:23:VAL:HG13	48:Ad:41:LEU:HD21	2.03	0.40
1:A:1821:A:H2'	1:A:1822:A:C8	2.55	0.40
1:A:1743:A:C2	1:A:1744:A:C4	3.09	0.40
34:AA:866:C:H5'	59:AS:70:HIS:CE1	2.55	0.40
34:AA:2649:A:H61	34:AA:3342:C:H5	1.66	0.40
60:AO:28:HIS:CE1	60:AO:32:ARG:HH11	2.39	0.40
1:A:953:C:H2'	1:A:954:G:C8	2.55	0.40
7:K:2:VAL:HG22	7:K:3:ARG:H	1.86	0.40
21:F:161:ARG:HE	21:F:171:GLU:CD	2.28	0.40
52:Ah:54:ILE:HD12	69:AD:50:HIS:HD1	1.86	0.40
73:AU:6:ASP:CG	73:AU:8:SER:H	2.30	0.40
1:A:310:U:H2'	1:A:311:C:C6	2.56	0.40
34:AA:495:U:H2'	34:AA:496:C:C6	2.57	0.40
34:AA:1791:A:C4	34:AA:1798:A:C6	3.09	0.40
51:AP:140:HIS:CD2	51:AP:142:ALA:H	2.39	0.40

There are no symmetry-related clashes.

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	D	149/209 (71%)	144 (97%)	3 (2%)	2 (1%)	9	41
4	E	183/185 (99%)	175 (96%)	6 (3%)	2 (1%)	11	45
5	G	222/224 (99%)	206 (93%)	14 (6%)	2 (1%)	14	49
6	I	176/189 (93%)	161 (92%)	12 (7%)	3 (2%)	7	35
7	K	127/129 (98%)	118 (93%)	7 (6%)	2 (2%)	7	37
8	M	136/138 (99%)	127 (93%)	5 (4%)	4 (3%)	3	23
9	W	91/108 (84%)	84 (92%)	6 (7%)	1 (1%)	11	45
10	R	92/114 (81%)	80 (87%)	10 (11%)	2 (2%)	5	28
11	O	77/79 (98%)	67 (87%)	4 (5%)	6 (8%)	1	10
12	Y	152/154 (99%)	137 (90%)	11 (7%)	4 (3%)	4	25
13	Z	70/72 (97%)	65 (93%)	4 (6%)	1 (1%)	9	39
14	1	118/120 (98%)	111 (94%)	4 (3%)	3 (2%)	4	26
15	2	35/68 (52%)	31 (89%)	3 (9%)	1 (3%)	3	23
16	3	93/95 (98%)	81 (87%)	11 (12%)	1 (1%)	11	45
17	4	74/76 (97%)	65 (88%)	7 (10%)	2 (3%)	4	25
18	5	54/65 (83%)	53 (98%)	1 (2%)	0	100	100
19	6	41/43 (95%)	35 (85%)	5 (12%)	1 (2%)	4	27
20	B	208/210 (99%)	186 (89%)	19 (9%)	3 (1%)	9	39
21	F	255/257 (99%)	238 (93%)	13 (5%)	4 (2%)	7	37
22	H	200/214 (94%)	191 (96%)	8 (4%)	1 (0%)	24	63
23	J	186/188 (99%)	176 (95%)	5 (3%)	5 (3%)	4	25
24	L	165/214 (77%)	147 (89%)	14 (8%)	4 (2%)	4	27
25	N	96/98 (98%)	91 (95%)	3 (3%)	2 (2%)	5	29
26	P	125/127 (98%)	114 (91%)	8 (6%)	3 (2%)	4	27
27	Q	142/144 (99%)	130 (92%)	7 (5%)	5 (4%)	3	20
28	S	126/128 (98%)	108 (86%)	14 (11%)	4 (3%)	3	21
29	T	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
30	U	147/149 (99%)	142 (97%)	4 (3%)	1 (1%)	18	55
31	V	142/156 (91%)	129 (91%)	10 (7%)	3 (2%)	5	29
32	X	92/103 (89%)	78 (85%)	10 (11%)	4 (4%)	2	17
33	C	193/195 (99%)	181 (94%)	9 (5%)	3 (2%)	7	37
37	AL	209/211 (99%)	190 (91%)	16 (8%)	3 (1%)	9	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	A1	136/145 (94%)	127 (93%)	7 (5%)	2 (2%)	8	38
39	A2	96/118 (81%)	89 (93%)	5 (5%)	2 (2%)	5	29
40	A4	64/66 (97%)	58 (91%)	4 (6%)	2 (3%)	3	21
41	A6	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
42	A7	92/102 (90%)	89 (97%)	3 (3%)	0	100	100
43	AN	144/146 (99%)	140 (97%)	2 (1%)	2 (1%)	9	39
44	A8	123/125 (98%)	114 (93%)	8 (6%)	1 (1%)	16	53
45	A9	101/103 (98%)	92 (91%)	9 (9%)	0	100	100
46	Aa	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
47	Ab	91/105 (87%)	85 (93%)	5 (6%)	1 (1%)	11	45
48	Ad	68/76 (90%)	68 (100%)	0	0	100	100
49	Ae	39/50 (78%)	39 (100%)	0	0	100	100
50	Af	49/51 (96%)	46 (94%)	3 (6%)	0	100	100
51	AP	202/204 (99%)	183 (91%)	14 (7%)	5 (2%)	4	26
52	Ah	83/85 (98%)	76 (92%)	5 (6%)	2 (2%)	4	27
53	Ai	93/95 (98%)	87 (94%)	5 (5%)	1 (1%)	11	45
54	AI	203/213 (95%)	187 (92%)	14 (7%)	2 (1%)	12	47
55	AJ	216/244 (88%)	196 (91%)	13 (6%)	7 (3%)	3	21
56	Ac	87/89 (98%)	74 (85%)	12 (14%)	1 (1%)	11	45
57	AK	199/201 (99%)	191 (96%)	6 (3%)	2 (1%)	12	47
58	AM	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
59	AS	184/186 (99%)	171 (93%)	12 (6%)	1 (0%)	24	63
60	AO	145/147 (99%)	132 (91%)	10 (7%)	3 (2%)	5	29
61	AQ	185/205 (90%)	170 (92%)	12 (6%)	3 (2%)	7	37
62	AR	244/289 (84%)	224 (92%)	13 (5%)	7 (3%)	3	23
63	AW	149/170 (88%)	135 (91%)	12 (8%)	2 (1%)	9	41
64	AY	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
65	AT	179/181 (99%)	173 (97%)	5 (3%)	1 (1%)	21	59
66	AZ	119/121 (98%)	113 (95%)	5 (4%)	1 (1%)	16	53
67	A3	117/119 (98%)	108 (92%)	9 (8%)	0	100	100
68	A5	221/223 (99%)	201 (91%)	15 (7%)	5 (2%)	5	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	AD	245/247 (99%)	230 (94%)	14 (6%)	1 (0%)	30	67
70	AE	378/380 (100%)	346 (92%)	26 (7%)	6 (2%)	7	37
71	AF	388/390 (100%)	363 (94%)	21 (5%)	4 (1%)	12	47
72	AG	116/159 (73%)	107 (92%)	6 (5%)	3 (3%)	4	25
73	AU	178/180 (99%)	167 (94%)	9 (5%)	2 (1%)	11	45
74	AH	183/185 (99%)	168 (92%)	12 (7%)	3 (2%)	7	37
75	AV	153/155 (99%)	141 (92%)	9 (6%)	3 (2%)	6	31
76	Ag	35/37 (95%)	29 (83%)	5 (14%)	1 (3%)	3	23
77	AX	95/97 (98%)	90 (95%)	4 (4%)	1 (1%)	11	45
78	A0	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	7	35
All	All	10111/10698 (94%)	9361 (93%)	590 (6%)	160 (2%)	10	37

All (160) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	K	120	HIS
8	M	41	GLU
9	W	4	VAL
10	R	42	ILE
12	Y	55	LYS
22	H	25	LEU
24	L	9	HIS
27	Q	137	LYS
28	S	101	ILE
30	U	62	GLN
32	X	51	LYS
32	X	52	LYS
44	A8	64	LYS
51	AP	188	SER
60	AO	25	HIS
62	AR	152	ILE
70	AE	196	LEU
70	AE	247	ALA
71	AF	267	ILE
6	I	174	GLU
11	O	34	VAL
12	Y	68	LEU
14	1	117	LYS

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Mol	Chain	Res	Type
20	B	146	ARG
27	Q	138	GLU
31	V	41	VAL
32	X	49	ILE
32	X	112	ILE
33	C	27	LYS
37	AL	169	PRO
39	A2	95	GLN
40	A4	3	LYS
51	AP	150	ASN
52	Ah	42	CYS
55	AJ	75	ILE
55	AJ	219	SER
60	AO	15	VAL
61	AQ	35	ASP
62	AR	44	TYR
62	AR	59	GLN
62	AR	229	ASN
63	AW	20	VAL
70	AE	300	LYS
73	AU	10	ASN
75	AV	133	THR
4	E	16	LYS
5	G	101	GLN
5	G	121	GLY
6	I	49	LYS
6	I	70	HIS
7	K	58	SER
8	M	130	PHE
11	O	15	PRO
11	O	76	TYR
12	Y	60	VAL
16	3	92	ARG
17	4	18	LYS
20	B	130	LEU
23	J	31	SER
23	J	112	ILE
24	L	61	ASP
25	N	67	SER
25	N	117	ASP
26	P	100	SER
26	P	134	PRO

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Mol	Chain	Res	Type
27	Q	118	PRO
27	Q	141	GLU
28	S	24	GLY
31	V	56	TYR
37	AL	61	THR
38	A1	42	LEU
43	AN	25	VAL
51	AP	149	ILE
53	Ai	85	LYS
55	AJ	64	ASP
56	Ac	29	SER
61	AQ	24	ARG
62	AR	172	GLY
65	AT	129	ASN
72	AG	10	ARG
72	AG	125	MET
74	AH	42	PRO
74	AH	115	ASN
75	AV	130	LYS
75	AV	132	LYS
78	A0	18	TYR
3	D	29	LEU
4	E	169	PRO
10	R	63	CYS
11	O	41	PRO
12	Y	27	ASN
13	Z	30	GLY
19	6	11	ALA
21	F	195	ILE
23	J	165	ILE
24	L	8	ARG
26	P	57	THR
28	S	18	LEU
31	V	9	HIS
37	AL	129	LYS
39	A2	17	ASN
47	Ab	8	LYS
51	AP	70	ASP
55	AJ	59	VAL
60	AO	58	MET
63	AW	106	ASN
70	AE	221	HIS

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Mol	Chain	Res	Type
70	AE	254	PRO
71	AF	19	VAL
71	AF	155	SER
72	AG	141	ARG
74	AH	53	TYR
76	Ag	13	ALA
77	AX	78	LYS
8	M	98	VAL
11	O	72	TRP
14	1	11	LYS
17	4	47	HIS
20	B	75	ASN
21	F	21	ASN
21	F	189	VAL
23	J	57	LYS
23	J	132	SER
27	Q	67	ALA
28	S	92	LEU
33	C	28	ASN
33	C	143	VAL
38	A1	104	SER
54	AI	19	VAL
54	AI	25	ALA
55	AJ	41	ASP
55	AJ	63	LYS
62	AR	58	SER
66	AZ	70	VAL
68	A5	116	ARG
68	A5	171	TYR
68	A5	229	ALA
8	M	57	GLY
11	O	12	SER
14	1	104	ALA
40	A4	36	ASP
51	AP	80	VAL
61	AQ	60	ILE
62	AR	89	PRO
68	A5	177	GLN
69	AD	29	LEU
73	AU	134	ARG
24	L	202	GLY
43	AN	46	VAL

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Mol	Chain	Res	Type
68	A5	100	GLY
71	AF	216	GLY
15	2	60	THR
21	F	239	PRO
52	Ah	9	GLY
57	AK	88	PRO
59	AS	82	VAL
55	AJ	72	PRO
57	AK	64	ASN
3	D	162	GLY
70	AE	297	ILE

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	D	132/177 (75%)	131 (99%)	1 (1%)	73	78
4	E	161/164 (98%)	159 (99%)	2 (1%)	63	74
5	G	191/191 (100%)	187 (98%)	4 (2%)	47	65
6	I	154/160 (96%)	149 (97%)	5 (3%)	34	56
7	K	115/115 (100%)	111 (96%)	4 (4%)	32	54
8	M	116/116 (100%)	114 (98%)	2 (2%)	53	68
9	W	86/99 (87%)	86 (100%)	0	100	100
10	R	83/97 (86%)	83 (100%)	0	100	100
11	O	76/76 (100%)	73 (96%)	3 (4%)	28	50
12	Y	137/137 (100%)	133 (97%)	4 (3%)	37	58
13	Z	60/60 (100%)	60 (100%)	0	100	100
14	1	104/104 (100%)	101 (97%)	3 (3%)	37	58
15	2	35/61 (57%)	34 (97%)	1 (3%)	37	58
16	3	87/87 (100%)	87 (100%)	0	100	100
17	4	70/70 (100%)	68 (97%)	2 (3%)	37	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	5	47/52 (90%)	45 (96%)	2 (4%)	26	48
19	6	36/36 (100%)	36 (100%)	0	100	100
20	B	195/195 (100%)	192 (98%)	3 (2%)	57	71
21	F	233/233 (100%)	229 (98%)	4 (2%)	53	68
22	H	182/190 (96%)	179 (98%)	3 (2%)	55	69
23	J	177/177 (100%)	176 (99%)	1 (1%)	78	81
24	L	151/190 (80%)	149 (99%)	2 (1%)	61	72
25	N	91/91 (100%)	89 (98%)	2 (2%)	45	64
26	P	99/99 (100%)	96 (97%)	3 (3%)	36	57
27	Q	120/120 (100%)	119 (99%)	1 (1%)	73	78
28	S	114/114 (100%)	109 (96%)	5 (4%)	25	47
29	T	43/43 (100%)	42 (98%)	1 (2%)	44	64
30	U	132/132 (100%)	130 (98%)	2 (2%)	57	71
31	V	131/140 (94%)	129 (98%)	2 (2%)	57	71
32	X	88/94 (94%)	88 (100%)	0	100	100
33	C	167/167 (100%)	162 (97%)	5 (3%)	36	57
37	AL	190/190 (100%)	187 (98%)	3 (2%)	55	69
38	A1	127/131 (97%)	124 (98%)	3 (2%)	43	63
39	A2	97/109 (89%)	95 (98%)	2 (2%)	47	65
40	A4	60/60 (100%)	60 (100%)	0	100	100
41	A6	83/83 (100%)	82 (99%)	1 (1%)	63	74
42	A7	90/96 (94%)	89 (99%)	1 (1%)	65	74
43	AN	135/135 (100%)	134 (99%)	1 (1%)	76	79
44	A8	114/114 (100%)	110 (96%)	4 (4%)	32	54
45	A9	90/90 (100%)	90 (100%)	0	100	100
46	Aa	89/89 (100%)	85 (96%)	4 (4%)	24	47
47	Ab	82/92 (89%)	80 (98%)	2 (2%)	43	63
48	Ad	69/73 (94%)	68 (99%)	1 (1%)	59	72
49	Ae	40/47 (85%)	39 (98%)	1 (2%)	42	62
50	Af	45/45 (100%)	45 (100%)	0	100	100
51	AP	179/179 (100%)	174 (97%)	5 (3%)	38	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	Ah	70/70 (100%)	69 (99%)	1 (1%)	59	72
53	Ai	87/87 (100%)	85 (98%)	2 (2%)	44	64
54	AI	189/195 (97%)	187 (99%)	2 (1%)	65	74
55	AJ	204/224 (91%)	200 (98%)	4 (2%)	48	66
56	Ac	74/74 (100%)	73 (99%)	1 (1%)	59	72
57	AK	181/181 (100%)	180 (99%)	1 (1%)	78	81
58	AM	106/106 (100%)	106 (100%)	0	100	100
59	AS	158/158 (100%)	156 (99%)	2 (1%)	61	72
60	AO	121/121 (100%)	114 (94%)	7 (6%)	18	40
61	AQ	165/176 (94%)	163 (99%)	2 (1%)	63	74
62	AR	215/250 (86%)	213 (99%)	2 (1%)	70	77
63	AW	128/128 (100%)	125 (98%)	3 (2%)	44	64
64	AY	90/90 (100%)	89 (99%)	1 (1%)	65	74
65	AT	162/162 (100%)	162 (100%)	0	100	100
66	AZ	111/111 (100%)	109 (98%)	2 (2%)	51	67
67	A3	110/110 (100%)	109 (99%)	1 (1%)	70	77
68	A5	201/201 (100%)	197 (98%)	4 (2%)	48	66
69	AD	191/191 (100%)	185 (97%)	6 (3%)	35	56
70	AE	335/335 (100%)	327 (98%)	8 (2%)	43	63
71	AF	336/336 (100%)	329 (98%)	7 (2%)	47	65
72	AG	110/142 (78%)	109 (99%)	1 (1%)	70	77
73	AU	162/162 (100%)	157 (97%)	5 (3%)	35	56
74	AH	168/168 (100%)	164 (98%)	4 (2%)	43	63
75	AV	140/140 (100%)	138 (99%)	2 (1%)	59	72
76	Ag	34/34 (100%)	34 (100%)	0	100	100
77	AX	92/92 (100%)	92 (100%)	0	100	100
78	A0	53/53 (100%)	52 (98%)	1 (2%)	50	66
All	All	9096/9417 (97%)	8932 (98%)	164 (2%)	51	67

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	107	ARG

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Mol	Chain	Res	Type
4	E	91	GLU
4	E	104	LEU
5	G	182	VAL
5	G	215	LYS
5	G	219	LYS
5	G	242	TRP
6	I	16	TYR
6	I	17	GLU
6	I	61	GLU
6	I	62	ARG
6	I	79	LYS
7	K	52	ILE
7	K	60	LYS
7	K	110	ILE
7	K	115	GLU
8	M	56	ILE
8	M	100	GLU
11	O	20	LYS
11	O	35	GLU
11	O	75	GLN
12	Y	30	LYS
12	Y	32	VAL
12	Y	64	LYS
12	Y	105	LYS
14	1	4	GLN
14	1	116	ARG
14	1	118	LYS
15	2	38	HIS
17	4	12	GLU
17	4	40	GLN
18	5	2	GLU
18	5	49	ARG
20	B	119	THR
20	B	151	LYS
20	B	210	VAL
21	F	114	ILE
21	F	174	LYS
21	F	227	VAL
21	F	233	LYS
22	H	13	GLN
22	H	120	GLU
22	H	158	ILE

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Mol	Chain	Res	Type
23	J	149	ARG
24	L	198	TYR
24	L	213	ASP
25	N	71	GLU
25	N	88	ILE
26	P	25	GLU
26	P	93	ILE
26	P	117	ARG
27	Q	87	VAL
28	S	12	GLN
28	S	36	LYS
28	S	62	THR
28	S	93	LYS
28	S	120	ARG
29	T	31	LYS
30	U	3	ARG
30	U	149	LEU
31	V	89	ILE
31	V	107	HIS
33	C	58	GLN
33	C	63	ILE
33	C	75	VAL
33	C	121	LEU
33	C	168	GLU
37	AL	75	THR
37	AL	181	LYS
37	AL	202	ARG
38	A1	43	VAL
38	A1	46	ILE
38	A1	135	LYS
39	A2	34	ASP
39	A2	82	LYS
41	A6	44	LEU
42	A7	15	PRO
43	AN	56	VAL
44	A8	77	LYS
44	A8	82	MET
44	A8	94	VAL
44	A8	115	MET
46	Aa	32	ILE
46	Aa	52	GLN
46	Aa	66	ARG

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Mol	Chain	Res	Type
46	Aa	80	ILE
47	Ab	18	ASN
47	Ab	88	LYS
48	Ad	47	LYS
49	Ae	42	ARG
51	AP	13	LYS
51	AP	19	MET
51	AP	85	LYS
51	AP	95	THR
51	AP	162	LEU
52	Ah	47	THR
53	Ai	32	GLU
53	Ai	79	LYS
54	AI	63	LEU
54	AI	83	LEU
55	AJ	121	LYS
55	AJ	129	LEU
55	AJ	179	LEU
55	AJ	218	GLU
56	Ac	66	ARG
57	AK	153	LYS
59	AS	18	HIS
59	AS	149	LYS
60	AO	27	LYS
60	AO	32	ARG
60	AO	59	ARG
60	AO	62	ASN
60	AO	63	LEU
60	AO	87	LYS
60	AO	102	VAL
61	AQ	49	VAL
61	AQ	156	LYS
62	AR	56	THR
62	AR	73	LYS
63	AW	22	LEU
63	AW	67	VAL
63	AW	131	LYS
64	AY	111	ILE
66	AZ	37	GLU
66	AZ	88	LYS
67	A3	119	LEU
68	A5	149	THR

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Mol	Chain	Res	Type
68	A5	169	ARG
68	A5	219	LYS
68	A5	224	ARG
69	AD	54	ARG
69	AD	159	ASP
69	AD	163	ARG
69	AD	209	HIS
69	AD	218	HIS
69	AD	242	ARG
70	AE	39	LYS
70	AE	56	ILE
70	AE	237	ARG
70	AE	334	THR
70	AE	338	ASN
70	AE	361	LYS
70	AE	366	ARG
70	AE	380	LEU
71	AF	6	PRO
71	AF	55	LYS
71	AF	109	ARG
71	AF	222	ARG
71	AF	232	VAL
71	AF	254	GLU
71	AF	347	ILE
72	AG	43	GLN
73	AU	7	ASN
73	AU	56	LYS
73	AU	108	LYS
73	AU	157	ARG
73	AU	174	PHE
74	AH	14	GLU
74	AH	46	ARG
74	AH	54	ILE
74	AH	131	VAL
75	AV	15	LYS
75	AV	30	LYS
78	A0	26	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	22	ASN

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Mol	Chain	Res	Type
3	D	126	HIS
4	E	123	HIS
4	E	131	GLN
4	E	133	HIS
5	G	80	GLN
5	G	86	HIS
5	G	106	GLN
5	G	120	ASN
6	I	20	ASN
6	I	105	ASN
7	K	56	HIS
7	K	64	ASN
7	K	113	HIS
8	M	75	GLN
9	W	56	HIS
10	R	87	GLN
11	O	50	ASN
12	Y	26	ASN
12	Y	72	ASN
12	Y	132	ASN
12	Y	139	ASN
12	Y	153	ASN
12	Y	163	ASN
13	Z	81	GLN
13	Z	82	ASN
17	4	47	HIS
17	4	50	ASN
17	4	58	ASN
20	B	148	ASN
20	B	149	GLN
22	H	104	GLN
22	H	192	GLN
24	L	21	HIS
24	L	115	ASN
28	S	127	HIS
30	U	62	GLN
30	U	105	ASN
31	V	81	ASN
31	V	107	HIS
31	V	144	HIS
32	X	46	GLN
32	X	104	ASN

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Mol	Chain	Res	Type
33	C	23	HIS
33	C	46	HIS
33	C	110	GLN
33	C	179	GLN
37	AL	130	ASN
39	A2	37	ASN
39	A2	96	HIS
40	A4	51	GLN
41	A6	12	ASN
41	A6	14	ASN
42	A7	74	ASN
44	A8	107	GLN
45	A9	73	HIS
46	Aa	12	HIS
49	Ae	25	HIS
50	Af	16	GLN
50	Af	44	GLN
51	AP	20	HIS
54	AI	161	ASN
55	AJ	42	ASN
55	AJ	78	GLN
55	AJ	208	HIS
57	AK	62	ASN
57	AK	71	HIS
57	AK	194	GLN
58	AM	42	GLN
58	AM	83	GLN
58	AM	90	HIS
59	AS	14	HIS
60	AO	28	HIS
60	AO	60	HIS
61	AQ	86	HIS
62	AR	180	ASN
62	AR	211	GLN
62	AR	223	ASN
63	AW	80	GLN
65	AT	57	HIS
65	AT	142	GLN
66	AZ	102	ASN
67	A3	39	ASN
68	A5	51	ASN
68	A5	185	HIS

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Mol	Chain	Res	Type
69	AD	118	HIS
69	AD	233	GLN
70	AE	11	HIS
70	AE	162	GLN
70	AE	240	HIS
70	AE	264	HIS
70	AE	310	HIS
71	AF	34	ASN
71	AF	181	ASN
71	AF	362	GLN
72	AG	15	ASN
72	AG	164	GLN
73	AU	114	GLN
73	AU	162	HIS
74	AH	40	HIS
75	AV	23	HIS
75	AV	96	HIS
77	AX	114	HIS
78	A0	49	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1586/1608 (98%)	487 (30%)	89 (5%)
2	7	75/76 (98%)	13 (17%)	2 (2%)
34	AA	3168/3193 (99%)	993 (31%)	187 (5%)
35	AC	148/151 (98%)	50 (33%)	9 (6%)
36	AB	117/118 (99%)	27 (23%)	1 (0%)
All	All	5094/5146 (98%)	1570 (30%)	288 (5%)

All (1570) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	3	C
1	A	5	U
1	A	17	C
1	A	25	C
1	A	26	A
1	A	27	U
1	A	34	G
1	A	35	U

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Mol	Chain	Res	Type
1	A	42	G
1	A	45	U
1	A	47	A
1	A	50	C
1	A	57	G
1	A	59	G
1	A	60	A
1	A	67	A
1	A	68	U
1	A	71	A
1	A	79	U
1	A	81	U
1	A	82	G
1	A	84	A
1	A	97	G
1	A	106	A
1	A	107	A
1	A	108	A
1	A	111	G
1	A	113	U
1	A	116	A
1	A	125	G
1	A	128	A
1	A	129	U
1	A	130	U
1	A	138	U
1	A	139	A
1	A	140	A
1	A	142	G
1	A	143	A
1	A	144	U
1	A	151	G
1	A	157	G
1	A	159	U
1	A	161	U
1	A	164	C
1	A	165	U
1	A	169	A
1	A	182	U
1	A	183	C
1	A	186	U
1	A	205	A

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Mol	Chain	Res	Type
1	A	206	A
1	A	207	G
1	A	208	U
1	A	209	A
1	A	217	G
1	A	247	G
1	A	251	U
1	A	252	U
1	A	254	U
1	A	255	A
1	A	258	A
1	A	260	A
1	A	262	A
1	A	264	G
1	A	266	A
1	A	267	A
1	A	272	U
1	A	273	A
1	A	292	G
1	A	305	G
1	A	308	U
1	A	320	C
1	A	322	G
1	A	323	C
1	A	326	U
1	A	327	U
1	A	330	U
1	A	335	G
1	A	339	A
1	A	342	G
1	A	343	G
1	A	344	C
1	A	345	C
1	A	350	A
1	A	357	U
1	A	358	G
1	A	361	G
1	A	365	A
1	A	367	C
1	A	375	U
1	A	378	A
1	A	379	G

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Mol	Chain	Res	Type
1	A	384	A
1	A	386	U
1	A	396	G
1	A	399	C
1	A	405	A
1	A	406	A
1	A	407	A
1	A	408	U
1	A	409	A
1	A	410	G
1	A	422	A
1	A	423	A
1	A	424	G
1	A	425	G
1	A	430	C
1	A	431	A
1	A	432	G
1	A	433	C
1	A	434	A
1	A	440	G
1	A	445	U
1	A	446	U
1	A	450	C
1	A	451	A
1	A	454	U
1	A	458	A
1	A	459	A
1	A	460	G
1	A	461	A
1	A	462	A
1	A	466	A
1	A	467	G
1	A	470	A
1	A	483	A
1	A	484	A
1	A	488	U
1	A	508	U
1	A	509	U
1	A	515	U
1	A	516	G
1	A	521	G
1	A	526	G

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Mol	Chain	Res	Type
1	A	527	A
1	A	543	A
1	A	545	A
1	A	546	G
1	A	548	A
1	A	549	A
1	A	562	A
1	A	564	G
1	A	565	U
1	A	566	C
1	A	568	G
1	A	572	C
1	A	575	G
1	A	578	G
1	A	584	G
1	A	587	A
1	A	588	U
1	A	589	U
1	A	590	C
1	A	601	A
1	A	602	G
1	A	614	A
1	A	615	U
1	A	616	U
1	A	617	G
1	A	618	U
1	A	626	A
1	A	627	A
1	A	629	A
1	A	630	C
1	A	631	G
1	A	642	A
1	A	645	U
1	A	646	U
1	A	648	A
1	A	752	U
1	A	753	U
1	A	756	A
1	A	760	C
1	A	790	U
1	A	791	U
1	A	792	U

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Mol	Chain	Res	Type
1	A	793	G
1	A	794	U
1	A	800	U
1	A	801	G
1	A	804	U
1	A	805	A
1	A	806	A
1	A	816	U
1	A	817	U
1	A	818	C
1	A	819	A
1	A	821	A
1	A	824	A
1	A	828	A
1	A	832	A
1	A	833	A
1	A	837	A
1	A	844	G
1	A	845	U
1	A	846	G
1	A	849	U
1	A	852	A
1	A	853	U
1	A	856	U
1	A	857	A
1	A	858	U
1	A	866	A
1	A	867	A
1	A	869	A
1	A	870	A
1	A	874	A
1	A	875	A
1	A	876	U
1	A	877	U
1	A	879	A
1	A	880	A
1	A	881	C
1	A	882	A
1	A	887	A
1	A	888	A
1	A	896	U
1	A	906	U

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Mol	Chain	Res	Type
1	A	908	U
1	A	915	G
1	A	917	C
1	A	920	A
1	A	921	G
1	A	922	U
1	A	924	A
1	A	928	U
1	A	929	U
1	A	931	A
1	A	941	C
1	A	942	U
1	A	945	G
1	A	962	A
1	A	965	U
1	A	966	C
1	A	967	A
1	A	973	G
1	A	974	A
1	A	982	A
1	A	983	G
1	A	984	A
1	A	990	U
1	A	998	A
1	A	1002	A
1	A	1004	U
1	A	1011	G
1	A	1013	A
1	A	1021	A
1	A	1029	U
1	A	1035	A
1	A	1038	C
1	A	1051	U
1	A	1056	G
1	A	1061	A
1	A	1062	A
1	A	1065	C
1	A	1067	A
1	A	1071	G
1	A	1072	A
1	A	1073	U
1	A	1074	A

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Mol	Chain	Res	Type
1	A	1082	A
1	A	1089	A
1	A	1090	C
1	A	1092	A
1	A	1093	U
1	A	1094	A
1	A	1095	A
1	A	1097	C
1	A	1099	A
1	A	1101	G
1	A	1107	U
1	A	1108	A
1	A	1109	G
1	A	1112	G
1	A	1116	G
1	A	1119	G
1	A	1175	G
1	A	1177	A
1	A	1183	U
1	A	1193	A
1	A	1194	A
1	A	1195	G
1	A	1197	C
1	A	1199	U
1	A	1209	G
1	A	1210	G
1	A	1212	C
1	A	1214	A
1	A	1227	G
1	A	1230	A
1	A	1239	A
1	A	1247	G
1	A	1251	G
1	A	1255	G
1	A	1259	C
1	A	1260	C
1	A	1261	A
1	A	1265	G
1	A	1268	G
1	A	1271	G
1	A	1284	A
1	A	1286	U

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Mol	Chain	Res	Type
1	A	1287	U
1	A	1292	U
1	A	1293	C
1	A	1295	A
1	A	1296	C
1	A	1297	A
1	A	1301	G
1	A	1302	G
1	A	1304	A
1	A	1306	C
1	A	1307	U
1	A	1309	A
1	A	1315	U
1	A	1317	A
1	A	1318	A
1	A	1319	G
1	A	1321	C
1	A	1363	U
1	A	1366	A
1	A	1367	U
1	A	1370	U
1	A	1374	G
1	A	1375	C
1	A	1382	G
1	A	1383	U
1	A	1384	U
1	A	1385	U
1	A	1387	U
1	A	1388	A
1	A	1409	U
1	A	1414	A
1	A	1416	U
1	A	1417	U
1	A	1423	A
1	A	1427	A
1	A	1431	A
1	A	1432	G
1	A	1437	U
1	A	1443	G
1	A	1444	C
1	A	1445	U
1	A	1449	U

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Mol	Chain	Res	Type
1	A	1450	A
1	A	1451	G
1	A	1453	G
1	A	1454	G
1	A	1456	G
1	A	1459	U
1	A	1463	C
1	A	1464	U
1	A	1607	U
1	A	1623	U
1	A	1624	U
1	A	1626	U
1	A	1635	C
1	A	1636	A
1	A	1644	U
1	A	1645	C
1	A	1646	U
1	A	1648	A
1	A	1649	C
1	A	1656	A
1	A	1659	U
1	A	1660	U
1	A	1664	G
1	A	1667	A
1	A	1668	A
1	A	1673	A
1	A	1674	G
1	A	1677	C
1	A	1678	U
1	A	1679	G
1	A	1691	G
1	A	1692	A
1	A	1693	U
1	A	1702	C
1	A	1703	U
1	A	1704	G
1	A	1705	C
1	A	1706	A
1	A	1715	A
1	A	1716	C
1	A	1717	A
1	A	1718	C

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Mol	Chain	Res	Type
1	A	1720	G
1	A	1721	A
1	A	1723	A
1	A	1727	A
1	A	1728	U
1	A	1732	G
1	A	1735	U
1	A	1749	C
1	A	1787	U
1	A	1790	C
1	A	1792	U
1	A	1795	G
1	A	1796	C
1	A	1799	A
1	A	1801	A
1	A	1802	G
1	A	1806	U
1	A	1811	A
1	A	1812	A
1	A	1813	U
1	A	1817	U
1	A	1818	A
1	A	1819	U
1	A	1820	C
1	A	1824	A
1	A	1825	U
1	A	1830	C
1	A	1832	U
1	A	1833	G
1	A	1834	A
1	A	1835	U
1	A	1837	G
1	A	1844	A
1	A	1846	U
1	A	1850	G
1	A	1854	U
1	A	1855	U
1	A	1856	A
1	A	1861	U
1	A	1863	U
1	A	1866	A
1	A	1868	C

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Mol	Chain	Res	Type
1	A	1870	A
1	A	1871	G
1	A	1872	G
1	A	1881	G
1	A	1882	U
1	A	1883	A
1	A	1887	A
1	A	1892	U
1	A	1897	A
1	A	1898	G
1	A	1899	A
1	A	1902	G
1	A	1904	G
1	A	1907	A
1	A	1908	A
1	A	1911	A
1	A	1912	C
1	A	1913	G
1	A	1915	C
1	A	1916	C
1	A	1927	U
1	A	1928	A
1	A	1929	C
1	A	1930	A
1	A	1934	C
1	A	1935	G
1	A	1938	C
1	A	1944	U
1	A	1954	U
1	A	1955	G
1	A	1961	U
1	A	1977	G
1	A	1978	A
1	A	1979	C
1	A	1980	A
1	A	1981	A
1	A	1982	G
1	A	2012	G
1	A	2019	C
1	A	2020	G
1	A	2021	U
1	A	2028	U

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Mol	Chain	Res	Type
1	A	2034	U
1	A	2042	A
1	A	2048	A
1	A	2049	G
1	A	2053	U
1	A	2054	A
1	A	2060	G
1	A	2061	U
1	A	2072	G
1	A	2073	A
1	A	2075	C
1	A	2084	G
1	A	2085	G
1	A	2086	A
1	A	2088	C
1	A	2089	A
1	A	2090	U
2	7	4	G
2	7	5	G
2	7	8	U
2	7	18	G
2	7	19	G
2	7	21	A
2	7	34	C
2	7	47	U
2	7	48	C
2	7	63	G
2	7	71	C
2	7	75	C
2	7	76	A
34	AA	11	A
34	AA	12	U
34	AA	13	G
34	AA	14	U
34	AA	16	A
34	AA	18	G
34	AA	25	A
34	AA	26	A
34	AA	30	G
34	AA	32	C
34	AA	34	A
34	AA	40	A

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Mol	Chain	Res	Type
34	AA	43	A
34	AA	44	U
34	AA	45	A
34	AA	49	U
34	AA	55	G
34	AA	57	A
34	AA	59	G
34	AA	60	A
34	AA	63	A
34	AA	66	A
34	AA	69	U
34	AA	73	U
34	AA	75	U
34	AA	83	U
34	AA	85	A
34	AA	87	U
34	AA	92	G
34	AA	105	G
34	AA	108	C
34	AA	109	A
34	AA	110	G
34	AA	111	C
34	AA	122	A
34	AA	124	U
34	AA	125	C
34	AA	130	G
34	AA	133	U
34	AA	134	G
34	AA	135	G
34	AA	136	U
34	AA	139	A
34	AA	144	U
34	AA	145	U
34	AA	147	C
34	AA	148	G
34	AA	149	A
34	AA	152	G
34	AA	156	U
34	AA	157	G
34	AA	163	G
34	AA	165	A
34	AA	167	U

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Mol	Chain	Res	Type
34	AA	168	A
34	AA	172	C
34	AA	173	A
34	AA	174	U
34	AA	175	G
34	AA	182	U
34	AA	183	U
34	AA	185	A
34	AA	186	A
34	AA	189	U
34	AA	190	G
34	AA	191	A
34	AA	192	G
34	AA	195	A
34	AA	197	G
34	AA	198	U
34	AA	199	G
34	AA	200	A
34	AA	201	G
34	AA	207	A
34	AA	208	U
34	AA	211	U
34	AA	214	C
34	AA	215	C
34	AA	216	C
34	AA	219	A
34	AA	220	G
34	AA	221	A
34	AA	226	G
34	AA	227	A
34	AA	228	A
34	AA	229	A
34	AA	231	G
34	AA	235	A
34	AA	239	U
34	AA	242	U
34	AA	246	U
34	AA	247	A
34	AA	250	U
34	AA	255	C
34	AA	257	U
34	AA	258	U

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Mol	Chain	Res	Type
34	AA	263	U
34	AA	265	U
34	AA	268	C
34	AA	269	A
34	AA	271	G
34	AA	276	G
34	AA	277	U
34	AA	290	G
34	AA	292	U
34	AA	293	U
34	AA	302	A
34	AA	303	A
34	AA	304	U
34	AA	305	A
34	AA	307	G
34	AA	308	U
34	AA	309	G
34	AA	310	U
34	AA	313	U
34	AA	315	C
34	AA	317	U
34	AA	319	U
34	AA	324	U
34	AA	325	A
34	AA	336	U
34	AA	337	A
34	AA	338	U
34	AA	342	G
34	AA	344	A
34	AA	347	C
34	AA	351	U
34	AA	354	C
34	AA	356	A
34	AA	359	A
34	AA	362	U
34	AA	378	U
34	AA	382	A
34	AA	384	A
34	AA	385	G
34	AA	386	U
34	AA	392	G
34	AA	395	A

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Mol	Chain	Res	Type
34	AA	396	U
34	AA	400	C
34	AA	401	A
34	AA	402	A
34	AA	405	A
34	AA	409	A
34	AA	411	U
34	AA	412	A
34	AA	413	C
34	AA	416	G
34	AA	417	A
34	AA	431	G
34	AA	432	A
34	AA	433	A
34	AA	434	C
34	AA	439	U
34	AA	442	G
34	AA	444	G
34	AA	447	A
34	AA	448	A
34	AA	449	A
34	AA	450	A
34	AA	451	C
34	AA	458	A
34	AA	459	G
34	AA	462	G
34	AA	463	G
34	AA	489	U
34	AA	490	U
34	AA	494	U
34	AA	495	U
34	AA	497	U
34	AA	498	U
34	AA	499	U
34	AA	500	A
34	AA	501	U
34	AA	502	U
34	AA	503	A
34	AA	504	A
34	AA	505	A
34	AA	506	A
34	AA	509	A

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Mol	Chain	Res	Type
34	AA	510	A
34	AA	514	C
34	AA	521	U
34	AA	522	A
34	AA	523	A
34	AA	527	A
34	AA	531	U
34	AA	532	C
34	AA	534	A
34	AA	536	A
34	AA	538	A
34	AA	539	G
34	AA	542	A
34	AA	543	U
34	AA	544	C
34	AA	545	C
34	AA	546	C
34	AA	547	C
34	AA	549	G
34	AA	573	U
34	AA	575	U
34	AA	579	C
34	AA	580	A
34	AA	581	C
34	AA	582	U
34	AA	583	U
34	AA	585	C
34	AA	586	U
34	AA	592	C
34	AA	594	C
34	AA	595	U
34	AA	597	A
34	AA	598	U
34	AA	599	G
34	AA	601	G
34	AA	604	G
34	AA	605	A
34	AA	608	A
34	AA	610	U
34	AA	615	U
34	AA	617	A
34	AA	618	U

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Mol	Chain	Res	Type
34	AA	620	U
34	AA	621	C
34	AA	622	U
34	AA	623	U
34	AA	628	U
34	AA	631	U
34	AA	636	U
34	AA	637	U
34	AA	641	G
34	AA	642	A
34	AA	643	G
34	AA	644	G
34	AA	645	A
34	AA	646	A
34	AA	649	U
34	AA	653	A
34	AA	658	U
34	AA	659	U
34	AA	662	A
34	AA	665	U
34	AA	666	U
34	AA	671	U
34	AA	672	C
34	AA	674	U
34	AA	675	A
34	AA	677	A
34	AA	678	A
34	AA	679	U
34	AA	681	U
34	AA	682	A
34	AA	683	A
34	AA	684	G
34	AA	685	U
34	AA	694	U
34	AA	697	A
34	AA	698	G
34	AA	699	U
34	AA	704	U
34	AA	707	U
34	AA	708	A
34	AA	714	C
34	AA	715	U

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Mol	Chain	Res	Type
34	AA	716	C
34	AA	727	A
34	AA	729	G
34	AA	738	A
34	AA	755	A
34	AA	760	A
34	AA	761	U
34	AA	763	U
34	AA	765	A
34	AA	766	U
34	AA	767	U
34	AA	769	U
34	AA	773	A
34	AA	774	A
34	AA	778	U
34	AA	779	U
34	AA	793	A
34	AA	794	C
34	AA	799	A
34	AA	804	A
34	AA	806	G
34	AA	809	A
34	AA	810	U
34	AA	811	A
34	AA	812	U
34	AA	813	G
34	AA	822	A
34	AA	825	G
34	AA	833	G
34	AA	834	U
34	AA	835	G
34	AA	857	C
34	AA	859	C
34	AA	860	A
34	AA	862	U
34	AA	866	C
34	AA	873	U
34	AA	874	A
34	AA	880	A
34	AA	889	U
34	AA	890	G
34	AA	893	U

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Mol	Chain	Res	Type
34	AA	894	U
34	AA	896	U
34	AA	900	G
34	AA	903	C
34	AA	905	A
34	AA	918	G
34	AA	920	A
34	AA	925	A
34	AA	927	A
34	AA	934	G
34	AA	936	A
34	AA	937	C
34	AA	945	G
34	AA	946	A
34	AA	951	A
34	AA	956	A
34	AA	966	A
34	AA	968	G
34	AA	970	C
34	AA	976	G
34	AA	980	A
34	AA	984	A
34	AA	988	G
34	AA	990	U
34	AA	993	U
34	AA	998	U
34	AA	999	G
34	AA	1000	C
34	AA	1013	U
34	AA	1014	C
34	AA	1015	A
34	AA	1016	A
34	AA	1024	U
34	AA	1026	G
34	AA	1027	G
34	AA	1028	G
34	AA	1033	A
34	AA	1034	A
34	AA	1035	G
34	AA	1036	A
34	AA	1042	C
34	AA	1043	G

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Mol	Chain	Res	Type
34	AA	1052	A
34	AA	1053	U
34	AA	1056	G
34	AA	1063	A
34	AA	1070	A
34	AA	1072	A
34	AA	1073	G
34	AA	1078	C
34	AA	1079	U
34	AA	1086	C
34	AA	1087	G
34	AA	1092	A
34	AA	1098	U
34	AA	1099	U
34	AA	1101	A
34	AA	1102	U
34	AA	1106	A
34	AA	1109	U
34	AA	1111	A
34	AA	1113	C
34	AA	1114	A
34	AA	1115	G
34	AA	1116	G
34	AA	1121	G
34	AA	1122	A
34	AA	1123	U
34	AA	1124	A
34	AA	1128	A
34	AA	1132	G
34	AA	1136	A
34	AA	1158	G
34	AA	1164	U
34	AA	1168	C
34	AA	1169	A
34	AA	1170	A
34	AA	1172	C
34	AA	1174	C
34	AA	1186	A
34	AA	1193	G
34	AA	1194	A
34	AA	1196	A
34	AA	1197	U

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Mol	Chain	Res	Type
34	AA	1198	A
34	AA	1199	A
34	AA	1200	C
34	AA	1203	A
34	AA	1204	A
34	AA	1205	U
34	AA	1206	U
34	AA	1207	U
34	AA	1210	A
34	AA	1215	A
34	AA	1217	U
34	AA	1218	C
34	AA	1219	A
34	AA	1221	A
34	AA	1222	U
34	AA	1224	A
34	AA	1225	A
34	AA	1226	A
34	AA	1229	A
34	AA	1230	A
34	AA	1231	A
34	AA	1232	U
34	AA	1233	A
34	AA	1234	A
34	AA	1235	C
34	AA	1239	A
34	AA	1240	A
34	AA	1244	G
34	AA	1245	G
34	AA	1259	G
34	AA	1263	A
34	AA	1272	U
34	AA	1273	G
34	AA	1281	C
34	AA	1283	C
34	AA	1287	A
34	AA	1288	C
34	AA	1291	U
34	AA	1295	A
34	AA	1299	G
34	AA	1300	G
34	AA	1306	A

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Mol	Chain	Res	Type
34	AA	1309	U
34	AA	1310	A
34	AA	1313	C
34	AA	1314	G
34	AA	1320	G
34	AA	1321	A
34	AA	1324	U
34	AA	1325	C
34	AA	1329	U
34	AA	1330	A
34	AA	1334	G
34	AA	1337	G
34	AA	1340	G
34	AA	1341	G
34	AA	1344	C
34	AA	1345	A
34	AA	1346	U
34	AA	1416	U
34	AA	1418	A
34	AA	1420	C
34	AA	1431	A
34	AA	1432	A
34	AA	1433	U
34	AA	1435	G
34	AA	1436	A
34	AA	1437	U
34	AA	1441	G
34	AA	1444	A
34	AA	1445	A
34	AA	1450	G
34	AA	1451	A
34	AA	1453	U
34	AA	1458	A
34	AA	1460	A
34	AA	1473	A
34	AA	1476	A
34	AA	1480	G
34	AA	1481	A
34	AA	1486	A
34	AA	1498	U
34	AA	1499	U
34	AA	1503	A

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Mol	Chain	Res	Type
34	AA	1504	A
34	AA	1505	U
34	AA	1506	C
34	AA	1524	U
34	AA	1535	G
34	AA	1537	G
34	AA	1539	U
34	AA	1540	G
34	AA	1549	U
34	AA	1550	A
34	AA	1556	G
34	AA	1565	G
34	AA	1566	A
34	AA	1567	A
34	AA	1569	A
34	AA	1571	C
34	AA	1572	U
34	AA	1575	C
34	AA	1583	G
34	AA	1586	C
34	AA	1587	U
34	AA	1592	G
34	AA	1595	A
34	AA	1599	G
34	AA	1603	C
34	AA	1604	U
34	AA	1605	A
34	AA	1619	U
34	AA	1624	A
34	AA	1626	A
34	AA	1630	A
34	AA	1631	A
34	AA	1632	G
34	AA	1633	U
34	AA	1635	G
34	AA	1636	A
34	AA	1637	G
34	AA	1643	U
34	AA	1649	G
34	AA	1651	C
34	AA	1657	U
34	AA	1661	U

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Mol	Chain	Res	Type
34	AA	1668	G
34	AA	1676	C
34	AA	1677	G
34	AA	1685	G
34	AA	1688	A
34	AA	1691	G
34	AA	1693	U
34	AA	1703	U
34	AA	1704	U
34	AA	1705	A
34	AA	1706	A
34	AA	1707	A
34	AA	1721	C
34	AA	1725	U
34	AA	1730	A
34	AA	1732	A
34	AA	1736	A
34	AA	1737	A
34	AA	1748	A
34	AA	1750	U
34	AA	1751	C
34	AA	1756	G
34	AA	1760	A
34	AA	1761	U
34	AA	1762	A
34	AA	1763	G
34	AA	1766	U
34	AA	1767	U
34	AA	1768	A
34	AA	1769	U
34	AA	1770	G
34	AA	1771	A
34	AA	1774	U
34	AA	1780	G
34	AA	1781	A
34	AA	1782	U
34	AA	1783	G
34	AA	1788	C
34	AA	1797	A
34	AA	1798	A
34	AA	1800	U
34	AA	1801	G

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Mol	Chain	Res	Type
34	AA	1805	U
34	AA	1806	C
34	AA	1812	C
34	AA	1817	G
34	AA	1832	U
34	AA	1842	U
34	AA	1850	U
34	AA	1852	C
34	AA	1855	U
34	AA	1856	U
34	AA	1857	A
34	AA	1871	A
34	AA	1872	A
34	AA	1873	U
34	AA	1874	C
34	AA	1881	C
34	AA	1882	U
34	AA	1887	G
34	AA	1888	A
34	AA	1898	U
34	AA	1899	U
34	AA	1900	G
34	AA	1902	A
34	AA	1904	U
34	AA	1905	C
34	AA	1914	A
34	AA	1963	U
34	AA	1964	G
34	AA	1965	U
34	AA	1966	A
34	AA	1969	A
34	AA	1970	A
34	AA	1971	U
34	AA	1976	A
34	AA	1978	U
34	AA	1980	G
34	AA	1981	U
34	AA	1990	A
34	AA	1991	U
34	AA	1996	C
34	AA	1997	G
34	AA	1998	A

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Mol	Chain	Res	Type
34	AA	1999	A
34	AA	2000	G
34	AA	2003	G
34	AA	2010	C
34	AA	2016	U
34	AA	2017	U
34	AA	2018	G
34	AA	2019	A
34	AA	2030	G
34	AA	2034	G
34	AA	2072	U
34	AA	2082	C
34	AA	2084	U
34	AA	2090	U
34	AA	2092	G
34	AA	2094	A
34	AA	2096	G
34	AA	2102	A
34	AA	2106	A
34	AA	2107	C
34	AA	2108	A
34	AA	2109	A
34	AA	2113	C
34	AA	2114	A
34	AA	2115	U
34	AA	2125	A
34	AA	2136	C
34	AA	2145	A
34	AA	2146	A
34	AA	2147	A
34	AA	2148	U
34	AA	2149	A
34	AA	2160	G
34	AA	2161	G
34	AA	2169	A
34	AA	2170	G
34	AA	2171	U
34	AA	2172	C
34	AA	2174	G
34	AA	2186	C
34	AA	2203	G
34	AA	2218	C

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Mol	Chain	Res	Type
34	AA	2219	A
34	AA	2220	U
34	AA	2221	U
34	AA	2389	G
34	AA	2394	C
34	AA	2395	U
34	AA	2403	G
34	AA	2404	A
34	AA	2406	A
34	AA	2409	G
34	AA	2411	C
34	AA	2414	G
34	AA	2415	G
34	AA	2419	A
34	AA	2424	A
34	AA	2427	G
34	AA	2434	U
34	AA	2435	A
34	AA	2437	A
34	AA	2438	A
34	AA	2451	A
34	AA	2453	A
34	AA	2463	U
34	AA	2464	G
34	AA	2465	G
34	AA	2477	U
34	AA	2486	U
34	AA	2489	C
34	AA	2500	A
34	AA	2501	A
34	AA	2510	U
34	AA	2516	A
34	AA	2518	U
34	AA	2521	A
34	AA	2524	C
34	AA	2536	A
34	AA	2537	A
34	AA	2539	G
34	AA	2542	G
34	AA	2544	G
34	AA	2545	A
34	AA	2548	A

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Mol	Chain	Res	Type
34	AA	2549	A
34	AA	2550	C
34	AA	2551	U
34	AA	2552	A
34	AA	2555	A
34	AA	2556	C
34	AA	2563	A
34	AA	2565	G
34	AA	2566	G
34	AA	2573	A
34	AA	2574	A
34	AA	2575	U
34	AA	2576	G
34	AA	2580	C
34	AA	2581	G
34	AA	2584	A
34	AA	2588	A
34	AA	2589	A
34	AA	2591	U
34	AA	2596	A
34	AA	2599	C
34	AA	2600	G
34	AA	2601	C
34	AA	2602	A
34	AA	2603	U
34	AA	2606	A
34	AA	2607	U
34	AA	2608	G
34	AA	2627	U
34	AA	2628	G
34	AA	2629	U
34	AA	2640	U
34	AA	2656	A
34	AA	2667	C
34	AA	2668	G
34	AA	2671	C
34	AA	2676	C
34	AA	2681	U
34	AA	2684	G
34	AA	2686	G
34	AA	2690	A
34	AA	2694	A

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Mol	Chain	Res	Type
34	AA	2695	A
34	AA	2696	G
34	AA	2697	A
34	AA	2698	C
34	AA	2703	U
34	AA	2704	U
34	AA	2705	G
34	AA	2710	U
34	AA	2711	U
34	AA	2712	A
34	AA	2727	U
34	AA	2728	G
34	AA	2730	G
34	AA	2745	G
34	AA	2746	U
34	AA	2747	G
34	AA	2809	A
34	AA	2811	A
34	AA	2817	U
34	AA	2822	U
34	AA	2823	U
34	AA	2833	U
34	AA	2834	A
34	AA	2835	G
34	AA	2837	G
34	AA	2884	G
34	AA	2885	A
34	AA	2886	A
34	AA	2887	U
34	AA	2888	U
34	AA	2926	A
34	AA	2928	G
34	AA	2932	A
34	AA	2933	C
34	AA	2945	G
34	AA	2946	G
34	AA	2953	G
34	AA	2958	G
34	AA	2959	G
34	AA	2960	G
34	AA	2967	A
34	AA	2968	U

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Mol	Chain	Res	Type
34	AA	2980	U
34	AA	2981	A
34	AA	2987	G
34	AA	2990	G
34	AA	2991	U
34	AA	2994	A
34	AA	2995	A
34	AA	2996	A
34	AA	3005	C
34	AA	3011	G
34	AA	3013	A
34	AA	3016	G
34	AA	3017	A
34	AA	3018	A
34	AA	3019	A
34	AA	3020	U
34	AA	3028	A
34	AA	3029	G
34	AA	3030	A
34	AA	3033	A
34	AA	3034	A
34	AA	3035	A
34	AA	3053	G
34	AA	3067	G
34	AA	3068	A
34	AA	3073	G
34	AA	3076	G
34	AA	3079	A
34	AA	3081	C
34	AA	3088	G
34	AA	3091	U
34	AA	3092	G
34	AA	3093	G
34	AA	3094	C
34	AA	3100	G
34	AA	3108	A
34	AA	3111	U
34	AA	3113	U
34	AA	3116	A
34	AA	3118	A
34	AA	3121	G
34	AA	3123	C

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Mol	Chain	Res	Type
34	AA	3124	G
34	AA	3126	A
34	AA	3127	A
34	AA	3130	U
34	AA	3131	A
34	AA	3135	A
34	AA	3138	A
34	AA	3140	U
34	AA	3141	G
34	AA	3146	U
34	AA	3155	G
34	AA	3158	U
34	AA	3159	G
34	AA	3160	A
34	AA	3161	A
34	AA	3169	C
34	AA	3173	G
34	AA	3175	G
34	AA	3176	A
34	AA	3177	U
34	AA	3180	C
34	AA	3193	G
34	AA	3201	C
34	AA	3202	U
34	AA	3204	C
34	AA	3208	C
34	AA	3209	G
34	AA	3212	G
34	AA	3219	U
34	AA	3220	U
34	AA	3222	G
34	AA	3225	C
34	AA	3229	C
34	AA	3230	G
34	AA	3231	A
34	AA	3232	U
34	AA	3235	C
34	AA	3245	U
34	AA	3246	A
34	AA	3248	C
34	AA	3253	G
34	AA	3257	G

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Mol	Chain	Res	Type
34	AA	3258	C
34	AA	3262	A
34	AA	3269	A
34	AA	3277	G
34	AA	3281	G
34	AA	3282	U
34	AA	3287	C
34	AA	3292	A
34	AA	3293	A
34	AA	3294	U
34	AA	3295	A
34	AA	3297	G
34	AA	3301	C
34	AA	3302	G
34	AA	3304	G
34	AA	3305	A
34	AA	3306	G
34	AA	3312	U
34	AA	3313	U
34	AA	3330	A
34	AA	3336	G
34	AA	3338	U
34	AA	3342	C
34	AA	3343	C
34	AA	3349	G
34	AA	3351	U
34	AA	3353	A
34	AA	3354	A
34	AA	3358	U
34	AA	3359	A
34	AA	3361	U
34	AA	3362	A
34	AA	3374	U
34	AA	3375	A
34	AA	3378	C
34	AA	3380	U
34	AA	3381	A
34	AA	3382	U
34	AA	3383	A
34	AA	3389	G
34	AA	3391	G
34	AA	3398	A

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Mol	Chain	Res	Type
34	AA	3415	A
34	AA	3416	G
34	AA	3418	A
34	AA	3421	A
34	AA	3432	A
34	AA	3434	A
34	AA	3435	A
34	AA	3436	U
34	AA	3442	C
34	AA	3443	A
34	AA	3444	G
34	AA	3445	C
34	AA	3459	A
34	AA	3463	G
34	AA	3464	U
34	AA	3468	G
34	AA	3471	A
34	AA	3472	A
34	AA	3476	A
34	AA	3477	A
34	AA	3483	U
34	AA	3488	U
34	AA	3493	G
34	AA	3500	G
34	AA	3507	A
34	AA	3510	C
34	AA	3513	G
34	AA	3515	A
34	AA	3516	A
34	AA	3527	U
34	AA	3530	A
34	AA	3571	A
34	AA	3573	U
34	AA	3575	U
34	AA	3576	A
34	AA	3577	A
34	AA	3578	A
34	AA	3580	G
34	AA	3581	A
34	AA	3582	G
34	AA	3585	A
34	AA	3586	U

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Mol	Chain	Res	Type
34	AA	3588	A
34	AA	3589	U
34	AA	3590	A
34	AA	3591	U
34	AA	3594	G
34	AA	3597	C
34	AA	3612	U
34	AA	3615	A
34	AA	3616	U
34	AA	3617	A
34	AA	3618	A
34	AA	3624	U
34	AA	3625	C
34	AA	3626	A
34	AA	3627	C
34	AA	3628	C
34	AA	3632	U
34	AA	3658	G
34	AA	3659	C
34	AA	3662	U
34	AA	3663	A
34	AA	3664	G
34	AA	3665	U
34	AA	3667	C
34	AA	3668	U
34	AA	3670	U
34	AA	3671	A
34	AA	3672	A
34	AA	3677	A
34	AA	3680	A
34	AA	3683	G
34	AA	3689	C
34	AA	3697	G
34	AA	3698	U
34	AA	3707	U
34	AA	3712	G
34	AA	3716	C
34	AA	3727	A
34	AA	3728	A
34	AA	3732	U
34	AA	3733	G
34	AA	3736	A

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Mol	Chain	Res	Type
34	AA	3737	G
34	AA	3739	A
34	AA	3740	A
34	AA	3741	A
34	AA	3752	C
34	AA	3761	G
34	AA	3767	U
34	AA	3768	A
34	AA	3770	C
34	AA	3774	A
34	AA	3775	G
34	AA	3778	G
34	AA	3779	U
34	AA	3782	A
34	AA	3783	G
35	AC	5	A
35	AC	6	C
35	AC	25	C
35	AC	36	C
35	AC	38	G
35	AC	39	C
35	AC	43	G
35	AC	44	A
35	AC	50	G
35	AC	53	G
35	AC	55	A
35	AC	57	A
35	AC	58	A
35	AC	63	A
35	AC	64	U
35	AC	65	A
35	AC	66	C
35	AC	67	G
35	AC	73	A
35	AC	75	A
35	AC	80	C
35	AC	85	A
35	AC	90	G
35	AC	92	A
35	AC	94	C
35	AC	98	A
35	AC	99	G

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Mol	Chain	Res	Type
35	AC	107	A
35	AC	108	A
35	AC	109	U
35	AC	111	U
35	AC	112	A
35	AC	114	A
35	AC	115	C
35	AC	116	U
35	AC	117	A
35	AC	119	A
35	AC	122	A
35	AC	123	A
35	AC	135	G
35	AC	136	A
35	AC	137	A
35	AC	138	U
35	AC	139	A
35	AC	140	G
35	AC	142	G
35	AC	145	A
35	AC	146	C
35	AC	149	C
35	AC	157	A
36	AB	3	A
36	AB	7	G
36	AB	13	A
36	AB	16	A
36	AB	18	A
36	AB	22	G
36	AB	25	A
36	AB	26	C
36	AB	27	A
36	AB	33	U
36	AB	38	U
36	AB	48	G
36	AB	51	G
36	AB	53	U
36	AB	54	A
36	AB	63	A
36	AB	64	A
36	AB	69	U
36	AB	71	G

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Mol	Chain	Res	Type
36	AB	74	A
36	AB	84	U
36	AB	85	G
36	AB	93	G
36	AB	97	G
36	AB	100	A
36	AB	110	G
36	AB	119	G

All (288) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2	A
1	A	25	C
1	A	44	U
1	A	45	U
1	A	96	C
1	A	105	A
1	A	139	A
1	A	156	A
1	A	161	U
1	A	206	A
1	A	246	A
1	A	250	A
1	A	251	U
1	A	358	G
1	A	383	G
1	A	406	A
1	A	422	A
1	A	423	A
1	A	461	A
1	A	474	A
1	A	525	G
1	A	544	G
1	A	547	U
1	A	577	A
1	A	588	U
1	A	614	A
1	A	752	U
1	A	753	U
1	A	789	U
1	A	790	U

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Mol	Chain	Res	Type
1	A	793	G
1	A	803	G
1	A	805	A
1	A	818	C
1	A	844	G
1	A	874	A
1	A	876	U
1	A	879	A
1	A	919	U
1	A	973	G
1	A	981	U
1	A	983	G
1	A	1028	U
1	A	1055	G
1	A	1070	A
1	A	1098	U
1	A	1100	U
1	A	1182	A
1	A	1183	U
1	A	1198	U
1	A	1209	G
1	A	1259	C
1	A	1291	C
1	A	1292	U
1	A	1295	A
1	A	1301	G
1	A	1305	A
1	A	1370	U
1	A	1381	C
1	A	1383	U
1	A	1413	U
1	A	1423	A
1	A	1430	G
1	A	1431	A
1	A	1448	U
1	A	1455	C
1	A	1659	U
1	A	1667	A
1	A	1672	C
1	A	1691	G
1	A	1692	A
1	A	1704	G

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Mol	Chain	Res	Type
1	A	1705	C
1	A	1719	U
1	A	1786	U
1	A	1818	A
1	A	1819	U
1	A	1834	A
1	A	1865	G
1	A	1870	A
1	A	1871	G
1	A	1897	A
1	A	1898	G
1	A	1912	C
1	A	1934	C
1	A	1976	G
1	A	1977	G
1	A	2053	U
1	A	2071	U
2	7	17	C
2	7	75	C
34	AA	10	G
34	AA	11	A
34	AA	25	A
34	AA	62	A
34	AA	65	A
34	AA	124	U
34	AA	138	C
34	AA	149	A
34	AA	156	U
34	AA	162	U
34	AA	181	C
34	AA	198	U
34	AA	215	C
34	AA	228	A
34	AA	257	U
34	AA	270	U
34	AA	289	A
34	AA	337	A
34	AA	344	A
34	AA	411	U
34	AA	416	G
34	AA	432	A
34	AA	497	U

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Mol	Chain	Res	Type
34	AA	500	A
34	AA	501	U
34	AA	504	A
34	AA	505	A
34	AA	573	U
34	AA	579	C
34	AA	580	A
34	AA	581	C
34	AA	593	A
34	AA	594	C
34	AA	596	A
34	AA	597	A
34	AA	607	A
34	AA	620	U
34	AA	621	C
34	AA	641	G
34	AA	645	A
34	AA	652	A
34	AA	667	U
34	AA	674	U
34	AA	681	U
34	AA	683	A
34	AA	697	A
34	AA	698	G
34	AA	703	U
34	AA	715	U
34	AA	764	G
34	AA	768	C
34	AA	803	A
34	AA	809	A
34	AA	810	U
34	AA	811	A
34	AA	859	C
34	AA	888	A
34	AA	889	U
34	AA	904	G
34	AA	935	A
34	AA	998	U
34	AA	999	G
34	AA	1027	G
34	AA	1035	G
34	AA	1080	C

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Mol	Chain	Res	Type
34	AA	1099	U
34	AA	1101	A
34	AA	1115	G
34	AA	1197	U
34	AA	1204	A
34	AA	1206	U
34	AA	1217	U
34	AA	1224	A
34	AA	1234	A
34	AA	1243	G
34	AA	1272	U
34	AA	1277	G
34	AA	1415	A
34	AA	1422	A
34	AA	1431	A
34	AA	1435	G
34	AA	1457	G
34	AA	1459	U
34	AA	1479	A
34	AA	1503	A
34	AA	1538	U
34	AA	1539	U
34	AA	1566	A
34	AA	1574	C
34	AA	1602	A
34	AA	1603	C
34	AA	1632	G
34	AA	1642	G
34	AA	1643	U
34	AA	1703	U
34	AA	1705	A
34	AA	1735	G
34	AA	1748	A
34	AA	1750	U
34	AA	1779	A
34	AA	1805	U
34	AA	1872	A
34	AA	1873	U
34	AA	1881	C
34	AA	1898	U
34	AA	1964	G
34	AA	1965	U

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Mol	Chain	Res	Type
34	AA	1989	A
34	AA	1990	A
34	AA	1996	C
34	AA	1999	A
34	AA	2015	C
34	AA	2033	C
34	AA	2096	G
34	AA	2107	C
34	AA	2146	A
34	AA	2193	U
34	AA	2219	A
34	AA	2394	C
34	AA	2403	G
34	AA	2405	A
34	AA	2434	U
34	AA	2437	A
34	AA	2506	A
34	AA	2523	U
34	AA	2575	U
34	AA	2665	A
34	AA	2693	G
34	AA	2694	A
34	AA	2727	U
34	AA	2746	U
34	AA	2810	A
34	AA	2816	U
34	AA	2822	U
34	AA	2832	A
34	AA	2883	U
34	AA	2884	G
34	AA	2886	A
34	AA	2932	A
34	AA	2959	G
34	AA	2966	C
34	AA	2994	A
34	AA	3016	G
34	AA	3018	A
34	AA	3034	A
34	AA	3129	U
34	AA	3130	U
34	AA	3137	U
34	AA	3140	U

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Mol	Chain	Res	Type
34	AA	3158	U
34	AA	3229	C
34	AA	3230	G
34	AA	3231	A
34	AA	3245	U
34	AA	3309	G
34	AA	3332	G
34	AA	3337	U
34	AA	3342	C
34	AA	3361	U
34	AA	3379	A
34	AA	3381	A
34	AA	3382	U
34	AA	3414	G
34	AA	3434	A
34	AA	3435	A
34	AA	3476	A
34	AA	3505	U
34	AA	3526	U
34	AA	3575	U
34	AA	3576	A
34	AA	3577	A
34	AA	3581	A
34	AA	3588	A
34	AA	3589	U
34	AA	3590	A
34	AA	3624	U
34	AA	3627	C
34	AA	3658	G
34	AA	3662	U
34	AA	3664	G
34	AA	3667	C
34	AA	3668	U
34	AA	3671	A
34	AA	3711	U
34	AA	3767	U
34	AA	3774	A
34	AA	3782	A
35	AC	35	A
35	AC	37	A
35	AC	57	A
35	AC	75	A

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Mol	Chain	Res	Type
35	AC	108	A
35	AC	114	A
35	AC	134	G
35	AC	139	A
35	AC	145	A
36	AB	84	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
63	AW	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AW	154:ASN	C	197:UNK	N	33.92

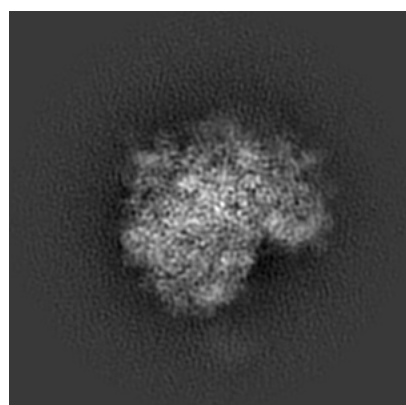
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6456. These allow visual inspection of the internal detail of the map and identification of artifacts.

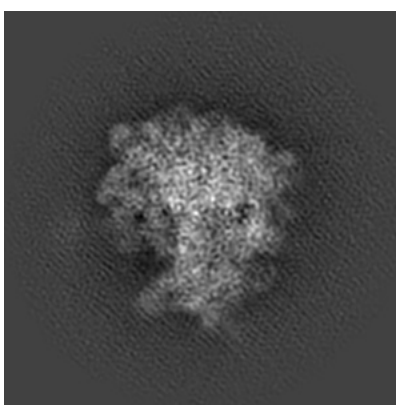
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

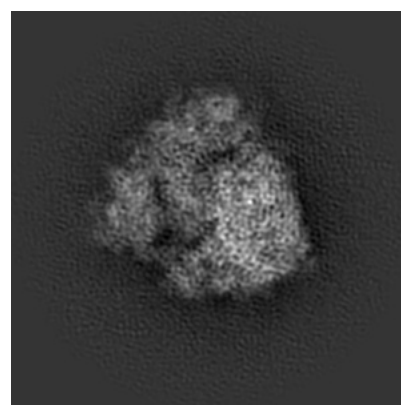
6.1.1 Primary map



X



Y

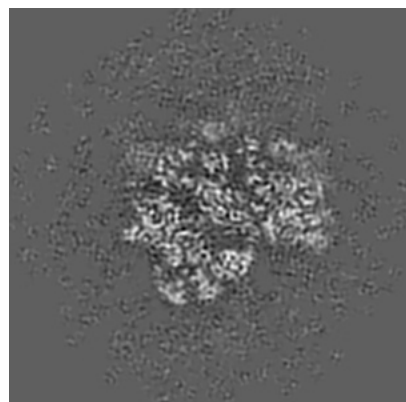


Z

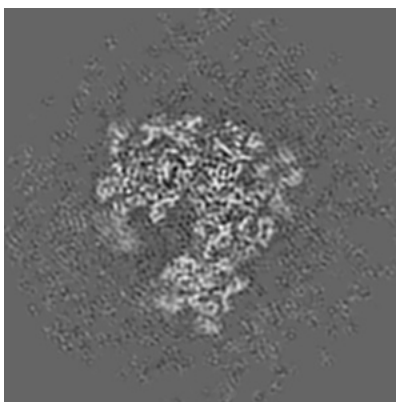
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

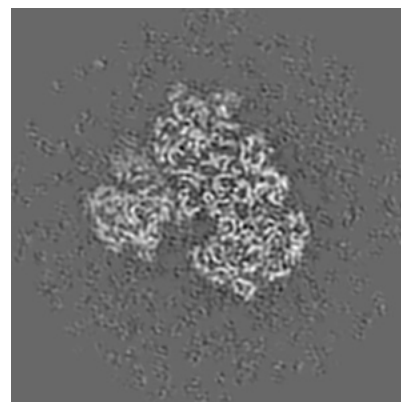
6.2.1 Primary map



X Index: 148



Y Index: 148

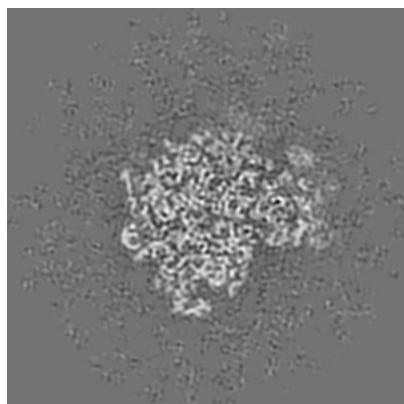


Z Index: 148

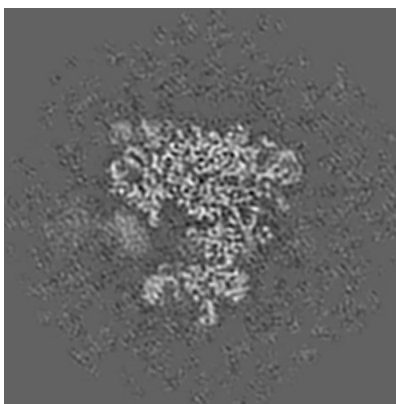
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

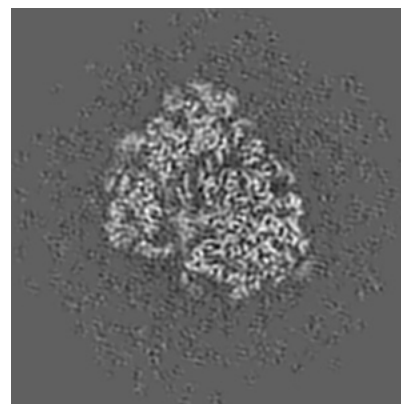
6.3.1 Primary map



X Index: 156



Y Index: 158

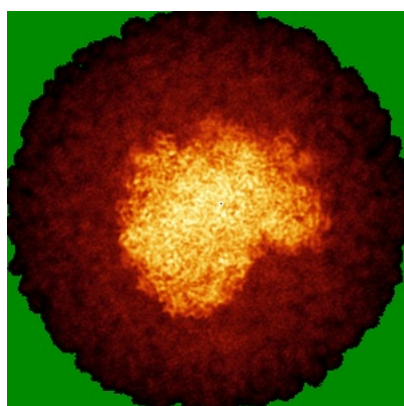


Z Index: 140

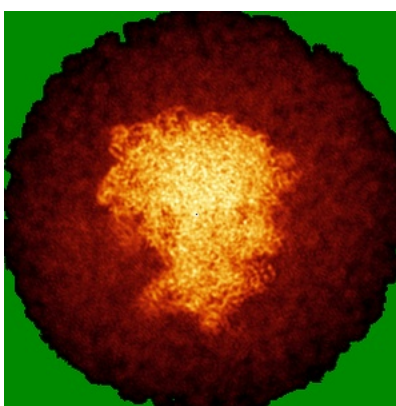
The images above show the largest variance slices of the map in three orthogonal directions.

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

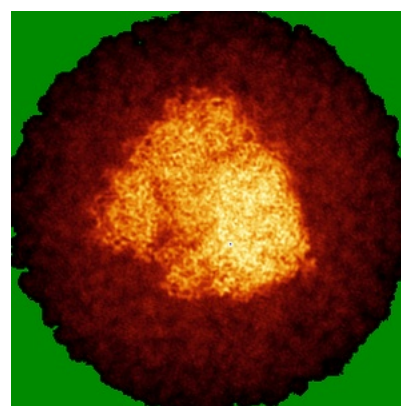
6.4.1 Primary map



X



Y

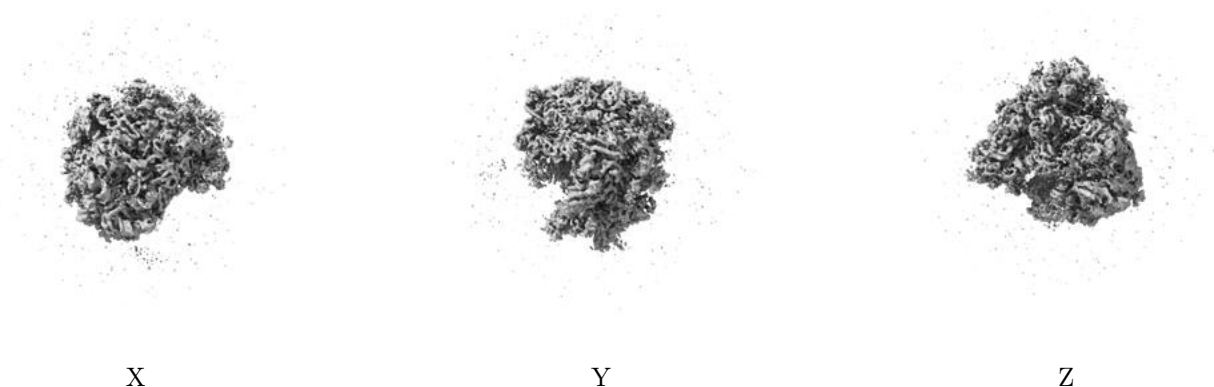


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

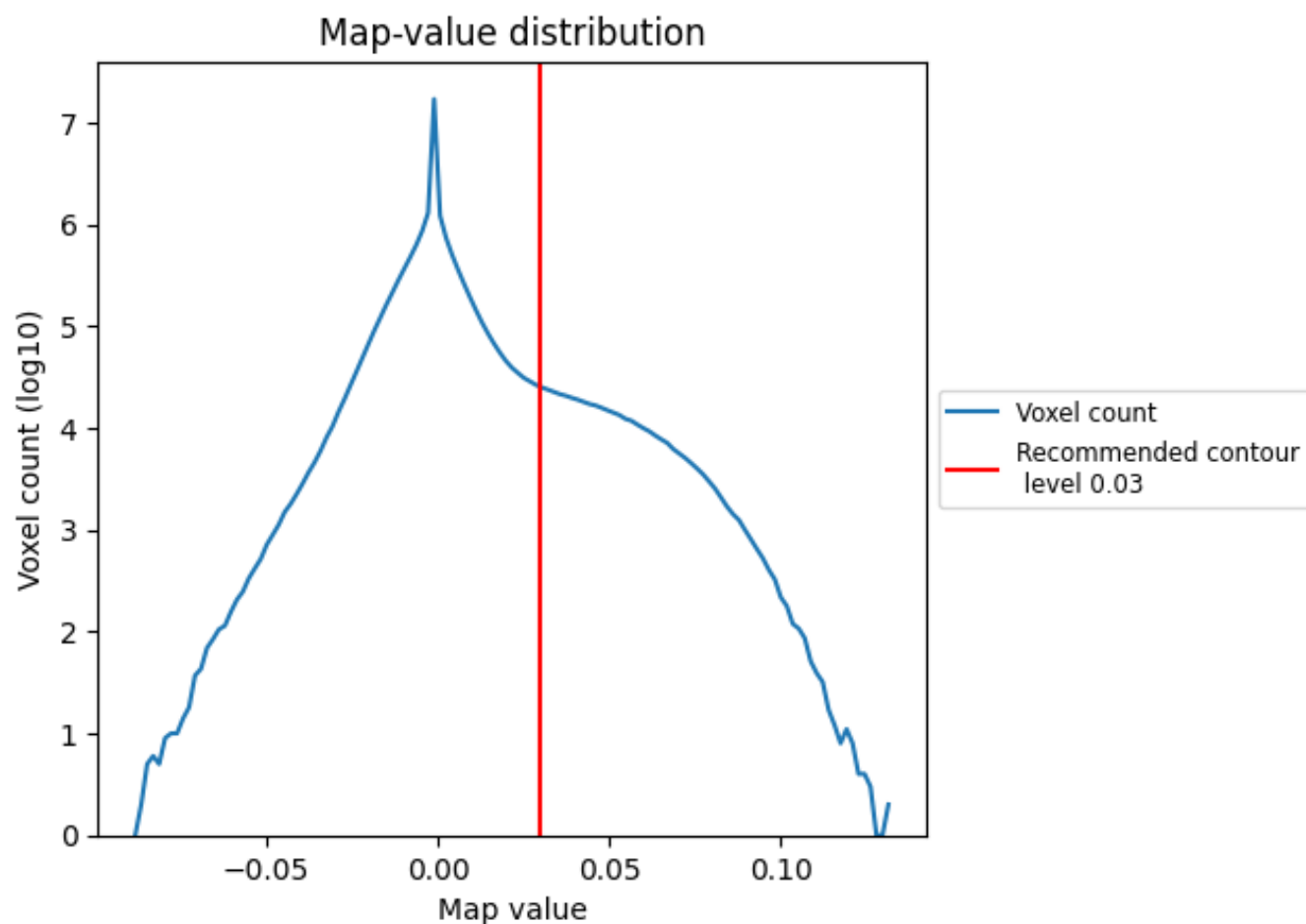
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

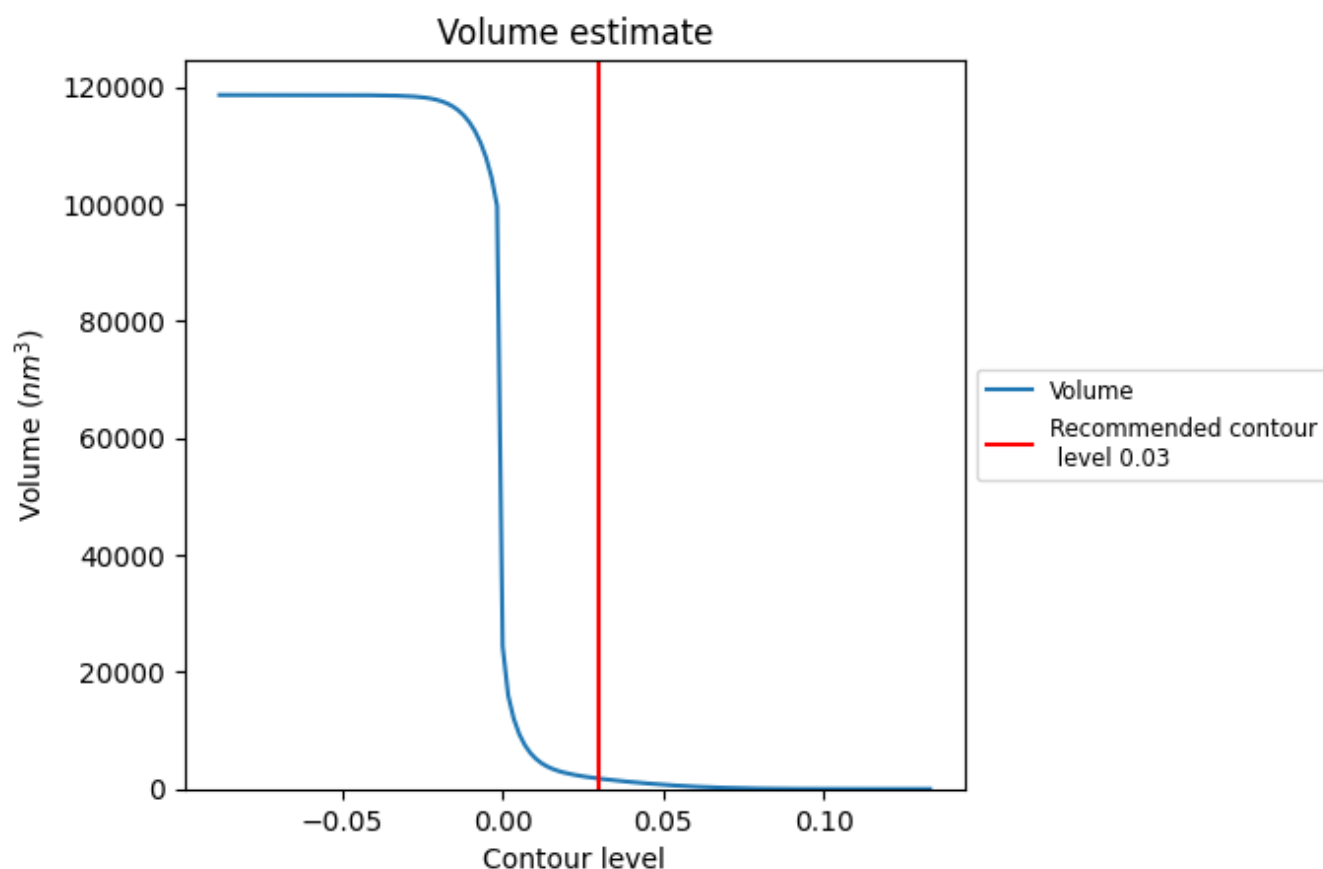
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

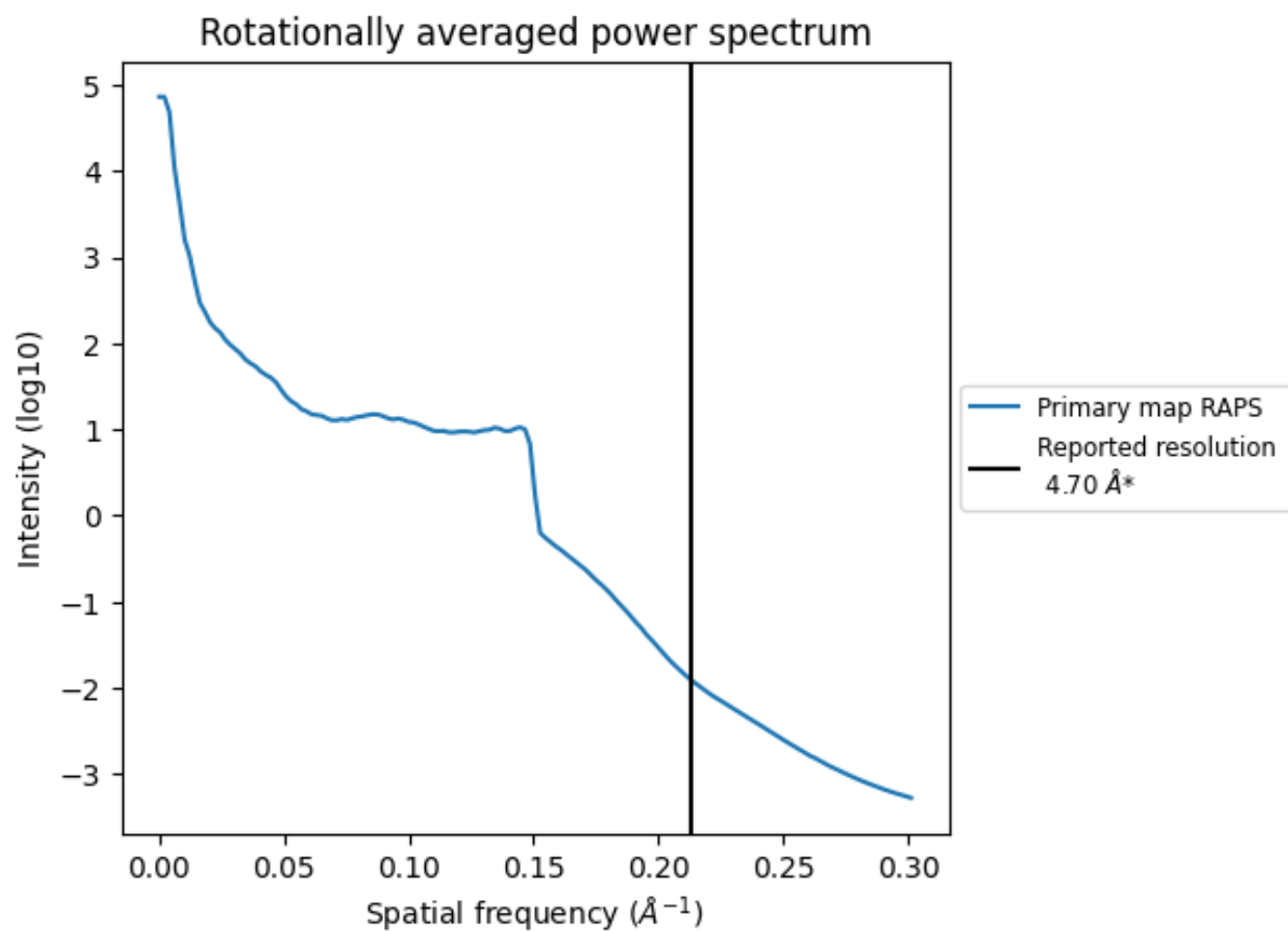
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1785 nm^3 ; this corresponds to an approximate mass of 1612 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 0.213 Å⁻¹

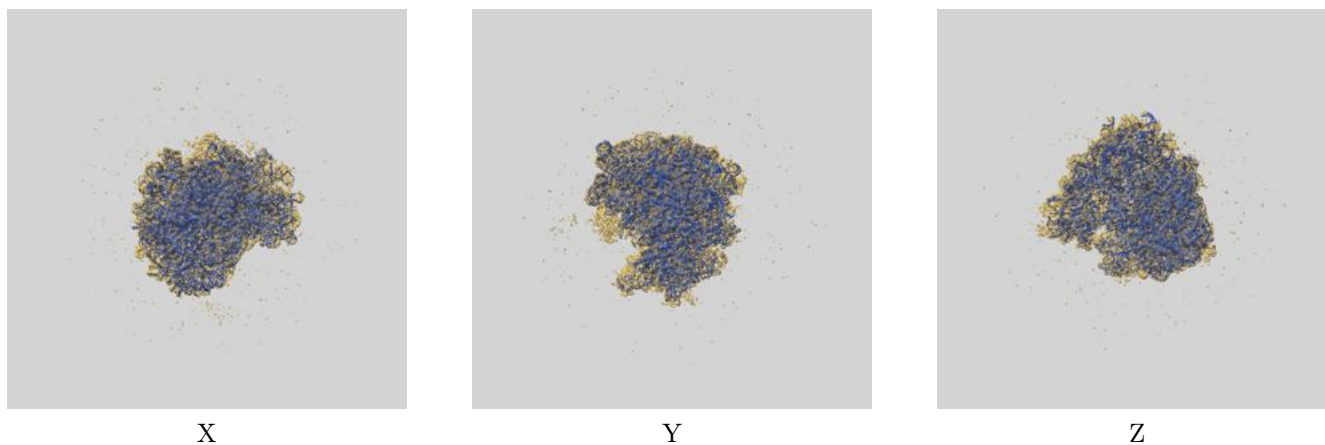
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

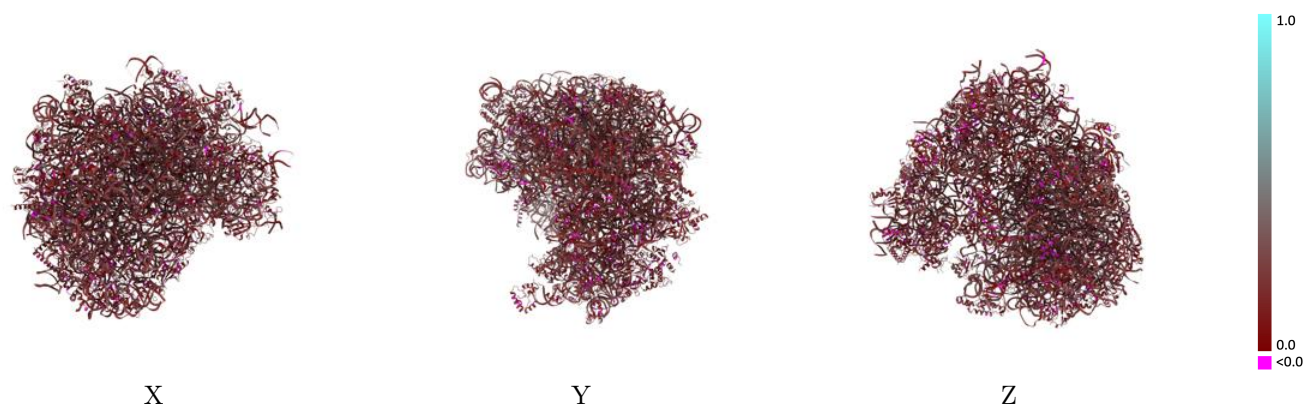
This section contains information regarding the fit between EMDB map EMD-6456 and PDB model 3JBN. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



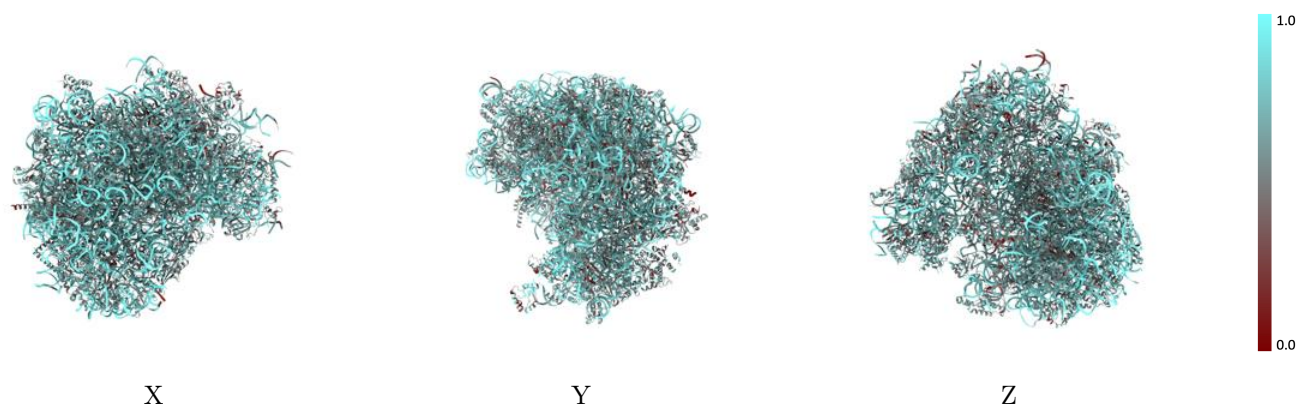
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



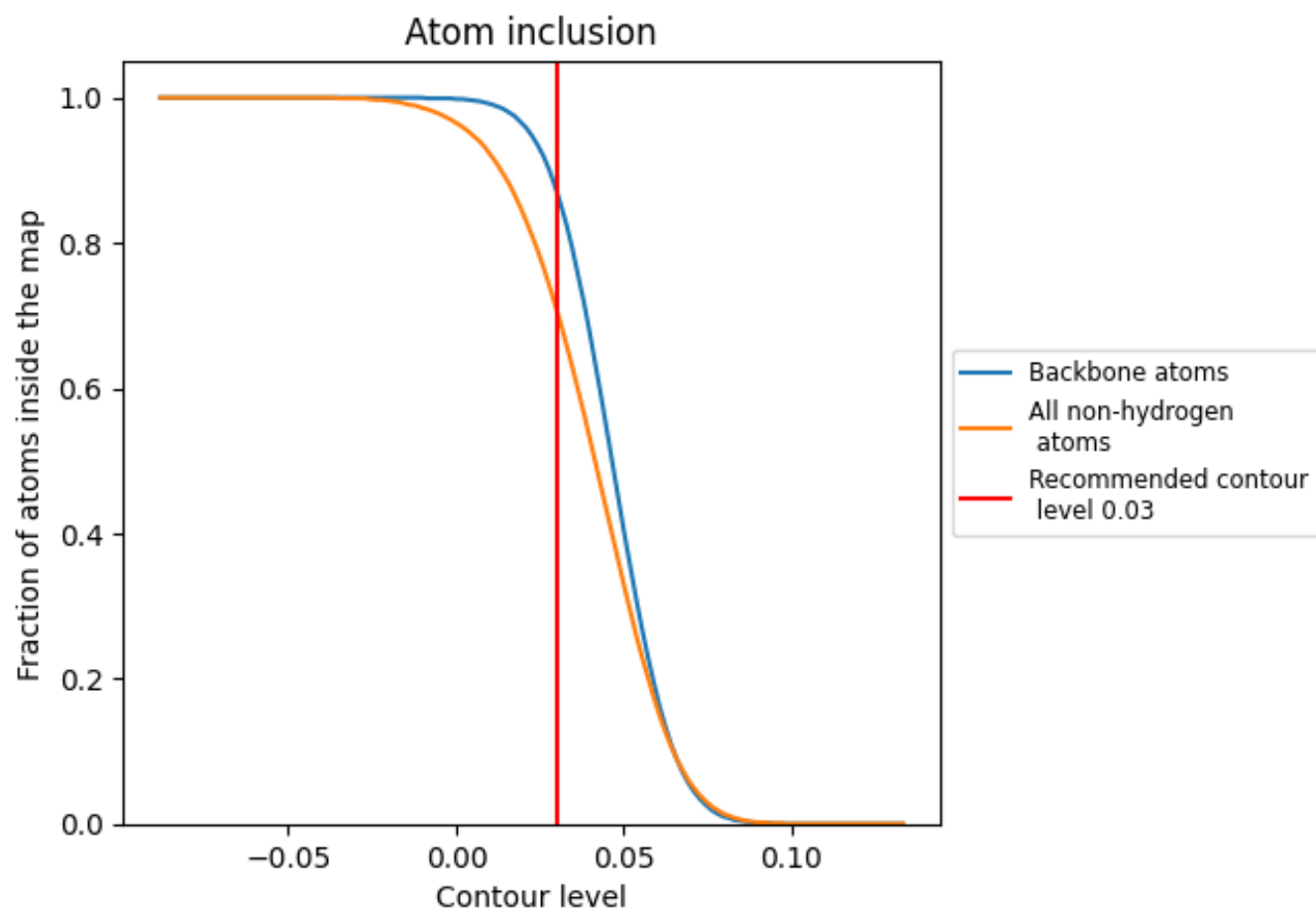
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 71% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7080	 0.2120
1	 0.5850	 0.1930
2	 0.7290	 0.2350
3	 0.4950	 0.1840
4	 0.5710	 0.2280
5	 0.4950	 0.1860
6	 0.5460	 0.1990
7	 0.6700	 0.2120
A	 0.8290	 0.2330
A0	 0.5330	 0.1800
A1	 0.5520	 0.1910
A2	 0.6370	 0.2100
A3	 0.5860	 0.1640
A4	 0.4910	 0.1830
A5	 0.5400	 0.1560
A6	 0.5510	 0.2030
A7	 0.5580	 0.1850
A8	 0.4910	 0.1730
A9	 0.4950	 0.1550
AA	 0.8210	 0.2360
AB	 0.8970	 0.2400
AC	 0.8610	 0.2440
AD	 0.4260	 0.1490
AE	 0.5310	 0.1710
AF	 0.5550	 0.1790
AG	 0.6190	 0.2110
AH	 0.6090	 0.1900
AI	 0.5930	 0.1790
AJ	 0.5790	 0.2010
AK	 0.5350	 0.1640
AL	 0.5900	 0.1900
AM	 0.4910	 0.1930
AN	 0.6040	 0.1820
AO	 0.5410	 0.1770
AP	 0.5180	 0.1530



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Chain	Atom inclusion	Q-score
AQ	0.5370	0.1970
AR	0.5980	0.1730
AS	0.5480	0.1720
AT	0.5010	0.1720
AU	0.5450	0.1820
AV	0.5240	0.1930
AW	0.5850	0.1890
AX	0.5490	0.1860
AY	0.5510	0.2110
AZ	0.6220	0.1780
Aa	0.5290	0.1780
Ab	0.6080	0.2020
Ac	0.5390	0.1680
Ad	0.5830	0.1920
Ae	0.5450	0.1830
Af	0.5950	0.1760
Ag	0.4750	0.1480
Ah	0.5110	0.1640
Ai	0.5070	0.1740
B	0.5040	0.1720
C	0.5800	0.1910
D	0.5820	0.2060
E	0.5540	0.1730
F	0.5390	0.1770
G	0.5940	0.1880
H	0.5530	0.1770
I	0.5730	0.1790
J	0.5150	0.1920
K	0.5340	0.1530
L	0.5330	0.1870
M	0.5380	0.1580
N	0.5780	0.1910
O	0.6180	0.1990
P	0.4790	0.1660
Q	0.4680	0.1880
R	0.6860	0.2090
S	0.6040	0.1890
T	0.4510	0.1400
U	0.5260	0.1820
V	0.4960	0.1890
W	0.6020	0.1990
X	0.6320	0.2110

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Chain	Atom inclusion	Q-score
Y	0.5970	0.1700
Z	0.5730	0.1940